



## Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 10:54 pm BST

PDB ID : 7BGL  
EMDB ID : EMD-12183  
Title : Salmonella LP ring 26 mer refined in C26 map  
Authors : Johnson, S.; Furlong, E.; Lea, S.M.  
Deposited on : 2021-01-07  
Resolution : 2.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

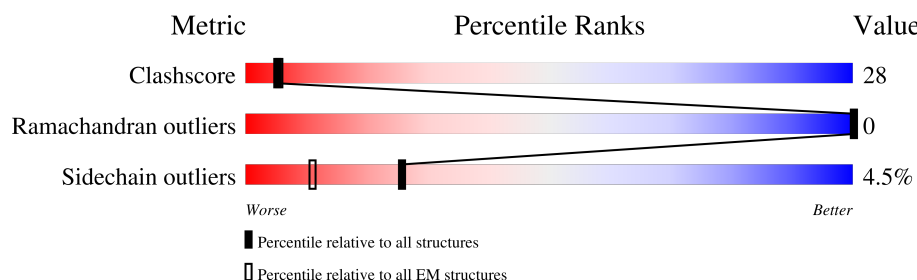
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.









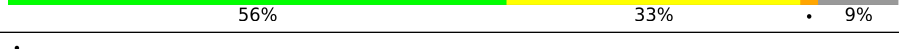
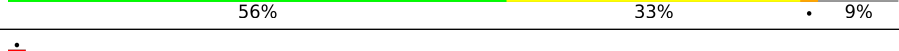
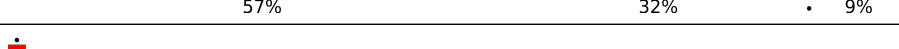
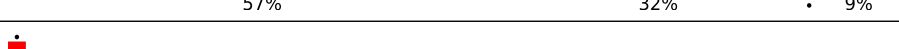
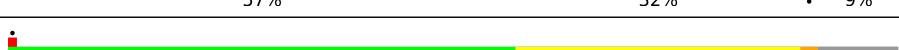

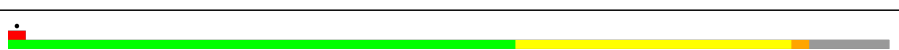

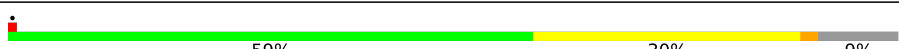





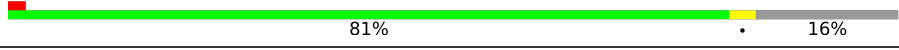
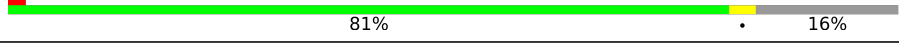



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	232	
1	B	232	
1	C	232	
1	D	232	
1	E	232	
1	F	232	
1	G	232	
1	H	232	







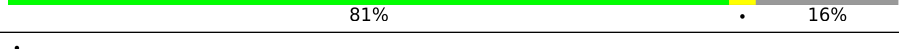
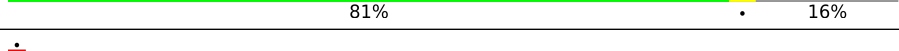
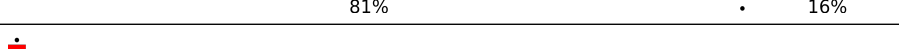
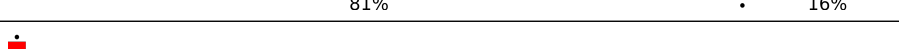
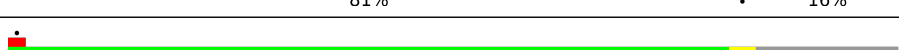

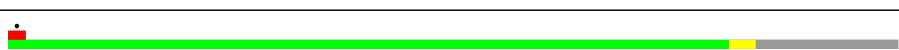

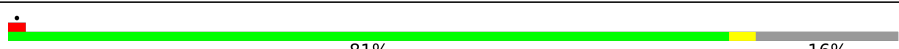



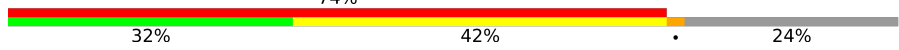
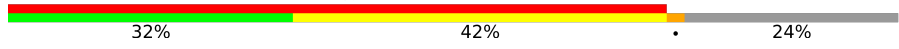
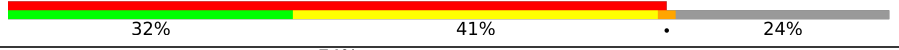
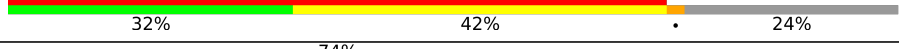
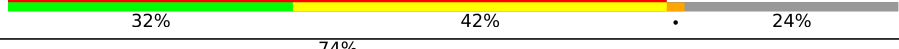
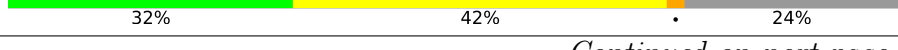

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Mol	Chain	Length	Quality of chain
1	I	232	
1	J	232	
1	K	232	
1	L	232	
1	M	232	
1	N	232	
1	O	232	
1	P	232	
1	Q	232	
1	R	232	
1	S	232	
1	T	232	
1	U	232	
1	V	232	
1	W	232	
1	X	232	
1	Y	232	
1	Z	232	
2	a	365	
2	b	365	
2	c	365	
2	d	365	
2	e	365	
2	f	365	
2	g	365	

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Mol	Chain	Length	Quality of chain
2	h	365	
2	i	365	
2	j	365	
2	k	365	
2	l	365	
2	m	365	
2	n	365	
2	o	365	
2	p	365	
2	q	365	
2	r	365	
2	s	365	
2	t	365	
2	u	365	
2	v	365	
2	w	365	
2	x	365	
2	y	365	
2	z	365	
3	1	111	
3	10	111	
3	11	111	
3	12	111	
3	13	111	
3	14	111	

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Mol	Chain	Length	Quality of chain			
3	15	111	74%	32%	42%	24%
3	16	111	74%	32%	42%	24%
3	17	111	74%	32%	41%	24%
3	18	111	74%	32%	42%	24%
3	19	111	74%	32%	42%	24%
3	2	111	74%	32%	42%	24%
3	20	111	74%	32%	42%	24%
3	21	111	74%	32%	42%	24%
3	22	111	74%	32%	42%	24%
3	23	111	74%	32%	42%	24%
3	24	111	74%	31%	43%	24%
3	25	111	74%	32%	42%	24%
3	26	111	74%	32%	42%	24%
3	3	111	74%	32%	42%	24%
3	4	111	74%	32%	41%	24%
3	5	111	74%	32%	41%	24%
3	6	111	74%	32%	42%	24%
3	7	111	74%	32%	41%	24%
3	8	111	74%	32%	41%	24%
3	9	111	74%	32%	42%	24%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TLW	A	301	X	-	-	-
4	TLW	A	303	X	-	-	-
4	TLW	B	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TLW	C	302	X	-	-	-
4	TLW	D	302	X	-	-	-
4	TLW	E	302	X	-	-	-
4	TLW	F	302	X	-	-	-
4	TLW	G	302	X	-	-	-
4	TLW	H	302	X	-	-	-
4	TLW	I	302	X	-	-	-
4	TLW	J	302	X	-	-	-
4	TLW	K	302	X	-	-	-
4	TLW	L	302	X	-	-	-
4	TLW	M	302	X	-	-	-
4	TLW	N	302	X	-	-	-
4	TLW	O	302	X	-	-	-
4	TLW	P	302	X	-	-	-
4	TLW	Q	302	X	-	-	-
4	TLW	R	302	X	-	-	-
4	TLW	S	302	X	-	-	-
4	TLW	T	302	X	-	-	-
4	TLW	U	302	X	-	-	-
4	TLW	V	302	X	-	-	-
4	TLW	W	302	X	-	-	-
4	TLW	X	302	X	-	-	-
4	TLW	Y	302	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 126022 atoms, of which 5538 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Flagellar L-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	B	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	C	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	D	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	E	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	F	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	G	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	H	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	I	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	J	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	K	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	L	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	M	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	N	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	O	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	P	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	Q	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	S	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	T	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	U	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	V	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	W	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	X	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	Y	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		
1	Z	211	Total	C	N	O	S	0	0
			1581	985	282	310	4		

- Molecule 2 is a protein called Flagellar P-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	306	Total	C	N	O	S	0	0
			2251	1378	409	451	13		
2	b	306	Total	C	N	O	S	0	0
			2251	1378	409	451	13		
2	c	306	Total	C	N	O	S	0	0
			2251	1378	409	451	13		
2	d	306	Total	C	N	O	S	0	0
			2251	1378	409	451	13		
2	e	306	Total	C	N	O	S	0	0
			2251	1378	409	451	13		
2	f	306	Total	C	N	O	S	0	0
			2251	1378	409	451	13		
2	g	306	Total	C	N	O	S	0	0
			2251	1378	409	451	13		
2	h	306	Total	C	N	O	S	0	0
			2251	1378	409	451	13		
2	i	306	Total	C	N	O	S	0	0
			2251	1378	409	451	13		
2	j	306	Total	C	N	O	S	0	0
			2251	1378	409	451	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	k	306	Total 2251	C 1378	N 409	O 451	S 13	0	0
2	l	306	Total 2251	C 1378	N 409	O 451	S 13	0	0
2	m	306	Total 2251	C 1378	N 409	O 451	S 13	0	0
2	n	306	Total 2251	C 1378	N 409	O 451	S 13	0	0
2	o	306	Total 2251	C 1378	N 409	O 451	S 13	0	0
2	p	306	Total 2251	C 1378	N 409	O 451	S 13	0	0
2	q	306	Total 2251	C 1378	N 409	O 451	S 13	0	0
2	r	306	Total 2251	C 1378	N 409	O 451	S 13	0	0
2	s	306	Total 2251	C 1378	N 409	O 451	S 13	0	0
2	t	306	Total 2251	C 1378	N 409	O 451	S 13	0	0
2	u	306	Total 2251	C 1378	N 409	O 451	S 13	0	0
2	v	306	Total 2251	C 1378	N 409	O 451	S 13	0	0
2	w	306	Total 2251	C 1378	N 409	O 451	S 13	0	0
2	x	306	Total 2251	C 1378	N 409	O 451	S 13	0	0
2	y	306	Total 2251	C 1378	N 409	O 451	S 13	0	0
2	z	306	Total 2251	C 1378	N 409	O 451	S 13	0	0

- Molecule 3 is a protein called YecR.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	2	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	3	84	Total 647	C 401	N 114	O 126	S 6	0	0

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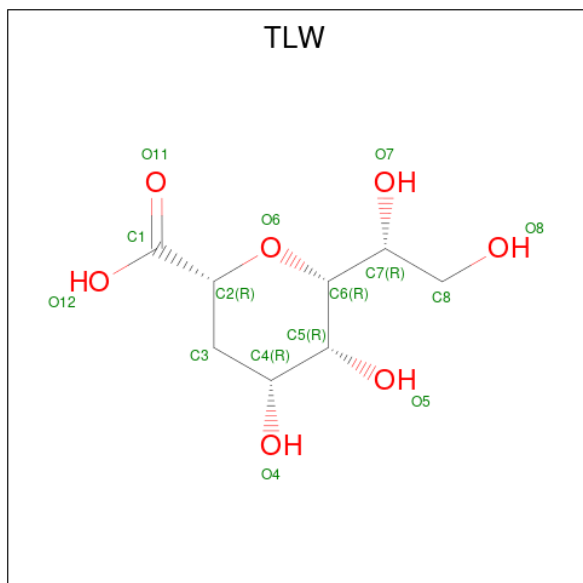
Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	5	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	6	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	7	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	8	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	9	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	10	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	11	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	12	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	13	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	14	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	15	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	16	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	17	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	18	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	19	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	20	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	21	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	22	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	23	84	Total 647	C 401	N 114	O 126	S 6	0	0
3	24	84	Total 647	C 401	N 114	O 126	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	25	84	Total	C	N	O	S	0	0
			647	401	114	126	6		
3	26	84	Total	C	N	O	S	0	0
			647	401	114	126	6		

- Molecule 4 is (2 {R},4 {R},5 {R},6 {R})-6-[(1 {R})-1,2-bis(oxidanyl)ethyl]-4,5-bis(oxidanyl)oxane-2-carboxylic acid (three-letter code: TLW) (formula: C<sub>8</sub>H<sub>14</sub>O<sub>7</sub>).



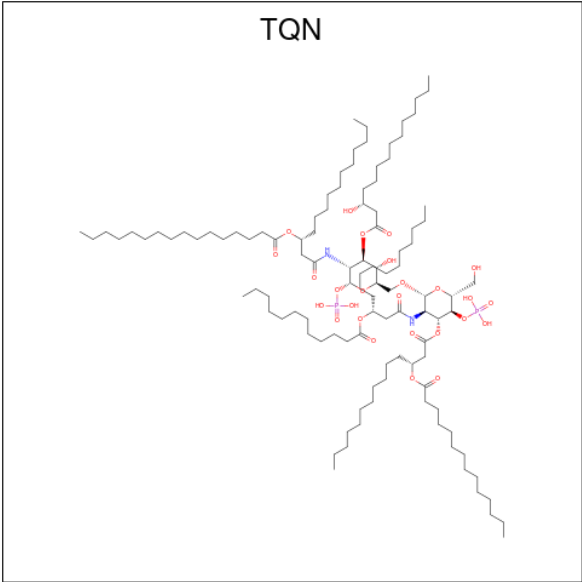
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	H	O	0
			25	8	10	7	
4	A	1	Total	C	H	O	0
			25	8	10	7	
4	B	1	Total	C	H	O	0
			25	8	10	7	
4	C	1	Total	C	H	O	0
			25	8	10	7	
4	D	1	Total	C	H	O	0
			25	8	10	7	
4	E	1	Total	C	H	O	0
			25	8	10	7	
4	F	1	Total	C	H	O	0
			25	8	10	7	
4	G	1	Total	C	H	O	0
			25	8	10	7	
4	H	1	Total	C	H	O	0
			25	8	10	7	

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Mol	Chain	Residues	Atoms				AltConf
4	I	1	Total	C	H	O	0
			25	8	10	7	
4	J	1	Total	C	H	O	0
			25	8	10	7	
4	K	1	Total	C	H	O	0
			25	8	10	7	
4	L	1	Total	C	H	O	0
			25	8	10	7	
4	M	1	Total	C	H	O	0
			25	8	10	7	
4	N	1	Total	C	H	O	0
			25	8	10	7	
4	O	1	Total	C	H	O	0
			25	8	10	7	
4	P	1	Total	C	H	O	0
			25	8	10	7	
4	Q	1	Total	C	H	O	0
			25	8	10	7	
4	R	1	Total	C	H	O	0
			25	8	10	7	
4	S	1	Total	C	H	O	0
			25	8	10	7	
4	T	1	Total	C	H	O	0
			25	8	10	7	
4	U	1	Total	C	H	O	0
			25	8	10	7	
4	V	1	Total	C	H	O	0
			25	8	10	7	
4	W	1	Total	C	H	O	0
			25	8	10	7	
4	X	1	Total	C	H	O	0
			25	8	10	7	
4	Y	1	Total	C	H	O	0
			25	8	10	7	

- Molecule 5 is [(3 {R})-1-[[[(2 {R},3 {R},4 {R},5 {S},6 {R})-6-[[[(2 {R},3 {R},4 {R},5 {S},6 {R})-3-[[[(3 {R})-3-dodecanoyloxytetradecanoyl]amino]-6-(hydroxymethyl)-5-phosphonooxy-4-[(3 {R})-3-tetradecanoyloxytetradecanoyl]oxy-oxan-2-yl]oxymethyl]-5-oxidanyl-4-[(3 {R})-3-oxidanyltetradecanoyl]oxy-2-phosphonooxy-oxan-3-yl]amino]-1-oxidanylidene-tetradecan-3-yl] hexadecanoate (three-letter code: TQN) (formula: C<sub>110</sub>H<sub>208</sub>N<sub>2</sub>O<sub>26</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			343	110	203	2	26	2	
5	B	1	Total	C	H	N	O	P	0
			343	110	203	2	26	2	
5	C	1	Total	C	H	N	O	P	0
			343	110	203	2	26	2	
5	D	1	Total	C	H	N	O	P	0
			343	110	203	2	26	2	
5	E	1	Total	C	H	N	O	P	0
			343	110	203	2	26	2	
5	F	1	Total	C	H	N	O	P	0
			343	110	203	2	26	2	
5	G	1	Total	C	H	N	O	P	0
			343	110	203	2	26	2	
5	H	1	Total	C	H	N	O	P	0
			343	110	203	2	26	2	
5	I	1	Total	C	H	N	O	P	0
			343	110	203	2	26	2	
5	J	1	Total	C	H	N	O	P	0
			343	110	203	2	26	2	
5	K	1	Total	C	H	N	O	P	0
			343	110	203	2	26	2	
5	L	1	Total	C	H	N	O	P	0
			343	110	203	2	26	2	
5	M	1	Total	C	H	N	O	P	0
			343	110	203	2	26	2	
5	N	1	Total	C	H	N	O	P	0
			343	110	203	2	26	2	

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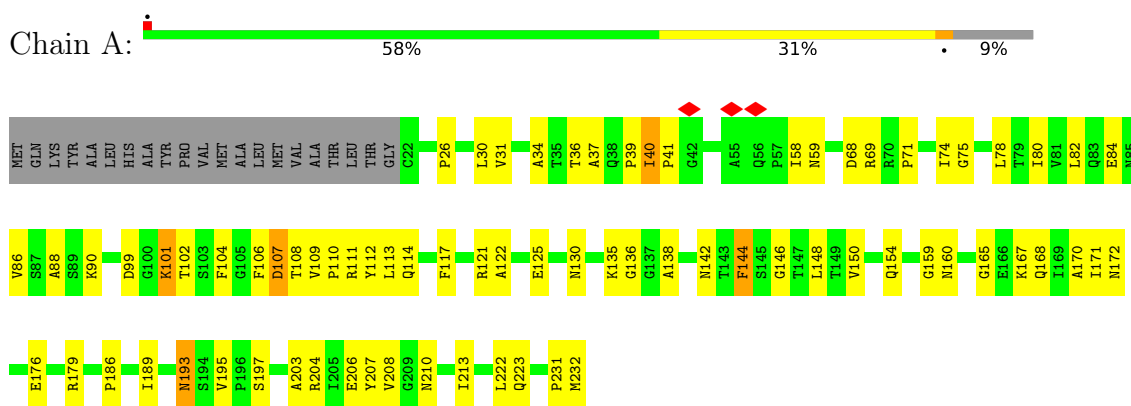
*Continued from previous page...*

Mol	Chain	Residues	Atoms						AltConf
5	O	1	Total 343	C 110	H 203	N 2	O 26	P 2	0
5	P	1	Total 343	C 110	H 203	N 2	O 26	P 2	0
5	Q	1	Total 343	C 110	H 203	N 2	O 26	P 2	0
5	R	1	Total 343	C 110	H 203	N 2	O 26	P 2	0
5	S	1	Total 343	C 110	H 203	N 2	O 26	P 2	0
5	T	1	Total 343	C 110	H 203	N 2	O 26	P 2	0
5	U	1	Total 343	C 110	H 203	N 2	O 26	P 2	0
5	V	1	Total 343	C 110	H 203	N 2	O 26	P 2	0
5	W	1	Total 343	C 110	H 203	N 2	O 26	P 2	0
5	X	1	Total 343	C 110	H 203	N 2	O 26	P 2	0
5	Y	1	Total 343	C 110	H 203	N 2	O 26	P 2	0
5	Z	1	Total 343	C 110	H 203	N 2	O 26	P 2	0

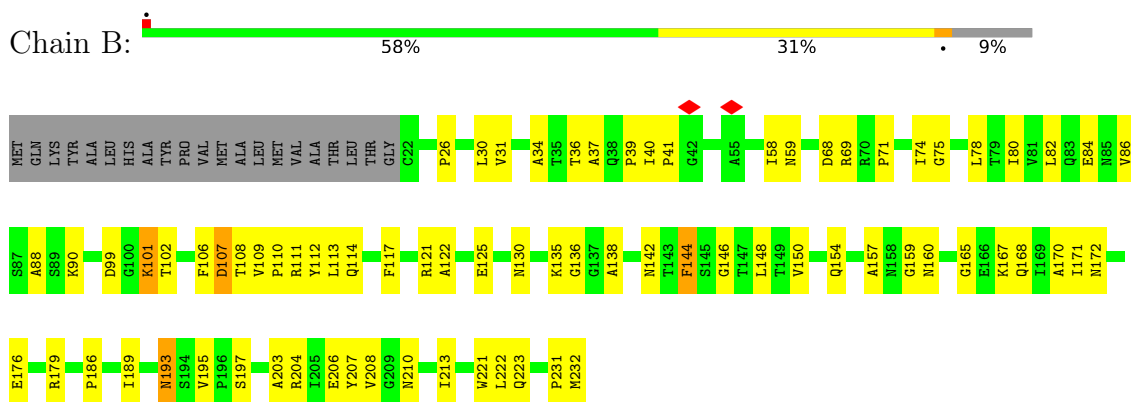
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

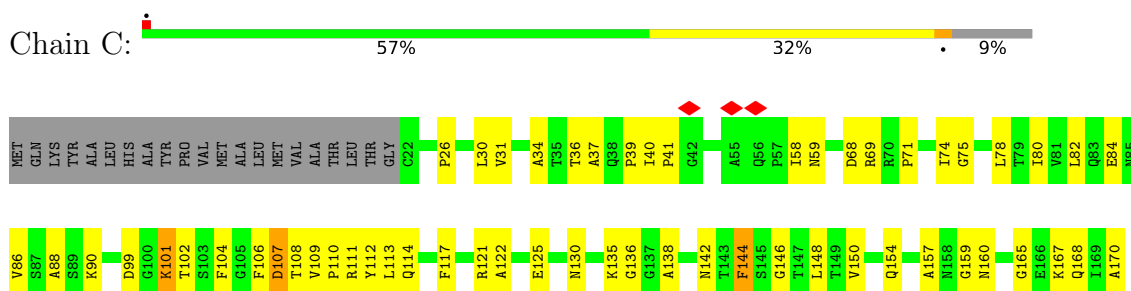
#### • Molecule 1: Flagellar L-ring protein



#### • Molecule 1: Flagellar L-ring protein



#### • Molecule 1: Flagellar L-ring protein

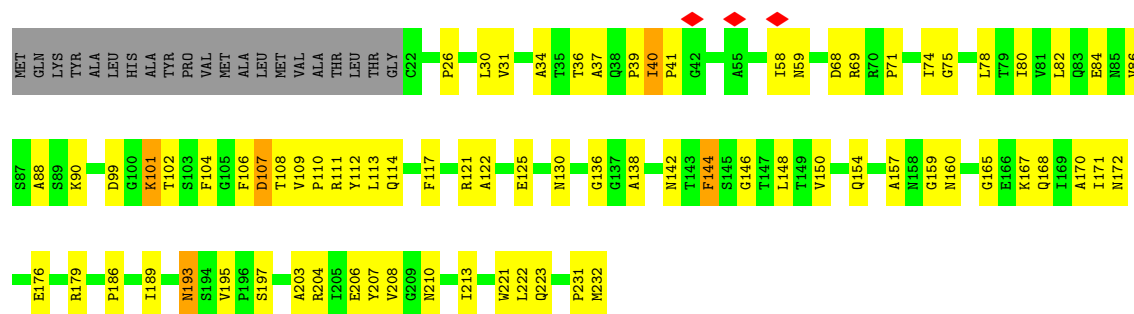




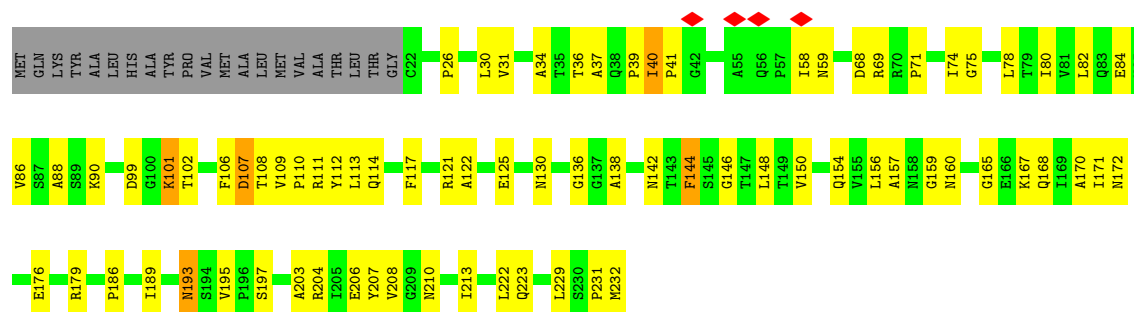




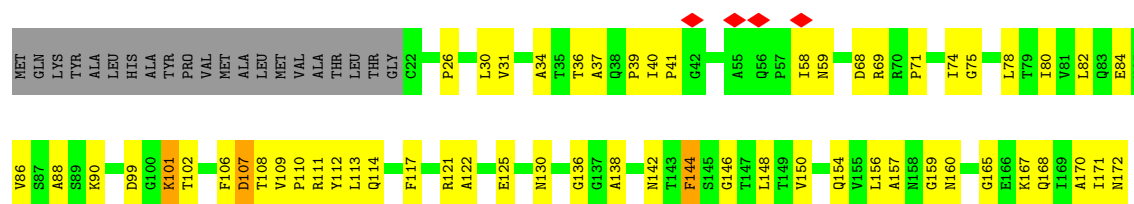
• Molecule 1: Flagellar L-ring protein



• Molecule 1: Flagellar L-ring protein

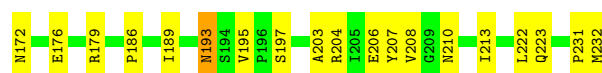
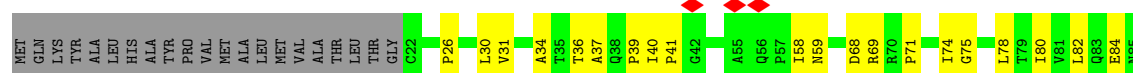


• Molecule 1: Flagellar L-ring protein





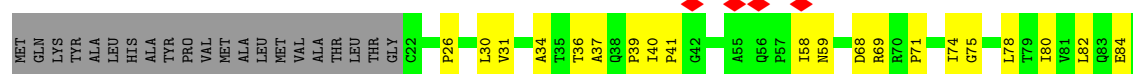
• Molecule 1: Flagellar L-ring protein



• Molecule 1: Flagellar L-ring protein

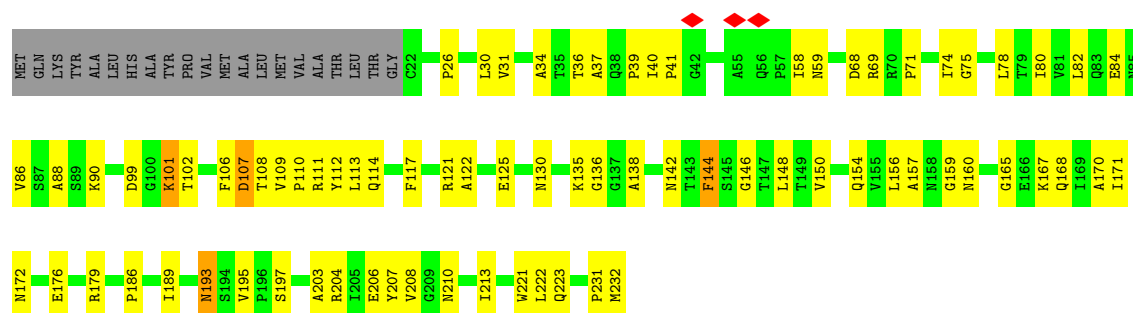


• Molecule 1: Flagellar L-ring protein

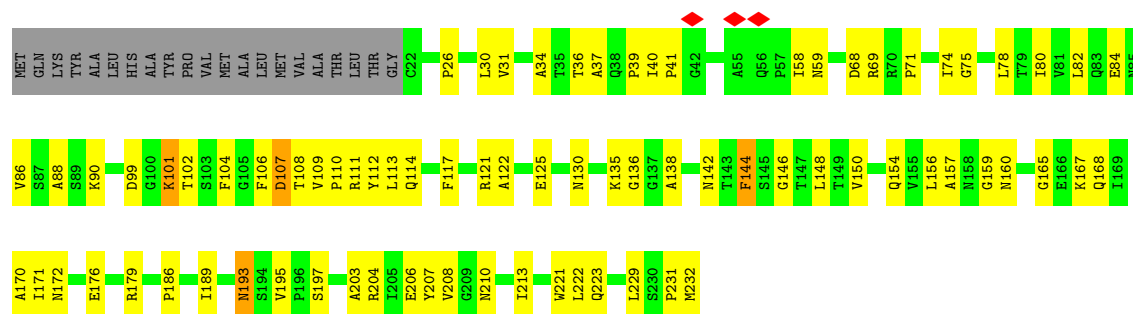


• Molecule 1: Flagellar L-ring protein

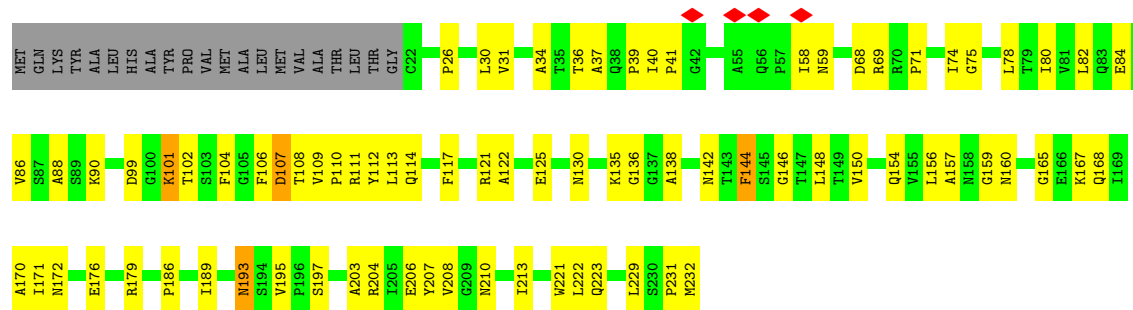




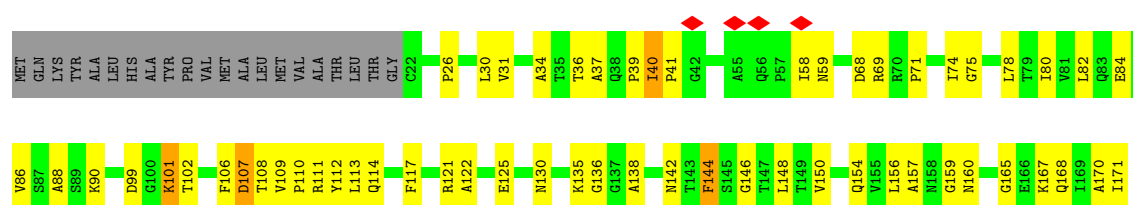
• Molecule 1: Flagellar L-ring protein



• Molecule 1: Flagellar L-ring protein



• Molecule 1: Flagellar L-ring protein





• Molecule 1: Flagellar L-ring protein



• Molecule 1: Flagellar L-ring protein

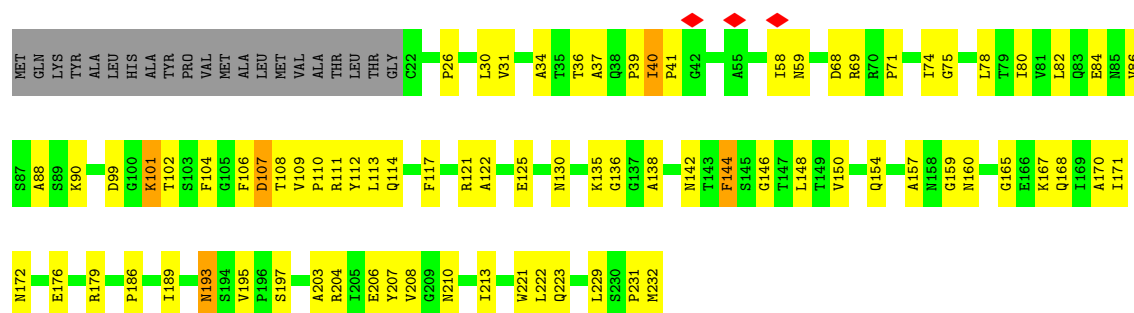


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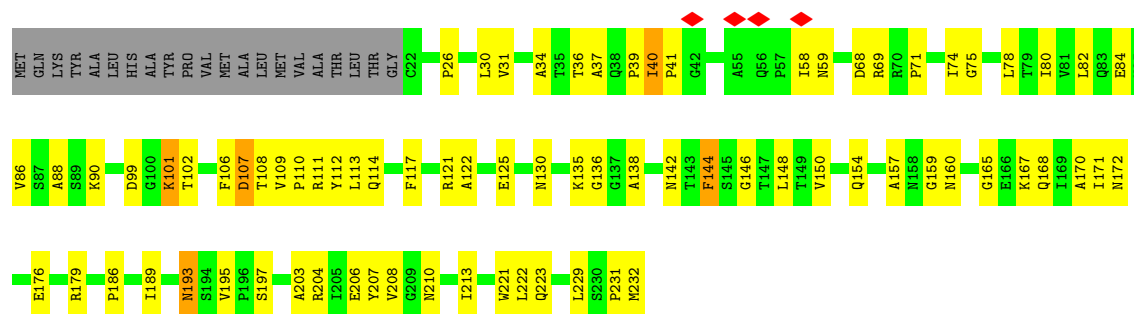


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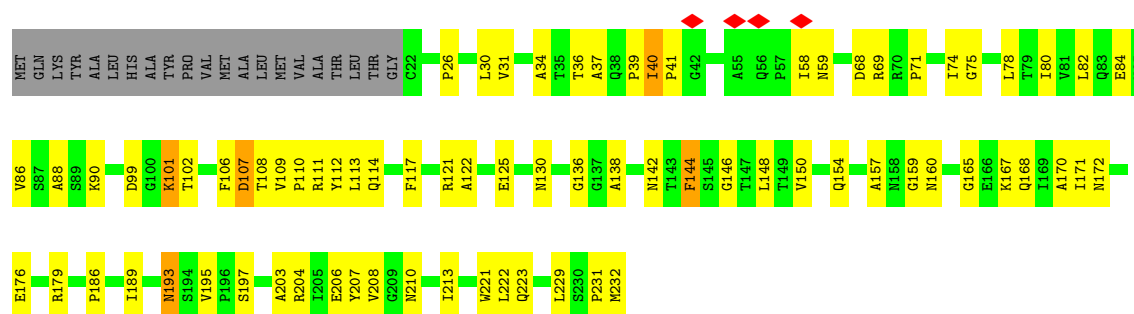




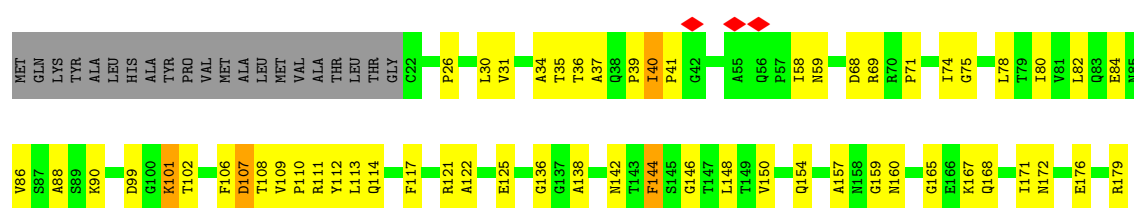
• Molecule 1: Flagellar L-ring protein



• Molecule 1: Flagellar L-ring protein

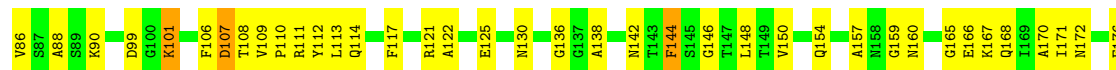


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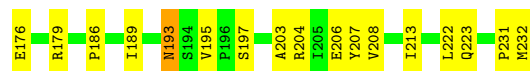




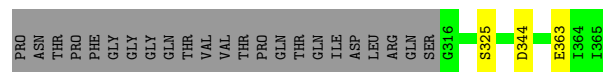
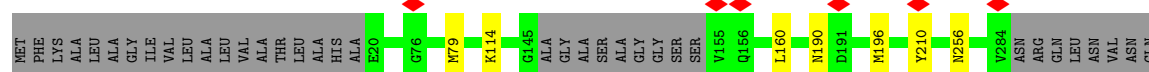
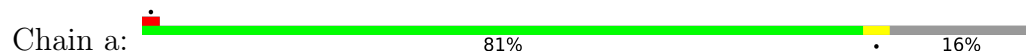
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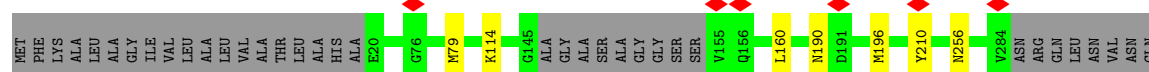
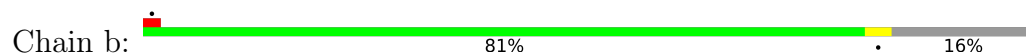
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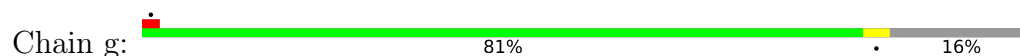


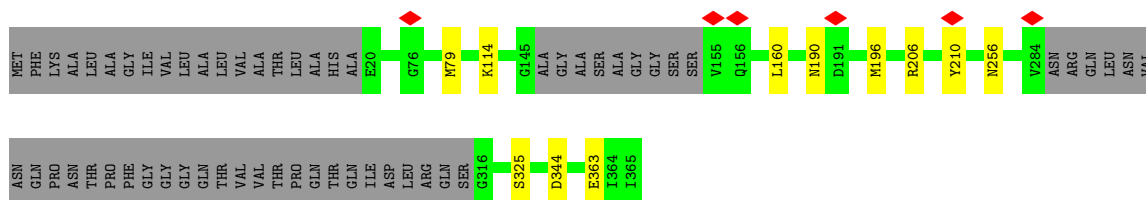
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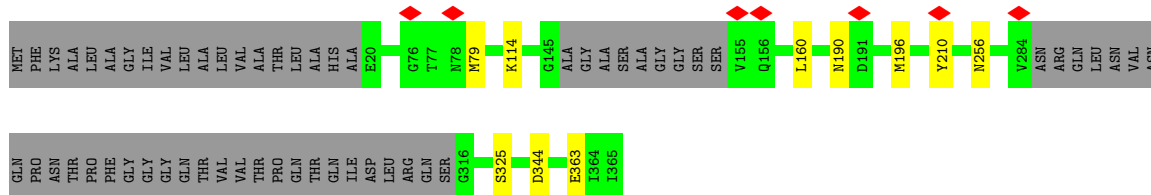
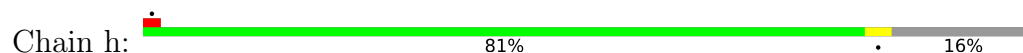
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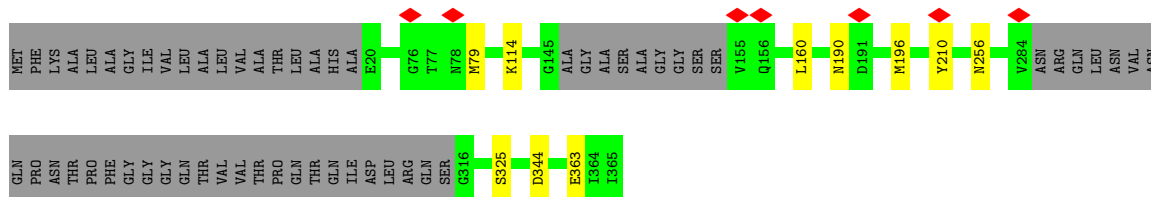
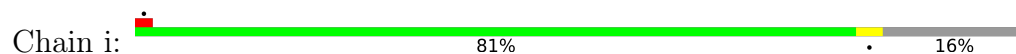




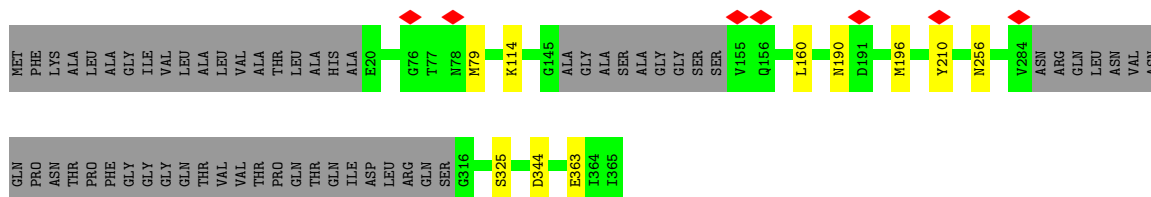
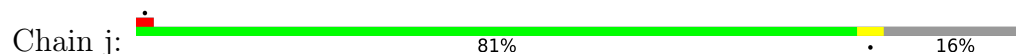
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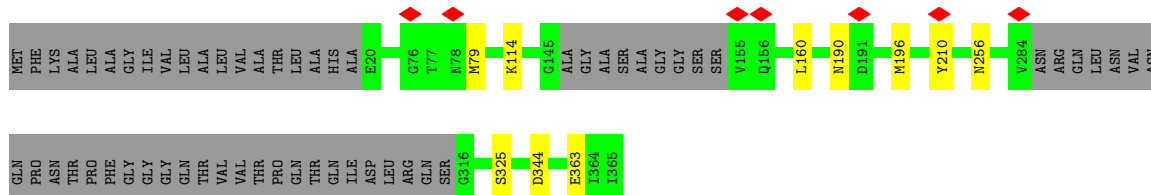
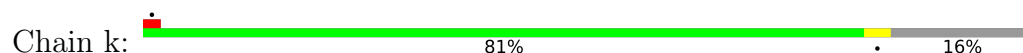
• Molecule 2: Flagellar P-ring protein



• Molecule 2: Flagellar P-ring protein

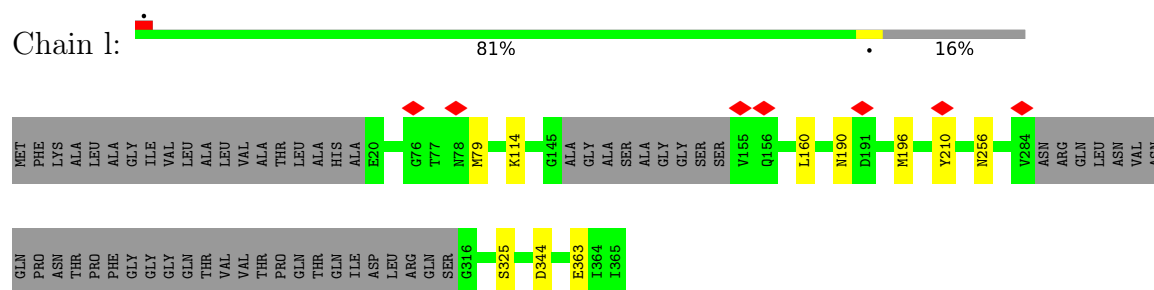


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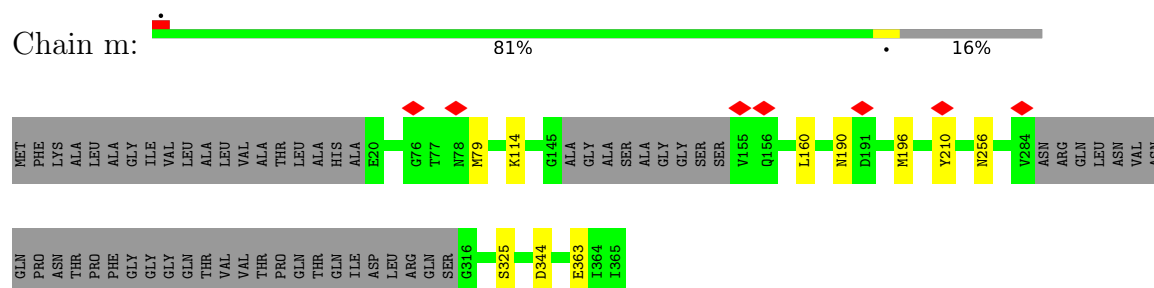




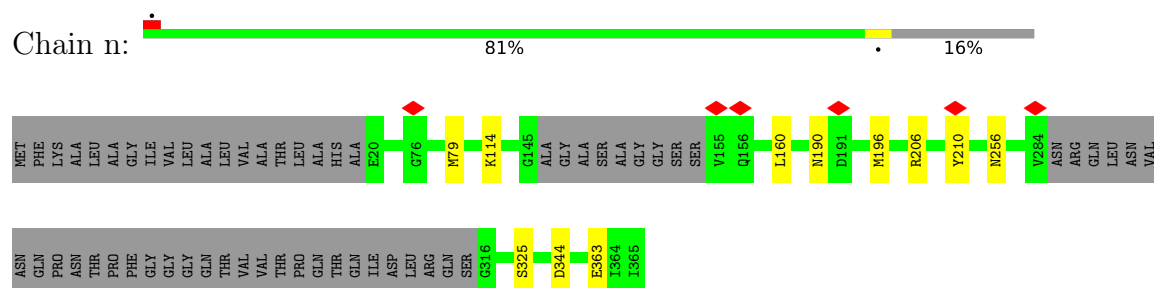
- Molecule 2: Flagellar P-ring protein



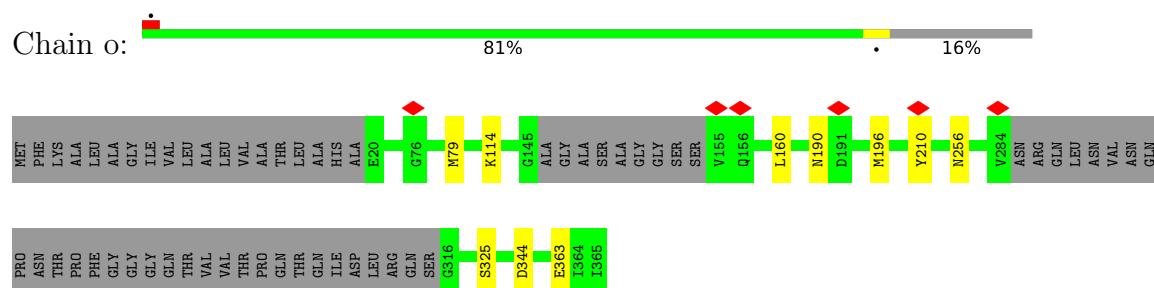
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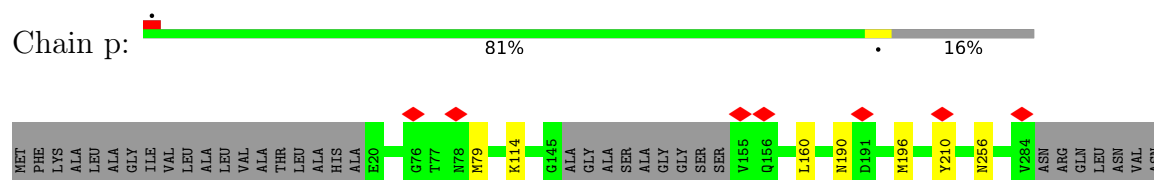
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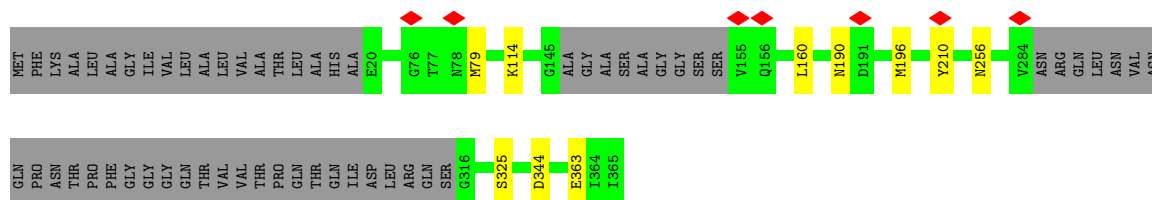
- Molecule 2: Flagellar P-ring protein



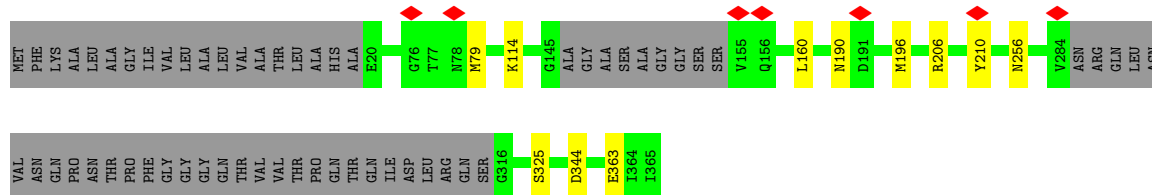
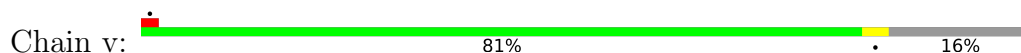
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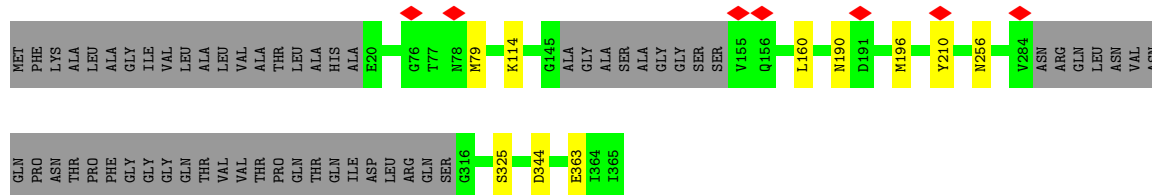
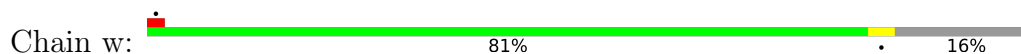




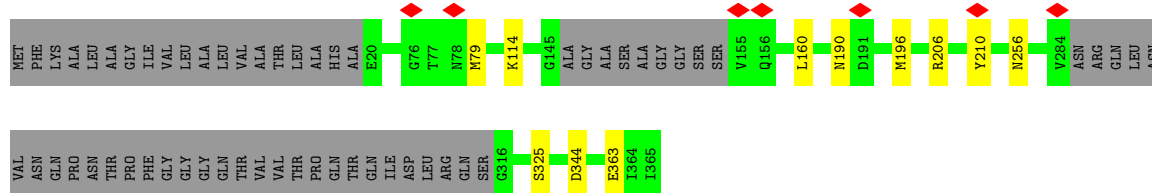
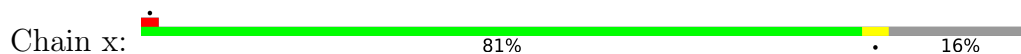
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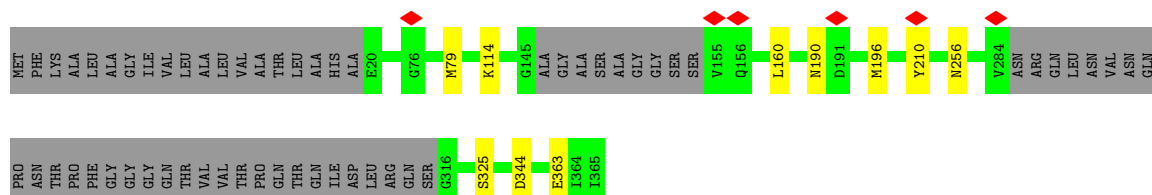
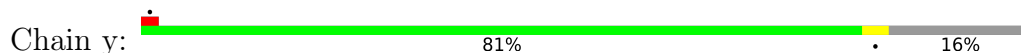
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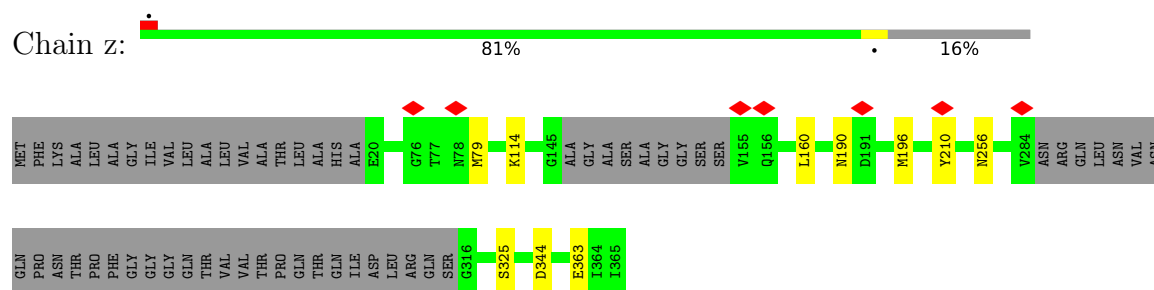
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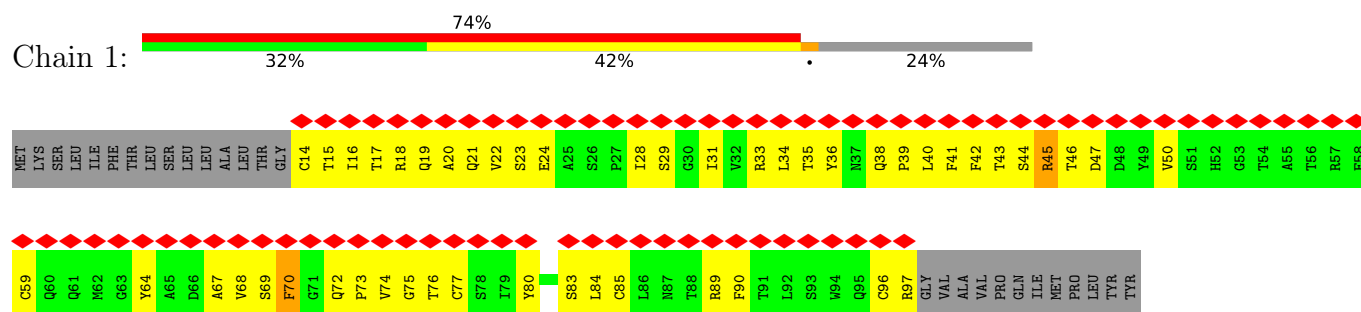
• Molecule 2: Flagellar P-ring protein



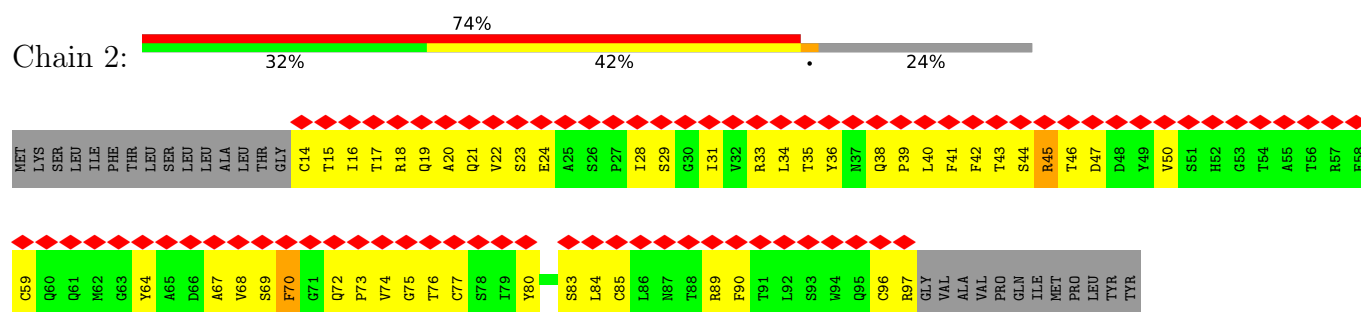
- Molecule 2: Flagellar P-ring protein



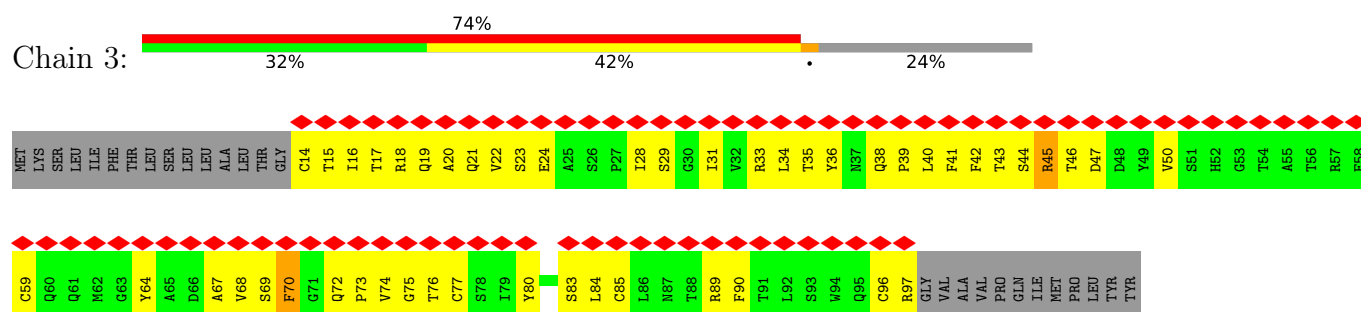
- Molecule 3: YecR



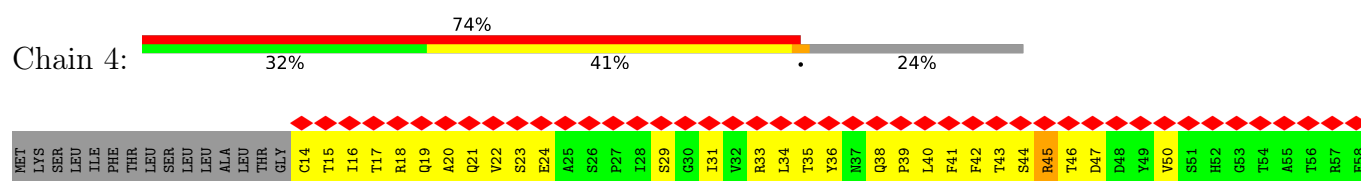
- Molecule 3: YecR

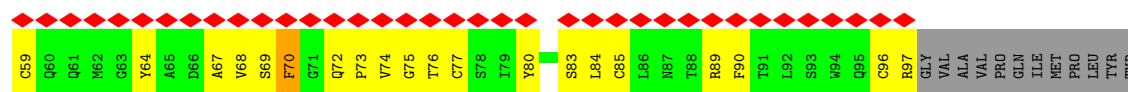


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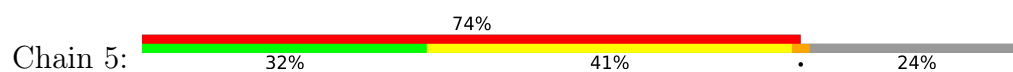


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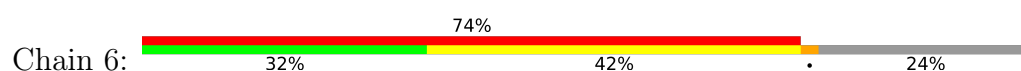




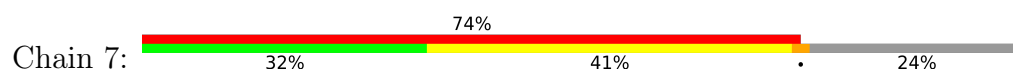
## • Molecule 3: YecR



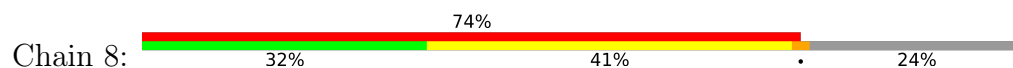
## • Molecule 3: YecR



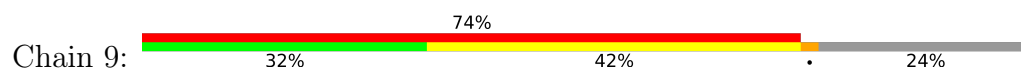
## • Molecule 3: YecR



## • Molecule 3: YecR

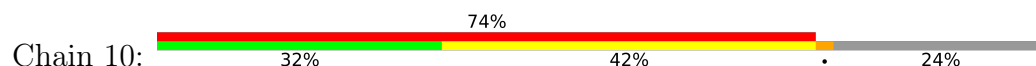


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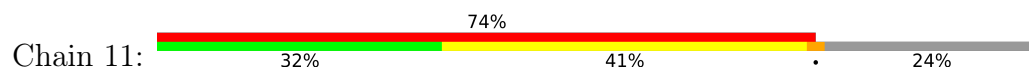




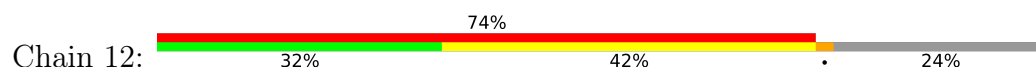
### • Molecule 3: YecR



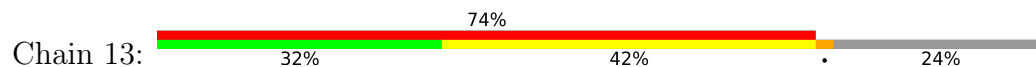
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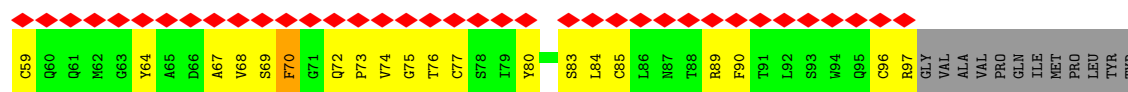
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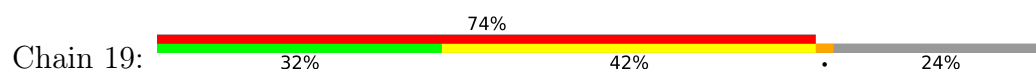
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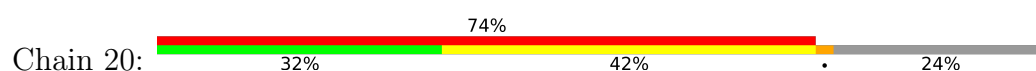
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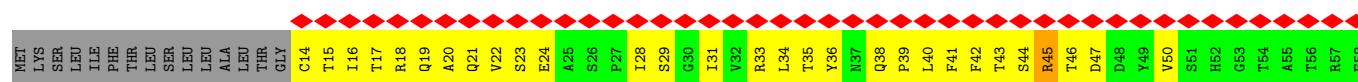
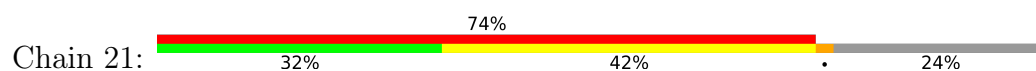
## • Molecule 3: YecR



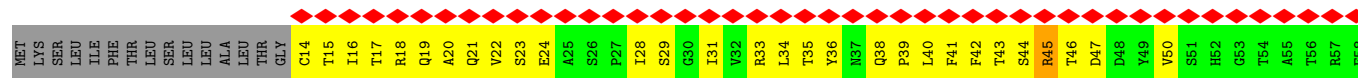
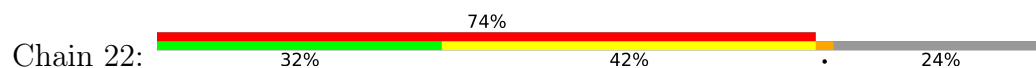
## • Molecule 3: YecR



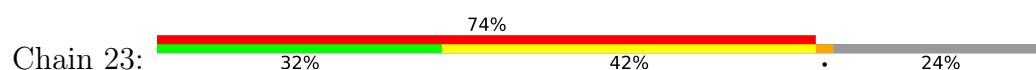
## • Molecule 3: YecR



## • Molecule 3: YecR



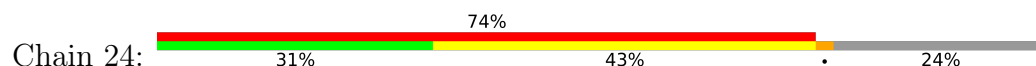
## • Molecule 3: YecR



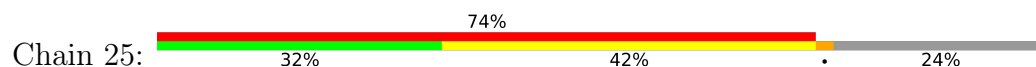




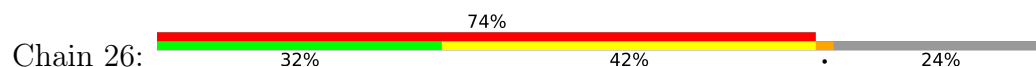
### • Molecule 3: YecR



### • Molecule 3: YecR



### • Molecule 3: YecR



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C26	Depositor
Number of particles used	31643	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	59	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	359.424, 359.424, 359.424	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TLW, TQN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.26	0/1614	0.49	0/2194
1	B	0.25	0/1614	0.49	0/2194
1	C	0.25	0/1614	0.49	0/2194
1	D	0.25	0/1614	0.49	0/2194
1	E	0.25	0/1614	0.49	0/2194
1	F	0.25	0/1614	0.49	0/2194
1	G	0.25	0/1614	0.49	0/2194
1	H	0.25	0/1614	0.49	0/2194
1	I	0.25	0/1614	0.49	0/2194
1	J	0.26	0/1614	0.49	0/2194
1	K	0.25	0/1614	0.49	0/2194
1	L	0.25	0/1614	0.49	0/2194
1	M	0.25	0/1614	0.49	0/2194
1	N	0.25	0/1614	0.49	0/2194
1	O	0.25	0/1614	0.49	0/2194
1	P	0.25	0/1614	0.49	0/2194
1	Q	0.25	0/1614	0.49	0/2194
1	R	0.26	0/1614	0.49	0/2194
1	S	0.25	0/1614	0.49	0/2194
1	T	0.25	0/1614	0.49	0/2194
1	U	0.25	0/1614	0.49	0/2194
1	V	0.25	0/1614	0.49	0/2194
1	W	0.25	0/1614	0.49	0/2194
1	X	0.25	0/1614	0.49	0/2194
1	Y	0.25	0/1614	0.49	0/2194
1	Z	0.25	0/1614	0.49	0/2194
2	a	0.24	0/2266	0.50	0/3071
2	b	0.24	0/2266	0.50	0/3071
2	c	0.24	0/2266	0.50	0/3071
2	d	0.24	0/2266	0.50	0/3071
2	e	0.24	0/2266	0.50	0/3071
2	f	0.24	0/2266	0.50	0/3071

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	g	0.24	0/2266	0.50	0/3071
2	h	0.24	0/2266	0.50	0/3071
2	i	0.24	0/2266	0.50	0/3071
2	j	0.24	0/2266	0.50	0/3071
2	k	0.24	0/2266	0.50	0/3071
2	l	0.24	0/2266	0.50	0/3071
2	m	0.24	0/2266	0.50	0/3071
2	n	0.24	0/2266	0.50	0/3071
2	o	0.24	0/2266	0.50	0/3071
2	p	0.24	0/2266	0.50	0/3071
2	q	0.24	0/2266	0.50	0/3071
2	r	0.24	0/2266	0.50	0/3071
2	s	0.24	0/2266	0.50	0/3071
2	t	0.24	0/2266	0.50	0/3071
2	u	0.24	0/2266	0.50	0/3071
2	v	0.24	0/2266	0.50	0/3071
2	w	0.24	0/2266	0.50	0/3071
2	x	0.24	0/2266	0.50	0/3071
2	y	0.24	0/2266	0.50	0/3071
2	z	0.24	0/2266	0.50	0/3071
3	1	0.24	0/660	0.53	0/897
3	10	0.24	0/660	0.53	0/897
3	11	0.24	0/660	0.53	0/897
3	12	0.24	0/660	0.53	0/897
3	13	0.24	0/660	0.53	0/897
3	14	0.23	0/660	0.53	0/897
3	15	0.23	0/660	0.53	0/897
3	16	0.24	0/660	0.53	0/897
3	17	0.23	0/660	0.53	0/897
3	18	0.23	0/660	0.53	0/897
3	19	0.24	0/660	0.53	0/897
3	2	0.24	0/660	0.53	0/897
3	20	0.23	0/660	0.53	0/897
3	21	0.24	0/660	0.53	0/897
3	22	0.24	0/660	0.53	0/897
3	23	0.23	0/660	0.53	0/897
3	24	0.24	0/660	0.53	0/897
3	25	0.24	0/660	0.53	0/897
3	26	0.24	0/660	0.53	0/897
3	3	0.23	0/660	0.53	0/897
3	4	0.24	0/660	0.53	0/897
3	5	0.23	0/660	0.53	0/897
3	6	0.23	0/660	0.53	0/897

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	7	0.24	0/660	0.53	0/897
3	8	0.24	0/660	0.53	0/897
3	9	0.23	0/660	0.53	0/897
All	All	0.25	0/118040	0.50	0/160212

