



Full wwPDB EM Validation Report ⓘ

Sep 14, 2026 – 01:44 PM EDT

PDB ID : 37CY / pdb_000037cy
EMDB ID : EMD-78079
Title : Cryo-EM structure of Nitrogenase MoFe protein from Methanosarcina acetivorans bound to the NifI inhibitor complex in strictly anaerobic condition
Authors : Kashyap, R.; Antony, E.
Deposited on : 2026-07-14
Resolution : 3.80 Å(reported)
Based on initial model : .

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

We welcome your comments at 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>.

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

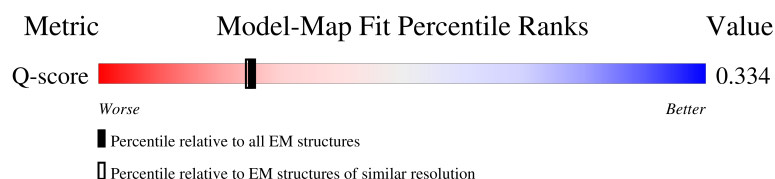
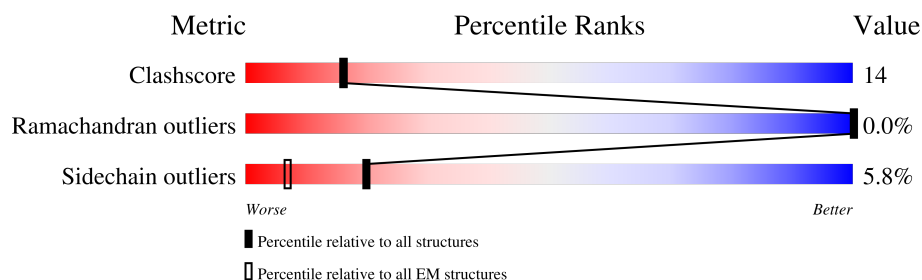
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

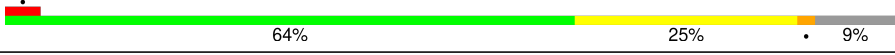
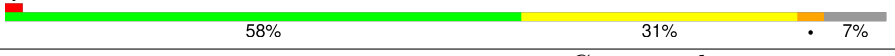
The reported resolution of this entry is 3.80 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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 ≥ 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	559	
1	C	559	
1	K	559	
1	L	559	

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Mol	Chain	Length	Quality of chain
1	U	559	
1	V	559	
2	B	456	
2	D	456	
2	M	456	
2	N	456	
2	W	456	
2	X	456	
3	F	105	
3	H	105	
3	I	105	
3	J	105	
3	P	105	
3	R	105	
3	S	105	
3	T	105	
3	Z	105	
3	b	105	
3	c	105	
3	d	105	
4	E	125	
4	G	125	
4	O	125	
4	Q	125	
4	Y	125	

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Mol	Chain	Length	Quality of chain
4	a	125	

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
5	CLF	A	601	-	-	X	-
5	CLF	D	601	-	-	X	-
5	CLF	L	603	-	-	X	-
5	CLF	M	501	-	-	X	-
5	CLF	V	601	-	-	X	-
5	CLF	W	601	-	-	X	-
6	ICS	A	602	-	-	X	-
6	ICS	C	601	-	-	X	-
6	ICS	K	601	-	-	X	-
6	ICS	L	602	-	-	X	-
6	ICS	U	601	-	-	X	-
6	ICS	V	602	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 58733 atoms, of which 0 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 Nitrogenase protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	496	Total	C	N	O	S	0	0
			3944	2505	680	739	20		
1	C	519	Total	C	N	O	S	0	0
			4137	2625	713	778	21		
1	K	508	Total	C	N	O	S	0	0
			4049	2572	699	758	20		
1	V	510	Total	C	N	O	S	0	0
			4054	2572	701	760	21		
1	L	519	Total	C	N	O	S	0	0
			4133	2624	713	776	20		
1	U	511	Total	C	N	O	S	0	0
			4070	2583	702	765	20		

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	initiating methionine	UNP Q8TJ90
A	-29	TRP	-	expression tag	UNP Q8TJ90
A	-28	SER	-	expression tag	UNP Q8TJ90
A	-27	HIS	-	expression tag	UNP Q8TJ90
A	-26	PRO	-	expression tag	UNP Q8TJ90
A	-25	GLN	-	expression tag	UNP Q8TJ90
A	-24	PHE	-	expression tag	UNP Q8TJ90
A	-23	GLU	-	expression tag	UNP Q8TJ90
A	-22	LYS	-	expression tag	UNP Q8TJ90
A	-21	GLY	-	expression tag	UNP Q8TJ90
A	-20	GLY	-	expression tag	UNP Q8TJ90
A	-19	GLY	-	expression tag	UNP Q8TJ90
A	-18	SER	-	expression tag	UNP Q8TJ90
A	-17	GLY	-	expression tag	UNP Q8TJ90
A	-16	GLY	-	expression tag	UNP Q8TJ90
A	-15	GLY	-	expression tag	UNP Q8TJ90
A	-14	SER	-	expression tag	UNP Q8TJ90
A	-13	GLY	-	expression tag	UNP Q8TJ90