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1581	0	1534	95	0
1	B	1581	0	1534	96	0
1	C	1581	0	1534	95	0
1	D	1581	0	1534	93	0
1	E	1581	0	1534	97	0
1	F	1581	0	1534	95	0
1	G	1581	0	1534	94	0
1	H	1581	0	1534	93	0
1	I	1581	0	1534	94	0
1	J	1581	0	1534	91	0
1	K	1581	0	1534	91	0
1	L	1581	0	1534	90	0
1	M	1581	0	1534	92	0
1	N	1581	0	1534	93	0
1	O	1581	0	1534	94	0
1	P	1581	0	1534	96	0
1	Q	1581	0	1534	96	0
1	R	1581	0	1534	97	0
1	S	1581	0	1534	97	0
1	T	1581	0	1534	97	0
1	U	1581	0	1534	96	0
1	V	1581	0	1534	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	1581	0	1534	94	0
1	X	1581	0	1534	92	0
1	Y	1581	0	1534	92	0
1	Z	1581	0	1534	90	0
2	a	2251	0	2289	0	0
2	b	2251	0	2289	0	0
2	c	2251	0	2289	0	0
2	d	2251	0	2289	0	0
2	e	2251	0	2289	0	0
2	f	2251	0	2289	0	0
2	g	2251	0	2289	0	0
2	h	2251	0	2289	0	0
2	i	2251	0	2289	0	0
2	j	2251	0	2289	0	0
2	k	2251	0	2289	0	0
2	l	2251	0	2289	0	0
2	m	2251	0	2289	0	0
2	n	2251	0	2289	0	0
2	o	2251	0	2289	0	0
2	p	2251	0	2289	0	0
2	q	2251	0	2289	0	0
2	r	2251	0	2289	0	0
2	s	2251	0	2289	0	0
2	t	2251	0	2289	0	0
2	u	2251	0	2289	0	0
2	v	2251	0	2289	0	0
2	w	2251	0	2289	0	0
2	x	2251	0	2289	0	0
2	y	2251	0	2289	0	0
2	z	2251	0	2289	0	0
3	1	647	0	616	47	0
3	10	647	0	616	46	0
3	11	647	0	616	44	0
3	12	647	0	616	45	0
3	13	647	0	616	46	0
3	14	647	0	616	46	0
3	15	647	0	616	46	0
3	16	647	0	616	46	0
3	17	647	0	616	47	0
3	18	647	0	616	47	0
3	19	647	0	616	47	0
3	2	647	0	616	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	20	647	0	616	47	0
3	21	647	0	616	48	0
3	22	647	0	616	45	0
3	23	647	0	616	46	0
3	24	647	0	616	48	0
3	25	647	0	616	45	0
3	26	647	0	616	46	0
3	3	647	0	616	47	0
3	4	647	0	616	44	0
3	5	647	0	616	45	0
3	6	647	0	616	46	0
3	7	647	0	616	45	0
3	8	647	0	616	45	0
3	9	647	0	616	45	0
4	A	30	20	0	0	0
4	B	15	10	0	0	0
4	C	15	10	0	0	0
4	D	15	10	0	0	0
4	E	15	10	0	0	0
4	F	15	10	0	0	0
4	G	15	10	0	0	0
4	H	15	10	0	0	0
4	I	15	10	0	0	0
4	J	15	10	0	0	0
4	K	15	10	0	0	0
4	L	15	10	0	0	0
4	M	15	10	0	0	0
4	N	15	10	0	0	0
4	O	15	10	0	0	0
4	P	15	10	0	0	0
4	Q	15	10	0	0	0
4	R	15	10	0	0	0
4	S	15	10	0	0	0
4	T	15	10	0	0	0
4	U	15	10	0	0	0
4	V	15	10	0	0	0
4	W	15	10	0	0	0
4	X	15	10	0	0	0
4	Y	15	10	0	0	0
5	A	140	203	0	2	0
5	B	140	203	0	2	0
5	C	140	203	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	140	203	0	2	0
5	E	140	203	0	2	0
5	F	140	203	0	2	0
5	G	140	203	0	2	0
5	H	140	203	0	2	0
5	I	140	203	0	2	0
5	J	140	203	0	2	0
5	K	140	203	0	2	0
5	L	140	203	0	2	0
5	M	140	203	0	2	0
5	N	140	203	0	2	0
5	O	140	203	0	2	0
5	P	140	203	0	2	0
5	Q	140	203	0	2	0
5	R	140	203	0	2	0
5	S	140	203	0	2	0
5	T	140	203	0	2	0
5	U	140	203	0	2	0
5	V	140	203	0	2	0
5	W	140	203	0	2	0
5	X	140	203	0	2	0
5	Y	140	203	0	2	0
5	Z	140	203	0	2	0
All	All	120484	5538	115414	2873	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (2873) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:171:ILE:HD12	1:O:88:ALA:HB1	1.48	0.96
1:N:171:ILE:HD12	1:P:88:ALA:HB1	1.48	0.96
1:L:171:ILE:HD12	1:N:88:ALA:HB1	1.48	0.96
1:O:171:ILE:HD12	1:Q:88:ALA:HB1	1.48	0.95
1:I:171:ILE:HD12	1:K:88:ALA:HB1	1.48	0.95
1:J:171:ILE:HD12	1:L:88:ALA:HB1	1.49	0.95
1:K:171:ILE:HD12	1:M:88:ALA:HB1	1.49	0.95
1:B:88:ALA:HB1	1:Z:171:ILE:HD12	1.46	0.94
1:P:171:ILE:HD12	1:R:88:ALA:HB1	1.49	0.94
1:X:171:ILE:HD12	1:Z:88:ALA:HB1	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:171:ILE:HD12	1:J:88:ALA:HB1	1.48	0.94
1:Q:171:ILE:HD12	1:S:88:ALA:HB1	1.49	0.94
1:R:171:ILE:HD12	1:T:88:ALA:HB1	1.48	0.94
1:A:171:ILE:HD12	1:C:88:ALA:HB1	1.48	0.93
1:S:171:ILE:HD12	1:U:88:ALA:HB1	1.47	0.93
1:B:171:ILE:HD12	1:D:88:ALA:HB1	1.48	0.93
1:G:171:ILE:HD12	1:I:88:ALA:HB1	1.47	0.93
1:T:171:ILE:HD12	1:V:88:ALA:HB1	1.48	0.92
1:U:171:ILE:HD12	1:W:88:ALA:HB1	1.48	0.92
1:V:171:ILE:HD12	1:X:88:ALA:HB1	1.49	0.92
1:C:171:ILE:HD12	1:E:88:ALA:HB1	1.48	0.92
1:W:171:ILE:HD12	1:Y:88:ALA:HB1	1.48	0.92
1:D:171:ILE:HD12	1:F:88:ALA:HB1	1.49	0.92
1:F:171:ILE:HD12	1:H:88:ALA:HB1	1.47	0.92
1:E:171:ILE:HD12	1:G:88:ALA:HB1	1.48	0.91
1:A:88:ALA:HB1	1:Y:171:ILE:HD12	1.52	0.89
3:6:22:VAL:HG22	3:6:34:LEU:HD22	1.56	0.88
3:23:22:VAL:HG22	3:23:34:LEU:HD22	1.56	0.88
3:7:22:VAL:HG22	3:7:34:LEU:HD22	1.56	0.88
3:24:22:VAL:HG22	3:24:34:LEU:HD22	1.56	0.88
3:10:22:VAL:HG22	3:10:34:LEU:HD22	1.56	0.88
3:11:22:VAL:HG22	3:11:34:LEU:HD22	1.56	0.88
3:20:22:VAL:HG22	3:20:34:LEU:HD22	1.56	0.88
3:2:22:VAL:HG22	3:2:34:LEU:HD22	1.56	0.88
3:5:22:VAL:HG22	3:5:34:LEU:HD22	1.56	0.88
3:19:22:VAL:HG22	3:19:34:LEU:HD22	1.56	0.88
3:9:22:VAL:HG22	3:9:34:LEU:HD22	1.56	0.88
3:1:22:VAL:HG22	3:1:34:LEU:HD22	1.56	0.88
3:3:22:VAL:HG22	3:3:34:LEU:HD22	1.56	0.88
3:21:22:VAL:HG22	3:21:34:LEU:HD22	1.56	0.88
3:22:22:VAL:HG22	3:22:34:LEU:HD22	1.56	0.88
3:25:22:VAL:HG22	3:25:34:LEU:HD22	1.56	0.88
3:8:22:VAL:HG22	3:8:34:LEU:HD22	1.56	0.88
3:12:22:VAL:HG22	3:12:34:LEU:HD22	1.56	0.88
3:14:22:VAL:HG22	3:14:34:LEU:HD22	1.56	0.88
3:15:22:VAL:HG22	3:15:34:LEU:HD22	1.56	0.88
3:18:22:VAL:HG22	3:18:34:LEU:HD22	1.56	0.88
3:4:22:VAL:HG22	3:4:34:LEU:HD22	1.56	0.87
3:16:22:VAL:HG22	3:16:34:LEU:HD22	1.56	0.87
3:13:22:VAL:HG22	3:13:34:LEU:HD22	1.56	0.87
3:26:22:VAL:HG22	3:26:34:LEU:HD22	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:17:22:VAL:HG22	3:17:34:LEU:HD22	1.56	0.87
3:9:17:THR:OG1	3:9:43:THR:O	1.98	0.82
3:21:17:THR:OG1	3:21:43:THR:O	1.98	0.82
3:20:17:THR:OG1	3:20:43:THR:O	1.98	0.82
3:8:17:THR:OG1	3:8:43:THR:O	1.98	0.82
3:10:17:THR:OG1	3:10:43:THR:O	1.98	0.82
3:25:17:THR:OG1	3:25:43:THR:O	1.98	0.82
3:15:17:THR:OG1	3:15:43:THR:O	1.98	0.81
3:26:17:THR:OG1	3:26:43:THR:O	1.98	0.81
3:4:17:THR:OG1	3:4:43:THR:O	1.98	0.81
3:14:17:THR:OG1	3:14:43:THR:O	1.98	0.81
3:5:17:THR:OG1	3:5:43:THR:O	1.98	0.81
3:19:17:THR:OG1	3:19:43:THR:O	1.98	0.81
3:22:17:THR:OG1	3:22:43:THR:O	1.98	0.81
3:13:17:THR:OG1	3:13:43:THR:O	1.98	0.81
3:16:17:THR:OG1	3:16:43:THR:O	1.98	0.81
3:3:17:THR:OG1	3:3:43:THR:O	1.98	0.81
3:24:17:THR:OG1	3:24:43:THR:O	1.98	0.81
1:W:172:ASN:OD1	1:Y:138:ALA:HB1	1.81	0.81
3:11:17:THR:OG1	3:11:43:THR:O	1.98	0.81
3:1:17:THR:OG1	3:1:43:THR:O	1.98	0.81
3:7:17:THR:OG1	3:7:43:THR:O	1.98	0.81
3:6:17:THR:OG1	3:6:43:THR:O	1.98	0.80
3:17:17:THR:OG1	3:17:43:THR:O	1.98	0.80
1:Y:167:LYS:HD3	1:Z:203:ALA:HB3	1.62	0.80
3:12:17:THR:OG1	3:12:43:THR:O	1.98	0.80
3:18:17:THR:OG1	3:18:43:THR:O	1.98	0.80
3:23:17:THR:OG1	3:23:43:THR:O	1.98	0.80
1:B:138:ALA:HB1	1:Z:172:ASN:OD1	1.82	0.80
3:2:17:THR:OG1	3:2:43:THR:O	1.98	0.79
1:M:82:LEU:HA	1:M:197:SER:HB3	1.64	0.79
1:O:82:LEU:HA	1:O:197:SER:HB3	1.64	0.79
3:16:68:VAL:HG21	3:16:97:ARG:HH21	1.48	0.79
1:N:82:LEU:HA	1:N:197:SER:HB3	1.65	0.79
1:Q:82:LEU:HA	1:Q:197:SER:HB3	1.64	0.79
1:L:82:LEU:HA	1:L:197:SER:HB3	1.65	0.79
1:P:82:LEU:HA	1:P:197:SER:HB3	1.65	0.79
1:J:82:LEU:HA	1:J:197:SER:HB3	1.64	0.79
1:K:82:LEU:HA	1:K:197:SER:HB3	1.65	0.79
1:R:82:LEU:HA	1:R:197:SER:HB3	1.65	0.79
1:S:82:LEU:HA	1:S:197:SER:HB3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:82:LEU:HA	1:T:197:SER:HB3	1.64	0.79
1:U:82:LEU:HA	1:U:197:SER:HB3	1.64	0.79
3:14:68:VAL:HG21	3:14:97:ARG:HH21	1.48	0.79
5:G:301:TQN:C15	1:H:112:TYR:HB2	2.13	0.79
5:W:301:TQN:C15	1:X:112:TYR:HB2	2.13	0.79
5:Y:301:TQN:C15	1:Z:112:TYR:HB2	2.13	0.79
1:A:112:TYR:HB2	5:Z:301:TQN:C15	2.13	0.79
5:A:302:TQN:C15	1:B:112:TYR:HB2	2.13	0.79
5:V:301:TQN:C15	1:W:112:TYR:HB2	2.13	0.79
5:X:301:TQN:C15	1:Y:112:TYR:HB2	2.13	0.79
3:18:68:VAL:HG21	3:18:97:ARG:HH21	1.48	0.78
3:21:68:VAL:HG21	3:21:97:ARG:HH21	1.48	0.78
5:B:301:TQN:C15	1:C:112:TYR:HB2	2.13	0.78
1:I:82:LEU:HA	1:I:197:SER:HB3	1.64	0.78
1:V:82:LEU:HA	1:V:197:SER:HB3	1.65	0.78
5:C:301:TQN:C15	1:D:112:TYR:HB2	2.13	0.78
5:D:301:TQN:C15	1:E:112:TYR:HB2	2.13	0.78
5:U:301:TQN:C15	1:V:112:TYR:HB2	2.13	0.78
3:14:47:ASP:OD1	3:14:50:VAL:N	2.13	0.78
3:19:68:VAL:HG21	3:19:97:ARG:HH21	1.48	0.78
1:H:82:LEU:HA	1:H:197:SER:HB3	1.64	0.78
1:W:82:LEU:HA	1:W:197:SER:HB3	1.65	0.78
3:1:68:VAL:HG21	3:1:97:ARG:HH21	1.48	0.78
3:11:68:VAL:HG21	3:11:97:ARG:HH21	1.48	0.78
5:E:301:TQN:C15	1:F:112:TYR:HB2	2.13	0.78
5:J:301:TQN:C15	1:K:112:TYR:HB2	2.13	0.78
5:T:301:TQN:C15	1:U:112:TYR:HB2	2.13	0.78
3:5:68:VAL:HG21	3:5:97:ARG:HH21	1.48	0.78
3:13:47:ASP:OD1	3:13:50:VAL:N	2.13	0.78
1:X:82:LEU:HA	1:X:197:SER:HB3	1.65	0.78
3:13:68:VAL:HG21	3:13:97:ARG:HH21	1.48	0.78
3:23:68:VAL:HG21	3:23:97:ARG:HH21	1.48	0.78
5:S:301:TQN:C15	1:T:112:TYR:HB2	2.13	0.78
3:9:68:VAL:HG21	3:9:97:ARG:HH21	1.48	0.78
1:G:82:LEU:HA	1:G:197:SER:HB3	1.64	0.78
5:I:301:TQN:C15	1:J:112:TYR:HB2	2.13	0.78
5:R:301:TQN:C15	1:S:112:TYR:HB2	2.13	0.78
1:T:172:ASN:OD1	1:V:138:ALA:HB1	1.84	0.78
5:F:301:TQN:C15	1:G:112:TYR:HB2	2.13	0.78
1:A:172:ASN:OD1	1:C:138:ALA:HB1	1.83	0.78
3:12:68:VAL:HG21	3:12:97:ARG:HH21	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:301:TQN:C15	1:M:112:TYR:HB2	2.13	0.78
5:Q:301:TQN:C15	1:R:112:TYR:HB2	2.13	0.78
1:Y:82:LEU:HA	1:Y:197:SER:HB3	1.65	0.78
5:H:301:TQN:C15	1:I:112:TYR:HB2	2.13	0.77
5:P:301:TQN:C15	1:Q:112:TYR:HB2	2.13	0.77
5:O:301:TQN:C15	1:P:112:TYR:HB2	2.13	0.77
1:Z:82:LEU:HA	1:Z:197:SER:HB3	1.64	0.77
3:2:68:VAL:HG21	3:2:97:ARG:HH21	1.48	0.77
3:4:68:VAL:HG21	3:4:97:ARG:HH21	1.48	0.77
1:C:82:LEU:HA	1:C:197:SER:HB3	1.64	0.77
5:K:301:TQN:C15	1:L:112:TYR:HB2	2.13	0.77
5:M:301:TQN:C15	1:N:112:TYR:HB2	2.13	0.77
5:N:301:TQN:C15	1:O:112:TYR:HB2	2.13	0.77
1:B:82:LEU:HA	1:B:197:SER:HB3	1.65	0.77
1:F:82:LEU:HA	1:F:197:SER:HB3	1.65	0.77
1:A:82:LEU:HA	1:A:197:SER:HB3	1.64	0.77
3:23:47:ASP:OD1	3:23:50:VAL:N	2.13	0.77
1:D:82:LEU:HA	1:D:197:SER:HB3	1.65	0.77
3:15:47:ASP:OD1	3:15:50:VAL:N	2.13	0.77
3:24:47:ASP:OD1	3:24:50:VAL:N	2.13	0.77
1:S:172:ASN:OD1	1:U:138:ALA:HB1	1.84	0.77
3:6:68:VAL:HG21	3:6:97:ARG:HH21	1.48	0.77
3:7:68:VAL:HG21	3:7:97:ARG:HH21	1.48	0.77
3:17:68:VAL:HG21	3:17:97:ARG:HH21	1.48	0.77
3:20:68:VAL:HG21	3:20:97:ARG:HH21	1.48	0.77
1:E:82:LEU:HA	1:E:197:SER:HB3	1.65	0.77
1:U:172:ASN:OD1	1:W:138:ALA:HB1	1.85	0.77
3:22:47:ASP:OD1	3:22:50:VAL:N	2.13	0.77
3:25:68:VAL:HG21	3:25:97:ARG:HH21	1.48	0.77
3:19:47:ASP:OD1	3:19:50:VAL:N	2.13	0.77
3:8:47:ASP:OD1	3:8:50:VAL:N	2.13	0.76
3:26:68:VAL:HG21	3:26:97:ARG:HH21	1.48	0.76
1:F:172:ASN:OD1	1:H:138:ALA:HB1	1.84	0.76
3:24:68:VAL:HG21	3:24:97:ARG:HH21	1.48	0.76
1:N:172:ASN:OD1	1:P:138:ALA:HB1	1.84	0.76
1:Q:172:ASN:OD1	1:S:138:ALA:HB1	1.85	0.76
1:V:172:ASN:OD1	1:X:138:ALA:HB1	1.86	0.76
3:8:68:VAL:HG21	3:8:97:ARG:HH21	1.48	0.76
3:12:47:ASP:OD1	3:12:50:VAL:N	2.13	0.76
3:15:68:VAL:HG21	3:15:97:ARG:HH21	1.48	0.76
1:O:172:ASN:OD1	1:Q:138:ALA:HB1	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:10:47:ASP:OD1	3:10:50:VAL:N	2.13	0.76
3:11:47:ASP:OD1	3:11:50:VAL:N	2.13	0.76
1:B:172:ASN:OD1	1:D:138:ALA:HB1	1.84	0.76
1:H:172:ASN:OD1	1:J:138:ALA:HB1	1.84	0.76
3:10:68:VAL:HG21	3:10:97:ARG:HH21	1.48	0.76
1:G:172:ASN:OD1	1:I:138:ALA:HB1	1.84	0.76
1:M:172:ASN:OD1	1:O:138:ALA:HB1	1.84	0.76
1:E:172:ASN:OD1	1:G:138:ALA:HB1	1.84	0.76
3:3:68:VAL:HG21	3:3:97:ARG:HH21	1.48	0.76
1:C:172:ASN:OD1	1:E:138:ALA:HB1	1.85	0.76
1:L:172:ASN:OD1	1:N:138:ALA:HB1	1.84	0.76
3:18:47:ASP:OD1	3:18:50:VAL:N	2.13	0.76
1:U:125:GLU:HB3	1:V:108:THR:HB	1.68	0.76
1:M:125:GLU:HB3	1:N:108:THR:HB	1.68	0.75
1:P:172:ASN:OD1	1:R:138:ALA:HB1	1.85	0.75
1:Q:125:GLU:HB3	1:R:108:THR:HB	1.69	0.75
1:T:179:ARG:HG3	1:T:206:GLU:HB3	1.69	0.75
1:Y:179:ARG:HG3	1:Y:206:GLU:HB3	1.69	0.75
3:2:47:ASP:OD1	3:2:50:VAL:N	2.13	0.75
3:22:68:VAL:HG21	3:22:97:ARG:HH21	1.48	0.75
3:25:47:ASP:OD1	3:25:50:VAL:N	2.13	0.75
1:R:172:ASN:OD1	1:T:138:ALA:HB1	1.85	0.75
1:S:179:ARG:HG3	1:S:206:GLU:HB3	1.68	0.75
1:Z:179:ARG:HG3	1:Z:206:GLU:HB3	1.68	0.75
1:A:108:THR:HB	1:Z:125:GLU:HB3	1.68	0.75
1:X:125:GLU:HB3	1:Y:108:THR:HB	1.68	0.75
1:X:179:ARG:HG3	1:X:206:GLU:HB3	1.69	0.75
1:R:125:GLU:HB3	1:S:108:THR:HB	1.69	0.75
1:W:125:GLU:HB3	1:X:108:THR:HB	1.69	0.75
1:A:125:GLU:HB3	1:B:108:THR:HB	1.68	0.75
3:1:47:ASP:OD1	3:1:50:VAL:N	2.13	0.75
1:I:172:ASN:OD1	1:K:138:ALA:HB1	1.85	0.75
1:S:125:GLU:HB3	1:T:108:THR:HB	1.68	0.75
1:T:125:GLU:HB3	1:U:108:THR:HB	1.69	0.75
1:U:179:ARG:HG3	1:U:206:GLU:HB3	1.68	0.75
1:D:172:ASN:OD1	1:F:138:ALA:HB1	1.85	0.75
1:J:172:ASN:OD1	1:L:138:ALA:HB1	1.85	0.75
1:K:172:ASN:OD1	1:M:138:ALA:HB1	1.85	0.75
1:N:125:GLU:HB3	1:O:108:THR:HB	1.69	0.75
1:O:125:GLU:HB3	1:P:108:THR:HB	1.69	0.75
1:B:136:GLY:HA3	1:Z:213:ILE:HG23	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:ARG:HG3	1:E:206:GLU:HB3	1.68	0.75
1:Q:30:LEU:HD23	1:Q:30:LEU:H	1.52	0.75
3:9:47:ASP:OD1	3:9:50:VAL:N	2.13	0.75
3:16:47:ASP:OD1	3:16:50:VAL:N	2.13	0.75
1:D:179:ARG:HG3	1:D:206:GLU:HB3	1.69	0.75
1:M:30:LEU:HD23	1:M:30:LEU:H	1.52	0.75
1:N:30:LEU:HD23	1:N:30:LEU:H	1.52	0.75
3:26:47:ASP:OD1	3:26:50:VAL:N	2.13	0.74
1:K:125:GLU:HB3	1:L:108:THR:HB	1.69	0.74
1:O:30:LEU:HD23	1:O:30:LEU:H	1.52	0.74
1:R:30:LEU:HD23	1:R:30:LEU:H	1.52	0.74
1:R:179:ARG:HG3	1:R:206:GLU:HB3	1.69	0.74
3:20:47:ASP:OD1	3:20:50:VAL:N	2.13	0.74
1:B:125:GLU:HB3	1:C:108:THR:HB	1.69	0.74
1:P:30:LEU:H	1:P:30:LEU:HD23	1.52	0.74
1:A:179:ARG:HG3	1:A:206:GLU:HB3	1.68	0.74
3:7:47:ASP:OD1	3:7:50:VAL:N	2.13	0.74
1:C:179:ARG:HG3	1:C:206:GLU:HB3	1.69	0.74
1:L:125:GLU:HB3	1:M:108:THR:HB	1.69	0.74
1:S:30:LEU:HD23	1:S:30:LEU:H	1.52	0.74
1:W:179:ARG:HG3	1:W:206:GLU:HB3	1.69	0.74
1:C:125:GLU:HB3	1:D:108:THR:HB	1.69	0.74
1:E:125:GLU:HB3	1:F:108:THR:HB	1.69	0.74
1:F:179:ARG:HG3	1:F:206:GLU:HB3	1.69	0.74
1:N:179:ARG:HG3	1:N:206:GLU:HB3	1.69	0.74
1:T:30:LEU:HD23	1:T:30:LEU:H	1.52	0.74
1:M:179:ARG:HG3	1:M:206:GLU:HB3	1.68	0.74
1:O:179:ARG:HG3	1:O:206:GLU:HB3	1.69	0.74
1:U:30:LEU:HD23	1:U:30:LEU:H	1.52	0.74
1:X:172:ASN:OD1	1:Z:138:ALA:HB1	1.87	0.74
1:G:125:GLU:HB3	1:H:108:THR:HB	1.69	0.74
1:H:125:GLU:HB3	1:I:108:THR:HB	1.69	0.74
1:I:125:GLU:HB3	1:J:108:THR:HB	1.69	0.74
1:L:30:LEU:HD23	1:L:30:LEU:H	1.52	0.74
1:V:167:LYS:HD3	1:W:203:ALA:HB3	1.70	0.74
1:V:179:ARG:HG3	1:V:206:GLU:HB3	1.68	0.74
3:4:47:ASP:OD1	3:4:50:VAL:N	2.13	0.74
1:V:125:GLU:HB3	1:W:108:THR:HB	1.70	0.74
1:W:167:LYS:HD3	1:X:203:ALA:HB3	1.70	0.74
1:L:179:ARG:HG3	1:L:206:GLU:HB3	1.68	0.74
1:P:125:GLU:HB3	1:Q:108:THR:HB	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:30:LEU:HD23	1:V:30:LEU:H	1.52	0.74
1:P:179:ARG:HG3	1:P:206:GLU:HB3	1.68	0.73
1:W:213:ILE:HG23	1:Y:136:GLY:HA3	1.70	0.73
1:G:179:ARG:HG3	1:G:206:GLU:HB3	1.69	0.73
3:21:47:ASP:OD1	3:21:50:VAL:N	2.13	0.73
1:B:179:ARG:HG3	1:B:206:GLU:HB3	1.68	0.73
1:K:30:LEU:HD23	1:K:30:LEU:H	1.52	0.73
1:W:30:LEU:HD23	1:W:30:LEU:H	1.52	0.73
1:F:30:LEU:HD23	1:F:30:LEU:H	1.52	0.73
1:Q:179:ARG:HG3	1:Q:206:GLU:HB3	1.69	0.73
3:3:47:ASP:OD1	3:3:50:VAL:N	2.13	0.73
3:6:47:ASP:OD1	3:6:50:VAL:N	2.13	0.73
1:G:30:LEU:HD23	1:G:30:LEU:H	1.52	0.73
1:D:167:LYS:HD3	1:E:203:ALA:HB3	1.70	0.73
1:J:30:LEU:HD23	1:J:30:LEU:H	1.52	0.73
1:K:179:ARG:HG3	1:K:206:GLU:HB3	1.69	0.73
1:S:213:ILE:HG23	1:U:136:GLY:HA3	1.71	0.73
1:X:30:LEU:HD23	1:X:30:LEU:H	1.52	0.73
1:Y:30:LEU:HD23	1:Y:30:LEU:H	1.52	0.73
1:Z:30:LEU:HD23	1:Z:30:LEU:H	1.52	0.73
3:5:47:ASP:OD1	3:5:50:VAL:N	2.13	0.73
1:A:30:LEU:HD23	1:A:30:LEU:H	1.52	0.73
1:B:30:LEU:HD23	1:B:30:LEU:H	1.52	0.73
1:C:30:LEU:HD23	1:C:30:LEU:H	1.52	0.73
1:D:30:LEU:HD23	1:D:30:LEU:H	1.52	0.73
1:E:30:LEU:HD23	1:E:30:LEU:H	1.52	0.73
1:J:125:GLU:HB3	1:K:108:THR:HB	1.70	0.73
1:R:213:ILE:HG23	1:T:136:GLY:HA3	1.71	0.73
1:U:167:LYS:HD3	1:V:203:ALA:HB3	1.71	0.73
1:B:167:LYS:HD3	1:C:203:ALA:HB3	1.71	0.73
1:E:167:LYS:HD3	1:F:203:ALA:HB3	1.70	0.73
1:H:30:LEU:H	1:H:30:LEU:HD23	1.52	0.73
1:I:30:LEU:HD23	1:I:30:LEU:H	1.52	0.73
1:I:179:ARG:HG3	1:I:206:GLU:HB3	1.69	0.73
1:T:213:ILE:HG23	1:V:136:GLY:HA3	1.71	0.73
1:A:213:ILE:HG23	1:C:136:GLY:HA3	1.70	0.72
1:J:179:ARG:HG3	1:J:206:GLU:HB3	1.69	0.72
1:G:213:ILE:HG23	1:I:136:GLY:HA3	1.71	0.72
1:H:179:ARG:HG3	1:H:206:GLU:HB3	1.69	0.72
1:Q:167:LYS:HD3	1:R:203:ALA:HB3	1.70	0.72
3:17:47:ASP:OD1	3:17:50:VAL:N	2.13	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:GLU:HB3	1:E:108:THR:HB	1.70	0.72
1:F:125:GLU:HB3	1:G:108:THR:HB	1.70	0.72
1:R:167:LYS:HD3	1:S:203:ALA:HB3	1.70	0.72
1:T:167:LYS:HD3	1:U:203:ALA:HB3	1.70	0.72
1:U:213:ILE:HG23	1:W:136:GLY:HA3	1.72	0.72
1:C:167:LYS:HD3	1:D:203:ALA:HB3	1.71	0.72
1:F:167:LYS:HD3	1:G:203:ALA:HB3	1.70	0.72
1:F:213:ILE:HG23	1:H:136:GLY:HA3	1.71	0.72
1:P:167:LYS:HD3	1:Q:203:ALA:HB3	1.70	0.72
1:V:213:ILE:HG23	1:X:136:GLY:HA3	1.72	0.72
1:Q:213:ILE:HG23	1:S:136:GLY:HA3	1.71	0.72
1:S:167:LYS:HD3	1:T:203:ALA:HB3	1.71	0.72
3:12:72:GLN:HG2	3:12:73:PRO:HD2	1.72	0.71
1:H:213:ILE:HG23	1:J:136:GLY:HA3	1.71	0.71
1:J:167:LYS:HD3	1:K:203:ALA:HB3	1.70	0.71
1:A:167:LYS:HD3	1:B:203:ALA:HB3	1.72	0.71
3:10:72:GLN:HG2	3:10:73:PRO:HD2	1.72	0.71
3:15:72:GLN:HG2	3:15:73:PRO:HD2	1.72	0.71
3:16:72:GLN:HG2	3:16:73:PRO:HD2	1.72	0.71
1:Y:125:GLU:HB3	1:Z:108:THR:HB	1.73	0.71
3:11:72:GLN:HG2	3:11:73:PRO:HD2	1.73	0.71
3:13:72:GLN:HG2	3:13:73:PRO:HD2	1.72	0.71
3:17:72:GLN:HG2	3:17:73:PRO:HD2	1.72	0.71
3:14:72:GLN:HG2	3:14:73:PRO:HD2	1.72	0.71
1:E:213:ILE:HG23	1:G:136:GLY:HA3	1.72	0.71
1:H:167:LYS:HD3	1:I:203:ALA:HB3	1.71	0.71
3:8:72:GLN:HG2	3:8:73:PRO:HD2	1.72	0.71
1:B:213:ILE:HG23	1:D:136:GLY:HA3	1.71	0.71
1:K:167:LYS:HD3	1:L:203:ALA:HB3	1.70	0.71
1:N:167:LYS:HD3	1:O:203:ALA:HB3	1.70	0.71
1:A:203:ALA:HB3	1:Z:167:LYS:HD3	1.73	0.71
3:9:72:GLN:HG2	3:9:73:PRO:HD2	1.72	0.71
1:E:179:ARG:HD2	1:E:206:GLU:OE1	1.91	0.71
1:F:179:ARG:HD2	1:F:206:GLU:OE1	1.91	0.71
1:I:167:LYS:HD3	1:J:203:ALA:HB3	1.71	0.71
1:O:167:LYS:HD3	1:P:203:ALA:HB3	1.71	0.71
1:A:138:ALA:HB1	1:Y:172:ASN:OD1	1.91	0.71
3:19:72:GLN:HG2	3:19:73:PRO:HD2	1.72	0.71
3:20:72:GLN:HG2	3:20:73:PRO:HD2	1.72	0.71
1:C:213:ILE:HG23	1:E:136:GLY:HA3	1.72	0.71
1:D:213:ILE:HG23	1:F:136:GLY:HA3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:LYS:HD3	1:H:203:ALA:HB3	1.71	0.71
1:I:213:ILE:HG23	1:K:136:GLY:HA3	1.72	0.71
1:L:179:ARG:HD2	1:L:206:GLU:OE1	1.91	0.71
3:7:72:GLN:HG2	3:7:73:PRO:HD2	1.73	0.71
1:M:179:ARG:HD2	1:M:206:GLU:OE1	1.91	0.71
3:18:72:GLN:HG2	3:18:73:PRO:HD2	1.73	0.70
1:D:179:ARG:HD2	1:D:206:GLU:OE1	1.91	0.70
1:P:213:ILE:HG23	1:R:136:GLY:HA3	1.72	0.70
1:G:179:ARG:HD2	1:G:206:GLU:OE1	1.91	0.70
1:L:213:ILE:HG23	1:N:136:GLY:HA3	1.71	0.70
1:M:213:ILE:HG23	1:O:136:GLY:HA3	1.71	0.70
3:6:72:GLN:HG2	3:6:73:PRO:HD2	1.73	0.70
1:K:179:ARG:HD2	1:K:206:GLU:OE1	1.91	0.70
1:N:179:ARG:HD2	1:N:206:GLU:OE1	1.91	0.70
3:21:72:GLN:HG2	3:21:73:PRO:HD2	1.72	0.70
1:C:179:ARG:HD2	1:C:206:GLU:OE1	1.91	0.70
1:J:213:ILE:HG23	1:L:136:GLY:HA3	1.72	0.70
1:K:213:ILE:HG23	1:M:136:GLY:HA3	1.72	0.70
1:L:167:LYS:HD3	1:M:203:ALA:HB3	1.70	0.70
1:M:167:LYS:HD3	1:N:203:ALA:HB3	1.71	0.70
1:H:179:ARG:HD2	1:H:206:GLU:OE1	1.91	0.70
1:Y:179:ARG:HD2	1:Y:206:GLU:OE1	1.91	0.70
1:N:213:ILE:HG23	1:P:136:GLY:HA3	1.71	0.70
3:5:72:GLN:HG2	3:5:73:PRO:HD2	1.73	0.70
1:J:179:ARG:HD2	1:J:206:GLU:OE1	1.91	0.70
1:O:179:ARG:HD2	1:O:206:GLU:OE1	1.91	0.70
1:O:213:ILE:HG23	1:Q:136:GLY:HA3	1.72	0.70
1:P:179:ARG:HD2	1:P:206:GLU:OE1	1.91	0.70
1:Q:179:ARG:HD2	1:Q:206:GLU:OE1	1.91	0.70
1:X:179:ARG:HD2	1:X:206:GLU:OE1	1.91	0.70
1:X:213:ILE:HG23	1:Z:136:GLY:HA3	1.73	0.70
3:1:72:GLN:HG2	3:1:73:PRO:HD2	1.72	0.70
1:Z:179:ARG:HD2	1:Z:206:GLU:OE1	1.91	0.70
3:3:72:GLN:HG2	3:3:73:PRO:HD2	1.72	0.69
3:22:72:GLN:HG2	3:22:73:PRO:HD2	1.72	0.69
3:26:72:GLN:HG2	3:26:73:PRO:HD2	1.72	0.69
1:R:179:ARG:HD2	1:R:206:GLU:OE1	1.91	0.69
1:S:179:ARG:HD2	1:S:206:GLU:OE1	1.91	0.69
1:X:167:LYS:HD3	1:Y:203:ALA:HB3	1.74	0.69
3:2:72:GLN:HG2	3:2:73:PRO:HD2	1.72	0.69
3:4:72:GLN:HG2	3:4:73:PRO:HD2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:25:72:GLN:HG2	3:25:73:PRO:HD2	1.72	0.69
1:T:179:ARG:HD2	1:T:206:GLU:OE1	1.91	0.69
1:V:179:ARG:HD2	1:V:206:GLU:OE1	1.91	0.69
3:23:72:GLN:HG2	3:23:73:PRO:HD2	1.72	0.69
3:24:72:GLN:HG2	3:24:73:PRO:HD2	1.72	0.69
1:I:179:ARG:HD2	1:I:206:GLU:OE1	1.91	0.69
1:U:179:ARG:HD2	1:U:206:GLU:OE1	1.91	0.69
1:W:179:ARG:HD2	1:W:206:GLU:OE1	1.91	0.69
1:B:179:ARG:HD2	1:B:206:GLU:OE1	1.91	0.69
1:A:179:ARG:HD2	1:A:206:GLU:OE1	1.91	0.69
3:17:18:ARG:HE	3:17:46:THR:HA	1.58	0.69
3:21:18:ARG:HE	3:21:46:THR:HA	1.58	0.69
3:14:18:ARG:HE	3:14:46:THR:HA	1.58	0.69
3:24:18:ARG:HE	3:24:46:THR:HA	1.58	0.69
1:L:86:VAL:HB	1:L:142:ASN:OD1	1.93	0.69
1:V:86:VAL:HB	1:V:142:ASN:OD1	1.93	0.69
1:W:86:VAL:HB	1:W:142:ASN:OD1	1.93	0.69
1:Y:167:LYS:HD3	1:Z:203:ALA:CB	2.23	0.69
3:2:18:ARG:HE	3:2:46:THR:HA	1.58	0.69
3:5:18:ARG:HE	3:5:46:THR:HA	1.58	0.69
3:7:18:ARG:HE	3:7:46:THR:HA	1.58	0.69
3:10:18:ARG:HE	3:10:46:THR:HA	1.58	0.69
1:M:86:VAL:HB	1:M:142:ASN:OD1	1.93	0.69
1:U:86:VAL:HB	1:U:142:ASN:OD1	1.93	0.69
1:X:86:VAL:HB	1:X:142:ASN:OD1	1.93	0.69
3:1:18:ARG:HE	3:1:46:THR:HA	1.58	0.68
3:18:18:ARG:HE	3:18:46:THR:HA	1.58	0.68
1:E:86:VAL:HB	1:E:142:ASN:OD1	1.93	0.68
1:G:86:VAL:HB	1:G:142:ASN:OD1	1.93	0.68
1:K:86:VAL:HB	1:K:142:ASN:OD1	1.93	0.68
3:20:18:ARG:HE	3:20:46:THR:HA	1.58	0.68
1:D:86:VAL:HB	1:D:142:ASN:OD1	1.93	0.68
1:F:86:VAL:HB	1:F:142:ASN:OD1	1.93	0.68
1:T:86:VAL:HB	1:T:142:ASN:OD1	1.93	0.68
1:Y:86:VAL:HB	1:Y:142:ASN:OD1	1.93	0.68
3:15:18:ARG:HE	3:15:46:THR:HA	1.58	0.68
1:N:86:VAL:HB	1:N:142:ASN:OD1	1.93	0.68
1:S:86:VAL:HB	1:S:142:ASN:OD1	1.93	0.68
3:4:18:ARG:HE	3:4:46:THR:HA	1.58	0.68
3:8:18:ARG:HE	3:8:46:THR:HA	1.58	0.68
3:11:18:ARG:HE	3:11:46:THR:HA	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:12:18:ARG:HE	3:12:46:THR:HA	1.58	0.68
1:H:86:VAL:HB	1:H:142:ASN:OD1	1.93	0.68
1:Z:86:VAL:HB	1:Z:142:ASN:OD1	1.93	0.68
3:23:18:ARG:HE	3:23:46:THR:HA	1.58	0.68
1:R:86:VAL:HB	1:R:142:ASN:OD1	1.93	0.68
3:3:18:ARG:HE	3:3:46:THR:HA	1.58	0.68
3:13:18:ARG:HE	3:13:46:THR:HA	1.58	0.68
3:26:18:ARG:HE	3:26:46:THR:HA	1.58	0.68
1:C:86:VAL:HB	1:C:142:ASN:OD1	1.93	0.68
1:J:86:VAL:HB	1:J:142:ASN:OD1	1.93	0.68
3:9:18:ARG:HE	3:9:46:THR:HA	1.58	0.68
3:6:18:ARG:HE	3:6:46:THR:HA	1.58	0.68
3:25:18:ARG:HE	3:25:46:THR:HA	1.58	0.68
1:B:86:VAL:HB	1:B:142:ASN:OD1	1.93	0.68
1:A:86:VAL:HB	1:A:142:ASN:OD1	1.93	0.68
1:O:86:VAL:HB	1:O:142:ASN:OD1	1.93	0.68
1:Q:86:VAL:HB	1:Q:142:ASN:OD1	1.93	0.67
3:16:18:ARG:HE	3:16:46:THR:HA	1.58	0.67
1:I:86:VAL:HB	1:I:142:ASN:OD1	1.93	0.67
3:22:18:ARG:HE	3:22:46:THR:HA	1.58	0.67
1:P:86:VAL:HB	1:P:142:ASN:OD1	1.93	0.67
1:A:136:GLY:HA3	1:Y:213:ILE:HG23	1.76	0.67
3:19:18:ARG:HE	3:19:46:THR:HA	1.58	0.67
3:25:76:THR:HG21	1:Y:34:ALA:HA	1.78	0.66
1:T:82:LEU:HD13	1:T:144:PHE:CD1	2.31	0.66
1:R:82:LEU:HD13	1:R:144:PHE:CD1	2.31	0.66
1:B:82:LEU:HD13	1:B:144:PHE:CD1	2.31	0.66
1:W:82:LEU:HD13	1:W:144:PHE:CD1	2.31	0.66
1:Y:82:LEU:HD13	1:Y:144:PHE:CD1	2.31	0.66
1:A:82:LEU:HD13	1:A:144:PHE:CD1	2.31	0.66
3:12:76:THR:HG21	1:L:34:ALA:HA	1.78	0.66
3:24:76:THR:HG21	1:X:34:ALA:HA	1.78	0.66
1:E:82:LEU:HD13	1:E:144:PHE:CD1	2.31	0.66
1:Q:82:LEU:HD13	1:Q:144:PHE:CD1	2.31	0.66
1:S:82:LEU:HD13	1:S:144:PHE:CD1	2.31	0.66
3:11:76:THR:HG21	1:K:34:ALA:HA	1.78	0.66
3:16:76:THR:HG21	1:P:34:ALA:HA	1.78	0.66
3:20:76:THR:HG21	1:T:34:ALA:HA	1.78	0.66
1:O:37:ALA:HB1	1:P:74:ILE:HG22	1.78	0.66
3:15:76:THR:HG21	1:O:34:ALA:HA	1.78	0.66
3:19:76:THR:HG21	1:S:34:ALA:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:21:76:THR:HG21	1:U:34:ALA:HA	1.78	0.66
3:23:76:THR:HG21	1:W:34:ALA:HA	1.78	0.66
1:C:82:LEU:HD13	1:C:144:PHE:CD1	2.31	0.66
1:L:37:ALA:HB1	1:M:74:ILE:HG22	1.78	0.66
1:Z:82:LEU:HD13	1:Z:144:PHE:CD1	2.31	0.66
3:10:76:THR:HG21	1:J:34:ALA:HA	1.78	0.66
1:D:82:LEU:HD13	1:D:144:PHE:CD1	2.31	0.66
1:O:82:LEU:HD13	1:O:144:PHE:CD1	2.31	0.66
1:P:82:LEU:HD13	1:P:144:PHE:CD1	2.31	0.66
1:V:82:LEU:HD13	1:V:144:PHE:CD1	2.31	0.66
3:8:76:THR:HG21	1:H:34:ALA:HA	1.78	0.65
3:17:76:THR:HG21	1:Q:34:ALA:HA	1.78	0.65
3:18:76:THR:HG21	1:R:34:ALA:HA	1.78	0.65
1:H:82:LEU:HD13	1:H:144:PHE:CD1	2.31	0.65
1:N:82:LEU:HD13	1:N:144:PHE:CD1	2.31	0.65
1:U:82:LEU:HD13	1:U:144:PHE:CD1	2.31	0.65
3:2:76:THR:HG21	1:B:34:ALA:HA	1.78	0.65
3:9:76:THR:HG21	1:I:34:ALA:HA	1.78	0.65
3:13:76:THR:HG21	1:M:34:ALA:HA	1.78	0.65
3:22:76:THR:HG21	1:V:34:ALA:HA	1.78	0.65
1:K:82:LEU:HD13	1:K:144:PHE:CD1	2.31	0.65
1:P:37:ALA:HB1	1:Q:74:ILE:HG22	1.79	0.65
3:3:76:THR:HG21	1:C:34:ALA:HA	1.78	0.65
3:7:76:THR:HG21	1:G:34:ALA:HA	1.78	0.65
3:14:76:THR:HG21	1:N:34:ALA:HA	1.78	0.65
1:G:82:LEU:HD13	1:G:144:PHE:CD1	2.31	0.65
3:6:76:THR:HG21	1:F:34:ALA:HA	1.78	0.65
3:7:45:ARG:O	3:7:45:ARG:HG2	1.97	0.65
3:10:45:ARG:HG2	3:10:45:ARG:O	1.97	0.65
3:8:45:ARG:HG2	3:8:45:ARG:O	1.97	0.65
3:25:45:ARG:HG2	3:25:45:ARG:O	1.97	0.65
3:26:45:ARG:O	3:26:45:ARG:HG2	1.97	0.65
1:L:82:LEU:HD13	1:L:144:PHE:CD1	2.31	0.65
3:4:45:ARG:O	3:4:45:ARG:HG2	1.97	0.65
3:4:76:THR:HG21	1:D:34:ALA:HA	1.78	0.65
3:23:45:ARG:O	3:23:45:ARG:HG2	1.97	0.65
3:17:45:ARG:O	3:17:45:ARG:HG2	1.97	0.65
3:18:45:ARG:HG2	3:18:45:ARG:O	1.97	0.65
1:H:37:ALA:HB1	1:I:74:ILE:HG22	1.79	0.65
1:K:37:ALA:HB1	1:L:74:ILE:HG22	1.79	0.65
1:X:37:ALA:HB1	1:Y:74:ILE:HG22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:45:ARG:O	3:1:45:ARG:HG2	1.97	0.65
3:3:45:ARG:HG2	3:3:45:ARG:O	1.97	0.65
3:13:45:ARG:HG2	3:13:45:ARG:O	1.97	0.65
3:16:45:ARG:HG2	3:16:45:ARG:O	1.97	0.65
3:24:45:ARG:O	3:24:45:ARG:HG2	1.97	0.65
3:26:76:THR:HG21	1:Z:34:ALA:HA	1.79	0.65
1:F:82:LEU:HD13	1:F:144:PHE:CD1	2.31	0.65
1:I:37:ALA:HB1	1:J:74:ILE:HG22	1.78	0.65
1:I:82:LEU:HD13	1:I:144:PHE:CD1	2.31	0.65
1:T:37:ALA:HB1	1:U:74:ILE:HG22	1.79	0.65
3:5:76:THR:HG21	1:E:34:ALA:HA	1.78	0.65
1:J:82:LEU:HD13	1:J:144:PHE:CD1	2.31	0.65
1:S:37:ALA:HB1	1:T:74:ILE:HG22	1.79	0.65
1:A:34:ALA:HA	3:1:76:THR:HG21	1.79	0.65
3:20:45:ARG:O	3:20:45:ARG:HG2	1.97	0.65
1:X:82:LEU:HD13	1:X:144:PHE:CD1	2.31	0.65
3:6:45:ARG:HG2	3:6:45:ARG:O	1.97	0.64
3:11:45:ARG:O	3:11:45:ARG:HG2	1.97	0.64
1:M:82:LEU:HD13	1:M:144:PHE:CD1	2.31	0.64
3:14:45:ARG:O	3:14:45:ARG:HG2	1.97	0.64
3:15:45:ARG:O	3:15:45:ARG:HG2	1.97	0.64
1:C:37:ALA:HB1	1:D:74:ILE:HG22	1.78	0.64
3:9:45:ARG:O	3:9:45:ARG:HG2	1.97	0.64
3:22:45:ARG:HG2	3:22:45:ARG:O	1.97	0.64
1:M:37:ALA:HB1	1:N:74:ILE:HG22	1.79	0.64
1:D:37:ALA:HB1	1:E:74:ILE:HG22	1.78	0.64
1:G:37:ALA:HB1	1:H:74:ILE:HG22	1.79	0.64
1:L:82:LEU:HD12	1:L:146:GLY:CA	2.28	0.64
1:N:37:ALA:HB1	1:O:74:ILE:HG22	1.79	0.64
1:U:82:LEU:HD12	1:U:146:GLY:CA	2.28	0.64
1:Y:37:ALA:HB1	1:Z:74:ILE:HG22	1.80	0.64
3:19:45:ARG:HG2	3:19:45:ARG:O	1.97	0.64
1:M:82:LEU:HD12	1:M:146:GLY:CA	2.28	0.64
1:T:82:LEU:HD12	1:T:146:GLY:CA	2.28	0.64
1:K:82:LEU:HD12	1:K:146:GLY:CA	2.28	0.64
1:V:82:LEU:HD12	1:V:146:GLY:CA	2.28	0.64
1:R:82:LEU:HD12	1:R:146:GLY:CA	2.28	0.64
3:21:45:ARG:O	3:21:45:ARG:HG2	1.97	0.64
1:N:82:LEU:HD12	1:N:146:GLY:CA	2.28	0.64
1:Q:37:ALA:HB1	1:R:74:ILE:HG22	1.79	0.64
1:U:37:ALA:HB1	1:V:74:ILE:HG22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:82:LEU:HD12	1:W:146:GLY:CA	2.28	0.64
1:F:37:ALA:HB1	1:G:74:ILE:HG22	1.78	0.64
1:J:82:LEU:HD12	1:J:146:GLY:CA	2.28	0.64
1:P:82:LEU:HD12	1:P:146:GLY:CA	2.28	0.64
1:S:82:LEU:HD12	1:S:146:GLY:CA	2.28	0.64
3:5:45:ARG:O	3:5:45:ARG:HG2	1.97	0.63
3:12:45:ARG:O	3:12:45:ARG:HG2	1.97	0.63
1:O:82:LEU:HD12	1:O:146:GLY:CA	2.28	0.63
3:2:45:ARG:O	3:2:45:ARG:HG2	1.97	0.63
1:C:82:LEU:HD12	1:C:146:GLY:CA	2.28	0.63
1:W:37:ALA:HB1	1:X:74:ILE:HG22	1.79	0.63
1:D:82:LEU:HD12	1:D:146:GLY:CA	2.28	0.63
1:E:82:LEU:HD12	1:E:146:GLY:CA	2.28	0.63
1:J:37:ALA:HB1	1:K:74:ILE:HG22	1.79	0.63
1:X:82:LEU:HD12	1:X:146:GLY:CA	2.28	0.63
1:B:37:ALA:HB1	1:C:74:ILE:HG22	1.79	0.63
1:B:82:LEU:HD12	1:B:146:GLY:CA	2.28	0.63
1:A:74:ILE:HG22	1:Z:37:ALA:HB1	1.79	0.63
1:F:82:LEU:HD12	1:F:146:GLY:CA	2.28	0.63
1:I:82:LEU:HD12	1:I:146:GLY:CA	2.28	0.63
1:A:82:LEU:HD12	1:A:146:GLY:CA	2.28	0.63
1:R:37:ALA:HB1	1:S:74:ILE:HG22	1.80	0.63
3:22:18:ARG:NH2	3:22:45:ARG:O	2.32	0.63
3:24:18:ARG:NH2	3:24:45:ARG:O	2.32	0.63
1:Q:82:LEU:HD12	1:Q:146:GLY:CA	2.28	0.63
3:20:18:ARG:NH2	3:20:45:ARG:O	2.32	0.63
3:21:18:ARG:NH2	3:21:45:ARG:O	2.32	0.63
3:26:18:ARG:NH2	3:26:45:ARG:O	2.32	0.63
1:E:37:ALA:HB1	1:F:74:ILE:HG22	1.79	0.63
1:G:82:LEU:HD12	1:G:146:GLY:CA	2.28	0.63
3:18:18:ARG:NH2	3:18:45:ARG:O	2.32	0.62
3:19:18:ARG:NH2	3:19:45:ARG:O	2.32	0.62
3:23:18:ARG:NH2	3:23:45:ARG:O	2.32	0.62
3:25:18:ARG:NH2	3:25:45:ARG:O	2.32	0.62
1:Y:82:LEU:HD12	1:Y:146:GLY:CA	2.28	0.62
1:Z:82:LEU:HD12	1:Z:146:GLY:CA	2.28	0.62
3:16:18:ARG:NH2	3:16:45:ARG:O	2.32	0.62
3:1:18:ARG:NH2	3:1:45:ARG:O	2.32	0.62
1:H:82:LEU:HD12	1:H:146:GLY:CA	2.28	0.62
1:V:167:LYS:HD3	1:W:203:ALA:CB	2.30	0.62
3:2:18:ARG:NH2	3:2:45:ARG:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:18:ARG:NH2	3:3:45:ARG:O	2.32	0.62
3:17:18:ARG:NH2	3:17:45:ARG:O	2.32	0.62
1:V:37:ALA:HB1	1:W:74:ILE:HG22	1.79	0.62
3:14:18:ARG:NH2	3:14:45:ARG:O	2.32	0.62
1:A:37:ALA:HB1	1:B:74:ILE:HG22	1.80	0.62
3:5:18:ARG:NH2	3:5:45:ARG:O	2.32	0.62
3:10:18:ARG:NH2	3:10:45:ARG:O	2.32	0.62
1:W:167:LYS:HD3	1:X:203:ALA:CB	2.30	0.62
3:7:18:ARG:NH2	3:7:45:ARG:O	2.32	0.62
3:9:18:ARG:NH2	3:9:45:ARG:O	2.32	0.61
3:12:18:ARG:NH2	3:12:45:ARG:O	2.32	0.61
3:4:18:ARG:NH2	3:4:45:ARG:O	2.32	0.61
3:15:18:ARG:NH2	3:15:45:ARG:O	2.32	0.61
1:J:167:LYS:HD3	1:K:203:ALA:CB	2.30	0.61
1:T:167:LYS:HD3	1:U:203:ALA:CB	2.30	0.61
3:8:18:ARG:NH2	3:8:45:ARG:O	2.32	0.61
3:13:18:ARG:NH2	3:13:45:ARG:O	2.32	0.61
1:U:167:LYS:HD3	1:V:203:ALA:CB	2.31	0.61
3:1:77:CYS:HB3	3:1:80:TYR:HE1	1.66	0.61
3:26:77:CYS:HB3	3:26:80:TYR:HE1	1.66	0.61
3:6:47:ASP:OD2	3:6:50:VAL:HG23	2.01	0.61
3:25:77:CYS:HB3	3:25:80:TYR:HE1	1.66	0.61
1:D:167:LYS:HD3	1:E:203:ALA:CB	2.30	0.61
3:3:47:ASP:OD2	3:3:50:VAL:HG23	2.01	0.61
3:6:18:ARG:NH2	3:6:45:ARG:O	2.32	0.61
1:B:167:LYS:HD3	1:C:203:ALA:CB	2.31	0.61
3:2:77:CYS:HB3	3:2:80:TYR:HE1	1.66	0.61
3:7:47:ASP:OD2	3:7:50:VAL:HG23	2.01	0.61
3:16:77:CYS:HB3	3:16:80:TYR:HE1	1.66	0.61
3:17:77:CYS:HB3	3:17:80:TYR:HE1	1.66	0.61
3:24:77:CYS:HB3	3:24:80:TYR:HE1	1.66	0.61
1:K:167:LYS:HD3	1:L:203:ALA:CB	2.30	0.61
1:P:167:LYS:HD3	1:Q:203:ALA:CB	2.30	0.61
1:R:167:LYS:HD3	1:S:203:ALA:CB	2.30	0.61
3:10:47:ASP:OD2	3:10:50:VAL:HG23	2.01	0.61
3:11:18:ARG:NH2	3:11:45:ARG:O	2.32	0.61
3:15:77:CYS:HB3	3:15:80:TYR:HE1	1.66	0.61
3:20:47:ASP:OD2	3:20:50:VAL:HG23	2.01	0.61
1:Q:167:LYS:HD3	1:R:203:ALA:CB	2.30	0.61
3:5:47:ASP:OD2	3:5:50:VAL:HG23	2.01	0.60
3:14:77:CYS:HB3	3:14:80:TYR:HE1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:18:77:CYS:HB3	3:18:80:TYR:HE1	1.66	0.60
1:C:58:ILE:HG13	1:C:59:ASN:H	1.66	0.60
1:I:58:ILE:HG13	1:I:59:ASN:H	1.66	0.60
1:S:167:LYS:HD3	1:T:203:ALA:CB	2.31	0.60
3:3:77:CYS:HB3	3:3:80:TYR:HE1	1.66	0.60
3:19:47:ASP:OD2	3:19:50:VAL:HG23	2.01	0.60
3:21:47:ASP:OD2	3:21:50:VAL:HG23	2.01	0.60
3:23:77:CYS:HB3	3:23:80:TYR:HE1	1.66	0.60
1:D:58:ILE:HG13	1:D:59:ASN:H	1.67	0.60
1:H:58:ILE:HG13	1:H:59:ASN:H	1.66	0.60
1:X:58:ILE:HG13	1:X:59:ASN:H	1.66	0.60
3:2:47:ASP:OD2	3:2:50:VAL:HG23	2.01	0.60
3:4:47:ASP:OD2	3:4:50:VAL:HG23	2.01	0.60
1:H:167:LYS:HD3	1:I:203:ALA:CB	2.30	0.60
1:L:167:LYS:HD3	1:M:203:ALA:CB	2.31	0.60
1:N:58:ILE:HG13	1:N:59:ASN:H	1.67	0.60
1:Q:58:ILE:HG13	1:Q:59:ASN:H	1.66	0.60
3:9:47:ASP:OD2	3:9:50:VAL:HG23	2.01	0.60
1:F:167:LYS:HD3	1:G:203:ALA:CB	2.30	0.60
1:N:167:LYS:HD3	1:O:203:ALA:CB	2.30	0.60
1:Y:58:ILE:HG13	1:Y:59:ASN:H	1.66	0.60
3:12:77:CYS:HB3	3:12:80:TYR:HE1	1.66	0.60
3:13:77:CYS:HB3	3:13:80:TYR:HE1	1.66	0.60
3:20:77:CYS:HB3	3:20:80:TYR:HE1	1.66	0.60
3:22:47:ASP:OD2	3:22:50:VAL:HG23	2.01	0.60
1:C:167:LYS:HD3	1:D:203:ALA:CB	2.31	0.60
1:I:167:LYS:HD3	1:J:203:ALA:CB	2.31	0.60
1:J:58:ILE:HG13	1:J:59:ASN:H	1.66	0.60
1:T:58:ILE:HG13	1:T:59:ASN:H	1.67	0.60
3:18:47:ASP:OD2	3:18:50:VAL:HG23	2.01	0.60
3:19:77:CYS:HB3	3:19:80:TYR:HE1	1.66	0.60
3:21:77:CYS:HB3	3:21:80:TYR:HE1	1.66	0.60
1:B:58:ILE:HG13	1:B:59:ASN:H	1.66	0.60
1:E:167:LYS:HD3	1:F:203:ALA:CB	2.30	0.60
1:R:58:ILE:HG13	1:R:59:ASN:H	1.66	0.60
3:25:47:ASP:OD2	3:25:50:VAL:HG23	2.01	0.60
3:26:47:ASP:OD2	3:26:50:VAL:HG23	2.01	0.60
1:K:58:ILE:HG13	1:K:59:ASN:H	1.67	0.60
1:W:58:ILE:HG13	1:W:59:ASN:H	1.67	0.60
3:4:77:CYS:HB3	3:4:80:TYR:HE1	1.66	0.60
3:8:47:ASP:OD2	3:8:50:VAL:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:10:72:GLN:CG	3:10:73:PRO:HD2	2.32	0.60
3:11:47:ASP:OD2	3:11:50:VAL:HG23	2.01	0.60
1:U:58:ILE:HG13	1:U:59:ASN:H	1.66	0.60
1:X:39:PRO:HB3	1:Y:75:GLY:HA3	1.84	0.60
3:9:72:GLN:CG	3:9:73:PRO:HD2	2.32	0.60
3:12:72:GLN:CG	3:12:73:PRO:HD2	2.32	0.60
3:17:47:ASP:OD2	3:17:50:VAL:HG23	2.01	0.60
1:E:58:ILE:HG13	1:E:59:ASN:H	1.66	0.60
1:M:167:LYS:HD3	1:N:203:ALA:CB	2.31	0.60
1:O:58:ILE:HG13	1:O:59:ASN:H	1.66	0.60
3:8:72:GLN:CG	3:8:73:PRO:HD2	2.32	0.60
3:10:77:CYS:HB3	3:10:80:TYR:HE1	1.66	0.60
3:11:72:GLN:CG	3:11:73:PRO:HD2	2.32	0.60
3:13:47:ASP:OD2	3:13:50:VAL:HG23	2.01	0.60
3:13:72:GLN:CG	3:13:73:PRO:HD2	2.32	0.60
3:22:77:CYS:HB3	3:22:80:TYR:HE1	1.66	0.60
1:G:167:LYS:HD3	1:H:203:ALA:CB	2.31	0.60
3:9:77:CYS:HB3	3:9:80:TYR:HE1	1.66	0.59
3:11:77:CYS:HB3	3:11:80:TYR:HE1	1.66	0.59
3:15:72:GLN:CG	3:15:73:PRO:HD2	2.32	0.59
3:23:47:ASP:OD2	3:23:50:VAL:HG23	2.01	0.59
3:24:80:TYR:O	1:X:26:PRO:HA	2.02	0.59
3:5:77:CYS:HB3	3:5:80:TYR:HE1	1.66	0.59
3:7:72:GLN:CG	3:7:73:PRO:HD2	2.32	0.59
3:8:77:CYS:HB3	3:8:80:TYR:HE1	1.66	0.59
3:8:80:TYR:O	1:H:26:PRO:HA	2.03	0.59
3:9:80:TYR:O	1:I:26:PRO:HA	2.03	0.59
3:14:47:ASP:OD2	3:14:50:VAL:HG23	2.01	0.59
3:14:72:GLN:CG	3:14:73:PRO:HD2	2.32	0.59
1:G:58:ILE:HG13	1:G:59:ASN:H	1.66	0.59
1:L:58:ILE:HG13	1:L:59:ASN:H	1.66	0.59
1:O:167:LYS:HD3	1:P:203:ALA:CB	2.31	0.59
1:V:58:ILE:HG13	1:V:59:ASN:H	1.66	0.59
1:A:39:PRO:HB3	1:B:75:GLY:HA3	1.85	0.59
1:A:167:LYS:HD3	1:B:203:ALA:CB	2.32	0.59
3:1:47:ASP:OD2	3:1:50:VAL:HG23	2.01	0.59
3:6:72:GLN:CG	3:6:73:PRO:HD2	2.32	0.59
3:16:72:GLN:CG	3:16:73:PRO:HD2	2.32	0.59
3:23:80:TYR:O	1:W:26:PRO:HA	2.03	0.59
1:Z:58:ILE:HG13	1:Z:59:ASN:H	1.66	0.59
1:A:75:GLY:HA3	1:Z:39:PRO:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ALA:CB	1:Z:167:LYS:HD3	2.33	0.59
3:5:72:GLN:CG	3:5:73:PRO:HD2	2.32	0.59
3:7:77:CYS:HB3	3:7:80:TYR:HE1	1.66	0.59
3:12:47:ASP:OD2	3:12:50:VAL:HG23	2.01	0.59
3:15:80:TYR:O	1:O:26:PRO:HA	2.03	0.59
3:17:72:GLN:CG	3:17:73:PRO:HD2	2.32	0.59
3:25:80:TYR:O	1:Y:26:PRO:HA	2.02	0.59
3:3:72:GLN:CG	3:3:73:PRO:HD2	2.32	0.59
3:4:72:GLN:CG	3:4:73:PRO:HD2	2.32	0.59
3:10:80:TYR:O	1:J:26:PRO:HA	2.03	0.59
3:15:47:ASP:OD2	3:15:50:VAL:HG23	2.01	0.59
3:22:80:TYR:O	1:V:26:PRO:HA	2.03	0.59
1:P:58:ILE:HG13	1:P:59:ASN:H	1.66	0.59
3:2:72:GLN:CG	3:2:73:PRO:HD2	2.32	0.59
3:16:47:ASP:OD2	3:16:50:VAL:HG23	2.01	0.59
3:18:72:GLN:CG	3:18:73:PRO:HD2	2.32	0.59
3:24:47:ASP:OD2	3:24:50:VAL:HG23	2.01	0.59
3:26:80:TYR:O	1:Z:26:PRO:HA	2.03	0.59
1:M:58:ILE:HG13	1:M:59:ASN:H	1.66	0.59
3:14:80:TYR:O	1:N:26:PRO:HA	2.03	0.59
3:19:72:GLN:CG	3:19:73:PRO:HD2	2.32	0.59
3:26:72:GLN:CG	3:26:73:PRO:HD2	2.32	0.59
3:1:72:GLN:CG	3:1:73:PRO:HD2	2.32	0.59
3:6:80:TYR:O	1:F:26:PRO:HA	2.02	0.59
3:20:72:GLN:CG	3:20:73:PRO:HD2	2.32	0.59
3:20:80:TYR:O	1:T:26:PRO:HA	2.03	0.59
3:25:72:GLN:CG	3:25:73:PRO:HD2	2.32	0.59
1:E:160:ASN:HA	1:E:186:PRO:HD3	1.85	0.59
1:H:223:GLN:HB2	1:I:232:MET:HG3	1.85	0.59
1:N:223:GLN:HB2	1:O:232:MET:HG3	1.85	0.59
3:6:77:CYS:HB3	3:6:80:TYR:HE1	1.66	0.59
3:7:80:TYR:O	1:G:26:PRO:HA	2.03	0.59
3:16:80:TYR:O	1:P:26:PRO:HA	2.03	0.59
3:21:80:TYR:O	1:U:26:PRO:HA	2.03	0.59
3:24:72:GLN:CG	3:24:73:PRO:HD2	2.32	0.59
1:F:160:ASN:HA	1:F:186:PRO:HD3	1.85	0.59
1:X:160:ASN:HA	1:X:186:PRO:HD3	1.85	0.59
3:11:80:TYR:O	1:K:26:PRO:HA	2.03	0.59
3:21:72:GLN:CG	3:21:73:PRO:HD2	2.32	0.59
3:22:72:GLN:CG	3:22:73:PRO:HD2	2.32	0.59
3:23:72:GLN:CG	3:23:73:PRO:HD2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:58:ILE:HG13	1:S:59:ASN:H	1.66	0.59
3:17:80:TYR:O	1:Q:26:PRO:HA	2.03	0.58
1:D:160:ASN:HA	1:D:186:PRO:HD3	1.85	0.58
1:F:58:ILE:HG13	1:F:59:ASN:H	1.67	0.58
1:W:160:ASN:HA	1:W:186:PRO:HD3	1.85	0.58
1:Y:160:ASN:HA	1:Y:186:PRO:HD3	1.85	0.58
3:19:80:TYR:O	1:S:26:PRO:HA	2.03	0.58
1:B:223:GLN:HB2	1:C:232:MET:HG3	1.85	0.58
1:T:223:GLN:HB2	1:U:232:MET:HG3	1.85	0.58
1:A:58:ILE:HG13	1:A:59:ASN:H	1.67	0.58
3:18:80:TYR:O	1:R:26:PRO:HA	2.03	0.58
1:V:223:GLN:HB2	1:W:232:MET:HG3	1.86	0.58
1:A:232:MET:HG3	1:Z:223:GLN:HB2	1.85	0.58
3:2:80:TYR:O	1:B:26:PRO:HA	2.02	0.58
3:4:80:TYR:O	1:D:26:PRO:HA	2.03	0.58
1:G:160:ASN:HA	1:G:186:PRO:HD3	1.85	0.58
1:W:223:GLN:HB2	1:X:232:MET:HG3	1.85	0.58
1:X:167:LYS:HD3	1:Y:203:ALA:CB	2.34	0.58
3:5:80:TYR:O	1:E:26:PRO:HA	2.03	0.58
1:G:223:GLN:HB2	1:H:232:MET:HG3	1.86	0.58
1:M:223:GLN:HB2	1:N:232:MET:HG3	1.86	0.58
1:A:223:GLN:HB2	1:B:232:MET:HG3	1.86	0.58
3:7:70:PHE:CD1	1:G:41:PRO:HD3	2.39	0.58
3:12:80:TYR:O	1:L:26:PRO:HA	2.02	0.58
3:13:80:TYR:O	1:M:26:PRO:HA	2.03	0.58
3:25:70:PHE:CD1	1:Y:41:PRO:HD3	2.39	0.58
1:O:39:PRO:HB3	1:P:75:GLY:HA3	1.86	0.58
1:S:39:PRO:HB3	1:T:75:GLY:HA3	1.86	0.58
1:V:160:ASN:HA	1:V:186:PRO:HD3	1.85	0.58
1:Z:160:ASN:HA	1:Z:186:PRO:HD3	1.85	0.58
1:C:160:ASN:HA	1:C:186:PRO:HD3	1.85	0.58
1:Q:39:PRO:HB3	1:R:75:GLY:HA3	1.86	0.58
1:R:39:PRO:HB3	1:S:75:GLY:HA3	1.86	0.58
1:U:39:PRO:HB3	1:V:75:GLY:HA3	1.86	0.58
1:A:26:PRO:HA	3:1:80:TYR:O	2.03	0.58
1:A:41:PRO:HD3	3:1:70:PHE:CD1	2.38	0.58
3:4:70:PHE:CD1	1:D:41:PRO:HD3	2.39	0.58
3:10:70:PHE:CD1	1:J:41:PRO:HD3	2.39	0.58
1:H:160:ASN:HA	1:H:186:PRO:HD3	1.85	0.58
1:K:160:ASN:HA	1:K:186:PRO:HD3	1.85	0.58
1:L:160:ASN:HA	1:L:186:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:39:PRO:HB3	1:N:75:GLY:HA3	1.86	0.58
1:R:160:ASN:HA	1:R:186:PRO:HD3	1.85	0.58
1:W:39:PRO:HB3	1:X:75:GLY:HA3	1.86	0.58
1:C:39:PRO:HB3	1:D:75:GLY:HA3	1.86	0.58
1:P:223:GLN:HB2	1:Q:232:MET:HG3	1.86	0.58
1:Q:160:ASN:HA	1:Q:186:PRO:HD3	1.85	0.58
3:3:80:TYR:O	1:C:26:PRO:HA	2.03	0.57
1:B:39:PRO:HB3	1:C:75:GLY:HA3	1.86	0.57
1:M:160:ASN:HA	1:M:186:PRO:HD3	1.85	0.57
1:Q:223:GLN:HB2	1:R:232:MET:HG3	1.85	0.57
1:S:160:ASN:HA	1:S:186:PRO:HD3	1.85	0.57
3:2:70:PHE:CD1	1:B:41:PRO:HD3	2.39	0.57
3:6:70:PHE:CD1	1:F:41:PRO:HD3	2.40	0.57
3:22:70:PHE:CD1	1:V:41:PRO:HD3	2.39	0.57
1:U:223:GLN:HB2	1:V:232:MET:HG3	1.87	0.57
1:A:160:ASN:HA	1:A:186:PRO:HD3	1.85	0.57
3:3:70:PHE:CD1	1:C:41:PRO:HD3	2.39	0.57
3:8:70:PHE:CD1	1:H:41:PRO:HD3	2.40	0.57
1:L:223:GLN:HB2	1:M:232:MET:HG3	1.86	0.57
1:N:39:PRO:HB3	1:O:75:GLY:HA3	1.86	0.57
3:11:70:PHE:CD1	1:K:41:PRO:HD3	2.39	0.57
3:16:24:GLU:HB3	3:16:33:ARG:HB2	1.87	0.57
3:20:24:GLU:HB3	3:20:33:ARG:HB2	1.87	0.57
3:21:24:GLU:HB3	3:21:33:ARG:HB2	1.87	0.57
3:24:70:PHE:CD1	1:X:41:PRO:HD3	2.39	0.57
3:26:70:PHE:CD1	1:Z:41:PRO:HD3	2.40	0.57
1:B:160:ASN:HA	1:B:186:PRO:HD3	1.85	0.57
1:J:160:ASN:HA	1:J:186:PRO:HD3	1.85	0.57
1:K:223:GLN:HB2	1:L:232:MET:HG3	1.86	0.57
1:L:39:PRO:HB3	1:M:75:GLY:HA3	1.86	0.57
1:S:223:GLN:HB2	1:T:232:MET:HG3	1.86	0.57
1:T:39:PRO:HB3	1:U:75:GLY:HA3	1.86	0.57
3:13:70:PHE:CD1	1:M:41:PRO:HD3	2.39	0.57
3:17:24:GLU:HB3	3:17:33:ARG:HB2	1.87	0.57
3:19:18:ARG:NE	3:19:46:THR:HA	2.20	0.57
3:22:18:ARG:NE	3:22:46:THR:HA	2.20	0.57
3:22:24:GLU:HB3	3:22:33:ARG:HB2	1.87	0.57
1:F:223:GLN:HB2	1:G:232:MET:HG3	1.86	0.57
1:I:39:PRO:HB3	1:J:75:GLY:HA3	1.86	0.57
1:K:39:PRO:HB3	1:L:75:GLY:HA3	1.86	0.57
1:O:223:GLN:HB2	1:P:232:MET:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:13:24:GLU:HB3	3:13:33:ARG:HB2	1.87	0.57
3:19:70:PHE:CD1	1:S:41:PRO:HD3	2.39	0.57
3:23:70:PHE:CD1	1:W:41:PRO:HD3	2.39	0.57
3:24:24:GLU:HB3	3:24:33:ARG:HB2	1.87	0.57
3:25:24:GLU:HB3	3:25:33:ARG:HB2	1.87	0.57
1:E:39:PRO:HB3	1:F:75:GLY:HA3	1.86	0.57
1:E:223:GLN:HB2	1:F:232:MET:HG3	1.86	0.57
1:G:39:PRO:HB3	1:H:75:GLY:HA3	1.86	0.57
1:P:160:ASN:HA	1:P:186:PRO:HD3	1.85	0.57
1:U:160:ASN:HA	1:U:186:PRO:HD3	1.85	0.57
3:5:70:PHE:CD1	1:E:41:PRO:HD3	2.39	0.57
3:12:24:GLU:HB3	3:12:33:ARG:HB2	1.87	0.57
3:14:24:GLU:HB3	3:14:33:ARG:HB2	1.87	0.57
3:16:18:ARG:NE	3:16:46:THR:HA	2.20	0.57
3:18:24:GLU:HB3	3:18:33:ARG:HB2	1.87	0.57
3:19:24:GLU:HB3	3:19:33:ARG:HB2	1.87	0.57
3:21:70:PHE:CD1	1:U:41:PRO:HD3	2.39	0.57
3:26:24:GLU:HB3	3:26:33:ARG:HB2	1.87	0.57
1:R:223:GLN:HB2	1:S:232:MET:HG3	1.85	0.57
3:12:70:PHE:CD1	1:L:41:PRO:HD3	2.40	0.57
3:15:24:GLU:HB3	3:15:33:ARG:HB2	1.87	0.57
3:25:18:ARG:NE	3:25:46:THR:HA	2.20	0.57
3:26:18:ARG:NE	3:26:46:THR:HA	2.20	0.57
1:P:39:PRO:HB3	1:Q:75:GLY:HA3	1.87	0.57
3:2:18:ARG:NE	3:2:46:THR:HA	2.20	0.57
3:11:24:GLU:HB3	3:11:33:ARG:HB2	1.87	0.57
3:16:70:PHE:CD1	1:P:41:PRO:HD3	2.39	0.57
3:17:70:PHE:CD1	1:Q:41:PRO:HD3	2.39	0.57
3:23:18:ARG:NE	3:23:46:THR:HA	2.20	0.57
3:23:24:GLU:HB3	3:23:33:ARG:HB2	1.87	0.57
1:I:223:GLN:HB2	1:J:232:MET:HG3	1.87	0.57
1:J:223:GLN:HB2	1:K:232:MET:HG3	1.86	0.57
1:T:160:ASN:HA	1:T:186:PRO:HD3	1.85	0.57
1:V:39:PRO:HB3	1:W:75:GLY:HA3	1.87	0.57
3:1:24:GLU:HB3	3:1:33:ARG:HB2	1.87	0.57
3:20:18:ARG:NE	3:20:46:THR:HA	2.20	0.57
1:C:223:GLN:HB2	1:D:232:MET:HG3	1.86	0.57
1:H:39:PRO:HB3	1:I:75:GLY:HA3	1.86	0.57
3:2:24:GLU:HB3	3:2:33:ARG:HB2	1.87	0.56
3:3:24:GLU:HB3	3:3:33:ARG:HB2	1.87	0.56
3:9:24:GLU:HB3	3:9:33:ARG:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:9:70:PHE:CD1	1:I:41:PRO:HD3	2.39	0.56
1:N:160:ASN:HA	1:N:186:PRO:HD3	1.85	0.56
3:8:24:GLU:HB3	3:8:33:ARG:HB2	1.87	0.56
3:14:70:PHE:CD1	1:N:41:PRO:HD3	2.40	0.56
1:D:223:GLN:HB2	1:E:232:MET:HG3	1.86	0.56
1:F:39:PRO:HB3	1:G:75:GLY:HA3	1.86	0.56
1:I:160:ASN:HA	1:I:186:PRO:HD3	1.85	0.56
3:3:18:ARG:NE	3:3:46:THR:HA	2.20	0.56
3:4:24:GLU:HB3	3:4:33:ARG:HB2	1.87	0.56
3:7:24:GLU:HB3	3:7:33:ARG:HB2	1.87	0.56
3:8:39:PRO:HB2	3:8:42:PHE:CD1	2.41	0.56
3:9:39:PRO:HB2	3:9:42:PHE:CD1	2.41	0.56
3:10:24:GLU:HB3	3:10:33:ARG:HB2	1.87	0.56
3:10:39:PRO:HB2	3:10:42:PHE:CD1	2.41	0.56
3:11:39:PRO:HB2	3:11:42:PHE:CD1	2.41	0.56
3:13:18:ARG:NE	3:13:46:THR:HA	2.20	0.56
3:14:39:PRO:HB2	3:14:42:PHE:CD1	2.41	0.56
3:15:70:PHE:CD1	1:O:41:PRO:HD3	2.39	0.56
3:16:39:PRO:HB2	3:16:42:PHE:CD1	2.41	0.56
3:17:18:ARG:NE	3:17:46:THR:HA	2.20	0.56
3:18:18:ARG:NE	3:18:46:THR:HA	2.20	0.56
3:21:18:ARG:NE	3:21:46:THR:HA	2.20	0.56
1:D:39:PRO:HB3	1:E:75:GLY:HA3	1.87	0.56
1:Y:223:GLN:HB2	1:Z:232:MET:HG3	1.86	0.56
3:1:39:PRO:HB2	3:1:42:PHE:CD1	2.41	0.56
3:5:18:ARG:NE	3:5:46:THR:HA	2.20	0.56
3:12:39:PRO:HB2	3:12:42:PHE:CD1	2.41	0.56
1:J:39:PRO:HB3	1:K:75:GLY:HA3	1.87	0.56
3:5:24:GLU:HB3	3:5:33:ARG:HB2	1.87	0.56
3:7:39:PRO:HB2	3:7:42:PHE:CD1	2.41	0.56
3:25:39:PRO:HB2	3:25:42:PHE:CD1	2.41	0.56
1:O:160:ASN:HA	1:O:186:PRO:HD3	1.85	0.56
3:4:39:PRO:HB2	3:4:42:PHE:CD1	2.41	0.56
3:6:24:GLU:HB3	3:6:33:ARG:HB2	1.87	0.56
3:6:39:PRO:HB2	3:6:42:PHE:CD1	2.41	0.56
3:8:22:VAL:HG22	3:8:34:LEU:CD2	2.34	0.56
3:15:18:ARG:NE	3:15:46:THR:HA	2.20	0.56
3:20:70:PHE:CD1	1:T:41:PRO:HD3	2.39	0.56
3:3:39:PRO:HB2	3:3:42:PHE:CD1	2.41	0.56
3:13:39:PRO:HB2	3:13:42:PHE:CD1	2.41	0.56
3:18:70:PHE:CD1	1:R:41:PRO:HD3	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:39:PRO:HB2	3:2:42:PHE:CD1	2.41	0.56
3:8:18:ARG:NE	3:8:46:THR:HA	2.20	0.56
3:9:22:VAL:HG22	3:9:34:LEU:CD2	2.34	0.56
3:10:18:ARG:NE	3:10:46:THR:HA	2.20	0.56
3:11:18:ARG:NE	3:11:46:THR:HA	2.20	0.56
3:18:23:SER:OG	3:18:35:THR:HG23	2.06	0.56
3:18:39:PRO:HB2	3:18:42:PHE:CD1	2.41	0.56
3:19:23:SER:OG	3:19:35:THR:HG23	2.06	0.56
3:20:23:SER:OG	3:20:35:THR:HG23	2.06	0.56
3:21:23:SER:OG	3:21:35:THR:HG23	2.06	0.56
3:23:39:PRO:HB2	3:23:42:PHE:CD1	2.41	0.56
3:3:59:CYS:SG	3:3:67:ALA:HB2	2.46	0.56
3:5:39:PRO:HB2	3:5:42:PHE:CD1	2.41	0.56
3:13:59:CYS:SG	3:13:67:ALA:HB2	2.46	0.56
3:14:59:CYS:SG	3:14:67:ALA:HB2	2.46	0.56
3:17:23:SER:OG	3:17:35:THR:HG23	2.06	0.56
3:24:18:ARG:NE	3:24:46:THR:HA	2.20	0.56
3:24:59:CYS:SG	3:24:67:ALA:HB2	2.46	0.56
3:25:59:CYS:SG	3:25:67:ALA:HB2	2.46	0.56
3:26:59:CYS:SG	3:26:67:ALA:HB2	2.46	0.56
1:O:80:ILE:HD13	1:O:195:VAL:HG13	1.88	0.56
1:P:80:ILE:HD13	1:P:195:VAL:HG13	1.88	0.56
1:X:223:GLN:HB2	1:Y:232:MET:HG3	1.87	0.56
3:1:59:CYS:SG	3:1:67:ALA:HB2	2.46	0.56
3:6:59:CYS:SG	3:6:67:ALA:HB2	2.46	0.56
3:9:59:CYS:SG	3:9:67:ALA:HB2	2.46	0.56
3:11:59:CYS:SG	3:11:67:ALA:HB2	2.46	0.56
3:12:59:CYS:SG	3:12:67:ALA:HB2	2.46	0.56
1:C:80:ILE:HD13	1:C:195:VAL:HG13	1.88	0.56
1:D:80:ILE:HD13	1:D:195:VAL:HG13	1.88	0.56
3:10:22:VAL:HG22	3:10:34:LEU:CD2	2.34	0.55
3:15:59:CYS:SG	3:15:67:ALA:HB2	2.46	0.55
3:21:39:PRO:HB2	3:21:42:PHE:CD1	2.41	0.55
3:23:59:CYS:SG	3:23:67:ALA:HB2	2.46	0.55
3:26:39:PRO:HB2	3:26:42:PHE:CD1	2.41	0.55
1:V:80:ILE:HD13	1:V:195:VAL:HG13	1.88	0.55
1:W:80:ILE:HD13	1:W:195:VAL:HG13	1.88	0.55
3:1:18:ARG:NE	3:1:46:THR:HA	2.20	0.55
3:2:59:CYS:SG	3:2:67:ALA:HB2	2.46	0.55
3:9:18:ARG:NE	3:9:46:THR:HA	2.20	0.55
3:16:23:SER:OG	3:16:35:THR:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:16:59:CYS:SG	3:16:67:ALA:HB2	2.46	0.55
3:19:39:PRO:HB2	3:19:42:PHE:CD1	2.41	0.55
3:22:23:SER:OG	3:22:35:THR:HG23	2.06	0.55
3:7:18:ARG:NE	3:7:46:THR:HA	2.20	0.55
3:8:59:CYS:SG	3:8:67:ALA:HB2	2.46	0.55
3:15:23:SER:OG	3:15:35:THR:HG23	2.06	0.55
3:15:39:PRO:HB2	3:15:42:PHE:CD1	2.41	0.55
3:22:59:CYS:SG	3:22:67:ALA:HB2	2.46	0.55
3:23:23:SER:OG	3:23:35:THR:HG23	2.06	0.55
1:E:80:ILE:HD13	1:E:195:VAL:HG13	1.88	0.55
1:J:80:ILE:HD13	1:J:195:VAL:HG13	1.88	0.55
1:N:80:ILE:HD13	1:N:195:VAL:HG13	1.88	0.55
1:U:80:ILE:HD13	1:U:195:VAL:HG13	1.88	0.55
1:X:80:ILE:HD13	1:X:195:VAL:HG13	1.88	0.55
3:4:18:ARG:NE	3:4:46:THR:HA	2.20	0.55
3:4:59:CYS:SG	3:4:67:ALA:HB2	2.46	0.55
3:10:59:CYS:SG	3:10:67:ALA:HB2	2.46	0.55
3:17:39:PRO:HB2	3:17:42:PHE:CD1	2.41	0.55
3:19:74:VAL:O	3:19:90:PHE:HA	2.07	0.55
3:24:39:PRO:HB2	3:24:42:PHE:CD1	2.41	0.55
1:I:80:ILE:HD13	1:I:195:VAL:HG13	1.88	0.55
1:Q:80:ILE:HD13	1:Q:195:VAL:HG13	1.88	0.55
3:3:19:GLN:O	3:3:21:GLN:NE2	2.40	0.55
3:6:74:VAL:O	3:6:90:PHE:HA	2.07	0.55
3:7:23:SER:OG	3:7:35:THR:HG23	2.06	0.55
3:8:19:GLN:O	3:8:21:GLN:NE2	2.40	0.55
3:8:23:SER:OG	3:8:35:THR:HG23	2.06	0.55
3:11:22:VAL:HG22	3:11:34:LEU:CD2	2.34	0.55
3:12:74:VAL:O	3:12:90:PHE:HA	2.07	0.55
3:13:74:VAL:O	3:13:90:PHE:HA	2.07	0.55
3:17:59:CYS:SG	3:17:67:ALA:HB2	2.46	0.55
3:20:39:PRO:HB2	3:20:42:PHE:CD1	2.41	0.55
3:20:74:VAL:O	3:20:90:PHE:HA	2.07	0.55
3:22:39:PRO:HB2	3:22:42:PHE:CD1	2.41	0.55
3:24:23:SER:OG	3:24:35:THR:HG23	2.06	0.55
1:B:80:ILE:HD13	1:B:195:VAL:HG13	1.88	0.55
1:W:176:GLU:OE1	1:W:207:TYR:OH	2.21	0.55
1:Y:176:GLU:OE1	1:Y:207:TYR:OH	2.21	0.55
3:1:19:GLN:O	3:1:21:GLN:NE2	2.40	0.55
3:6:19:GLN:O	3:6:21:GLN:NE2	2.40	0.55
3:6:23:SER:OG	3:6:35:THR:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:19:GLN:O	3:7:21:GLN:NE2	2.40	0.55
3:12:18:ARG:NE	3:12:46:THR:HA	2.20	0.55
1:T:80:ILE:HD13	1:T:195:VAL:HG13	1.88	0.55
3:5:59:CYS:SG	3:5:67:ALA:HB2	2.46	0.55
3:5:74:VAL:O	3:5:90:PHE:HA	2.07	0.55
3:7:74:VAL:O	3:7:90:PHE:HA	2.07	0.55
3:9:23:SER:OG	3:9:35:THR:HG23	2.06	0.55
3:11:19:GLN:O	3:11:21:GLN:NE2	2.40	0.55
3:12:22:VAL:HG22	3:12:34:LEU:CD2	2.34	0.55
3:14:23:SER:OG	3:14:35:THR:HG23	2.06	0.55
3:18:74:VAL:O	3:18:90:PHE:HA	2.07	0.55
3:24:74:VAL:O	3:24:90:PHE:HA	2.07	0.55
1:Y:80:ILE:HD13	1:Y:195:VAL:HG13	1.88	0.55
1:Z:176:GLU:OE1	1:Z:207:TYR:OH	2.21	0.55
3:1:74:VAL:O	3:1:90:PHE:HA	2.07	0.55
3:4:19:GLN:O	3:4:21:GLN:NE2	2.40	0.55
3:5:23:SER:OG	3:5:35:THR:HG23	2.06	0.55
3:14:74:VAL:O	3:14:90:PHE:HA	2.07	0.55
3:21:59:CYS:SG	3:21:67:ALA:HB2	2.47	0.55
3:21:74:VAL:O	3:21:90:PHE:HA	2.07	0.55
3:22:22:VAL:HG22	3:22:34:LEU:CD2	2.34	0.55
3:23:22:VAL:HG22	3:23:34:LEU:CD2	2.34	0.55
1:K:80:ILE:HD13	1:K:195:VAL:HG13	1.88	0.55
3:4:74:VAL:O	3:4:90:PHE:HA	2.07	0.55
3:7:59:CYS:SG	3:7:67:ALA:HB2	2.46	0.55
3:10:19:GLN:O	3:10:21:GLN:NE2	2.40	0.55
3:10:23:SER:OG	3:10:35:THR:HG23	2.06	0.55
3:18:59:CYS:SG	3:18:67:ALA:HB2	2.46	0.55
3:24:19:GLN:O	3:24:21:GLN:NE2	2.40	0.55
3:24:22:VAL:HG22	3:24:34:LEU:CD2	2.34	0.55
3:25:22:VAL:HG22	3:25:34:LEU:CD2	2.34	0.55
3:25:23:SER:OG	3:25:35:THR:HG23	2.06	0.55
1:H:80:ILE:HD13	1:H:195:VAL:HG13	1.88	0.55
3:1:22:VAL:HG22	3:1:34:LEU:CD2	2.34	0.55
3:9:19:GLN:O	3:9:21:GLN:NE2	2.40	0.55
3:11:74:VAL:O	3:11:90:PHE:HA	2.07	0.55
3:13:22:VAL:HG22	3:13:34:LEU:CD2	2.34	0.55
3:26:19:GLN:O	3:26:21:GLN:NE2	2.40	0.55
3:26:22:VAL:HG22	3:26:34:LEU:CD2	2.34	0.55
3:2:22:VAL:HG22	3:2:34:LEU:CD2	2.34	0.54
3:5:19:GLN:O	3:5:21:GLN:NE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:11:23:SER:OG	3:11:35:THR:HG23	2.06	0.54
3:13:23:SER:OG	3:13:35:THR:HG23	2.06	0.54
3:14:18:ARG:NE	3:14:46:THR:HA	2.20	0.54
3:20:59:CYS:SG	3:20:67:ALA:HB2	2.46	0.54
1:F:80:ILE:HD13	1:F:195:VAL:HG13	1.88	0.54
1:M:80:ILE:HD13	1:M:195:VAL:HG13	1.88	0.54
3:2:74:VAL:O	3:2:90:PHE:HA	2.07	0.54
3:4:23:SER:OG	3:4:35:THR:HG23	2.06	0.54
3:8:74:VAL:O	3:8:90:PHE:HA	2.07	0.54
3:13:19:GLN:O	3:13:21:GLN:NE2	2.40	0.54
3:17:74:VAL:O	3:17:90:PHE:HA	2.07	0.54
3:21:22:VAL:HG22	3:21:34:LEU:CD2	2.34	0.54
1:J:68:ASP:O	1:J:69:ARG:HG2	2.08	0.54
1:M:68:ASP:O	1:M:69:ARG:HG2	2.08	0.54
1:R:80:ILE:HD13	1:R:195:VAL:HG13	1.88	0.54
1:Z:68:ASP:O	1:Z:69:ARG:HG2	2.08	0.54
1:Z:80:ILE:HD13	1:Z:195:VAL:HG13	1.88	0.54
3:3:74:VAL:O	3:3:90:PHE:HA	2.07	0.54
3:6:18:ARG:NE	3:6:46:THR:HA	2.20	0.54
3:14:22:VAL:HG22	3:14:34:LEU:CD2	2.34	0.54
3:15:74:VAL:O	3:15:90:PHE:HA	2.07	0.54
3:19:22:VAL:HG22	3:19:34:LEU:CD2	2.34	0.54
3:20:22:VAL:HG22	3:20:34:LEU:CD2	2.34	0.54
3:25:19:GLN:O	3:25:21:GLN:NE2	2.40	0.54
3:26:23:SER:OG	3:26:35:THR:HG23	2.06	0.54
1:N:68:ASP:O	1:N:69:ARG:HG2	2.08	0.54
1:S:80:ILE:HD13	1:S:195:VAL:HG13	1.88	0.54
1:V:68:ASP:O	1:V:69:ARG:HG2	2.08	0.54
1:A:80:ILE:HD13	1:A:195:VAL:HG13	1.89	0.54
3:1:23:SER:OG	3:1:35:THR:HG23	2.06	0.54
3:3:22:VAL:HG22	3:3:34:LEU:CD2	2.34	0.54
3:12:23:SER:OG	3:12:35:THR:HG23	2.06	0.54
3:15:22:VAL:HG22	3:15:34:LEU:CD2	2.34	0.54
3:16:22:VAL:HG22	3:16:34:LEU:CD2	2.34	0.54
3:17:22:VAL:HG22	3:17:34:LEU:CD2	2.34	0.54
3:19:59:CYS:SG	3:19:67:ALA:HB2	2.46	0.54
3:22:19:GLN:O	3:22:21:GLN:NE2	2.40	0.54
3:22:74:VAL:O	3:22:90:PHE:HA	2.07	0.54
3:23:28:ILE:O	3:23:29:SER:OG	2.21	0.54
3:25:74:VAL:O	3:25:90:PHE:HA	2.07	0.54
1:O:68:ASP:O	1:O:69:ARG:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:68:ASP:O	1:U:69:ARG:HG2	2.08	0.54
1:W:68:ASP:O	1:W:69:ARG:HG2	2.08	0.54
3:2:19:GLN:O	3:2:21:GLN:NE2	2.40	0.54
3:3:23:SER:OG	3:3:35:THR:HG23	2.06	0.54
3:10:74:VAL:O	3:10:90:PHE:HA	2.07	0.54
3:14:19:GLN:O	3:14:21:GLN:NE2	2.40	0.54
3:18:22:VAL:HG22	3:18:34:LEU:CD2	2.34	0.54
1:C:68:ASP:O	1:C:69:ARG:HG2	2.08	0.54
1:D:68:ASP:O	1:D:69:ARG:HG2	2.08	0.54
1:G:68:ASP:O	1:G:69:ARG:HG2	2.08	0.54
1:R:176:GLU:OE1	1:R:207:TYR:OH	2.21	0.54
3:4:22:VAL:HG22	3:4:34:LEU:CD2	2.34	0.54
3:16:19:GLN:O	3:16:21:GLN:NE2	2.40	0.54
3:16:74:VAL:O	3:16:90:PHE:HA	2.07	0.54
3:18:19:GLN:O	3:18:21:GLN:NE2	2.40	0.54
1:E:68:ASP:O	1:E:69:ARG:HG2	2.08	0.54
1:L:68:ASP:O	1:L:69:ARG:HG2	2.08	0.54
1:P:68:ASP:O	1:P:69:ARG:HG2	2.08	0.54
1:X:68:ASP:O	1:X:69:ARG:HG2	2.08	0.54
1:A:68:ASP:O	1:A:69:ARG:HG2	2.08	0.54
3:17:19:GLN:O	3:17:21:GLN:NE2	2.40	0.54
3:23:74:VAL:O	3:23:90:PHE:HA	2.07	0.54
1:F:68:ASP:O	1:F:69:ARG:HG2	2.08	0.54
1:K:68:ASP:O	1:K:69:ARG:HG2	2.08	0.54
1:Q:68:ASP:O	1:Q:69:ARG:HG2	2.08	0.54
1:T:68:ASP:O	1:T:69:ARG:HG2	2.08	0.54
1:Y:121:ARG:HA	1:Z:111:ARG:HB2	1.90	0.54
3:2:23:SER:OG	3:2:35:THR:HG23	2.06	0.54
3:19:19:GLN:O	3:19:21:GLN:NE2	2.40	0.54
3:20:19:GLN:O	3:20:21:GLN:NE2	2.40	0.54
3:21:19:GLN:O	3:21:21:GLN:NE2	2.40	0.54
1:L:80:ILE:HD13	1:L:195:VAL:HG13	1.88	0.54
3:5:22:VAL:HG22	3:5:34:LEU:CD2	2.34	0.54
3:26:74:VAL:O	3:26:90:PHE:HA	2.07	0.54
1:B:121:ARG:HA	1:C:111:ARG:HB2	1.90	0.54
1:G:80:ILE:HD13	1:G:195:VAL:HG13	1.88	0.54
3:9:74:VAL:O	3:9:90:PHE:HA	2.07	0.54
3:12:19:GLN:O	3:12:21:GLN:NE2	2.40	0.54
3:23:19:GLN:O	3:23:21:GLN:NE2	2.40	0.54
1:B:68:ASP:O	1:B:69:ARG:HG2	2.08	0.54
1:Y:68:ASP:O	1:Y:69:ARG:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:68:ASP:O	1:I:69:ARG:HG2	2.08	0.53
1:S:68:ASP:O	1:S:69:ARG:HG2	2.08	0.53
1:X:121:ARG:HA	1:Y:111:ARG:HB2	1.90	0.53
3:15:19:GLN:O	3:15:21:GLN:NE2	2.40	0.53
1:F:37:ALA:HB1	1:G:74:ILE:CG2	2.39	0.53
3:6:22:VAL:HG22	3:6:34:LEU:CD2	2.34	0.53
1:E:121:ARG:HA	1:F:111:ARG:HB2	1.90	0.53
1:H:68:ASP:O	1:H:69:ARG:HG2	2.08	0.53
1:S:176:GLU:OE1	1:S:207:TYR:OH	2.21	0.53
1:A:121:ARG:HA	1:B:111:ARG:HB2	1.91	0.53
1:C:37:ALA:HB1	1:D:74:ILE:CG2	2.39	0.53
1:I:37:ALA:HB1	1:J:74:ILE:CG2	2.39	0.53
1:T:121:ARG:HA	1:U:111:ARG:HB2	1.90	0.53
1:W:121:ARG:HA	1:X:111:ARG:HB2	1.90	0.53
1:X:37:ALA:HB1	1:Y:74:ILE:CG2	2.39	0.53
1:H:121:ARG:HA	1:I:111:ARG:HB2	1.90	0.53
1:N:121:ARG:HA	1:O:111:ARG:HB2	1.90	0.53
1:U:37:ALA:HB1	1:V:74:ILE:CG2	2.39	0.53
1:C:121:ARG:HA	1:D:111:ARG:HB2	1.90	0.53
1:M:121:ARG:HA	1:N:111:ARG:HB2	1.90	0.53
3:5:64:TYR:HB2	3:5:96:CYS:HB3	1.91	0.53
1:G:121:ARG:HA	1:H:111:ARG:HB2	1.90	0.53
1:P:206:GLU:HG2	1:P:208:VAL:HG13	1.91	0.53
1:S:121:ARG:HA	1:T:111:ARG:HB2	1.90	0.53
1:A:111:ARG:HB2	1:Z:121:ARG:HA	1.91	0.53
3:1:28:ILE:O	3:1:29:SER:OG	2.21	0.53
3:7:22:VAL:HG22	3:7:34:LEU:CD2	2.34	0.53
3:7:64:TYR:HB2	3:7:96:CYS:HB3	1.91	0.53
3:20:28:ILE:O	3:20:29:SER:OG	2.21	0.53
1:K:121:ARG:HA	1:L:111:ARG:HB2	1.90	0.53
1:O:37:ALA:HB1	1:P:74:ILE:CG2	2.39	0.53
1:O:121:ARG:HA	1:P:111:ARG:HB2	1.90	0.53
1:Q:121:ARG:HA	1:R:111:ARG:HB2	1.90	0.53
1:R:206:GLU:HG2	1:R:208:VAL:HG13	1.91	0.53
1:A:69:ARG:HG3	1:A:69:ARG:O	2.10	0.52
3:4:64:TYR:HB2	3:4:96:CYS:HB3	1.91	0.52
3:6:64:TYR:HB2	3:6:96:CYS:HB3	1.91	0.52
3:19:70:PHE:HD1	1:S:41:PRO:HD3	1.74	0.52
3:20:70:PHE:HD1	1:T:41:PRO:HD3	1.74	0.52
3:25:70:PHE:HD1	1:Y:41:PRO:HD3	1.74	0.52
1:D:37:ALA:HB1	1:E:74:ILE:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:206:GLU:HG2	1:L:208:VAL:HG13	1.91	0.52
1:N:206:GLU:HG2	1:N:208:VAL:HG13	1.91	0.52
1:R:68:ASP:O	1:R:69:ARG:HG2	2.08	0.52
1:U:121:ARG:HA	1:V:111:ARG:HB2	1.90	0.52
3:3:64:TYR:HB2	3:3:96:CYS:HB3	1.91	0.52
3:14:70:PHE:HD1	1:N:41:PRO:HD3	1.74	0.52
3:15:70:PHE:HD1	1:O:41:PRO:HD3	1.74	0.52
1:D:69:ARG:HG3	1:D:69:ARG:O	2.09	0.52
1:E:69:ARG:HG3	1:E:69:ARG:O	2.10	0.52
1:L:37:ALA:HB1	1:M:74:ILE:CG2	2.39	0.52
1:T:206:GLU:HG2	1:T:208:VAL:HG13	1.91	0.52
3:8:64:TYR:HB2	3:8:96:CYS:HB3	1.92	0.52
1:F:121:ARG:HA	1:G:111:ARG:HB2	1.91	0.52
1:H:84:GLU:HG2	1:H:197:SER:OG	2.10	0.52
1:N:84:GLU:HG2	1:N:197:SER:OG	2.10	0.52
1:Q:84:GLU:HG2	1:Q:197:SER:OG	2.10	0.52
1:V:37:ALA:HB1	1:W:74:ILE:CG2	2.39	0.52
3:13:70:PHE:HD1	1:M:41:PRO:HD3	1.74	0.52
3:21:70:PHE:HD1	1:U:41:PRO:HD3	1.74	0.52
1:E:84:GLU:HG2	1:E:197:SER:OG	2.10	0.52
1:H:69:ARG:O	1:H:69:ARG:HG3	2.09	0.52
1:K:84:GLU:HG2	1:K:197:SER:OG	2.10	0.52
3:2:64:TYR:HB2	3:2:96:CYS:HB3	1.91	0.52
3:9:64:TYR:HB2	3:9:96:CYS:HB3	1.92	0.52
3:16:70:PHE:HD1	1:P:41:PRO:HD3	1.74	0.52
1:B:176:GLU:OE1	1:B:207:TYR:OH	2.21	0.52
1:G:84:GLU:HG2	1:G:197:SER:OG	2.10	0.52
1:X:69:ARG:O	1:X:69:ARG:HG3	2.10	0.52
1:Z:69:ARG:HG3	1:Z:69:ARG:O	2.10	0.52
3:5:21:GLN:O	3:5:34:LEU:HB3	2.10	0.52
3:15:21:GLN:O	3:15:34:LEU:HB3	2.10	0.52
3:23:21:GLN:O	3:23:34:LEU:HB3	2.10	0.52
1:B:69:ARG:HG3	1:B:69:ARG:O	2.10	0.52
1:B:84:GLU:HG2	1:B:197:SER:OG	2.10	0.52
1:I:121:ARG:HA	1:J:111:ARG:HB2	1.90	0.52
1:J:31:VAL:HB	1:K:179:ARG:HD3	1.92	0.52
1:J:206:GLU:HG2	1:J:208:VAL:HG13	1.91	0.52
1:L:121:ARG:HA	1:M:111:ARG:HB2	1.90	0.52
1:R:31:VAL:HB	1:S:179:ARG:HD3	1.92	0.52
1:R:121:ARG:HA	1:S:111:ARG:HB2	1.90	0.52
1:T:84:GLU:HG2	1:T:197:SER:OG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:69:ARG:HG3	1:W:69:ARG:O	2.10	0.52
3:9:21:GLN:O	3:9:34:LEU:HB3	2.10	0.52
3:10:70:PHE:HD1	1:J:41:PRO:HD3	1.74	0.52
3:18:21:GLN:O	3:18:34:LEU:HB3	2.10	0.52
3:20:21:GLN:O	3:20:34:LEU:HB3	2.10	0.52
1:D:84:GLU:HG2	1:D:197:SER:OG	2.10	0.52
1:J:84:GLU:HG2	1:J:197:SER:OG	2.10	0.52
1:K:37:ALA:HB1	1:L:74:ILE:CG2	2.39	0.52
1:N:31:VAL:HB	1:O:179:ARG:HD3	1.92	0.52
1:S:37:ALA:HB1	1:T:74:ILE:CG2	2.40	0.52
1:V:206:GLU:HG2	1:V:208:VAL:HG13	1.91	0.52
1:Y:37:ALA:HB1	1:Z:74:ILE:CG2	2.39	0.52
1:Y:69:ARG:HG3	1:Y:69:ARG:O	2.10	0.52
1:A:84:GLU:HG2	1:A:197:SER:OG	2.10	0.52
1:A:179:ARG:HD3	1:Z:31:VAL:HB	1.92	0.52
3:1:64:TYR:HB2	3:1:96:CYS:HB3	1.91	0.52
3:10:64:TYR:HB2	3:10:96:CYS:HB3	1.92	0.52
3:12:21:GLN:O	3:12:34:LEU:HB3	2.10	0.52
1:C:69:ARG:HG3	1:C:69:ARG:O	2.10	0.52
1:H:37:ALA:HB1	1:I:74:ILE:CG2	2.40	0.52
1:P:31:VAL:HB	1:Q:179:ARG:HD3	1.92	0.52
1:Z:84:GLU:HG2	1:Z:197:SER:OG	2.10	0.52
3:1:21:GLN:O	3:1:34:LEU:HB3	2.10	0.52
3:2:21:GLN:O	3:2:34:LEU:HB3	2.10	0.52
3:26:21:GLN:O	3:26:34:LEU:HB3	2.10	0.52
1:E:37:ALA:HB1	1:F:74:ILE:CG2	2.39	0.52
1:H:31:VAL:HB	1:I:179:ARG:HD3	1.92	0.52
1:I:69:ARG:HG3	1:I:69:ARG:O	2.09	0.52
1:L:84:GLU:HG2	1:L:197:SER:OG	2.10	0.52
1:M:31:VAL:HB	1:N:179:ARG:HD3	1.92	0.52
1:O:84:GLU:HG2	1:O:197:SER:OG	2.10	0.52
1:X:206:GLU:HG2	1:X:208:VAL:HG13	1.91	0.52
1:Y:31:VAL:HB	1:Z:179:ARG:HD3	1.92	0.52
1:Y:84:GLU:HG2	1:Y:197:SER:OG	2.10	0.52
1:A:37:ALA:HB1	1:B:74:ILE:CG2	2.40	0.52
3:6:21:GLN:O	3:6:34:LEU:HB3	2.10	0.52
3:8:21:GLN:O	3:8:34:LEU:HB3	2.10	0.52
3:11:64:TYR:HB2	3:11:96:CYS:HB3	1.91	0.52
3:17:21:GLN:O	3:17:34:LEU:HB3	2.10	0.52
1:B:31:VAL:HB	1:C:179:ARG:HD3	1.92	0.52
1:G:37:ALA:HB1	1:H:74:ILE:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:37:ALA:HB1	1:K:74:ILE:CG2	2.39	0.52
1:M:84:GLU:HG2	1:M:197:SER:OG	2.10	0.52
1:P:37:ALA:HB1	1:Q:74:ILE:CG2	2.39	0.52
1:R:84:GLU:HG2	1:R:197:SER:OG	2.10	0.52
1:U:84:GLU:HG2	1:U:197:SER:OG	2.10	0.52
1:V:31:VAL:HB	1:W:179:ARG:HD3	1.92	0.52
1:Y:39:PRO:HB3	1:Z:75:GLY:HA3	1.92	0.52
1:Y:171:ILE:O	1:Z:207:TYR:O	2.27	0.52
3:10:21:GLN:O	3:10:34:LEU:HB3	2.10	0.51
3:13:21:GLN:O	3:13:34:LEU:HB3	2.10	0.51
3:17:28:ILE:O	3:17:29:SER:OG	2.21	0.51
3:18:70:PHE:HD1	1:R:41:PRO:HD3	1.74	0.51
3:21:21:GLN:O	3:21:34:LEU:HB3	2.10	0.51
3:24:70:PHE:HD1	1:X:41:PRO:HD3	1.74	0.51
3:25:21:GLN:O	3:25:34:LEU:HB3	2.10	0.51
3:26:64:TYR:HB2	3:26:96:CYS:HB3	1.91	0.51
1:G:69:ARG:HG3	1:G:69:ARG:O	2.10	0.51
1:T:31:VAL:HB	1:U:179:ARG:HD3	1.92	0.51
1:W:37:ALA:HB1	1:X:74:ILE:CG2	2.39	0.51
1:W:84:GLU:HG2	1:W:197:SER:OG	2.10	0.51
3:3:21:GLN:O	3:3:34:LEU:HB3	2.10	0.51
3:4:21:GLN:O	3:4:34:LEU:HB3	2.10	0.51
3:9:70:PHE:HD1	1:I:41:PRO:HD3	1.74	0.51
3:11:70:PHE:HD1	1:K:41:PRO:HD3	1.74	0.51
3:17:70:PHE:HD1	1:Q:41:PRO:HD3	1.74	0.51
3:24:21:GLN:O	3:24:34:LEU:HB3	2.10	0.51
1:F:176:GLU:OE1	1:F:207:TYR:OH	2.21	0.51
1:P:84:GLU:HG2	1:P:197:SER:OG	2.10	0.51
1:S:84:GLU:HG2	1:S:197:SER:OG	2.10	0.51
1:V:84:GLU:HG2	1:V:197:SER:OG	2.10	0.51
1:A:41:PRO:HD3	3:1:70:PHE:HD1	1.73	0.51
3:16:21:GLN:O	3:16:34:LEU:HB3	2.10	0.51
3:22:70:PHE:HD1	1:V:41:PRO:HD3	1.74	0.51
1:B:37:ALA:HB1	1:C:74:ILE:CG2	2.40	0.51
1:F:69:ARG:HG3	1:F:69:ARG:O	2.10	0.51
1:K:31:VAL:HB	1:L:179:ARG:HD3	1.93	0.51
1:L:31:VAL:HB	1:M:179:ARG:HD3	1.93	0.51
1:P:121:ARG:HA	1:Q:111:ARG:HB2	1.91	0.51
1:Q:206:GLU:HG2	1:Q:208:VAL:HG13	1.91	0.51
1:S:31:VAL:HB	1:T:179:ARG:HD3	1.92	0.51
1:T:69:ARG:HG3	1:T:69:ARG:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:31:VAL:HB	1:X:179:ARG:HD3	1.92	0.51
1:A:74:ILE:CG2	1:Z:37:ALA:HB1	2.40	0.51
3:21:72:GLN:HG2	3:21:73:PRO:CD	2.41	0.51
3:22:21:GLN:O	3:22:34:LEU:HB3	2.10	0.51
3:22:72:GLN:HG2	3:22:73:PRO:CD	2.41	0.51
3:23:70:PHE:HD1	1:W:41:PRO:HD3	1.74	0.51
3:24:28:ILE:O	3:24:29:SER:OG	2.21	0.51
1:D:121:ARG:HA	1:E:111:ARG:HB2	1.91	0.51
1:D:206:GLU:HG2	1:D:208:VAL:HG13	1.91	0.51
1:G:31:VAL:HB	1:H:179:ARG:HD3	1.92	0.51
1:I:74:ILE:CD1	1:I:154:GLN:HA	2.41	0.51
1:K:74:ILE:CD1	1:K:154:GLN:HA	2.41	0.51
1:M:37:ALA:HB1	1:N:74:ILE:CG2	2.40	0.51
1:M:74:ILE:CD1	1:M:154:GLN:HA	2.41	0.51
1:M:206:GLU:HG2	1:M:208:VAL:HG13	1.91	0.51
1:N:37:ALA:HB1	1:O:74:ILE:CG2	2.40	0.51
1:O:206:GLU:HG2	1:O:208:VAL:HG13	1.91	0.51
1:Q:31:VAL:HB	1:R:179:ARG:HD3	1.93	0.51
1:A:31:VAL:HB	1:B:179:ARG:HD3	1.92	0.51
3:4:70:PHE:HD1	1:D:41:PRO:HD3	1.74	0.51
3:7:72:GLN:HG2	3:7:73:PRO:CD	2.41	0.51
3:14:28:ILE:O	3:14:29:SER:OG	2.21	0.51
1:B:74:ILE:CD1	1:B:154:GLN:HA	2.41	0.51
1:C:74:ILE:CD1	1:C:154:GLN:HA	2.41	0.51
1:D:31:VAL:HB	1:E:179:ARG:HD3	1.92	0.51
1:E:74:ILE:CD1	1:E:154:GLN:HA	2.41	0.51
1:G:74:ILE:CD1	1:G:154:GLN:HA	2.41	0.51
1:H:206:GLU:HG2	1:H:208:VAL:HG13	1.91	0.51
1:I:84:GLU:HG2	1:I:197:SER:OG	2.10	0.51
1:K:69:ARG:HG3	1:K:69:ARG:O	2.09	0.51
1:L:69:ARG:HG3	1:L:69:ARG:O	2.10	0.51
1:N:74:ILE:CD1	1:N:154:GLN:HA	2.41	0.51
1:A:74:ILE:CD1	1:A:154:GLN:HA	2.41	0.51
3:7:21:GLN:O	3:7:34:LEU:HB3	2.10	0.51
3:7:70:PHE:HD1	1:G:41:PRO:HD3	1.74	0.51
3:8:72:GLN:HG2	3:8:73:PRO:CD	2.41	0.51
3:14:21:GLN:O	3:14:34:LEU:HB3	2.10	0.51
3:20:64:TYR:HB2	3:20:96:CYS:HB3	1.91	0.51
3:21:64:TYR:HB2	3:21:96:CYS:HB3	1.91	0.51
3:23:72:GLN:HG2	3:23:73:PRO:CD	2.41	0.51
1:D:74:ILE:CD1	1:D:154:GLN:HA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:206:GLU:HG2	1:G:208:VAL:HG13	1.91	0.51
1:I:206:GLU:HG2	1:I:208:VAL:HG13	1.91	0.51
1:K:206:GLU:HG2	1:K:208:VAL:HG13	1.91	0.51
1:L:176:GLU:OE1	1:L:207:TYR:OH	2.21	0.51
1:O:74:ILE:CD1	1:O:154:GLN:HA	2.41	0.51
1:P:74:ILE:CD1	1:P:154:GLN:HA	2.41	0.51
1:Q:37:ALA:HB1	1:R:74:ILE:CG2	2.39	0.51
1:Q:74:ILE:CD1	1:Q:154:GLN:HA	2.41	0.51
1:Q:176:GLU:OE1	1:Q:207:TYR:OH	2.21	0.51
1:S:206:GLU:HG2	1:S:208:VAL:HG13	1.91	0.51
1:T:37:ALA:HB1	1:U:74:ILE:CG2	2.40	0.51
1:A:90:LYS:HD3	1:Y:176:GLU:OE2	2.10	0.51
3:3:70:PHE:HD1	1:C:41:PRO:HD3	1.74	0.51
3:5:70:PHE:HD1	1:E:41:PRO:HD3	1.74	0.51
3:9:72:GLN:HG2	3:9:73:PRO:CD	2.41	0.51
3:12:64:TYR:HB2	3:12:96:CYS:HB3	1.91	0.51
3:17:64:TYR:HB2	3:17:96:CYS:HB3	1.91	0.51
3:18:64:TYR:HB2	3:18:96:CYS:HB3	1.91	0.51
3:19:64:TYR:HB2	3:19:96:CYS:HB3	1.91	0.51
3:22:64:TYR:HB2	3:22:96:CYS:HB3	1.91	0.51
1:C:84:GLU:HG2	1:C:197:SER:OG	2.10	0.51
1:E:206:GLU:HG2	1:E:208:VAL:HG13	1.91	0.51
1:F:74:ILE:HD13	1:F:154:GLN:HA	1.93	0.51
1:F:84:GLU:HG2	1:F:197:SER:OG	2.10	0.51
1:H:74:ILE:HD13	1:H:154:GLN:HA	1.93	0.51
1:J:69:ARG:HG3	1:J:69:ARG:O	2.10	0.51
1:J:121:ARG:HA	1:K:111:ARG:HB2	1.91	0.51
1:Q:69:ARG:HG3	1:Q:69:ARG:O	2.10	0.51
1:R:37:ALA:HB1	1:S:74:ILE:CG2	2.41	0.51
1:X:84:GLU:HG2	1:X:197:SER:OG	2.10	0.51
1:Z:74:ILE:CD1	1:Z:154:GLN:HA	2.41	0.51
1:Z:206:GLU:HG2	1:Z:208:VAL:HG13	1.91	0.51
1:A:206:GLU:HG2	1:A:208:VAL:HG13	1.91	0.51
3:12:70:PHE:HD1	1:L:41:PRO:HD3	1.75	0.51
3:25:64:TYR:HB2	3:25:96:CYS:HB3	1.91	0.51
1:B:206:GLU:HG2	1:B:208:VAL:HG13	1.91	0.51
1:C:206:GLU:HG2	1:C:208:VAL:HG13	1.91	0.51
1:D:74:ILE:HD13	1:D:154:GLN:HA	1.93	0.51
1:P:69:ARG:O	1:P:69:ARG:HG3	2.10	0.51
1:R:74:ILE:CD1	1:R:154:GLN:HA	2.41	0.51
1:S:69:ARG:O	1:S:69:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:69:ARG:HG3	1:U:69:ARG:O	2.09	0.51
1:V:69:ARG:HG3	1:V:69:ARG:O	2.10	0.51
1:Y:74:ILE:CD1	1:Y:154:GLN:HA	2.41	0.51
1:Y:170:ALA:HB3	1:Z:206:GLU:HG3	1.92	0.51
3:11:21:GLN:O	3:11:34:LEU:HB3	2.10	0.51
3:16:64:TYR:HB2	3:16:96:CYS:HB3	1.91	0.51
3:24:72:GLN:HG2	3:24:73:PRO:CD	2.41	0.51
1:C:74:ILE:HD13	1:C:154:GLN:HA	1.93	0.51
1:E:74:ILE:HD13	1:E:154:GLN:HA	1.93	0.51
1:G:74:ILE:HD13	1:G:154:GLN:HA	1.93	0.51
1:I:74:ILE:HD13	1:I:154:GLN:HA	1.93	0.51
1:J:74:ILE:HD13	1:J:154:GLN:HA	1.93	0.51
1:K:176:GLU:OE1	1:K:207:TYR:OH	2.21	0.51
1:M:69:ARG:HG3	1:M:69:ARG:O	2.10	0.51
1:S:74:ILE:CD1	1:S:154:GLN:HA	2.41	0.51
1:V:121:ARG:HA	1:W:111:ARG:HB2	1.91	0.51
3:8:70:PHE:HD1	1:H:41:PRO:HD3	1.74	0.51
3:10:72:GLN:HG2	3:10:73:PRO:CD	2.41	0.51
1:I:31:VAL:HB	1:J:179:ARG:HD3	1.93	0.51
1:O:31:VAL:HB	1:P:179:ARG:HD3	1.93	0.51
1:U:206:GLU:HG2	1:U:208:VAL:HG13	1.91	0.51
3:2:70:PHE:HD1	1:B:41:PRO:HD3	1.74	0.50
3:6:70:PHE:HD1	1:F:41:PRO:HD3	1.74	0.50
3:23:64:TYR:HB2	3:23:96:CYS:HB3	1.92	0.50
1:B:74:ILE:HD13	1:B:154:GLN:HA	1.93	0.50
1:E:31:VAL:HB	1:F:179:ARG:HD3	1.92	0.50
1:F:31:VAL:HB	1:G:179:ARG:HD3	1.93	0.50
1:J:176:GLU:OE1	1:J:207:TYR:OH	2.21	0.50
1:K:74:ILE:HD13	1:K:154:GLN:HA	1.93	0.50
1:L:74:ILE:CD1	1:L:154:GLN:HA	2.41	0.50
1:N:69:ARG:HG3	1:N:69:ARG:O	2.09	0.50
1:X:74:ILE:CD1	1:X:154:GLN:HA	2.41	0.50
1:A:74:ILE:HD13	1:A:154:GLN:HA	1.93	0.50
3:15:64:TYR:HB2	3:15:96:CYS:HB3	1.92	0.50
3:24:83:SER:HA	1:Y:210:ASN:ND2	2.25	0.50
3:25:72:GLN:HG2	3:25:73:PRO:CD	2.41	0.50
1:F:74:ILE:CD1	1:F:154:GLN:HA	2.41	0.50
1:F:206:GLU:HG2	1:F:208:VAL:HG13	1.91	0.50
1:I:176:GLU:OE1	1:I:207:TYR:OH	2.21	0.50
1:U:31:VAL:HB	1:V:179:ARG:HD3	1.93	0.50
1:Y:206:GLU:HG2	1:Y:208:VAL:HG13	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:19:21:GLN:O	3:19:34:LEU:HB3	2.10	0.50
3:24:64:TYR:HB2	3:24:96:CYS:HB3	1.91	0.50
1:L:74:ILE:HD13	1:L:154:GLN:HA	1.93	0.50
1:T:74:ILE:CD1	1:T:154:GLN:HA	2.41	0.50
1:V:58:ILE:HG13	1:V:59:ASN:N	2.26	0.50
1:X:31:VAL:HB	1:Y:179:ARG:HD3	1.94	0.50
3:14:64:TYR:HB2	3:14:96:CYS:HB3	1.91	0.50
3:26:70:PHE:HD1	1:Z:41:PRO:HD3	1.75	0.50
1:O:69:ARG:HG3	1:O:69:ARG:O	2.10	0.50
1:T:58:ILE:HG13	1:T:59:ASN:N	2.26	0.50
1:U:58:ILE:HG13	1:U:59:ASN:N	2.26	0.50
1:W:74:ILE:CD1	1:W:154:GLN:HA	2.41	0.50
1:Z:74:ILE:HD13	1:Z:154:GLN:HA	1.93	0.50
3:11:72:GLN:HG2	3:11:73:PRO:CD	2.41	0.50
3:21:28:ILE:O	3:21:29:SER:OG	2.21	0.50
1:R:58:ILE:HG13	1:R:59:ASN:N	2.26	0.50
1:S:58:ILE:HG13	1:S:59:ASN:N	2.26	0.50
1:W:58:ILE:HG13	1:W:59:ASN:N	2.26	0.50
1:W:101:LYS:HZ2	1:W:101:LYS:HB3	1.76	0.50
1:W:206:GLU:HG2	1:W:208:VAL:HG13	1.91	0.50
1:X:58:ILE:HG13	1:X:59:ASN:N	2.26	0.50
1:Y:58:ILE:HG13	1:Y:59:ASN:N	2.26	0.50
1:Y:168:GLN:HG3	1:Z:204:ARG:NE	2.27	0.50
3:13:64:TYR:HB2	3:13:96:CYS:HB3	1.92	0.50
1:C:31:VAL:HB	1:D:179:ARG:HD3	1.93	0.50
1:H:74:ILE:CD1	1:H:154:GLN:HA	2.41	0.50
1:M:74:ILE:HD13	1:M:154:GLN:HA	1.93	0.50
1:P:58:ILE:HG13	1:P:59:ASN:N	2.26	0.50
1:Q:58:ILE:HG13	1:Q:59:ASN:N	2.26	0.50
1:T:80:ILE:HD13	1:T:195:VAL:CG1	2.42	0.50
1:U:74:ILE:CD1	1:U:154:GLN:HA	2.41	0.50
1:V:80:ILE:HD13	1:V:195:VAL:CG1	2.42	0.50
1:X:80:ILE:HD13	1:X:195:VAL:CG1	2.42	0.50
1:Z:58:ILE:HG13	1:Z:59:ASN:N	2.26	0.50
3:26:72:GLN:HG2	3:26:73:PRO:CD	2.41	0.50
1:B:101:LYS:HB3	1:B:101:LYS:HZ2	1.76	0.50
1:O:58:ILE:HG13	1:O:59:ASN:N	2.26	0.50
1:Q:80:ILE:HD13	1:Q:195:VAL:CG1	2.42	0.50
1:V:74:ILE:CD1	1:V:154:GLN:HA	2.41	0.50
1:Y:101:LYS:HZ2	1:Y:101:LYS:HB3	1.77	0.50
1:Z:80:ILE:HD13	1:Z:195:VAL:CG1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ILE:HG13	1:A:59:ASN:N	2.26	0.50
3:12:72:GLN:HG2	3:12:73:PRO:CD	2.41	0.50
1:B:58:ILE:HG13	1:B:59:ASN:N	2.26	0.50
1:B:80:ILE:HD13	1:B:195:VAL:CG1	2.42	0.50
1:J:74:ILE:CD1	1:J:154:GLN:HA	2.41	0.50
1:N:58:ILE:HG13	1:N:59:ASN:N	2.26	0.50
1:N:74:ILE:HD13	1:N:154:GLN:HA	1.93	0.50
1:P:80:ILE:HD13	1:P:195:VAL:CG1	2.42	0.50
1:R:80:ILE:HD13	1:R:195:VAL:CG1	2.42	0.50
1:U:80:ILE:HD13	1:U:195:VAL:CG1	2.42	0.50
1:Y:74:ILE:HD13	1:Y:154:GLN:HA	1.93	0.50
1:Y:80:ILE:HD13	1:Y:195:VAL:CG1	2.42	0.50
1:C:58:ILE:HG13	1:C:59:ASN:N	2.26	0.50
1:L:167:LYS:NZ	1:M:84:GLU:OE2	2.42	0.50
1:O:74:ILE:HD13	1:O:154:GLN:HA	1.93	0.50
1:D:58:ILE:HG13	1:D:59:ASN:N	2.26	0.49
1:M:58:ILE:HG13	1:M:59:ASN:N	2.26	0.49
1:P:74:ILE:HD13	1:P:154:GLN:HA	1.93	0.49
1:Q:74:ILE:HD13	1:Q:154:GLN:HA	1.93	0.49
3:1:72:GLN:HG2	3:1:73:PRO:CD	2.41	0.49
3:13:72:GLN:HG2	3:13:73:PRO:CD	2.41	0.49
1:E:58:ILE:HG13	1:E:59:ASN:N	2.26	0.49
1:L:58:ILE:HG13	1:L:59:ASN:N	2.26	0.49
1:R:69:ARG:HG3	1:R:69:ARG:O	2.10	0.49
1:X:74:ILE:HD13	1:X:154:GLN:HA	1.93	0.49
1:A:80:ILE:HD13	1:A:195:VAL:CG1	2.42	0.49
3:6:40:LEU:HG	3:6:85:CYS:O	2.13	0.49
3:12:40:LEU:HG	3:12:85:CYS:O	2.13	0.49
3:13:40:LEU:HG	3:13:85:CYS:O	2.13	0.49
1:F:58:ILE:HG13	1:F:59:ASN:N	2.26	0.49
1:G:58:ILE:HG13	1:G:59:ASN:N	2.26	0.49
1:S:74:ILE:HD13	1:S:154:GLN:HA	1.93	0.49
1:S:80:ILE:HD13	1:S:195:VAL:CG1	2.42	0.49
3:5:40:LEU:HG	3:5:85:CYS:O	2.13	0.49
1:D:80:ILE:HD13	1:D:195:VAL:CG1	2.42	0.49
1:H:58:ILE:HG13	1:H:59:ASN:N	2.26	0.49
1:K:58:ILE:HG13	1:K:59:ASN:N	2.26	0.49
1:R:74:ILE:HD13	1:R:154:GLN:HA	1.93	0.49
1:U:176:GLU:OE1	1:U:207:TYR:OH	2.21	0.49
1:H:167:LYS:NZ	1:I:84:GLU:OE2	2.42	0.49
1:I:58:ILE:HG13	1:I:59:ASN:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:80:ILE:HD13	1:N:195:VAL:CG1	2.42	0.49
1:U:74:ILE:HD13	1:U:154:GLN:HA	1.93	0.49
1:W:80:ILE:HD13	1:W:195:VAL:CG1	2.42	0.49
3:11:40:LEU:HG	3:11:85:CYS:O	2.13	0.49
3:14:40:LEU:HG	3:14:85:CYS:O	2.13	0.49
3:21:40:LEU:HG	3:21:85:CYS:O	2.13	0.49
3:24:40:LEU:HG	3:24:85:CYS:O	2.13	0.49
3:25:40:LEU:HG	3:25:85:CYS:O	2.13	0.49
3:26:40:LEU:HG	3:26:85:CYS:O	2.13	0.49
1:D:101:LYS:HZ2	1:D:101:LYS:HB3	1.76	0.49
1:J:58:ILE:HG13	1:J:59:ASN:N	2.26	0.49
1:R:176:GLU:OE2	1:T:90:LYS:HD3	2.13	0.49
1:T:74:ILE:HD13	1:T:154:GLN:HA	1.93	0.49
3:4:40:LEU:HG	3:4:85:CYS:O	2.13	0.49
3:7:40:LEU:HG	3:7:85:CYS:O	2.13	0.49
3:14:72:GLN:HG2	3:14:73:PRO:CD	2.41	0.49
3:18:40:LEU:HG	3:18:85:CYS:O	2.13	0.49
1:Q:176:GLU:OE2	1:S:90:LYS:HD3	2.13	0.49
1:W:74:ILE:HD13	1:W:154:GLN:HA	1.93	0.49
3:23:40:LEU:HG	3:23:85:CYS:O	2.13	0.49
1:I:80:ILE:HD13	1:I:195:VAL:CG1	2.42	0.49
1:K:80:ILE:HD13	1:K:195:VAL:CG1	2.42	0.49
1:M:80:ILE:HD13	1:M:195:VAL:CG1	2.42	0.49
1:V:74:ILE:HD13	1:V:154:GLN:HA	1.93	0.49
3:2:28:ILE:O	3:2:29:SER:OG	2.21	0.49
3:2:72:GLN:HG2	3:2:73:PRO:CD	2.41	0.49
1:G:176:GLU:OE2	1:I:90:LYS:HD3	2.13	0.49
1:O:80:ILE:HD13	1:O:195:VAL:CG1	2.42	0.49
1:R:167:LYS:NZ	1:S:84:GLU:OE2	2.41	0.49
1:S:101:LYS:HZ2	1:S:101:LYS:HB3	1.78	0.49
3:1:40:LEU:HG	3:1:85:CYS:O	2.13	0.49
3:10:40:LEU:HG	3:10:85:CYS:O	2.13	0.49
3:15:40:LEU:HG	3:15:85:CYS:O	2.13	0.49
3:17:40:LEU:HG	3:17:85:CYS:O	2.13	0.49
1:F:80:ILE:HD13	1:F:195:VAL:CG1	2.42	0.49
1:G:80:ILE:HD13	1:G:195:VAL:CG1	2.42	0.49
1:M:176:GLU:OE2	1:O:90:LYS:HD3	2.13	0.49
1:S:176:GLU:OE2	1:U:90:LYS:HD3	2.13	0.49
1:W:167:LYS:NZ	1:X:84:GLU:OE2	2.42	0.49
1:A:210:ASN:ND2	3:26:83:SER:HA	2.28	0.48
3:15:72:GLN:HG2	3:15:73:PRO:CD	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:22:40:LEU:HG	3:22:85:CYS:O	2.13	0.48
1:P:167:LYS:NZ	1:Q:84:GLU:OE2	2.41	0.48
3:6:75:GLY:HA2	3:6:89:ARG:O	2.14	0.48
3:20:40:LEU:HG	3:20:85:CYS:O	2.13	0.48
1:C:80:ILE:HD13	1:C:195:VAL:CG1	2.42	0.48
1:E:80:ILE:HD13	1:E:195:VAL:CG1	2.42	0.48
1:J:101:LYS:HB3	1:J:101:LYS:HZ2	1.77	0.48
3:8:40:LEU:HG	3:8:85:CYS:O	2.13	0.48
1:H:80:ILE:HD13	1:H:195:VAL:CG1	2.42	0.48
1:L:80:ILE:HD13	1:L:195:VAL:CG1	2.42	0.48
1:P:176:GLU:OE2	1:R:90:LYS:HD3	2.13	0.48
1:Q:101:LYS:HZ2	1:Q:101:LYS:HB3	1.78	0.48
1:V:101:LYS:HZ2	1:V:101:LYS:HB3	1.79	0.48
1:A:176:GLU:OE2	1:C:90:LYS:HD3	2.14	0.48
3:2:75:GLY:HA2	3:2:89:ARG:O	2.14	0.48
3:3:40:LEU:HG	3:3:85:CYS:O	2.13	0.48
1:K:101:LYS:HZ2	1:K:101:LYS:HB3	1.77	0.48
1:T:101:LYS:HZ2	1:T:101:LYS:HB3	1.79	0.48
3:1:75:GLY:HA2	3:1:89:ARG:O	2.14	0.48
3:7:75:GLY:HA2	3:7:89:ARG:O	2.14	0.48
3:9:40:LEU:HG	3:9:85:CYS:O	2.13	0.48
1:F:101:LYS:HZ2	1:F:101:LYS:HB3	1.77	0.48
1:N:176:GLU:OE1	1:N:207:TYR:OH	2.21	0.48
1:V:176:GLU:OE2	1:X:90:LYS:HD3	2.13	0.48
1:X:176:GLU:OE2	1:Z:90:LYS:HD3	2.12	0.48
3:2:40:LEU:HG	3:2:85:CYS:O	2.13	0.48
3:16:40:LEU:HG	3:16:85:CYS:O	2.13	0.48
3:16:72:GLN:HG2	3:16:73:PRO:CD	2.41	0.48
3:19:40:LEU:HG	3:19:85:CYS:O	2.13	0.48
3:3:72:GLN:HG2	3:3:73:PRO:CD	2.41	0.48
3:19:75:GLY:HA2	3:19:89:ARG:O	2.14	0.48
1:C:101:LYS:HZ2	1:C:101:LYS:HB3	1.79	0.48
1:E:101:LYS:HZ2	1:E:101:LYS:HB3	1.78	0.48
1:L:176:GLU:OE2	1:N:90:LYS:HD3	2.14	0.48
1:N:167:LYS:NZ	1:O:84:GLU:OE2	2.42	0.48
1:Z:101:LYS:HZ2	1:Z:101:LYS:HB3	1.79	0.48
3:20:75:GLY:HA2	3:20:89:ARG:O	2.14	0.48
1:D:176:GLU:OE2	1:F:90:LYS:HD3	2.13	0.48
1:E:167:LYS:NZ	1:F:84:GLU:OE2	2.42	0.48
1:J:80:ILE:HD13	1:J:195:VAL:CG1	2.42	0.48
3:3:75:GLY:HA2	3:3:89:ARG:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:75:GLY:HA2	3:5:89:ARG:O	2.14	0.48
3:18:28:ILE:O	3:18:29:SER:OG	2.21	0.48
3:21:75:GLY:HA2	3:21:89:ARG:O	2.14	0.48
3:25:28:ILE:O	3:25:29:SER:OG	2.21	0.48
1:J:109:VAL:HG21	1:J:117:PHE:O	2.14	0.48
1:K:109:VAL:HG21	1:K:117:PHE:O	2.14	0.48
1:N:109:VAL:HG21	1:N:117:PHE:O	2.14	0.48
1:O:109:VAL:HG21	1:O:117:PHE:O	2.14	0.48
1:P:101:LYS:HZ2	1:P:101:LYS:HB3	1.77	0.48
3:11:75:GLY:HA2	3:11:89:ARG:O	2.14	0.48
3:17:22:VAL:HG13	3:17:34:LEU:HD23	1.96	0.48
3:17:72:GLN:HG2	3:17:73:PRO:CD	2.41	0.48
3:17:75:GLY:HA2	3:17:89:ARG:O	2.14	0.48
3:18:22:VAL:HG13	3:18:34:LEU:HD23	1.96	0.48
3:18:75:GLY:HA2	3:18:89:ARG:O	2.14	0.48
3:22:75:GLY:HA2	3:22:89:ARG:O	2.14	0.48
1:G:101:LYS:HZ2	1:G:101:LYS:HB3	1.77	0.48
1:L:109:VAL:HG21	1:L:117:PHE:O	2.14	0.48
1:Q:109:VAL:HG21	1:Q:117:PHE:O	2.14	0.48
1:R:109:VAL:HG21	1:R:117:PHE:O	2.14	0.48
1:A:159:GLY:O	1:A:186:PRO:HG3	2.14	0.47
3:14:22:VAL:HG13	3:14:34:LEU:HD23	1.96	0.47
3:22:22:VAL:HG13	3:22:34:LEU:HD23	1.96	0.47
1:B:176:GLU:OE2	1:D:90:LYS:HD3	2.14	0.47
1:H:109:VAL:HG21	1:H:117:PHE:O	2.14	0.47
1:H:176:GLU:OE2	1:J:90:LYS:HD3	2.14	0.47
1:I:109:VAL:HG21	1:I:117:PHE:O	2.14	0.47
1:S:109:VAL:HG21	1:S:117:PHE:O	2.14	0.47
3:8:75:GLY:HA2	3:8:89:ARG:O	2.14	0.47
3:10:75:GLY:HA2	3:10:89:ARG:O	2.14	0.47
3:16:22:VAL:HG13	3:16:34:LEU:HD23	1.96	0.47
3:16:75:GLY:HA2	3:16:89:ARG:O	2.14	0.47
3:18:72:GLN:HG2	3:18:73:PRO:CD	2.41	0.47
3:19:22:VAL:HG13	3:19:34:LEU:HD23	1.96	0.47
3:23:75:GLY:HA2	3:23:89:ARG:O	2.14	0.47
1:J:176:GLU:OE2	1:L:90:LYS:HD3	2.13	0.47
1:K:176:GLU:OE2	1:M:90:LYS:HD3	2.14	0.47
1:P:109:VAL:HG21	1:P:117:PHE:O	2.14	0.47
1:T:176:GLU:OE2	1:V:90:LYS:HD3	2.14	0.47
3:13:22:VAL:HG13	3:13:34:LEU:HD23	1.96	0.47
3:15:22:VAL:HG13	3:15:34:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:21:22:VAL:HG13	3:21:34:LEU:HD23	1.96	0.47
3:23:22:VAL:HG13	3:23:34:LEU:HD23	1.96	0.47
3:24:75:GLY:HA2	3:24:89:ARG:O	2.14	0.47
3:26:75:GLY:HA2	3:26:89:ARG:O	2.14	0.47
1:B:159:GLY:O	1:B:186:PRO:HG3	2.14	0.47
1:B:167:LYS:NZ	1:C:84:GLU:OE2	2.42	0.47
1:C:159:GLY:O	1:C:186:PRO:HG3	2.14	0.47
1:H:101:LYS:HZ2	1:H:101:LYS:HB3	1.77	0.47
1:N:176:GLU:OE2	1:P:90:LYS:HD3	2.14	0.47
1:S:159:GLY:O	1:S:186:PRO:HG3	2.14	0.47
1:T:159:GLY:O	1:T:186:PRO:HG3	2.14	0.47
1:U:101:LYS:HB3	1:U:101:LYS:HZ2	1.80	0.47
1:Z:159:GLY:O	1:Z:186:PRO:HG3	2.14	0.47
3:4:72:GLN:HG2	3:4:73:PRO:CD	2.41	0.47
3:6:83:SER:HA	1:G:210:ASN:ND2	2.30	0.47
3:12:75:GLY:HA2	3:12:89:ARG:O	2.14	0.47
1:B:90:LYS:HD3	1:Z:176:GLU:OE2	2.15	0.47
1:C:176:GLU:OE2	1:E:90:LYS:HD3	2.14	0.47
1:I:101:LYS:HZ2	1:I:101:LYS:HB3	1.78	0.47
1:R:159:GLY:O	1:R:186:PRO:HG3	2.14	0.47
1:R:171:ILE:HD12	1:T:88:ALA:CB	2.34	0.47
1:U:109:VAL:HG21	1:U:117:PHE:O	2.14	0.47
1:U:159:GLY:O	1:U:186:PRO:HG3	2.14	0.47
1:U:176:GLU:OE2	1:W:90:LYS:HD3	2.14	0.47
3:6:39:PRO:HD2	3:6:42:PHE:CB	2.45	0.47
3:8:39:PRO:HD2	3:8:42:PHE:CB	2.45	0.47
3:15:75:GLY:HA2	3:15:89:ARG:O	2.14	0.47
1:D:159:GLY:O	1:D:186:PRO:HG3	2.14	0.47
1:F:159:GLY:O	1:F:186:PRO:HG3	2.14	0.47
1:F:176:GLU:OE2	1:H:90:LYS:HD3	2.15	0.47
1:G:159:GLY:O	1:G:186:PRO:HG3	2.14	0.47
1:H:159:GLY:O	1:H:186:PRO:HG3	2.14	0.47
1:Y:40:ILE:H	1:Y:40:ILE:HG12	1.49	0.47
1:Y:159:GLY:O	1:Y:186:PRO:HG3	2.14	0.47
3:9:83:SER:HA	1:J:210:ASN:ND2	2.30	0.47
3:11:17:THR:O	3:11:18:ARG:NE	2.48	0.47
3:12:17:THR:O	3:12:18:ARG:NE	2.48	0.47
3:12:22:VAL:HG13	3:12:34:LEU:HD23	1.96	0.47
3:20:22:VAL:HG13	3:20:34:LEU:HD23	1.96	0.47
3:23:17:THR:O	3:23:18:ARG:NE	2.48	0.47
3:24:17:THR:O	3:24:18:ARG:NE	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:25:17:THR:O	3:25:18:ARG:NE	2.48	0.47
3:26:17:THR:O	3:26:18:ARG:NE	2.48	0.47
1:E:159:GLY:O	1:E:186:PRO:HG3	2.14	0.47
1:I:159:GLY:O	1:I:186:PRO:HG3	2.14	0.47
1:I:176:GLU:OE2	1:K:90:LYS:HD3	2.14	0.47
1:J:159:GLY:O	1:J:186:PRO:HG3	2.14	0.47
1:O:101:LYS:HZ2	1:O:101:LYS:HB3	1.77	0.47
1:Q:159:GLY:O	1:Q:186:PRO:HG3	2.14	0.47
1:T:109:VAL:HG21	1:T:117:PHE:O	2.14	0.47
1:V:159:GLY:O	1:V:186:PRO:HG3	2.14	0.47
3:1:17:THR:O	3:1:18:ARG:NE	2.48	0.47
3:2:17:THR:O	3:2:18:ARG:NE	2.48	0.47
3:3:83:SER:HA	1:D:210:ASN:ND2	2.30	0.47
3:4:39:PRO:HD2	3:4:42:PHE:CB	2.45	0.47
3:5:77:CYS:HB3	3:5:80:TYR:CE1	2.48	0.47
3:6:77:CYS:HB3	3:6:80:TYR:CE1	2.48	0.47
3:7:77:CYS:HB3	3:7:80:TYR:CE1	2.48	0.47
3:9:17:THR:O	3:9:18:ARG:NE	2.48	0.47
3:10:17:THR:O	3:10:18:ARG:NE	2.48	0.47
3:13:17:THR:O	3:13:18:ARG:NE	2.48	0.47
3:15:28:ILE:O	3:15:29:SER:OG	2.21	0.47
3:17:39:PRO:HD2	3:17:42:PHE:CB	2.45	0.47
3:21:17:THR:O	3:21:18:ARG:NE	2.48	0.47
3:22:17:THR:O	3:22:18:ARG:NE	2.48	0.47
3:25:22:VAL:HG13	3:25:34:LEU:HD23	1.96	0.47
1:E:109:VAL:HG21	1:E:117:PHE:O	2.14	0.47
1:G:109:VAL:HG21	1:G:117:PHE:O	2.14	0.47
1:K:159:GLY:O	1:K:186:PRO:HG3	2.14	0.47
1:O:176:GLU:OE2	1:Q:90:LYS:HD3	2.14	0.47
1:P:159:GLY:O	1:P:186:PRO:HG3	2.14	0.47
1:V:150:VAL:HG12	1:V:165:GLY:HA3	1.97	0.47
1:W:159:GLY:O	1:W:186:PRO:HG3	2.14	0.47
1:X:159:GLY:O	1:X:186:PRO:HG3	2.14	0.47
1:A:101:LYS:HZ2	1:A:101:LYS:HB3	1.80	0.47
3:3:17:THR:O	3:3:18:ARG:NE	2.48	0.47
3:3:39:PRO:HD2	3:3:42:PHE:CB	2.45	0.47
3:4:75:GLY:HA2	3:4:89:ARG:O	2.14	0.47
3:10:22:VAL:HG13	3:10:34:LEU:HD23	1.96	0.47
3:10:39:PRO:HD2	3:10:42:PHE:CB	2.45	0.47
3:14:17:THR:O	3:14:18:ARG:NE	2.48	0.47
3:19:39:PRO:HD2	3:19:42:PHE:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:19:72:GLN:HG2	3:19:73:PRO:CD	2.41	0.47
3:20:17:THR:O	3:20:18:ARG:NE	2.48	0.47
3:24:22:VAL:HG13	3:24:34:LEU:HD23	1.96	0.47
3:26:22:VAL:HG13	3:26:34:LEU:HD23	1.96	0.47
1:F:171:ILE:HD12	1:H:88:ALA:CB	2.34	0.47
1:M:109:VAL:HG21	1:M:117:PHE:O	2.14	0.47
1:W:150:VAL:HG12	1:W:165:GLY:HA3	1.97	0.47
1:X:150:VAL:HG12	1:X:165:GLY:HA3	1.97	0.47
1:Y:150:VAL:HG12	1:Y:165:GLY:HA3	1.97	0.47
3:4:17:THR:O	3:4:18:ARG:NE	2.48	0.47
3:4:77:CYS:HB3	3:4:80:TYR:CE1	2.48	0.47
3:8:17:THR:O	3:8:18:ARG:NE	2.48	0.47
3:9:22:VAL:HG13	3:9:34:LEU:HD23	1.96	0.47
3:9:75:GLY:HA2	3:9:89:ARG:O	2.14	0.47
3:11:22:VAL:HG13	3:11:34:LEU:HD23	1.96	0.47
3:14:75:GLY:HA2	3:14:89:ARG:O	2.14	0.47
3:19:17:THR:O	3:19:18:ARG:NE	2.48	0.47
3:25:75:GLY:HA2	3:25:89:ARG:O	2.14	0.47
1:Q:167:LYS:NZ	1:R:84:GLU:OE2	2.42	0.47
1:Y:222:LEU:HB2	1:Z:231:PRO:HB3	1.97	0.47
3:1:39:PRO:HD2	3:1:42:PHE:CB	2.45	0.47
3:3:77:CYS:HB3	3:3:80:TYR:CE1	2.48	0.47
3:5:39:PRO:HD2	3:5:42:PHE:CB	2.45	0.47
3:7:83:SER:HA	1:H:210:ASN:ND2	2.30	0.47
3:8:15:THR:HG23	3:8:43:THR:HG21	1.97	0.47
3:8:83:SER:HA	1:I:210:ASN:ND2	2.30	0.47
3:11:77:CYS:HB3	3:11:80:TYR:CE1	2.48	0.47
3:12:77:CYS:HB3	3:12:80:TYR:CE1	2.48	0.47
3:15:17:THR:O	3:15:18:ARG:NE	2.48	0.47
3:16:15:THR:HG23	3:16:43:THR:HG21	1.98	0.47
3:20:39:PRO:HD2	3:20:42:PHE:CB	2.45	0.47
3:21:39:PRO:HD2	3:21:42:PHE:CB	2.45	0.47
3:21:83:SER:HA	1:V:210:ASN:ND2	2.30	0.47
1:E:176:GLU:OE2	1:G:90:LYS:HD3	2.14	0.47
1:J:150:VAL:HG12	1:J:165:GLY:HA3	1.97	0.47
1:L:159:GLY:O	1:L:186:PRO:HG3	2.14	0.47
1:O:159:GLY:O	1:O:186:PRO:HG3	2.14	0.47
1:S:171:ILE:HD12	1:U:88:ALA:CB	2.34	0.47
1:U:150:VAL:HG12	1:U:165:GLY:HA3	1.97	0.47
1:A:150:VAL:HG12	1:A:165:GLY:HA3	1.97	0.46
3:1:22:VAL:HG13	3:1:34:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:39:PRO:HD2	3:2:42:PHE:CB	2.45	0.46
3:5:17:THR:O	3:5:18:ARG:NE	2.48	0.46
3:5:72:GLN:HG2	3:5:73:PRO:CD	2.41	0.46
3:7:17:THR:O	3:7:18:ARG:NE	2.48	0.46
3:9:15:THR:HG23	3:9:43:THR:HG21	1.98	0.46
3:10:15:THR:HG23	3:10:43:THR:HG21	1.98	0.46
3:11:15:THR:HG23	3:11:43:THR:HG21	1.97	0.46
3:12:28:ILE:O	3:12:29:SER:OG	2.21	0.46
3:13:75:GLY:HA2	3:13:89:ARG:O	2.14	0.46
3:14:15:THR:HG23	3:14:43:THR:HG21	1.97	0.46
3:15:15:THR:HG23	3:15:43:THR:HG21	1.98	0.46
3:15:39:PRO:HD2	3:15:42:PHE:CB	2.45	0.46
3:17:15:THR:HG23	3:17:43:THR:HG21	1.97	0.46
3:18:17:THR:O	3:18:18:ARG:NE	2.48	0.46
3:23:39:PRO:HD2	3:23:42:PHE:CB	2.45	0.46
1:K:150:VAL:HG12	1:K:165:GLY:HA3	1.97	0.46
1:M:150:VAL:HG12	1:M:165:GLY:HA3	1.97	0.46
1:V:109:VAL:HG21	1:V:117:PHE:O	2.14	0.46
1:X:40:ILE:H	1:X:40:ILE:HG12	1.49	0.46
1:X:109:VAL:HG21	1:X:117:PHE:O	2.14	0.46
1:Z:109:VAL:HG21	1:Z:117:PHE:O	2.14	0.46
1:Z:150:VAL:HG12	1:Z:165:GLY:HA3	1.97	0.46
1:A:109:VAL:HG21	1:A:117:PHE:O	2.14	0.46
3:1:83:SER:HA	1:B:210:ASN:ND2	2.30	0.46
3:5:83:SER:HA	1:F:210:ASN:ND2	2.31	0.46
3:6:15:THR:HG23	3:6:43:THR:HG21	1.97	0.46
3:7:15:THR:HG23	3:7:43:THR:HG21	1.98	0.46
3:7:39:PRO:HD2	3:7:42:PHE:CB	2.45	0.46
3:8:22:VAL:HG13	3:8:34:LEU:HD23	1.96	0.46
3:10:77:CYS:HB3	3:10:80:TYR:CE1	2.48	0.46
3:13:15:THR:HG23	3:13:43:THR:HG21	1.97	0.46
3:16:17:THR:O	3:16:18:ARG:NE	2.48	0.46
3:18:15:THR:HG23	3:18:43:THR:HG21	1.98	0.46
3:18:39:PRO:HD2	3:18:42:PHE:CB	2.45	0.46
3:20:83:SER:HA	1:U:210:ASN:ND2	2.30	0.46
3:22:39:PRO:HD2	3:22:42:PHE:CB	2.45	0.46
3:24:39:PRO:HD2	3:24:42:PHE:CB	2.45	0.46
3:25:39:PRO:HD2	3:25:42:PHE:CB	2.45	0.46
1:E:112:TYR:CE1	1:E:113:LEU:HG	2.51	0.46
1:I:40:ILE:H	1:I:40:ILE:HG12	1.49	0.46
1:L:150:VAL:HG12	1:L:165:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:150:VAL:HG12	1:T:165:GLY:HA3	1.97	0.46
1:Y:121:ARG:HB3	1:Z:111:ARG:HB3	1.96	0.46
1:A:106:PHE:O	1:A:107:ASP:HB2	2.16	0.46
3:2:77:CYS:HB3	3:2:80:TYR:CE1	2.48	0.46
3:2:83:SER:HA	1:C:210:ASN:ND2	2.30	0.46
3:12:15:THR:HG23	3:12:43:THR:HG21	1.98	0.46
3:19:83:SER:HA	1:T:210:ASN:ND2	2.30	0.46
3:26:39:PRO:HD2	3:26:42:PHE:CB	2.45	0.46
1:B:109:VAL:HG21	1:B:117:PHE:O	2.14	0.46
1:B:150:VAL:HG12	1:B:165:GLY:HA3	1.97	0.46
1:D:109:VAL:HG21	1:D:117:PHE:O	2.14	0.46
1:F:106:PHE:O	1:F:107:ASP:HB2	2.16	0.46
1:F:109:VAL:HG21	1:F:117:PHE:O	2.14	0.46
1:G:82:LEU:HD12	1:G:146:GLY:HA3	1.97	0.46
1:I:71:PRO:HD2	1:I:189:ILE:HD13	1.98	0.46
1:J:71:PRO:HD2	1:J:189:ILE:HD13	1.98	0.46
1:L:101:LYS:HZ2	1:L:101:LYS:HB3	1.79	0.46
1:N:101:LYS:HZ2	1:N:101:LYS:HB3	1.78	0.46
1:N:110:PRO:O	1:N:114:GLN:HG2	2.16	0.46
1:N:159:GLY:O	1:N:186:PRO:HG3	2.14	0.46
1:Q:112:TYR:CE1	1:Q:113:LEU:HG	2.51	0.46
1:S:112:TYR:CE1	1:S:113:LEU:HG	2.51	0.46
1:S:150:VAL:HG12	1:S:165:GLY:HA3	1.97	0.46
1:T:106:PHE:O	1:T:107:ASP:HB2	2.16	0.46
1:W:101:LYS:HZ2	1:W:101:LYS:CB	2.28	0.46
1:Y:109:VAL:HG21	1:Y:117:PHE:O	2.14	0.46
3:4:22:VAL:HG13	3:4:34:LEU:HD23	1.96	0.46
3:4:83:SER:HA	1:E:210:ASN:ND2	2.31	0.46
3:6:17:THR:O	3:6:18:ARG:NE	2.48	0.46
3:15:83:SER:HA	1:P:210:ASN:ND2	2.30	0.46
3:16:39:PRO:HD2	3:16:42:PHE:CB	2.45	0.46
3:17:17:THR:O	3:17:18:ARG:NE	2.48	0.46
3:23:83:SER:HA	1:X:210:ASN:ND2	2.31	0.46
1:C:109:VAL:HG21	1:C:117:PHE:O	2.14	0.46
1:C:112:TYR:CE1	1:C:113:LEU:HG	2.51	0.46
1:F:82:LEU:HD12	1:F:146:GLY:HA3	1.98	0.46
1:F:110:PRO:O	1:F:114:GLN:HG2	2.16	0.46
1:H:71:PRO:HD2	1:H:189:ILE:HD13	1.98	0.46
1:I:110:PRO:O	1:I:114:GLN:HG2	2.16	0.46
1:I:150:VAL:HG12	1:I:165:GLY:HA3	1.97	0.46
1:K:110:PRO:O	1:K:114:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:71:PRO:HD2	1:L:189:ILE:HD13	1.98	0.46
1:L:110:PRO:O	1:L:114:GLN:HG2	2.16	0.46
1:N:106:PHE:O	1:N:107:ASP:HB2	2.16	0.46
1:N:150:VAL:HG12	1:N:165:GLY:HA3	1.97	0.46
1:S:106:PHE:O	1:S:107:ASP:HB2	2.16	0.46
1:U:106:PHE:O	1:U:107:ASP:HB2	2.16	0.46
1:V:106:PHE:O	1:V:107:ASP:HB2	2.16	0.46
1:V:112:TYR:CE1	1:V:113:LEU:HG	2.51	0.46
1:W:112:TYR:CE1	1:W:113:LEU:HG	2.51	0.46
1:X:101:LYS:HZ2	1:X:101:LYS:HB3	1.81	0.46
1:Z:106:PHE:O	1:Z:107:ASP:HB2	2.16	0.46
3:2:22:VAL:HG13	3:2:34:LEU:HD23	1.96	0.46
3:5:15:THR:HG23	3:5:43:THR:HG21	1.98	0.46
3:5:22:VAL:HG13	3:5:34:LEU:HD23	1.96	0.46
3:12:39:PRO:HD2	3:12:42:PHE:CB	2.45	0.46
3:13:77:CYS:HB3	3:13:80:TYR:CE1	2.48	0.46
3:14:39:PRO:HD2	3:14:42:PHE:CB	2.45	0.46
3:19:15:THR:HG23	3:19:43:THR:HG21	1.98	0.46
1:G:71:PRO:HD2	1:G:189:ILE:HD13	1.98	0.46
1:G:106:PHE:O	1:G:107:ASP:HB2	2.16	0.46
1:J:171:ILE:O	1:K:207:TYR:O	2.34	0.46
1:K:71:PRO:HD2	1:K:189:ILE:HD13	1.98	0.46
1:L:112:TYR:CE1	1:L:113:LEU:HG	2.51	0.46
1:M:71:PRO:HD2	1:M:189:ILE:HD13	1.98	0.46
1:M:159:GLY:O	1:M:186:PRO:HG3	2.14	0.46
1:N:71:PRO:HD2	1:N:189:ILE:HD13	1.98	0.46
1:P:106:PHE:O	1:P:107:ASP:HB2	2.16	0.46
1:Q:106:PHE:O	1:Q:107:ASP:HB2	2.16	0.46
1:U:112:TYR:CE1	1:U:113:LEU:HG	2.51	0.46
1:W:106:PHE:O	1:W:107:ASP:HB2	2.16	0.46
1:W:110:PRO:O	1:W:114:GLN:HG2	2.16	0.46
1:X:106:PHE:O	1:X:107:ASP:HB2	2.16	0.46
1:X:112:TYR:CE1	1:X:113:LEU:HG	2.51	0.46
1:Y:110:PRO:O	1:Y:114:GLN:HG2	2.16	0.46
1:Y:130:ASN:CG	1:Z:102:THR:HG22	2.36	0.46
3:6:22:VAL:HG13	3:6:34:LEU:HD23	1.96	0.46
3:9:39:PRO:HD2	3:9:42:PHE:CB	2.45	0.46
3:9:77:CYS:HB3	3:9:80:TYR:CE1	2.48	0.46
3:12:83:SER:HA	1:M:210:ASN:ND2	2.30	0.46
3:20:15:THR:HG23	3:20:43:THR:HG21	1.98	0.46
3:20:72:GLN:HG2	3:20:73:PRO:CD	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:PHE:O	1:E:107:ASP:HB2	2.16	0.46
1:F:71:PRO:HD2	1:F:189:ILE:HD13	1.98	0.46
1:H:110:PRO:O	1:H:114:GLN:HG2	2.16	0.46
1:H:150:VAL:HG12	1:H:165:GLY:HA3	1.97	0.46
1:N:112:TYR:CE1	1:N:113:LEU:HG	2.51	0.46
1:R:101:LYS:HZ2	1:R:101:LYS:HB3	1.81	0.46
1:R:106:PHE:O	1:R:107:ASP:HB2	2.16	0.46
1:R:150:VAL:HG12	1:R:165:GLY:HA3	1.97	0.46
1:U:110:PRO:O	1:U:114:GLN:HG2	2.16	0.46
1:Y:106:PHE:O	1:Y:107:ASP:HB2	2.16	0.46
3:1:77:CYS:HB3	3:1:80:TYR:CE1	2.48	0.46
3:3:22:VAL:HG13	3:3:34:LEU:HD23	1.96	0.46
3:7:22:VAL:HG13	3:7:34:LEU:HD23	1.96	0.46
1:C:150:VAL:HG12	1:C:165:GLY:HA3	1.97	0.46
1:D:176:GLU:OE1	1:D:207:TYR:OH	2.21	0.46
1:G:112:TYR:CE1	1:G:113:LEU:HG	2.51	0.46
1:H:82:LEU:HD12	1:H:146:GLY:HA3	1.98	0.46
1:J:112:TYR:CE1	1:J:113:LEU:HG	2.51	0.46
1:M:106:PHE:O	1:M:107:ASP:HB2	2.16	0.46
1:O:106:PHE:O	1:O:107:ASP:HB2	2.16	0.46
1:O:110:PRO:O	1:O:114:GLN:HG2	2.16	0.46
1:O:112:TYR:CE1	1:O:113:LEU:HG	2.51	0.46
1:O:150:VAL:HG12	1:O:165:GLY:HA3	1.97	0.46
1:A:110:PRO:O	1:A:114:GLN:HG2	2.16	0.46
3:4:15:THR:HG23	3:4:43:THR:HG21	1.98	0.46
3:11:83:SER:HA	1:L:210:ASN:ND2	2.31	0.46
1:C:110:PRO:O	1:C:114:GLN:HG2	2.16	0.46
1:D:171:ILE:O	1:E:207:TYR:O	2.34	0.46
1:E:71:PRO:HD2	1:E:189:ILE:HD13	1.98	0.46
1:E:110:PRO:O	1:E:114:GLN:HG2	2.16	0.46
1:H:112:TYR:CE1	1:H:113:LEU:HG	2.51	0.46
1:K:106:PHE:O	1:K:107:ASP:HB2	2.16	0.46
1:L:78:LEU:HD12	1:L:193:ASN:O	2.16	0.46
1:O:71:PRO:HD2	1:O:189:ILE:HD13	1.98	0.46
1:O:78:LEU:HD12	1:O:193:ASN:O	2.16	0.46
1:P:112:TYR:CE1	1:P:113:LEU:HG	2.51	0.46
1:Q:110:PRO:O	1:Q:114:GLN:HG2	2.16	0.46
1:S:110:PRO:O	1:S:114:GLN:HG2	2.16	0.46
1:T:112:TYR:CE1	1:T:113:LEU:HG	2.51	0.46
1:W:109:VAL:HG21	1:W:117:PHE:O	2.14	0.46
1:Y:112:TYR:CE1	1:Y:113:LEU:HG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:72:GLN:HG2	3:6:73:PRO:CD	2.41	0.46
3:10:83:SER:HA	1:K:210:ASN:ND2	2.31	0.46
3:11:39:PRO:HD2	3:11:42:PHE:CB	2.45	0.46
3:17:83:SER:HA	1:R:210:ASN:ND2	2.31	0.46
3:21:15:THR:HG23	3:21:43:THR:HG21	1.98	0.46
3:22:83:SER:HA	1:W:210:ASN:ND2	2.31	0.46
1:B:106:PHE:O	1:B:107:ASP:HB2	2.16	0.46
1:D:71:PRO:HD2	1:D:189:ILE:HD13	1.98	0.46
1:E:176:GLU:OE1	1:E:207:TYR:OH	2.21	0.46
1:H:106:PHE:O	1:H:107:ASP:HB2	2.16	0.46
1:K:78:LEU:HD12	1:K:193:ASN:O	2.16	0.46
1:L:106:PHE:O	1:L:107:ASP:HB2	2.16	0.46
1:R:78:LEU:HD12	1:R:193:ASN:O	2.16	0.46
1:T:78:LEU:HD12	1:T:193:ASN:O	2.16	0.46
1:U:78:LEU:HD12	1:U:193:ASN:O	2.16	0.46
1:A:112:TYR:CE1	1:A:113:LEU:HG	2.51	0.46
3:2:15:THR:HG23	3:2:43:THR:HG21	1.97	0.46
3:3:15:THR:HG23	3:3:43:THR:HG21	1.98	0.46
3:14:83:SER:HA	1:O:210:ASN:ND2	2.30	0.46
3:22:15:THR:HG23	3:22:43:THR:HG21	1.98	0.46
3:23:15:THR:HG23	3:23:43:THR:HG21	1.97	0.46
1:F:112:TYR:CE1	1:F:113:LEU:HG	2.51	0.46
1:G:150:VAL:HG12	1:G:165:GLY:HA3	1.97	0.46
1:M:78:LEU:HD12	1:M:193:ASN:O	2.16	0.46
1:O:148:LEU:HD13	1:O:167:LYS:HE2	1.99	0.46
1:S:148:LEU:HD13	1:S:167:LYS:HE2	1.98	0.46
1:T:148:LEU:HD13	1:T:167:LYS:HE2	1.99	0.46
1:X:167:LYS:NZ	1:Y:84:GLU:OE2	2.44	0.46
1:Y:82:LEU:HD12	1:Y:146:GLY:HA3	1.97	0.46
1:Z:112:TYR:CE1	1:Z:113:LEU:HG	2.51	0.46
3:1:15:THR:HG23	3:1:43:THR:HG21	1.98	0.45
3:13:83:SER:HA	1:N:210:ASN:ND2	2.30	0.45
3:22:28:ILE:O	3:22:29:SER:OG	2.21	0.45
1:D:150:VAL:HG12	1:D:165:GLY:HA3	1.97	0.45
1:H:171:ILE:O	1:I:207:TYR:O	2.35	0.45
1:J:78:LEU:HD12	1:J:193:ASN:O	2.16	0.45
1:J:106:PHE:O	1:J:107:ASP:HB2	2.16	0.45
1:K:112:TYR:CE1	1:K:113:LEU:HG	2.51	0.45
1:K:171:ILE:O	1:L:207:TYR:O	2.34	0.45
1:L:148:LEU:HD13	1:L:167:LYS:HE2	1.98	0.45
1:M:101:LYS:HB3	1:M:101:LYS:HZ2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:112:TYR:CE1	1:M:113:LEU:HG	2.51	0.45
1:P:71:PRO:HD2	1:P:189:ILE:HD13	1.98	0.45
1:P:148:LEU:HD13	1:P:167:LYS:HE2	1.99	0.45
1:Q:150:VAL:HG12	1:Q:165:GLY:HA3	1.97	0.45
1:R:110:PRO:O	1:R:114:GLN:HG2	2.16	0.45
1:S:78:LEU:HD12	1:S:193:ASN:O	2.16	0.45
1:A:82:LEU:HA	1:A:197:SER:CB	2.43	0.45
3:2:15:THR:HG23	3:2:43:THR:CG2	2.47	0.45
3:8:15:THR:HG23	3:8:43:THR:CG2	2.47	0.45
3:9:15:THR:HG23	3:9:43:THR:CG2	2.47	0.45
3:10:15:THR:HG23	3:10:43:THR:CG2	2.47	0.45
3:13:39:PRO:HD2	3:13:42:PHE:CB	2.45	0.45
3:14:77:CYS:HB3	3:14:80:TYR:CE1	2.48	0.45
3:16:83:SER:HA	1:Q:210:ASN:ND2	2.31	0.45
3:18:83:SER:HA	1:S:210:ASN:ND2	2.31	0.45
3:22:64:TYR:CB	3:22:96:CYS:HB3	2.47	0.45
3:24:15:THR:HG23	3:24:43:THR:HG21	1.98	0.45
3:25:15:THR:HG23	3:25:43:THR:HG21	1.97	0.45
3:26:15:THR:HG23	3:26:43:THR:HG21	1.98	0.45
3:26:77:CYS:HB3	3:26:80:TYR:CE1	2.48	0.45
1:B:101:LYS:HZ2	1:B:101:LYS:CB	2.28	0.45
1:B:110:PRO:O	1:B:114:GLN:HG2	2.16	0.45
1:B:112:TYR:CE1	1:B:113:LEU:HG	2.51	0.45
1:E:171:ILE:O	1:F:207:TYR:O	2.34	0.45
1:F:167:LYS:NZ	1:G:84:GLU:OE2	2.42	0.45
1:F:171:ILE:O	1:G:207:TYR:O	2.35	0.45
1:I:82:LEU:HD12	1:I:146:GLY:HA3	1.98	0.45
1:I:171:ILE:HD12	1:K:88:ALA:CB	2.34	0.45
1:N:78:LEU:HD12	1:N:193:ASN:O	2.16	0.45
1:P:150:VAL:HG12	1:P:165:GLY:HA3	1.97	0.45
1:V:78:LEU:HD12	1:V:193:ASN:O	2.16	0.45
1:W:148:LEU:HD13	1:W:167:LYS:HE2	1.99	0.45
1:X:148:LEU:HD13	1:X:167:LYS:HE2	1.98	0.45
3:7:15:THR:HG23	3:7:43:THR:CG2	2.47	0.45
3:11:15:THR:HG23	3:11:43:THR:CG2	2.47	0.45
3:12:15:THR:HG23	3:12:43:THR:CG2	2.47	0.45
3:24:83:SER:HA	1:Y:210:ASN:HD22	1.82	0.45
3:26:15:THR:HG23	3:26:43:THR:CG2	2.47	0.45
1:C:71:PRO:HD2	1:C:189:ILE:HD13	1.98	0.45
1:G:171:ILE:HD12	1:I:88:ALA:CB	2.34	0.45
1:I:112:TYR:CE1	1:I:113:LEU:HG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:148:LEU:HD13	1:M:167:LYS:HE2	1.98	0.45
1:N:148:LEU:HD13	1:N:167:LYS:HE2	1.99	0.45
1:Q:148:LEU:HD13	1:Q:167:LYS:HE2	1.99	0.45
1:U:148:LEU:HD13	1:U:167:LYS:HE2	1.99	0.45
1:Z:82:LEU:HD12	1:Z:146:GLY:HA3	1.98	0.45
1:A:71:PRO:HD2	1:A:189:ILE:HD13	1.98	0.45
3:2:64:TYR:CB	3:2:96:CYS:HB3	2.47	0.45
3:3:64:TYR:CB	3:3:96:CYS:HB3	2.47	0.45
3:5:64:TYR:CB	3:5:96:CYS:HB3	2.47	0.45
3:6:15:THR:HG23	3:6:43:THR:CG2	2.47	0.45
3:7:64:TYR:CB	3:7:96:CYS:HB3	2.47	0.45
3:8:64:TYR:CB	3:8:96:CYS:HB3	2.47	0.45
3:8:77:CYS:HB3	3:8:80:TYR:CE1	2.48	0.45
3:13:64:TYR:CB	3:13:96:CYS:HB3	2.47	0.45
3:14:64:TYR:CB	3:14:96:CYS:HB3	2.47	0.45
1:B:71:PRO:HD2	1:B:189:ILE:HD13	1.98	0.45
1:B:221:TRP:NE1	1:C:229:LEU:O	2.39	0.45
1:D:101:LYS:HZ2	1:D:101:LYS:CB	2.29	0.45
1:D:106:PHE:O	1:D:107:ASP:HB2	2.16	0.45
1:G:110:PRO:O	1:G:114:GLN:HG2	2.16	0.45
1:I:78:LEU:HD12	1:I:193:ASN:O	2.16	0.45
1:J:110:PRO:O	1:J:114:GLN:HG2	2.16	0.45
1:K:148:LEU:HD13	1:K:167:LYS:HE2	1.99	0.45
1:Q:71:PRO:HD2	1:Q:189:ILE:HD13	1.98	0.45
1:R:148:LEU:HD13	1:R:167:LYS:HE2	1.98	0.45
1:U:167:LYS:NZ	1:V:84:GLU:OE2	2.43	0.45
1:V:148:LEU:HD13	1:V:167:LYS:HE2	1.99	0.45
1:Y:148:LEU:HD13	1:Y:167:LYS:HE2	1.98	0.45
3:1:64:TYR:CB	3:1:96:CYS:HB3	2.47	0.45
3:4:15:THR:HG23	3:4:43:THR:CG2	2.47	0.45
3:6:28:ILE:O	3:6:29:SER:OG	2.21	0.45
3:13:15:THR:HG23	3:13:43:THR:CG2	2.47	0.45
3:17:15:THR:HG23	3:17:43:THR:CG2	2.47	0.45
3:19:15:THR:HG23	3:19:43:THR:CG2	2.47	0.45
3:21:64:TYR:CB	3:21:96:CYS:HB3	2.47	0.45
3:22:15:THR:HG23	3:22:43:THR:CG2	2.47	0.45
3:23:64:TYR:CB	3:23:96:CYS:HB3	2.47	0.45
3:24:15:THR:HG23	3:24:43:THR:CG2	2.47	0.45
1:D:110:PRO:O	1:D:114:GLN:HG2	2.16	0.45
1:H:78:LEU:HD12	1:H:193:ASN:O	2.16	0.45
1:H:176:GLU:OE1	1:H:207:TYR:OH	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:106:PHE:O	1:I:107:ASP:HB2	2.16	0.45
1:L:171:ILE:O	1:M:207:TYR:O	2.35	0.45
1:V:171:ILE:O	1:W:207:TYR:O	2.34	0.45
1:A:82:LEU:HD12	1:A:146:GLY:HA3	1.98	0.45
3:5:15:THR:HG23	3:5:43:THR:CG2	2.47	0.45
3:6:64:TYR:CB	3:6:96:CYS:HB3	2.47	0.45
3:12:64:TYR:CB	3:12:96:CYS:HB3	2.47	0.45
3:15:64:TYR:CB	3:15:96:CYS:HB3	2.47	0.45
3:20:15:THR:HG23	3:20:43:THR:CG2	2.47	0.45
3:21:15:THR:HG23	3:21:43:THR:CG2	2.47	0.45
1:C:106:PHE:O	1:C:107:ASP:HB2	2.16	0.45
1:D:112:TYR:CE1	1:D:113:LEU:HG	2.51	0.45
1:E:150:VAL:HG12	1:E:165:GLY:HA3	1.97	0.45
1:F:150:VAL:HG12	1:F:165:GLY:HA3	1.97	0.45
1:J:148:LEU:HD13	1:J:167:LYS:HE2	1.99	0.45
1:J:170:ALA:HB3	1:K:206:GLU:HG3	1.98	0.45
1:N:171:ILE:O	1:O:207:TYR:O	2.35	0.45
1:P:171:ILE:O	1:Q:207:TYR:O	2.34	0.45
1:Q:78:LEU:HD12	1:Q:193:ASN:O	2.16	0.45
1:R:112:TYR:CE1	1:R:113:LEU:HG	2.51	0.45
1:W:78:LEU:HD12	1:W:193:ASN:O	2.16	0.45
3:4:64:TYR:CB	3:4:96:CYS:HB3	2.47	0.45
3:9:64:TYR:CB	3:9:96:CYS:HB3	2.47	0.45
3:14:15:THR:HG23	3:14:43:THR:CG2	2.47	0.45
3:18:15:THR:HG23	3:18:43:THR:CG2	2.47	0.45
3:20:64:TYR:CB	3:20:96:CYS:HB3	2.47	0.45
3:24:64:TYR:CB	3:24:96:CYS:HB3	2.47	0.45
3:25:77:CYS:HB3	3:25:80:TYR:CE1	2.48	0.45
1:C:78:LEU:HD12	1:C:193:ASN:O	2.16	0.45
1:D:78:LEU:HD12	1:D:193:ASN:O	2.16	0.45
1:D:168:GLN:HG3	1:E:204:ARG:NE	2.32	0.45
1:G:171:ILE:O	1:H:207:TYR:O	2.35	0.45
1:H:121:ARG:HB3	1:I:111:ARG:HB3	1.99	0.45
1:M:82:LEU:HD12	1:M:146:GLY:HA3	1.97	0.45
1:M:110:PRO:O	1:M:114:GLN:HG2	2.16	0.45
1:M:171:ILE:O	1:N:207:TYR:O	2.35	0.45
1:N:82:LEU:HD12	1:N:146:GLY:HA3	1.98	0.45
1:U:82:LEU:HD12	1:U:146:GLY:HA3	1.97	0.45
1:Z:71:PRO:HD2	1:Z:189:ILE:HD13	1.98	0.45
1:Z:110:PRO:O	1:Z:114:GLN:HG2	2.16	0.45
3:19:28:ILE:O	3:19:29:SER:OG	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:23:15:THR:HG23	3:23:43:THR:CG2	2.47	0.45
1:B:82:LEU:HA	1:B:197:SER:CB	2.43	0.45
1:D:170:ALA:HB3	1:E:206:GLU:HG3	1.98	0.45
1:E:78:LEU:HD12	1:E:193:ASN:O	2.16	0.45
1:H:170:ALA:HB3	1:I:206:GLU:HG3	1.99	0.45
1:J:82:LEU:HD12	1:J:146:GLY:HA3	1.97	0.45
1:K:121:ARG:HB3	1:L:111:ARG:HB3	1.99	0.45
1:P:78:LEU:HD12	1:P:193:ASN:O	2.16	0.45
1:R:71:PRO:HD2	1:R:189:ILE:HD13	1.98	0.45
1:T:171:ILE:HD12	1:V:88:ALA:CB	2.34	0.45
1:V:170:ALA:HB3	1:W:206:GLU:HG3	1.98	0.45
1:Y:71:PRO:HD2	1:Y:189:ILE:HD13	1.98	0.45
1:A:148:LEU:HD13	1:A:167:LYS:HE2	1.99	0.45
3:16:64:TYR:CB	3:16:96:CYS:HB3	2.47	0.45
3:17:77:CYS:HB3	3:17:80:TYR:CE1	2.48	0.45
3:25:15:THR:HG23	3:25:43:THR:CG2	2.47	0.45
3:26:64:TYR:CB	3:26:96:CYS:HB3	2.47	0.45
1:B:78:LEU:HD12	1:B:193:ASN:O	2.16	0.45
1:B:148:LEU:HD13	1:B:167:LYS:HE2	1.99	0.45
1:B:222:LEU:HB2	1:C:231:PRO:HB3	1.99	0.45
1:F:148:LEU:HD13	1:F:167:LYS:HE2	1.98	0.45
1:G:148:LEU:HD13	1:G:167:LYS:HE2	1.99	0.45
1:H:148:LEU:HD13	1:H:167:LYS:HE2	1.99	0.45
1:I:171:ILE:O	1:J:207:TYR:O	2.35	0.45
1:J:82:LEU:HA	1:J:197:SER:CB	2.43	0.45
1:K:170:ALA:HB3	1:L:206:GLU:HG3	1.99	0.45
1:N:121:ARG:HB3	1:O:111:ARG:HB3	1.99	0.45
1:O:82:LEU:HD12	1:O:146:GLY:HA3	1.98	0.45
1:P:110:PRO:O	1:P:114:GLN:HG2	2.16	0.45
1:T:82:LEU:HD12	1:T:146:GLY:HA3	1.97	0.45
1:V:82:LEU:HD12	1:V:146:GLY:HA3	1.98	0.45
1:V:168:GLN:HG3	1:W:204:ARG:NE	2.32	0.45
1:W:40:ILE:H	1:W:40:ILE:HG12	1.49	0.45
1:W:71:PRO:HD2	1:W:189:ILE:HD13	1.98	0.45
1:X:71:PRO:HD2	1:X:189:ILE:HD13	1.98	0.45
3:14:36:TYR:HE2	3:14:44:SER:HG	1.64	0.45
3:15:15:THR:HG23	3:15:43:THR:CG2	2.47	0.45
3:16:15:THR:HG23	3:16:43:THR:CG2	2.47	0.45
3:16:77:CYS:HB3	3:16:80:TYR:CE1	2.48	0.45
1:B:171:ILE:O	1:C:207:TYR:O	2.35	0.45
1:C:148:LEU:HD13	1:C:167:LYS:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:222:LEU:HB2	1:I:231:PRO:HB3	1.99	0.45
1:I:148:LEU:HD13	1:I:167:LYS:HE2	1.99	0.45
1:J:222:LEU:HB2	1:K:231:PRO:HB3	2.00	0.45
1:L:82:LEU:HD12	1:L:146:GLY:HA3	1.97	0.45
1:Q:171:ILE:O	1:R:207:TYR:O	2.34	0.45
1:T:110:PRO:O	1:T:114:GLN:HG2	2.16	0.45
1:T:168:GLN:HG3	1:U:204:ARG:NE	2.32	0.45
1:V:71:PRO:HD2	1:V:189:ILE:HD13	1.98	0.45
1:V:110:PRO:O	1:V:114:GLN:HG2	2.16	0.45
1:W:82:LEU:HD12	1:W:146:GLY:HA3	1.97	0.45
1:X:78:LEU:HD12	1:X:193:ASN:O	2.16	0.45
1:A:78:LEU:HD12	1:A:193:ASN:O	2.16	0.44
3:1:15:THR:HG23	3:1:43:THR:CG2	2.47	0.44
3:10:64:TYR:CB	3:10:96:CYS:HB3	2.47	0.44
3:11:64:TYR:CB	3:11:96:CYS:HB3	2.47	0.44
3:18:77:CYS:HB3	3:18:80:TYR:CE1	2.48	0.44
1:C:82:LEU:HA	1:C:197:SER:CB	2.43	0.44
1:E:170:ALA:HB3	1:F:206:GLU:HG3	1.99	0.44
1:N:222:LEU:HB2	1:O:231:PRO:HB3	1.99	0.44
1:P:82:LEU:HD12	1:P:146:GLY:HA3	1.98	0.44
1:Q:121:ARG:HB3	1:R:111:ARG:HB3	1.99	0.44
1:X:110:PRO:O	1:X:114:GLN:HG2	2.16	0.44
1:Y:78:LEU:HD12	1:Y:193:ASN:O	2.16	0.44
1:Z:148:LEU:HD13	1:Z:167:LYS:HE2	1.99	0.44
3:1:36:TYR:CE2	3:1:90:PHE:HB2	2.53	0.44
3:2:36:TYR:CE2	3:2:90:PHE:HB2	2.53	0.44
3:3:15:THR:HG23	3:3:43:THR:CG2	2.47	0.44
3:5:36:TYR:CE2	3:5:90:PHE:HB2	2.53	0.44
3:15:77:CYS:HB3	3:15:80:TYR:CE1	2.48	0.44
3:17:64:TYR:CB	3:17:96:CYS:HB3	2.47	0.44
3:18:36:TYR:CE2	3:18:90:PHE:HB2	2.53	0.44
3:19:36:TYR:CE2	3:19:90:PHE:HB2	2.53	0.44
3:20:36:TYR:CE2	3:20:90:PHE:HB2	2.53	0.44
1:B:82:LEU:HD12	1:B:146:GLY:HA3	1.98	0.44
1:C:171:ILE:O	1:D:207:TYR:O	2.35	0.44
1:E:148:LEU:HD13	1:E:167:LYS:HE2	1.98	0.44
1:F:78:LEU:HD12	1:F:193:ASN:O	2.16	0.44
1:H:40:ILE:H	1:H:40:ILE:HG12	1.49	0.44
1:M:121:ARG:HB3	1:N:111:ARG:HB3	2.00	0.44
1:O:111:ARG:NH1	1:O:111:ARG:HG2	2.33	0.44
1:O:167:LYS:NZ	1:P:84:GLU:OE2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:71:PRO:HD2	1:S:189:ILE:HD13	1.98	0.44
1:S:82:LEU:HD12	1:S:146:GLY:HA3	1.98	0.44
1:T:111:ARG:NH1	1:T:111:ARG:HG2	2.33	0.44
1:U:71:PRO:HD2	1:U:189:ILE:HD13	1.98	0.44
1:Y:111:ARG:NH1	1:Y:111:ARG:HG2	2.33	0.44
3:3:36:TYR:CE2	3:3:90:PHE:HB2	2.53	0.44
3:19:64:TYR:CB	3:19:96:CYS:HB3	2.47	0.44
3:24:77:CYS:HB3	3:24:80:TYR:CE1	2.48	0.44
1:B:157:ALA:HB1	1:Z:41:PRO:HA	1.98	0.44
1:D:111:ARG:NH1	1:D:111:ARG:HG2	2.33	0.44
1:D:148:LEU:HD13	1:D:167:LYS:HE2	1.99	0.44
1:D:222:LEU:HB2	1:E:231:PRO:HB3	2.00	0.44
1:E:111:ARG:HG2	1:E:111:ARG:NH1	2.33	0.44
1:E:121:ARG:HB3	1:F:111:ARG:HB3	1.99	0.44
1:G:170:ALA:HB3	1:H:206:GLU:HG3	1.99	0.44
1:P:111:ARG:HG2	1:P:111:ARG:NH1	2.33	0.44
1:P:168:GLN:HG3	1:Q:204:ARG:NE	2.32	0.44
1:Z:111:ARG:NH1	1:Z:111:ARG:HG2	2.33	0.44
3:15:36:TYR:CE2	3:15:90:PHE:HB2	2.53	0.44
3:21:36:TYR:CE2	3:21:90:PHE:HB2	2.53	0.44
3:25:64:TYR:CB	3:25:96:CYS:HB3	2.47	0.44
3:26:36:TYR:CE2	3:26:90:PHE:HB2	2.53	0.44
1:E:168:GLN:HG3	1:F:204:ARG:NE	2.32	0.44
1:L:121:ARG:HB3	1:M:111:ARG:HB3	2.00	0.44
1:L:170:ALA:HB3	1:M:206:GLU:HG3	1.99	0.44
1:O:171:ILE:O	1:P:207:TYR:O	2.35	0.44
1:Q:82:LEU:HD12	1:Q:146:GLY:HA3	1.98	0.44
1:S:168:GLN:HG3	1:T:204:ARG:NE	2.33	0.44
1:E:222:LEU:HB2	1:F:231:PRO:HB3	2.00	0.44
1:F:168:GLN:HG3	1:G:204:ARG:NE	2.32	0.44
1:I:121:ARG:HB3	1:J:111:ARG:HB3	2.00	0.44
1:K:82:LEU:HD12	1:K:146:GLY:HA3	1.98	0.44
1:M:41:PRO:HA	1:O:157:ALA:HB1	2.00	0.44
1:N:82:LEU:HD13	1:N:144:PHE:CE1	2.53	0.44
1:N:168:GLN:HG3	1:O:204:ARG:NE	2.32	0.44
1:O:82:LEU:HD13	1:O:144:PHE:CE1	2.53	0.44
1:P:82:LEU:HD13	1:P:144:PHE:CE1	2.53	0.44
1:Q:82:LEU:HD13	1:Q:144:PHE:CE1	2.53	0.44
1:S:111:ARG:HG2	1:S:111:ARG:NH1	2.33	0.44
1:T:71:PRO:HD2	1:T:189:ILE:HD13	1.98	0.44
1:T:170:ALA:HB3	1:U:206:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:222:LEU:HB2	1:U:231:PRO:HB3	1.99	0.44
1:U:111:ARG:HA	1:U:111:ARG:HD3	1.90	0.44
1:V:222:LEU:HB2	1:W:231:PRO:HB3	2.00	0.44
1:X:82:LEU:HD12	1:X:146:GLY:HA3	1.98	0.44
1:Z:78:LEU:HD12	1:Z:193:ASN:O	2.16	0.44
1:A:41:PRO:HA	1:C:157:ALA:HB1	1.99	0.44
1:A:171:ILE:HD12	1:C:88:ALA:CB	2.34	0.44
3:19:77:CYS:HB3	3:19:80:TYR:CE1	2.48	0.44
3:22:36:TYR:CE2	3:22:90:PHE:HB2	2.53	0.44
1:G:78:LEU:HD12	1:G:193:ASN:O	2.16	0.44
1:G:121:ARG:HB3	1:H:111:ARG:HB3	2.00	0.44
1:H:111:ARG:HG2	1:H:111:ARG:NH1	2.33	0.44
1:J:168:GLN:HG3	1:K:204:ARG:NE	2.32	0.44
1:K:222:LEU:HB2	1:L:231:PRO:HB3	2.00	0.44
1:L:111:ARG:NH1	1:L:111:ARG:HG2	2.33	0.44
1:M:82:LEU:HD13	1:M:144:PHE:CE1	2.52	0.44
1:M:170:ALA:HB3	1:N:206:GLU:HG3	1.99	0.44
1:N:170:ALA:HB3	1:O:206:GLU:HG3	1.99	0.44
1:P:121:ARG:HB3	1:Q:111:ARG:HB3	2.00	0.44
1:P:170:ALA:HB3	1:Q:206:GLU:HG3	1.99	0.44
1:R:82:LEU:HD13	1:R:144:PHE:CE1	2.53	0.44
1:R:168:GLN:HG3	1:S:204:ARG:NE	2.33	0.44
1:R:171:ILE:O	1:S:207:TYR:O	2.35	0.44
1:U:111:ARG:HG2	1:U:111:ARG:NH1	2.33	0.44
1:U:168:GLN:HG3	1:V:204:ARG:NE	2.33	0.44
1:W:168:GLN:HG3	1:X:204:ARG:NE	2.32	0.44
1:W:222:LEU:HB2	1:X:231:PRO:HB3	2.00	0.44
1:A:111:ARG:NH1	1:A:111:ARG:HG2	2.33	0.44
3:4:36:TYR:CE2	3:4:90:PHE:HB2	2.53	0.44
3:13:36:TYR:CE2	3:13:90:PHE:HB2	2.53	0.44
3:16:36:TYR:CE2	3:16:90:PHE:HB2	2.53	0.44
3:17:36:TYR:CE2	3:17:90:PHE:HB2	2.53	0.44
3:18:64:TYR:CB	3:18:96:CYS:HB3	2.47	0.44
3:23:36:TYR:CE2	3:23:90:PHE:HB2	2.53	0.44
3:24:82:GLY:O	1:Y:210:ASN:ND2	2.50	0.44
1:D:82:LEU:HD13	1:D:144:PHE:CE1	2.53	0.44
1:F:101:LYS:HZ2	1:F:101:LYS:CB	2.31	0.44
1:F:170:ALA:HB3	1:G:206:GLU:HG3	1.99	0.44
1:I:170:ALA:HB3	1:J:206:GLU:HG3	2.00	0.44
1:Q:168:GLN:HG3	1:R:204:ARG:NE	2.32	0.44
1:S:82:LEU:HD13	1:S:144:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:121:ARG:HB3	1:U:111:ARG:HB3	1.99	0.44
1:W:170:ALA:HB3	1:X:206:GLU:HG3	1.99	0.44
1:W:171:ILE:O	1:X:207:TYR:O	2.34	0.44
1:X:111:ARG:HG2	1:X:111:ARG:NH1	2.33	0.44
3:7:36:TYR:CE2	3:7:90:PHE:HB2	2.53	0.44
3:25:36:TYR:CE2	3:25:90:PHE:HB2	2.53	0.44
3:25:38:GLN:HG2	3:25:44:SER:HB3	2.00	0.44
1:C:82:LEU:HD12	1:C:146:GLY:HA3	1.97	0.44
1:E:82:LEU:HD13	1:E:144:PHE:CE1	2.53	0.44
1:F:82:LEU:HD13	1:F:144:PHE:CE1	2.53	0.44
1:J:121:ARG:HB3	1:K:111:ARG:HB3	2.00	0.44
1:K:111:ARG:HG2	1:K:111:ARG:NH1	2.33	0.44
1:L:82:LEU:HD13	1:L:144:PHE:CE1	2.53	0.44
1:O:135:LYS:HB2	1:O:135:LYS:HE2	1.73	0.44
1:P:222:LEU:HB2	1:Q:231:PRO:HB3	2.00	0.44
1:R:82:LEU:HD12	1:R:146:GLY:HA3	1.98	0.44
1:S:171:ILE:O	1:T:207:TYR:O	2.35	0.44
1:T:82:LEU:HD13	1:T:144:PHE:CE1	2.53	0.44
1:Z:82:LEU:HD13	1:Z:144:PHE:CE1	2.53	0.44
1:A:82:LEU:HD13	1:A:144:PHE:CE1	2.53	0.44
3:8:36:TYR:CE2	3:8:90:PHE:HB2	2.53	0.44
3:10:36:TYR:CE2	3:10:90:PHE:HB2	2.53	0.44
3:23:77:CYS:HB3	3:23:80:TYR:CE1	2.48	0.44
1:B:121:ARG:HB3	1:C:111:ARG:HB3	1.99	0.44
1:C:111:ARG:HG2	1:C:111:ARG:NH1	2.33	0.44
1:C:168:GLN:HG3	1:D:204:ARG:NE	2.33	0.44
1:D:121:ARG:HB3	1:E:111:ARG:HB3	2.00	0.44
1:E:82:LEU:O	1:E:197:SER:OG	2.28	0.44
1:H:171:ILE:HD12	1:J:88:ALA:CB	2.34	0.44
1:I:111:ARG:NH1	1:I:111:ARG:HG2	2.33	0.44
1:J:171:ILE:HD12	1:L:88:ALA:CB	2.35	0.44
1:N:111:ARG:NH1	1:N:111:ARG:HG2	2.33	0.44
1:N:135:LYS:HE2	1:N:135:LYS:HB2	1.73	0.44
1:O:121:ARG:HB3	1:P:111:ARG:HB3	2.00	0.44
1:R:170:ALA:HB3	1:S:206:GLU:HG3	1.99	0.44
1:U:171:ILE:O	1:V:207:TYR:O	2.35	0.44
1:X:82:LEU:HD13	1:X:144:PHE:CE1	2.53	0.44
1:Y:82:LEU:HD13	1:Y:144:PHE:CE1	2.53	0.44
1:A:231:PRO:HB3	1:Z:222:LEU:HB2	2.00	0.43
3:1:38:GLN:HG2	3:1:44:SER:HB3	2.00	0.43
3:9:36:TYR:CE2	3:9:90:PHE:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:11:36:TYR:CE2	3:11:90:PHE:HB2	2.53	0.43
3:12:36:TYR:CE2	3:12:90:PHE:HB2	2.53	0.43
3:26:38:GLN:HG2	3:26:44:SER:HB3	2.00	0.43
1:F:111:ARG:NH1	1:F:111:ARG:HG2	2.33	0.43
1:F:121:ARG:HB3	1:G:111:ARG:HB3	2.00	0.43
1:G:82:LEU:HD13	1:G:144:PHE:CE1	2.53	0.43
1:K:82:LEU:HA	1:K:197:SER:CB	2.43	0.43
1:K:82:LEU:HD13	1:K:144:PHE:CE1	2.53	0.43
1:M:222:LEU:HB2	1:N:231:PRO:HB3	2.00	0.43
1:O:168:GLN:HG3	1:P:204:ARG:NE	2.33	0.43
1:Q:90:LYS:HE2	1:Q:138:ALA:HB3	2.00	0.43
1:Q:170:ALA:HB3	1:R:206:GLU:HG3	1.99	0.43
1:Q:222:LEU:HB2	1:R:231:PRO:HB3	2.00	0.43
1:U:82:LEU:HD13	1:U:144:PHE:CE1	2.53	0.43
1:U:170:ALA:HB3	1:V:206:GLU:HG3	2.00	0.43
1:W:176:GLU:OE2	1:Y:90:LYS:HD3	2.18	0.43
3:2:38:GLN:HG2	3:2:44:SER:HB3	2.00	0.43
3:19:36:TYR:HE2	3:19:44:SER:HG	1.64	0.43
3:24:38:GLN:HG2	3:24:44:SER:HB3	2.00	0.43
1:C:121:ARG:HB3	1:D:111:ARG:HB3	2.00	0.43
1:C:167:LYS:NZ	1:D:84:GLU:OE2	2.43	0.43
1:D:82:LEU:HA	1:D:197:SER:CB	2.43	0.43
1:F:222:LEU:HB2	1:G:231:PRO:HB3	2.00	0.43
1:L:168:GLN:HG3	1:M:204:ARG:NE	2.32	0.43
1:M:90:LYS:HE2	1:M:138:ALA:HB3	2.01	0.43
1:N:90:LYS:HE2	1:N:138:ALA:HB3	2.01	0.43
1:O:101:LYS:HZ2	1:O:101:LYS:CB	2.31	0.43
1:Q:111:ARG:NH1	1:Q:111:ARG:HG2	2.33	0.43
1:R:111:ARG:NH1	1:R:111:ARG:HG2	2.33	0.43
1:R:121:ARG:HB3	1:S:111:ARG:HB3	2.00	0.43
1:S:41:PRO:HA	1:U:157:ALA:HB1	2.00	0.43
1:T:171:ILE:O	1:U:207:TYR:O	2.34	0.43
1:A:84:GLU:OE2	1:Z:167:LYS:NZ	2.41	0.43
3:9:28:ILE:O	3:9:29:SER:OG	2.21	0.43
1:B:82:LEU:HD13	1:B:144:PHE:CE1	2.53	0.43
1:G:222:LEU:HB2	1:H:231:PRO:HB3	2.00	0.43
1:I:168:GLN:HG3	1:J:204:ARG:NE	2.33	0.43
1:L:41:PRO:HA	1:N:157:ALA:HB1	2.00	0.43
1:L:90:LYS:HE2	1:L:138:ALA:HB3	2.01	0.43
1:N:171:ILE:O	1:N:172:ASN:HB3	2.19	0.43
1:O:90:LYS:HE2	1:O:138:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:90:LYS:HE2	1:P:138:ALA:HB3	2.01	0.43
1:P:171:ILE:O	1:P:172:ASN:HB3	2.19	0.43
1:R:90:LYS:HE2	1:R:138:ALA:HB3	2.01	0.43
1:R:171:ILE:O	1:R:172:ASN:HB3	2.19	0.43
1:R:222:LEU:HB2	1:S:231:PRO:HB3	2.00	0.43
1:T:90:LYS:HE2	1:T:138:ALA:HB3	2.01	0.43
1:T:221:TRP:NE1	1:U:229:LEU:O	2.39	0.43
1:V:171:ILE:HD12	1:X:88:ALA:CB	2.35	0.43
3:4:29:SER:OG	3:4:31:ILE:HG12	2.19	0.43
3:9:29:SER:OG	3:9:31:ILE:HG12	2.19	0.43
3:15:29:SER:OG	3:15:31:ILE:HG12	2.19	0.43
3:20:77:CYS:HB3	3:20:80:TYR:CE1	2.48	0.43
3:23:38:GLN:HG2	3:23:44:SER:HB3	2.00	0.43
1:B:168:GLN:HG3	1:C:204:ARG:NE	2.32	0.43
1:C:82:LEU:HD13	1:C:144:PHE:CE1	2.53	0.43
1:G:101:LYS:HZ2	1:G:101:LYS:CB	2.32	0.43
1:G:111:ARG:NH1	1:G:111:ARG:HG2	2.33	0.43
1:J:82:LEU:HD13	1:J:144:PHE:CE1	2.53	0.43
1:K:101:LYS:HZ2	1:K:101:LYS:CB	2.31	0.43
1:K:168:GLN:HG3	1:L:204:ARG:NE	2.32	0.43
1:L:171:ILE:O	1:L:172:ASN:HB3	2.19	0.43
1:R:41:PRO:HA	1:T:157:ALA:HB1	2.00	0.43
1:S:90:LYS:HE2	1:S:138:ALA:HB3	2.01	0.43
1:S:135:LYS:HE2	1:S:135:LYS:HB2	1.73	0.43
1:S:170:ALA:HB3	1:T:206:GLU:HG3	1.99	0.43
1:T:171:ILE:O	1:T:172:ASN:HB3	2.19	0.43
1:U:90:LYS:HE2	1:U:138:ALA:HB3	2.01	0.43
1:V:40:ILE:H	1:V:40:ILE:HG12	1.49	0.43
1:V:111:ARG:NH1	1:V:111:ARG:HG2	2.33	0.43
1:V:167:LYS:NZ	1:W:84:GLU:OE2	2.42	0.43
3:3:38:GLN:HG2	3:3:44:SER:HB3	2.00	0.43
3:14:29:SER:OG	3:14:31:ILE:HG12	2.19	0.43
3:14:36:TYR:CE2	3:14:90:PHE:HB2	2.53	0.43
3:24:36:TYR:CE2	3:24:90:PHE:HB2	2.53	0.43
1:B:170:ALA:HB3	1:C:206:GLU:HG3	1.99	0.43
1:C:170:ALA:HB3	1:D:206:GLU:HG3	2.00	0.43
1:H:221:TRP:NE1	1:I:229:LEU:O	2.39	0.43
1:I:82:LEU:HD13	1:I:144:PHE:CE1	2.53	0.43
1:K:90:LYS:HE2	1:K:138:ALA:HB3	2.01	0.43
1:M:111:ARG:HG2	1:M:111:ARG:NH1	2.33	0.43
1:M:168:GLN:HG3	1:N:204:ARG:NE	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:82:LEU:HA	1:P:197:SER:CB	2.43	0.43
1:P:101:LYS:HZ2	1:P:101:LYS:CB	2.32	0.43
1:S:121:ARG:HB3	1:T:111:ARG:HB3	2.00	0.43
1:V:82:LEU:HD13	1:V:144:PHE:CE1	2.53	0.43
1:V:171:ILE:O	1:V:172:ASN:HB3	2.19	0.43
1:W:111:ARG:NH1	1:W:111:ARG:HG2	2.33	0.43
1:A:88:ALA:CB	1:Y:171:ILE:HD12	2.37	0.43
1:A:171:ILE:O	1:B:207:TYR:O	2.36	0.43
3:3:29:SER:OG	3:3:31:ILE:HG12	2.19	0.43
3:5:36:TYR:HE2	3:5:44:SER:HG	1.65	0.43
3:6:36:TYR:CE2	3:6:90:PHE:HB2	2.53	0.43
3:10:29:SER:OG	3:10:31:ILE:HG12	2.19	0.43
3:11:38:GLN:HG2	3:11:44:SER:HB3	2.00	0.43
3:12:38:GLN:HG2	3:12:44:SER:HB3	2.00	0.43
3:13:38:GLN:HG2	3:13:44:SER:HB3	2.00	0.43
3:14:38:GLN:HG2	3:14:44:SER:HB3	2.00	0.43
3:22:38:GLN:HG2	3:22:44:SER:HB3	2.00	0.43
1:E:130:ASN:CG	1:F:102:THR:HG22	2.39	0.43
1:H:30:LEU:HD21	1:I:206:GLU:HG3	2.01	0.43
1:H:82:LEU:HD13	1:H:144:PHE:CE1	2.53	0.43
1:H:168:GLN:HG3	1:I:204:ARG:NE	2.32	0.43
1:J:90:LYS:HE2	1:J:138:ALA:HB3	2.01	0.43
1:M:135:LYS:HB2	1:M:135:LYS:HE2	1.73	0.43
1:P:135:LYS:HE2	1:P:135:LYS:HB2	1.73	0.43
1:U:121:ARG:HB3	1:V:111:ARG:HB3	2.00	0.43
1:W:121:ARG:HB3	1:X:111:ARG:HB3	1.99	0.43
3:16:29:SER:OG	3:16:31:ILE:HG12	2.19	0.43
3:25:36:TYR:HE2	3:25:44:SER:HG	1.63	0.43
1:B:111:ARG:HG2	1:B:111:ARG:NH1	2.33	0.43
1:E:221:TRP:NE1	1:F:229:LEU:O	2.39	0.43
1:G:168:GLN:HG3	1:H:204:ARG:NE	2.33	0.43
1:I:90:LYS:HE2	1:I:138:ALA:HB3	2.01	0.43
1:J:171:ILE:O	1:J:172:ASN:HB3	2.19	0.43
1:L:222:LEU:HB2	1:M:231:PRO:HB3	2.01	0.43
1:Q:82:LEU:HA	1:Q:197:SER:CB	2.43	0.43
1:S:222:LEU:HB2	1:T:231:PRO:HB3	2.00	0.43
1:V:90:LYS:HE2	1:V:138:ALA:HB3	2.01	0.43
1:W:82:LEU:HD13	1:W:144:PHE:CE1	2.53	0.43
1:X:90:LYS:HE2	1:X:138:ALA:HB3	2.00	0.43
1:A:204:ARG:NE	1:Z:168:GLN:HG3	2.34	0.43
3:8:29:SER:OG	3:8:31:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:10:38:GLN:HG2	3:10:44:SER:HB3	2.00	0.43
3:10:69:SER:O	3:10:70:PHE:CD2	2.72	0.43
3:15:38:GLN:HG2	3:15:44:SER:HB3	2.00	0.43
3:22:77:CYS:HB3	3:22:80:TYR:CE1	2.49	0.43
3:25:29:SER:OG	3:25:31:ILE:HG12	2.19	0.43
1:B:135:LYS:HE2	1:B:135:LYS:HB2	1.73	0.43
1:B:171:ILE:O	1:B:172:ASN:HB3	2.19	0.43
1:E:171:ILE:O	1:E:172:ASN:HB3	2.19	0.43
1:G:41:PRO:HA	1:I:157:ALA:HB1	2.00	0.43
1:I:222:LEU:HB2	1:J:231:PRO:HB3	2.01	0.43
1:K:130:ASN:CG	1:L:102:THR:HG22	2.39	0.43
1:N:41:PRO:HA	1:P:157:ALA:HB1	2.01	0.43
1:O:170:ALA:HB3	1:P:206:GLU:HG3	2.00	0.43
1:P:221:TRP:NE1	1:Q:229:LEU:O	2.39	0.43
1:W:90:LYS:HE2	1:W:138:ALA:HB3	2.01	0.43
1:X:171:ILE:O	1:X:172:ASN:HB3	2.19	0.43
3:2:29:SER:OG	3:2:31:ILE:HG12	2.19	0.43
3:3:36:TYR:HE2	3:3:44:SER:HG	1.64	0.43
3:5:29:SER:OG	3:5:31:ILE:HG12	2.19	0.43
3:5:69:SER:O	3:5:70:PHE:CD2	2.72	0.43
3:11:29:SER:OG	3:11:31:ILE:HG12	2.19	0.43
3:16:38:GLN:HG2	3:16:44:SER:HB3	2.00	0.43
1:B:130:ASN:CG	1:C:102:THR:HG22	2.40	0.43
1:D:82:LEU:HD12	1:D:146:GLY:HA3	1.97	0.43
1:G:30:LEU:HD21	1:H:206:GLU:HG3	2.01	0.43
1:J:111:ARG:HG2	1:J:111:ARG:NH1	2.33	0.43
1:R:135:LYS:HE2	1:R:135:LYS:HB2	1.73	0.43
1:Y:90:LYS:HE2	1:Y:138:ALA:HB3	2.01	0.43
1:Z:90:LYS:HE2	1:Z:138:ALA:HB3	2.01	0.43
1:A:90:LYS:HE2	1:A:138:ALA:HB3	2.01	0.43
3:1:69:SER:O	3:1:70:PHE:CD2	2.72	0.43
3:4:38:GLN:HG2	3:4:44:SER:HB3	2.00	0.43
3:6:69:SER:O	3:6:70:PHE:CD2	2.72	0.43
3:9:38:GLN:HG2	3:9:44:SER:HB3	2.00	0.43
3:9:69:SER:O	3:9:70:PHE:CD2	2.72	0.43
3:13:69:SER:O	3:13:70:PHE:CD2	2.72	0.43
3:14:22:VAL:HG13	3:14:34:LEU:CD2	2.49	0.43
3:14:69:SER:O	3:14:70:PHE:CD2	2.72	0.43
3:20:29:SER:OG	3:20:31:ILE:HG12	2.19	0.43
3:21:38:GLN:HG2	3:21:44:SER:HB3	2.00	0.43
1:C:104:PHE:CZ	1:Z:231:PRO:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:LEU:HD12	1:E:146:GLY:HA3	1.97	0.43
1:G:171:ILE:O	1:G:172:ASN:HB3	2.19	0.43
1:H:90:LYS:HE2	1:H:138:ALA:HB3	2.01	0.43
1:O:222:LEU:HB2	1:P:231:PRO:HB3	2.01	0.43
1:V:121:ARG:HB3	1:W:111:ARG:HB3	2.00	0.43
1:W:111:ARG:HA	1:W:111:ARG:HD3	1.90	0.43
1:Y:101:LYS:HZ2	1:Y:101:LYS:CB	2.31	0.43
1:Y:171:ILE:O	1:Y:172:ASN:HB3	2.19	0.43
1:A:207:TYR:O	1:Z:171:ILE:O	2.36	0.42
1:A:222:LEU:HB2	1:B:231:PRO:HB3	2.02	0.42
3:1:29:SER:OG	3:1:31:ILE:HG12	2.19	0.42
3:2:69:SER:O	3:2:70:PHE:CD2	2.72	0.42
3:16:22:VAL:HG13	3:16:34:LEU:CD2	2.49	0.42
3:17:38:GLN:HG2	3:17:44:SER:HB3	2.00	0.42
3:21:39:PRO:HD2	3:21:42:PHE:HB2	2.01	0.42
3:22:39:PRO:HD2	3:22:42:PHE:HB2	2.01	0.42
3:23:22:VAL:HG13	3:23:34:LEU:CD2	2.49	0.42
3:24:29:SER:OG	3:24:31:ILE:HG12	2.19	0.42
3:26:29:SER:OG	3:26:31:ILE:HG12	2.19	0.42
1:B:90:LYS:HE2	1:B:138:ALA:HB3	2.01	0.42
1:E:82:LEU:HA	1:E:197:SER:CB	2.43	0.42
5:G:301:TQN:C14	1:H:112:TYR:HB2	2.49	0.42
5:H:301:TQN:C14	1:I:112:TYR:HB2	2.49	0.42
1:Q:130:ASN:CG	1:R:102:THR:HG22	2.39	0.42
1:Q:171:ILE:O	1:Q:172:ASN:HB3	2.19	0.42
5:Q:301:TQN:C14	1:R:112:TYR:HB2	2.49	0.42
1:S:171:ILE:O	1:S:172:ASN:HB3	2.19	0.42
1:U:171:ILE:HD12	1:W:88:ALA:CB	2.34	0.42
1:V:135:LYS:HE2	1:V:135:LYS:HB2	1.73	0.42
5:X:301:TQN:C14	1:Y:112:TYR:HB2	2.49	0.42
5:Y:301:TQN:C14	1:Z:112:TYR:HB2	2.49	0.42
1:A:102:THR:HG22	1:Z:130:ASN:CG	2.40	0.42
1:A:206:GLU:HG3	1:Z:30:LEU:HD21	2.00	0.42
1:A:210:ASN:HD22	3:26:83:SER:HA	1.84	0.42
3:8:38:GLN:HG2	3:8:44:SER:HB3	2.00	0.42
3:10:36:TYR:HE2	3:10:44:SER:HG	1.65	0.42
3:13:29:SER:OG	3:13:31:ILE:HG12	2.19	0.42
3:15:22:VAL:HG13	3:15:34:LEU:CD2	2.49	0.42
3:19:29:SER:OG	3:19:31:ILE:HG12	2.19	0.42
3:20:39:PRO:HD2	3:20:42:PHE:HB2	2.01	0.42
3:21:22:VAL:HG13	3:21:34:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:23:39:PRO:HD2	3:23:42:PHE:HB2	2.02	0.42
3:24:22:VAL:HG13	3:24:34:LEU:CD2	2.49	0.42
1:C:90:LYS:HE2	1:C:138:ALA:HB3	2.01	0.42
1:C:222:LEU:HB2	1:D:231:PRO:HB3	2.01	0.42
1:D:171:ILE:O	1:D:172:ASN:HB3	2.19	0.42
1:H:171:ILE:O	1:H:172:ASN:HB3	2.19	0.42
1:I:171:ILE:O	1:I:172:ASN:HB3	2.19	0.42
5:I:301:TQN:C14	1:J:112:TYR:HB2	2.49	0.42
1:K:171:ILE:HD12	1:M:88:ALA:CB	2.35	0.42
1:K:171:ILE:O	1:K:172:ASN:HB3	2.19	0.42
1:M:171:ILE:O	1:M:172:ASN:HB3	2.19	0.42
1:O:41:PRO:HA	1:Q:157:ALA:HB1	2.01	0.42
1:O:171:ILE:O	1:O:172:ASN:HB3	2.19	0.42
5:O:301:TQN:C14	1:P:112:TYR:HB2	2.49	0.42
5:P:301:TQN:C14	1:Q:112:TYR:HB2	2.49	0.42
1:R:82:LEU:HA	1:R:197:SER:CB	2.43	0.42
1:S:221:TRP:NE1	1:T:229:LEU:O	2.40	0.42
1:T:41:PRO:HA	1:V:157:ALA:HB1	2.01	0.42
1:A:112:TYR:HB2	5:Z:301:TQN:C14	2.49	0.42
1:A:168:GLN:HG3	1:B:204:ARG:NE	2.34	0.42
3:4:69:SER:O	3:4:70:PHE:CD2	2.72	0.42
3:6:29:SER:OG	3:6:31:ILE:HG12	2.19	0.42
3:11:69:SER:O	3:11:70:PHE:CD2	2.72	0.42
3:15:39:PRO:HD2	3:15:42:PHE:HB2	2.01	0.42
3:17:39:PRO:HD2	3:17:42:PHE:HB2	2.01	0.42
3:19:22:VAL:HG13	3:19:34:LEU:CD2	2.49	0.42
3:19:39:PRO:HD2	3:19:42:PHE:HB2	2.02	0.42
3:22:22:VAL:HG13	3:22:34:LEU:CD2	2.49	0.42
3:24:36:TYR:HE2	3:24:44:SER:HG	1.65	0.42
3:25:22:VAL:HG13	3:25:34:LEU:CD2	2.49	0.42
3:25:39:PRO:HD2	3:25:42:PHE:HB2	2.01	0.42
3:26:22:VAL:HG13	3:26:34:LEU:CD2	2.49	0.42
1:B:171:ILE:HD12	1:D:88:ALA:CB	2.34	0.42
1:C:171:ILE:O	1:C:172:ASN:HB3	2.19	0.42
1:D:30:LEU:HD21	1:E:206:GLU:HG3	2.01	0.42
5:F:301:TQN:C14	1:G:112:TYR:HB2	2.49	0.42
1:G:90:LYS:HE2	1:G:138:ALA:HB3	2.01	0.42
1:H:130:ASN:CG	1:I:102:THR:HG22	2.39	0.42
1:J:30:LEU:HD21	1:K:206:GLU:HG3	2.01	0.42
1:L:82:LEU:HA	1:L:197:SER:CB	2.43	0.42
1:M:167:LYS:NZ	1:N:84:GLU:OE2	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:130:ASN:CG	1:S:102:THR:HG22	2.39	0.42
5:R:301:TQN:C14	1:S:112:TYR:HB2	2.49	0.42
1:S:167:LYS:NZ	1:T:84:GLU:OE2	2.42	0.42
1:U:40:ILE:H	1:U:40:ILE:HG12	1.49	0.42
5:W:301:TQN:C14	1:X:112:TYR:HB2	2.49	0.42
1:Z:171:ILE:O	1:Z:172:ASN:HB3	2.19	0.42
3:5:38:GLN:HG2	3:5:44:SER:HB3	2.00	0.42
3:7:29:SER:OG	3:7:31:ILE:HG12	2.19	0.42
3:13:39:PRO:HD2	3:13:42:PHE:HB2	2.01	0.42
3:14:39:PRO:HD2	3:14:42:PHE:HB2	2.01	0.42
3:17:22:VAL:HG13	3:17:34:LEU:CD2	2.50	0.42
3:18:38:GLN:HG2	3:18:44:SER:HB3	2.00	0.42
3:18:39:PRO:HD2	3:18:42:PHE:HB2	2.02	0.42
3:20:83:SER:O	3:20:84:LEU:HD23	2.20	0.42
3:21:29:SER:OG	3:21:31:ILE:HG12	2.19	0.42
3:21:77:CYS:HB3	3:21:80:TYR:CE1	2.48	0.42
3:23:29:SER:OG	3:23:31:ILE:HG12	2.19	0.42
3:23:83:SER:O	3:23:84:LEU:HD23	2.20	0.42
3:24:39:PRO:HD2	3:24:42:PHE:HB2	2.02	0.42
1:D:90:LYS:HE2	1:D:138:ALA:HB3	2.01	0.42
1:F:30:LEU:HD21	1:G:206:GLU:HG3	2.01	0.42
3:1:83:SER:O	3:1:84:LEU:HD23	2.20	0.42
3:7:38:GLN:HG2	3:7:44:SER:HB3	2.00	0.42
3:8:39:PRO:HD2	3:8:42:PHE:HB2	2.01	0.42
3:9:39:PRO:HD2	3:9:42:PHE:HB2	2.01	0.42
3:10:39:PRO:HD2	3:10:42:PHE:HB2	2.01	0.42
3:11:39:PRO:HD2	3:11:42:PHE:HB2	2.01	0.42
3:15:69:SER:O	3:15:70:PHE:CD2	2.72	0.42
3:16:39:PRO:HD2	3:16:42:PHE:HB2	2.02	0.42
3:17:69:SER:O	3:17:70:PHE:CD2	2.72	0.42
3:22:29:SER:OG	3:22:31:ILE:HG12	2.19	0.42
3:24:69:SER:O	3:24:70:PHE:CD2	2.72	0.42
3:24:83:SER:O	3:24:84:LEU:HD23	2.20	0.42
3:26:39:PRO:HD2	3:26:42:PHE:HB2	2.01	0.42
1:B:30:LEU:HD21	1:C:206:GLU:HG3	2.01	0.42
1:E:90:LYS:HE2	1:E:138:ALA:HB3	2.01	0.42
1:F:41:PRO:HA	1:H:157:ALA:HB1	2.00	0.42
1:G:40:ILE:H	1:G:40:ILE:HG12	1.49	0.42
1:L:171:ILE:HD12	1:N:88:ALA:CB	2.34	0.42
5:N:301:TQN:C14	1:O:112:TYR:HB2	2.49	0.42
1:Q:101:LYS:HZ2	1:Q:101:LYS:CB	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:135:LYS:HE2	1:Q:135:LYS:HB2	1.73	0.42
1:U:171:ILE:O	1:U:172:ASN:HB3	2.19	0.42
1:U:222:LEU:HB2	1:V:231:PRO:HB3	2.01	0.42
5:A:302:TQN:C14	1:B:112:TYR:HB2	2.49	0.42
3:2:22:VAL:HG13	3:2:34:LEU:CD2	2.49	0.42
3:7:39:PRO:HD2	3:7:42:PHE:HB2	2.01	0.42
3:11:20:ALA:HA	3:11:36:TYR:HB3	2.02	0.42
3:12:29:SER:OG	3:12:31:ILE:HG12	2.19	0.42
3:17:29:SER:OG	3:17:31:ILE:HG12	2.19	0.42
3:19:38:GLN:HG2	3:19:44:SER:HB3	2.00	0.42
3:22:20:ALA:HA	3:22:36:TYR:HB3	2.02	0.42
3:23:20:ALA:HA	3:23:36:TYR:HB3	2.02	0.42
1:B:41:PRO:HA	1:D:157:ALA:HB1	2.01	0.42
1:D:130:ASN:CG	1:E:102:THR:HG22	2.40	0.42
1:E:30:LEU:HD21	1:F:206:GLU:HG3	2.02	0.42
5:E:301:TQN:C14	1:F:112:TYR:HB2	2.49	0.42
1:F:90:LYS:HE2	1:F:138:ALA:HB3	2.01	0.42
1:H:30:LEU:HD21	1:I:206:GLU:CG	2.50	0.42
5:J:301:TQN:C14	1:K:112:TYR:HB2	2.49	0.42
1:N:130:ASN:CG	1:O:102:THR:HG22	2.39	0.42
1:R:30:LEU:H	1:R:30:LEU:CD2	2.29	0.42
1:S:130:ASN:CG	1:T:102:THR:HG22	2.39	0.42
5:V:301:TQN:C14	1:W:112:TYR:HB2	2.49	0.42
1:W:130:ASN:CG	1:X:102:THR:HG22	2.39	0.42
1:X:168:GLN:HG3	1:Y:204:ARG:NE	2.35	0.42
1:A:171:ILE:O	1:A:172:ASN:HB3	2.19	0.42
1:A:206:GLU:HG3	1:Z:170:ALA:HB3	2.01	0.42
3:6:20:ALA:HA	3:6:36:TYR:HB3	2.02	0.42
3:6:38:GLN:HG2	3:6:44:SER:HB3	2.00	0.42
3:6:39:PRO:HD2	3:6:42:PHE:HB2	2.01	0.42
3:8:69:SER:O	3:8:70:PHE:CD2	2.72	0.42
3:9:20:ALA:HA	3:9:36:TYR:HB3	2.02	0.42
3:10:20:ALA:HA	3:10:36:TYR:HB3	2.02	0.42
3:12:22:VAL:HG13	3:12:34:LEU:CD2	2.50	0.42
3:12:39:PRO:HD2	3:12:42:PHE:HB2	2.02	0.42
3:16:28:ILE:O	3:16:29:SER:OG	2.21	0.42
3:19:20:ALA:HA	3:19:36:TYR:HB3	2.02	0.42
3:20:36:TYR:HE2	3:20:44:SER:HG	1.65	0.42
3:20:38:GLN:HG2	3:20:44:SER:HB3	2.00	0.42
3:26:69:SER:O	3:26:70:PHE:CD2	2.72	0.42
1:C:117:PHE:HD1	1:C:122:ALA:CB	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:ASN:CG	1:H:102:THR:HG22	2.40	0.42
1:G:167:LYS:NZ	1:H:84:GLU:OE2	2.42	0.42
1:I:117:PHE:HD1	1:I:122:ALA:CB	2.33	0.42
1:J:130:ASN:CG	1:K:102:THR:HG22	2.40	0.42
1:L:135:LYS:HB2	1:L:135:LYS:HE2	1.73	0.42
1:P:111:ARG:HA	1:P:111:ARG:HD3	1.90	0.42
1:S:82:LEU:HA	1:S:197:SER:CB	2.43	0.42
5:S:301:TQN:C14	1:T:112:TYR:HB2	2.49	0.42
1:T:30:LEU:HD21	1:U:206:GLU:HG3	2.01	0.42
1:T:130:ASN:CG	1:U:102:THR:HG22	2.39	0.42
1:T:135:LYS:HB2	1:T:135:LYS:HE2	1.73	0.42
1:U:41:PRO:HA	1:W:157:ALA:HB1	2.01	0.42
1:V:30:LEU:HD21	1:W:206:GLU:HG3	2.01	0.42
1:A:117:PHE:HD1	1:A:122:ALA:CB	2.33	0.42
3:5:20:ALA:HA	3:5:36:TYR:HB3	2.02	0.42
3:7:69:SER:O	3:7:70:PHE:CD2	2.72	0.42
3:12:69:SER:O	3:12:70:PHE:CD2	2.72	0.42
3:13:22:VAL:HG13	3:13:34:LEU:CD2	2.50	0.42
3:14:20:ALA:HA	3:14:36:TYR:HB3	2.02	0.42
3:16:69:SER:O	3:16:70:PHE:CD2	2.72	0.42
3:18:20:ALA:HA	3:18:36:TYR:HB3	2.02	0.42
3:18:22:VAL:HG13	3:18:34:LEU:CD2	2.50	0.42
3:18:69:SER:O	3:18:70:PHE:CD2	2.72	0.42
3:19:83:SER:O	3:19:84:LEU:HD23	2.20	0.42
3:21:20:ALA:HA	3:21:36:TYR:HB3	2.02	0.42
3:21:83:SER:O	3:21:84:LEU:HD23	2.20	0.42
3:26:83:SER:O	3:26:84:LEU:HD23	2.20	0.42
1:B:117:PHE:HD1	1:B:122:ALA:CB	2.33	0.42
1:D:41:PRO:HA	1:F:157:ALA:HB1	2.01	0.42
1:D:117:PHE:HD1	1:D:122:ALA:CB	2.33	0.42
1:E:101:LYS:HZ2	1:E:101:LYS:CB	2.33	0.42
1:F:30:LEU:H	1:F:30:LEU:CD2	2.29	0.42
1:I:101:LYS:HZ2	1:I:101:LYS:CB	2.33	0.42
5:M:301:TQN:C14	1:N:112:TYR:HB2	2.49	0.42
1:N:30:LEU:HD21	1:O:206:GLU:HG3	2.01	0.42
1:N:117:PHE:HD1	1:N:122:ALA:CB	2.33	0.42
1:Q:221:TRP:NE1	1:R:229:LEU:O	2.39	0.42
1:W:171:ILE:O	1:W:172:ASN:HB3	2.19	0.42
1:Y:117:PHE:HD1	1:Y:122:ALA:CB	2.33	0.42
1:Z:117:PHE:HD1	1:Z:122:ALA:CB	2.33	0.42
1:A:130:ASN:CG	1:B:102:THR:HG22	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ALA:HB3	1:B:206:GLU:HG3	2.01	0.42
3:1:39:PRO:HD2	3:1:42:PHE:HB2	2.01	0.42
3:2:36:TYR:HE2	3:2:44:SER:HG	1.65	0.42
3:3:69:SER:O	3:3:70:PHE:CD2	2.72	0.42
3:4:39:PRO:HD2	3:4:42:PHE:HB2	2.01	0.42
3:5:39:PRO:HD2	3:5:42:PHE:HB2	2.02	0.42
3:9:22:VAL:HG13	3:9:34:LEU:CD2	2.49	0.42
3:11:22:VAL:HG13	3:11:34:LEU:CD2	2.50	0.42
3:13:20:ALA:HA	3:13:36:TYR:HB3	2.02	0.42
3:15:20:ALA:HA	3:15:36:TYR:HB3	2.02	0.42
3:18:29:SER:OG	3:18:31:ILE:HG12	2.19	0.42
3:19:69:SER:O	3:19:70:PHE:CD2	2.72	0.42
3:20:20:ALA:HA	3:20:36:TYR:HB3	2.02	0.42
3:21:69:SER:O	3:21:70:PHE:CD2	2.72	0.42
3:23:69:SER:O	3:23:70:PHE:CD2	2.72	0.42
3:25:69:SER:O	3:25:70:PHE:CD2	2.72	0.42
1:C:41:PRO:HA	1:E:157:ALA:HB1	2.01	0.42
1:E:117:PHE:HD1	1:E:122:ALA:CB	2.33	0.42
1:F:171:ILE:O	1:F:172:ASN:HB3	2.19	0.42
1:G:117:PHE:HD1	1:G:122:ALA:CB	2.33	0.42
1:I:30:LEU:HD21	1:J:206:GLU:HG3	2.02	0.42
1:K:41:PRO:HA	1:M:157:ALA:HB1	2.01	0.42
1:K:117:PHE:HD1	1:K:122:ALA:CB	2.33	0.42
1:P:41:PRO:HA	1:R:157:ALA:HB1	2.01	0.42
1:X:117:PHE:HD1	1:X:122:ALA:CB	2.33	0.42
1:X:222:LEU:HB2	1:Y:231:PRO:HB3	2.02	0.42
1:A:206:GLU:CG	1:Z:30:LEU:HD21	2.50	0.42
1:A:210:ASN:ND2	3:26:82:GLY:O	2.53	0.42
3:1:20:ALA:HA	3:1:36:TYR:HB3	2.02	0.42
3:2:20:ALA:HA	3:2:36:TYR:HB3	2.02	0.42
3:4:20:ALA:HA	3:4:36:TYR:HB3	2.02	0.42
3:4:83:SER:O	3:4:84:LEU:HD23	2.20	0.42
3:7:20:ALA:HA	3:7:36:TYR:HB3	2.02	0.42
3:8:20:ALA:HA	3:8:36:TYR:HB3	2.02	0.42
3:10:83:SER:O	3:10:84:LEU:HD23	2.20	0.42
3:17:20:ALA:HA	3:17:36:TYR:HB3	2.02	0.42
3:20:69:SER:O	3:20:70:PHE:CD2	2.72	0.42
3:22:69:SER:O	3:22:70:PHE:CD2	2.72	0.42
3:22:83:SER:O	3:22:84:LEU:HD23	2.20	0.42
3:24:20:ALA:HA	3:24:36:TYR:HB3	2.02	0.42
1:C:130:ASN:CG	1:D:102:THR:HG22	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:PHE:HD1	1:F:122:ALA:CB	2.33	0.42
5:K:301:TQN:C14	1:L:112:TYR:HB2	2.49	0.42
1:L:130:ASN:CG	1:M:102:THR:HG22	2.40	0.42
1:M:130:ASN:CG	1:N:102:THR:HG22	2.39	0.42
1:P:30:LEU:HD21	1:Q:206:GLU:HG3	2.01	0.42
1:P:117:PHE:HD1	1:P:122:ALA:CB	2.33	0.42
1:Q:41:PRO:HA	1:S:157:ALA:HB1	2.00	0.42
1:R:30:LEU:HD21	1:S:206:GLU:HG3	2.01	0.42
1:T:82:LEU:O	1:T:197:SER:OG	2.28	0.42
5:T:301:TQN:C14	1:U:112:TYR:HB2	2.49	0.42
1:X:30:LEU:HD21	1:Y:206:GLU:HG3	2.01	0.42
3:2:83:SER:O	3:2:84:LEU:HD23	2.20	0.41
3:3:39:PRO:HD2	3:3:42:PHE:HB2	2.01	0.41
3:5:83:SER:O	3:5:84:LEU:HD23	2.20	0.41
3:6:22:VAL:HG13	3:6:34:LEU:CD2	2.49	0.41
3:7:22:VAL:HG13	3:7:34:LEU:CD2	2.49	0.41
3:11:83:SER:O	3:11:84:LEU:HD23	2.20	0.41
3:20:22:VAL:HG13	3:20:34:LEU:CD2	2.50	0.41
3:26:20:ALA:HA	3:26:36:TYR:HB3	2.02	0.41
5:B:301:TQN:C14	1:C:112:TYR:HB2	2.49	0.41
1:D:30:LEU:HD21	1:E:206:GLU:CG	2.50	0.41
1:H:41:PRO:HA	1:J:157:ALA:HB1	2.01	0.41
1:P:130:ASN:CG	1:Q:102:THR:HG22	2.40	0.41
1:S:30:LEU:H	1:S:30:LEU:CD2	2.29	0.41
1:T:82:LEU:HA	1:T:197:SER:CB	2.43	0.41
1:V:117:PHE:HD1	1:V:122:ALA:CB	2.33	0.41
1:V:221:TRP:NE1	1:W:229:LEU:O	2.39	0.41
1:W:30:LEU:HD21	1:X:206:GLU:HG3	2.01	0.41
1:W:117:PHE:HD1	1:W:122:ALA:CB	2.33	0.41
1:X:171:ILE:HD12	1:Z:88:ALA:CB	2.33	0.41
1:Y:30:LEU:HD21	1:Z:206:GLU:CG	2.50	0.41
1:A:30:LEU:HD21	1:B:206:GLU:HG3	2.01	0.41
3:4:22:VAL:HG13	3:4:34:LEU:CD2	2.49	0.41
3:12:20:ALA:HA	3:12:36:TYR:HB3	2.02	0.41
3:12:83:SER:O	3:12:84:LEU:HD23	2.20	0.41
3:16:20:ALA:HA	3:16:36:TYR:HB3	2.02	0.41
3:16:83:SER:O	3:16:84:LEU:HD23	2.20	0.41
5:D:301:TQN:C14	1:E:112:TYR:HB2	2.49	0.41
1:G:30:LEU:HD21	1:H:206:GLU:CG	2.51	0.41
1:H:117:PHE:HD1	1:H:122:ALA:CB	2.33	0.41
5:L:301:TQN:C14	1:M:112:TYR:HB2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:40:ILE:H	1:T:40:ILE:HG12	1.49	0.41
1:U:117:PHE:HD1	1:U:122:ALA:CB	2.33	0.41
1:X:41:PRO:HA	1:Z:157:ALA:HB1	2.01	0.41
1:Y:111:ARG:HA	1:Y:111:ARG:HD3	1.90	0.41
1:A:111:ARG:HB3	1:Z:121:ARG:HB3	2.01	0.41
3:3:20:ALA:HA	3:3:36:TYR:HB3	2.02	0.41
3:5:22:VAL:HG13	3:5:34:LEU:CD2	2.49	0.41
3:9:83:SER:O	3:9:84:LEU:HD23	2.20	0.41
3:18:83:SER:O	3:18:84:LEU:HD23	2.20	0.41
3:23:36:TYR:HE2	3:23:44:SER:HG	1.64	0.41
1:F:82:LEU:HA	1:F:197:SER:CB	2.43	0.41
1:F:130:ASN:CG	1:G:102:THR:HG22	2.41	0.41
1:G:111:ARG:HA	1:G:111:ARG:HD3	1.90	0.41
1:J:30:LEU:HD21	1:K:206:GLU:CG	2.50	0.41
1:K:30:LEU:HD21	1:L:206:GLU:HG3	2.02	0.41
1:L:117:PHE:HD1	1:L:122:ALA:CB	2.33	0.41
1:M:117:PHE:HD1	1:M:122:ALA:CB	2.33	0.41
1:R:221:TRP:NE1	1:S:229:LEU:O	2.40	0.41
1:S:30:LEU:HD21	1:T:206:GLU:HG3	2.01	0.41
5:U:301:TQN:C14	1:V:112:TYR:HB2	2.49	0.41
1:V:41:PRO:HA	1:X:157:ALA:HB1	2.01	0.41
1:X:35:THR:HG21	1:Y:166:GLU:HB2	2.02	0.41
1:X:111:ARG:HA	1:X:111:ARG:HD3	1.90	0.41
1:X:121:ARG:HB3	1:Y:111:ARG:HB3	2.01	0.41
3:2:39:PRO:HD2	3:2:42:PHE:HB2	2.02	0.41
3:3:83:SER:O	3:3:84:LEU:HD23	2.20	0.41
3:8:22:VAL:HG13	3:8:34:LEU:CD2	2.50	0.41
3:8:36:TYR:HE2	3:8:44:SER:HG	1.65	0.41
3:8:83:SER:O	3:8:84:LEU:HD23	2.20	0.41
3:13:28:ILE:O	3:13:29:SER:OG	2.21	0.41
3:13:36:TYR:HE2	3:13:44:SER:HG	1.64	0.41
3:17:83:SER:O	3:17:84:LEU:HD23	2.20	0.41
3:21:36:TYR:HE2	3:21:44:SER:HG	1.65	0.41
3:25:20:ALA:HA	3:25:36:TYR:HB3	2.02	0.41
1:E:111:ARG:HA	1:E:111:ARG:HD3	1.90	0.41
1:I:130:ASN:CG	1:J:102:THR:HG22	2.40	0.41
1:M:30:LEU:HD21	1:N:206:GLU:HG3	2.01	0.41
1:T:117:PHE:HD1	1:T:122:ALA:CB	2.33	0.41
1:A:121:ARG:HB3	1:B:111:ARG:HB3	2.01	0.41
1:A:231:PRO:HG2	1:D:104:PHE:CZ	2.56	0.41
3:1:22:VAL:HG13	3:1:34:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:10:22:VAL:HG13	3:10:34:LEU:CD2	2.49	0.41
1:B:30:LEU:HD21	1:C:206:GLU:CG	2.50	0.41
1:C:30:LEU:HD21	1:D:206:GLU:HG3	2.02	0.41
1:C:135:LYS:HB2	1:C:135:LYS:HE2	1.73	0.41
1:F:30:LEU:HD21	1:G:206:GLU:CG	2.51	0.41
1:J:117:PHE:HD1	1:J:122:ALA:CB	2.33	0.41
1:M:171:ILE:HD12	1:O:88:ALA:CB	2.34	0.41
1:N:30:LEU:HD21	1:O:206:GLU:CG	2.50	0.41
1:O:130:ASN:CG	1:P:102:THR:HG22	2.40	0.41
1:R:117:PHE:HD1	1:R:122:ALA:CB	2.33	0.41
1:S:117:PHE:HD1	1:S:122:ALA:CB	2.33	0.41
1:T:30:LEU:HD21	1:U:206:GLU:CG	2.50	0.41
1:T:176:GLU:OE1	1:T:207:TYR:OH	2.21	0.41
1:A:111:ARG:HA	1:A:111:ARG:HD3	1.90	0.41
3:13:83:SER:O	3:13:84:LEU:HD23	2.20	0.41
1:C:111:ARG:HA	1:C:111:ARG:HD3	1.90	0.41
1:J:41:PRO:HA	1:L:157:ALA:HB1	2.01	0.41
1:M:82:LEU:HA	1:M:197:SER:CB	2.43	0.41
1:P:30:LEU:HD21	1:Q:206:GLU:CG	2.50	0.41
1:S:101:LYS:HZ2	1:S:101:LYS:CB	2.34	0.41
1:T:30:LEU:H	1:T:30:LEU:CD2	2.29	0.41
1:U:30:LEU:HD21	1:V:206:GLU:HG3	2.02	0.41
1:V:30:LEU:HD21	1:W:206:GLU:CG	2.50	0.41
1:A:135:LYS:HE2	1:A:135:LYS:HB2	1.73	0.41
3:3:22:VAL:HG13	3:3:34:LEU:CD2	2.49	0.41
5:C:301:TQN:C14	1:D:112:TYR:HB2	2.49	0.41
1:G:30:LEU:H	1:G:30:LEU:CD2	2.29	0.41
1:I:111:ARG:HA	1:I:111:ARG:HD3	1.90	0.41
1:L:30:LEU:HD21	1:M:206:GLU:HG3	2.01	0.41
1:L:231:PRO:HG2	1:O:104:PHE:CZ	2.56	0.41
1:Q:30:LEU:HD21	1:R:206:GLU:HG3	2.01	0.41
1:U:82:LEU:HA	1:U:197:SER:CB	2.43	0.41
1:A:104:PHE:CZ	1:X:231:PRO:HG2	2.55	0.41
3:6:36:TYR:HE2	3:6:44:SER:HG	1.64	0.41
3:25:83:SER:O	3:25:84:LEU:HD23	2.20	0.41
1:Q:117:PHE:HD1	1:Q:122:ALA:CB	2.33	0.41
1:S:30:LEU:HD21	1:T:206:GLU:CG	2.51	0.41
3:6:83:SER:O	3:6:84:LEU:HD23	2.20	0.41
3:7:83:SER:O	3:7:84:LEU:HD23	2.20	0.41
3:15:83:SER:O	3:15:84:LEU:HD23	2.20	0.41
1:B:88:ALA:CB	1:Z:171:ILE:HD12	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:LEU:HD21	1:F:206:GLU:CG	2.51	0.41
1:E:41:PRO:HA	1:G:157:ALA:HB1	2.01	0.41
1:I:41:PRO:HA	1:K:157:ALA:HB1	2.01	0.41
1:J:101:LYS:HZ2	1:J:101:LYS:CB	2.31	0.41
1:O:30:LEU:HD21	1:P:206:GLU:HG3	2.02	0.41
1:P:231:PRO:HG2	1:S:104:PHE:CZ	2.56	0.41
1:Q:30:LEU:HD21	1:R:206:GLU:CG	2.51	0.41
1:Q:231:PRO:HG2	1:T:104:PHE:CZ	2.55	0.41
1:R:30:LEU:HD21	1:S:206:GLU:CG	2.50	0.41
1:R:231:PRO:HG2	1:U:104:PHE:CZ	2.55	0.41
1:S:40:ILE:H	1:S:40:ILE:HG12	1.49	0.41
1:U:135:LYS:HE2	1:U:135:LYS:HB2	1.73	0.41
1:W:30:LEU:HD21	1:X:206:GLU:CG	2.51	0.41
1:W:221:TRP:NE1	1:X:229:LEU:O	2.39	0.41
1:Y:167:LYS:NZ	1:Z:84:GLU:OE2	2.40	0.41
1:A:30:LEU:HD21	1:B:206:GLU:CG	2.51	0.41
3:10:28:ILE:O	3:10:29:SER:OG	2.21	0.41
1:M:231:PRO:HG2	1:P:104:PHE:CZ	2.56	0.41
1:N:101:LYS:HZ2	1:N:101:LYS:CB	2.34	0.41
1:O:117:PHE:HD1	1:O:122:ALA:CB	2.33	0.41
1:O:221:TRP:NE1	1:P:229:LEU:O	2.41	0.41
1:U:221:TRP:NE1	1:V:229:LEU:O	2.41	0.41
1:B:101:LYS:O	1:B:101:LYS:NZ	2.54	0.40
1:D:167:LYS:NZ	1:E:84:GLU:OE2	2.42	0.40
1:I:30:LEU:HD21	1:J:206:GLU:CG	2.51	0.40
1:K:135:LYS:HB2	1:K:135:LYS:HE2	1.73	0.40
1:M:30:LEU:HD21	1:N:206:GLU:CG	2.51	0.40
1:U:30:LEU:H	1:U:30:LEU:CD2	2.29	0.40
1:U:130:ASN:CG	1:V:102:THR:HG22	2.40	0.40
3:1:83:SER:HA	1:B:210:ASN:HD22	1.87	0.40
3:17:64:TYR:HB2	3:17:96:CYS:CB	2.51	0.40
1:C:171:ILE:HD12	1:E:88:ALA:CB	2.34	0.40
1:E:101:LYS:O	1:E:101:LYS:NZ	2.55	0.40
1:J:156:LEU:HD12	1:J:160:ASN:HB2	2.03	0.40
1:N:221:TRP:NE1	1:O:229:LEU:O	2.39	0.40
1:R:40:ILE:H	1:R:40:ILE:HG12	1.49	0.40
1:V:130:ASN:CG	1:W:102:THR:HG22	2.40	0.40
1:X:113:LEU:HD23	1:X:113:LEU:HA	1.95	0.40
3:7:70:PHE:CD1	1:G:40:ILE:HA	2.57	0.40
3:14:83:SER:O	3:14:84:LEU:HD23	2.20	0.40
3:18:64:TYR:HB2	3:18:96:CYS:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:21:64:TYR:HB2	3:21:96:CYS:CB	2.51	0.40
1:D:101:LYS:NZ	1:D:101:LYS:O	2.55	0.40
1:F:101:LYS:O	1:F:101:LYS:NZ	2.55	0.40
1:G:82:LEU:HA	1:G:197:SER:CB	2.43	0.40
1:N:156:LEU:HD12	1:N:160:ASN:HB2	2.04	0.40
1:V:82:LEU:HA	1:V:197:SER:CB	2.43	0.40
1:W:41:PRO:HA	1:Y:157:ALA:HB1	2.01	0.40
1:Y:30:LEU:HD21	1:Z:206:GLU:HG3	2.03	0.40
1:Y:101:LYS:O	1:Y:101:LYS:NZ	2.55	0.40
1:A:40:ILE:HA	3:1:70:PHE:CD1	2.57	0.40
3:17:16:ILE:H	3:17:16:ILE:HG12	1.83	0.40
3:18:47:ASP:CG	3:18:50:VAL:H	2.14	0.40
3:19:64:TYR:HB2	3:19:96:CYS:CB	2.51	0.40
3:20:64:TYR:HB2	3:20:96:CYS:CB	2.51	0.40
1:D:82:LEU:O	1:D:197:SER:OG	2.28	0.40
1:K:156:LEU:HD12	1:K:160:ASN:HB2	2.04	0.40
1:M:156:LEU:HD12	1:M:160:ASN:HB2	2.04	0.40
1:O:30:LEU:HD21	1:P:206:GLU:CG	2.51	0.40
1:O:156:LEU:HD12	1:O:160:ASN:HB2	2.04	0.40
1:P:156:LEU:HD12	1:P:160:ASN:HB2	2.04	0.40
1:Q:156:LEU:HD12	1:Q:160:ASN:HB2	2.03	0.40
1:R:156:LEU:HD12	1:R:160:ASN:HB2	2.04	0.40
3:3:28:ILE:O	3:3:29:SER:OG	2.21	0.40
3:3:47:ASP:CG	3:3:50:VAL:H	2.14	0.40
3:15:64:TYR:HB2	3:15:96:CYS:CB	2.51	0.40
3:16:64:TYR:HB2	3:16:96:CYS:CB	2.51	0.40
3:21:83:SER:HA	1:V:210:ASN:HD22	1.87	0.40
1:B:231:PRO:HG2	1:E:104:PHE:CZ	2.57	0.40
1:C:101:LYS:O	1:C:101:LYS:NZ	2.55	0.40
1:C:231:PRO:HG2	1:F:104:PHE:CZ	2.57	0.40
1:E:231:PRO:HG2	1:H:104:PHE:CZ	2.56	0.40
1:I:156:LEU:HD12	1:I:160:ASN:HB2	2.04	0.40
1:Q:40:ILE:H	1:Q:40:ILE:HG12	1.49	0.40
1:X:30:LEU:HD21	1:Y:206:GLU:CG	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	B	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	C	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	D	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	E	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	F	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	G	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	H	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	I	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	J	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	K	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	L	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	M	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	N	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	O	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	P	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	Q	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	R	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	S	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	T	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	U	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	V	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	W	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	X	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
1	Y	209/232 (90%)	193 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
2	a	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	b	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	c	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	d	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	e	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	f	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	g	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	h	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	i	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	j	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	k	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	l	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	m	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	n	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	o	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	p	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	q	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	r	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	s	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	t	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	u	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	v	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	w	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	x	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	y	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
2	z	300/365 (82%)	287 (96%)	13 (4%)	0	100	100
3	1	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	10	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	11	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	12	82/111 (74%)	68 (83%)	14 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	13	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	14	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	15	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	16	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	17	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	18	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	19	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	2	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	20	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	21	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	22	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	23	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	24	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	25	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	26	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	3	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	4	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	5	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	6	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	7	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	8	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
3	9	82/111 (74%)	68 (83%)	14 (17%)	0	100	100
All	All	15366/18408 (84%)	14248 (93%)	1118 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	B	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	C	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	D	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	E	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	F	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	G	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	H	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	I	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	J	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	K	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	L	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	M	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	N	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	O	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	P	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	Q	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	R	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	S	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	T	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	U	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	V	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	W	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	X	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	Y	170/186 (91%)	163 (96%)	7 (4%)	26	34
1	Z	170/186 (91%)	163 (96%)	7 (4%)	26	34
2	a	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	b	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	c	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	d	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	e	251/294 (85%)	240 (96%)	11 (4%)	24	31
2	f	251/294 (85%)	241 (96%)	10 (4%)	27	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	g	251/294 (85%)	240 (96%)	11 (4%)	24	31
2	h	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	i	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	j	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	k	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	l	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	m	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	n	251/294 (85%)	240 (96%)	11 (4%)	24	31
2	o	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	p	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	q	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	r	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	s	251/294 (85%)	240 (96%)	11 (4%)	24	31
2	t	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	u	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	v	251/294 (85%)	240 (96%)	11 (4%)	24	31
2	w	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	x	251/294 (85%)	240 (96%)	11 (4%)	24	31
2	y	251/294 (85%)	241 (96%)	10 (4%)	27	35
2	z	251/294 (85%)	241 (96%)	10 (4%)	27	35
3	1	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	10	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	11	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	12	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	13	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	14	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	15	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	16	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	17	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	18	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	19	72/95 (76%)	67 (93%)	5 (7%)	13	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	20	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	21	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	22	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	23	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	24	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	25	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	26	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	3	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	4	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	5	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	6	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	7	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	8	72/95 (76%)	67 (93%)	5 (7%)	13	14
3	9	72/95 (76%)	67 (93%)	5 (7%)	13	14
All	All	12818/14950 (86%)	12240 (96%)	578 (4%)	26	30