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	GLY	-	expression tag	UNP Q8TJ90
A	-11	GLY	-	expression tag	UNP Q8TJ90
A	-10	SER	-	expression tag	UNP Q8TJ90
A	-9	TRP	-	expression tag	UNP Q8TJ90
A	-8	SER	-	expression tag	UNP Q8TJ90
A	-7	HIS	-	expression tag	UNP Q8TJ90
A	-6	PRO	-	expression tag	UNP Q8TJ90
A	-5	GLN	-	expression tag	UNP Q8TJ90
A	-4	PHE	-	expression tag	UNP Q8TJ90
A	-3	GLU	-	expression tag	UNP Q8TJ90
A	-2	LYS	-	expression tag	UNP Q8TJ90
A	-1	SER	-	expression tag	UNP Q8TJ90
A	0	GLY	-	expression tag	UNP Q8TJ90
C	-30	MET	-	initiating methionine	UNP Q8TJ90
C	-29	TRP	-	expression tag	UNP Q8TJ90
C	-28	SER	-	expression tag	UNP Q8TJ90
C	-27	HIS	-	expression tag	UNP Q8TJ90
C	-26	PRO	-	expression tag	UNP Q8TJ90
C	-25	GLN	-	expression tag	UNP Q8TJ90
C	-24	PHE	-	expression tag	UNP Q8TJ90
C	-23	GLU	-	expression tag	UNP Q8TJ90
C	-22	LYS	-	expression tag	UNP Q8TJ90
C	-21	GLY	-	expression tag	UNP Q8TJ90
C	-20	GLY	-	expression tag	UNP Q8TJ90
C	-19	GLY	-	expression tag	UNP Q8TJ90
C	-18	SER	-	expression tag	UNP Q8TJ90
C	-17	GLY	-	expression tag	UNP Q8TJ90
C	-16	GLY	-	expression tag	UNP Q8TJ90
C	-15	GLY	-	expression tag	UNP Q8TJ90
C	-14	SER	-	expression tag	UNP Q8TJ90
C	-13	GLY	-	expression tag	UNP Q8TJ90
C	-12	GLY	-	expression tag	UNP Q8TJ90
C	-11	GLY	-	expression tag	UNP Q8TJ90
C	-10	SER	-	expression tag	UNP Q8TJ90
C	-9	TRP	-	expression tag	UNP Q8TJ90
C	-8	SER	-	expression tag	UNP Q8TJ90
C	-7	HIS	-	expression tag	UNP Q8TJ90
C	-6	PRO	-	expression tag	UNP Q8TJ90
C	-5	GLN	-	expression tag	UNP Q8TJ90
C	-4	PHE	-	expression tag	UNP Q8TJ90
C	-3	GLU	-	expression tag	UNP Q8TJ90
C	-2	LYS	-	expression tag	UNP Q8TJ90

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP Q8TJ90
C	0	GLY	-	expression tag	UNP Q8TJ90
K	-30	MET	-	initiating methionine	UNP Q8TJ90
K	-29	TRP	-	expression tag	UNP Q8TJ90
K	-28	SER	-	expression tag	UNP Q8TJ90
K	-27	HIS	-	expression tag	UNP Q8TJ90
K	-26	PRO	-	expression tag	UNP Q8TJ90
K	-25	GLN	-	expression tag	UNP Q8TJ90
K	-24	PHE	-	expression tag	UNP Q8TJ90
K	-23	GLU	-	expression tag	UNP Q8TJ90
K	-22	LYS	-	expression tag	UNP Q8TJ90
K	-21	GLY	-	expression tag	UNP Q8TJ90
K	-20	GLY	-	expression tag	UNP Q8TJ90
K	-19	GLY	-	expression tag	UNP Q8TJ90
K	-18	SER	-	expression tag	UNP Q8TJ90
K	-17	GLY	-	expression tag	UNP Q8TJ90
K	-16	GLY	-	expression tag	UNP Q8TJ90
K	-15	GLY	-	expression tag	UNP Q8TJ90
K	-14	SER	-	expression tag	UNP Q8TJ90
K	-13	GLY	-	expression tag	UNP Q8TJ90
K	-12	GLY	-	expression tag	UNP Q8TJ90
K	-11	GLY	-	expression tag	UNP Q8TJ90
K	-10	SER	-	expression tag	UNP Q8TJ90
K	-9	TRP	-	expression tag	UNP Q8TJ90
K	-8	SER	-	expression tag	UNP Q8TJ90
K	-7	HIS	-	expression tag	UNP Q8TJ90
K	-6	PRO	-	expression tag	UNP Q8TJ90
K	-5	GLN	-	expression tag	UNP Q8TJ90
K	-4	PHE	-	expression tag	UNP Q8TJ90
K	-3	GLU	-	expression tag	UNP Q8TJ90
K	-2	LYS	-	expression tag	UNP Q8TJ90
K	-1	SER	-	expression tag	UNP Q8TJ90
K	0	GLY	-	expression tag	UNP Q8TJ90
V	-30	MET	-	initiating methionine	UNP Q8TJ90
V	-29	TRP	-	expression tag	UNP Q8TJ90
V	-28	SER	-	expression tag	UNP Q8TJ90
V	-27	HIS	-	expression tag	UNP Q8TJ90
V	-26	PRO	-	expression tag	UNP Q8TJ90
V	-25	GLN	-	expression tag	UNP Q8TJ90
V	-24	PHE	-	expression tag	UNP Q8TJ90
V	-23	GLU	-	expression tag	UNP Q8TJ90
V	-22	LYS	-	expression tag	UNP Q8TJ90

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Chain	Residue	Modelled	Actual	Comment	Reference
V	-21	GLY	-	expression tag	UNP Q8TJ90
V	-20	GLY	-	expression tag	UNP Q8TJ90
V	-19	GLY	-	expression tag	UNP Q8TJ90
V	-18	SER	-	expression tag	UNP Q8TJ90
V	-17	GLY	-	expression tag	UNP Q8TJ90
V	-16	GLY	-	expression tag	UNP Q8TJ90
V	-15	GLY	-	expression tag	UNP Q8TJ90
V	-14	SER	-	expression tag	UNP Q8TJ90
V	-13	GLY	-	expression tag	UNP Q8TJ90
V	-12	GLY	-	expression tag	UNP Q8TJ90
V	-11	GLY	-	expression tag	UNP Q8TJ90
V	-10	SER	-	expression tag	UNP Q8TJ90
V	-9	TRP	-	expression tag	UNP Q8TJ90
V	-8	SER	-	expression tag	UNP Q8TJ90
V	-7	HIS	-	expression tag	UNP Q8TJ90
V	-6	PRO	-	expression tag	UNP Q8TJ90
V	-5	GLN	-	expression tag	UNP Q8TJ90
V	-4	PHE	-	expression tag	UNP Q8TJ90
V	-3	GLU	-	expression tag	UNP Q8TJ90
V	-2	LYS	-	expression tag	UNP Q8TJ90
V	-1	SER	-	expression tag	UNP Q8TJ90
V	0	GLY	-	expression tag	UNP Q8TJ90
L	-30	MET	-	initiating methionine	UNP Q8TJ90
L	-29	TRP	-	expression tag	UNP Q8TJ90
L	-28	SER	-	expression tag	UNP Q8TJ90
L	-27	HIS	-	expression tag	UNP Q8TJ90
L	-26	PRO	-	expression tag	UNP Q8TJ90
L	-25	GLN	-	expression tag	UNP Q8TJ90
L	-24	PHE	-	expression tag	UNP Q8TJ90
L	-23	GLU	-	expression tag	UNP Q8TJ90
L	-22	LYS	-	expression tag	UNP Q8TJ90
L	-21	GLY	-	expression tag	UNP Q8TJ90
L	-20	GLY	-	expression tag	UNP Q8TJ90
L	-19	GLY	-	expression tag	UNP Q8TJ90
L	-18	SER	-	expression tag	UNP Q8TJ90
L	-17	GLY	-	expression tag	UNP Q8TJ90
L	-16	GLY	-	expression tag	UNP Q8TJ90
L	-15	GLY	-	expression tag	UNP Q8TJ90
L	-14	SER	-	expression tag	UNP Q8TJ90
L	-13	GLY	-	expression tag	UNP Q8TJ90
L	-12	GLY	-	expression tag	UNP Q8TJ90
L	-11	GLY	-	expression tag	UNP Q8TJ90