All (578) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	THR
1	A	40	ILE
1	A	99	ASP
1	A	101	LYS
1	A	107	ASP
1	A	144	PHE
1	A	193	ASN
2	a	79	MET
2	a	114	LYS
2	a	160	LEU
2	a	190	ASN
2	a	196	MET
2	a	210	TYR
2	a	256	ASN
2	a	325	SER
2	a	344	ASP
2	a	363	GLU

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Mol	Chain	Res	Type
3	1	14	CYS
3	1	16	ILE
3	1	41	PHE
3	1	45	ARG
3	1	70	PHE
2	b	79	MET
2	b	114	LYS
2	b	160	LEU
2	b	190	ASN
2	b	196	MET
2	b	210	TYR
2	b	256	ASN
2	b	325	SER
2	b	344	ASP
2	b	363	GLU
2	c	79	MET
2	c	114	LYS
2	c	160	LEU
2	c	190	ASN
2	c	196	MET
2	c	210	TYR
2	c	256	ASN
2	c	325	SER
2	c	344	ASP
2	c	363	GLU
2	d	79	MET
2	d	114	LYS
2	d	160	LEU
2	d	190	ASN
2	d	196	MET
2	d	210	TYR
2	d	256	ASN
2	d	325	SER
2	d	344	ASP
2	d	363	GLU
2	e	79	MET
2	e	114	LYS
2	e	160	LEU
2	e	190	ASN
2	e	196	MET
2	e	206	ARG
2	e	210	TYR

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Mol	Chain	Res	Type
2	e	256	ASN
2	e	325	SER
2	e	344	ASP
2	e	363	GLU
2	f	79	MET
2	f	114	LYS
2	f	160	LEU
2	f	190	ASN
2	f	196	MET
2	f	210	TYR
2	f	256	ASN
2	f	325	SER
2	f	344	ASP
2	f	363	GLU
2	g	79	MET
2	g	114	LYS
2	g	160	LEU
2	g	190	ASN
2	g	196	MET
2	g	206	ARG
2	g	210	TYR
2	g	256	ASN
2	g	325	SER
2	g	344	ASP
2	g	363	GLU
2	h	79	MET
2	h	114	LYS
2	h	160	LEU
2	h	190	ASN
2	h	196	MET
2	h	210	TYR
2	h	256	ASN
2	h	325	SER
2	h	344	ASP
2	h	363	GLU
2	i	79	MET
2	i	114	LYS
2	i	160	LEU
2	i	190	ASN
2	i	196	MET
2	i	210	TYR
2	i	256	ASN

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Mol	Chain	Res	Type
2	i	325	SER
2	i	344	ASP
2	i	363	GLU
2	j	79	MET
2	j	114	LYS
2	j	160	LEU
2	j	190	ASN
2	j	196	MET
2	j	210	TYR
2	j	256	ASN
2	j	325	SER
2	j	344	ASP
2	j	363	GLU
2	k	79	MET
2	k	114	LYS
2	k	160	LEU
2	k	190	ASN
2	k	196	MET
2	k	210	TYR
2	k	256	ASN
2	k	325	SER
2	k	344	ASP
2	k	363	GLU
2	l	79	MET
2	l	114	LYS
2	l	160	LEU
2	l	190	ASN
2	l	196	MET
2	l	210	TYR
2	l	256	ASN
2	l	325	SER
2	l	344	ASP
2	l	363	GLU
2	m	79	MET
2	m	114	LYS
2	m	160	LEU
2	m	190	ASN
2	m	196	MET
2	m	210	TYR
2	m	256	ASN
2	m	325	SER
2	m	344	ASP

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Mol	Chain	Res	Type
2	m	363	GLU
2	n	79	MET
2	n	114	LYS
2	n	160	LEU
2	n	190	ASN
2	n	196	MET
2	n	206	ARG
2	n	210	TYR
2	n	256	ASN
2	n	325	SER
2	n	344	ASP
2	n	363	GLU
2	o	79	MET
2	o	114	LYS
2	o	160	LEU
2	o	190	ASN
2	o	196	MET
2	o	210	TYR
2	o	256	ASN
2	o	325	SER
2	o	344	ASP
2	o	363	GLU
2	p	79	MET
2	p	114	LYS
2	p	160	LEU
2	p	190	ASN
2	p	196	MET
2	p	210	TYR
2	p	256	ASN
2	p	325	SER
2	p	344	ASP
2	p	363	GLU
2	q	79	MET
2	q	114	LYS
2	q	160	LEU
2	q	190	ASN
2	q	196	MET
2	q	210	TYR
2	q	256	ASN
2	q	325	SER
2	q	344	ASP
2	q	363	GLU

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Mol	Chain	Res	Type
2	r	79	MET
2	r	114	LYS
2	r	160	LEU
2	r	190	ASN
2	r	196	MET
2	r	210	TYR
2	r	256	ASN
2	r	325	SER
2	r	344	ASP
2	r	363	GLU
2	s	79	MET
2	s	114	LYS
2	s	160	LEU
2	s	190	ASN
2	s	196	MET
2	s	206	ARG
2	s	210	TYR
2	s	256	ASN
2	s	325	SER
2	s	344	ASP
2	s	363	GLU
2	t	79	MET
2	t	114	LYS
2	t	160	LEU
2	t	190	ASN
2	t	196	MET
2	t	210	TYR
2	t	256	ASN
2	t	325	SER
2	t	344	ASP
2	t	363	GLU
2	u	79	MET
2	u	114	LYS
2	u	160	LEU
2	u	190	ASN
2	u	196	MET
2	u	210	TYR
2	u	256	ASN
2	u	325	SER
2	u	344	ASP
2	u	363	GLU
2	v	79	MET

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Mol	Chain	Res	Type
2	v	114	LYS
2	v	160	LEU
2	v	190	ASN
2	v	196	MET
2	v	206	ARG
2	v	210	TYR
2	v	256	ASN
2	v	325	SER
2	v	344	ASP
2	v	363	GLU
2	w	79	MET
2	w	114	LYS
2	w	160	LEU
2	w	190	ASN
2	w	196	MET
2	w	210	TYR
2	w	256	ASN
2	w	325	SER
2	w	344	ASP
2	w	363	GLU
2	x	79	MET
2	x	114	LYS
2	x	160	LEU
2	x	190	ASN
2	x	196	MET
2	x	206	ARG
2	x	210	TYR
2	x	256	ASN
2	x	325	SER
2	x	344	ASP
2	x	363	GLU
2	y	79	MET
2	y	114	LYS
2	y	160	LEU
2	y	190	ASN
2	y	196	MET
2	y	210	TYR
2	y	256	ASN
2	y	325	SER
2	y	344	ASP
2	y	363	GLU
2	z	79	MET

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Mol	Chain	Res	Type
2	z	114	LYS
2	z	160	LEU
2	z	190	ASN
2	z	196	MET
2	z	210	TYR
2	z	256	ASN
2	z	325	SER
2	z	344	ASP
2	z	363	GLU
3	2	14	CYS
3	2	16	ILE
3	2	41	PHE
3	2	45	ARG
3	2	70	PHE
3	3	14	CYS
3	3	16	ILE
3	3	41	PHE
3	3	45	ARG
3	3	70	PHE
3	4	14	CYS
3	4	16	ILE
3	4	41	PHE
3	4	45	ARG
3	4	70	PHE
3	5	14	CYS
3	5	16	ILE
3	5	41	PHE
3	5	45	ARG
3	5	70	PHE
3	6	14	CYS
3	6	16	ILE
3	6	41	PHE
3	6	45	ARG
3	6	70	PHE
3	7	14	CYS
3	7	16	ILE
3	7	41	PHE
3	7	45	ARG
3	7	70	PHE
3	8	14	CYS
3	8	16	ILE
3	8	41	PHE

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Mol	Chain	Res	Type
3	8	45	ARG
3	8	70	PHE
3	9	14	CYS
3	9	16	ILE
3	9	41	PHE
3	9	45	ARG
3	9	70	PHE
3	10	14	CYS
3	10	16	ILE
3	10	41	PHE
3	10	45	ARG
3	10	70	PHE
3	11	14	CYS
3	11	16	ILE
3	11	41	PHE
3	11	45	ARG
3	11	70	PHE
3	12	14	CYS
3	12	16	ILE
3	12	41	PHE
3	12	45	ARG
3	12	70	PHE
3	13	14	CYS
3	13	16	ILE
3	13	41	PHE
3	13	45	ARG
3	13	70	PHE
3	14	14	CYS
3	14	16	ILE
3	14	41	PHE
3	14	45	ARG
3	14	70	PHE
3	15	14	CYS
3	15	16	ILE
3	15	41	PHE
3	15	45	ARG
3	15	70	PHE
3	16	14	CYS
3	16	16	ILE
3	16	41	PHE
3	16	45	ARG
3	16	70	PHE