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-10	SER	-	expression tag	UNP Q8TJ90
L	-9	TRP	-	expression tag	UNP Q8TJ90
L	-8	SER	-	expression tag	UNP Q8TJ90
L	-7	HIS	-	expression tag	UNP Q8TJ90
L	-6	PRO	-	expression tag	UNP Q8TJ90
L	-5	GLN	-	expression tag	UNP Q8TJ90
L	-4	PHE	-	expression tag	UNP Q8TJ90
L	-3	GLU	-	expression tag	UNP Q8TJ90
L	-2	LYS	-	expression tag	UNP Q8TJ90
L	-1	SER	-	expression tag	UNP Q8TJ90
L	0	GLY	-	expression tag	UNP Q8TJ90
U	-30	MET	-	initiating methionine	UNP Q8TJ90
U	-29	TRP	-	expression tag	UNP Q8TJ90
U	-28	SER	-	expression tag	UNP Q8TJ90
U	-27	HIS	-	expression tag	UNP Q8TJ90
U	-26	PRO	-	expression tag	UNP Q8TJ90
U	-25	GLN	-	expression tag	UNP Q8TJ90
U	-24	PHE	-	expression tag	UNP Q8TJ90
U	-23	GLU	-	expression tag	UNP Q8TJ90
U	-22	LYS	-	expression tag	UNP Q8TJ90
U	-21	GLY	-	expression tag	UNP Q8TJ90
U	-20	GLY	-	expression tag	UNP Q8TJ90
U	-19	GLY	-	expression tag	UNP Q8TJ90
U	-18	SER	-	expression tag	UNP Q8TJ90
U	-17	GLY	-	expression tag	UNP Q8TJ90
U	-16	GLY	-	expression tag	UNP Q8TJ90
U	-15	GLY	-	expression tag	UNP Q8TJ90
U	-14	SER	-	expression tag	UNP Q8TJ90
U	-13	GLY	-	expression tag	UNP Q8TJ90
U	-12	GLY	-	expression tag	UNP Q8TJ90
U	-11	GLY	-	expression tag	UNP Q8TJ90
U	-10	SER	-	expression tag	UNP Q8TJ90
U	-9	TRP	-	expression tag	UNP Q8TJ90
U	-8	SER	-	expression tag	UNP Q8TJ90
U	-7	HIS	-	expression tag	UNP Q8TJ90
U	-6	PRO	-	expression tag	UNP Q8TJ90
U	-5	GLN	-	expression tag	UNP Q8TJ90
U	-4	PHE	-	expression tag	UNP Q8TJ90
U	-3	GLU	-	expression tag	UNP Q8TJ90
U	-2	LYS	-	expression tag	UNP Q8TJ90
U	-1	SER	-	expression tag	UNP Q8TJ90
U	0	GLY	-	expression tag	UNP Q8TJ90

- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	456	Total	C	N	O	S	1	0
			3474	2202	585	665	22		
2	D	456	Total	C	N	O	S	0	0
			3467	2197	583	665	22		
2	M	456	Total	C	N	O	S	0	0
			3467	2197	583	665	22		
2	W	456	Total	C	N	O	S	0	0
			3467	2197	583	665	22		
2	X	456	Total	C	N	O	S	0	0
			3467	2197	583	665	22		
2	N	456	Total	C	N	O	S	0	0
			3467	2197	583	665	22		

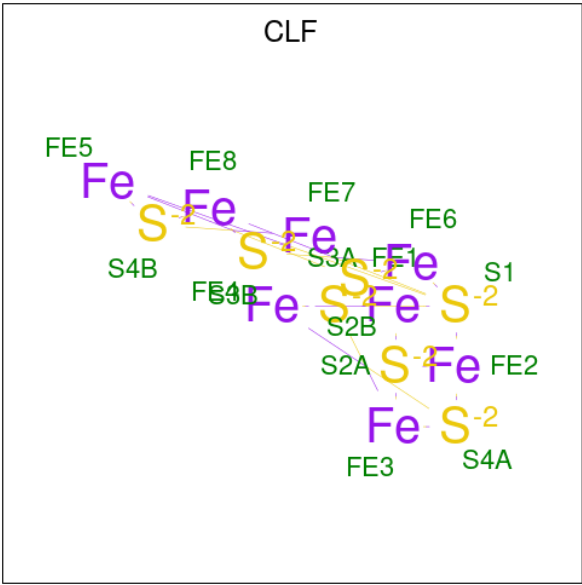
- Molecule 3 is a protein called P-II family nitrogen regulatory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	87	Total	C	N	O	S	0	0
			681	429	116	127	9		
3	J	95	Total	C	N	O	S	0	0
			747	469	129	140	9		
3	R	97	Total	C	N	O	S	0	0
			757	475	134	139	9		
3	T	90	Total	C	N	O	S	0	0
			704	443	122	130	9		
3	b	86	Total	C	N	O	S	0	0
			668	420	115	125	8		
3	d	97	Total	C	N	O	S	0	0
			763	479	132	143	9		
3	F	90	Total	C	N	O	S	0	0
			704	443	122	130	9		
3	I	90	Total	C	N	O	S	0	0
			700	437	121	133	9		
3	P	90	Total	C	N	O	S	0	0
			704	443	122	130	9		
3	S	99	Total	C	N	O	S	0	0
			781	490	135	147	9		
3	Z	90	Total	C	N	O	S	0	0
			704	443	122	130	9		
3	c	89	Total	C	N	O	S	0	0
			691	431	120	131	9		

- Molecule 4 is a protein called P-II family nitrogen regulatory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	92	Total	C	N	O	S	0	0
			723	453	137	128	5		
4	E	109	Total	C	N	O	S	1	0
			858	543	155	154	6		
4	Q	98	Total	C	N	O	S	0	0
			763	475	143	140	5		
4	O	101	Total	C	N	O	S	0	0
			783	489	146	143	5		
4	a	94	Total	C	N	O	S	0	0
			735	461	139	130	5		
4	Y	101	Total	C	N	O	S	0	0
			789	493	147	144	5		

- Molecule 5 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe₈S₇) (labeled as "Ligand of Interest" by depositor).



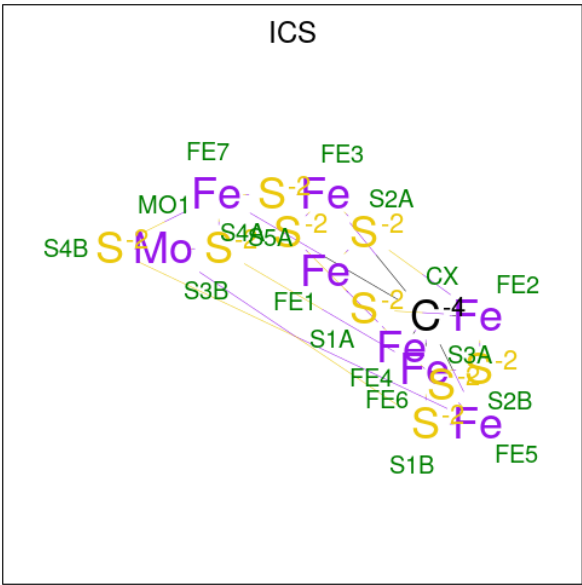
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Fe	S	0
			15	8	7	
5	D	1	Total	Fe	S	0
			15	8	7	
5	M	1	Total	Fe	S	0
			15	8	7	
5	V	1	Total	Fe	S	0
			15	8	7	
5	W	1	Total	Fe	S	0
			15	8	7	

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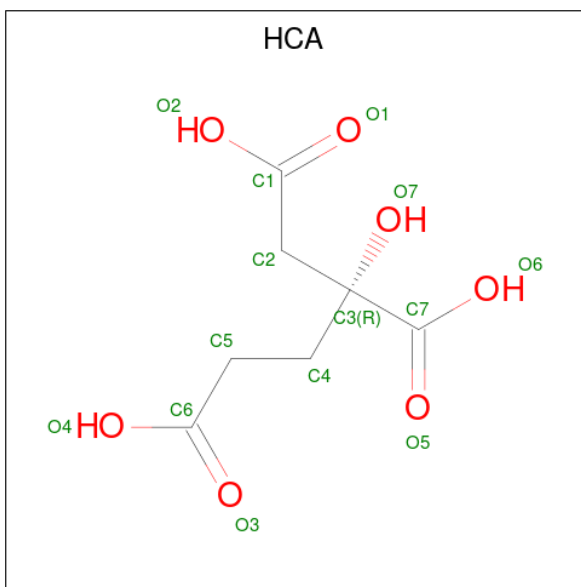
Mol	Chain	Residues	Atoms			AltConf
5	L	1	Total	Fe	S	0
			15	8	7	

- Molecule 6 is iron-sulfur-molybdenum cluster with interstitial carbon (CCD ID: ICS) (formula: CFe₇MoS₉) (labeled as "Ligand of Interest" by depositor).

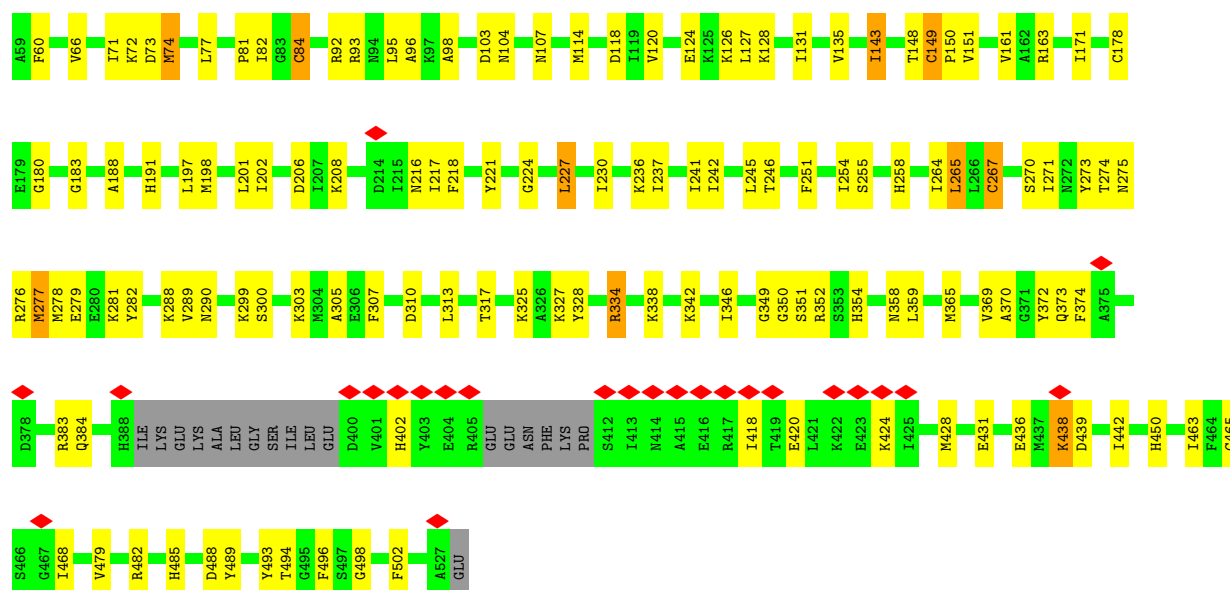


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	
6	C	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	
6	K	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	
6	V	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	
6	L	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	
6	U	1	Total	C	Fe	Mo	S	0
			18	1	7	1	9	