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Mol	Chain	Res	Type
3	17	14	CYS
3	17	16	ILE
3	17	41	PHE
3	17	45	ARG
3	17	70	PHE
3	18	14	CYS
3	18	16	ILE
3	18	41	PHE
3	18	45	ARG
3	18	70	PHE
3	19	14	CYS
3	19	16	ILE
3	19	41	PHE
3	19	45	ARG
3	19	70	PHE
3	20	14	CYS
3	20	16	ILE
3	20	41	PHE
3	20	45	ARG
3	20	70	PHE
3	21	14	CYS
3	21	16	ILE
3	21	41	PHE
3	21	45	ARG
3	21	70	PHE
3	22	14	CYS
3	22	16	ILE
3	22	41	PHE
3	22	45	ARG
3	22	70	PHE
3	23	14	CYS
3	23	16	ILE
3	23	41	PHE
3	23	45	ARG
3	23	70	PHE
3	24	14	CYS
3	24	16	ILE
3	24	41	PHE
3	24	45	ARG
3	24	70	PHE
3	25	14	CYS
3	25	16	ILE

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Mol	Chain	Res	Type
3	25	41	PHE
3	25	45	ARG
3	25	70	PHE
3	26	14	CYS
3	26	16	ILE
3	26	41	PHE
3	26	45	ARG
3	26	70	PHE
1	B	36	THR
1	B	40	ILE
1	B	99	ASP
1	B	101	LYS
1	B	107	ASP
1	B	144	PHE
1	B	193	ASN
1	C	36	THR
1	C	40	ILE
1	C	99	ASP
1	C	101	LYS
1	C	107	ASP
1	C	144	PHE
1	C	193	ASN
1	D	36	THR
1	D	40	ILE
1	D	99	ASP
1	D	101	LYS
1	D	107	ASP
1	D	144	PHE
1	D	193	ASN
1	E	36	THR
1	E	40	ILE
1	E	99	ASP
1	E	101	LYS
1	E	107	ASP
1	E	144	PHE
1	E	193	ASN
1	F	36	THR
1	F	40	ILE
1	F	99	ASP
1	F	101	LYS
1	F	107	ASP
1	F	144	PHE

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Mol	Chain	Res	Type
1	F	193	ASN
1	G	36	THR
1	G	40	ILE
1	G	99	ASP
1	G	101	LYS
1	G	107	ASP
1	G	144	PHE
1	G	193	ASN
1	H	36	THR
1	H	40	ILE
1	H	99	ASP
1	H	101	LYS
1	H	107	ASP
1	H	144	PHE
1	H	193	ASN
1	I	36	THR
1	I	40	ILE
1	I	99	ASP
1	I	101	LYS
1	I	107	ASP
1	I	144	PHE
1	I	193	ASN
1	J	36	THR
1	J	40	ILE
1	J	99	ASP
1	J	101	LYS
1	J	107	ASP
1	J	144	PHE
1	J	193	ASN
1	K	36	THR
1	K	40	ILE
1	K	99	ASP
1	K	101	LYS
1	K	107	ASP
1	K	144	PHE
1	K	193	ASN
1	L	36	THR
1	L	40	ILE
1	L	99	ASP
1	L	101	LYS
1	L	107	ASP
1	L	144	PHE

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Mol	Chain	Res	Type
1	L	193	ASN
1	M	36	THR
1	M	40	ILE
1	M	99	ASP
1	M	101	LYS
1	M	107	ASP
1	M	144	PHE
1	M	193	ASN
1	N	36	THR
1	N	40	ILE
1	N	99	ASP
1	N	101	LYS
1	N	107	ASP
1	N	144	PHE
1	N	193	ASN
1	O	36	THR
1	O	40	ILE
1	O	99	ASP
1	O	101	LYS
1	O	107	ASP
1	O	144	PHE
1	O	193	ASN
1	P	36	THR
1	P	40	ILE
1	P	99	ASP
1	P	101	LYS
1	P	107	ASP
1	P	144	PHE
1	P	193	ASN
1	Q	36	THR
1	Q	40	ILE
1	Q	99	ASP
1	Q	101	LYS
1	Q	107	ASP
1	Q	144	PHE
1	Q	193	ASN
1	R	36	THR
1	R	40	ILE
1	R	99	ASP
1	R	101	LYS
1	R	107	ASP
1	R	144	PHE

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Mol	Chain	Res	Type
1	R	193	ASN
1	S	36	THR
1	S	40	ILE
1	S	99	ASP
1	S	101	LYS
1	S	107	ASP
1	S	144	PHE
1	S	193	ASN
1	T	36	THR
1	T	40	ILE
1	T	99	ASP
1	T	101	LYS
1	T	107	ASP
1	T	144	PHE
1	T	193	ASN
1	U	36	THR
1	U	40	ILE
1	U	99	ASP
1	U	101	LYS
1	U	107	ASP
1	U	144	PHE
1	U	193	ASN
1	V	36	THR
1	V	40	ILE
1	V	99	ASP
1	V	101	LYS
1	V	107	ASP
1	V	144	PHE
1	V	193	ASN
1	W	36	THR
1	W	40	ILE
1	W	99	ASP
1	W	101	LYS
1	W	107	ASP
1	W	144	PHE
1	W	193	ASN
1	X	36	THR
1	X	40	ILE
1	X	99	ASP
1	X	101	LYS
1	X	107	ASP
1	X	144	PHE

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Mol	Chain	Res	Type
1	X	193	ASN
1	Y	36	THR
1	Y	40	ILE
1	Y	99	ASP
1	Y	101	LYS
1	Y	107	ASP
1	Y	144	PHE
1	Y	193	ASN
1	Z	36	THR
1	Z	40	ILE
1	Z	99	ASP
1	Z	101	LYS
1	Z	107	ASP
1	Z	144	PHE
1	Z	193	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
2	a	99	GLN
2	a	161	ASN
2	a	350	GLN
2	b	99	GLN
2	b	161	ASN
2	b	350	GLN
2	c	99	GLN
2	c	161	ASN
2	c	350	GLN
2	d	99	GLN
2	d	161	ASN
2	d	350	GLN
2	e	99	GLN
2	e	161	ASN
2	e	350	GLN
2	f	99	GLN
2	f	161	ASN
2	f	350	GLN
2	g	99	GLN
2	g	161	ASN
2	g	350	GLN
2	h	99	GLN
2	h	161	ASN

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Mol	Chain	Res	Type
2	h	350	GLN
2	i	99	GLN
2	i	161	ASN
2	i	350	GLN
2	j	99	GLN
2	j	161	ASN
2	j	350	GLN
2	k	99	GLN
2	k	161	ASN
2	k	350	GLN
2	l	99	GLN
2	l	161	ASN
2	l	350	GLN
2	m	99	GLN
2	m	161	ASN
2	m	350	GLN
2	n	99	GLN
2	n	161	ASN
2	n	350	GLN
2	o	99	GLN
2	o	161	ASN
2	o	350	GLN
2	p	99	GLN
2	p	161	ASN
2	p	350	GLN
2	q	161	ASN
2	q	350	GLN
2	r	99	GLN
2	r	161	ASN
2	r	350	GLN
2	s	99	GLN
2	s	161	ASN
2	s	350	GLN
2	t	99	GLN
2	t	161	ASN
2	t	350	GLN
2	u	99	GLN
2	u	161	ASN
2	u	350	GLN
2	v	161	ASN
2	v	350	GLN
2	w	99	GLN

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Mol	Chain	Res	Type
2	w	161	ASN
2	w	350	GLN
2	x	99	GLN
2	x	161	ASN
2	x	350	GLN
2	y	161	ASN
2	y	350	GLN
2	z	99	GLN
2	z	161	ASN
2	z	350	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

52 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	TLW	H	302	-	15,15,15	1.19	2 (13%)	19,21,21	2.11	4 (21%)
4	TLW	A	303	-	15,15,15	1.21	2 (13%)	19,21,21	2.10	4 (21%)
5	TQN	A	302	-	140,141,141	1.67	26 (18%)	160,169,169	1.36	11 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	TQN	E	301	-	140,141,141	1.67	27 (19%)	160,169,169	1.36	11 (6%)
4	TLW	N	302	-	15,15,15	1.19	2 (13%)	19,21,21	2.10	4 (21%)
5	TQN	I	301	-	140,141,141	1.67	27 (19%)	160,169,169	1.36	11 (6%)
5	TQN	C	301	-	140,141,141	1.67	28 (20%)	160,169,169	1.36	11 (6%)
4	TLW	L	302	-	15,15,15	1.20	1 (6%)	19,21,21	2.10	4 (21%)
4	TLW	Y	302	-	15,15,15	1.20	1 (6%)	19,21,21	2.10	4 (21%)
4	TLW	X	302	-	15,15,15	1.19	1 (6%)	19,21,21	2.10	4 (21%)
5	TQN	Q	301	-	140,141,141	1.67	27 (19%)	160,169,169	1.36	11 (6%)
5	TQN	J	301	-	140,141,141	1.68	27 (19%)	160,169,169	1.36	11 (6%)
4	TLW	B	302	-	15,15,15	1.19	1 (6%)	19,21,21	2.11	4 (21%)
5	TQN	T	301	-	140,141,141	1.67	27 (19%)	160,169,169	1.36	11 (6%)
4	TLW	F	302	-	15,15,15	1.20	2 (13%)	19,21,21	2.10	4 (21%)
4	TLW	R	302	-	15,15,15	1.19	1 (6%)	19,21,21	2.10	4 (21%)
5	TQN	Z	301	-	140,141,141	1.67	27 (19%)	160,169,169	1.36	11 (6%)
5	TQN	S	301	-	140,141,141	1.67	28 (20%)	160,169,169	1.36	11 (6%)
4	TLW	S	302	-	15,15,15	1.19	2 (13%)	19,21,21	2.11	4 (21%)
4	TLW	J	302	-	15,15,15	1.20	1 (6%)	19,21,21	2.10	4 (21%)
4	TLW	T	302	-	15,15,15	1.19	2 (13%)	19,21,21	2.10	4 (21%)
4	TLW	V	302	-	15,15,15	1.20	1 (6%)	19,21,21	2.10	4 (21%)
4	TLW	D	302	-	15,15,15	1.19	1 (6%)	19,21,21	2.10	4 (21%)
4	TLW	E	302	-	15,15,15	1.19	1 (6%)	19,21,21	2.10	4 (21%)
4	TLW	G	302	-	15,15,15	1.19	1 (6%)	19,21,21	2.11	4 (21%)
5	TQN	U	301	-	140,141,141	1.67	27 (19%)	160,169,169	1.36	11 (6%)
4	TLW	W	302	-	15,15,15	1.18	1 (6%)	19,21,21	2.10	4 (21%)
5	TQN	D	301	-	140,141,141	1.67	27 (19%)	160,169,169	1.36	11 (6%)
5	TQN	L	301	-	140,141,141	1.67	28 (20%)	160,169,169	1.36	11 (6%)
5	TQN	X	301	-	140,141,141	1.67	28 (20%)	160,169,169	1.36	11 (6%)
4	TLW	I	302	-	15,15,15	1.21	2 (13%)	19,21,21	2.11	4 (21%)
4	TLW	C	302	-	15,15,15	1.19	1 (6%)	19,21,21	2.10	4 (21%)
4	TLW	Q	302	-	15,15,15	1.19	2 (13%)	19,21,21	2.10	4 (21%)
5	TQN	K	301	-	140,141,141	1.67	27 (19%)	160,169,169	1.36	11 (6%)
5	TQN	M	301	-	140,141,141	1.67	28 (20%)	160,169,169	1.36	12 (7%)
5	TQN	O	301	-	140,141,141	1.67	28 (20%)	160,169,169	1.36	11 (6%)
5	TQN	R	301	-	140,141,141	1.67	27 (19%)	160,169,169	1.36	11 (6%)
5	TQN	V	301	-	140,141,141	1.67	28 (20%)	160,169,169	1.36	11 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	TQN	H	301	-	140,141,141	1.67	27 (19%)	160,169,169	1.36	11 (6%)
4	TLW	A	301	-	15,15,15	1.20	2 (13%)	19,21,21	2.10	4 (21%)
4	TLW	P	302	-	15,15,15	1.20	1 (6%)	19,21,21	2.10	4 (21%)
4	TLW	M	302	-	15,15,15	1.19	1 (6%)	19,21,21	2.10	4 (21%)
4	TLW	U	302	-	15,15,15	1.20	2 (13%)	19,21,21	2.10	4 (21%)
5	TQN	N	301	-	140,141,141	1.67	27 (19%)	160,169,169	1.36	11 (6%)
5	TQN	P	301	-	140,141,141	1.67	27 (19%)	160,169,169	1.36	11 (6%)
5	TQN	Y	301	-	140,141,141	1.67	27 (19%)	160,169,169	1.36	11 (6%)
4	TLW	K	302	-	15,15,15	1.20	2 (13%)	19,21,21	2.10	4 (21%)
4	TLW	O	302	-	15,15,15	1.20	2 (13%)	19,21,21	2.10	4 (21%)
5	TQN	B	301	-	140,141,141	1.67	28 (20%)	160,169,169	1.36	11 (6%)
5	TQN	G	301	-	140,141,141	1.67	28 (20%)	160,169,169	1.36	12 (7%)
5	TQN	F	301	-	140,141,141	1.67	28 (20%)	160,169,169	1.36	11 (6%)
5	TQN	W	301	-	140,141,141	1.67	28 (20%)	160,169,169	1.36	11 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TLW	H	302	-	1/1/6/6	5/10/26/26	0/1/1/1
4	TLW	A	303	-	1/1/6/6	5/10/26/26	0/1/1/1
5	TQN	A	302	-	-	53/143/184/184	0/2/2/2
5	TQN	E	301	-	-	53/143/184/184	0/2/2/2
4	TLW	N	302	-	1/1/6/6	5/10/26/26	0/1/1/1
5	TQN	I	301	-	-	53/143/184/184	0/2/2/2
5	TQN	C	301	-	-	53/143/184/184	0/2/2/2
4	TLW	L	302	-	1/1/6/6	5/10/26/26	0/1/1/1
4	TLW	Y	302	-	1/1/6/6	5/10/26/26	0/1/1/1
4	TLW	X	302	-	1/1/6/6	5/10/26/26	0/1/1/1
5	TQN	Q	301	-	-	53/143/184/184	0/2/2/2
5	TQN	J	301	-	-	53/143/184/184	0/2/2/2
4	TLW	B	302	-	1/1/6/6	5/10/26/26	0/1/1/1
5	TQN	T	301	-	-	53/143/184/184	0/2/2/2
4	TLW	F	302	-	1/1/6/6	5/10/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TLW	R	302	-	1/1/6/6	5/10/26/26	0/1/1/1
5	TQN	Z	301	-	-	53/143/184/184	0/2/2/2
5	TQN	S	301	-	-	53/143/184/184	0/2/2/2
4	TLW	S	302	-	1/1/6/6	5/10/26/26	0/1/1/1
4	TLW	J	302	-	1/1/6/6	5/10/26/26	0/1/1/1
4	TLW	T	302	-	1/1/6/6	5/10/26/26	0/1/1/1
4	TLW	V	302	-	1/1/6/6	5/10/26/26	0/1/1/1
4	TLW	D	302	-	1/1/6/6	5/10/26/26	0/1/1/1
4	TLW	E	302	-	1/1/6/6	5/10/26/26	0/1/1/1
4	TLW	G	302	-	1/1/6/6	5/10/26/26	0/1/1/1
5	TQN	U	301	-	-	53/143/184/184	0/2/2/2
4	TLW	W	302	-	1/1/6/6	5/10/26/26	0/1/1/1
5	TQN	D	301	-	-	53/143/184/184	0/2/2/2
5	TQN	L	301	-	-	53/143/184/184	0/2/2/2
5	TQN	X	301	-	-	53/143/184/184	0/2/2/2
4	TLW	I	302	-	1/1/6/6	5/10/26/26	0/1/1/1
4	TLW	C	302	-	1/1/6/6	5/10/26/26	0/1/1/1
4	TLW	Q	302	-	1/1/6/6	5/10/26/26	0/1/1/1
5	TQN	K	301	-	-	53/143/184/184	0/2/2/2
5	TQN	M	301	-	-	53/143/184/184	0/2/2/2
5	TQN	O	301	-	-	53/143/184/184	0/2/2/2
5	TQN	R	301	-	-	53/143/184/184	0/2/2/2
5	TQN	V	301	-	-	53/143/184/184	0/2/2/2
5	TQN	H	301	-	-	54/143/184/184	0/2/2/2
4	TLW	A	301	-	1/1/6/6	5/10/26/26	0/1/1/1
4	TLW	P	302	-	1/1/6/6	5/10/26/26	0/1/1/1
4	TLW	M	302	-	1/1/6/6	5/10/26/26	0/1/1/1
4	TLW	U	302	-	1/1/6/6	5/10/26/26	0/1/1/1
5	TQN	N	301	-	-	53/143/184/184	0/2/2/2
5	TQN	P	301	-	-	53/143/184/184	0/2/2/2
5	TQN	Y	301	-	-	53/143/184/184	0/2/2/2
4	TLW	K	302	-	1/1/6/6	5/10/26/26	0/1/1/1
4	TLW	O	302	-	1/1/6/6	5/10/26/26	0/1/1/1
5	TQN	B	301	-	-	53/143/184/184	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TQN	G	301	-	-	53/143/184/184	0/2/2/2
5	TQN	F	301	-	-	53/143/184/184	0/2/2/2
5	TQN	W	301	-	-	53/143/184/184	0/2/2/2

All (750) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	301	TQN	C51-NB2	7.91	1.50	1.34
5	M	301	TQN	C51-NB2	7.91	1.50	1.34
5	O	301	TQN	C51-NB2	7.90	1.50	1.34
5	R	301	TQN	C51-NB2	7.90	1.50	1.34
5	J	301	TQN	C51-NB2	7.90	1.50	1.34
5	H	301	TQN	C51-NB2	7.89	1.50	1.34
5	C	301	TQN	C51-NB2	7.89	1.50	1.34
5	L	301	TQN	C51-NB2	7.89	1.50	1.34
5	U	301	TQN	C51-NB2	7.89	1.50	1.34
5	Y	301	TQN	C51-NB2	7.89	1.50	1.34
5	A	302	TQN	C51-NB2	7.88	1.50	1.34
5	D	301	TQN	C51-NB2	7.88	1.50	1.34
5	Q	301	TQN	C51-NB2	7.88	1.50	1.34
5	F	301	TQN	C51-NB2	7.87	1.50	1.34
5	S	301	TQN	C51-NB2	7.87	1.50	1.34
5	X	301	TQN	C51-NB2	7.87	1.50	1.34
5	P	301	TQN	C51-NB2	7.87	1.50	1.34
5	W	301	TQN	C51-NB2	7.87	1.50	1.34
5	I	301	TQN	C51-NB2	7.87	1.50	1.34
5	V	301	TQN	C51-NB2	7.87	1.50	1.34
5	Z	301	TQN	C51-NB2	7.86	1.50	1.34
5	T	301	TQN	C51-NB2	7.86	1.50	1.34
5	E	301	TQN	C51-NB2	7.86	1.50	1.34
5	B	301	TQN	C51-NB2	7.85	1.50	1.34
5	K	301	TQN	C51-NB2	7.85	1.50	1.34
5	N	301	TQN	C51-NB2	7.84	1.50	1.34
5	T	301	TQN	C11-NA2	7.73	1.50	1.34
5	J	301	TQN	C11-NA2	7.71	1.50	1.34
5	P	301	TQN	C11-NA2	7.71	1.50	1.34
5	G	301	TQN	C11-NA2	7.70	1.50	1.34
5	O	301	TQN	C11-NA2	7.70	1.50	1.34
5	Q	301	TQN	C11-NA2	7.70	1.50	1.34
5	I	301	TQN	C11-NA2	7.70	1.50	1.34
5	U	301	TQN	C11-NA2	7.70	1.50	1.34
5	Z	301	TQN	C11-NA2	7.69	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	301	TQN	C11-NA2	7.69	1.50	1.34
5	A	302	TQN	C11-NA2	7.69	1.50	1.34
5	K	301	TQN	C11-NA2	7.69	1.50	1.34
5	C	301	TQN	C11-NA2	7.68	1.50	1.34
5	V	301	TQN	C11-NA2	7.68	1.50	1.34
5	N	301	TQN	C11-NA2	7.68	1.50	1.34
5	B	301	TQN	C11-NA2	7.68	1.50	1.34
5	H	301	TQN	C11-NA2	7.68	1.50	1.34
5	D	301	TQN	C11-NA2	7.68	1.50	1.34
5	X	301	TQN	C11-NA2	7.68	1.50	1.34
5	Y	301	TQN	C11-NA2	7.67	1.50	1.34
5	W	301	TQN	C11-NA2	7.67	1.50	1.34
5	M	301	TQN	C11-NA2	7.67	1.50	1.34
5	F	301	TQN	C11-NA2	7.67	1.50	1.34
5	S	301	TQN	C11-NA2	7.67	1.50	1.34
5	L	301	TQN	C11-NA2	7.66	1.50	1.34
5	E	301	TQN	C11-NA2	7.64	1.50	1.34
5	O	301	TQN	OB6-CB6	-5.53	1.19	1.42
5	J	301	TQN	OB6-CB6	-5.53	1.19	1.42
5	B	301	TQN	OB6-CB6	-5.53	1.19	1.42
5	C	301	TQN	OB6-CB6	-5.53	1.19	1.42
5	V	301	TQN	OB6-CB6	-5.53	1.19	1.42
5	G	301	TQN	OB6-CB6	-5.53	1.19	1.42
5	D	301	TQN	OB6-CB6	-5.52	1.19	1.42
5	W	301	TQN	OB6-CB6	-5.52	1.19	1.42
5	X	301	TQN	OB6-CB6	-5.52	1.19	1.42
5	E	301	TQN	OB6-CB6	-5.51	1.19	1.42
5	K	301	TQN	OB6-CB6	-5.51	1.19	1.42
5	F	301	TQN	OB6-CB6	-5.51	1.19	1.42
5	P	301	TQN	OB6-CB6	-5.51	1.19	1.42
5	Y	301	TQN	OB6-CB6	-5.51	1.19	1.42
5	S	301	TQN	OB6-CB6	-5.51	1.19	1.42
5	A	302	TQN	OB6-CB6	-5.51	1.19	1.42
5	N	301	TQN	OB6-CB6	-5.51	1.19	1.42
5	T	301	TQN	OB6-CB6	-5.51	1.19	1.42
5	Q	301	TQN	OB6-CB6	-5.51	1.19	1.42
5	H	301	TQN	OB6-CB6	-5.51	1.19	1.42
5	U	301	TQN	OB6-CB6	-5.51	1.19	1.42
5	L	301	TQN	OB6-CB6	-5.50	1.19	1.42
5	R	301	TQN	OB6-CB6	-5.50	1.19	1.42
5	M	301	TQN	OB6-CB6	-5.50	1.19	1.42
5	I	301	TQN	OB6-CB6	-5.49	1.19	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Z	301	TQN	OB6-CB6	-5.49	1.19	1.42
5	L	301	TQN	CA2-NA2	4.01	1.52	1.45
5	M	301	TQN	CA2-NA2	3.99	1.52	1.45
5	W	301	TQN	CA2-NA2	3.99	1.52	1.45
5	U	301	TQN	CA2-NA2	3.99	1.52	1.45
5	E	301	TQN	CA2-NA2	3.99	1.52	1.45
5	N	301	TQN	CA2-NA2	3.99	1.52	1.45
5	V	301	TQN	CA2-NA2	3.97	1.52	1.45
5	G	301	TQN	CA2-NA2	3.96	1.52	1.45
5	T	301	TQN	CA2-NA2	3.96	1.52	1.45
5	Y	301	TQN	CA2-NA2	3.96	1.52	1.45
5	B	301	TQN	CA2-NA2	3.96	1.52	1.45
5	J	301	TQN	CA2-NA2	3.95	1.52	1.45
5	D	301	TQN	CA2-NA2	3.95	1.52	1.45
5	H	301	TQN	CA2-NA2	3.95	1.52	1.45
5	R	301	TQN	CA2-NA2	3.95	1.52	1.45
5	A	302	TQN	CA2-NA2	3.95	1.52	1.45
5	Z	301	TQN	CA2-NA2	3.95	1.52	1.45
5	X	301	TQN	CA2-NA2	3.94	1.52	1.45
5	Q	301	TQN	CA2-NA2	3.94	1.52	1.45
5	K	301	TQN	CA2-NA2	3.94	1.52	1.45
5	F	301	TQN	CA2-NA2	3.93	1.52	1.45
5	S	301	TQN	CA2-NA2	3.93	1.52	1.45
5	P	301	TQN	CA2-NA2	3.93	1.52	1.45
5	O	301	TQN	CA2-NA2	3.92	1.52	1.45
5	I	301	TQN	CA2-NA2	3.91	1.52	1.45
5	C	301	TQN	CA2-NA2	3.90	1.52	1.45
5	F	301	TQN	OB3-C71	3.76	1.44	1.34
5	P	301	TQN	OB3-C71	3.75	1.44	1.34
5	X	301	TQN	OB3-C71	3.74	1.44	1.34
5	V	301	TQN	OB3-C71	3.74	1.44	1.34
5	E	301	TQN	OB3-C71	3.74	1.44	1.34
5	Z	301	TQN	OB3-C71	3.74	1.44	1.34
5	J	301	TQN	OB3-C71	3.74	1.44	1.34
5	G	301	TQN	OB3-C71	3.73	1.44	1.34
5	L	301	TQN	OB3-C71	3.73	1.44	1.34
5	Y	301	TQN	OB3-C71	3.73	1.44	1.34
5	D	301	TQN	OB3-C71	3.73	1.44	1.34
5	Q	301	TQN	OB3-C71	3.73	1.44	1.34
5	I	301	TQN	OB3-C71	3.73	1.44	1.34
5	W	301	TQN	OB3-C71	3.73	1.44	1.34
5	B	301	TQN	OB3-C71	3.73	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	301	TQN	OB3-C71	3.73	1.44	1.34
5	A	302	TQN	OB3-C71	3.72	1.44	1.34
5	N	301	TQN	OB3-C71	3.72	1.44	1.34
5	C	301	TQN	OB3-C71	3.72	1.44	1.34
5	K	301	TQN	OB3-C71	3.72	1.44	1.34
5	M	301	TQN	OB3-C71	3.72	1.44	1.34
5	S	301	TQN	OB3-C71	3.72	1.44	1.34
5	R	301	TQN	OB3-C71	3.71	1.44	1.34
5	T	301	TQN	OB3-C71	3.71	1.44	1.34
5	H	301	TQN	OB3-C71	3.71	1.44	1.34
5	U	301	TQN	OB3-C71	3.71	1.44	1.34
5	N	301	TQN	O53-C61	3.47	1.44	1.34
5	F	301	TQN	O53-C61	3.47	1.44	1.34
5	C	301	TQN	O53-C61	3.47	1.44	1.34
5	H	301	TQN	O53-C61	3.47	1.44	1.34
5	X	301	TQN	O53-C61	3.47	1.44	1.34
5	U	301	TQN	O53-C61	3.47	1.44	1.34
5	V	301	TQN	O53-C61	3.47	1.44	1.34
5	T	301	TQN	O53-C61	3.47	1.44	1.34
5	B	301	TQN	O53-C61	3.47	1.44	1.34
5	E	301	TQN	O53-C61	3.46	1.44	1.34
5	L	301	TQN	O53-C61	3.46	1.44	1.34
5	R	301	TQN	O53-C61	3.46	1.44	1.34
5	Y	301	TQN	O53-C61	3.46	1.44	1.34
5	I	301	TQN	O53-C61	3.46	1.44	1.34
5	A	302	TQN	O53-C61	3.46	1.44	1.34
5	J	301	TQN	O53-C61	3.46	1.44	1.34
5	D	301	TQN	O53-C61	3.44	1.44	1.34
5	Q	301	TQN	O53-C61	3.44	1.44	1.34
5	O	301	TQN	O53-C61	3.44	1.44	1.34
5	P	301	TQN	O53-C61	3.44	1.44	1.34
5	K	301	TQN	O53-C61	3.44	1.44	1.34
5	G	301	TQN	O53-C61	3.44	1.44	1.34
5	M	301	TQN	O53-C61	3.43	1.44	1.34
5	Z	301	TQN	O53-C61	3.43	1.44	1.34
5	S	301	TQN	O53-C61	3.43	1.44	1.34
5	W	301	TQN	O53-C61	3.43	1.44	1.34
5	V	301	TQN	CA1-CA2	-3.37	1.47	1.53
5	G	301	TQN	CA1-CA2	-3.37	1.47	1.53
5	M	301	TQN	CA1-CA2	-3.37	1.47	1.53
5	Z	301	TQN	CA1-CA2	-3.37	1.47	1.53
5	A	302	TQN	CA1-CA2	-3.37	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	301	TQN	CA1-CA2	-3.37	1.47	1.53
5	Q	301	TQN	CA1-CA2	-3.37	1.47	1.53
5	P	301	TQN	CA1-CA2	-3.37	1.47	1.53
5	K	301	TQN	CA1-CA2	-3.36	1.47	1.53
5	Y	301	TQN	CA1-CA2	-3.36	1.47	1.53
5	T	301	TQN	CA1-CA2	-3.36	1.47	1.53
5	N	301	TQN	CA1-CA2	-3.36	1.47	1.53
5	J	301	TQN	CA1-CA2	-3.35	1.47	1.53
5	W	301	TQN	CA1-CA2	-3.35	1.47	1.53
5	L	301	TQN	CA1-CA2	-3.35	1.47	1.53
5	C	301	TQN	CA1-CA2	-3.32	1.47	1.53
5	S	301	TQN	CA1-CA2	-3.31	1.47	1.53
5	B	301	TQN	CA1-CA2	-3.31	1.47	1.53
5	O	301	TQN	CA1-CA2	-3.31	1.47	1.53
5	R	301	TQN	CA1-CA2	-3.31	1.47	1.53
5	D	301	TQN	CA1-CA2	-3.31	1.47	1.53
5	E	301	TQN	C12-C11	3.30	1.59	1.51
5	X	301	TQN	CA1-CA2	-3.30	1.47	1.53
5	J	301	TQN	C12-C11	3.30	1.59	1.51
5	H	301	TQN	CA1-CA2	-3.30	1.47	1.53
5	I	301	TQN	CA1-CA2	-3.30	1.47	1.53
5	U	301	TQN	CA1-CA2	-3.30	1.47	1.53
5	F	301	TQN	CA1-CA2	-3.30	1.47	1.53
5	V	301	TQN	C12-C11	3.30	1.59	1.51
5	M	301	TQN	C12-C11	3.29	1.59	1.51
5	C	301	TQN	C12-C11	3.28	1.59	1.51
5	G	301	TQN	C12-C11	3.28	1.59	1.51
5	N	301	TQN	C12-C11	3.28	1.59	1.51
5	Z	301	TQN	C12-C11	3.28	1.59	1.51
5	A	302	TQN	C12-C11	3.28	1.59	1.51
5	Y	301	TQN	C12-C11	3.28	1.59	1.51
5	S	301	TQN	C12-C11	3.27	1.59	1.51
5	I	301	TQN	C12-C11	3.27	1.59	1.51
5	L	301	TQN	C12-C11	3.27	1.59	1.51
5	R	301	TQN	C12-C11	3.27	1.59	1.51
5	W	301	TQN	C12-C11	3.27	1.59	1.51
5	X	301	TQN	C12-C11	3.27	1.59	1.51
5	F	301	TQN	C12-C11	3.27	1.59	1.51
5	B	301	TQN	C12-C11	3.26	1.59	1.51
5	O	301	TQN	C12-C11	3.26	1.59	1.51
5	P	301	TQN	C12-C11	3.26	1.59	1.51
5	T	301	TQN	C12-C11	3.26	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	301	TQN	C12-C11	3.25	1.59	1.51
5	H	301	TQN	C12-C11	3.25	1.59	1.51
5	D	301	TQN	C12-C11	3.24	1.59	1.51
5	Q	301	TQN	C12-C11	3.24	1.59	1.51
5	K	301	TQN	C12-C11	3.24	1.59	1.51
5	S	301	TQN	O73-C73	-3.18	1.38	1.46
5	D	301	TQN	O73-C73	-3.18	1.38	1.46
5	X	301	TQN	O73-C73	-3.18	1.38	1.46
5	W	301	TQN	O73-C73	-3.18	1.38	1.46
5	M	301	TQN	O73-C73	-3.18	1.38	1.46
5	Z	301	TQN	O73-C73	-3.18	1.38	1.46
5	V	301	TQN	O73-C73	-3.18	1.38	1.46
5	C	301	TQN	O73-C73	-3.18	1.38	1.46
5	Y	301	TQN	O73-C73	-3.17	1.38	1.46
5	A	302	TQN	O73-C73	-3.17	1.38	1.46
5	B	301	TQN	O73-C73	-3.16	1.38	1.46
5	P	301	TQN	O73-C73	-3.16	1.38	1.46
5	J	301	TQN	O73-C73	-3.16	1.38	1.46
5	K	301	TQN	O73-C73	-3.16	1.38	1.46
5	I	301	TQN	O73-C73	-3.15	1.38	1.46
5	N	301	TQN	O73-C73	-3.15	1.38	1.46
5	E	301	TQN	O73-C73	-3.15	1.38	1.46
5	Q	301	TQN	O73-C73	-3.15	1.38	1.46
5	F	301	TQN	O73-C73	-3.14	1.38	1.46
5	R	301	TQN	O73-C73	-3.14	1.38	1.46
5	O	301	TQN	O73-C73	-3.14	1.38	1.46
5	G	301	TQN	O73-C73	-3.13	1.38	1.46
5	T	301	TQN	O73-C73	-3.13	1.38	1.46
5	L	301	TQN	O73-C73	-3.13	1.38	1.46
5	H	301	TQN	O73-C73	-3.12	1.38	1.46
5	U	301	TQN	O73-C73	-3.12	1.38	1.46
5	O	301	TQN	OA3-CA3	-3.09	1.40	1.44
5	A	302	TQN	OA3-CA3	-3.08	1.40	1.44
5	K	301	TQN	OA3-CA3	-3.08	1.40	1.44
5	I	301	TQN	OA3-CA3	-3.08	1.40	1.44
5	R	301	TQN	OA3-CA3	-3.07	1.40	1.44
5	G	301	TQN	OA3-CA3	-3.07	1.40	1.44
5	B	301	TQN	OA3-CA3	-3.07	1.40	1.44
5	D	301	TQN	OA3-CA3	-3.05	1.40	1.44
5	U	301	TQN	OA3-CA3	-3.03	1.40	1.44
5	L	301	TQN	OA3-CA3	-3.02	1.40	1.44
5	E	301	TQN	OA3-CA3	-3.02	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	301	TQN	OA3-CA3	-3.02	1.40	1.44
5	C	301	TQN	OA3-CA3	-3.02	1.40	1.44
5	J	301	TQN	OA3-CA3	-3.02	1.40	1.44
5	M	301	TQN	OA3-CA3	-3.02	1.40	1.44
5	W	301	TQN	OA3-CA3	-3.02	1.40	1.44
5	V	301	TQN	OA3-CA3	-3.01	1.40	1.44
5	Q	301	TQN	OA3-CA3	-3.01	1.40	1.44
5	S	301	TQN	OA3-CA3	-3.01	1.40	1.44
5	X	301	TQN	OA3-CA3	-3.01	1.40	1.44
5	Y	301	TQN	OA3-CA3	-3.00	1.40	1.44
5	Z	301	TQN	OA3-CA3	-3.00	1.40	1.44
5	T	301	TQN	OA3-CA3	-3.00	1.40	1.44
5	P	301	TQN	OA3-CA3	-3.00	1.40	1.44
5	F	301	TQN	OA3-CA3	-2.99	1.40	1.44
5	N	301	TQN	OA3-CA3	-2.99	1.40	1.44
5	N	301	TQN	O13-C21	2.86	1.42	1.34
5	C	301	TQN	O13-C21	2.86	1.42	1.34
5	K	301	TQN	O13-C21	2.86	1.42	1.34
5	D	301	TQN	O13-C21	2.85	1.42	1.34
5	Q	301	TQN	O13-C21	2.85	1.42	1.34
5	Z	301	TQN	O13-C21	2.85	1.42	1.34
5	X	301	TQN	O13-C21	2.84	1.42	1.34
5	T	301	TQN	O13-C21	2.84	1.42	1.34
5	H	301	TQN	O13-C21	2.84	1.42	1.34
5	U	301	TQN	O13-C21	2.84	1.42	1.34
5	E	301	TQN	O13-C21	2.84	1.42	1.34
5	R	301	TQN	O13-C21	2.84	1.42	1.34
5	M	301	TQN	O13-C21	2.83	1.42	1.34
5	V	301	TQN	O13-C21	2.83	1.42	1.34
5	J	301	TQN	O13-C21	2.83	1.42	1.34
5	W	301	TQN	O13-C21	2.83	1.42	1.34
5	F	301	TQN	O13-C21	2.83	1.42	1.34
5	L	301	TQN	O13-C21	2.83	1.42	1.34
5	Y	301	TQN	O13-C21	2.83	1.42	1.34
5	I	301	TQN	O13-C21	2.83	1.42	1.34
5	S	301	TQN	O13-C21	2.83	1.42	1.34
5	G	301	TQN	O13-C21	2.83	1.42	1.34
5	B	301	TQN	O13-C21	2.83	1.42	1.34
5	A	302	TQN	O13-C21	2.82	1.42	1.34
5	O	301	TQN	O13-C21	2.82	1.42	1.34
5	P	301	TQN	O13-C21	2.82	1.42	1.34
5	X	301	TQN	PB-OB4	2.81	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	301	TQN	PB-OB4	2.81	1.64	1.59
5	L	301	TQN	PB-OB4	2.81	1.64	1.59
5	Z	301	TQN	PB-OB4	2.80	1.64	1.59
5	B	301	TQN	PB-OB4	2.80	1.64	1.59
5	G	301	TQN	PB-OB4	2.80	1.64	1.59
5	V	301	TQN	PB-OB4	2.79	1.64	1.59
5	D	301	TQN	PB-OB4	2.79	1.64	1.59
5	R	301	TQN	PB-OB4	2.79	1.64	1.59
5	C	301	TQN	PB-OB4	2.79	1.64	1.59
5	P	301	TQN	PB-OB4	2.79	1.64	1.59
5	S	301	TQN	PB-OB4	2.78	1.64	1.59
5	T	301	TQN	PB-OB4	2.78	1.64	1.59
5	J	301	TQN	PB-OB4	2.78	1.64	1.59
5	W	301	TQN	PB-OB4	2.78	1.64	1.59
5	A	302	TQN	PB-OB4	2.78	1.64	1.59
5	K	301	TQN	PB-OB4	2.78	1.64	1.59
5	Y	301	TQN	PB-OB4	2.77	1.64	1.59
5	A	302	TQN	C72-C71	2.77	1.56	1.50
5	J	301	TQN	C72-C71	2.77	1.56	1.50
5	U	301	TQN	PB-OB4	2.77	1.64	1.59
5	K	301	TQN	C72-C71	2.77	1.56	1.50
5	M	301	TQN	PB-OB4	2.77	1.64	1.59
5	G	301	TQN	C72-C71	2.76	1.56	1.50
5	B	301	TQN	C72-C71	2.76	1.56	1.50
5	E	301	TQN	C72-C71	2.76	1.56	1.50
5	R	301	TQN	C72-C71	2.76	1.56	1.50
5	E	301	TQN	PB-OB4	2.76	1.64	1.59
5	Q	301	TQN	PB-OB4	2.76	1.64	1.59
5	S	301	TQN	C72-C71	2.76	1.56	1.50
5	O	301	TQN	PB-OB4	2.76	1.64	1.59
5	O	301	TQN	C72-C71	2.76	1.56	1.50
5	L	301	TQN	C72-C71	2.75	1.56	1.50
5	H	301	TQN	C72-C71	2.75	1.56	1.50
5	F	301	TQN	PB-OB4	2.75	1.64	1.59
5	X	301	TQN	C72-C71	2.75	1.56	1.50
5	M	301	TQN	O53-C53	-2.75	1.39	1.46
5	Z	301	TQN	O53-C53	-2.75	1.39	1.46
5	I	301	TQN	PB-OB4	2.75	1.64	1.59
5	N	301	TQN	PB-OB4	2.75	1.64	1.59
5	D	301	TQN	C72-C71	2.75	1.56	1.50
5	Q	301	TQN	C72-C71	2.75	1.56	1.50
5	Y	301	TQN	O53-C53	-2.75	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	301	TQN	O53-C53	-2.75	1.39	1.46
5	C	301	TQN	O53-C53	-2.74	1.39	1.46
5	P	301	TQN	O53-C53	-2.74	1.39	1.46
5	C	301	TQN	C72-C71	2.74	1.56	1.50
5	P	301	TQN	C72-C71	2.74	1.56	1.50
5	N	301	TQN	C72-C71	2.74	1.56	1.50
5	A	302	TQN	O53-C53	-2.74	1.39	1.46
5	N	301	TQN	O53-C53	-2.74	1.39	1.46
5	V	301	TQN	O53-C53	-2.74	1.39	1.46
5	H	301	TQN	O53-C53	-2.74	1.39	1.46
5	U	301	TQN	C72-C71	2.74	1.56	1.50
5	V	301	TQN	C72-C71	2.74	1.56	1.50
5	G	301	TQN	O53-C53	-2.73	1.39	1.46
5	T	301	TQN	O53-C53	-2.73	1.39	1.46
5	I	301	TQN	C72-C71	2.73	1.56	1.50
5	J	301	TQN	O53-C53	-2.73	1.39	1.46
5	D	301	TQN	O53-C53	-2.73	1.39	1.46
5	Q	301	TQN	O53-C53	-2.73	1.39	1.46
5	B	301	TQN	O53-C53	-2.73	1.39	1.46
5	O	301	TQN	O53-C53	-2.73	1.39	1.46
5	R	301	TQN	O53-C53	-2.73	1.39	1.46
4	V	302	TLW	O6-C2	-2.72	1.40	1.43
5	L	301	TQN	O53-C53	-2.72	1.39	1.46
5	Y	301	TQN	C72-C71	2.72	1.56	1.50
5	W	301	TQN	C72-C71	2.72	1.56	1.50
5	M	301	TQN	C72-C71	2.72	1.56	1.50
5	Z	301	TQN	C72-C71	2.72	1.56	1.50
5	T	301	TQN	C72-C71	2.72	1.56	1.50
5	U	301	TQN	O53-C53	-2.72	1.39	1.46
5	F	301	TQN	C72-C71	2.72	1.56	1.50
5	F	301	TQN	O53-C53	-2.72	1.39	1.46
5	X	301	TQN	O53-C53	-2.72	1.39	1.46
5	K	301	TQN	O53-C53	-2.71	1.39	1.46
5	I	301	TQN	O53-C53	-2.71	1.39	1.46
5	S	301	TQN	O53-C53	-2.71	1.39	1.46
5	W	301	TQN	O53-C53	-2.71	1.39	1.46
4	A	303	TLW	O6-C2	-2.71	1.40	1.43
4	P	302	TLW	O6-C2	-2.71	1.40	1.43
4	U	302	TLW	O6-C2	-2.70	1.40	1.43
4	Y	302	TLW	O6-C2	-2.69	1.40	1.43
4	N	302	TLW	O6-C2	-2.69	1.40	1.43
4	O	302	TLW	O6-C2	-2.68	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	TLW	O6-C2	-2.68	1.40	1.43
4	I	302	TLW	O6-C2	-2.68	1.40	1.43
4	L	302	TLW	O6-C2	-2.67	1.40	1.43
4	G	302	TLW	O6-C2	-2.67	1.40	1.43
4	D	302	TLW	O6-C2	-2.67	1.40	1.43
4	J	302	TLW	O6-C2	-2.66	1.40	1.43
4	K	302	TLW	O6-C2	-2.66	1.40	1.43
4	R	302	TLW	O6-C2	-2.65	1.40	1.43
4	C	302	TLW	O6-C2	-2.65	1.40	1.43
4	A	301	TLW	O6-C2	-2.64	1.40	1.43
4	M	302	TLW	O6-C2	-2.64	1.40	1.43
4	H	302	TLW	O6-C2	-2.64	1.40	1.43
4	T	302	TLW	O6-C2	-2.64	1.40	1.43
4	X	302	TLW	O6-C2	-2.63	1.40	1.43
4	E	302	TLW	O6-C2	-2.63	1.40	1.43
4	F	302	TLW	O6-C2	-2.63	1.40	1.43
4	S	302	TLW	O6-C2	-2.63	1.40	1.43
4	Q	302	TLW	O6-C2	-2.62	1.40	1.43
4	W	302	TLW	O6-C2	-2.62	1.40	1.43
5	D	301	TQN	PA-OA1	2.55	1.64	1.59
5	S	301	TQN	PA-OA1	2.55	1.64	1.59
5	I	301	TQN	PA-OA1	2.55	1.64	1.59
5	B	301	TQN	PA-OA1	2.53	1.64	1.59
5	R	301	TQN	PA-OA1	2.53	1.64	1.59
5	J	301	TQN	PA-OA1	2.53	1.64	1.59
5	G	301	TQN	PA-OA1	2.53	1.64	1.59
5	Q	301	TQN	PA-OA1	2.52	1.64	1.59
5	Z	301	TQN	PA-OA1	2.51	1.64	1.59
5	U	301	TQN	PA-OA1	2.51	1.64	1.59
5	T	301	TQN	PA-OA1	2.51	1.64	1.59
5	F	301	TQN	PA-OA1	2.51	1.64	1.59
5	V	301	TQN	PA-OA1	2.51	1.64	1.59
5	A	302	TQN	PA-OA1	2.51	1.64	1.59
5	P	301	TQN	PA-OA1	2.51	1.64	1.59
5	K	301	TQN	PA-OA1	2.50	1.64	1.59
5	X	301	TQN	PA-OA1	2.50	1.64	1.59
5	E	301	TQN	PA-OA1	2.50	1.64	1.59
5	I	301	TQN	CB2-NB2	2.49	1.49	1.45
5	V	301	TQN	CB2-NB2	2.49	1.49	1.45
5	W	301	TQN	PA-OA1	2.49	1.64	1.59
5	P	301	TQN	CB2-NB2	2.49	1.49	1.45
5	L	301	TQN	PA-OA1	2.49	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	301	TQN	CB2-NB2	2.49	1.49	1.45
5	W	301	TQN	CB2-NB2	2.49	1.49	1.45
5	B	301	TQN	CB2-NB2	2.48	1.49	1.45
5	A	302	TQN	CB2-NB2	2.48	1.49	1.45
5	M	301	TQN	PA-OA1	2.48	1.64	1.59
5	N	301	TQN	PA-OA1	2.48	1.64	1.59
5	Y	301	TQN	PA-OA1	2.48	1.64	1.59
5	U	301	TQN	CB2-NB2	2.48	1.49	1.45
5	H	301	TQN	PA-OA1	2.48	1.64	1.59
5	Z	301	TQN	CB2-NB2	2.47	1.49	1.45
5	C	301	TQN	PA-OA1	2.47	1.64	1.59
5	K	301	TQN	CB2-NB2	2.47	1.49	1.45
5	X	301	TQN	CB2-NB2	2.47	1.49	1.45
5	O	301	TQN	PA-OA1	2.47	1.64	1.59
5	C	301	TQN	CB2-NB2	2.46	1.49	1.45
5	J	301	TQN	CB2-NB2	2.46	1.49	1.45
5	Q	301	TQN	CB2-NB2	2.46	1.49	1.45
5	L	301	TQN	CB2-NB2	2.46	1.49	1.45
5	Y	301	TQN	CB2-NB2	2.46	1.49	1.45
5	T	301	TQN	CB2-NB2	2.45	1.49	1.45
5	M	301	TQN	CB2-NB2	2.43	1.49	1.45
5	O	301	TQN	CB2-NB2	2.43	1.49	1.45
5	S	301	TQN	CB2-NB2	2.43	1.49	1.45
5	N	301	TQN	CB2-NB2	2.43	1.49	1.45
5	G	301	TQN	CB2-NB2	2.43	1.49	1.45
5	H	301	TQN	CB2-NB2	2.42	1.49	1.45
5	C	301	TQN	O73-C81	2.42	1.41	1.34
5	F	301	TQN	O73-C81	2.42	1.41	1.34
5	P	301	TQN	O73-C81	2.42	1.41	1.34
5	G	301	TQN	O73-C81	2.42	1.41	1.34
5	T	301	TQN	O73-C81	2.42	1.41	1.34
5	Z	301	TQN	O73-C81	2.42	1.41	1.34
5	E	301	TQN	O73-C81	2.42	1.41	1.34
5	K	301	TQN	O73-C81	2.42	1.41	1.34
5	X	301	TQN	O73-C81	2.42	1.41	1.34
5	F	301	TQN	CB2-NB2	2.42	1.49	1.45
5	N	301	TQN	O73-C81	2.41	1.41	1.34
5	E	301	TQN	CB2-NB2	2.41	1.49	1.45
5	Y	301	TQN	O73-C81	2.41	1.41	1.34
5	O	301	TQN	O73-C81	2.41	1.41	1.34
5	Q	301	TQN	O73-C81	2.41	1.41	1.34
5	R	301	TQN	CB2-NB2	2.40	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	301	TQN	O73-C81	2.39	1.41	1.34
5	V	301	TQN	O73-C81	2.39	1.41	1.34
5	B	301	TQN	O73-C81	2.39	1.41	1.34
5	W	301	TQN	O73-C81	2.39	1.41	1.34
5	J	301	TQN	O73-C81	2.39	1.41	1.34
5	A	302	TQN	O73-C81	2.39	1.41	1.34
5	L	301	TQN	O73-C81	2.39	1.41	1.34
5	D	301	TQN	O73-C81	2.39	1.41	1.34
5	M	301	TQN	O73-C81	2.39	1.41	1.34
5	R	301	TQN	O73-C81	2.39	1.41	1.34
5	H	301	TQN	O73-C81	2.39	1.41	1.34
5	I	301	TQN	O73-C81	2.38	1.41	1.34
5	U	301	TQN	O73-C81	2.38	1.41	1.34
5	S	301	TQN	OA3-C31	2.35	1.40	1.34
5	T	301	TQN	OA3-C31	2.35	1.40	1.34
5	G	301	TQN	OA3-C31	2.34	1.40	1.34
5	D	301	TQN	OA3-C31	2.34	1.40	1.34
5	W	301	TQN	OA3-C31	2.34	1.40	1.34
5	K	301	TQN	OA3-C31	2.34	1.40	1.34
5	R	301	TQN	OA3-C31	2.34	1.40	1.34
5	N	301	TQN	OA3-C31	2.34	1.40	1.34
5	A	302	TQN	OA3-C31	2.34	1.40	1.34
5	M	301	TQN	OA3-C31	2.34	1.40	1.34
5	P	301	TQN	OA3-C31	2.34	1.40	1.34
5	H	301	TQN	OA3-C31	2.34	1.40	1.34
5	U	301	TQN	OA3-C31	2.34	1.40	1.34
5	Y	301	TQN	OA3-C31	2.33	1.40	1.34
5	B	301	TQN	OA3-C31	2.33	1.40	1.34
5	O	301	TQN	OA3-C31	2.33	1.40	1.34
5	F	301	TQN	OA3-C31	2.33	1.40	1.34
5	I	301	TQN	OA3-C31	2.33	1.40	1.34
5	L	301	TQN	OA3-C31	2.33	1.40	1.34
5	E	301	TQN	OA3-C31	2.32	1.40	1.34
5	Z	301	TQN	OA3-C31	2.32	1.40	1.34
5	X	301	TQN	OA3-C31	2.32	1.40	1.34
5	V	301	TQN	OA3-C31	2.31	1.40	1.34
5	J	301	TQN	OA3-C31	2.31	1.40	1.34
5	C	301	TQN	OA3-C31	2.31	1.40	1.34
5	Y	301	TQN	C52-C51	2.31	1.56	1.51
5	Q	301	TQN	OA3-C31	2.30	1.40	1.34
5	I	301	TQN	C52-C51	2.30	1.56	1.51
5	V	301	TQN	C52-C51	2.30	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	301	TQN	C52-C51	2.29	1.56	1.51
5	X	301	TQN	C52-C51	2.29	1.56	1.51
5	Q	301	TQN	C52-C51	2.29	1.56	1.51
5	E	301	TQN	C52-C51	2.29	1.56	1.51
5	S	301	TQN	C52-C51	2.29	1.56	1.51
5	G	301	TQN	C52-C51	2.29	1.56	1.51
5	T	301	TQN	C52-C51	2.29	1.56	1.51
5	B	301	TQN	C52-C51	2.29	1.56	1.51
5	C	301	TQN	C52-C51	2.29	1.56	1.51
5	M	301	TQN	C52-C51	2.29	1.56	1.51
5	P	301	TQN	C52-C51	2.29	1.56	1.51
5	Z	301	TQN	C52-C51	2.29	1.56	1.51
5	L	301	TQN	C52-C51	2.29	1.56	1.51
5	H	301	TQN	C52-C51	2.28	1.56	1.51
5	U	301	TQN	C52-C51	2.28	1.56	1.51
5	A	302	TQN	C52-C51	2.28	1.56	1.51
5	N	301	TQN	C52-C51	2.28	1.56	1.51
5	O	301	TQN	C52-C51	2.28	1.56	1.51
5	R	301	TQN	C52-C51	2.27	1.56	1.51
5	D	301	TQN	C52-C51	2.27	1.56	1.51
5	F	301	TQN	C52-C51	2.27	1.56	1.51
5	J	301	TQN	C52-C51	2.27	1.56	1.51
5	W	301	TQN	C52-C51	2.27	1.56	1.51
5	R	301	TQN	PA-OP7	-2.26	1.46	1.54
5	E	301	TQN	PA-OP7	-2.25	1.46	1.54
5	D	301	TQN	PA-OP7	-2.25	1.46	1.54
5	F	301	TQN	PA-OP7	-2.25	1.46	1.54
5	S	301	TQN	PA-OP7	-2.25	1.46	1.54
5	Y	301	TQN	PA-OP7	-2.25	1.46	1.54
5	Q	301	TQN	PA-OP7	-2.25	1.46	1.54
5	G	301	TQN	PA-OP7	-2.25	1.46	1.54
5	H	301	TQN	PA-OP7	-2.25	1.46	1.54
5	J	301	TQN	PA-OP7	-2.25	1.46	1.54
5	U	301	TQN	PA-OP7	-2.25	1.46	1.54
5	I	301	TQN	PA-OP7	-2.25	1.46	1.54
5	V	301	TQN	PA-OP7	-2.25	1.46	1.54
5	X	301	TQN	PA-OP7	-2.25	1.46	1.54
5	K	301	TQN	PA-OP7	-2.24	1.46	1.54
5	B	301	TQN	PA-OP7	-2.24	1.46	1.54
5	C	301	TQN	PA-OP7	-2.24	1.46	1.54
5	O	301	TQN	PA-OP7	-2.24	1.46	1.54
5	P	301	TQN	PA-OP7	-2.24	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Z	301	TQN	PA-OP7	-2.24	1.46	1.54
5	F	301	TQN	O51-C51	-2.24	1.18	1.23
5	G	301	TQN	O51-C51	-2.24	1.18	1.23
5	L	301	TQN	PA-OP7	-2.24	1.46	1.54
5	M	301	TQN	PA-OP7	-2.24	1.46	1.54
5	W	301	TQN	PB-OP2	-2.23	1.46	1.54
5	P	301	TQN	O51-C51	-2.23	1.18	1.23
5	A	302	TQN	PA-OP7	-2.23	1.46	1.54
5	N	301	TQN	PA-OP7	-2.23	1.46	1.54
5	W	301	TQN	PA-OP7	-2.23	1.46	1.54
5	P	301	TQN	PB-OP2	-2.23	1.46	1.54
5	O	301	TQN	O51-C51	-2.23	1.18	1.23
5	M	301	TQN	PB-OP2	-2.23	1.46	1.54
5	S	301	TQN	PB-OP2	-2.23	1.46	1.54
5	T	301	TQN	PA-OP7	-2.23	1.46	1.54
5	M	301	TQN	O51-C51	-2.22	1.18	1.23
5	I	301	TQN	PB-OP2	-2.22	1.46	1.54
5	J	301	TQN	PB-OP2	-2.22	1.46	1.54
5	J	301	TQN	O51-C51	-2.22	1.18	1.23
5	R	301	TQN	O51-C51	-2.22	1.18	1.23
5	W	301	TQN	O51-C51	-2.22	1.18	1.23
5	D	301	TQN	PB-OP2	-2.22	1.46	1.54
5	H	301	TQN	O51-C51	-2.22	1.18	1.23
5	U	301	TQN	O51-C51	-2.22	1.18	1.23
5	H	301	TQN	PB-OP2	-2.22	1.46	1.54
5	X	301	TQN	PB-OP2	-2.22	1.46	1.54
5	L	301	TQN	PB-OP2	-2.22	1.46	1.54
5	A	302	TQN	O51-C51	-2.22	1.18	1.23
5	N	301	TQN	O51-C51	-2.22	1.18	1.23
5	T	301	TQN	PB-OP2	-2.22	1.46	1.54
5	U	301	TQN	PB-OP2	-2.22	1.46	1.54
5	D	301	TQN	O51-C51	-2.22	1.18	1.23
5	Q	301	TQN	O51-C51	-2.22	1.18	1.23
5	X	301	TQN	O51-C51	-2.22	1.18	1.23
5	I	301	TQN	O51-C51	-2.22	1.18	1.23
5	V	301	TQN	O51-C51	-2.22	1.18	1.23
5	Y	301	TQN	O51-C51	-2.22	1.18	1.23
5	Z	301	TQN	O51-C51	-2.21	1.18	1.23
5	R	301	TQN	PB-OP2	-2.21	1.46	1.54
5	Z	301	TQN	PB-OP2	-2.21	1.46	1.54
5	A	302	TQN	PB-OP2	-2.21	1.46	1.54
5	Y	301	TQN	PB-OP2	-2.21	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	301	TQN	PB-OP2	-2.21	1.46	1.54
5	K	301	TQN	PB-OP2	-2.21	1.46	1.54
5	O	301	TQN	PB-OP2	-2.21	1.46	1.54
5	V	301	TQN	PB-OP2	-2.21	1.46	1.54
5	L	301	TQN	O51-C51	-2.21	1.18	1.23
5	G	301	TQN	PB-OP2	-2.20	1.46	1.54
5	E	301	TQN	PB-OP2	-2.20	1.46	1.54
5	C	301	TQN	O51-C51	-2.20	1.18	1.23
5	E	301	TQN	O51-C51	-2.20	1.18	1.23
5	K	301	TQN	O51-C51	-2.20	1.18	1.23
5	B	301	TQN	O51-C51	-2.20	1.18	1.23
5	N	301	TQN	PB-OP2	-2.20	1.46	1.54
5	Q	301	TQN	PB-OP2	-2.20	1.46	1.54
5	F	301	TQN	PB-OP2	-2.20	1.46	1.54
5	C	301	TQN	PB-OP2	-2.19	1.46	1.54
5	J	301	TQN	O11-C11	-2.19	1.18	1.23
5	T	301	TQN	O51-C51	-2.19	1.18	1.23
5	Y	301	TQN	O11-C11	-2.18	1.18	1.23
5	K	301	TQN	O11-C11	-2.18	1.18	1.23
5	F	301	TQN	O11-C11	-2.17	1.18	1.23
5	S	301	TQN	O11-C11	-2.17	1.18	1.23
5	Z	301	TQN	PB-OP3	-2.17	1.46	1.54
5	F	301	TQN	PB-OP3	-2.17	1.46	1.54
5	H	301	TQN	O11-C11	-2.16	1.18	1.23
5	U	301	TQN	O11-C11	-2.16	1.18	1.23
5	A	302	TQN	O11-C11	-2.16	1.18	1.23
5	N	301	TQN	O11-C11	-2.16	1.18	1.23
5	O	301	TQN	PB-OP3	-2.16	1.46	1.54
5	D	301	TQN	O11-C11	-2.16	1.18	1.23
5	Q	301	TQN	O11-C11	-2.16	1.18	1.23
5	G	301	TQN	O11-C11	-2.16	1.18	1.23
5	C	301	TQN	O11-C11	-2.16	1.18	1.23
5	B	301	TQN	O11-C11	-2.16	1.18	1.23
5	O	301	TQN	O11-C11	-2.16	1.18	1.23
5	T	301	TQN	O11-C11	-2.16	1.18	1.23
5	P	301	TQN	O11-C11	-2.16	1.18	1.23
5	S	301	TQN	O51-C51	-2.15	1.18	1.23
5	H	301	TQN	PB-OP3	-2.15	1.46	1.54
5	M	301	TQN	PB-OP3	-2.15	1.46	1.54
5	W	301	TQN	PB-OP3	-2.15	1.46	1.54
5	E	301	TQN	O11-C11	-2.15	1.18	1.23
5	R	301	TQN	O11-C11	-2.15	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	301	TQN	PB-OP3	-2.15	1.46	1.54
5	R	301	TQN	PB-OP3	-2.15	1.46	1.54
5	X	301	TQN	O11-C11	-2.15	1.18	1.23
5	Y	301	TQN	PB-OP3	-2.15	1.46	1.54
5	N	301	TQN	PB-OP3	-2.14	1.46	1.54
5	E	301	TQN	PB-OP3	-2.14	1.46	1.54
5	Q	301	TQN	PB-OP3	-2.14	1.46	1.54
5	A	302	TQN	PB-OP3	-2.14	1.46	1.54
5	C	301	TQN	PB-OP3	-2.14	1.46	1.54
5	P	301	TQN	PB-OP3	-2.14	1.46	1.54
5	M	301	TQN	O11-C11	-2.14	1.18	1.23
5	Z	301	TQN	O11-C11	-2.14	1.18	1.23
5	X	301	TQN	PB-OP3	-2.14	1.46	1.54
5	S	301	TQN	PB-OP3	-2.14	1.46	1.54
5	B	301	TQN	PB-OP3	-2.14	1.46	1.54
5	V	301	TQN	PB-OP3	-2.14	1.46	1.54
5	U	301	TQN	PB-OP3	-2.14	1.46	1.54
5	L	301	TQN	O11-C11	-2.13	1.18	1.23
5	I	301	TQN	PB-OP3	-2.13	1.46	1.54
5	J	301	TQN	PB-OP3	-2.13	1.46	1.54
5	T	301	TQN	PA-OP6	-2.13	1.46	1.54
5	D	301	TQN	PA-OP6	-2.13	1.46	1.54
5	L	301	TQN	PB-OP3	-2.13	1.46	1.54
5	R	301	TQN	PA-OP6	-2.13	1.46	1.54
5	G	301	TQN	PB-OP3	-2.13	1.46	1.54
5	K	301	TQN	PB-OP3	-2.13	1.46	1.54
5	X	301	TQN	PA-OP6	-2.13	1.46	1.54
5	K	301	TQN	O13-C13	-2.13	1.41	1.46
5	L	301	TQN	PA-OP6	-2.13	1.46	1.54
5	D	301	TQN	PB-OP3	-2.13	1.46	1.54
5	M	301	TQN	PA-OP6	-2.12	1.46	1.54
5	W	301	TQN	O11-C11	-2.12	1.19	1.23
5	U	301	TQN	PA-OP6	-2.12	1.46	1.54
5	A	302	TQN	PA-OP6	-2.12	1.46	1.54
5	V	301	TQN	O11-C11	-2.12	1.19	1.23
5	J	301	TQN	PA-OP6	-2.12	1.46	1.54
5	W	301	TQN	PA-OP6	-2.12	1.46	1.54
5	I	301	TQN	O11-C11	-2.12	1.19	1.23
5	S	301	TQN	PA-OP6	-2.12	1.46	1.54
5	B	301	TQN	PA-OP6	-2.12	1.46	1.54
5	O	301	TQN	PA-OP6	-2.12	1.46	1.54
5	N	301	TQN	PA-OP6	-2.12	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Z	301	TQN	PA-OP6	-2.12	1.46	1.54
5	I	301	TQN	PA-OP6	-2.11	1.46	1.54
5	G	301	TQN	PA-OP6	-2.11	1.46	1.54
5	K	301	TQN	PA-OP6	-2.11	1.46	1.54
5	C	301	TQN	PA-OP6	-2.11	1.46	1.54
5	P	301	TQN	PA-OP6	-2.11	1.46	1.54
5	Y	301	TQN	PA-OP6	-2.11	1.46	1.54
5	F	301	TQN	PA-OP6	-2.11	1.46	1.54
5	V	301	TQN	PA-OP6	-2.10	1.46	1.54
5	Q	301	TQN	PA-OP6	-2.10	1.46	1.54
5	T	301	TQN	O13-C13	-2.10	1.41	1.46
5	E	301	TQN	PA-OP6	-2.10	1.46	1.54
5	H	301	TQN	PA-OP6	-2.09	1.46	1.54
5	D	301	TQN	O13-C13	-2.09	1.41	1.46
5	N	301	TQN	O13-C13	-2.09	1.41	1.46
5	Q	301	TQN	O13-C13	-2.08	1.41	1.46
5	E	301	TQN	O13-C13	-2.08	1.41	1.46
5	J	301	TQN	O13-C13	-2.08	1.41	1.46
5	V	301	TQN	O13-C13	-2.08	1.41	1.46
5	G	301	TQN	O13-C13	-2.08	1.41	1.46
5	C	301	TQN	O13-C13	-2.08	1.41	1.46
5	M	301	TQN	O13-C13	-2.07	1.41	1.46
5	Z	301	TQN	O13-C13	-2.07	1.41	1.46
5	W	301	TQN	O13-C13	-2.07	1.41	1.46
5	B	301	TQN	O13-C13	-2.07	1.41	1.46
5	O	301	TQN	O13-C13	-2.07	1.41	1.46
5	L	301	TQN	O13-C13	-2.07	1.41	1.46
5	A	302	TQN	O13-C13	-2.07	1.41	1.46
5	H	301	TQN	O13-C13	-2.07	1.41	1.46
5	U	301	TQN	O13-C13	-2.07	1.41	1.46
5	Y	301	TQN	O13-C13	-2.07	1.41	1.46
5	F	301	TQN	O13-C13	-2.06	1.41	1.46
5	S	301	TQN	O13-C13	-2.06	1.41	1.46
5	I	301	TQN	O13-C13	-2.06	1.41	1.46
5	R	301	TQN	O13-C13	-2.06	1.41	1.46
5	P	301	TQN	O13-C13	-2.06	1.41	1.46
5	X	301	TQN	O13-C13	-2.06	1.41	1.46
5	H	301	TQN	C62-C61	2.05	1.56	1.50
5	V	301	TQN	C62-C61	2.05	1.56	1.50
4	I	302	TLW	O6-C6	-2.04	1.40	1.44
5	B	301	TQN	C62-C61	2.04	1.56	1.50
5	F	301	TQN	C62-C61	2.04	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	301	TQN	C62-C61	2.04	1.56	1.50
5	Q	301	TQN	C62-C61	2.04	1.56	1.50
5	K	301	TQN	C62-C61	2.04	1.56	1.50
5	E	301	TQN	C62-C61	2.03	1.56	1.50
5	S	301	TQN	C62-C61	2.03	1.56	1.50
5	Z	301	TQN	C62-C61	2.03	1.56	1.50
5	N	301	TQN	C62-C61	2.03	1.56	1.50
4	O	302	TLW	O6-C6	-2.03	1.40	1.44
5	C	301	TQN	C62-C61	2.03	1.56	1.50
5	P	301	TQN	C62-C61	2.03	1.56	1.50
4	F	302	TLW	O6-C6	-2.03	1.40	1.44
5	O	301	TQN	C62-C61	2.02	1.56	1.50
5	U	301	TQN	C62-C61	2.02	1.56	1.50
4	K	302	TLW	O6-C6	-2.02	1.40	1.44
4	Q	302	TLW	O6-C6	-2.02	1.40	1.44
4	U	302	TLW	O6-C6	-2.02	1.40	1.44
4	A	301	TLW	O6-C6	-2.02	1.40	1.44
5	M	301	TQN	C62-C61	2.01	1.56	1.50
5	G	301	TQN	C62-C61	2.01	1.56	1.50
5	T	301	TQN	C62-C61	2.01	1.56	1.50
5	L	301	TQN	C62-C61	2.01	1.56	1.50
5	W	301	TQN	C22-C21	2.01	1.56	1.50
5	M	301	TQN	C22-C21	2.01	1.56	1.50
5	R	301	TQN	C62-C61	2.01	1.56	1.50
4	A	303	TLW	O6-C6	-2.01	1.40	1.44
4	N	302	TLW	O6-C6	-2.01	1.40	1.44
5	X	301	TQN	C22-C21	2.01	1.56	1.50
5	L	301	TQN	C22-C21	2.01	1.56	1.50
5	G	301	TQN	C22-C21	2.01	1.56	1.50
5	W	301	TQN	C62-C61	2.01	1.56	1.50
5	X	301	TQN	C62-C61	2.01	1.56	1.50
5	J	301	TQN	C62-C61	2.01	1.56	1.50
4	T	302	TLW	O6-C6	-2.01	1.40	1.44
5	I	301	TQN	C22-C21	2.01	1.56	1.50
5	V	301	TQN	C22-C21	2.01	1.56	1.50
5	F	301	TQN	C22-C21	2.00	1.56	1.50
5	S	301	TQN	C22-C21	2.00	1.56	1.50
5	C	301	TQN	C22-C21	2.00	1.56	1.50
5	Y	301	TQN	C62-C61	2.00	1.56	1.50
4	H	302	TLW	O6-C6	-2.00	1.40	1.44
5	B	301	TQN	C22-C21	2.00	1.56	1.50
5	O	301	TQN	C22-C21	2.00	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	302	TLW	O6-C6	-2.00	1.40	1.44

All (392) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	302	TLW	O6-C2-C1	7.72	122.85	107.70
4	H	302	TLW	O6-C2-C1	7.72	122.84	107.70
4	G	302	TLW	O6-C2-C1	7.72	122.84	107.70
4	P	302	TLW	O6-C2-C1	7.71	122.83	107.70
4	A	303	TLW	O6-C2-C1	7.71	122.83	107.70
4	V	302	TLW	O6-C2-C1	7.71	122.83	107.70
4	I	302	TLW	O6-C2-C1	7.71	122.82	107.70
4	N	302	TLW	O6-C2-C1	7.71	122.82	107.70
4	U	302	TLW	O6-C2-C1	7.71	122.82	107.70
4	S	302	TLW	O6-C2-C1	7.70	122.81	107.70
4	O	302	TLW	O6-C2-C1	7.70	122.81	107.70
4	R	302	TLW	O6-C2-C1	7.70	122.81	107.70
4	T	302	TLW	O6-C2-C1	7.70	122.81	107.70
4	W	302	TLW	O6-C2-C1	7.70	122.81	107.70
4	Y	302	TLW	O6-C2-C1	7.70	122.80	107.70
4	C	302	TLW	O6-C2-C1	7.70	122.80	107.70
4	K	302	TLW	O6-C2-C1	7.70	122.80	107.70
4	A	301	TLW	O6-C2-C1	7.70	122.80	107.70
4	J	302	TLW	O6-C2-C1	7.70	122.80	107.70
4	L	302	TLW	O6-C2-C1	7.70	122.79	107.70
4	F	302	TLW	O6-C2-C1	7.69	122.78	107.70
4	Q	302	TLW	O6-C2-C1	7.68	122.77	107.70
4	D	302	TLW	O6-C2-C1	7.68	122.77	107.70
4	X	302	TLW	O6-C2-C1	7.68	122.76	107.70
4	E	302	TLW	O6-C2-C1	7.67	122.74	107.70
4	M	302	TLW	O6-C2-C1	7.67	122.74	107.70
5	V	301	TQN	OB3-C71-C72	4.73	120.15	111.46
5	S	301	TQN	OB3-C71-C72	4.73	120.15	111.46
5	B	301	TQN	OB3-C71-C72	4.72	120.14	111.46
5	W	301	TQN	OB3-C71-C72	4.72	120.14	111.46
5	X	301	TQN	OB3-C71-C72	4.72	120.13	111.46
5	R	301	TQN	OB3-C71-C72	4.72	120.13	111.46
5	Z	301	TQN	OB3-C71-C72	4.72	120.13	111.46
5	E	301	TQN	OB3-C71-C72	4.72	120.13	111.46
5	O	301	TQN	OB3-C71-C72	4.72	120.13	111.46
5	T	301	TQN	OB3-C71-C72	4.71	120.12	111.46
5	G	301	TQN	OB3-C71-C72	4.71	120.12	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	301	TQN	OB3-C71-C72	4.71	120.12	111.46
5	D	301	TQN	OB3-C71-C72	4.71	120.12	111.46
5	Q	301	TQN	OB3-C71-C72	4.71	120.12	111.46
5	M	301	TQN	OB3-C71-C72	4.71	120.12	111.46
5	N	301	TQN	OB3-C71-C72	4.71	120.12	111.46
5	C	301	TQN	OB3-C71-C72	4.71	120.11	111.46
5	Y	301	TQN	OB3-C71-C72	4.71	120.11	111.46
5	H	301	TQN	OB3-C71-C72	4.70	120.10	111.46
5	P	301	TQN	OB3-C71-C72	4.70	120.10	111.46
5	I	301	TQN	OB3-C71-C72	4.70	120.10	111.46
5	L	301	TQN	OB3-C71-C72	4.70	120.10	111.46
5	A	302	TQN	OB3-C71-C72	4.70	120.09	111.46
5	U	301	TQN	OB3-C71-C72	4.69	120.08	111.46
5	K	301	TQN	OB3-C71-C72	4.69	120.08	111.46
5	F	301	TQN	OB3-C71-C72	4.69	120.08	111.46
5	I	301	TQN	OA3-C31-C32	4.28	119.32	111.46
5	G	301	TQN	OA3-C31-C32	4.26	119.29	111.46
5	L	301	TQN	OA3-C31-C32	4.26	119.29	111.46
5	V	301	TQN	OA3-C31-C32	4.26	119.29	111.46
5	C	301	TQN	OA3-C31-C32	4.26	119.28	111.46
5	K	301	TQN	OA3-C31-C32	4.26	119.28	111.46
5	J	301	TQN	OA3-C31-C32	4.26	119.28	111.46
5	A	302	TQN	OA3-C31-C32	4.25	119.27	111.46
5	N	301	TQN	OA3-C31-C32	4.25	119.27	111.46
5	E	301	TQN	OA3-C31-C32	4.25	119.27	111.46
5	M	301	TQN	OA3-C31-C32	4.25	119.27	111.46
5	P	301	TQN	OA3-C31-C32	4.25	119.27	111.46
5	B	301	TQN	OA3-C31-C32	4.25	119.26	111.46
5	O	301	TQN	OA3-C31-C32	4.25	119.26	111.46
5	W	301	TQN	OA3-C31-C32	4.25	119.26	111.46
5	Q	301	TQN	OA3-C31-C32	4.24	119.25	111.46
5	R	301	TQN	OA3-C31-C32	4.24	119.25	111.46
5	H	301	TQN	OA3-C31-C32	4.24	119.25	111.46
5	U	301	TQN	OA3-C31-C32	4.24	119.25	111.46
5	X	301	TQN	OA3-C31-C32	4.24	119.24	111.46
5	D	301	TQN	OA3-C31-C32	4.23	119.23	111.46
5	F	301	TQN	OA3-C31-C32	4.23	119.23	111.46
5	S	301	TQN	OA3-C31-C32	4.23	119.23	111.46
5	Y	301	TQN	OA3-C31-C32	4.22	119.21	111.46
5	T	301	TQN	OA3-C31-C32	4.22	119.21	111.46
5	Z	301	TQN	OA3-C31-C32	4.21	119.20	111.46
5	P	301	TQN	O13-C21-C22	4.13	120.40	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	301	TQN	O13-C21-C22	4.13	120.40	111.50
5	Q	301	TQN	O13-C21-C22	4.13	120.40	111.50
5	D	301	TQN	O13-C21-C22	4.12	120.39	111.50
5	Z	301	TQN	O13-C21-C22	4.12	120.39	111.50
5	B	301	TQN	O13-C21-C22	4.12	120.38	111.50
5	L	301	TQN	O13-C21-C22	4.12	120.38	111.50
5	E	301	TQN	O13-C21-C22	4.12	120.38	111.50
5	Y	301	TQN	O13-C21-C22	4.12	120.37	111.50
5	R	301	TQN	O13-C21-C22	4.12	120.37	111.50
5	S	301	TQN	O13-C21-C22	4.11	120.37	111.50
5	N	301	TQN	O13-C21-C22	4.11	120.37	111.50
5	J	301	TQN	O13-C21-C22	4.11	120.36	111.50
5	T	301	TQN	O13-C21-C22	4.11	120.36	111.50
5	K	301	TQN	O13-C21-C22	4.11	120.36	111.50
5	F	301	TQN	O13-C21-C22	4.11	120.36	111.50
5	V	301	TQN	O13-C21-C22	4.11	120.35	111.50
5	O	301	TQN	O13-C21-C22	4.11	120.35	111.50
5	M	301	TQN	O13-C21-C22	4.10	120.34	111.50
5	U	301	TQN	O13-C21-C22	4.10	120.34	111.50
5	W	301	TQN	O13-C21-C22	4.10	120.34	111.50
5	A	302	TQN	O13-C21-C22	4.10	120.33	111.50
5	R	301	TQN	O53-C61-C62	4.10	120.33	111.50
5	X	301	TQN	O13-C21-C22	4.10	120.33	111.50
5	H	301	TQN	O13-C21-C22	4.09	120.32	111.50
5	W	301	TQN	O53-C61-C62	4.09	120.32	111.50
5	T	301	TQN	O53-C61-C62	4.09	120.32	111.50
5	G	301	TQN	O13-C21-C22	4.09	120.31	111.50
5	C	301	TQN	O13-C21-C22	4.09	120.31	111.50
5	L	301	TQN	O53-C61-C62	4.09	120.31	111.50
5	Y	301	TQN	O53-C61-C62	4.09	120.31	111.50
5	X	301	TQN	O53-C61-C62	4.09	120.31	111.50
5	S	301	TQN	O53-C61-C62	4.09	120.31	111.50
5	G	301	TQN	O53-C61-C62	4.08	120.30	111.50
5	A	302	TQN	O53-C61-C62	4.08	120.30	111.50
5	M	301	TQN	O53-C61-C62	4.08	120.30	111.50
5	E	301	TQN	O53-C61-C62	4.08	120.30	111.50
5	I	301	TQN	O53-C61-C62	4.08	120.30	111.50
5	C	301	TQN	O53-C61-C62	4.08	120.29	111.50
5	J	301	TQN	O53-C61-C62	4.08	120.29	111.50
5	O	301	TQN	O53-C61-C62	4.07	120.28	111.50
5	P	301	TQN	O53-C61-C62	4.07	120.28	111.50
5	Z	301	TQN	O53-C61-C62	4.07	120.27	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	301	TQN	O53-C61-C62	4.07	120.27	111.50
5	V	301	TQN	O53-C61-C62	4.07	120.27	111.50
5	F	301	TQN	O53-C61-C62	4.07	120.26	111.50
5	B	301	TQN	O53-C61-C62	4.06	120.26	111.50
5	U	301	TQN	O53-C61-C62	4.06	120.25	111.50
5	H	301	TQN	O53-C61-C62	4.06	120.24	111.50
5	D	301	TQN	O53-C61-C62	4.05	120.24	111.50
5	Q	301	TQN	O53-C61-C62	4.05	120.24	111.50
5	K	301	TQN	O53-C61-C62	4.05	120.23	111.50
5	C	301	TQN	CE1-CD9-C59	3.84	133.94	114.42
5	G	301	TQN	CE1-CD9-C59	3.84	133.94	114.42
5	A	302	TQN	CE1-CD9-C59	3.84	133.93	114.42
5	I	301	TQN	CE1-CD9-C59	3.84	133.93	114.42
5	U	301	TQN	CE1-CD9-C59	3.84	133.93	114.42
5	N	301	TQN	CE1-CD9-C59	3.84	133.92	114.42
5	O	301	TQN	CE1-CD9-C59	3.84	133.92	114.42
5	T	301	TQN	CE1-CD9-C59	3.84	133.92	114.42
5	R	301	TQN	CE1-CD9-C59	3.84	133.91	114.42
5	P	301	TQN	CE1-CD9-C59	3.84	133.91	114.42
5	S	301	TQN	CE1-CD9-C59	3.84	133.91	114.42
5	Y	301	TQN	CE1-CD9-C59	3.84	133.91	114.42
5	B	301	TQN	CE1-CD9-C59	3.84	133.90	114.42
5	E	301	TQN	CE1-CD9-C59	3.84	133.90	114.42
5	K	301	TQN	CE1-CD9-C59	3.84	133.90	114.42
5	L	301	TQN	CE1-CD9-C59	3.83	133.89	114.42
5	D	301	TQN	CE1-CD9-C59	3.83	133.89	114.42
5	H	301	TQN	CE1-CD9-C59	3.83	133.89	114.42
5	J	301	TQN	CE1-CD9-C59	3.83	133.88	114.42
5	W	301	TQN	CE1-CD9-C59	3.83	133.88	114.42
5	Q	301	TQN	CE1-CD9-C59	3.83	133.87	114.42
5	X	301	TQN	CE1-CD9-C59	3.83	133.87	114.42
5	V	301	TQN	CE1-CD9-C59	3.83	133.86	114.42
5	M	301	TQN	CE1-CD9-C59	3.83	133.86	114.42
5	Z	301	TQN	CE1-CD9-C59	3.83	133.86	114.42
5	F	301	TQN	CE1-CD9-C59	3.83	133.85	114.42
5	I	301	TQN	O73-C81-C82	3.69	119.46	111.50
5	Y	301	TQN	O73-C81-C82	3.68	119.44	111.50
5	Q	301	TQN	O73-C81-C82	3.68	119.43	111.50
5	O	301	TQN	O73-C81-C82	3.68	119.43	111.50
5	U	301	TQN	O73-C81-C82	3.68	119.43	111.50
5	V	301	TQN	O73-C81-C82	3.67	119.42	111.50
5	K	301	TQN	O73-C81-C82	3.67	119.42	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	301	TQN	O73-C81-C82	3.67	119.41	111.50
5	A	302	TQN	O73-C81-C82	3.67	119.41	111.50
5	G	301	TQN	O73-C81-C82	3.67	119.40	111.50
5	T	301	TQN	O73-C81-C82	3.67	119.40	111.50
5	Z	301	TQN	O73-C81-C82	3.67	119.40	111.50
5	E	301	TQN	O73-C81-C82	3.66	119.40	111.50
5	M	301	TQN	O73-C81-C82	3.66	119.40	111.50
5	B	301	TQN	O73-C81-C82	3.66	119.39	111.50
5	D	301	TQN	O73-C81-C82	3.66	119.39	111.50
5	L	301	TQN	O73-C81-C82	3.66	119.39	111.50
5	F	301	TQN	O73-C81-C82	3.66	119.39	111.50
5	S	301	TQN	O73-C81-C82	3.66	119.39	111.50
5	R	301	TQN	O73-C81-C82	3.66	119.38	111.50
5	X	301	TQN	O73-C81-C82	3.66	119.38	111.50
5	N	301	TQN	O73-C81-C82	3.66	119.38	111.50
5	H	301	TQN	O73-C81-C82	3.66	119.38	111.50
5	C	301	TQN	O73-C81-C82	3.65	119.38	111.50
5	P	301	TQN	O73-C81-C82	3.65	119.37	111.50
5	W	301	TQN	O73-C81-C82	3.65	119.36	111.50
5	E	301	TQN	C52-C51-NB2	3.10	120.39	116.33
5	T	301	TQN	C52-C51-NB2	3.09	120.38	116.33
5	S	301	TQN	C52-C51-NB2	3.09	120.37	116.33
5	L	301	TQN	C52-C51-NB2	3.08	120.37	116.33
5	P	301	TQN	C52-C51-NB2	3.08	120.37	116.33
5	Z	301	TQN	C52-C51-NB2	3.08	120.36	116.33
5	J	301	TQN	C52-C51-NB2	3.08	120.36	116.33
5	M	301	TQN	C52-C51-NB2	3.08	120.36	116.33
5	Q	301	TQN	C52-C51-NB2	3.08	120.36	116.33
5	G	301	TQN	C52-C51-NB2	3.07	120.36	116.33
5	K	301	TQN	C52-C51-NB2	3.07	120.36	116.33
5	W	301	TQN	C52-C51-NB2	3.07	120.36	116.33
5	N	301	TQN	C52-C51-NB2	3.07	120.35	116.33
5	H	301	TQN	C52-C51-NB2	3.07	120.35	116.33
5	B	301	TQN	C52-C51-NB2	3.06	120.34	116.33
5	X	301	TQN	C52-C51-NB2	3.06	120.34	116.33
5	C	301	TQN	C52-C51-NB2	3.06	120.34	116.33
5	F	301	TQN	C52-C51-NB2	3.06	120.34	116.33
5	D	301	TQN	C52-C51-NB2	3.06	120.34	116.33
5	R	301	TQN	C52-C51-NB2	3.06	120.34	116.33
5	O	301	TQN	C52-C51-NB2	3.06	120.33	116.33
5	I	301	TQN	C52-C51-NB2	3.05	120.33	116.33
5	V	301	TQN	C52-C51-NB2	3.05	120.33	116.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	301	TQN	C52-C51-NB2	3.05	120.33	116.33
5	A	302	TQN	C52-C51-NB2	3.05	120.32	116.33
5	U	301	TQN	C52-C51-NB2	3.04	120.31	116.33
4	X	302	TLW	O12-C1-C2	2.44	120.01	113.03
4	Q	302	TLW	O12-C1-C2	2.44	120.00	113.03
4	A	303	TLW	O12-C1-C2	2.44	119.99	113.03
4	I	302	TLW	O12-C1-C2	2.44	119.98	113.03
4	O	302	TLW	O12-C1-C2	2.43	119.98	113.03
4	B	302	TLW	O12-C1-C2	2.43	119.98	113.03
4	U	302	TLW	O12-C1-C2	2.43	119.98	113.03
4	W	302	TLW	O12-C1-C2	2.43	119.98	113.03
4	C	302	TLW	O12-C1-C2	2.43	119.98	113.03
4	N	302	TLW	O12-C1-C2	2.43	119.98	113.03
4	P	302	TLW	O12-C1-C2	2.43	119.97	113.03
4	G	302	TLW	O12-C1-C2	2.43	119.97	113.03
4	E	302	TLW	O12-C1-C2	2.43	119.97	113.03
4	F	302	TLW	O12-C1-C2	2.43	119.97	113.03
4	D	302	TLW	O12-C1-C2	2.43	119.97	113.03
4	R	302	TLW	O12-C1-C2	2.43	119.97	113.03
4	T	302	TLW	O12-C1-C2	2.43	119.97	113.03
4	A	301	TLW	O12-C1-C2	2.43	119.97	113.03
4	M	302	TLW	O12-C1-C2	2.43	119.96	113.03
4	H	302	TLW	O12-C1-C2	2.43	119.96	113.03
4	L	302	TLW	O12-C1-C2	2.42	119.95	113.03
4	J	302	TLW	O12-C1-C2	2.42	119.95	113.03
4	S	302	TLW	O12-C1-C2	2.42	119.94	113.03
4	K	302	TLW	O12-C1-C2	2.42	119.94	113.03
4	V	302	TLW	O12-C1-C2	2.42	119.93	113.03
4	Y	302	TLW	O12-C1-C2	2.42	119.93	113.03
4	S	302	TLW	O6-C6-C5	2.28	111.07	107.87
4	D	302	TLW	O6-C6-C5	2.27	111.06	107.87
4	A	301	TLW	O6-C6-C5	2.26	111.04	107.87
4	R	302	TLW	O6-C6-C5	2.26	111.04	107.87
4	L	302	TLW	O6-C6-C5	2.25	111.03	107.87
4	X	302	TLW	O6-C6-C5	2.25	111.03	107.87
4	E	302	TLW	O6-C6-C5	2.25	111.03	107.87
4	V	302	TLW	O6-C6-C5	2.25	111.03	107.87
5	E	301	TQN	O71-C71-C72	-2.25	119.76	124.73
5	S	301	TQN	O71-C71-C72	-2.25	119.77	124.73
5	T	301	TQN	O71-C71-C72	-2.24	119.77	124.73
4	K	302	TLW	O6-C6-C5	2.24	111.02	107.87
5	J	301	TQN	O71-C71-C72	-2.24	119.77	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	301	TQN	C12-C11-NA2	2.24	119.26	116.33
4	Q	302	TLW	O6-C6-C5	2.24	111.02	107.87
4	M	302	TLW	O6-C6-C5	2.24	111.02	107.87
4	J	302	TLW	O6-C6-C5	2.24	111.01	107.87
4	I	302	TLW	O6-C6-C5	2.24	111.01	107.87
5	A	302	TQN	O71-C71-C72	-2.24	119.79	124.73
5	B	301	TQN	O71-C71-C72	-2.24	119.79	124.73
5	R	301	TQN	O71-C71-C72	-2.24	119.79	124.73
4	U	302	TLW	O6-C6-C5	2.24	111.01	107.87
5	I	301	TQN	C12-C11-NA2	2.23	119.26	116.33
4	F	302	TLW	O6-C6-C5	2.23	111.01	107.87
5	D	301	TQN	O71-C71-C72	-2.23	119.79	124.73
5	H	301	TQN	C12-C11-NA2	2.23	119.25	116.33
5	Q	301	TQN	O71-C71-C72	-2.23	119.80	124.73
4	Y	302	TLW	O6-C6-C5	2.23	111.00	107.87
5	V	301	TQN	O71-C71-C72	-2.23	119.80	124.73
4	T	302	TLW	O6-C6-C5	2.23	111.00	107.87
5	O	301	TQN	O71-C71-C72	-2.23	119.80	124.73
5	G	301	TQN	O71-C71-C72	-2.23	119.81	124.73
5	Z	301	TQN	O71-C71-C72	-2.23	119.81	124.73
4	H	302	TLW	O6-C6-C5	2.23	111.00	107.87
5	W	301	TQN	C12-C11-NA2	2.23	119.24	116.33
5	W	301	TQN	O71-C71-C72	-2.22	119.81	124.73
4	O	302	TLW	O6-C6-C5	2.22	110.99	107.87
5	H	301	TQN	O71-C71-C72	-2.22	119.82	124.73
4	P	302	TLW	O6-C6-C5	2.22	110.99	107.87
5	I	301	TQN	O71-C71-C72	-2.22	119.82	124.73
5	N	301	TQN	O71-C71-C72	-2.22	119.83	124.73
5	X	301	TQN	O71-C71-C72	-2.22	119.83	124.73
5	F	301	TQN	C12-C11-NA2	2.22	119.23	116.33
5	M	301	TQN	O71-C71-C72	-2.22	119.83	124.73
5	U	301	TQN	O71-C71-C72	-2.22	119.83	124.73
5	F	301	TQN	O71-C71-C72	-2.21	119.84	124.73
5	C	301	TQN	O71-C71-C72	-2.21	119.84	124.73
5	K	301	TQN	O71-C71-C72	-2.21	119.84	124.73
5	P	301	TQN	O71-C71-C72	-2.21	119.84	124.73
4	B	302	TLW	O6-C6-C5	2.21	110.98	107.87
5	P	301	TQN	C12-C11-NA2	2.21	119.23	116.33
5	S	301	TQN	C12-C11-NA2	2.21	119.23	116.33
5	X	301	TQN	C12-C11-NA2	2.21	119.23	116.33
4	N	302	TLW	O6-C6-C5	2.21	110.98	107.87
5	C	301	TQN	C12-C11-NA2	2.21	119.22	116.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	301	TQN	C12-C11-NA2	2.21	119.22	116.33
4	A	303	TLW	O6-C6-C5	2.21	110.97	107.87
5	Q	301	TQN	C12-C11-NA2	2.21	119.22	116.33
5	Y	301	TQN	O71-C71-C72	-2.21	119.85	124.73
5	R	301	TQN	C12-C11-NA2	2.21	119.22	116.33
4	G	302	TLW	O6-C6-C5	2.21	110.97	107.87
4	W	302	TLW	O6-C6-C5	2.21	110.97	107.87
5	M	301	TQN	C12-C11-NA2	2.21	119.22	116.33
5	V	301	TQN	C12-C11-NA2	2.21	119.22	116.33
5	K	301	TQN	C12-C11-NA2	2.20	119.22	116.33
5	L	301	TQN	O71-C71-C72	-2.20	119.86	124.73
5	B	301	TQN	C12-C11-NA2	2.20	119.21	116.33
5	D	301	TQN	C12-C11-NA2	2.20	119.21	116.33
5	E	301	TQN	C12-C11-NA2	2.20	119.21	116.33
4	C	302	TLW	O6-C6-C5	2.20	110.95	107.87
5	N	301	TQN	C12-C11-NA2	2.19	119.20	116.33
5	A	302	TQN	C12-C11-NA2	2.19	119.19	116.33
5	Z	301	TQN	C12-C11-NA2	2.18	119.19	116.33
5	J	301	TQN	C12-C11-NA2	2.18	119.18	116.33
5	U	301	TQN	C12-C11-NA2	2.18	119.18	116.33
5	Y	301	TQN	C12-C11-NA2	2.18	119.18	116.33
5	T	301	TQN	C12-C11-NA2	2.17	119.18	116.33
5	G	301	TQN	C12-C11-NA2	2.17	119.17	116.33
5	R	301	TQN	O31-C31-C32	-2.16	119.96	124.73
5	N	301	TQN	O31-C31-C32	-2.15	119.97	124.73
5	B	301	TQN	O31-C31-C32	-2.15	119.97	124.73
5	O	301	TQN	O31-C31-C32	-2.15	119.97	124.73
5	U	301	TQN	O31-C31-C32	-2.15	119.98	124.73
5	K	301	TQN	O31-C31-C32	-2.15	119.98	124.73
5	M	301	TQN	O31-C31-C32	-2.15	119.98	124.73
5	D	301	TQN	O31-C31-C32	-2.15	119.98	124.73
5	I	301	TQN	O31-C31-C32	-2.15	119.99	124.73
5	L	301	TQN	O31-C31-C32	-2.15	119.99	124.73
5	Q	301	TQN	O31-C31-C32	-2.15	119.99	124.73
5	V	301	TQN	O31-C31-C32	-2.15	119.99	124.73
5	Z	301	TQN	O31-C31-C32	-2.15	119.99	124.73
5	C	301	TQN	O31-C31-C32	-2.14	120.00	124.73
5	P	301	TQN	O31-C31-C32	-2.14	120.00	124.73
5	J	301	TQN	O31-C31-C32	-2.14	120.00	124.73
5	G	301	TQN	O31-C31-C32	-2.14	120.00	124.73
5	W	301	TQN	O31-C31-C32	-2.14	120.01	124.73
5	X	301	TQN	O31-C31-C32	-2.13	120.02	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	301	TQN	O31-C31-C32	-2.13	120.02	124.73
5	H	301	TQN	O31-C31-C32	-2.13	120.02	124.73
5	E	301	TQN	O31-C31-C32	-2.13	120.02	124.73
5	Y	301	TQN	O31-C31-C32	-2.13	120.03	124.73
5	A	302	TQN	O31-C31-C32	-2.13	120.03	124.73
5	S	301	TQN	O31-C31-C32	-2.13	120.03	124.73
5	T	301	TQN	O31-C31-C32	-2.11	120.07	124.73
4	H	302	TLW	C7-C6-C5	-2.09	110.57	114.03
4	A	301	TLW	C7-C6-C5	-2.08	110.59	114.03
4	O	302	TLW	C7-C6-C5	-2.07	110.59	114.03
4	K	302	TLW	C7-C6-C5	-2.07	110.59	114.03
4	T	302	TLW	C7-C6-C5	-2.07	110.60	114.03
4	F	302	TLW	C7-C6-C5	-2.07	110.60	114.03
4	N	302	TLW	C7-C6-C5	-2.07	110.60	114.03
4	J	302	TLW	C7-C6-C5	-2.07	110.60	114.03
4	S	302	TLW	C7-C6-C5	-2.07	110.61	114.03
5	K	301	TQN	C73-C72-C71	-2.07	108.65	113.36
5	S	301	TQN	C73-C72-C71	-2.06	108.65	113.36
4	V	302	TLW	C7-C6-C5	-2.06	110.61	114.03
4	A	303	TLW	C7-C6-C5	-2.06	110.61	114.03
5	L	301	TQN	C73-C72-C71	-2.06	108.65	113.36
4	U	302	TLW	C7-C6-C5	-2.06	110.61	114.03
4	I	302	TLW	C7-C6-C5	-2.06	110.62	114.03
4	Q	302	TLW	C7-C6-C5	-2.06	110.62	114.03
5	X	301	TQN	C73-C72-C71	-2.06	108.66	113.36
5	B	301	TQN	C73-C72-C71	-2.06	108.66	113.36
5	A	302	TQN	C73-C72-C71	-2.06	108.67	113.36
5	V	301	TQN	C73-C72-C71	-2.06	108.67	113.36
4	E	302	TLW	C7-C6-C5	-2.05	110.62	114.03
5	Y	301	TQN	C73-C72-C71	-2.05	108.67	113.36
5	N	301	TQN	C73-C72-C71	-2.05	108.67	113.36
4	X	302	TLW	C7-C6-C5	-2.05	110.63	114.03
5	F	301	TQN	C73-C72-C71	-2.05	108.67	113.36
4	L	302	TLW	C7-C6-C5	-2.05	110.63	114.03
4	Y	302	TLW	C7-C6-C5	-2.05	110.63	114.03
5	D	301	TQN	C73-C72-C71	-2.05	108.68	113.36
5	O	301	TQN	C73-C72-C71	-2.05	108.68	113.36
4	D	302	TLW	C7-C6-C5	-2.05	110.63	114.03
5	E	301	TQN	C73-C72-C71	-2.05	108.69	113.36
4	G	302	TLW	C7-C6-C5	-2.05	110.63	114.03
4	P	302	TLW	C7-C6-C5	-2.05	110.63	114.03
5	J	301	TQN	C73-C72-C71	-2.05	108.69	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	301	TQN	C73-C72-C71	-2.04	108.69	113.36
5	W	301	TQN	C73-C72-C71	-2.04	108.70	113.36
4	M	302	TLW	C7-C6-C5	-2.04	110.64	114.03
4	W	302	TLW	C7-C6-C5	-2.04	110.64	114.03
5	C	301	TQN	C73-C72-C71	-2.04	108.70	113.36
5	M	301	TQN	C73-C72-C71	-2.04	108.70	113.36
5	Z	301	TQN	C73-C72-C71	-2.04	108.70	113.36
5	H	301	TQN	C73-C72-C71	-2.04	108.70	113.36
4	R	302	TLW	C7-C6-C5	-2.04	110.65	114.03
5	G	301	TQN	C73-C72-C71	-2.04	108.70	113.36
5	Q	301	TQN	C73-C72-C71	-2.04	108.70	113.36
5	P	301	TQN	C73-C72-C71	-2.04	108.70	113.36
5	U	301	TQN	C73-C72-C71	-2.04	108.71	113.36
5	I	301	TQN	C73-C72-C71	-2.04	108.71	113.36
5	T	301	TQN	C73-C72-C71	-2.03	108.72	113.36
4	C	302	TLW	C7-C6-C5	-2.03	110.66	114.03
4	B	302	TLW	C7-C6-C5	-2.03	110.66	114.03
5	G	301	TQN	CA2-NA2-C11	-2.00	119.95	122.90
5	M	301	TQN	CA2-NA2-C11	-2.00	119.95	122.90

All (26) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	301	TLW	C2
4	A	303	TLW	C2
4	B	302	TLW	C2
4	C	302	TLW	C2
4	D	302	TLW	C2
4	E	302	TLW	C2
4	F	302	TLW	C2
4	G	302	TLW	C2
4	H	302	TLW	C2
4	I	302	TLW	C2
4	J	302	TLW	C2
4	K	302	TLW	C2
4	L	302	TLW	C2
4	M	302	TLW	C2
4	N	302	TLW	C2
4	O	302	TLW	C2
4	P	302	TLW	C2
4	Q	302	TLW	C2
4	R	302	TLW	C2

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Mol	Chain	Res	Type	Atom
4	S	302	TLW	C2
4	T	302	TLW	C2
4	U	302	TLW	C2
4	V	302	TLW	C2
4	W	302	TLW	C2
4	X	302	TLW	C2
4	Y	302	TLW	C2

All (1509) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	TLW	C5-C6-C7-C8
4	A	301	TLW	C5-C6-C7-O7
4	A	301	TLW	O6-C6-C7-C8
4	A	301	TLW	O6-C6-C7-O7
4	A	303	TLW	C5-C6-C7-C8
4	A	303	TLW	C5-C6-C7-O7
4	A	303	TLW	O6-C6-C7-C8
4	A	303	TLW	O6-C6-C7-O7
4	B	302	TLW	C5-C6-C7-C8
4	B	302	TLW	C5-C6-C7-O7
4	B	302	TLW	O6-C6-C7-C8
4	B	302	TLW	O6-C6-C7-O7
4	C	302	TLW	C5-C6-C7-C8
4	C	302	TLW	C5-C6-C7-O7
4	C	302	TLW	O6-C6-C7-C8
4	C	302	TLW	O6-C6-C7-O7
4	D	302	TLW	C5-C6-C7-C8
4	D	302	TLW	C5-C6-C7-O7
4	D	302	TLW	O6-C6-C7-C8
4	D	302	TLW	O6-C6-C7-O7
4	E	302	TLW	C5-C6-C7-C8
4	E	302	TLW	C5-C6-C7-O7
4	E	302	TLW	O6-C6-C7-C8
4	E	302	TLW	O6-C6-C7-O7
4	F	302	TLW	C5-C6-C7-C8
4	F	302	TLW	C5-C6-C7-O7
4	F	302	TLW	O6-C6-C7-C8
4	F	302	TLW	O6-C6-C7-O7
4	G	302	TLW	C5-C6-C7-C8
4	G	302	TLW	C5-C6-C7-O7
4	G	302	TLW	O6-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
4	G	302	TLW	O6-C6-C7-O7
4	H	302	TLW	C5-C6-C7-C8
4	H	302	TLW	C5-C6-C7-O7
4	H	302	TLW	O6-C6-C7-C8
4	H	302	TLW	O6-C6-C7-O7
4	I	302	TLW	C5-C6-C7-C8
4	I	302	TLW	C5-C6-C7-O7
4	I	302	TLW	O6-C6-C7-C8
4	I	302	TLW	O6-C6-C7-O7
4	J	302	TLW	C5-C6-C7-C8
4	J	302	TLW	C5-C6-C7-O7
4	J	302	TLW	O6-C6-C7-C8
4	J	302	TLW	O6-C6-C7-O7
4	K	302	TLW	C5-C6-C7-C8
4	K	302	TLW	C5-C6-C7-O7
4	K	302	TLW	O6-C6-C7-C8
4	K	302	TLW	O6-C6-C7-O7
4	L	302	TLW	C5-C6-C7-C8
4	L	302	TLW	C5-C6-C7-O7
4	L	302	TLW	O6-C6-C7-C8
4	L	302	TLW	O6-C6-C7-O7
4	M	302	TLW	C5-C6-C7-C8
4	M	302	TLW	C5-C6-C7-O7
4	M	302	TLW	O6-C6-C7-C8
4	M	302	TLW	O6-C6-C7-O7
4	N	302	TLW	C5-C6-C7-C8
4	N	302	TLW	C5-C6-C7-O7
4	N	302	TLW	O6-C6-C7-C8
4	N	302	TLW	O6-C6-C7-O7
4	O	302	TLW	C5-C6-C7-C8
4	O	302	TLW	C5-C6-C7-O7
4	O	302	TLW	O6-C6-C7-C8
4	O	302	TLW	O6-C6-C7-O7
4	P	302	TLW	C5-C6-C7-C8
4	P	302	TLW	C5-C6-C7-O7
4	P	302	TLW	O6-C6-C7-C8
4	P	302	TLW	O6-C6-C7-O7
4	Q	302	TLW	C5-C6-C7-C8
4	Q	302	TLW	C5-C6-C7-O7
4	Q	302	TLW	O6-C6-C7-C8
4	Q	302	TLW	O6-C6-C7-O7
4	R	302	TLW	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
4	R	302	TLW	C5-C6-C7-O7
4	R	302	TLW	O6-C6-C7-C8
4	R	302	TLW	O6-C6-C7-O7
4	S	302	TLW	C5-C6-C7-C8
4	S	302	TLW	C5-C6-C7-O7
4	S	302	TLW	O6-C6-C7-C8
4	S	302	TLW	O6-C6-C7-O7
4	T	302	TLW	C5-C6-C7-C8
4	T	302	TLW	C5-C6-C7-O7
4	T	302	TLW	O6-C6-C7-C8
4	T	302	TLW	O6-C6-C7-O7
4	U	302	TLW	C5-C6-C7-C8
4	U	302	TLW	C5-C6-C7-O7
4	U	302	TLW	O6-C6-C7-C8
4	U	302	TLW	O6-C6-C7-O7
4	V	302	TLW	C5-C6-C7-C8
4	V	302	TLW	C5-C6-C7-O7
4	V	302	TLW	O6-C6-C7-C8
4	V	302	TLW	O6-C6-C7-O7
4	W	302	TLW	C5-C6-C7-C8
4	W	302	TLW	C5-C6-C7-O7
4	W	302	TLW	O6-C6-C7-C8
4	W	302	TLW	O6-C6-C7-O7
4	X	302	TLW	C5-C6-C7-C8
4	X	302	TLW	C5-C6-C7-O7
4	X	302	TLW	O6-C6-C7-C8
4	X	302	TLW	O6-C6-C7-O7
4	Y	302	TLW	C5-C6-C7-C8
4	Y	302	TLW	C5-C6-C7-O7
4	Y	302	TLW	O6-C6-C7-C8
4	Y	302	TLW	O6-C6-C7-O7
5	A	302	TQN	C11-C12-C13-C14
5	A	302	TQN	C11-C12-C13-O13
5	A	302	TQN	C22-C21-O13-C13
5	A	302	TQN	O21-C21-O13-C13
5	A	302	TQN	C51-C52-C53-C54
5	A	302	TQN	C51-C52-C53-O53
5	A	302	TQN	C62-C61-O53-C53
5	A	302	TQN	O61-C61-O53-C53
5	A	302	TQN	C71-C72-C73-O73
5	A	302	TQN	C72-C73-O73-C81
5	A	302	TQN	C82-C81-O73-C73

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Mol	Chain	Res	Type	Atoms
5	A	302	TQN	O81-C81-O73-C73
5	A	302	TQN	CB4-OB4-PB-OP4
5	B	301	TQN	C11-C12-C13-C14
5	B	301	TQN	C11-C12-C13-O13
5	B	301	TQN	C22-C21-O13-C13
5	B	301	TQN	O21-C21-O13-C13
5	B	301	TQN	C51-C52-C53-C54
5	B	301	TQN	C51-C52-C53-O53
5	B	301	TQN	C62-C61-O53-C53
5	B	301	TQN	O61-C61-O53-C53
5	B	301	TQN	C71-C72-C73-O73
5	B	301	TQN	C72-C73-O73-C81
5	B	301	TQN	C82-C81-O73-C73
5	B	301	TQN	O81-C81-O73-C73
5	B	301	TQN	CB4-OB4-PB-OP4
5	C	301	TQN	C11-C12-C13-C14
5	C	301	TQN	C11-C12-C13-O13
5	C	301	TQN	C22-C21-O13-C13
5	C	301	TQN	O21-C21-O13-C13
5	C	301	TQN	C51-C52-C53-C54
5	C	301	TQN	C51-C52-C53-O53
5	C	301	TQN	C62-C61-O53-C53
5	C	301	TQN	O61-C61-O53-C53
5	C	301	TQN	C71-C72-C73-O73
5	C	301	TQN	C72-C73-O73-C81
5	C	301	TQN	C82-C81-O73-C73
5	C	301	TQN	O81-C81-O73-C73
5	C	301	TQN	CB4-OB4-PB-OP4
5	D	301	TQN	C11-C12-C13-C14
5	D	301	TQN	C11-C12-C13-O13
5	D	301	TQN	C22-C21-O13-C13
5	D	301	TQN	O21-C21-O13-C13
5	D	301	TQN	C51-C52-C53-C54
5	D	301	TQN	C51-C52-C53-O53
5	D	301	TQN	C62-C61-O53-C53
5	D	301	TQN	O61-C61-O53-C53
5	D	301	TQN	C71-C72-C73-O73
5	D	301	TQN	C72-C73-O73-C81
5	D	301	TQN	C82-C81-O73-C73
5	D	301	TQN	O81-C81-O73-C73
5	D	301	TQN	CB4-OB4-PB-OP4
5	E	301	TQN	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
5	E	301	TQN	C11-C12-C13-O13
5	E	301	TQN	C22-C21-O13-C13
5	E	301	TQN	O21-C21-O13-C13
5	E	301	TQN	C51-C52-C53-C54
5	E	301	TQN	C51-C52-C53-O53
5	E	301	TQN	C62-C61-O53-C53
5	E	301	TQN	O61-C61-O53-C53
5	E	301	TQN	C71-C72-C73-O73
5	E	301	TQN	C72-C73-O73-C81
5	E	301	TQN	C82-C81-O73-C73
5	E	301	TQN	O81-C81-O73-C73
5	E	301	TQN	CB4-OB4-PB-OP4
5	F	301	TQN	C11-C12-C13-C14
5	F	301	TQN	C11-C12-C13-O13
5	F	301	TQN	C22-C21-O13-C13
5	F	301	TQN	O21-C21-O13-C13
5	F	301	TQN	C51-C52-C53-C54
5	F	301	TQN	C51-C52-C53-O53
5	F	301	TQN	C62-C61-O53-C53
5	F	301	TQN	O61-C61-O53-C53
5	F	301	TQN	C71-C72-C73-O73
5	F	301	TQN	C72-C73-O73-C81
5	F	301	TQN	C82-C81-O73-C73
5	F	301	TQN	O81-C81-O73-C73
5	F	301	TQN	CB4-OB4-PB-OP4
5	G	301	TQN	C11-C12-C13-C14
5	G	301	TQN	C11-C12-C13-O13
5	G	301	TQN	C22-C21-O13-C13
5	G	301	TQN	O21-C21-O13-C13
5	G	301	TQN	C51-C52-C53-C54
5	G	301	TQN	C51-C52-C53-O53
5	G	301	TQN	C62-C61-O53-C53
5	G	301	TQN	O61-C61-O53-C53
5	G	301	TQN	C71-C72-C73-O73
5	G	301	TQN	C72-C73-O73-C81
5	G	301	TQN	C82-C81-O73-C73
5	G	301	TQN	O81-C81-O73-C73
5	G	301	TQN	CB4-OB4-PB-OP4
5	H	301	TQN	C11-C12-C13-C14
5	H	301	TQN	C11-C12-C13-O13
5	H	301	TQN	C22-C21-O13-C13
5	H	301	TQN	O21-C21-O13-C13

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Mol	Chain	Res	Type	Atoms
5	H	301	TQN	C51-C52-C53-C54
5	H	301	TQN	C51-C52-C53-O53
5	H	301	TQN	C62-C61-O53-C53
5	H	301	TQN	O61-C61-O53-C53
5	H	301	TQN	C71-C72-C73-O73
5	H	301	TQN	C72-C73-O73-C81
5	H	301	TQN	C82-C81-O73-C73
5	H	301	TQN	O81-C81-O73-C73
5	H	301	TQN	CB4-OB4-PB-OP4
5	I	301	TQN	C11-C12-C13-C14
5	I	301	TQN	C11-C12-C13-O13
5	I	301	TQN	C22-C21-O13-C13
5	I	301	TQN	O21-C21-O13-C13
5	I	301	TQN	C51-C52-C53-C54
5	I	301	TQN	C51-C52-C53-O53
5	I	301	TQN	C62-C61-O53-C53
5	I	301	TQN	O61-C61-O53-C53
5	I	301	TQN	C71-C72-C73-O73
5	I	301	TQN	C72-C73-O73-C81
5	I	301	TQN	C82-C81-O73-C73
5	I	301	TQN	O81-C81-O73-C73
5	I	301	TQN	CB4-OB4-PB-OP4
5	J	301	TQN	C11-C12-C13-C14
5	J	301	TQN	C11-C12-C13-O13
5	J	301	TQN	C22-C21-O13-C13
5	J	301	TQN	O21-C21-O13-C13
5	J	301	TQN	C51-C52-C53-C54
5	J	301	TQN	C51-C52-C53-O53
5	J	301	TQN	C62-C61-O53-C53
5	J	301	TQN	O61-C61-O53-C53
5	J	301	TQN	C71-C72-C73-O73
5	J	301	TQN	C72-C73-O73-C81
5	J	301	TQN	C82-C81-O73-C73
5	J	301	TQN	O81-C81-O73-C73
5	J	301	TQN	CB4-OB4-PB-OP4
5	K	301	TQN	C11-C12-C13-C14
5	K	301	TQN	C11-C12-C13-O13
5	K	301	TQN	C22-C21-O13-C13
5	K	301	TQN	O21-C21-O13-C13
5	K	301	TQN	C51-C52-C53-C54
5	K	301	TQN	C51-C52-C53-O53
5	K	301	TQN	C62-C61-O53-C53

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Mol	Chain	Res	Type	Atoms
5	K	301	TQN	O61-C61-O53-C53
5	K	301	TQN	C71-C72-C73-O73
5	K	301	TQN	C72-C73-O73-C81
5	K	301	TQN	C82-C81-O73-C73
5	K	301	TQN	O81-C81-O73-C73
5	K	301	TQN	CB4-OB4-PB-OP4
5	L	301	TQN	C11-C12-C13-C14
5	L	301	TQN	C11-C12-C13-O13
5	L	301	TQN	C22-C21-O13-C13
5	L	301	TQN	O21-C21-O13-C13
5	L	301	TQN	C51-C52-C53-C54
5	L	301	TQN	C51-C52-C53-O53
5	L	301	TQN	C62-C61-O53-C53
5	L	301	TQN	O61-C61-O53-C53
5	L	301	TQN	C71-C72-C73-O73
5	L	301	TQN	C72-C73-O73-C81
5	L	301	TQN	C82-C81-O73-C73
5	L	301	TQN	O81-C81-O73-C73
5	L	301	TQN	CB4-OB4-PB-OP4
5	M	301	TQN	C11-C12-C13-C14
5	M	301	TQN	C11-C12-C13-O13
5	M	301	TQN	C22-C21-O13-C13
5	M	301	TQN	O21-C21-O13-C13
5	M	301	TQN	C51-C52-C53-C54
5	M	301	TQN	C51-C52-C53-O53
5	M	301	TQN	C62-C61-O53-C53
5	M	301	TQN	O61-C61-O53-C53
5	M	301	TQN	C71-C72-C73-O73
5	M	301	TQN	C72-C73-O73-C81
5	M	301	TQN	C82-C81-O73-C73
5	M	301	TQN	O81-C81-O73-C73
5	M	301	TQN	CB4-OB4-PB-OP4
5	N	301	TQN	C11-C12-C13-C14
5	N	301	TQN	C11-C12-C13-O13
5	N	301	TQN	C22-C21-O13-C13
5	N	301	TQN	O21-C21-O13-C13
5	N	301	TQN	C51-C52-C53-C54
5	N	301	TQN	C51-C52-C53-O53
5	N	301	TQN	C62-C61-O53-C53
5	N	301	TQN	O61-C61-O53-C53
5	N	301	TQN	C71-C72-C73-O73
5	N	301	TQN	C72-C73-O73-C81

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Mol	Chain	Res	Type	Atoms
5	N	301	TQN	C82-C81-O73-C73
5	N	301	TQN	O81-C81-O73-C73
5	N	301	TQN	CB4-OB4-PB-OP4
5	O	301	TQN	C11-C12-C13-C14
5	O	301	TQN	C11-C12-C13-O13
5	O	301	TQN	C22-C21-O13-C13
5	O	301	TQN	O21-C21-O13-C13
5	O	301	TQN	C51-C52-C53-C54
5	O	301	TQN	C51-C52-C53-O53
5	O	301	TQN	C62-C61-O53-C53
5	O	301	TQN	O61-C61-O53-C53
5	O	301	TQN	C71-C72-C73-O73
5	O	301	TQN	C72-C73-O73-C81
5	O	301	TQN	C82-C81-O73-C73
5	O	301	TQN	O81-C81-O73-C73
5	O	301	TQN	CB4-OB4-PB-OP4
5	P	301	TQN	C11-C12-C13-C14
5	P	301	TQN	C11-C12-C13-O13
5	P	301	TQN	C22-C21-O13-C13
5	P	301	TQN	O21-C21-O13-C13
5	P	301	TQN	C51-C52-C53-C54
5	P	301	TQN	C51-C52-C53-O53
5	P	301	TQN	C62-C61-O53-C53
5	P	301	TQN	O61-C61-O53-C53
5	P	301	TQN	C71-C72-C73-O73
5	P	301	TQN	C72-C73-O73-C81
5	P	301	TQN	C82-C81-O73-C73
5	P	301	TQN	O81-C81-O73-C73
5	P	301	TQN	CB4-OB4-PB-OP4
5	Q	301	TQN	C11-C12-C13-C14
5	Q	301	TQN	C11-C12-C13-O13
5	Q	301	TQN	C22-C21-O13-C13
5	Q	301	TQN	O21-C21-O13-C13
5	Q	301	TQN	C51-C52-C53-C54
5	Q	301	TQN	C51-C52-C53-O53
5	Q	301	TQN	C62-C61-O53-C53
5	Q	301	TQN	O61-C61-O53-C53
5	Q	301	TQN	C71-C72-C73-O73
5	Q	301	TQN	C72-C73-O73-C81
5	Q	301	TQN	C82-C81-O73-C73
5	Q	301	TQN	O81-C81-O73-C73
5	Q	301	TQN	CB4-OB4-PB-OP4

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Mol	Chain	Res	Type	Atoms
5	R	301	TQN	C11-C12-C13-C14
5	R	301	TQN	C11-C12-C13-O13
5	R	301	TQN	C22-C21-O13-C13
5	R	301	TQN	O21-C21-O13-C13
5	R	301	TQN	C51-C52-C53-C54
5	R	301	TQN	C51-C52-C53-O53
5	R	301	TQN	C62-C61-O53-C53
5	R	301	TQN	O61-C61-O53-C53
5	R	301	TQN	C71-C72-C73-O73
5	R	301	TQN	C72-C73-O73-C81
5	R	301	TQN	O81-C81-O73-C73
5	R	301	TQN	CB4-OB4-PB-OP4
5	S	301	TQN	C11-C12-C13-C14
5	S	301	TQN	C11-C12-C13-O13
5	S	301	TQN	C22-C21-O13-C13
5	S	301	TQN	O21-C21-O13-C13
5	S	301	TQN	C51-C52-C53-C54
5	S	301	TQN	C51-C52-C53-O53
5	S	301	TQN	C62-C61-O53-C53
5	S	301	TQN	O61-C61-O53-C53
5	S	301	TQN	C71-C72-C73-O73
5	S	301	TQN	C72-C73-O73-C81
5	S	301	TQN	C82-C81-O73-C73
5	S	301	TQN	O81-C81-O73-C73
5	S	301	TQN	CB4-OB4-PB-OP4
5	T	301	TQN	C11-C12-C13-C14
5	T	301	TQN	C11-C12-C13-O13
5	T	301	TQN	C22-C21-O13-C13
5	T	301	TQN	O21-C21-O13-C13
5	T	301	TQN	C51-C52-C53-C54
5	T	301	TQN	C51-C52-C53-O53
5	T	301	TQN	C62-C61-O53-C53
5	T	301	TQN	O61-C61-O53-C53
5	T	301	TQN	C71-C72-C73-O73
5	T	301	TQN	C72-C73-O73-C81
5	T	301	TQN	C82-C81-O73-C73
5	T	301	TQN	O81-C81-O73-C73
5	T	301	TQN	CB4-OB4-PB-OP4
5	U	301	TQN	C11-C12-C13-C14
5	U	301	TQN	C11-C12-C13-O13
5	U	301	TQN	C22-C21-O13-C13
5	U	301	TQN	O21-C21-O13-C13

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Mol	Chain	Res	Type	Atoms
5	U	301	TQN	C51-C52-C53-C54
5	U	301	TQN	C51-C52-C53-O53
5	U	301	TQN	C62-C61-O53-C53
5	U	301	TQN	O61-C61-O53-C53
5	U	301	TQN	C71-C72-C73-O73
5	U	301	TQN	C72-C73-O73-C81
5	U	301	TQN	C82-C81-O73-C73
5	U	301	TQN	O81-C81-O73-C73
5	U	301	TQN	CB4-OB4-PB-OP4
5	V	301	TQN	C11-C12-C13-C14
5	V	301	TQN	C11-C12-C13-O13
5	V	301	TQN	C22-C21-O13-C13
5	V	301	TQN	O21-C21-O13-C13
5	V	301	TQN	C51-C52-C53-C54
5	V	301	TQN	C51-C52-C53-O53
5	V	301	TQN	C62-C61-O53-C53
5	V	301	TQN	O61-C61-O53-C53
5	V	301	TQN	C71-C72-C73-O73
5	V	301	TQN	C72-C73-O73-C81
5	V	301	TQN	C82-C81-O73-C73
5	V	301	TQN	O81-C81-O73-C73
5	V	301	TQN	CB4-OB4-PB-OP4
5	W	301	TQN	C11-C12-C13-C14
5	W	301	TQN	C11-C12-C13-O13
5	W	301	TQN	C22-C21-O13-C13
5	W	301	TQN	O21-C21-O13-C13
5	W	301	TQN	C51-C52-C53-C54
5	W	301	TQN	C51-C52-C53-O53
5	W	301	TQN	C62-C61-O53-C53
5	W	301	TQN	O61-C61-O53-C53
5	W	301	TQN	C71-C72-C73-O73
5	W	301	TQN	C72-C73-O73-C81
5	W	301	TQN	C82-C81-O73-C73
5	W	301	TQN	O81-C81-O73-C73
5	W	301	TQN	CB4-OB4-PB-OP4
5	X	301	TQN	C11-C12-C13-C14
5	X	301	TQN	C11-C12-C13-O13
5	X	301	TQN	C22-C21-O13-C13
5	X	301	TQN	O21-C21-O13-C13
5	X	301	TQN	C51-C52-C53-C54
5	X	301	TQN	C51-C52-C53-O53
5	X	301	TQN	C62-C61-O53-C53

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Mol	Chain	Res	Type	Atoms
5	X	301	TQN	O61-C61-O53-C53
5	X	301	TQN	C71-C72-C73-O73
5	X	301	TQN	C72-C73-O73-C81
5	X	301	TQN	C82-C81-O73-C73
5	X	301	TQN	O81-C81-O73-C73
5	X	301	TQN	CB4-OB4-PB-OP4
5	Y	301	TQN	C11-C12-C13-C14
5	Y	301	TQN	C11-C12-C13-O13
5	Y	301	TQN	C22-C21-O13-C13
5	Y	301	TQN	O21-C21-O13-C13
5	Y	301	TQN	C51-C52-C53-C54
5	Y	301	TQN	C51-C52-C53-O53
5	Y	301	TQN	C62-C61-O53-C53
5	Y	301	TQN	O61-C61-O53-C53
5	Y	301	TQN	C71-C72-C73-O73
5	Y	301	TQN	C72-C73-O73-C81
5	Y	301	TQN	C82-C81-O73-C73
5	Y	301	TQN	O81-C81-O73-C73
5	Y	301	TQN	CB4-OB4-PB-OP4
5	Z	301	TQN	C11-C12-C13-C14
5	Z	301	TQN	C11-C12-C13-O13
5	Z	301	TQN	C22-C21-O13-C13
5	Z	301	TQN	O21-C21-O13-C13
5	Z	301	TQN	C51-C52-C53-C54
5	Z	301	TQN	C51-C52-C53-O53
5	Z	301	TQN	C62-C61-O53-C53
5	Z	301	TQN	O61-C61-O53-C53
5	Z	301	TQN	C71-C72-C73-O73
5	Z	301	TQN	C72-C73-O73-C81
5	Z	301	TQN	C82-C81-O73-C73
5	Z	301	TQN	O81-C81-O73-C73
5	Z	301	TQN	CB4-OB4-PB-OP4
5	R	301	TQN	C82-C81-O73-C73
5	A	302	TQN	C59-CD9-CE1-CE2
5	B	301	TQN	C59-CD9-CE1-CE2
5	C	301	TQN	C59-CD9-CE1-CE2
5	D	301	TQN	C59-CD9-CE1-CE2
5	E	301	TQN	C59-CD9-CE1-CE2
5	F	301	TQN	C59-CD9-CE1-CE2
5	G	301	TQN	C59-CD9-CE1-CE2
5	H	301	TQN	C59-CD9-CE1-CE2
5	I	301	TQN	C59-CD9-CE1-CE2

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Mol	Chain	Res	Type	Atoms
5	J	301	TQN	C59-CD9-CE1-CE2
5	K	301	TQN	C59-CD9-CE1-CE2
5	L	301	TQN	C59-CD9-CE1-CE2
5	M	301	TQN	C59-CD9-CE1-CE2
5	N	301	TQN	C59-CD9-CE1-CE2
5	O	301	TQN	C59-CD9-CE1-CE2
5	P	301	TQN	C59-CD9-CE1-CE2
5	Q	301	TQN	C59-CD9-CE1-CE2
5	R	301	TQN	C59-CD9-CE1-CE2
5	S	301	TQN	C59-CD9-CE1-CE2
5	T	301	TQN	C59-CD9-CE1-CE2
5	U	301	TQN	C59-CD9-CE1-CE2
5	V	301	TQN	C59-CD9-CE1-CE2
5	W	301	TQN	C59-CD9-CE1-CE2
5	X	301	TQN	C59-CD9-CE1-CE2
5	Y	301	TQN	C59-CD9-CE1-CE2
5	Z	301	TQN	C59-CD9-CE1-CE2
5	A	302	TQN	C74-C73-O73-C81
5	B	301	TQN	C74-C73-O73-C81
5	C	301	TQN	C74-C73-O73-C81
5	D	301	TQN	C74-C73-O73-C81
5	E	301	TQN	C74-C73-O73-C81
5	F	301	TQN	C74-C73-O73-C81
5	G	301	TQN	C74-C73-O73-C81
5	H	301	TQN	C74-C73-O73-C81
5	I	301	TQN	C74-C73-O73-C81
5	J	301	TQN	C74-C73-O73-C81
5	K	301	TQN	C74-C73-O73-C81
5	L	301	TQN	C74-C73-O73-C81
5	M	301	TQN	C74-C73-O73-C81
5	N	301	TQN	C74-C73-O73-C81
5	O	301	TQN	C74-C73-O73-C81
5	P	301	TQN	C74-C73-O73-C81
5	Q	301	TQN	C74-C73-O73-C81
5	R	301	TQN	C74-C73-O73-C81
5	S	301	TQN	C74-C73-O73-C81
5	T	301	TQN	C74-C73-O73-C81
5	U	301	TQN	C74-C73-O73-C81
5	V	301	TQN	C74-C73-O73-C81
5	W	301	TQN	C74-C73-O73-C81
5	X	301	TQN	C74-C73-O73-C81
5	Y	301	TQN	C74-C73-O73-C81

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Mol	Chain	Res	Type	Atoms
5	Z	301	TQN	C74-C73-O73-C81
5	A	302	TQN	C72-C71-OB3-CB3
5	B	301	TQN	C72-C71-OB3-CB3
5	C	301	TQN	C72-C71-OB3-CB3
5	D	301	TQN	C72-C71-OB3-CB3
5	E	301	TQN	C72-C71-OB3-CB3
5	F	301	TQN	C72-C71-OB3-CB3
5	G	301	TQN	C72-C71-OB3-CB3
5	H	301	TQN	C72-C71-OB3-CB3
5	I	301	TQN	C72-C71-OB3-CB3
5	J	301	TQN	C72-C71-OB3-CB3
5	K	301	TQN	C72-C71-OB3-CB3
5	L	301	TQN	C72-C71-OB3-CB3
5	M	301	TQN	C72-C71-OB3-CB3
5	N	301	TQN	C72-C71-OB3-CB3
5	O	301	TQN	C72-C71-OB3-CB3
5	P	301	TQN	C72-C71-OB3-CB3
5	Q	301	TQN	C72-C71-OB3-CB3
5	R	301	TQN	C72-C71-OB3-CB3
5	S	301	TQN	C72-C71-OB3-CB3
5	T	301	TQN	C72-C71-OB3-CB3
5	U	301	TQN	C72-C71-OB3-CB3
5	V	301	TQN	C72-C71-OB3-CB3
5	W	301	TQN	C72-C71-OB3-CB3
5	X	301	TQN	C72-C71-OB3-CB3
5	Y	301	TQN	C72-C71-OB3-CB3
5	Z	301	TQN	C72-C71-OB3-CB3
5	D	301	TQN	C85-C86-C87-C88
5	E	301	TQN	C85-C86-C87-C88
5	F	301	TQN	C85-C86-C87-C88
5	J	301	TQN	C85-C86-C87-C88
5	U	301	TQN	C85-C86-C87-C88
5	V	301	TQN	C85-C86-C87-C88
5	W	301	TQN	C85-C86-C87-C88
5	A	302	TQN	C85-C86-C87-C88
5	B	301	TQN	C85-C86-C87-C88
5	C	301	TQN	C85-C86-C87-C88
5	G	301	TQN	C85-C86-C87-C88
5	H	301	TQN	C85-C86-C87-C88
5	I	301	TQN	C85-C86-C87-C88
5	K	301	TQN	C85-C86-C87-C88
5	L	301	TQN	C85-C86-C87-C88

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Mol	Chain	Res	Type	Atoms
5	M	301	TQN	C85-C86-C87-C88
5	N	301	TQN	C85-C86-C87-C88
5	O	301	TQN	C85-C86-C87-C88
5	P	301	TQN	C85-C86-C87-C88
5	Q	301	TQN	C85-C86-C87-C88
5	R	301	TQN	C85-C86-C87-C88
5	S	301	TQN	C85-C86-C87-C88
5	T	301	TQN	C85-C86-C87-C88
5	X	301	TQN	C85-C86-C87-C88
5	Y	301	TQN	C85-C86-C87-C88
5	Z	301	TQN	C85-C86-C87-C88
5	A	302	TQN	O71-C71-OB3-CB3
5	B	301	TQN	O71-C71-OB3-CB3
5	C	301	TQN	O71-C71-OB3-CB3
5	D	301	TQN	O71-C71-OB3-CB3
5	E	301	TQN	O71-C71-OB3-CB3
5	F	301	TQN	O71-C71-OB3-CB3
5	G	301	TQN	O71-C71-OB3-CB3
5	H	301	TQN	O71-C71-OB3-CB3
5	I	301	TQN	O71-C71-OB3-CB3
5	J	301	TQN	O71-C71-OB3-CB3
5	K	301	TQN	O71-C71-OB3-CB3
5	L	301	TQN	O71-C71-OB3-CB3
5	M	301	TQN	O71-C71-OB3-CB3
5	N	301	TQN	O71-C71-OB3-CB3
5	O	301	TQN	O71-C71-OB3-CB3
5	P	301	TQN	O71-C71-OB3-CB3
5	Q	301	TQN	O71-C71-OB3-CB3
5	R	301	TQN	O71-C71-OB3-CB3
5	S	301	TQN	O71-C71-OB3-CB3
5	T	301	TQN	O71-C71-OB3-CB3
5	U	301	TQN	O71-C71-OB3-CB3
5	V	301	TQN	O71-C71-OB3-CB3
5	W	301	TQN	O71-C71-OB3-CB3
5	X	301	TQN	O71-C71-OB3-CB3
5	Y	301	TQN	O71-C71-OB3-CB3
5	Z	301	TQN	O71-C71-OB3-CB3
5	A	302	TQN	C23-C24-C25-C26
5	A	302	TQN	C24-C25-C26-C27
5	B	301	TQN	C23-C24-C25-C26
5	B	301	TQN	C24-C25-C26-C27
5	C	301	TQN	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
5	C	301	TQN	C24-C25-C26-C27
5	D	301	TQN	C23-C24-C25-C26
5	D	301	TQN	C24-C25-C26-C27
5	E	301	TQN	C23-C24-C25-C26
5	E	301	TQN	C24-C25-C26-C27
5	F	301	TQN	C23-C24-C25-C26
5	F	301	TQN	C24-C25-C26-C27
5	G	301	TQN	C23-C24-C25-C26
5	G	301	TQN	C24-C25-C26-C27
5	H	301	TQN	C24-C25-C26-C27
5	I	301	TQN	C23-C24-C25-C26
5	I	301	TQN	C24-C25-C26-C27
5	J	301	TQN	C24-C25-C26-C27
5	K	301	TQN	C24-C25-C26-C27
5	L	301	TQN	C23-C24-C25-C26
5	L	301	TQN	C24-C25-C26-C27
5	M	301	TQN	C23-C24-C25-C26
5	M	301	TQN	C24-C25-C26-C27
5	N	301	TQN	C24-C25-C26-C27
5	O	301	TQN	C24-C25-C26-C27
5	P	301	TQN	C23-C24-C25-C26
5	P	301	TQN	C24-C25-C26-C27
5	Q	301	TQN	C23-C24-C25-C26
5	Q	301	TQN	C24-C25-C26-C27
5	R	301	TQN	C24-C25-C26-C27
5	S	301	TQN	C23-C24-C25-C26
5	S	301	TQN	C24-C25-C26-C27
5	T	301	TQN	C23-C24-C25-C26
5	T	301	TQN	C24-C25-C26-C27
5	U	301	TQN	C23-C24-C25-C26
5	U	301	TQN	C24-C25-C26-C27
5	V	301	TQN	C24-C25-C26-C27
5	W	301	TQN	C23-C24-C25-C26
5	W	301	TQN	C24-C25-C26-C27
5	X	301	TQN	C23-C24-C25-C26
5	X	301	TQN	C24-C25-C26-C27
5	Y	301	TQN	C24-C25-C26-C27
5	Z	301	TQN	C23-C24-C25-C26
5	Z	301	TQN	C24-C25-C26-C27
5	H	301	TQN	C23-C24-C25-C26
5	J	301	TQN	C23-C24-C25-C26
5	K	301	TQN	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
5	N	301	TQN	C23-C24-C25-C26
5	O	301	TQN	C23-C24-C25-C26
5	R	301	TQN	C23-C24-C25-C26
5	V	301	TQN	C23-C24-C25-C26
5	Y	301	TQN	C23-C24-C25-C26
5	A	302	TQN	C68-C69-CE5-CE6
5	B	301	TQN	C68-C69-CE5-CE6
5	C	301	TQN	C68-C69-CE5-CE6
5	D	301	TQN	C68-C69-CE5-CE6
5	E	301	TQN	C68-C69-CE5-CE6
5	F	301	TQN	C68-C69-CE5-CE6
5	G	301	TQN	C68-C69-CE5-CE6
5	H	301	TQN	C68-C69-CE5-CE6
5	I	301	TQN	C68-C69-CE5-CE6
5	J	301	TQN	C68-C69-CE5-CE6
5	K	301	TQN	C68-C69-CE5-CE6
5	L	301	TQN	C68-C69-CE5-CE6
5	M	301	TQN	C68-C69-CE5-CE6
5	N	301	TQN	C68-C69-CE5-CE6
5	O	301	TQN	C68-C69-CE5-CE6
5	P	301	TQN	C68-C69-CE5-CE6
5	Q	301	TQN	C68-C69-CE5-CE6
5	R	301	TQN	C68-C69-CE5-CE6
5	S	301	TQN	C68-C69-CE5-CE6
5	T	301	TQN	C68-C69-CE5-CE6
5	U	301	TQN	C68-C69-CE5-CE6
5	V	301	TQN	C68-C69-CE5-CE6
5	W	301	TQN	C68-C69-CE5-CE6
5	X	301	TQN	C68-C69-CE5-CE6
5	Y	301	TQN	C68-C69-CE5-CE6
5	Z	301	TQN	C68-C69-CE5-CE6
5	J	301	TQN	C55-C56-C57-C58
5	M	301	TQN	C55-C56-C57-C58
5	N	301	TQN	C55-C56-C57-C58
5	S	301	TQN	C55-C56-C57-C58
5	Z	301	TQN	C55-C56-C57-C58
5	A	302	TQN	C55-C56-C57-C58
5	B	301	TQN	C55-C56-C57-C58
5	C	301	TQN	C55-C56-C57-C58
5	D	301	TQN	C55-C56-C57-C58
5	E	301	TQN	C55-C56-C57-C58
5	F	301	TQN	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
5	G	301	TQN	C55-C56-C57-C58
5	H	301	TQN	C55-C56-C57-C58
5	I	301	TQN	C55-C56-C57-C58
5	K	301	TQN	C55-C56-C57-C58
5	L	301	TQN	C55-C56-C57-C58
5	O	301	TQN	C55-C56-C57-C58
5	P	301	TQN	C55-C56-C57-C58
5	Q	301	TQN	C55-C56-C57-C58
5	R	301	TQN	C55-C56-C57-C58
5	T	301	TQN	C55-C56-C57-C58
5	U	301	TQN	C55-C56-C57-C58
5	V	301	TQN	C55-C56-C57-C58
5	W	301	TQN	C55-C56-C57-C58
5	X	301	TQN	C55-C56-C57-C58
5	Y	301	TQN	C55-C56-C57-C58
5	K	301	TQN	C37-C38-C39-CD4
5	A	302	TQN	C37-C38-C39-CD4
5	B	301	TQN	C37-C38-C39-CD4
5	C	301	TQN	C37-C38-C39-CD4
5	D	301	TQN	C37-C38-C39-CD4
5	E	301	TQN	C37-C38-C39-CD4
5	F	301	TQN	C37-C38-C39-CD4
5	G	301	TQN	C37-C38-C39-CD4
5	H	301	TQN	C37-C38-C39-CD4
5	I	301	TQN	C37-C38-C39-CD4
5	J	301	TQN	C37-C38-C39-CD4
5	L	301	TQN	C37-C38-C39-CD4
5	M	301	TQN	C37-C38-C39-CD4
5	N	301	TQN	C37-C38-C39-CD4
5	O	301	TQN	C37-C38-C39-CD4
5	P	301	TQN	C37-C38-C39-CD4
5	Q	301	TQN	C37-C38-C39-CD4
5	R	301	TQN	C37-C38-C39-CD4
5	S	301	TQN	C37-C38-C39-CD4
5	T	301	TQN	C37-C38-C39-CD4
5	U	301	TQN	C37-C38-C39-CD4
5	V	301	TQN	C37-C38-C39-CD4
5	W	301	TQN	C37-C38-C39-CD4
5	X	301	TQN	C37-C38-C39-CD4
5	Y	301	TQN	C37-C38-C39-CD4
5	Z	301	TQN	C37-C38-C39-CD4
5	A	302	TQN	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
5	B	301	TQN	C54-C55-C56-C57
5	C	301	TQN	C54-C55-C56-C57
5	D	301	TQN	C54-C55-C56-C57
5	E	301	TQN	C54-C55-C56-C57
5	F	301	TQN	C54-C55-C56-C57
5	G	301	TQN	C54-C55-C56-C57
5	H	301	TQN	C54-C55-C56-C57
5	I	301	TQN	C54-C55-C56-C57
5	J	301	TQN	C54-C55-C56-C57
5	K	301	TQN	C54-C55-C56-C57
5	L	301	TQN	C54-C55-C56-C57
5	M	301	TQN	C54-C55-C56-C57
5	N	301	TQN	C54-C55-C56-C57
5	O	301	TQN	C54-C55-C56-C57
5	P	301	TQN	C54-C55-C56-C57
5	Q	301	TQN	C54-C55-C56-C57
5	R	301	TQN	C54-C55-C56-C57
5	S	301	TQN	C54-C55-C56-C57
5	T	301	TQN	C54-C55-C56-C57
5	U	301	TQN	C54-C55-C56-C57
5	V	301	TQN	C54-C55-C56-C57
5	W	301	TQN	C54-C55-C56-C57
5	X	301	TQN	C54-C55-C56-C57
5	Z	301	TQN	C54-C55-C56-C57
5	Y	301	TQN	C54-C55-C56-C57
5	U	301	TQN	C87-C88-C89-CF4
5	A	302	TQN	C87-C88-C89-CF4
5	B	301	TQN	C87-C88-C89-CF4
5	C	301	TQN	C87-C88-C89-CF4
5	D	301	TQN	C87-C88-C89-CF4
5	E	301	TQN	C87-C88-C89-CF4
5	F	301	TQN	C87-C88-C89-CF4
5	G	301	TQN	C87-C88-C89-CF4
5	H	301	TQN	C87-C88-C89-CF4
5	I	301	TQN	C87-C88-C89-CF4
5	J	301	TQN	C87-C88-C89-CF4
5	K	301	TQN	C87-C88-C89-CF4
5	L	301	TQN	C87-C88-C89-CF4
5	M	301	TQN	C87-C88-C89-CF4
5	N	301	TQN	C87-C88-C89-CF4
5	O	301	TQN	C87-C88-C89-CF4
5	P	301	TQN	C87-C88-C89-CF4

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Mol	Chain	Res	Type	Atoms
5	Q	301	TQN	C87-C88-C89-CF4
5	R	301	TQN	C87-C88-C89-CF4
5	S	301	TQN	C87-C88-C89-CF4
5	T	301	TQN	C87-C88-C89-CF4
5	V	301	TQN	C87-C88-C89-CF4
5	W	301	TQN	C87-C88-C89-CF4
5	X	301	TQN	C87-C88-C89-CF4
5	Y	301	TQN	C87-C88-C89-CF4
5	Z	301	TQN	C87-C88-C89-CF4
5	A	302	TQN	C74-C75-C76-C77
5	B	301	TQN	C74-C75-C76-C77
5	C	301	TQN	C74-C75-C76-C77
5	D	301	TQN	C74-C75-C76-C77
5	E	301	TQN	C74-C75-C76-C77
5	F	301	TQN	C74-C75-C76-C77
5	G	301	TQN	C74-C75-C76-C77
5	H	301	TQN	C74-C75-C76-C77
5	I	301	TQN	C74-C75-C76-C77
5	J	301	TQN	C74-C75-C76-C77
5	K	301	TQN	C74-C75-C76-C77
5	L	301	TQN	C74-C75-C76-C77
5	M	301	TQN	C74-C75-C76-C77
5	N	301	TQN	C74-C75-C76-C77
5	O	301	TQN	C74-C75-C76-C77
5	P	301	TQN	C74-C75-C76-C77
5	Q	301	TQN	C74-C75-C76-C77
5	R	301	TQN	C74-C75-C76-C77
5	S	301	TQN	C74-C75-C76-C77
5	T	301	TQN	C74-C75-C76-C77
5	U	301	TQN	C74-C75-C76-C77
5	V	301	TQN	C74-C75-C76-C77
5	W	301	TQN	C74-C75-C76-C77
5	X	301	TQN	C74-C75-C76-C77
5	Y	301	TQN	C74-C75-C76-C77
5	Z	301	TQN	C74-C75-C76-C77
5	A	302	TQN	C15-C16-C17-C18
5	B	301	TQN	C15-C16-C17-C18
5	C	301	TQN	C15-C16-C17-C18
5	D	301	TQN	C15-C16-C17-C18
5	E	301	TQN	C15-C16-C17-C18
5	F	301	TQN	C15-C16-C17-C18
5	G	301	TQN	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
5	H	301	TQN	C15-C16-C17-C18
5	I	301	TQN	C15-C16-C17-C18
5	J	301	TQN	C15-C16-C17-C18
5	K	301	TQN	C15-C16-C17-C18
5	L	301	TQN	C15-C16-C17-C18
5	M	301	TQN	C15-C16-C17-C18
5	N	301	TQN	C15-C16-C17-C18
5	O	301	TQN	C15-C16-C17-C18
5	P	301	TQN	C15-C16-C17-C18
5	Q	301	TQN	C15-C16-C17-C18
5	R	301	TQN	C15-C16-C17-C18
5	S	301	TQN	C15-C16-C17-C18
5	T	301	TQN	C15-C16-C17-C18
5	U	301	TQN	C15-C16-C17-C18
5	V	301	TQN	C15-C16-C17-C18
5	W	301	TQN	C15-C16-C17-C18
5	X	301	TQN	C15-C16-C17-C18
5	Y	301	TQN	C15-C16-C17-C18
5	Z	301	TQN	C15-C16-C17-C18
5	A	302	TQN	O73-C73-C74-C75
5	B	301	TQN	O73-C73-C74-C75
5	C	301	TQN	O73-C73-C74-C75
5	D	301	TQN	O73-C73-C74-C75
5	E	301	TQN	O73-C73-C74-C75
5	F	301	TQN	O73-C73-C74-C75
5	G	301	TQN	O73-C73-C74-C75
5	H	301	TQN	O73-C73-C74-C75
5	I	301	TQN	O73-C73-C74-C75
5	J	301	TQN	O73-C73-C74-C75
5	K	301	TQN	O73-C73-C74-C75
5	L	301	TQN	O73-C73-C74-C75
5	M	301	TQN	O73-C73-C74-C75
5	N	301	TQN	O73-C73-C74-C75
5	O	301	TQN	O73-C73-C74-C75
5	P	301	TQN	O73-C73-C74-C75
5	Q	301	TQN	O73-C73-C74-C75
5	R	301	TQN	O73-C73-C74-C75
5	S	301	TQN	O73-C73-C74-C75
5	T	301	TQN	O73-C73-C74-C75
5	U	301	TQN	O73-C73-C74-C75
5	V	301	TQN	O73-C73-C74-C75
5	W	301	TQN	O73-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
5	X	301	TQN	O73-C73-C74-C75
5	Y	301	TQN	O73-C73-C74-C75
5	Z	301	TQN	O73-C73-C74-C75
5	A	302	TQN	C18-C19-CC1-CC2
5	C	301	TQN	C18-C19-CC1-CC2
5	D	301	TQN	C18-C19-CC1-CC2
5	E	301	TQN	C18-C19-CC1-CC2
5	F	301	TQN	C18-C19-CC1-CC2
5	G	301	TQN	C18-C19-CC1-CC2
5	H	301	TQN	C18-C19-CC1-CC2
5	I	301	TQN	C18-C19-CC1-CC2
5	J	301	TQN	C18-C19-CC1-CC2
5	K	301	TQN	C18-C19-CC1-CC2
5	L	301	TQN	C18-C19-CC1-CC2
5	M	301	TQN	C18-C19-CC1-CC2
5	N	301	TQN	C18-C19-CC1-CC2
5	O	301	TQN	C18-C19-CC1-CC2
5	P	301	TQN	C18-C19-CC1-CC2
5	R	301	TQN	C18-C19-CC1-CC2
5	T	301	TQN	C18-C19-CC1-CC2
5	U	301	TQN	C18-C19-CC1-CC2
5	V	301	TQN	C18-C19-CC1-CC2
5	Y	301	TQN	C18-C19-CC1-CC2
5	Z	301	TQN	C18-C19-CC1-CC2
5	B	301	TQN	C18-C19-CC1-CC2
5	Q	301	TQN	C18-C19-CC1-CC2
5	S	301	TQN	C18-C19-CC1-CC2
5	W	301	TQN	C18-C19-CC1-CC2
5	X	301	TQN	C18-C19-CC1-CC2
5	A	302	TQN	C14-C13-O13-C21
5	B	301	TQN	C14-C13-O13-C21
5	C	301	TQN	C14-C13-O13-C21
5	D	301	TQN	C14-C13-O13-C21
5	E	301	TQN	C14-C13-O13-C21
5	F	301	TQN	C14-C13-O13-C21
5	G	301	TQN	C14-C13-O13-C21
5	H	301	TQN	C14-C13-O13-C21
5	J	301	TQN	C14-C13-O13-C21
5	K	301	TQN	C14-C13-O13-C21
5	M	301	TQN	C14-C13-O13-C21
5	N	301	TQN	C14-C13-O13-C21
5	O	301	TQN	C14-C13-O13-C21

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Mol	Chain	Res	Type	Atoms
5	P	301	TQN	C14-C13-O13-C21
5	R	301	TQN	C14-C13-O13-C21
5	U	301	TQN	C14-C13-O13-C21
5	V	301	TQN	C14-C13-O13-C21
5	W	301	TQN	C14-C13-O13-C21
5	X	301	TQN	C14-C13-O13-C21
4	A	301	TLW	O11-C1-C2-O6
4	A	303	TLW	O11-C1-C2-O6
4	B	302	TLW	O11-C1-C2-O6
4	C	302	TLW	O11-C1-C2-O6
4	D	302	TLW	O11-C1-C2-O6
4	E	302	TLW	O11-C1-C2-O6
4	F	302	TLW	O11-C1-C2-O6
4	G	302	TLW	O11-C1-C2-O6
4	H	302	TLW	O11-C1-C2-O6
4	I	302	TLW	O11-C1-C2-O6
4	J	302	TLW	O11-C1-C2-O6
4	K	302	TLW	O11-C1-C2-O6
4	L	302	TLW	O11-C1-C2-O6
4	M	302	TLW	O11-C1-C2-O6
4	N	302	TLW	O11-C1-C2-O6
4	O	302	TLW	O11-C1-C2-O6
4	P	302	TLW	O11-C1-C2-O6
4	Q	302	TLW	O11-C1-C2-O6
4	R	302	TLW	O11-C1-C2-O6
4	S	302	TLW	O11-C1-C2-O6
4	T	302	TLW	O11-C1-C2-O6
4	U	302	TLW	O11-C1-C2-O6
4	V	302	TLW	O11-C1-C2-O6
4	W	302	TLW	O11-C1-C2-O6
4	X	302	TLW	O11-C1-C2-O6
4	Y	302	TLW	O11-C1-C2-O6
5	C	301	TQN	C81-C82-C83-C84
5	G	301	TQN	C81-C82-C83-C84
5	L	301	TQN	C81-C82-C83-C84
5	R	301	TQN	C81-C82-C83-C84
5	X	301	TQN	C81-C82-C83-C84
5	B	301	TQN	C81-C82-C83-C84
5	E	301	TQN	C81-C82-C83-C84
5	H	301	TQN	C81-C82-C83-C84
5	M	301	TQN	C81-C82-C83-C84
5	N	301	TQN	C81-C82-C83-C84

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Mol	Chain	Res	Type	Atoms
5	O	301	TQN	C81-C82-C83-C84
5	Q	301	TQN	C81-C82-C83-C84
5	T	301	TQN	C81-C82-C83-C84
5	U	301	TQN	C81-C82-C83-C84
5	V	301	TQN	C81-C82-C83-C84
5	W	301	TQN	C81-C82-C83-C84
5	Y	301	TQN	C81-C82-C83-C84
5	A	302	TQN	C81-C82-C83-C84
5	D	301	TQN	C81-C82-C83-C84
5	F	301	TQN	C81-C82-C83-C84
5	I	301	TQN	C81-C82-C83-C84
5	J	301	TQN	C81-C82-C83-C84
5	K	301	TQN	C81-C82-C83-C84
5	P	301	TQN	C81-C82-C83-C84
5	S	301	TQN	C81-C82-C83-C84
5	Z	301	TQN	C81-C82-C83-C84
5	B	301	TQN	C36-C37-C38-C39
5	C	301	TQN	C36-C37-C38-C39
5	E	301	TQN	C36-C37-C38-C39
5	F	301	TQN	C36-C37-C38-C39
5	G	301	TQN	C36-C37-C38-C39
5	H	301	TQN	C36-C37-C38-C39
5	I	301	TQN	C36-C37-C38-C39
5	N	301	TQN	C36-C37-C38-C39
5	O	301	TQN	C36-C37-C38-C39
5	Q	301	TQN	C36-C37-C38-C39
5	R	301	TQN	C36-C37-C38-C39
5	S	301	TQN	C36-C37-C38-C39
5	T	301	TQN	C36-C37-C38-C39
5	X	301	TQN	C36-C37-C38-C39
5	Z	301	TQN	C36-C37-C38-C39
5	A	302	TQN	C36-C37-C38-C39
5	D	301	TQN	C36-C37-C38-C39
5	J	301	TQN	C36-C37-C38-C39
5	K	301	TQN	C36-C37-C38-C39
5	L	301	TQN	C36-C37-C38-C39
5	M	301	TQN	C36-C37-C38-C39
5	P	301	TQN	C36-C37-C38-C39
5	U	301	TQN	C36-C37-C38-C39
5	V	301	TQN	C36-C37-C38-C39
5	W	301	TQN	C36-C37-C38-C39
5	Y	301	TQN	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
5	I	301	TQN	C14-C13-O13-C21
5	L	301	TQN	C14-C13-O13-C21
5	Q	301	TQN	C14-C13-O13-C21
5	S	301	TQN	C14-C13-O13-C21
5	T	301	TQN	C14-C13-O13-C21
5	Y	301	TQN	C14-C13-O13-C21
5	Z	301	TQN	C14-C13-O13-C21
5	A	302	TQN	C72-C73-C74-C75
5	B	301	TQN	C72-C73-C74-C75
5	C	301	TQN	C72-C73-C74-C75
5	D	301	TQN	C72-C73-C74-C75
5	E	301	TQN	C72-C73-C74-C75
5	F	301	TQN	C72-C73-C74-C75
5	G	301	TQN	C72-C73-C74-C75
5	H	301	TQN	C72-C73-C74-C75
5	I	301	TQN	C72-C73-C74-C75
5	J	301	TQN	C72-C73-C74-C75
5	K	301	TQN	C72-C73-C74-C75
5	L	301	TQN	C72-C73-C74-C75
5	M	301	TQN	C72-C73-C74-C75
5	N	301	TQN	C72-C73-C74-C75
5	O	301	TQN	C72-C73-C74-C75
5	P	301	TQN	C72-C73-C74-C75
5	Q	301	TQN	C72-C73-C74-C75
5	R	301	TQN	C72-C73-C74-C75
5	S	301	TQN	C72-C73-C74-C75
5	T	301	TQN	C72-C73-C74-C75
5	U	301	TQN	C72-C73-C74-C75
5	V	301	TQN	C72-C73-C74-C75
5	W	301	TQN	C72-C73-C74-C75
5	X	301	TQN	C72-C73-C74-C75
5	Y	301	TQN	C72-C73-C74-C75
5	Z	301	TQN	C72-C73-C74-C75
5	B	301	TQN	CC8-CC9-CD1-CD2
5	E	301	TQN	CC8-CC9-CD1-CD2
5	F	301	TQN	CC8-CC9-CD1-CD2
5	K	301	TQN	CC8-CC9-CD1-CD2
5	O	301	TQN	CC8-CC9-CD1-CD2
5	U	301	TQN	CC8-CC9-CD1-CD2
5	V	301	TQN	CC8-CC9-CD1-CD2
5	Y	301	TQN	CC8-CC9-CD1-CD2
5	Z	301	TQN	CC8-CC9-CD1-CD2

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Mol	Chain	Res	Type	Atoms
5	C	301	TQN	CC8-CC9-CD1-CD2
5	D	301	TQN	CC8-CC9-CD1-CD2
5	G	301	TQN	CC8-CC9-CD1-CD2
5	H	301	TQN	CC8-CC9-CD1-CD2
5	I	301	TQN	CC8-CC9-CD1-CD2
5	J	301	TQN	CC8-CC9-CD1-CD2
5	L	301	TQN	CC8-CC9-CD1-CD2
5	M	301	TQN	CC8-CC9-CD1-CD2
5	N	301	TQN	CC8-CC9-CD1-CD2
5	P	301	TQN	CC8-CC9-CD1-CD2
5	Q	301	TQN	CC8-CC9-CD1-CD2
5	S	301	TQN	CC8-CC9-CD1-CD2
5	T	301	TQN	CC8-CC9-CD1-CD2
5	W	301	TQN	CC8-CC9-CD1-CD2
5	X	301	TQN	CC8-CC9-CD1-CD2
5	A	302	TQN	CC8-CC9-CD1-CD2
5	R	301	TQN	CC8-CC9-CD1-CD2
5	A	302	TQN	CE8-CE9-CF1-CF2
5	B	301	TQN	CE8-CE9-CF1-CF2
5	D	301	TQN	CE8-CE9-CF1-CF2
5	E	301	TQN	CE8-CE9-CF1-CF2
5	F	301	TQN	CE8-CE9-CF1-CF2
5	J	301	TQN	CE8-CE9-CF1-CF2
5	O	301	TQN	CE8-CE9-CF1-CF2
5	T	301	TQN	CE8-CE9-CF1-CF2
5	U	301	TQN	CE8-CE9-CF1-CF2
5	V	301	TQN	CE8-CE9-CF1-CF2
5	C	301	TQN	CE8-CE9-CF1-CF2
5	G	301	TQN	CE8-CE9-CF1-CF2
5	I	301	TQN	CE8-CE9-CF1-CF2
5	K	301	TQN	CE8-CE9-CF1-CF2
5	L	301	TQN	CE8-CE9-CF1-CF2
5	M	301	TQN	CE8-CE9-CF1-CF2
5	N	301	TQN	CE8-CE9-CF1-CF2
5	P	301	TQN	CE8-CE9-CF1-CF2
5	Q	301	TQN	CE8-CE9-CF1-CF2
5	R	301	TQN	CE8-CE9-CF1-CF2
5	S	301	TQN	CE8-CE9-CF1-CF2
5	W	301	TQN	CE8-CE9-CF1-CF2
5	X	301	TQN	CE8-CE9-CF1-CF2
5	Y	301	TQN	CE8-CE9-CF1-CF2
5	Z	301	TQN	CE8-CE9-CF1-CF2

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Mol	Chain	Res	Type	Atoms
5	H	301	TQN	CE8-CE9-CF1-CF2
5	A	302	TQN	C71-C72-C73-C74
5	B	301	TQN	C71-C72-C73-C74
5	C	301	TQN	C71-C72-C73-C74
5	D	301	TQN	C71-C72-C73-C74
5	E	301	TQN	C71-C72-C73-C74
5	F	301	TQN	C71-C72-C73-C74
5	G	301	TQN	C71-C72-C73-C74
5	H	301	TQN	C71-C72-C73-C74
5	I	301	TQN	C71-C72-C73-C74
5	J	301	TQN	C71-C72-C73-C74
5	K	301	TQN	C71-C72-C73-C74
5	L	301	TQN	C71-C72-C73-C74
5	M	301	TQN	C71-C72-C73-C74
5	N	301	TQN	C71-C72-C73-C74
5	O	301	TQN	C71-C72-C73-C74
5	P	301	TQN	C71-C72-C73-C74
5	Q	301	TQN	C71-C72-C73-C74
5	R	301	TQN	C71-C72-C73-C74
5	S	301	TQN	C71-C72-C73-C74
5	T	301	TQN	C71-C72-C73-C74
5	U	301	TQN	C71-C72-C73-C74
5	V	301	TQN	C71-C72-C73-C74
5	W	301	TQN	C71-C72-C73-C74
5	X	301	TQN	C71-C72-C73-C74
5	Y	301	TQN	C71-C72-C73-C74
5	Z	301	TQN	C71-C72-C73-C74
5	B	301	TQN	C16-C17-C18-C19
5	D	301	TQN	C16-C17-C18-C19
5	G	301	TQN	C16-C17-C18-C19
5	H	301	TQN	C16-C17-C18-C19
5	I	301	TQN	C16-C17-C18-C19
5	J	301	TQN	C16-C17-C18-C19
5	K	301	TQN	C16-C17-C18-C19
5	L	301	TQN	C16-C17-C18-C19
5	O	301	TQN	C16-C17-C18-C19
5	P	301	TQN	C16-C17-C18-C19
5	Q	301	TQN	C16-C17-C18-C19
5	R	301	TQN	C16-C17-C18-C19
5	S	301	TQN	C16-C17-C18-C19
5	V	301	TQN	C16-C17-C18-C19
5	X	301	TQN	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
5	A	302	TQN	C16-C17-C18-C19
5	C	301	TQN	C16-C17-C18-C19
5	E	301	TQN	C16-C17-C18-C19
5	F	301	TQN	C16-C17-C18-C19
5	M	301	TQN	C16-C17-C18-C19
5	N	301	TQN	C16-C17-C18-C19
5	T	301	TQN	C16-C17-C18-C19
5	U	301	TQN	C16-C17-C18-C19
5	W	301	TQN	C16-C17-C18-C19
5	Y	301	TQN	C16-C17-C18-C19
5	Z	301	TQN	C16-C17-C18-C19
5	Z	301	TQN	C19-CC1-CC2-CC3
5	A	302	TQN	C19-CC1-CC2-CC3
5	B	301	TQN	C19-CC1-CC2-CC3
5	I	301	TQN	C19-CC1-CC2-CC3
5	Q	301	TQN	C19-CC1-CC2-CC3
5	R	301	TQN	C19-CC1-CC2-CC3
5	S	301	TQN	C19-CC1-CC2-CC3
5	T	301	TQN	C19-CC1-CC2-CC3
5	W	301	TQN	C19-CC1-CC2-CC3
5	X	301	TQN	C19-CC1-CC2-CC3
5	C	301	TQN	C19-CC1-CC2-CC3
5	D	301	TQN	C19-CC1-CC2-CC3
5	E	301	TQN	C19-CC1-CC2-CC3
5	F	301	TQN	C19-CC1-CC2-CC3
5	H	301	TQN	C19-CC1-CC2-CC3
5	J	301	TQN	C19-CC1-CC2-CC3
5	K	301	TQN	C19-CC1-CC2-CC3
5	L	301	TQN	C19-CC1-CC2-CC3
5	M	301	TQN	C19-CC1-CC2-CC3
5	N	301	TQN	C19-CC1-CC2-CC3
5	O	301	TQN	C19-CC1-CC2-CC3
5	U	301	TQN	C19-CC1-CC2-CC3
5	Y	301	TQN	C19-CC1-CC2-CC3
5	A	302	TQN	CF4-CF5-CF6-CF7
5	B	301	TQN	CF4-CF5-CF6-CF7
5	C	301	TQN	CF4-CF5-CF6-CF7
5	D	301	TQN	CF4-CF5-CF6-CF7
5	G	301	TQN	C19-CC1-CC2-CC3
5	I	301	TQN	CF4-CF5-CF6-CF7
5	J	301	TQN	CF4-CF5-CF6-CF7
5	K	301	TQN	CF4-CF5-CF6-CF7