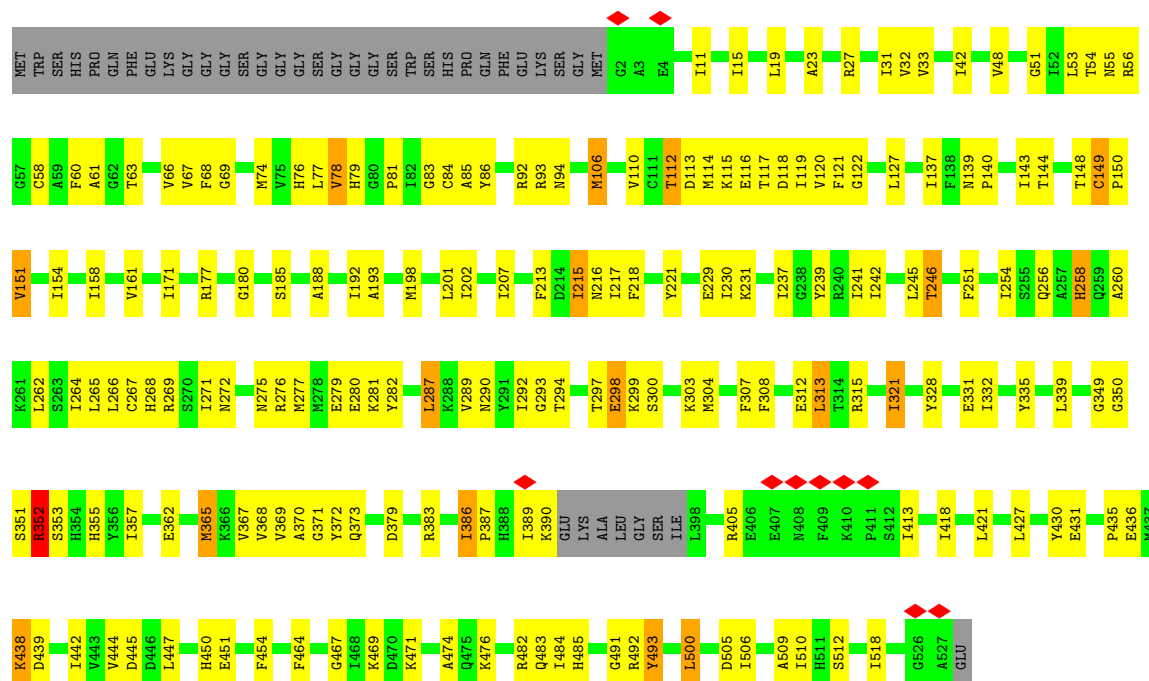
- Molecule 7 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: C₇H₁₀O₇) (labeled as "Ligand of Interest" by depositor).



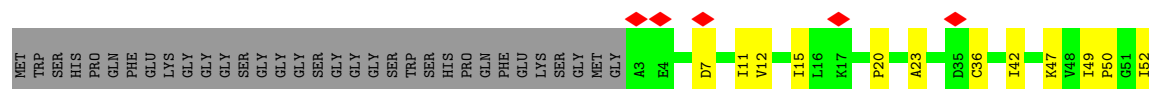
Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			14	7	7	
7	D	1	Total	C	O	0
			14	7	7	
7	K	1	Total	C	O	0
			14	7	7	
7	V	1	Total	C	O	0
			14	7	7	
7	L	1	Total	C	O	0
			14	7	7	
7	U	1	Total	C	O	0
			14	7	7	