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Mol	Chain	Res	Type	Atoms
5	L	301	TQN	CF4-CF5-CF6-CF7
5	N	301	TQN	CF4-CF5-CF6-CF7
5	O	301	TQN	CF4-CF5-CF6-CF7
5	P	301	TQN	C19-CC1-CC2-CC3
5	P	301	TQN	CF4-CF5-CF6-CF7
5	Q	301	TQN	CF4-CF5-CF6-CF7
5	T	301	TQN	CF4-CF5-CF6-CF7
5	V	301	TQN	C19-CC1-CC2-CC3
5	X	301	TQN	CF4-CF5-CF6-CF7
5	Y	301	TQN	CF4-CF5-CF6-CF7
5	Z	301	TQN	CF4-CF5-CF6-CF7
5	E	301	TQN	CF4-CF5-CF6-CF7
5	F	301	TQN	CF4-CF5-CF6-CF7
5	G	301	TQN	CF4-CF5-CF6-CF7
5	H	301	TQN	CF4-CF5-CF6-CF7
5	M	301	TQN	CF4-CF5-CF6-CF7
5	R	301	TQN	CF4-CF5-CF6-CF7
5	S	301	TQN	CF4-CF5-CF6-CF7
5	U	301	TQN	CF4-CF5-CF6-CF7
5	V	301	TQN	CF4-CF5-CF6-CF7
5	W	301	TQN	CF4-CF5-CF6-CF7
5	K	301	TQN	C75-C76-C77-C78
5	O	301	TQN	C75-C76-C77-C78
5	Q	301	TQN	C75-C76-C77-C78
5	B	301	TQN	C75-C76-C77-C78
5	C	301	TQN	C75-C76-C77-C78
5	G	301	TQN	C75-C76-C77-C78
5	I	301	TQN	C75-C76-C77-C78
5	J	301	TQN	C75-C76-C77-C78
5	M	301	TQN	C75-C76-C77-C78
5	P	301	TQN	C75-C76-C77-C78
5	R	301	TQN	C75-C76-C77-C78
5	S	301	TQN	C75-C76-C77-C78
5	V	301	TQN	C75-C76-C77-C78
5	X	301	TQN	C75-C76-C77-C78
5	D	301	TQN	C75-C76-C77-C78
5	E	301	TQN	C75-C76-C77-C78
5	F	301	TQN	C75-C76-C77-C78
5	H	301	TQN	C75-C76-C77-C78
5	L	301	TQN	C75-C76-C77-C78
5	T	301	TQN	C75-C76-C77-C78
5	W	301	TQN	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
5	Y	301	TQN	C75-C76-C77-C78
5	Z	301	TQN	C75-C76-C77-C78
5	A	302	TQN	C75-C76-C77-C78
5	N	301	TQN	C75-C76-C77-C78
5	U	301	TQN	C75-C76-C77-C78
5	B	301	TQN	CC6-CC7-CC8-CC9
5	D	301	TQN	C35-C36-C37-C38
5	J	301	TQN	C35-C36-C37-C38
5	L	301	TQN	C35-C36-C37-C38
5	M	301	TQN	C35-C36-C37-C38
5	N	301	TQN	C35-C36-C37-C38
5	O	301	TQN	C35-C36-C37-C38
5	S	301	TQN	C35-C36-C37-C38
5	U	301	TQN	CC6-CC7-CC8-CC9
5	V	301	TQN	C35-C36-C37-C38
5	X	301	TQN	C35-C36-C37-C38
5	A	302	TQN	C35-C36-C37-C38
5	B	301	TQN	C35-C36-C37-C38
5	C	301	TQN	C35-C36-C37-C38
5	E	301	TQN	C35-C36-C37-C38
5	E	301	TQN	CC6-CC7-CC8-CC9
5	F	301	TQN	C35-C36-C37-C38
5	F	301	TQN	CC6-CC7-CC8-CC9
5	G	301	TQN	C35-C36-C37-C38
5	G	301	TQN	CC6-CC7-CC8-CC9
5	H	301	TQN	C35-C36-C37-C38
5	H	301	TQN	CC6-CC7-CC8-CC9
5	K	301	TQN	C35-C36-C37-C38
5	L	301	TQN	CC6-CC7-CC8-CC9
5	P	301	TQN	C35-C36-C37-C38
5	Q	301	TQN	C35-C36-C37-C38
5	R	301	TQN	CC6-CC7-CC8-CC9
5	T	301	TQN	C35-C36-C37-C38
5	U	301	TQN	C35-C36-C37-C38
5	V	301	TQN	CC6-CC7-CC8-CC9
5	W	301	TQN	C35-C36-C37-C38
5	Z	301	TQN	C35-C36-C37-C38
5	Z	301	TQN	CC6-CC7-CC8-CC9
5	D	301	TQN	CC6-CC7-CC8-CC9
5	I	301	TQN	C35-C36-C37-C38
5	I	301	TQN	CC6-CC7-CC8-CC9
5	J	301	TQN	CC6-CC7-CC8-CC9

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Mol	Chain	Res	Type	Atoms
5	K	301	TQN	CC6-CC7-CC8-CC9
5	M	301	TQN	CC6-CC7-CC8-CC9
5	N	301	TQN	CC6-CC7-CC8-CC9
5	O	301	TQN	CC6-CC7-CC8-CC9
5	P	301	TQN	CC6-CC7-CC8-CC9
5	Q	301	TQN	CC6-CC7-CC8-CC9
5	R	301	TQN	C35-C36-C37-C38
5	S	301	TQN	CC6-CC7-CC8-CC9
5	T	301	TQN	CC6-CC7-CC8-CC9
5	W	301	TQN	CC6-CC7-CC8-CC9
5	X	301	TQN	CC6-CC7-CC8-CC9
5	Y	301	TQN	C35-C36-C37-C38
5	Y	301	TQN	CC6-CC7-CC8-CC9
5	A	302	TQN	CC6-CC7-CC8-CC9
5	C	301	TQN	CC6-CC7-CC8-CC9
5	B	301	TQN	C28-C29-CC6-CC7
5	R	301	TQN	C28-C29-CC6-CC7
5	A	302	TQN	C28-C29-CC6-CC7
5	E	301	TQN	C28-C29-CC6-CC7
5	F	301	TQN	C28-C29-CC6-CC7
5	G	301	TQN	C28-C29-CC6-CC7
5	H	301	TQN	C28-C29-CC6-CC7
5	J	301	TQN	C28-C29-CC6-CC7
5	K	301	TQN	C28-C29-CC6-CC7
5	L	301	TQN	C28-C29-CC6-CC7
5	M	301	TQN	C28-C29-CC6-CC7
5	N	301	TQN	C28-C29-CC6-CC7
5	O	301	TQN	C28-C29-CC6-CC7
5	P	301	TQN	C28-C29-CC6-CC7
5	Q	301	TQN	C28-C29-CC6-CC7
5	T	301	TQN	C28-C29-CC6-CC7
5	U	301	TQN	C28-C29-CC6-CC7
5	V	301	TQN	C28-C29-CC6-CC7
5	W	301	TQN	C28-C29-CC6-CC7
5	Z	301	TQN	C28-C29-CC6-CC7
5	C	301	TQN	C28-C29-CC6-CC7
5	I	301	TQN	C28-C29-CC6-CC7
5	S	301	TQN	C28-C29-CC6-CC7
5	Y	301	TQN	C28-C29-CC6-CC7
5	D	301	TQN	C28-C29-CC6-CC7
5	X	301	TQN	C28-C29-CC6-CC7
5	A	302	TQN	C12-C13-O13-C21

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Mol	Chain	Res	Type	Atoms
5	B	301	TQN	C12-C13-O13-C21
5	C	301	TQN	C12-C13-O13-C21
5	D	301	TQN	C12-C13-O13-C21
5	E	301	TQN	C12-C13-O13-C21
5	F	301	TQN	C12-C13-O13-C21
5	G	301	TQN	C12-C13-O13-C21
5	H	301	TQN	C12-C13-O13-C21
5	I	301	TQN	C12-C13-O13-C21
5	J	301	TQN	C12-C13-O13-C21
5	K	301	TQN	C12-C13-O13-C21
5	L	301	TQN	C12-C13-O13-C21
5	M	301	TQN	C12-C13-O13-C21
5	N	301	TQN	C12-C13-O13-C21
5	O	301	TQN	C12-C13-O13-C21
5	P	301	TQN	C12-C13-O13-C21
5	Q	301	TQN	C12-C13-O13-C21
5	R	301	TQN	C12-C13-O13-C21
5	S	301	TQN	C12-C13-O13-C21
5	T	301	TQN	C12-C13-O13-C21
5	U	301	TQN	C12-C13-O13-C21
5	V	301	TQN	C12-C13-O13-C21
5	W	301	TQN	C12-C13-O13-C21
5	X	301	TQN	C12-C13-O13-C21
5	Y	301	TQN	C12-C13-O13-C21
5	Z	301	TQN	C12-C13-O13-C21
5	A	302	TQN	CD5-CD6-CD7-CD8
5	B	301	TQN	CD5-CD6-CD7-CD8
5	E	301	TQN	CD5-CD6-CD7-CD8
5	F	301	TQN	CD5-CD6-CD7-CD8
5	I	301	TQN	CD5-CD6-CD7-CD8
5	L	301	TQN	CD5-CD6-CD7-CD8
5	O	301	TQN	CD5-CD6-CD7-CD8
5	Q	301	TQN	CD5-CD6-CD7-CD8
5	Z	301	TQN	CD5-CD6-CD7-CD8
5	C	301	TQN	CD5-CD6-CD7-CD8
5	D	301	TQN	CD5-CD6-CD7-CD8
5	G	301	TQN	CD5-CD6-CD7-CD8
5	H	301	TQN	CD5-CD6-CD7-CD8
5	J	301	TQN	CD5-CD6-CD7-CD8
5	M	301	TQN	CD5-CD6-CD7-CD8
5	N	301	TQN	CD5-CD6-CD7-CD8
5	P	301	TQN	CD5-CD6-CD7-CD8

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Mol	Chain	Res	Type	Atoms
5	S	301	TQN	CD5-CD6-CD7-CD8
5	T	301	TQN	CD5-CD6-CD7-CD8
5	U	301	TQN	CD5-CD6-CD7-CD8
5	V	301	TQN	CD5-CD6-CD7-CD8
5	W	301	TQN	CD5-CD6-CD7-CD8
5	X	301	TQN	CD5-CD6-CD7-CD8
5	Y	301	TQN	CD5-CD6-CD7-CD8
5	R	301	TQN	CD5-CD6-CD7-CD8
5	K	301	TQN	CD5-CD6-CD7-CD8
5	A	302	TQN	C39-CD4-CD5-CD6
5	B	301	TQN	C39-CD4-CD5-CD6
5	L	301	TQN	C39-CD4-CD5-CD6
5	M	301	TQN	C39-CD4-CD5-CD6
5	W	301	TQN	C39-CD4-CD5-CD6
5	Y	301	TQN	C39-CD4-CD5-CD6
5	C	301	TQN	C39-CD4-CD5-CD6
5	E	301	TQN	C39-CD4-CD5-CD6
5	F	301	TQN	C39-CD4-CD5-CD6
5	G	301	TQN	C39-CD4-CD5-CD6
5	H	301	TQN	C39-CD4-CD5-CD6
5	I	301	TQN	C39-CD4-CD5-CD6
5	Q	301	TQN	C39-CD4-CD5-CD6
5	S	301	TQN	C39-CD4-CD5-CD6
5	U	301	TQN	C39-CD4-CD5-CD6
5	Z	301	TQN	C39-CD4-CD5-CD6
5	D	301	TQN	C39-CD4-CD5-CD6
5	J	301	TQN	C39-CD4-CD5-CD6
5	N	301	TQN	C39-CD4-CD5-CD6
5	O	301	TQN	C39-CD4-CD5-CD6
5	P	301	TQN	C39-CD4-CD5-CD6
5	R	301	TQN	C39-CD4-CD5-CD6
5	T	301	TQN	C39-CD4-CD5-CD6
5	V	301	TQN	C39-CD4-CD5-CD6
5	X	301	TQN	C39-CD4-CD5-CD6
5	K	301	TQN	C39-CD4-CD5-CD6
5	B	301	TQN	C14-C15-C16-C17
5	C	301	TQN	C14-C15-C16-C17
5	E	301	TQN	C14-C15-C16-C17
5	F	301	TQN	C14-C15-C16-C17
5	H	301	TQN	C14-C15-C16-C17
5	L	301	TQN	C14-C15-C16-C17
5	M	301	TQN	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
5	N	301	TQN	C14-C15-C16-C17
5	R	301	TQN	C14-C15-C16-C17
5	T	301	TQN	C14-C15-C16-C17
5	U	301	TQN	C14-C15-C16-C17
5	V	301	TQN	C14-C15-C16-C17
5	W	301	TQN	C14-C15-C16-C17
5	X	301	TQN	C14-C15-C16-C17
5	Y	301	TQN	C14-C15-C16-C17
5	Z	301	TQN	C14-C15-C16-C17
5	K	301	TQN	C14-C15-C16-C17
5	P	301	TQN	C14-C15-C16-C17
5	Q	301	TQN	C14-C15-C16-C17
5	S	301	TQN	C14-C15-C16-C17
5	G	301	TQN	C14-C15-C16-C17
5	I	301	TQN	C14-C15-C16-C17
5	J	301	TQN	C14-C15-C16-C17
5	O	301	TQN	C14-C15-C16-C17
5	A	302	TQN	C14-C15-C16-C17
5	D	301	TQN	C14-C15-C16-C17
5	F	301	TQN	CD4-CD5-CD6-CD7
5	L	301	TQN	CD4-CD5-CD6-CD7
5	V	301	TQN	CD4-CD5-CD6-CD7
5	C	301	TQN	CD4-CD5-CD6-CD7
5	G	301	TQN	CD4-CD5-CD6-CD7
5	O	301	TQN	CD4-CD5-CD6-CD7
5	T	301	TQN	CD4-CD5-CD6-CD7
5	U	301	TQN	CD4-CD5-CD6-CD7
5	X	301	TQN	CD4-CD5-CD6-CD7
5	A	302	TQN	CD4-CD5-CD6-CD7
5	B	301	TQN	CD4-CD5-CD6-CD7
5	D	301	TQN	CD4-CD5-CD6-CD7
5	E	301	TQN	CD4-CD5-CD6-CD7
5	H	301	TQN	CD4-CD5-CD6-CD7
5	I	301	TQN	CD4-CD5-CD6-CD7
5	J	301	TQN	CD4-CD5-CD6-CD7
5	K	301	TQN	CD4-CD5-CD6-CD7
5	M	301	TQN	CD4-CD5-CD6-CD7
5	N	301	TQN	CD4-CD5-CD6-CD7
5	P	301	TQN	CD4-CD5-CD6-CD7
5	Q	301	TQN	CD4-CD5-CD6-CD7
5	R	301	TQN	CD4-CD5-CD6-CD7
5	S	301	TQN	CD4-CD5-CD6-CD7

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Mol	Chain	Res	Type	Atoms
5	W	301	TQN	CD4-CD5-CD6-CD7
5	Y	301	TQN	CD4-CD5-CD6-CD7
5	Z	301	TQN	CD4-CD5-CD6-CD7
5	A	302	TQN	C13-C14-C15-C16
5	B	301	TQN	C13-C14-C15-C16
5	C	301	TQN	C13-C14-C15-C16
5	D	301	TQN	C13-C14-C15-C16
5	E	301	TQN	C13-C14-C15-C16
5	F	301	TQN	C13-C14-C15-C16
5	G	301	TQN	C13-C14-C15-C16
5	H	301	TQN	C13-C14-C15-C16
5	I	301	TQN	C13-C14-C15-C16
5	J	301	TQN	C13-C14-C15-C16
5	K	301	TQN	C13-C14-C15-C16
5	L	301	TQN	C13-C14-C15-C16
5	M	301	TQN	C13-C14-C15-C16
5	N	301	TQN	C13-C14-C15-C16
5	O	301	TQN	C13-C14-C15-C16
5	P	301	TQN	C13-C14-C15-C16
5	Q	301	TQN	C13-C14-C15-C16
5	R	301	TQN	C13-C14-C15-C16
5	S	301	TQN	C13-C14-C15-C16
5	T	301	TQN	C13-C14-C15-C16
5	U	301	TQN	C13-C14-C15-C16
5	V	301	TQN	C13-C14-C15-C16
5	W	301	TQN	C13-C14-C15-C16
5	X	301	TQN	C13-C14-C15-C16
5	Y	301	TQN	C13-C14-C15-C16
5	Z	301	TQN	C13-C14-C15-C16
5	A	302	TQN	CA1-OA1-PA-OP6
5	A	302	TQN	CB4-OB4-PB-OP2
5	B	301	TQN	CA1-OA1-PA-OP6
5	B	301	TQN	CB4-OB4-PB-OP2
5	C	301	TQN	CA1-OA1-PA-OP6
5	C	301	TQN	CB4-OB4-PB-OP2
5	D	301	TQN	CA1-OA1-PA-OP6
5	D	301	TQN	CB4-OB4-PB-OP2
5	E	301	TQN	CA1-OA1-PA-OP6
5	E	301	TQN	CB4-OB4-PB-OP2
5	F	301	TQN	CA1-OA1-PA-OP6
5	F	301	TQN	CB4-OB4-PB-OP2
5	G	301	TQN	CA1-OA1-PA-OP6

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Mol	Chain	Res	Type	Atoms
5	G	301	TQN	CB4-OB4-PB-OP2
5	H	301	TQN	CA1-OA1-PA-OP6
5	H	301	TQN	CB4-OB4-PB-OP2
5	I	301	TQN	CA1-OA1-PA-OP6
5	I	301	TQN	CB4-OB4-PB-OP2
5	J	301	TQN	CA1-OA1-PA-OP6
5	J	301	TQN	CB4-OB4-PB-OP2
5	K	301	TQN	CA1-OA1-PA-OP6
5	K	301	TQN	CB4-OB4-PB-OP2
5	L	301	TQN	CA1-OA1-PA-OP6
5	L	301	TQN	CB4-OB4-PB-OP2
5	M	301	TQN	CA1-OA1-PA-OP6
5	M	301	TQN	CB4-OB4-PB-OP2
5	N	301	TQN	CA1-OA1-PA-OP6
5	N	301	TQN	CB4-OB4-PB-OP2
5	O	301	TQN	CA1-OA1-PA-OP6
5	O	301	TQN	CB4-OB4-PB-OP2
5	P	301	TQN	CA1-OA1-PA-OP6
5	P	301	TQN	CB4-OB4-PB-OP2
5	Q	301	TQN	CA1-OA1-PA-OP6
5	Q	301	TQN	CB4-OB4-PB-OP2
5	R	301	TQN	CA1-OA1-PA-OP6
5	R	301	TQN	CB4-OB4-PB-OP2
5	S	301	TQN	CA1-OA1-PA-OP6
5	S	301	TQN	CB4-OB4-PB-OP2
5	T	301	TQN	CA1-OA1-PA-OP6
5	T	301	TQN	CB4-OB4-PB-OP2
5	U	301	TQN	CA1-OA1-PA-OP6
5	U	301	TQN	CB4-OB4-PB-OP2
5	V	301	TQN	CA1-OA1-PA-OP6
5	V	301	TQN	CB4-OB4-PB-OP2
5	W	301	TQN	CA1-OA1-PA-OP6
5	W	301	TQN	CB4-OB4-PB-OP2
5	X	301	TQN	CA1-OA1-PA-OP6
5	X	301	TQN	CB4-OB4-PB-OP2
5	Y	301	TQN	CA1-OA1-PA-OP6
5	Y	301	TQN	CB4-OB4-PB-OP2
5	Z	301	TQN	CA1-OA1-PA-OP6
5	Z	301	TQN	CB4-OB4-PB-OP2
5	L	301	TQN	C82-C83-C84-C85
5	N	301	TQN	C82-C83-C84-C85
5	S	301	TQN	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
5	W	301	TQN	C82-C83-C84-C85
5	D	301	TQN	C82-C83-C84-C85
5	G	301	TQN	C82-C83-C84-C85
5	O	301	TQN	C82-C83-C84-C85
5	A	302	TQN	C82-C83-C84-C85
5	B	301	TQN	C82-C83-C84-C85
5	C	301	TQN	C82-C83-C84-C85
5	R	301	TQN	C82-C83-C84-C85
5	T	301	TQN	C82-C83-C84-C85
5	U	301	TQN	C82-C83-C84-C85
5	V	301	TQN	C82-C83-C84-C85
5	X	301	TQN	C82-C83-C84-C85
5	Y	301	TQN	C82-C83-C84-C85
5	F	301	TQN	C82-C83-C84-C85
5	H	301	TQN	C82-C83-C84-C85
5	K	301	TQN	C82-C83-C84-C85
5	Q	301	TQN	C82-C83-C84-C85
5	Z	301	TQN	C82-C83-C84-C85
5	I	301	TQN	C82-C83-C84-C85
5	M	301	TQN	C82-C83-C84-C85
5	P	301	TQN	C82-C83-C84-C85
5	J	301	TQN	C82-C83-C84-C85
5	E	301	TQN	C82-C83-C84-C85
5	A	302	TQN	O33-C33-C34-C35
5	B	301	TQN	O33-C33-C34-C35
5	C	301	TQN	O33-C33-C34-C35
5	D	301	TQN	O33-C33-C34-C35
5	E	301	TQN	O33-C33-C34-C35
5	F	301	TQN	O33-C33-C34-C35
5	G	301	TQN	O33-C33-C34-C35
5	H	301	TQN	O33-C33-C34-C35
5	I	301	TQN	O33-C33-C34-C35
5	J	301	TQN	O33-C33-C34-C35
5	K	301	TQN	O33-C33-C34-C35
5	L	301	TQN	O33-C33-C34-C35
5	M	301	TQN	O33-C33-C34-C35
5	N	301	TQN	O33-C33-C34-C35
5	O	301	TQN	O33-C33-C34-C35
5	P	301	TQN	O33-C33-C34-C35
5	Q	301	TQN	O33-C33-C34-C35
5	R	301	TQN	O33-C33-C34-C35
5	S	301	TQN	O33-C33-C34-C35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	T	301	TQN	O33-C33-C34-C35
5	U	301	TQN	O33-C33-C34-C35
5	V	301	TQN	O33-C33-C34-C35
5	W	301	TQN	O33-C33-C34-C35
5	X	301	TQN	O33-C33-C34-C35
5	Y	301	TQN	O33-C33-C34-C35
5	Z	301	TQN	O33-C33-C34-C35
5	H	301	TQN	C64-C65-C66-C67

There are no ring outliers.

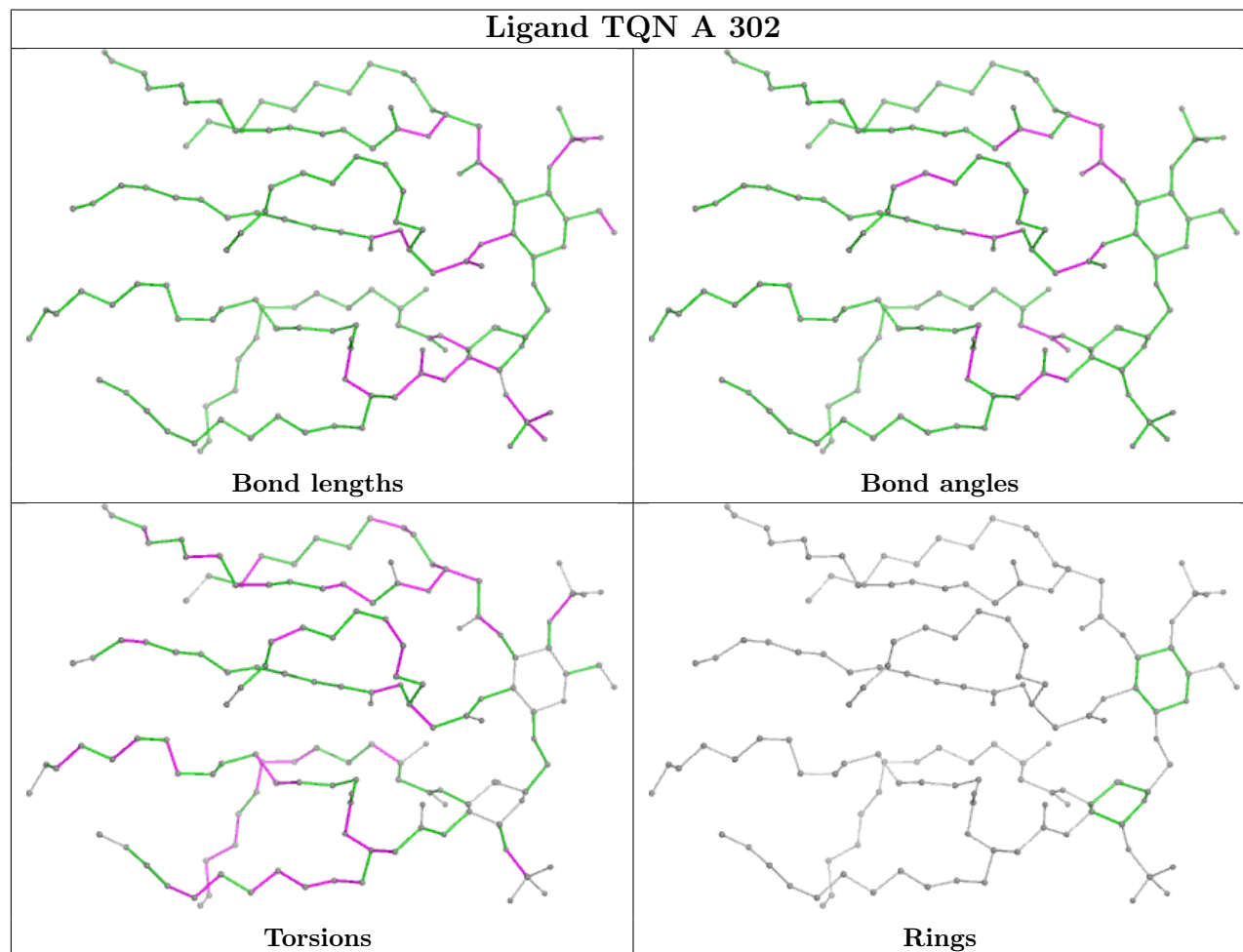
26 monomers are involved in 52 short contacts:

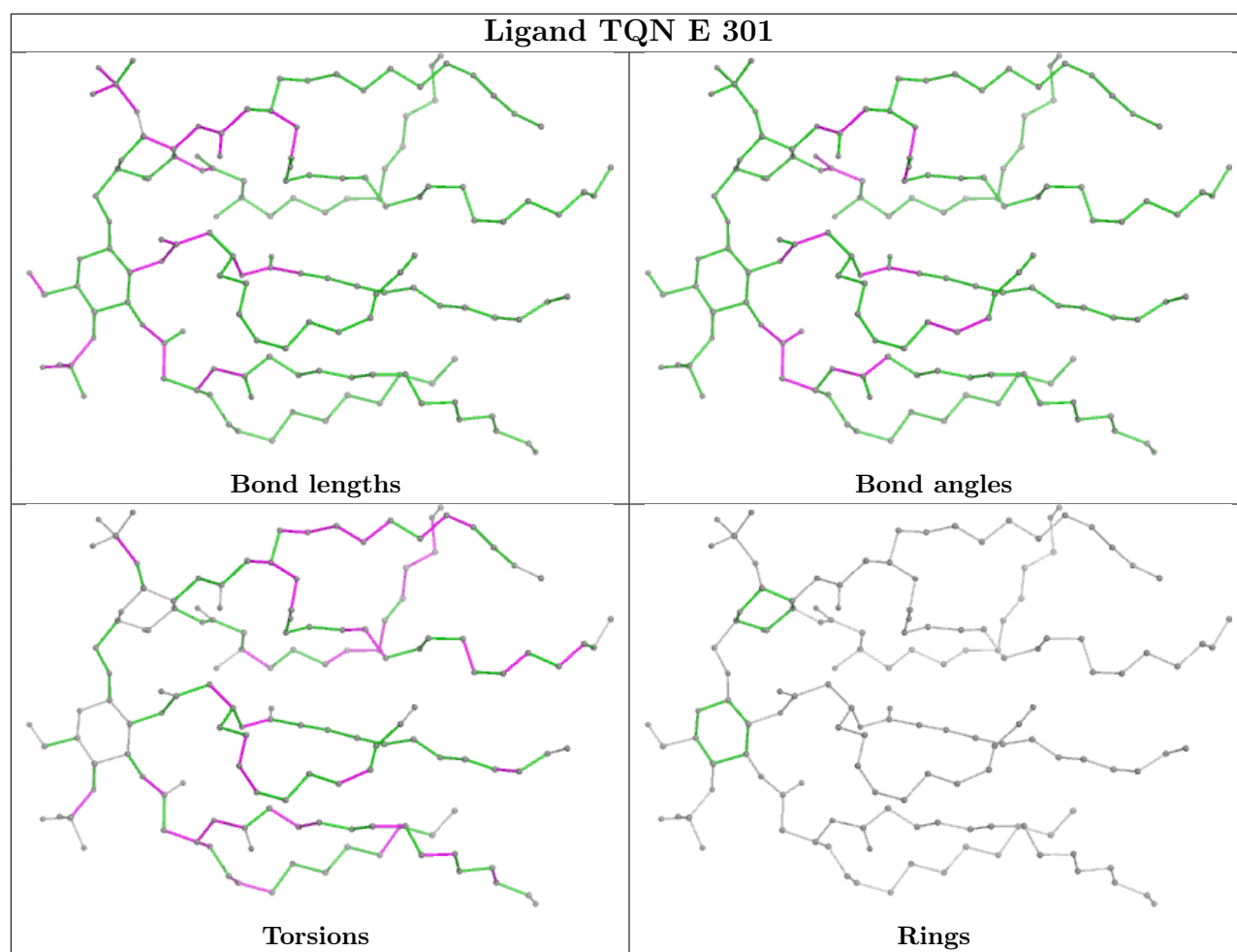
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	302	TQN	2	0
5	E	301	TQN	2	0
5	I	301	TQN	2	0
5	C	301	TQN	2	0
5	Q	301	TQN	2	0
5	J	301	TQN	2	0
5	T	301	TQN	2	0
5	Z	301	TQN	2	0
5	S	301	TQN	2	0
5	U	301	TQN	2	0
5	D	301	TQN	2	0
5	L	301	TQN	2	0
5	X	301	TQN	2	0
5	K	301	TQN	2	0
5	M	301	TQN	2	0
5	O	301	TQN	2	0
5	R	301	TQN	2	0
5	V	301	TQN	2	0
5	H	301	TQN	2	0
5	N	301	TQN	2	0
5	P	301	TQN	2	0
5	Y	301	TQN	2	0
5	B	301	TQN	2	0
5	G	301	TQN	2	0
5	F	301	TQN	2	0
5	W	301	TQN	2	0

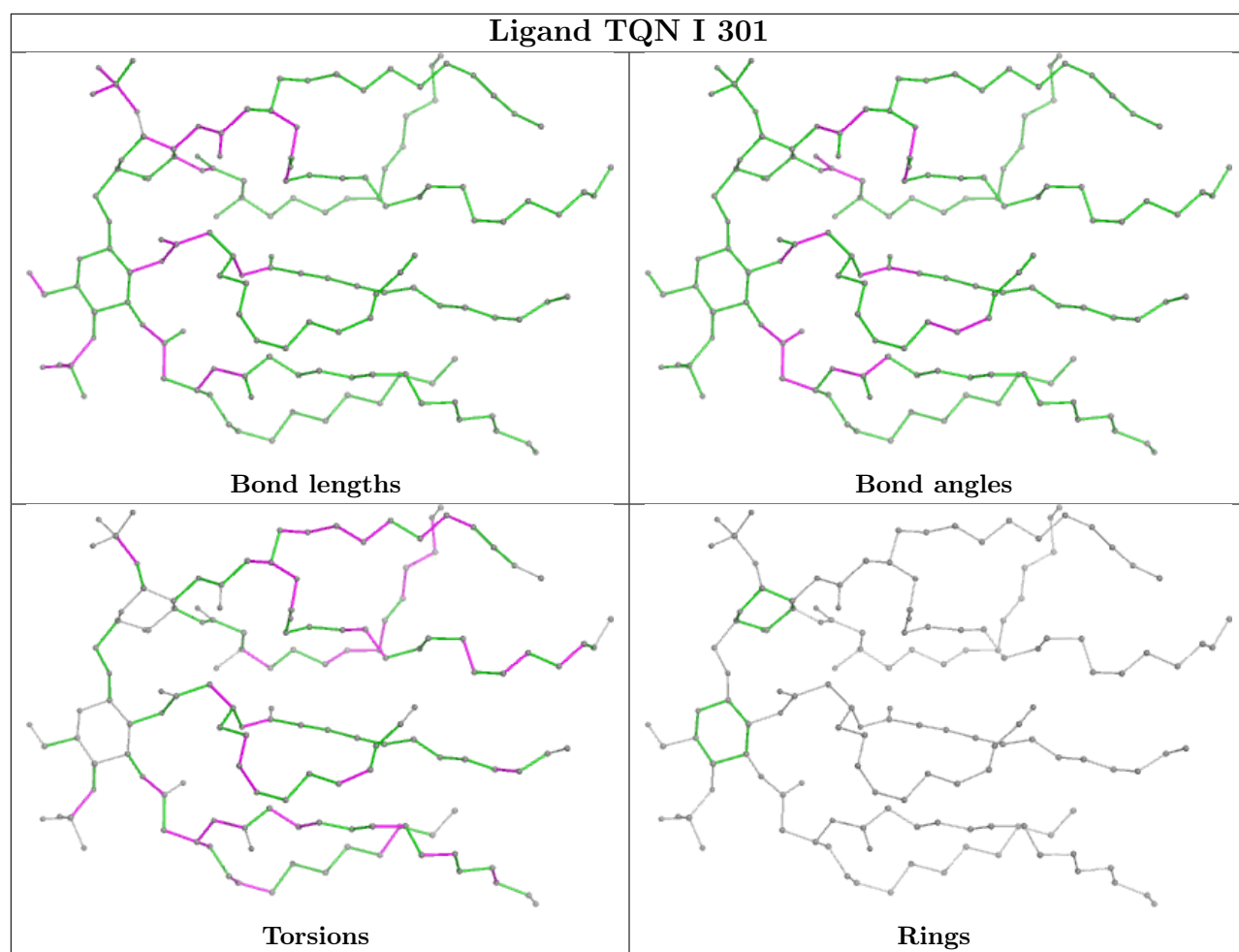
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

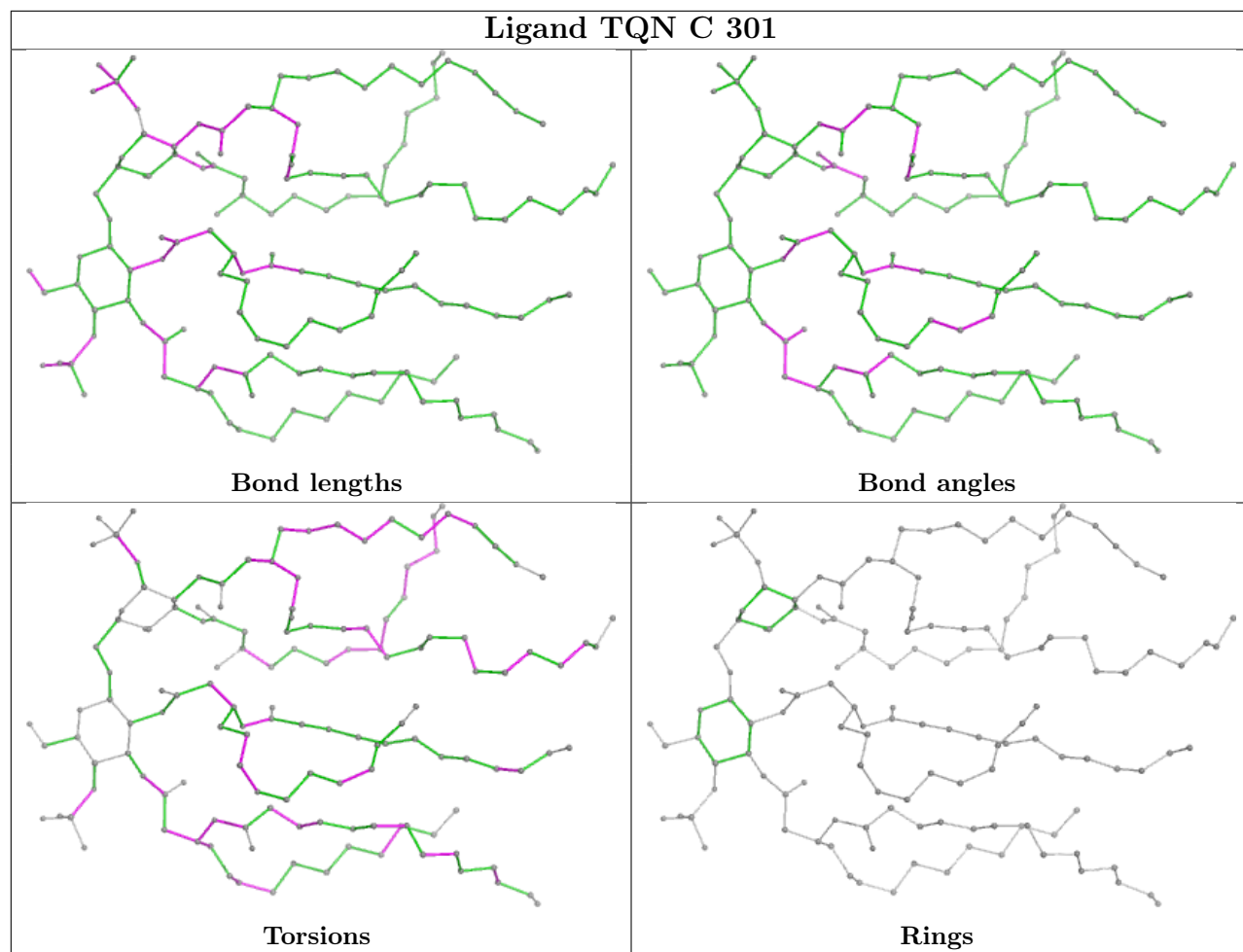


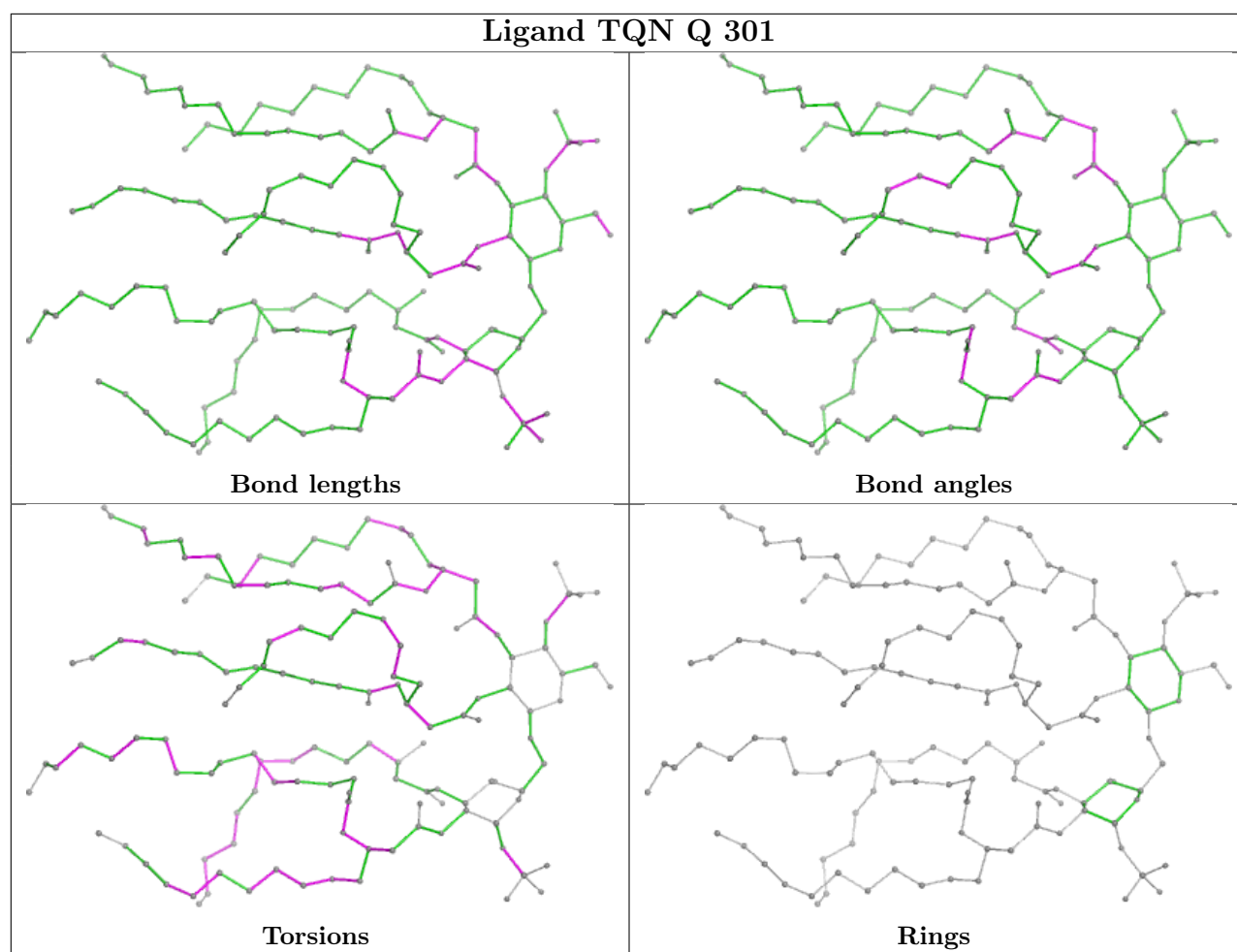
addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

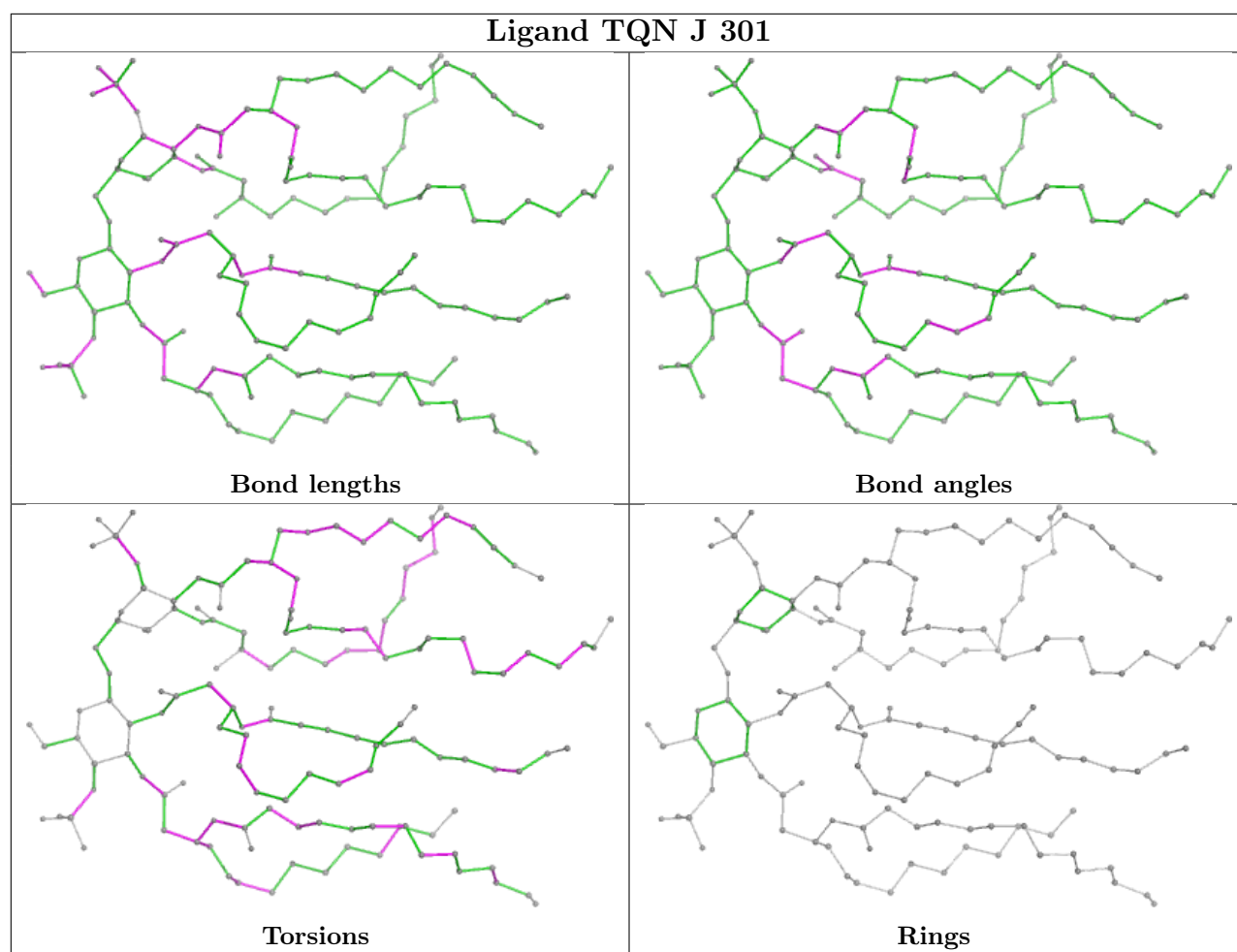


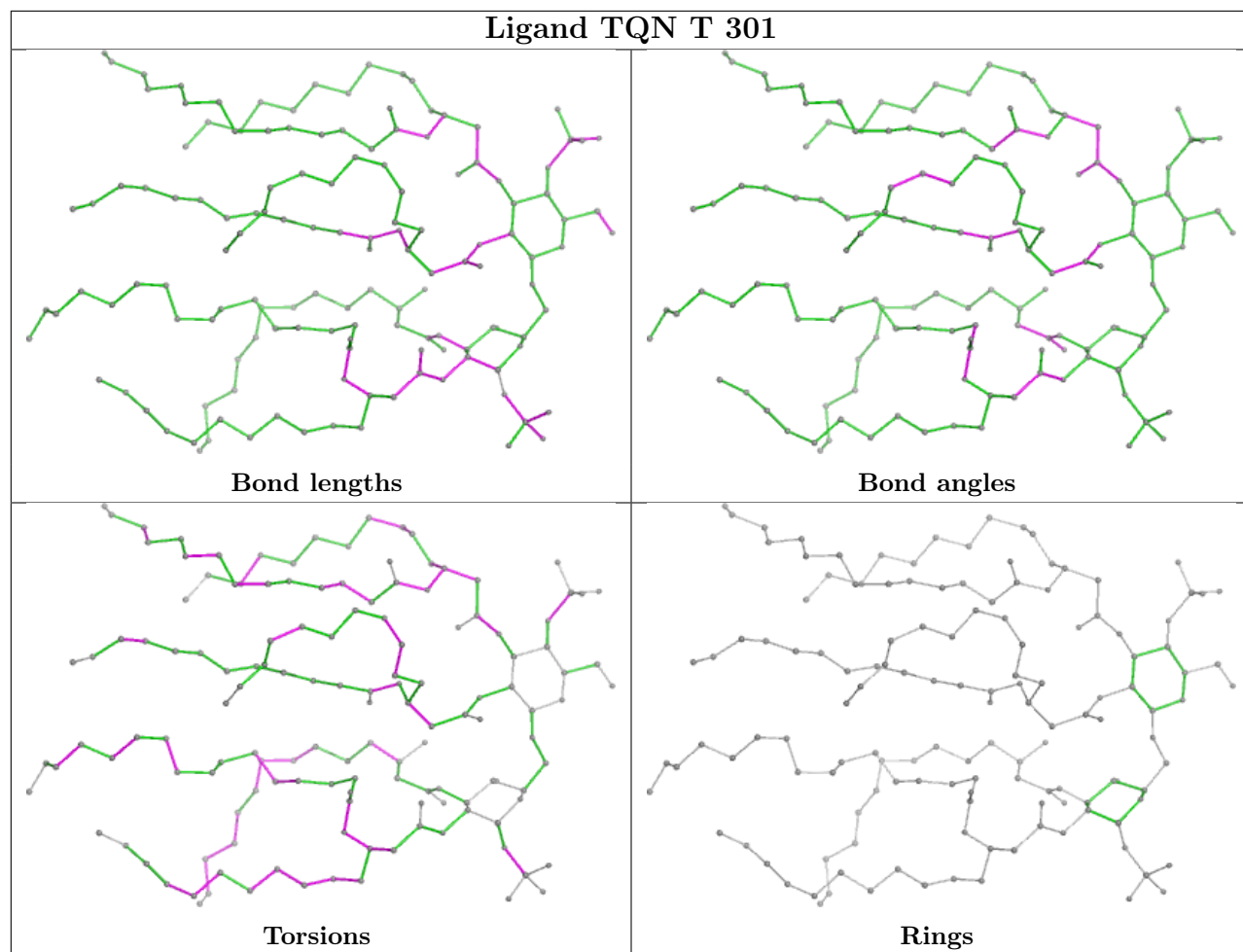


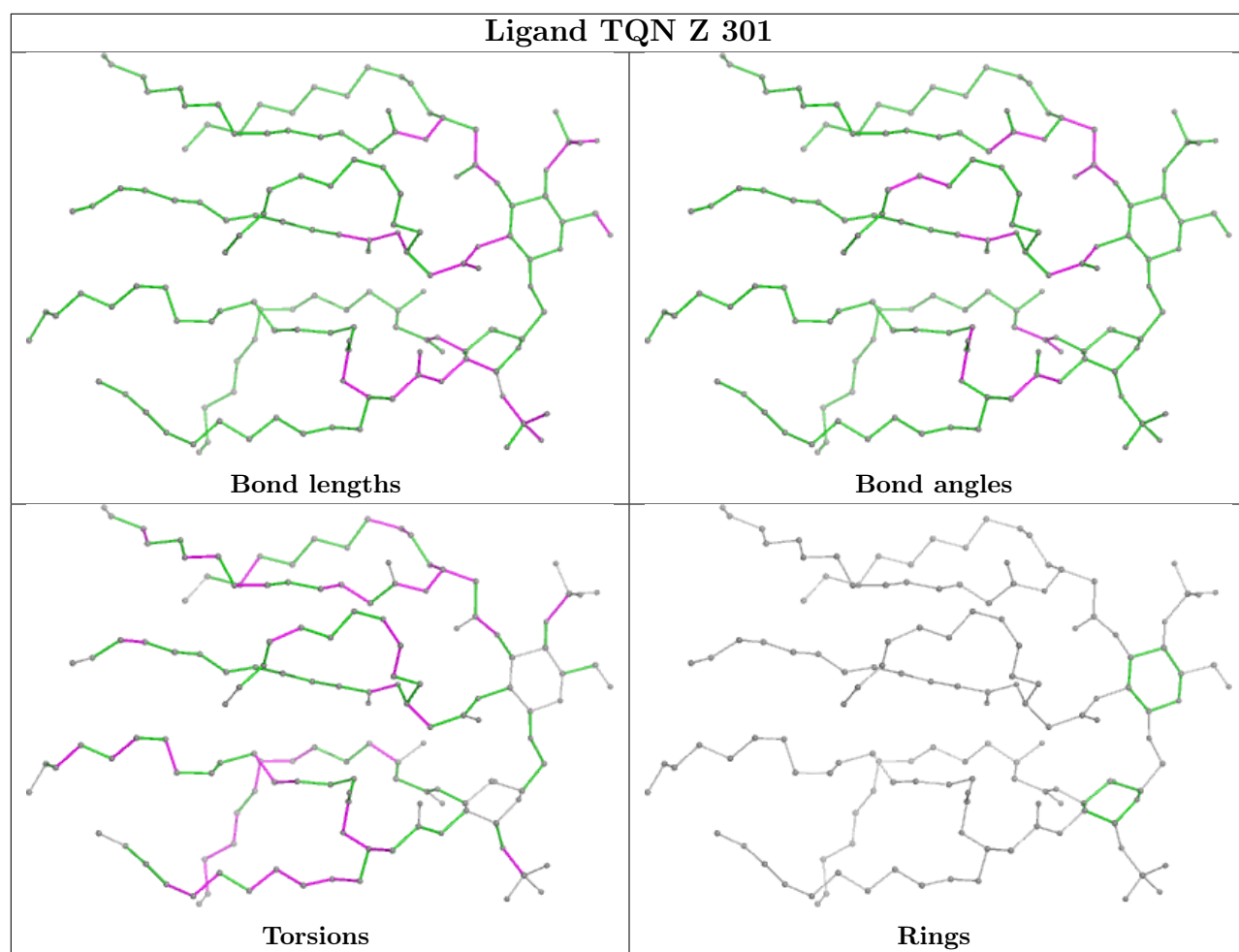




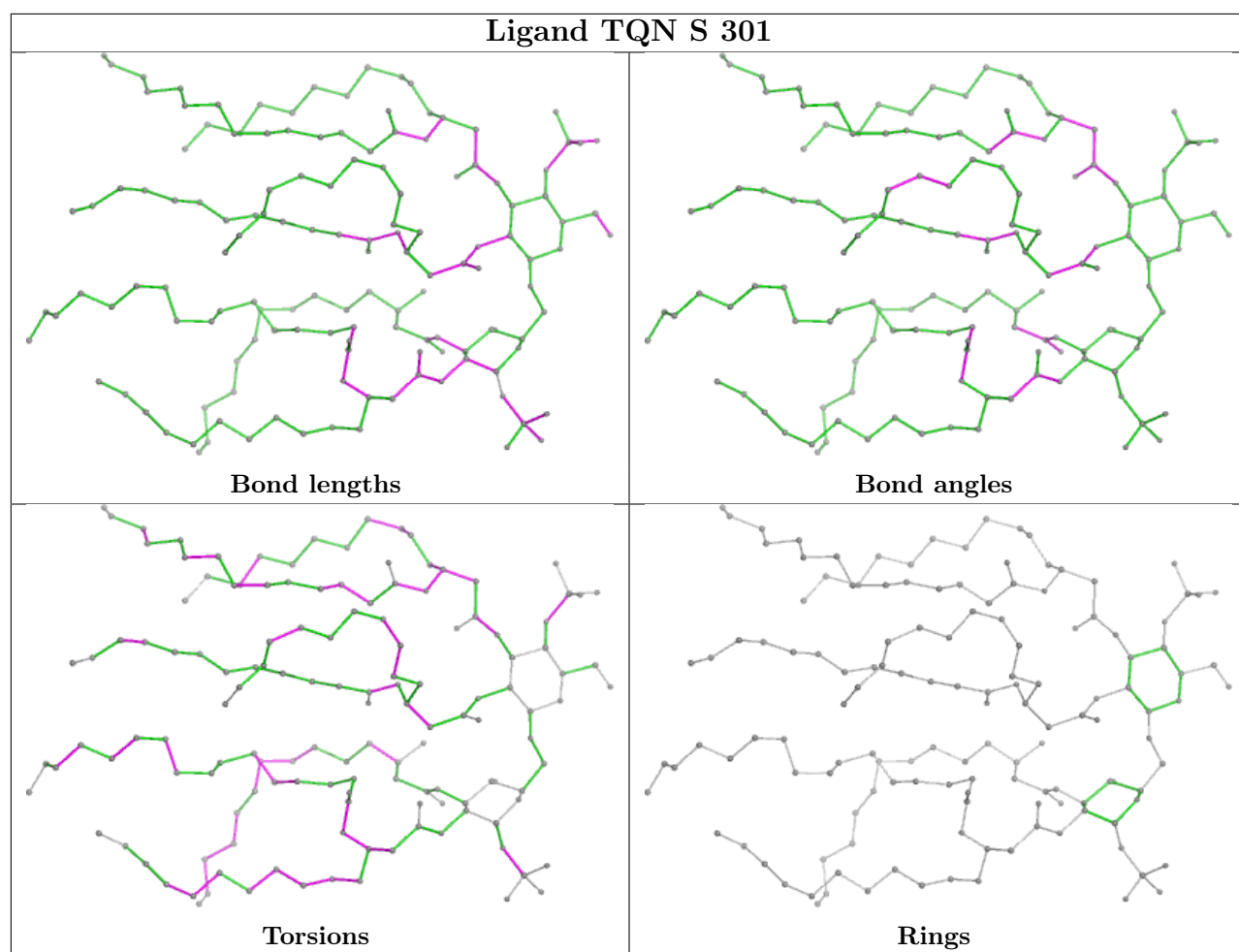


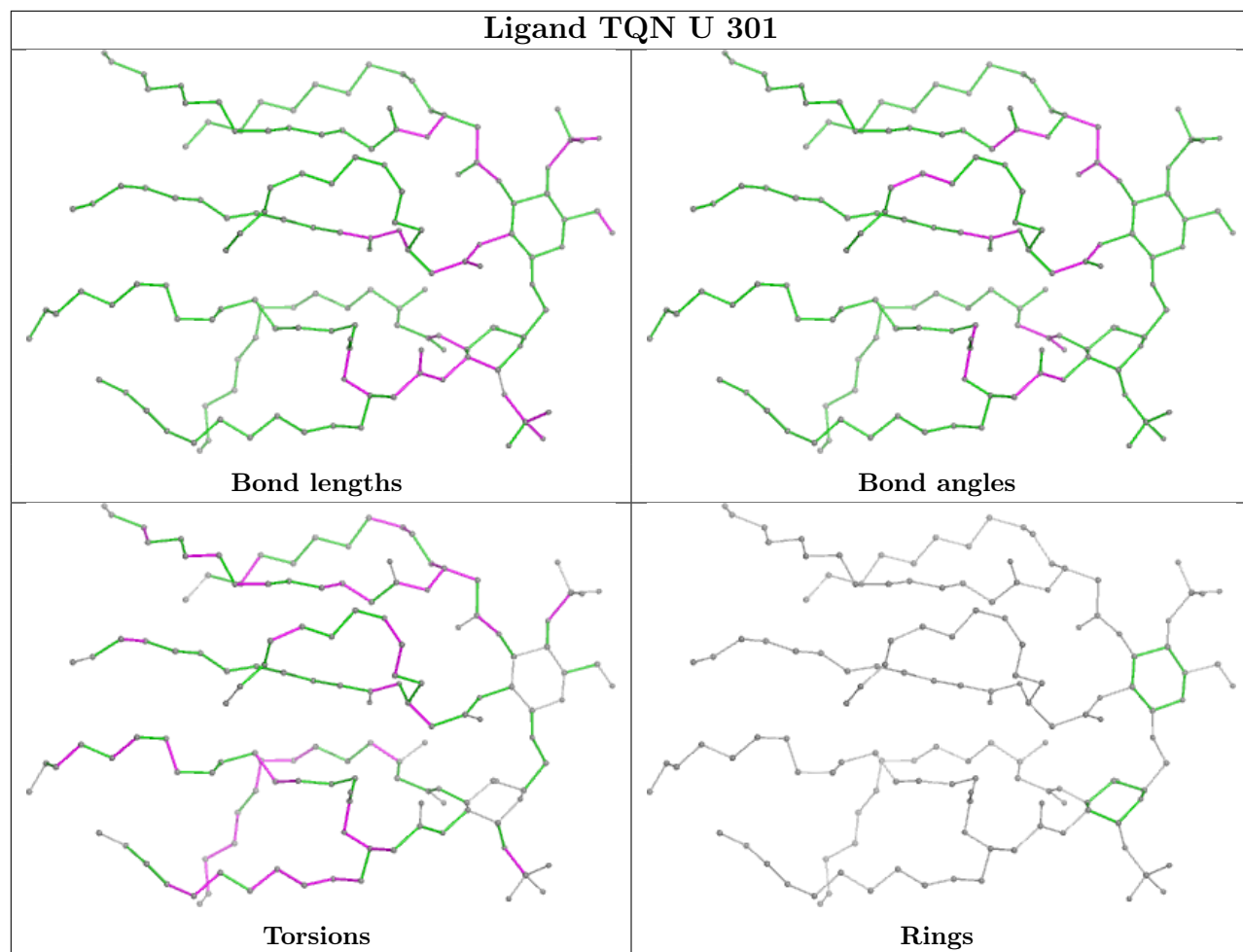


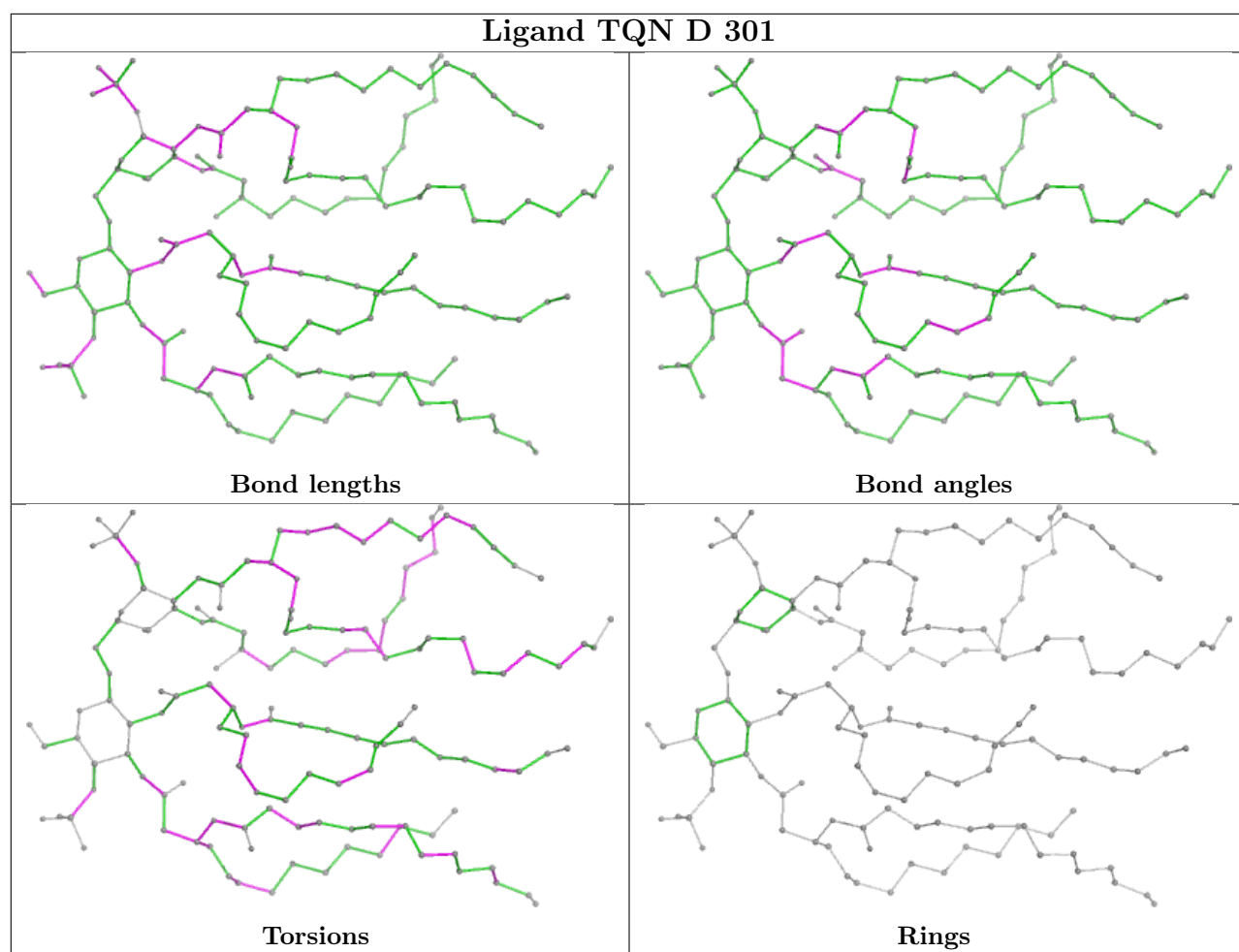


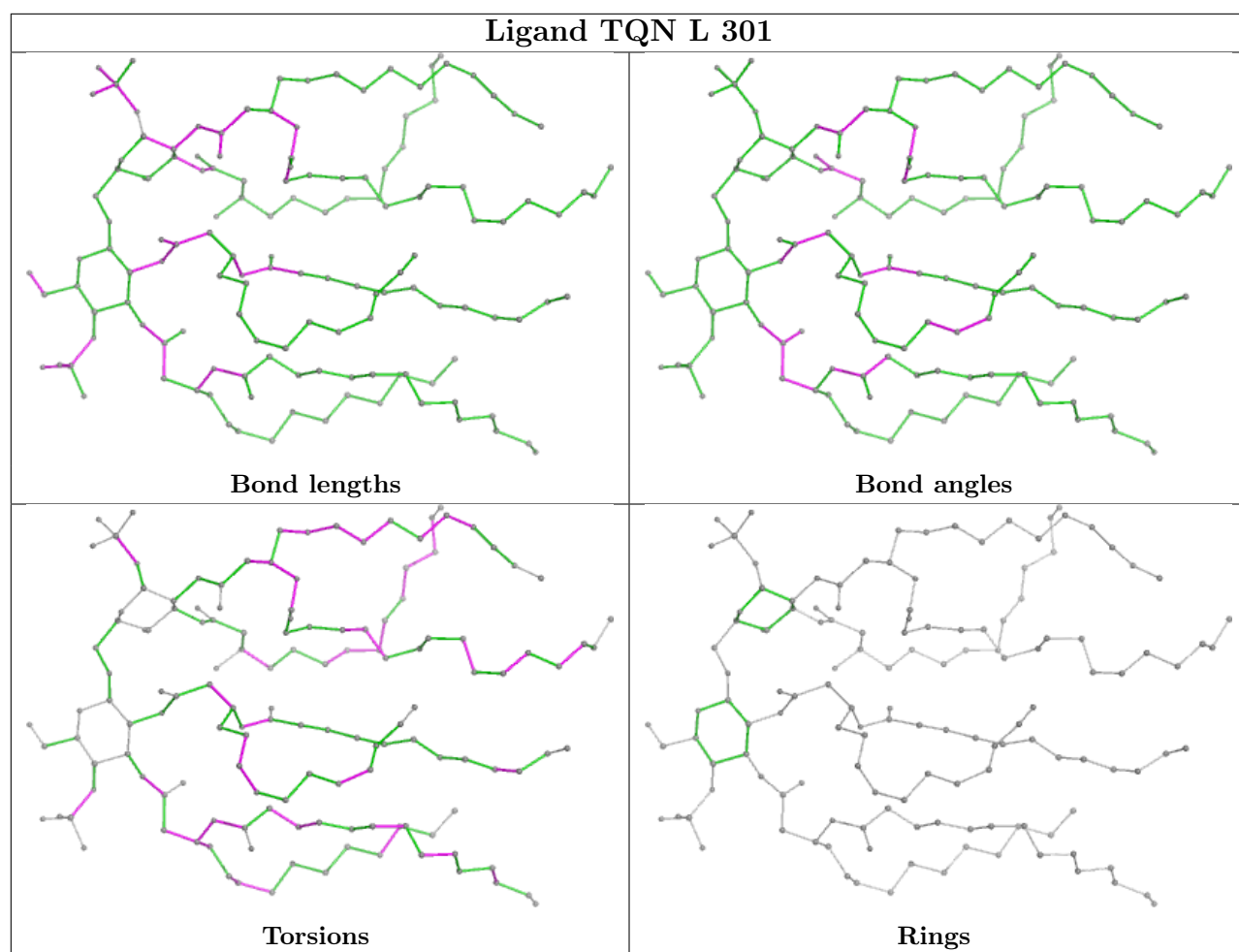


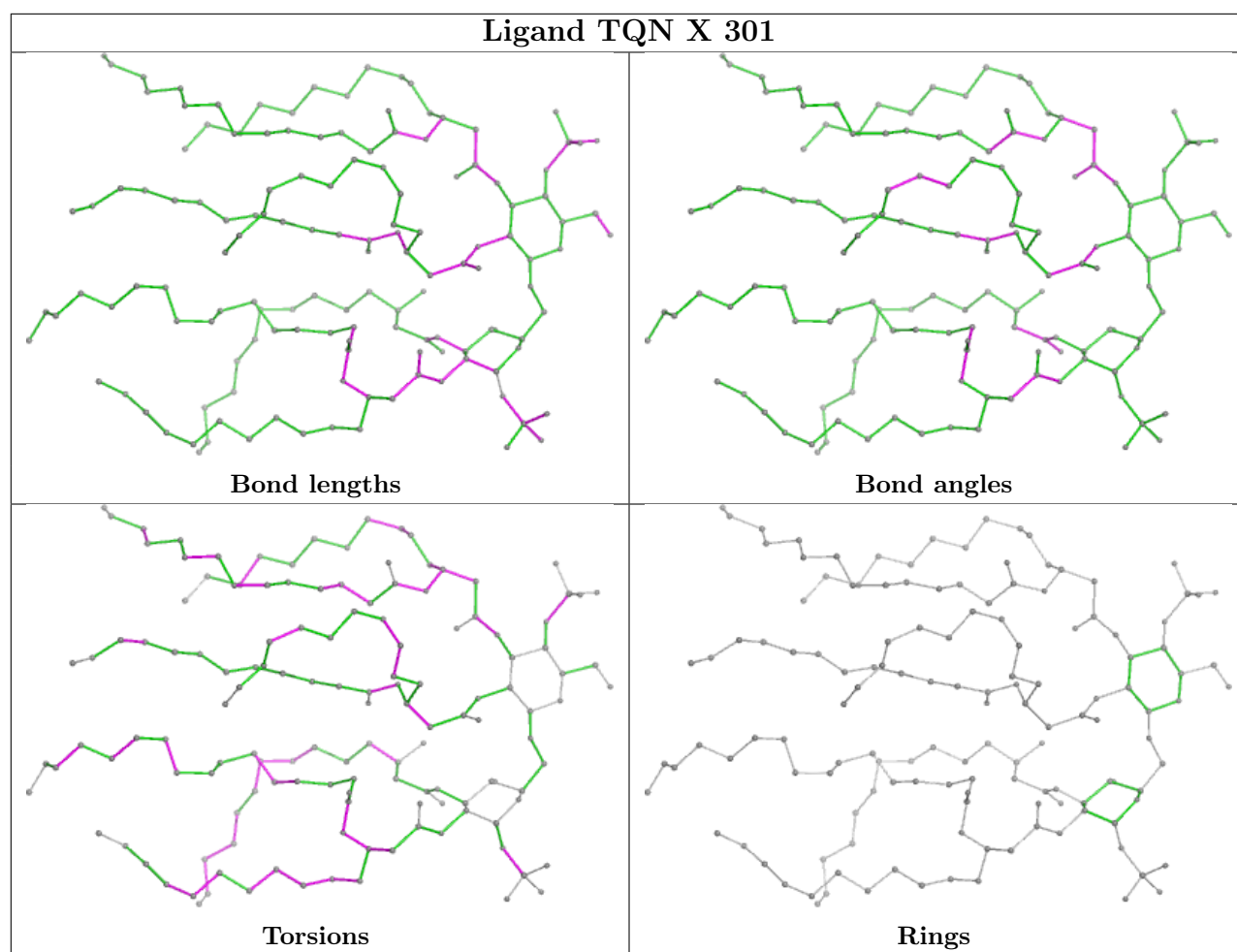


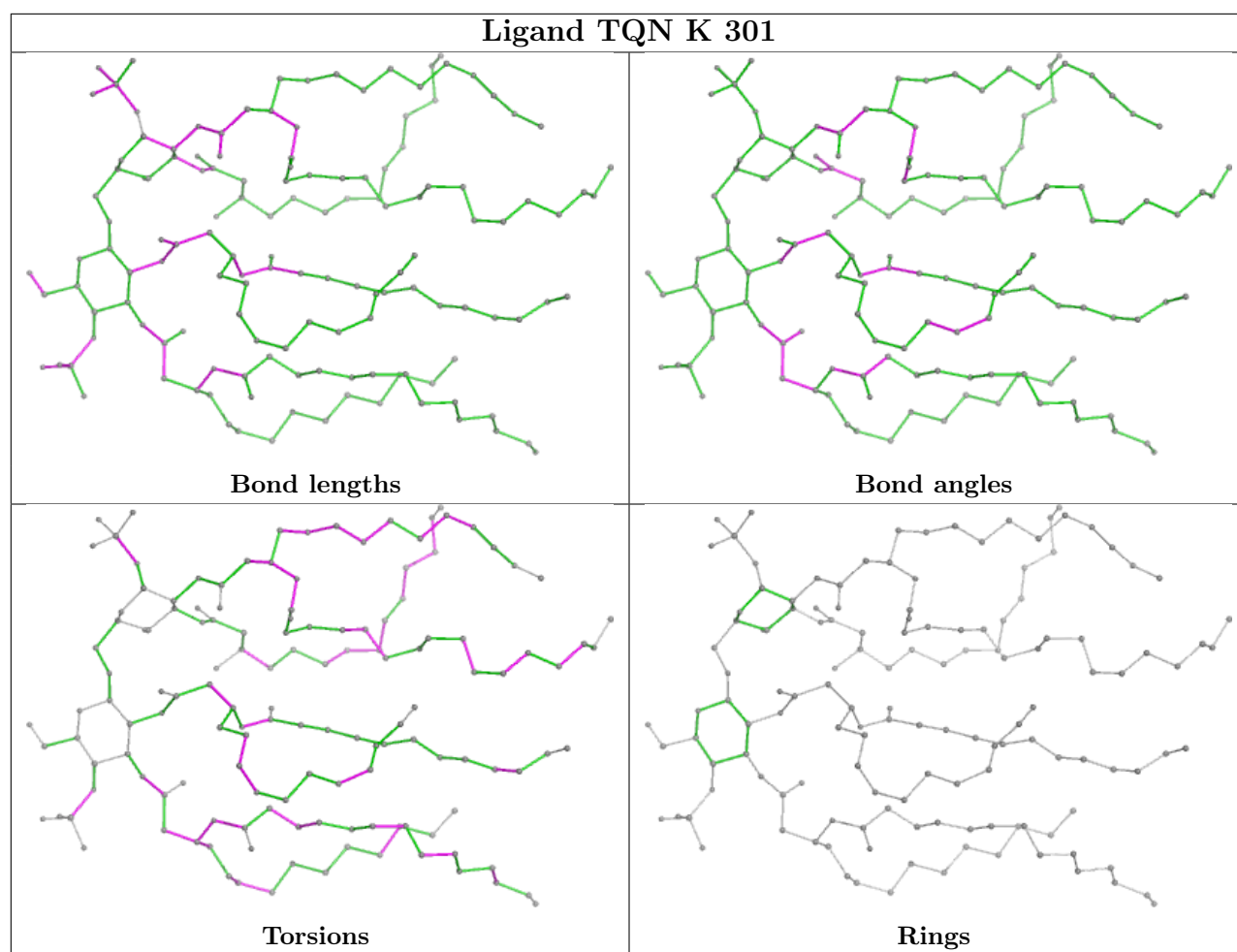


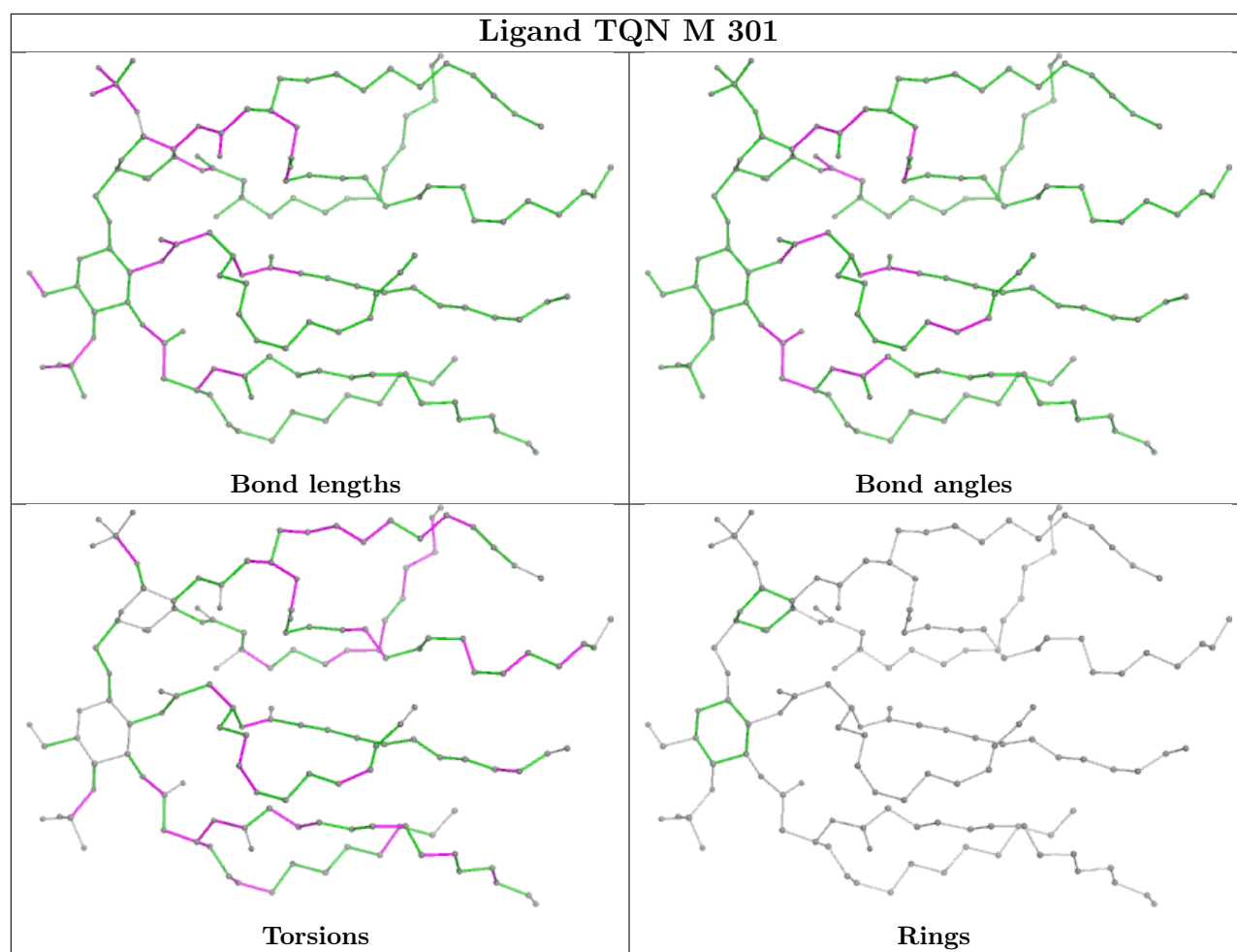


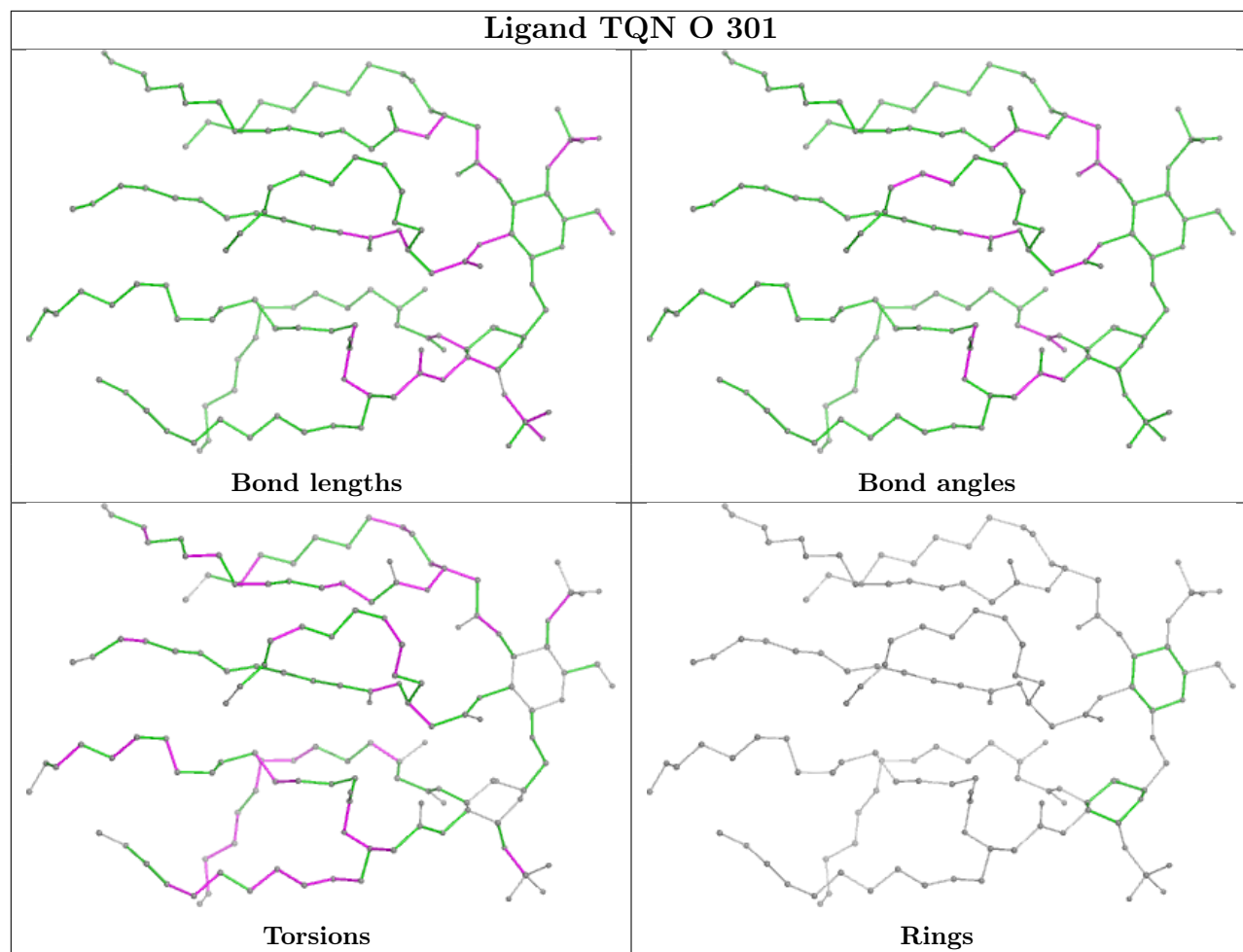




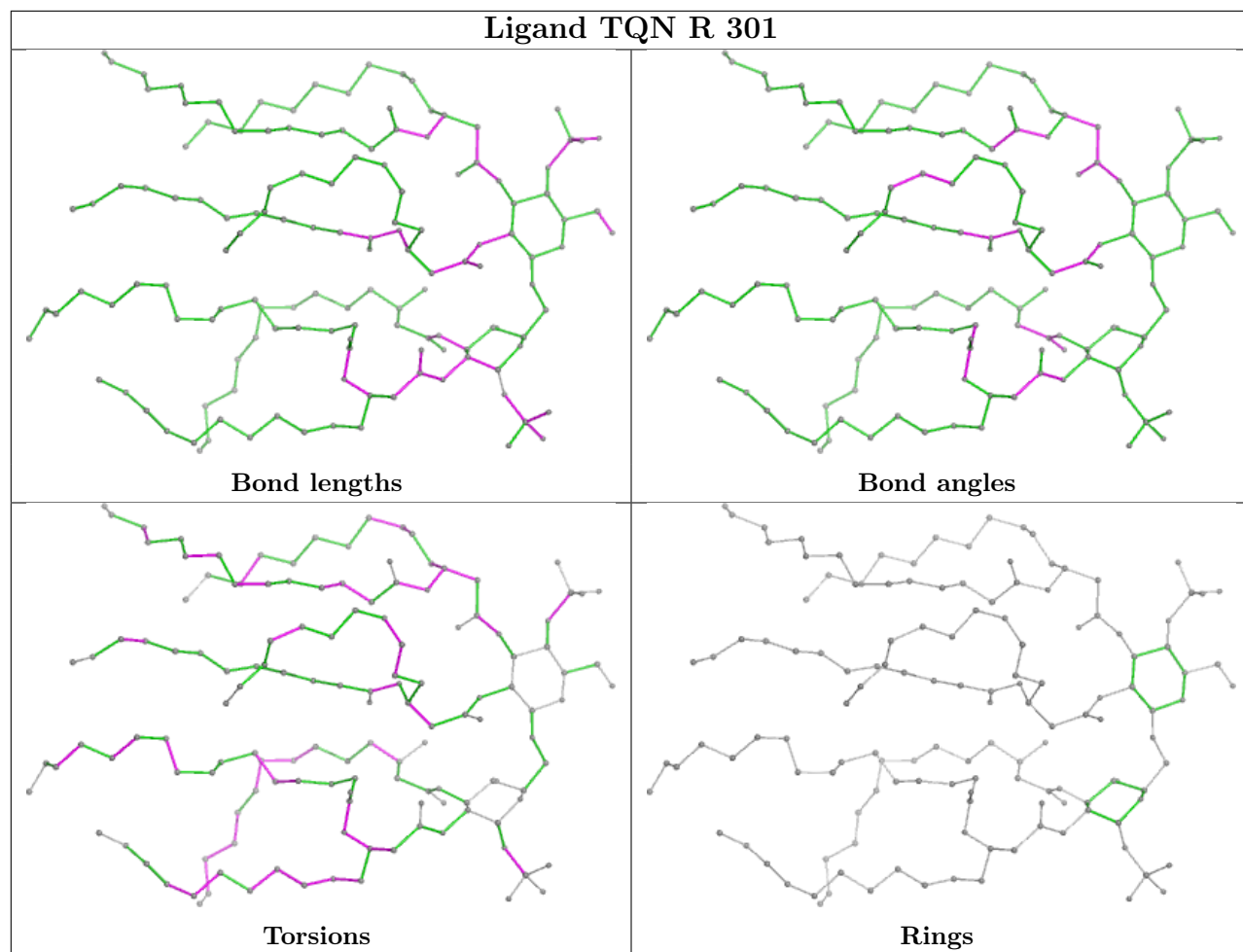


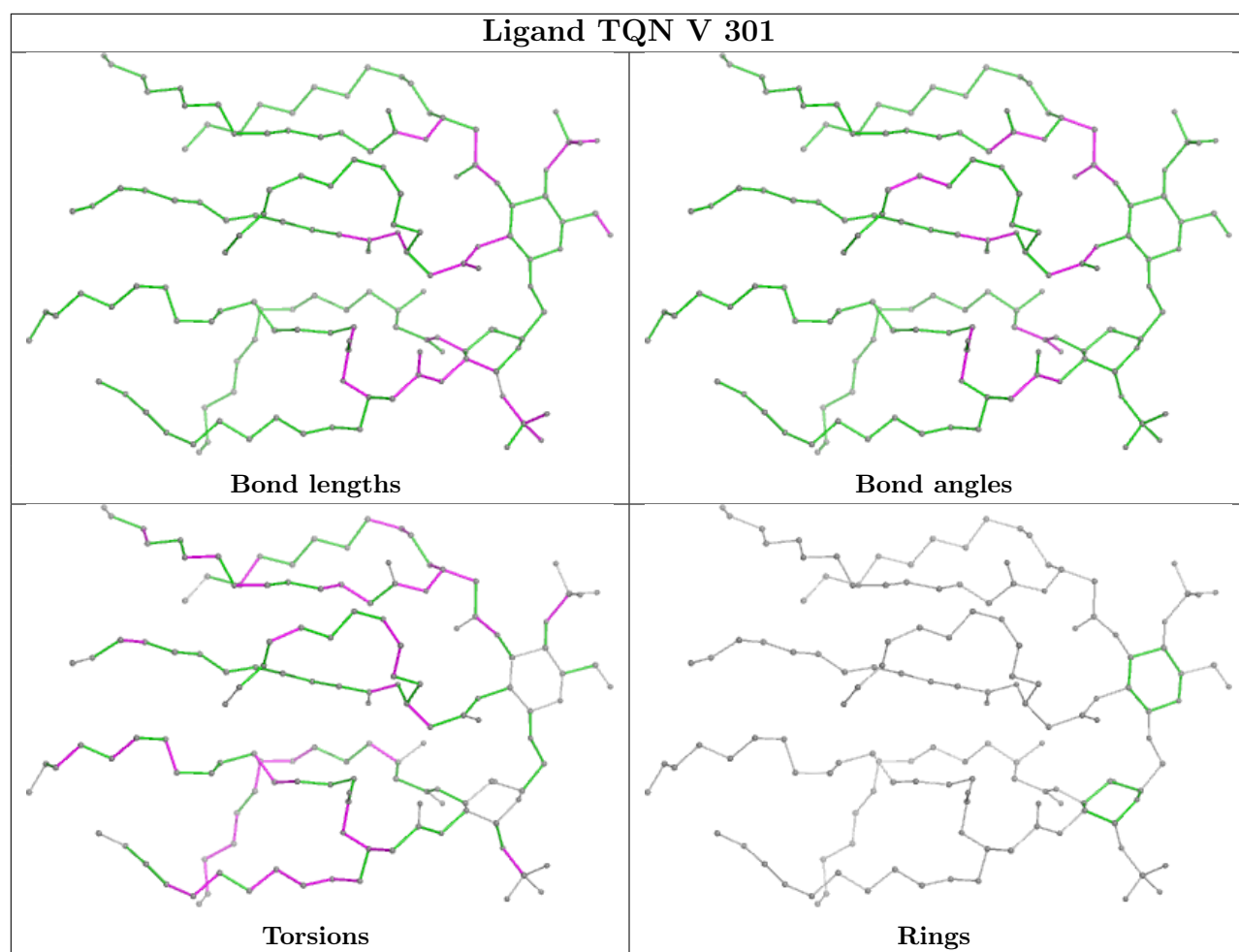


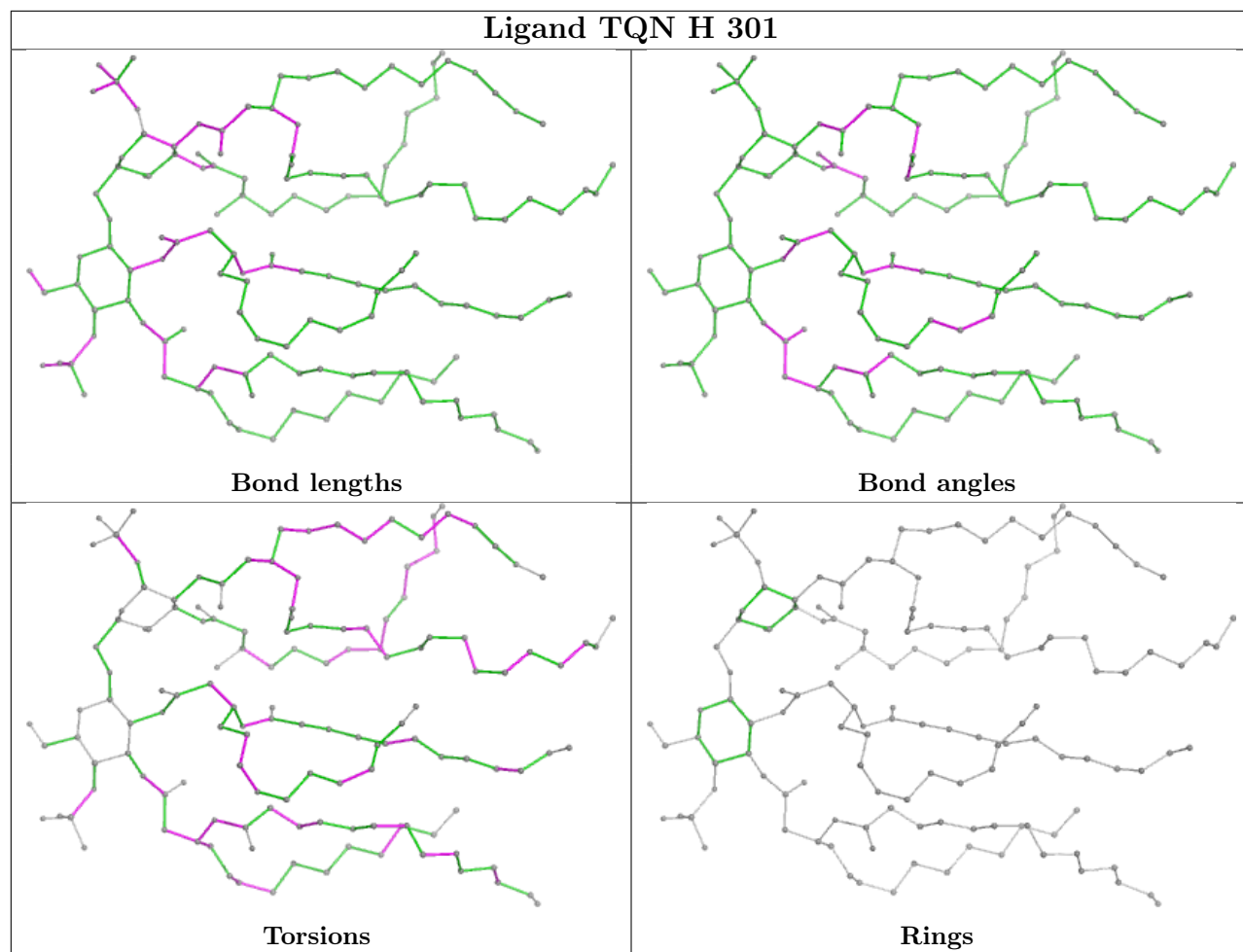


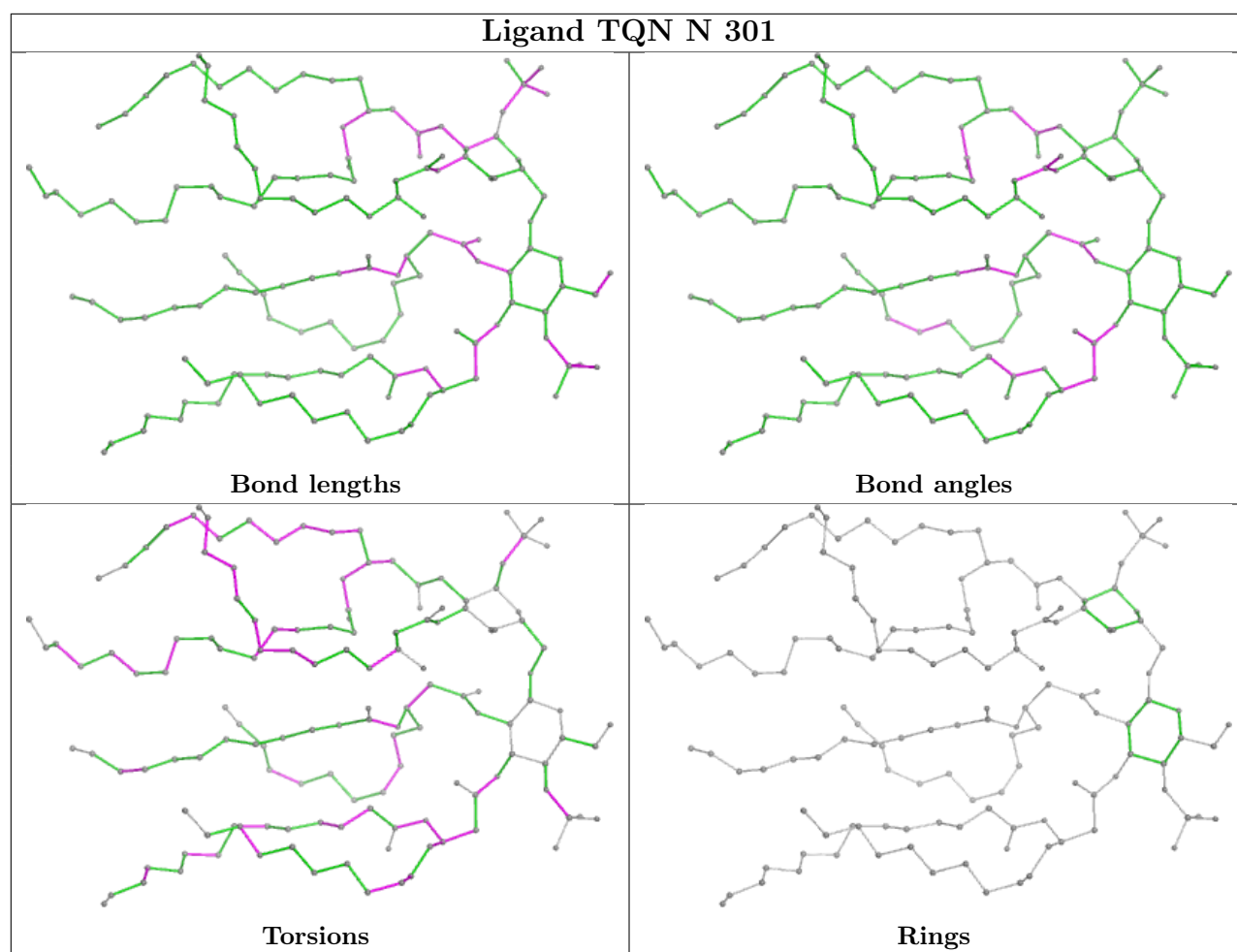


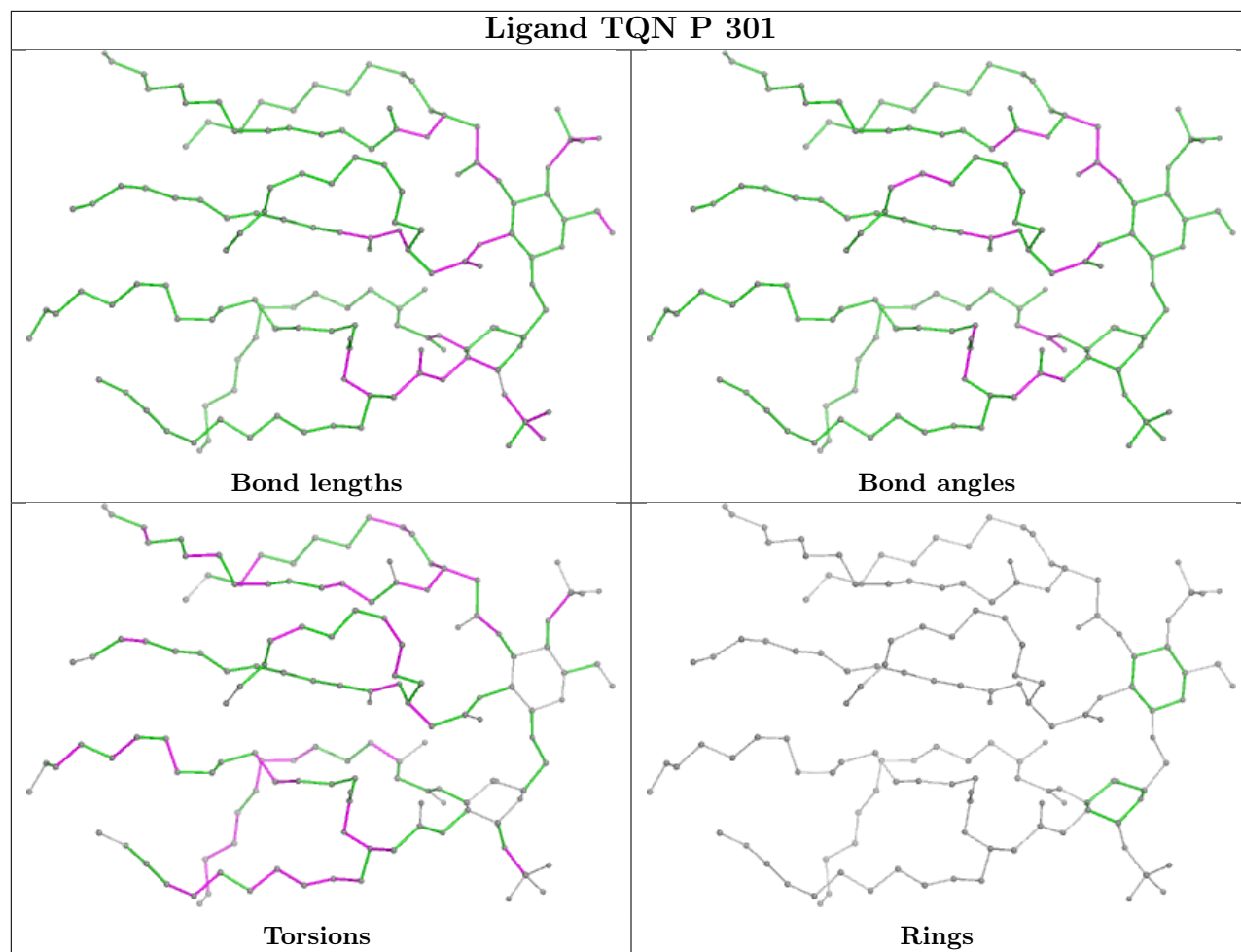


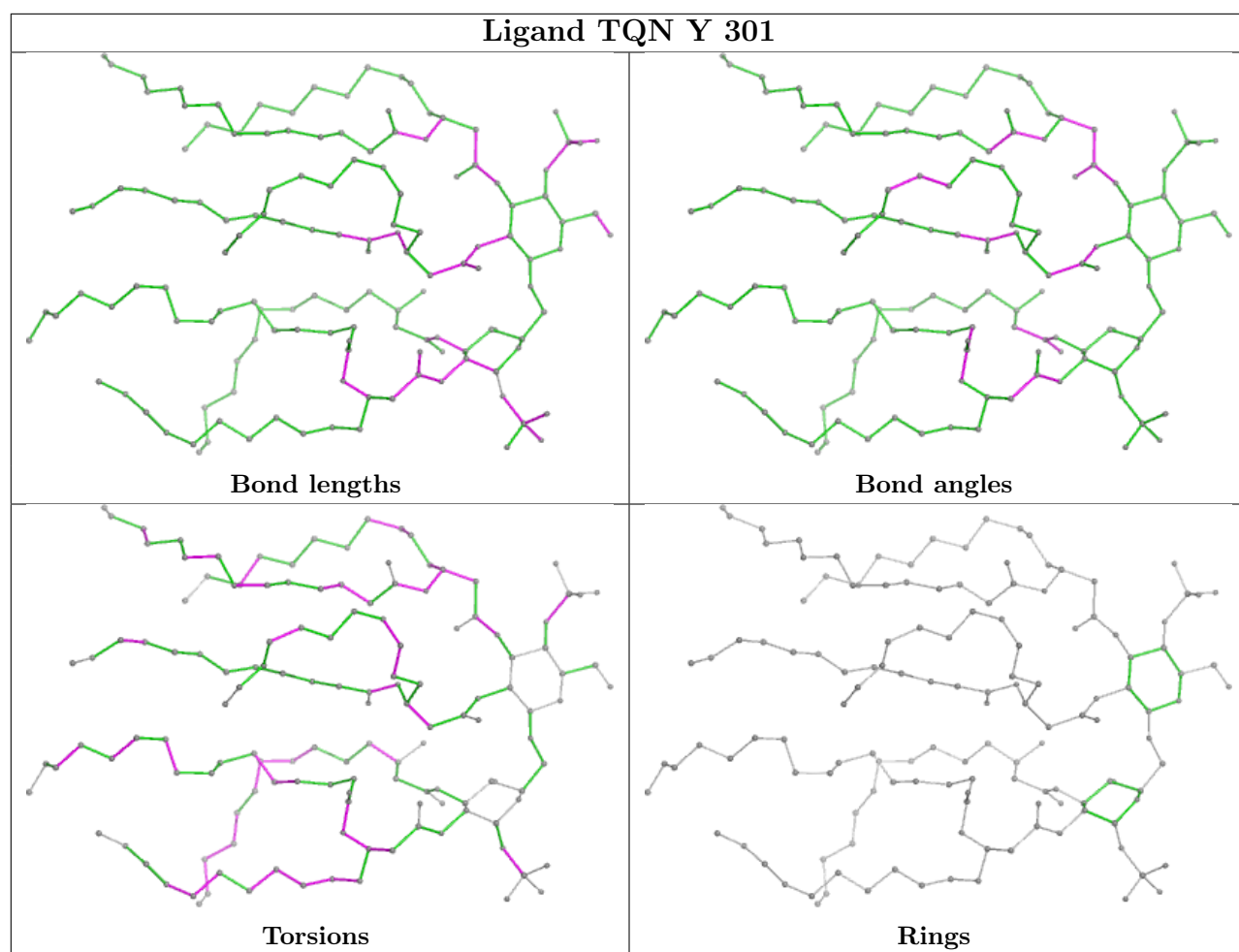


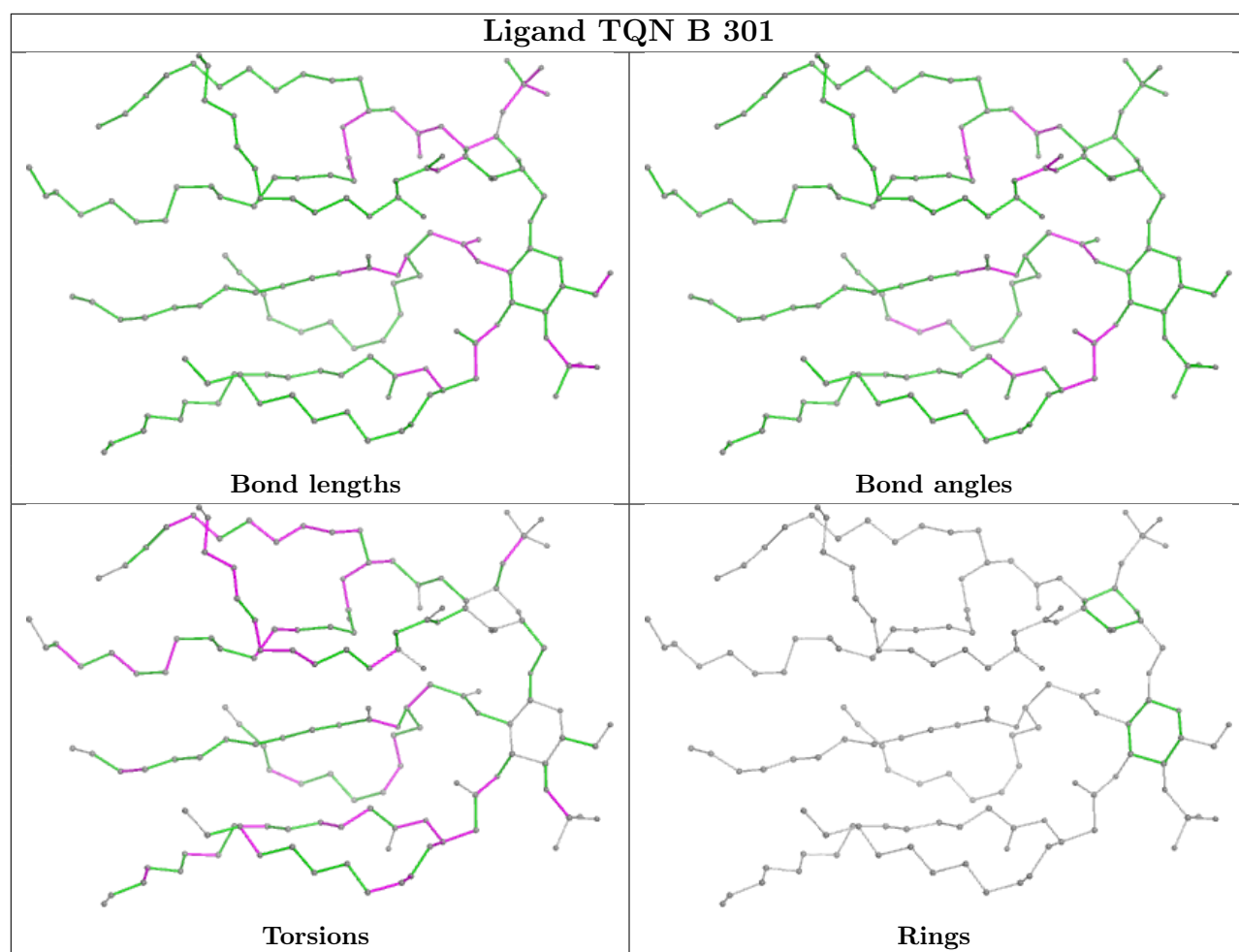


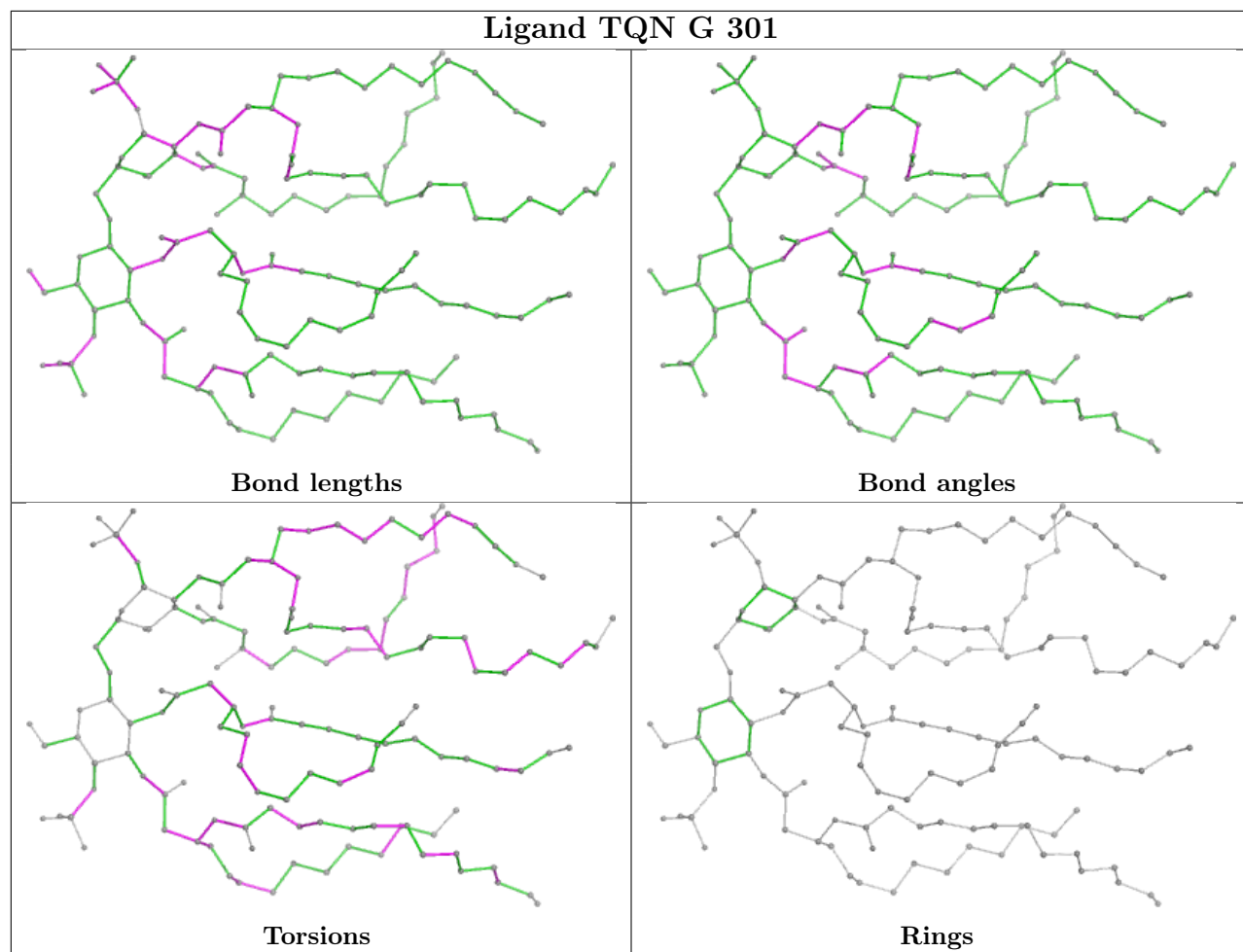




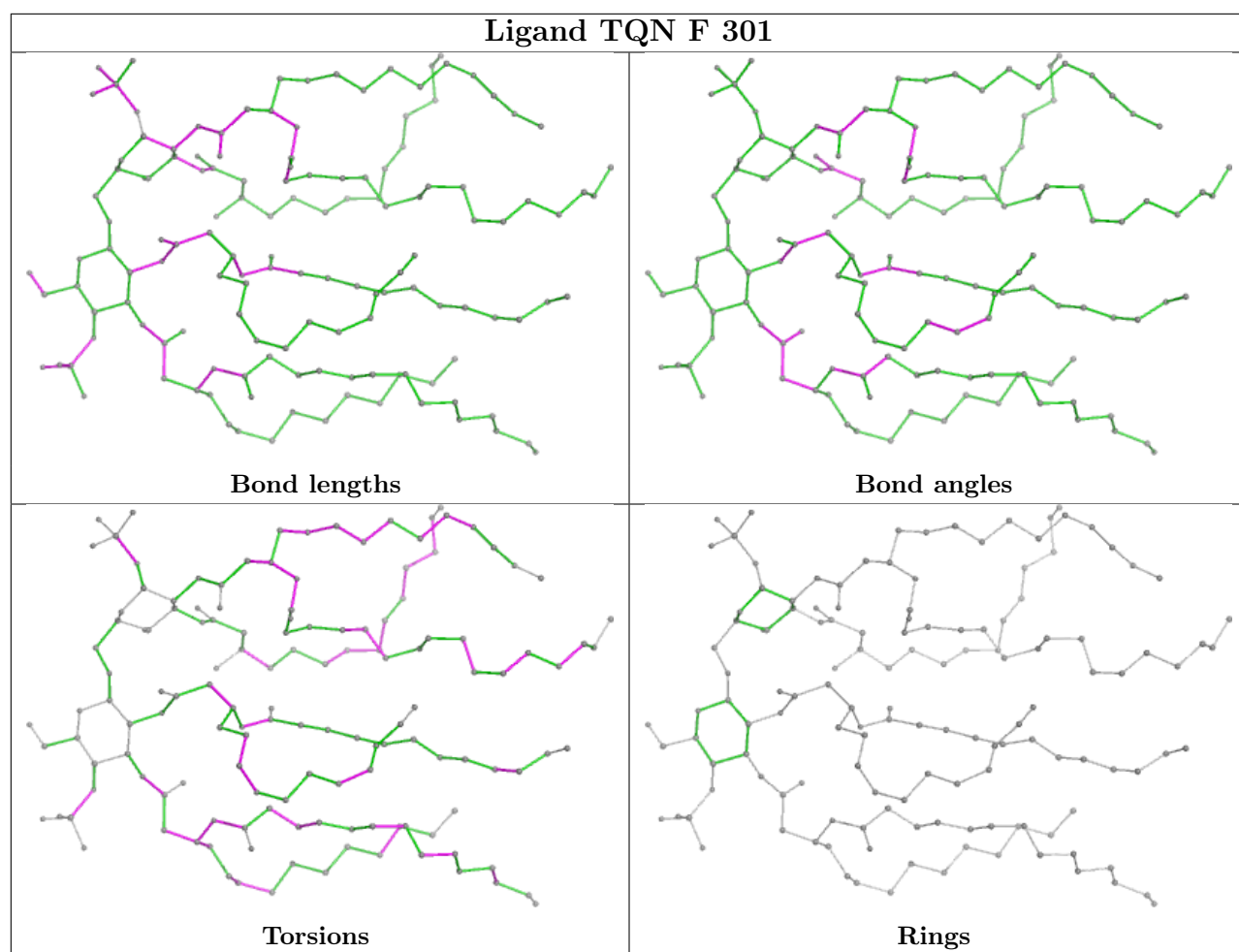


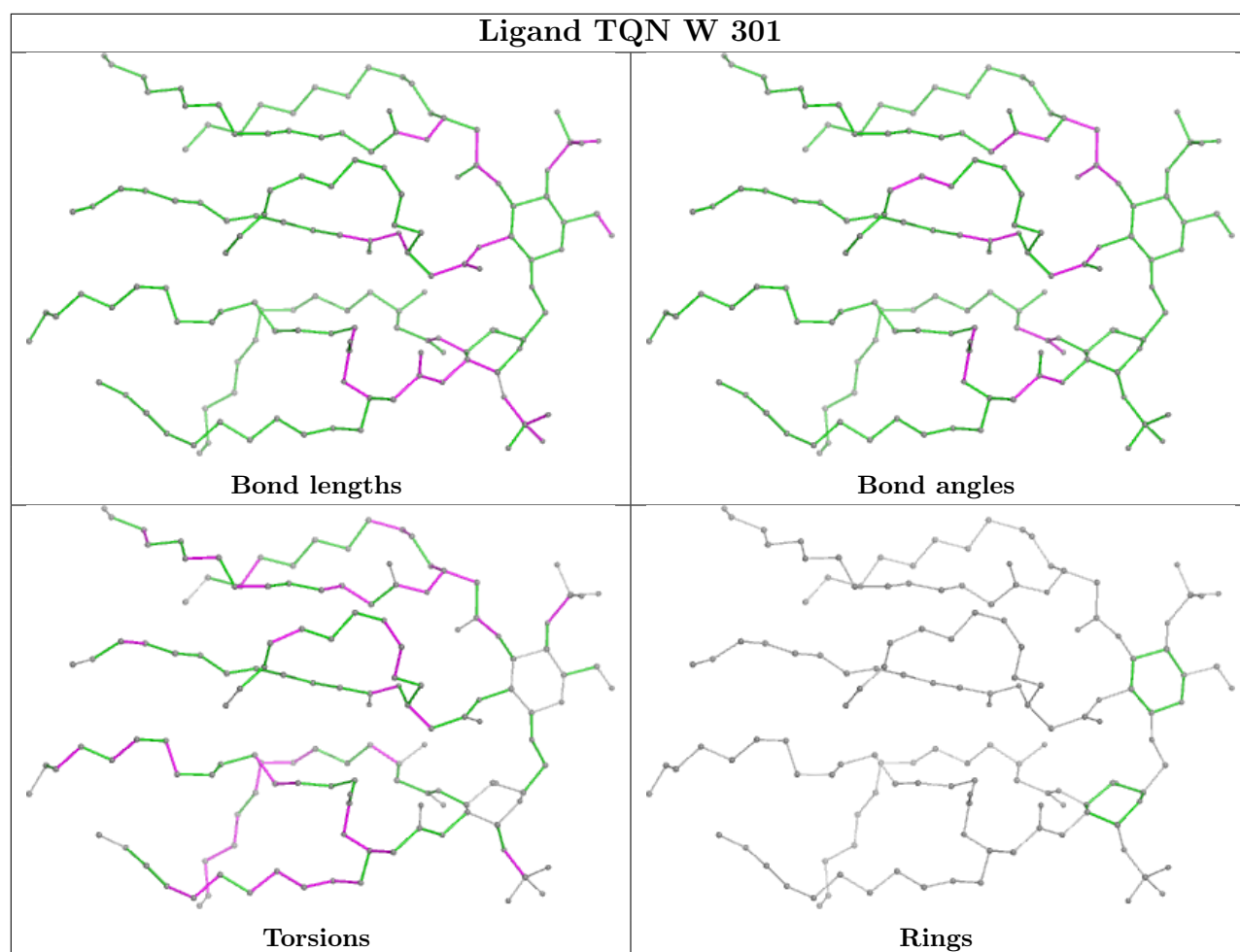












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

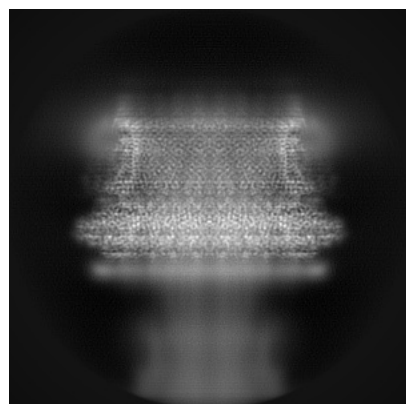
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12183. These allow visual inspection of the internal detail of the map and identification of artifacts.

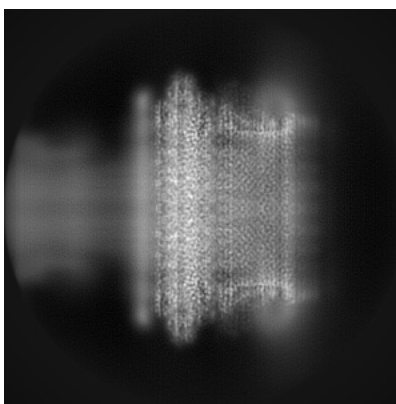
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

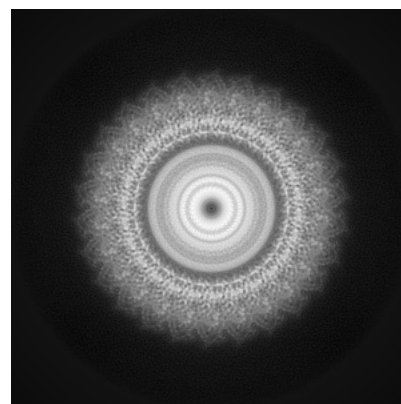
#### 6.1.1 Primary map



X

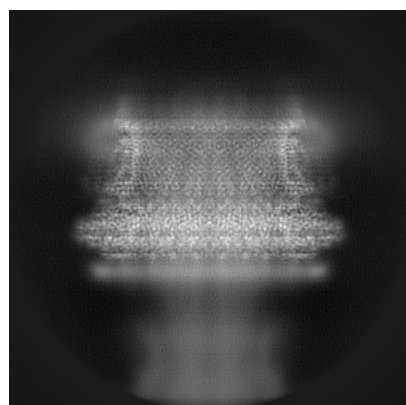


Y

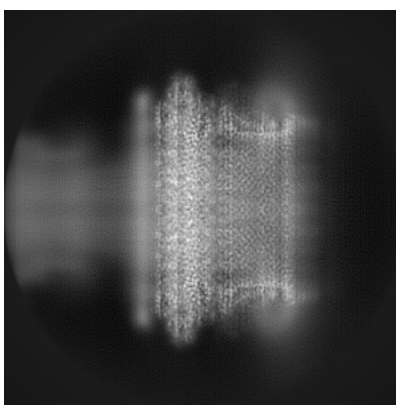


Z

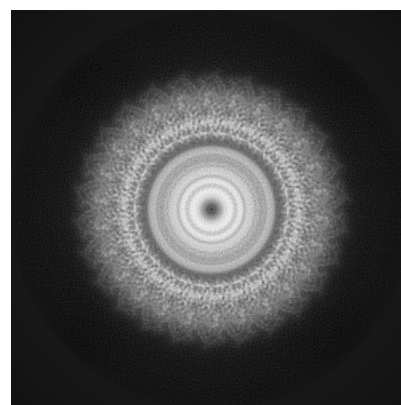
#### 6.1.2 Raw map



X



Y

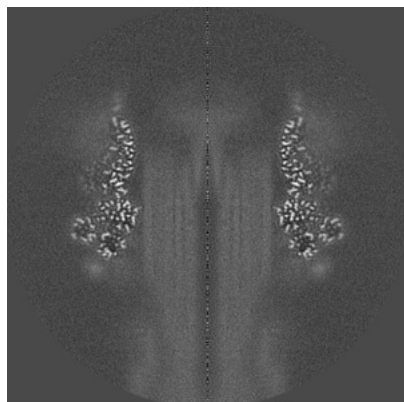


Z

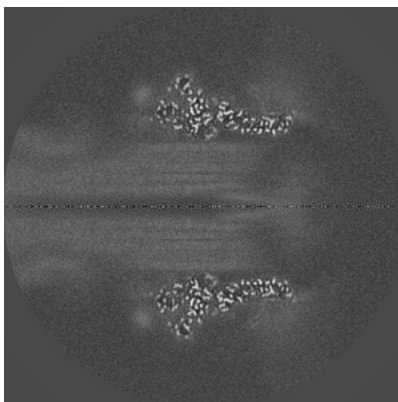
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

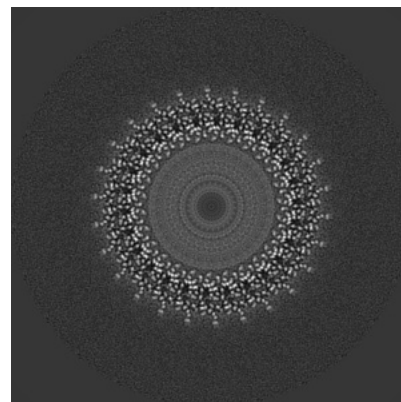
### 6.2.1 Primary map



X Index: 216

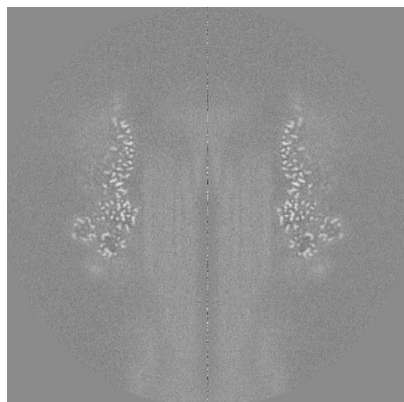


Y Index: 216

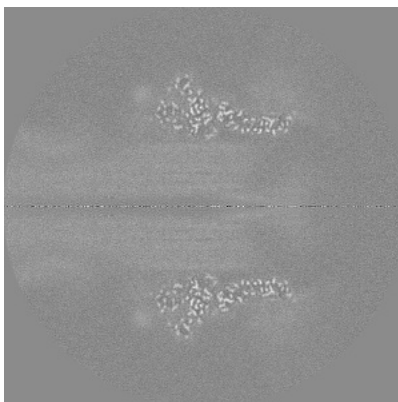


Z Index: 216

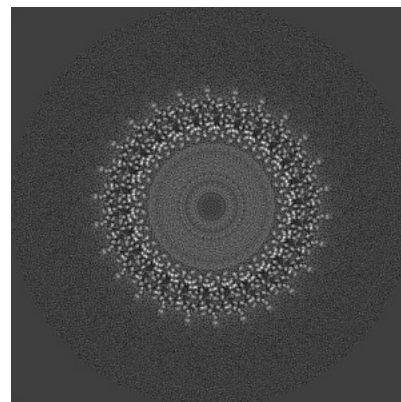
### 6.2.2 Raw map



X Index: 216



Y Index: 216

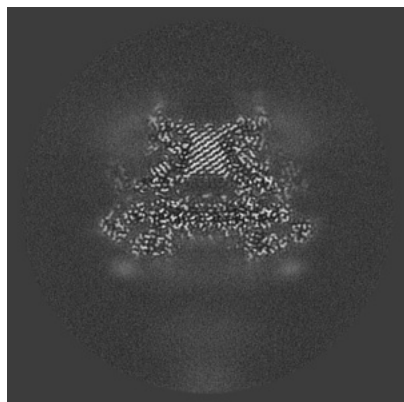


Z Index: 216

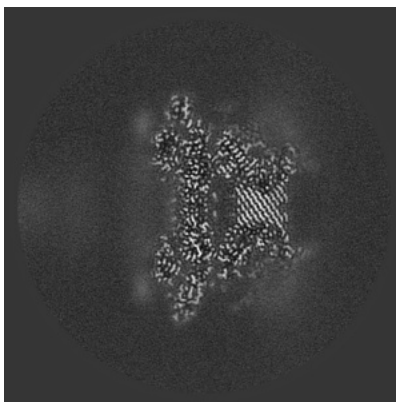
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

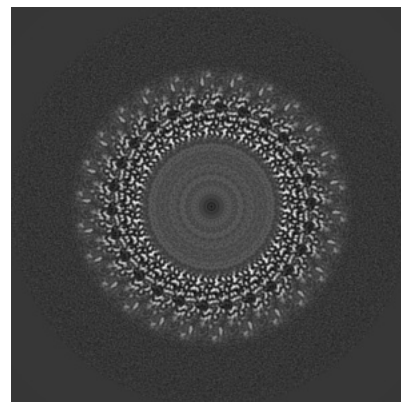
### 6.3.1 Primary map



X Index: 134

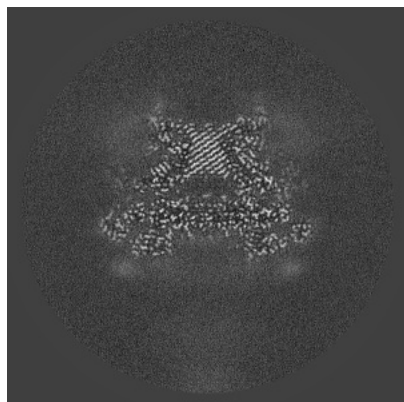


Y Index: 134

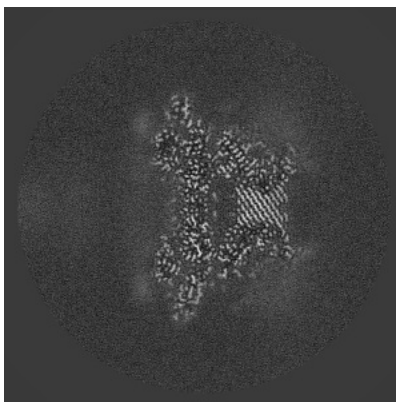


Z Index: 204

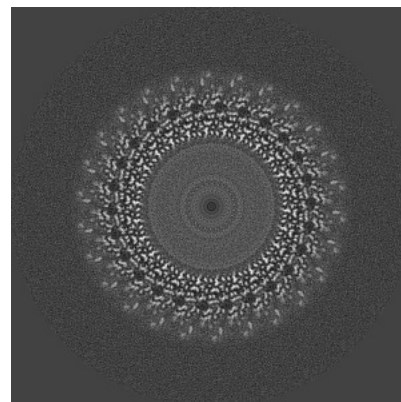
### 6.3.2 Raw map



X Index: 134



Y Index: 134



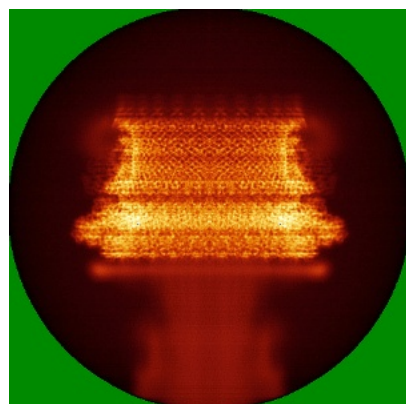
Z Index: 204

The images above show the largest variance slices of the map in three orthogonal directions.

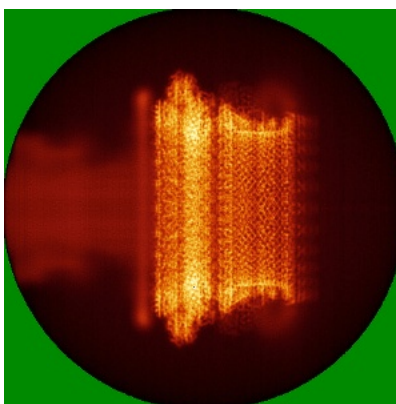


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

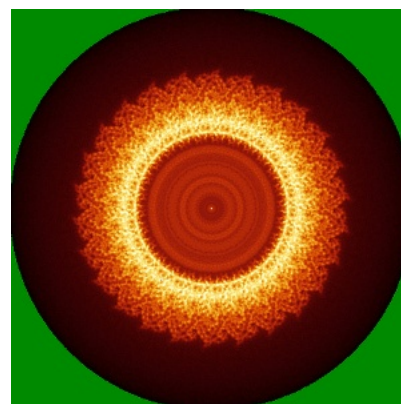
### 6.4.1 Primary map



X

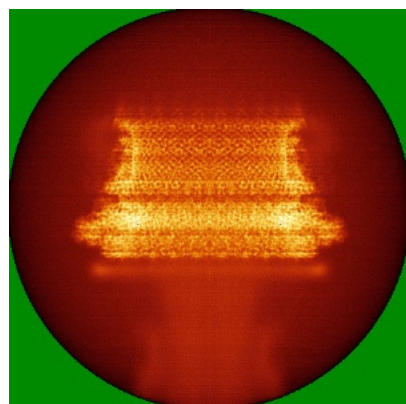


Y

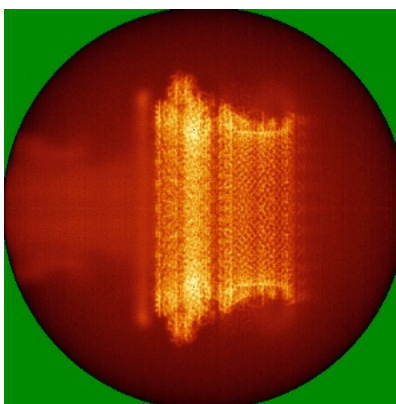


Z

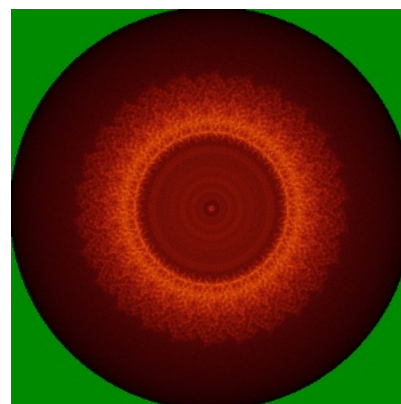
### 6.4.2 Raw map



X



Y

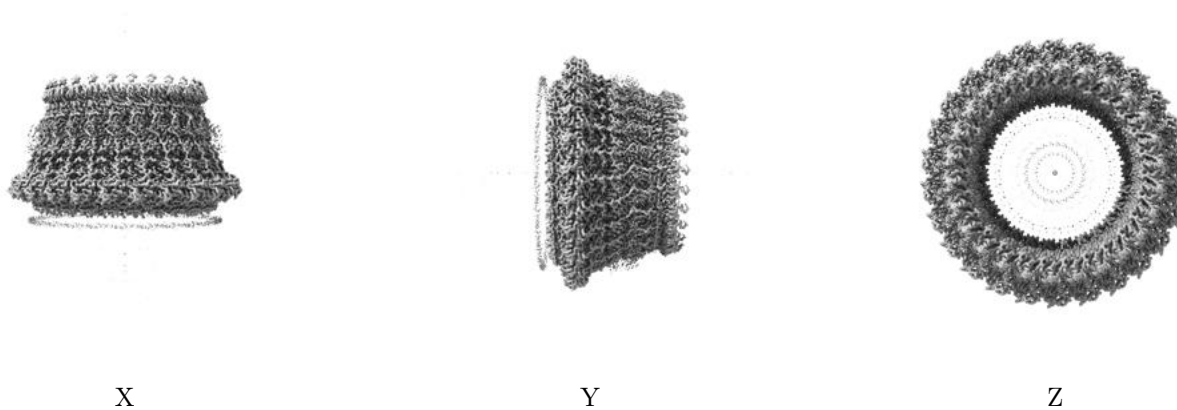


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

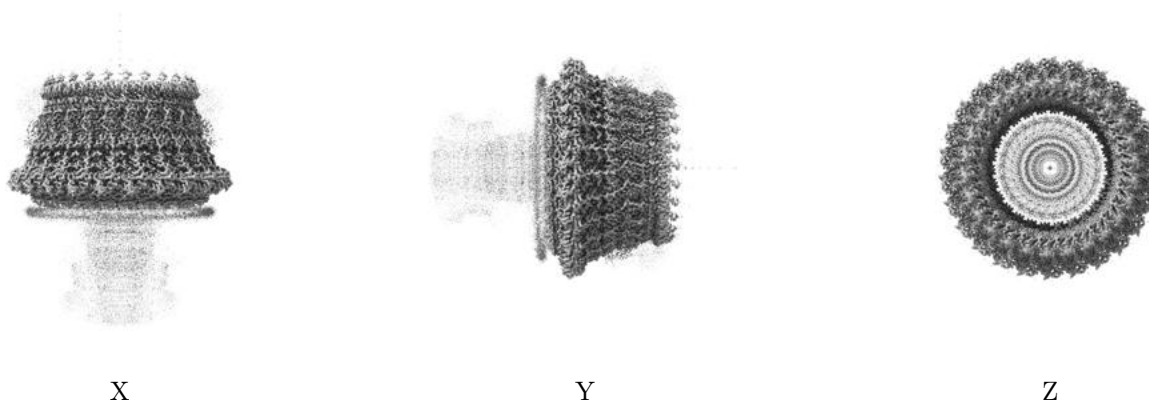
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

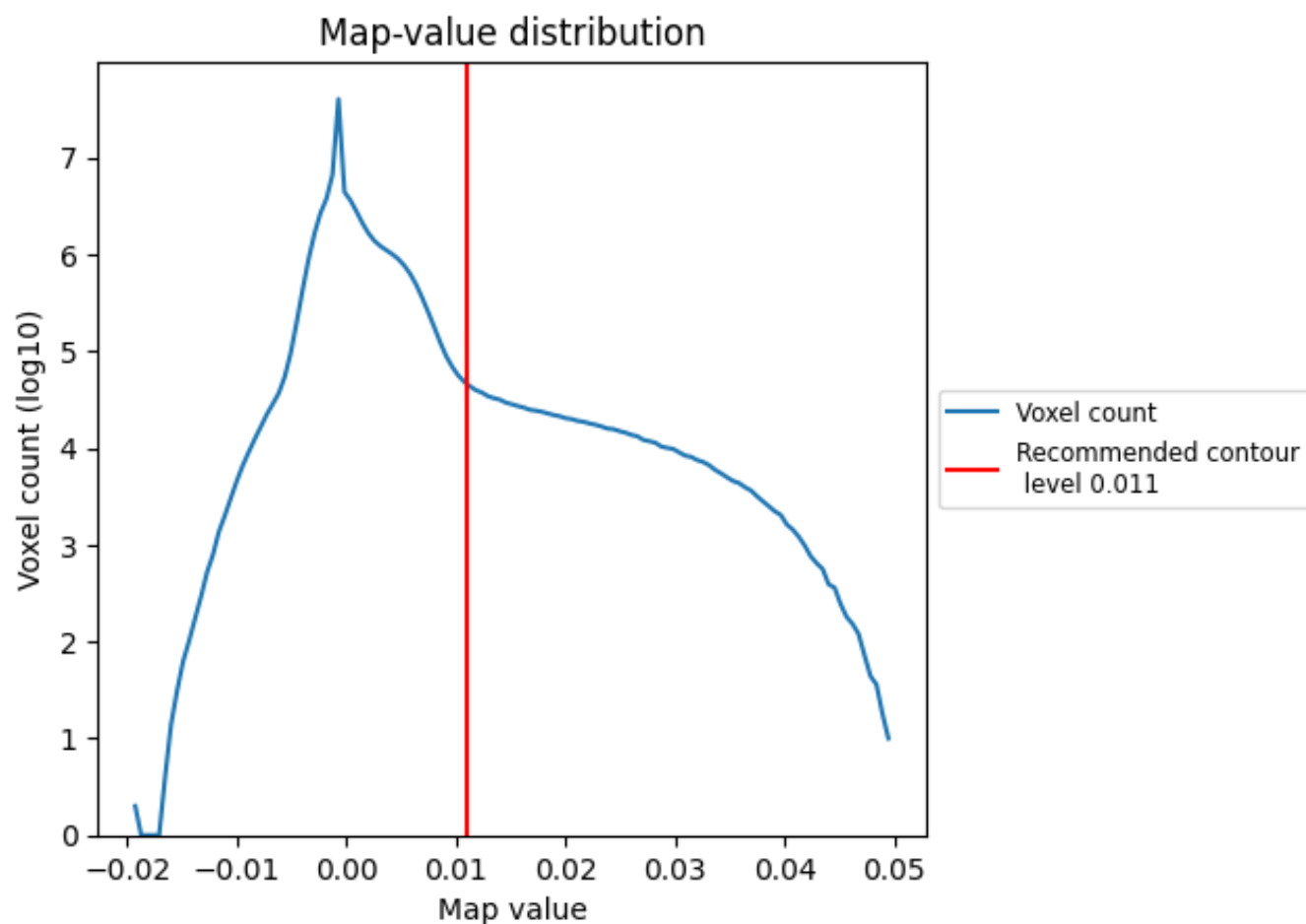
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

This section contains the results of statistical analysis of the map.

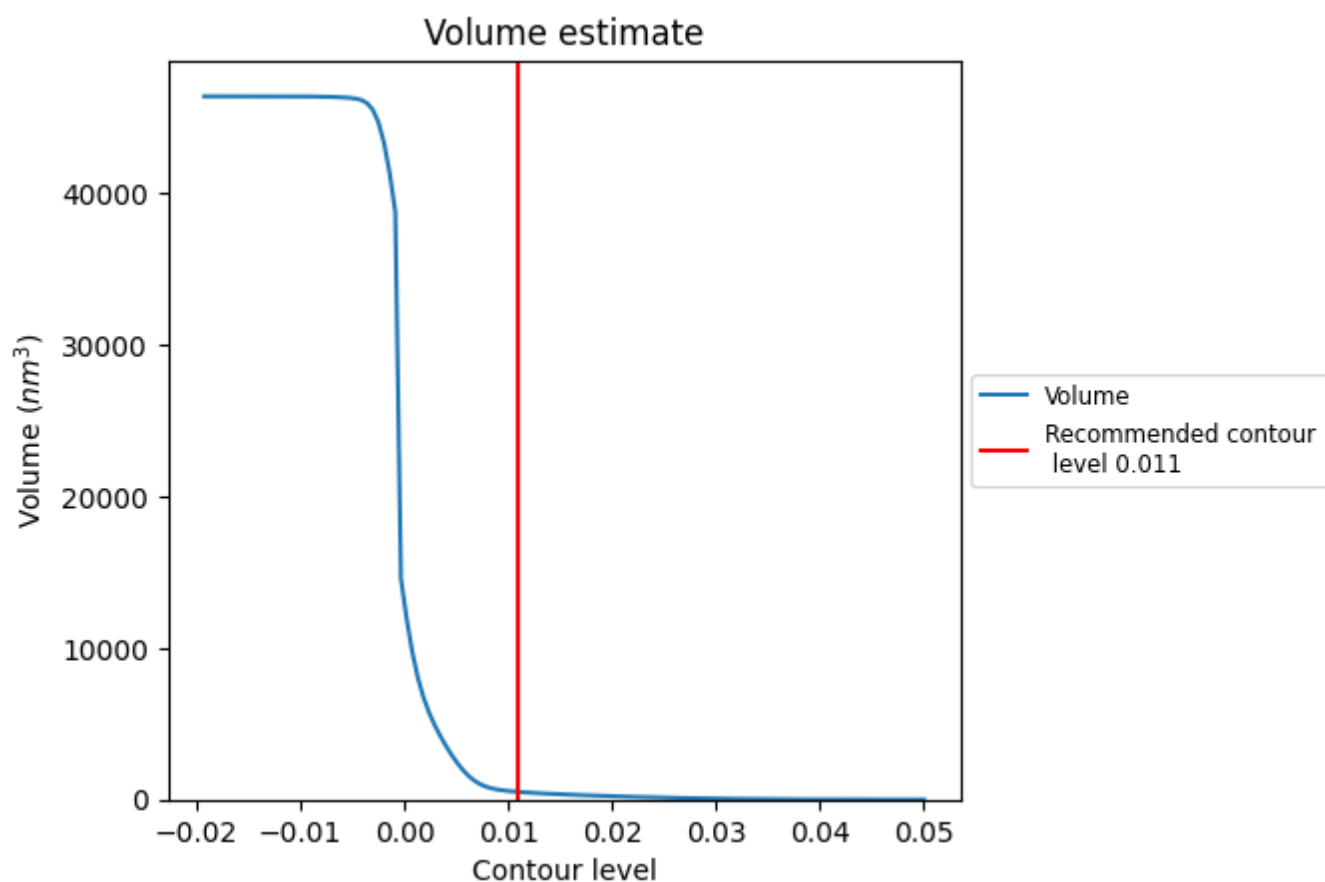
### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



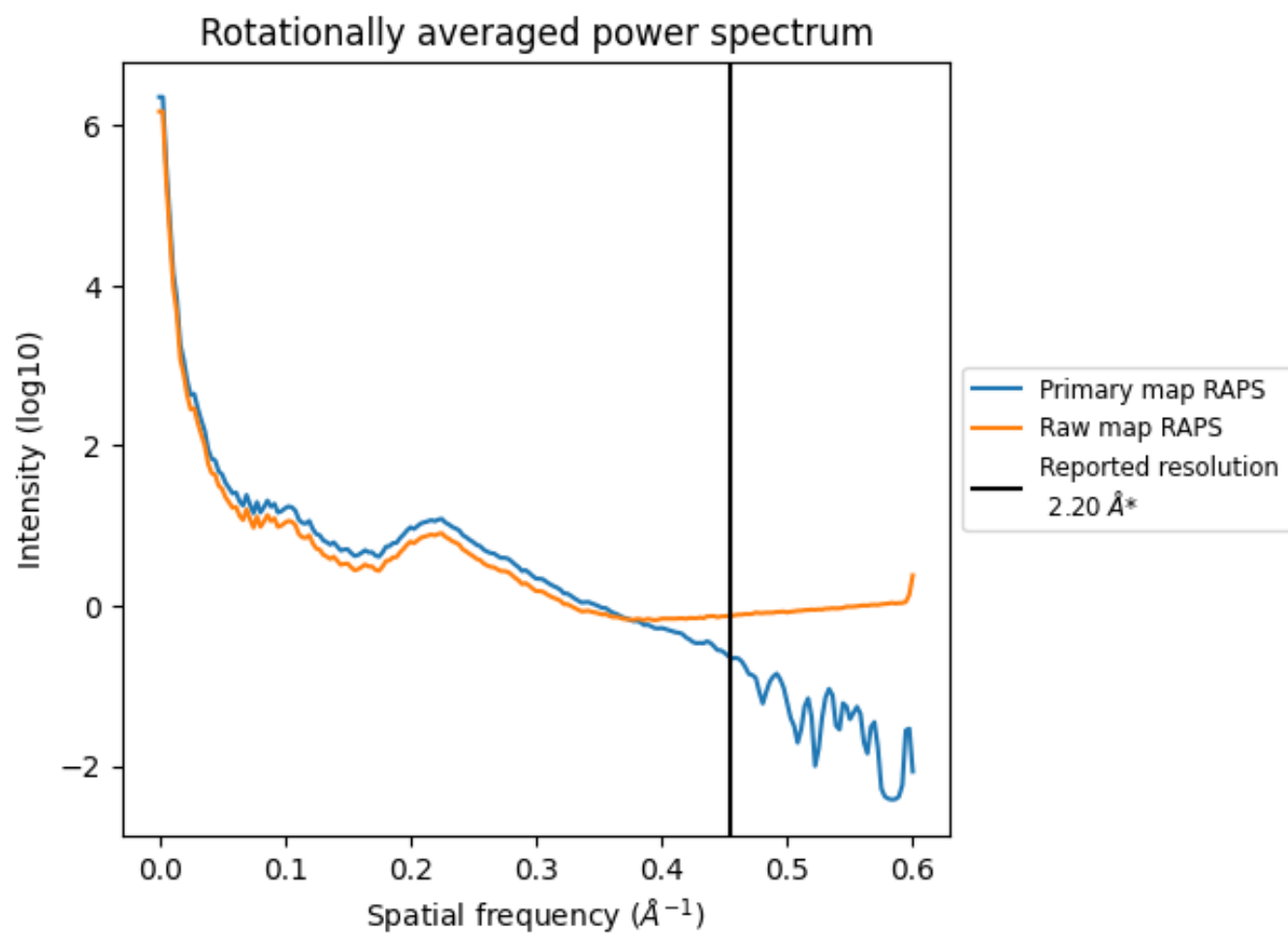
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 505 nm<sup>3</sup>; this corresponds to an approximate mass of 456 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

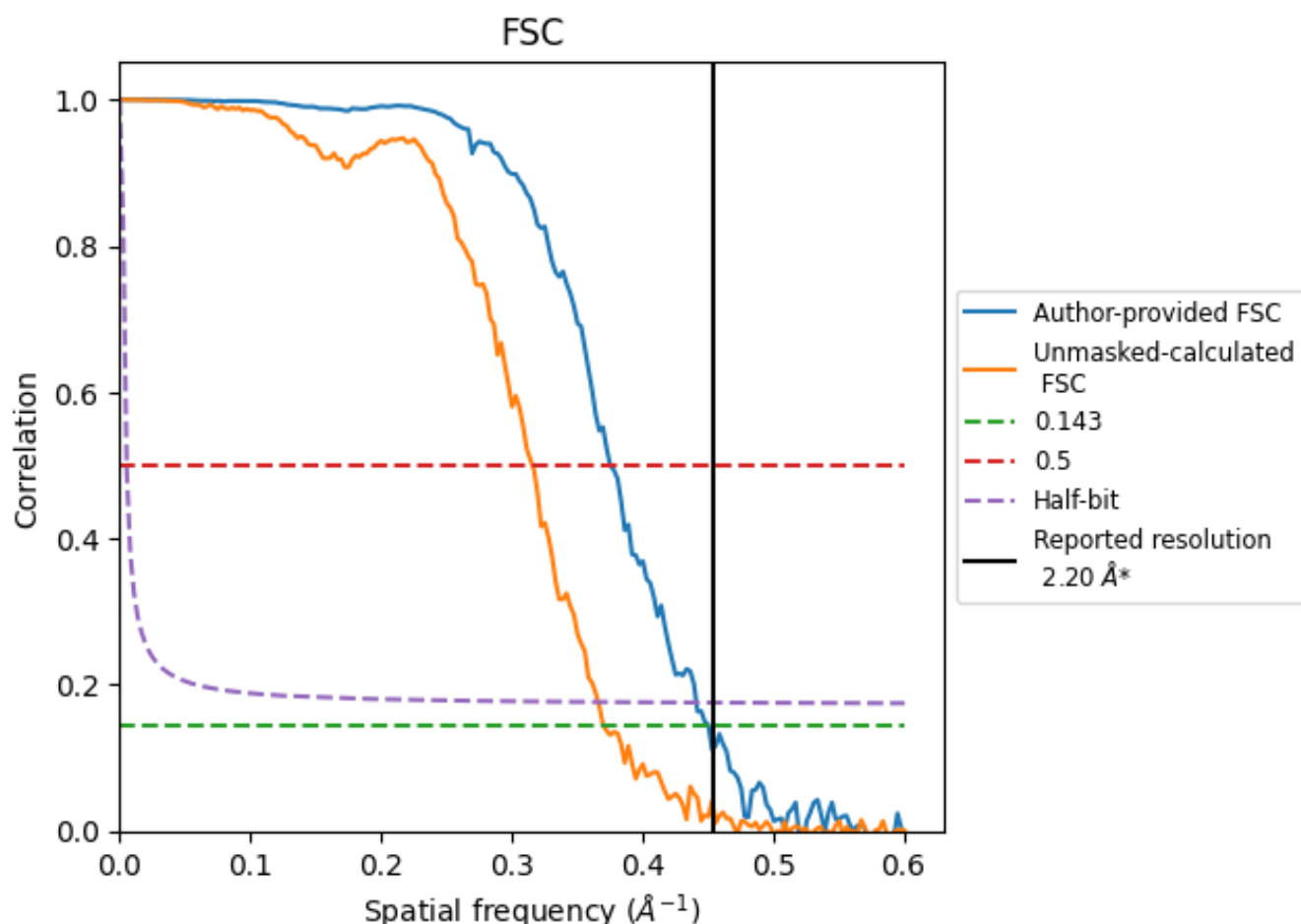


\*Reported resolution corresponds to spatial frequency of 0.455 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.455  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

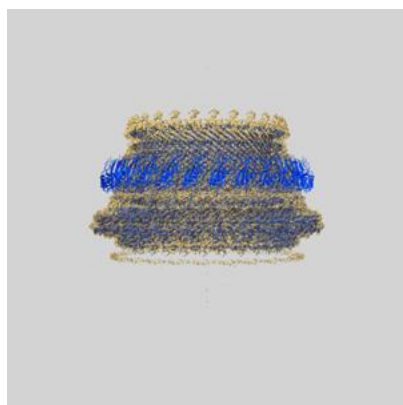
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.22	2.66	2.27
Unmasked-calculated*	2.70	3.16	2.73

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.70 differs from the reported value 2.2 by more than 10 %

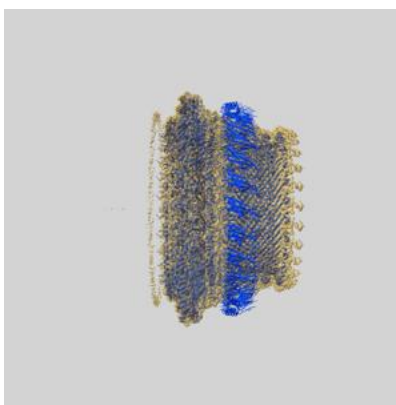
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12183 and PDB model 7BGL. Per-residue inclusion information can be found in section 3 on page 15.

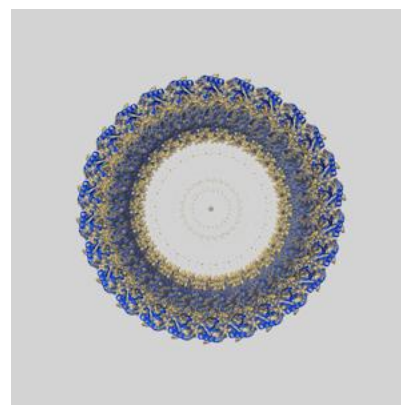
### 9.1 Map-model overlay [i](#)



X



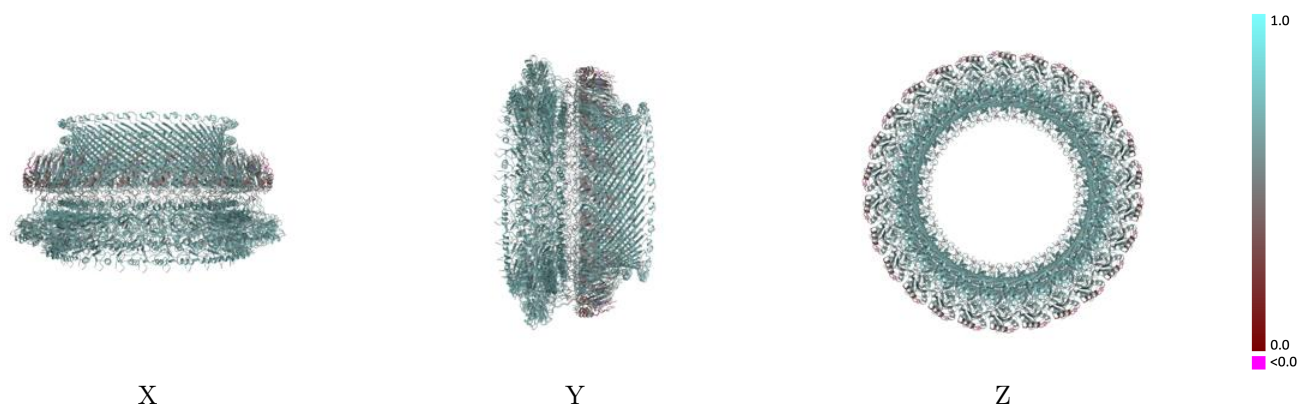
Y



Z

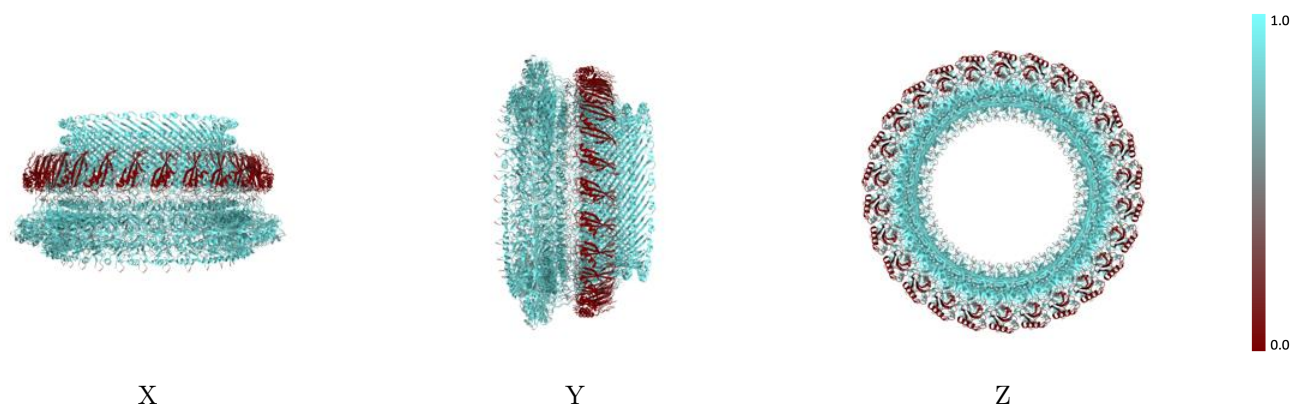
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



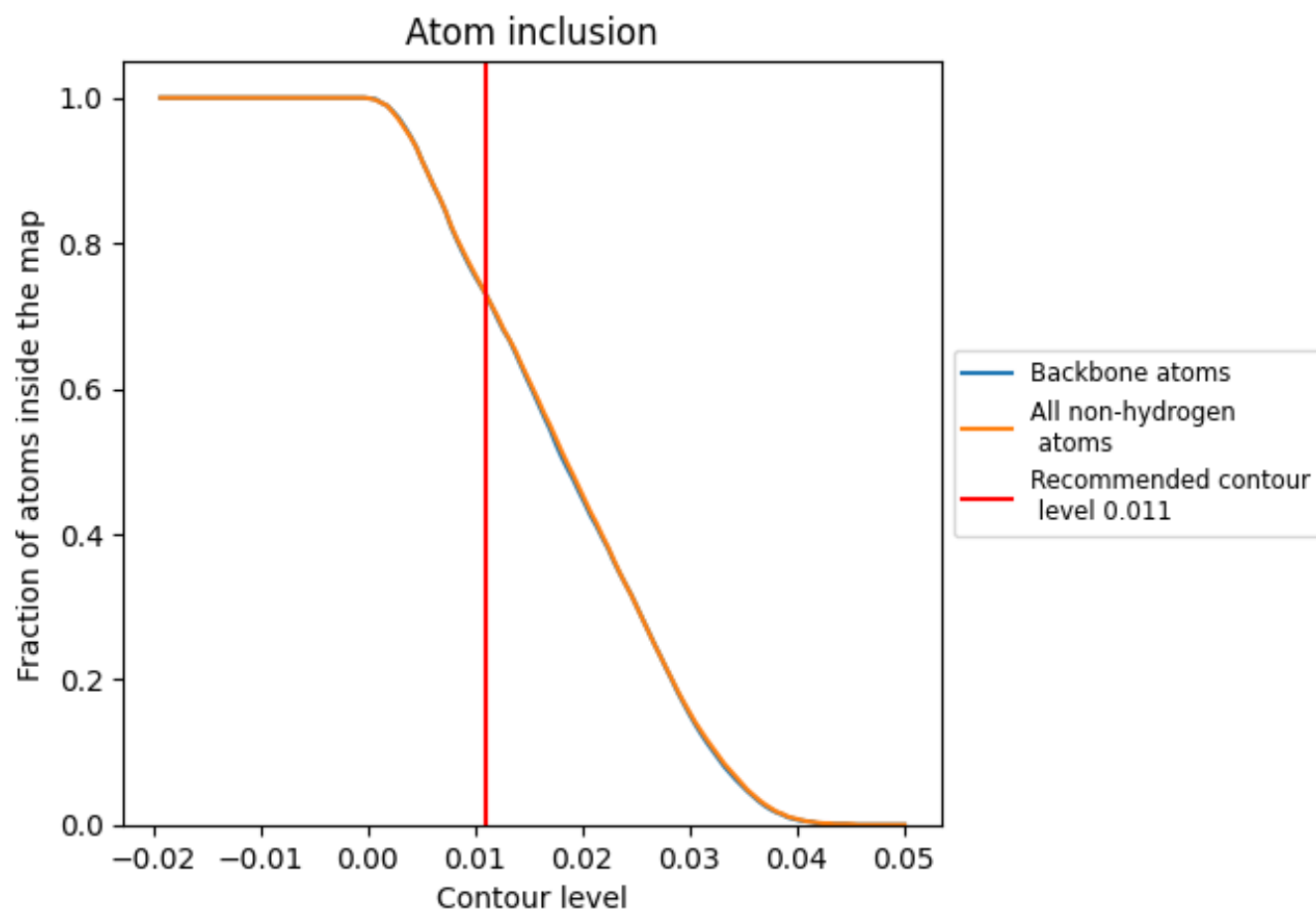
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.011).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.011) and Q-score for the entire model and for each chain.





















































































Chain	Atom inclusion	Q-score
All	 0.7300	 0.6030
1	 0.0440	 0.4570
10	 0.0460	 0.4580
11	 0.0480	 0.4580
12	 0.0460	 0.4610
13	 0.0460	 0.4630
14	 0.0440	 0.4600
15	 0.0460	 0.4590
16	 0.0490	 0.4600
17	 0.0460	 0.4600
18	 0.0460	 0.4580
19	 0.0460	 0.4580
2	 0.0460	 0.4580
20	 0.0520	 0.4590
21	 0.0490	 0.4590
22	 0.0480	 0.4610
23	 0.0460	 0.4590
24	 0.0480	 0.4550
25	 0.0460	 0.4580
26	 0.0480	 0.4570
3	 0.0490	 0.4570
4	 0.0460	 0.4570
5	 0.0460	 0.4570
6	 0.0460	 0.4590
7	 0.0520	 0.4610
8	 0.0490	 0.4620
9	 0.0480	 0.4610
A	 0.8390	 0.6140
B	 0.8460	 0.6150
C	 0.8410	 0.6140
D	 0.8370	 0.6140
E	 0.8410	 0.6140
F	 0.8400	 0.6140
G	 0.8420	 0.6140
H	 0.8410	 0.6140



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Chain	Atom inclusion	Q-score
I	 0.8400	 0.6140
J	 0.8410	 0.6150
K	 0.8430	 0.6160
L	 0.8400	 0.6160
M	 0.8430	 0.6150
N	 0.8380	 0.6160
O	 0.8440	 0.6160
P	 0.8390	 0.6160
Q	 0.8390	 0.6160
R	 0.8400	 0.6160
S	 0.8400	 0.6160
T	 0.8400	 0.6170
U	 0.8390	 0.6160
V	 0.8400	 0.6160
W	 0.8390	 0.6150
X	 0.8430	 0.6150
Y	 0.8400	 0.6160
Z	 0.8440	 0.6170
a	 0.8610	 0.6350
b	 0.8630	 0.6350
c	 0.8580	 0.6340
d	 0.8620	 0.6330
e	 0.8600	 0.6340
f	 0.8590	 0.6350
g	 0.8580	 0.6350
h	 0.8580	 0.6340
i	 0.8600	 0.6330
j	 0.8600	 0.6340
k	 0.8590	 0.6350
l	 0.8570	 0.6350
m	 0.8610	 0.6350
n	 0.8620	 0.6350
o	 0.8630	 0.6340
p	 0.8600	 0.6340
q	 0.8630	 0.6340
r	 0.8590	 0.6340
s	 0.8580	 0.6340
t	 0.8580	 0.6330
u	 0.8590	 0.6330
v	 0.8600	 0.6340
w	 0.8590	 0.6330
x	 0.8600	 0.6340

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Chain	Atom inclusion	Q-score
y	 0.8590	 0.6330
z	 0.8600	 0.6330