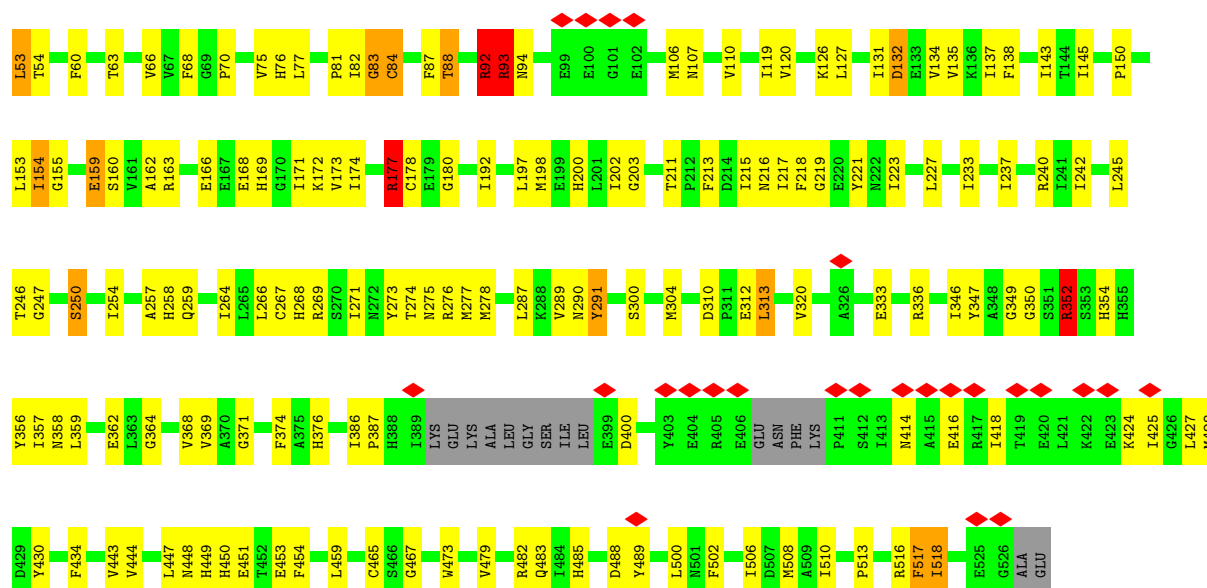


• Molecule 1: Nitrogenase protein alpha chain

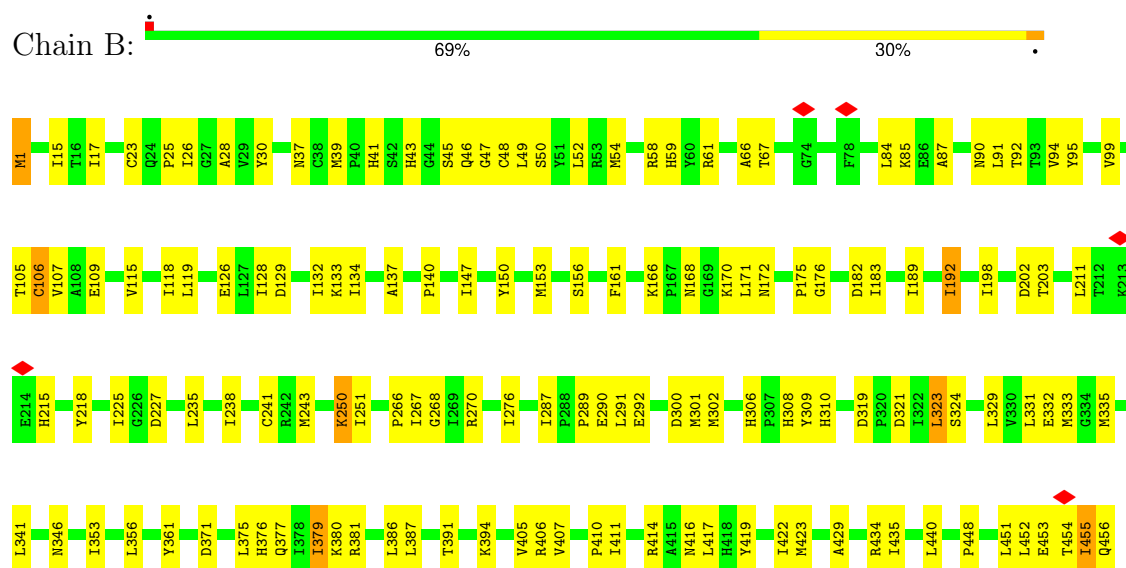


• Molecule 1: Nitrogenase protein alpha chain

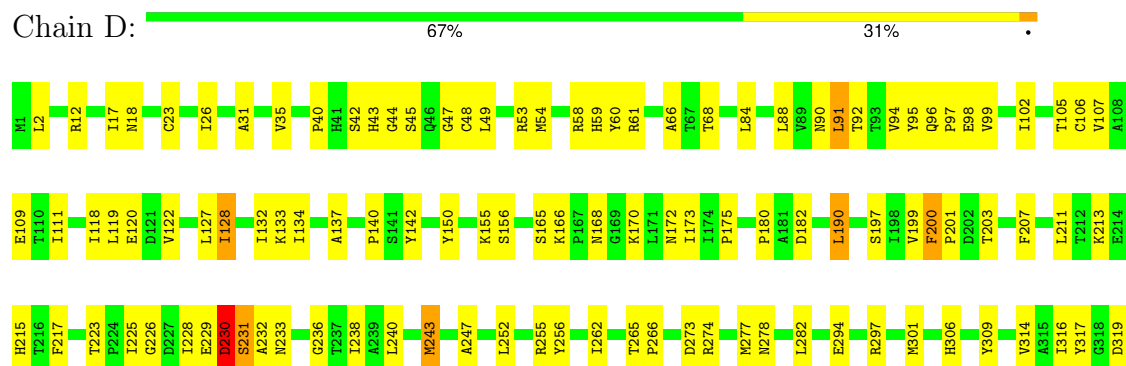


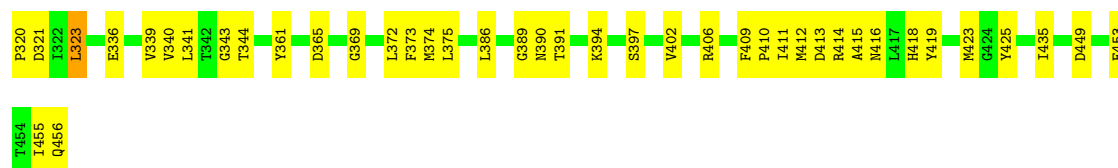


• Molecule 2: Nitrogenase molybdenum-iron protein beta chain



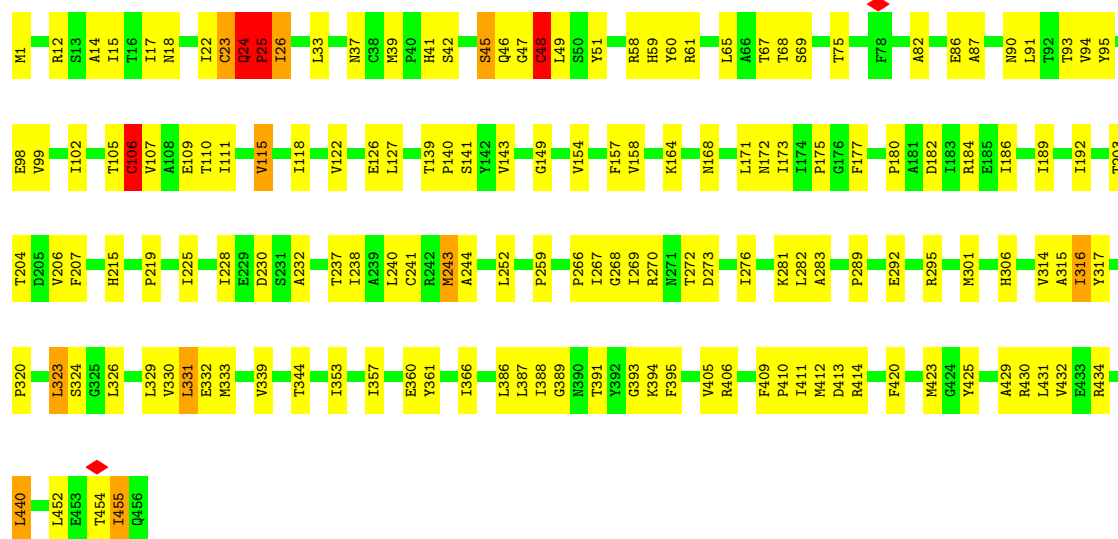
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain





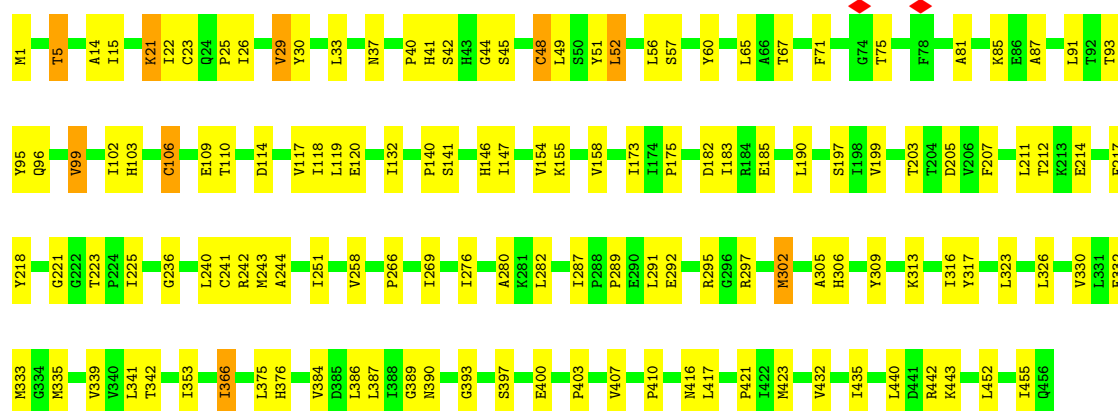
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain M: 66% 31% ..



• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

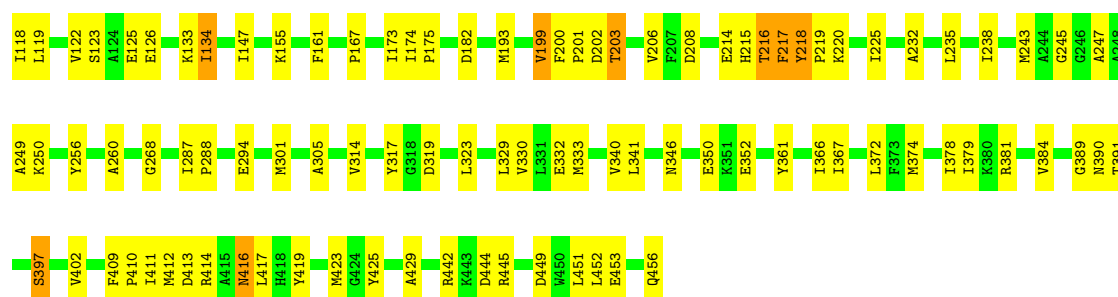
Chain W: 70% 28% .



• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

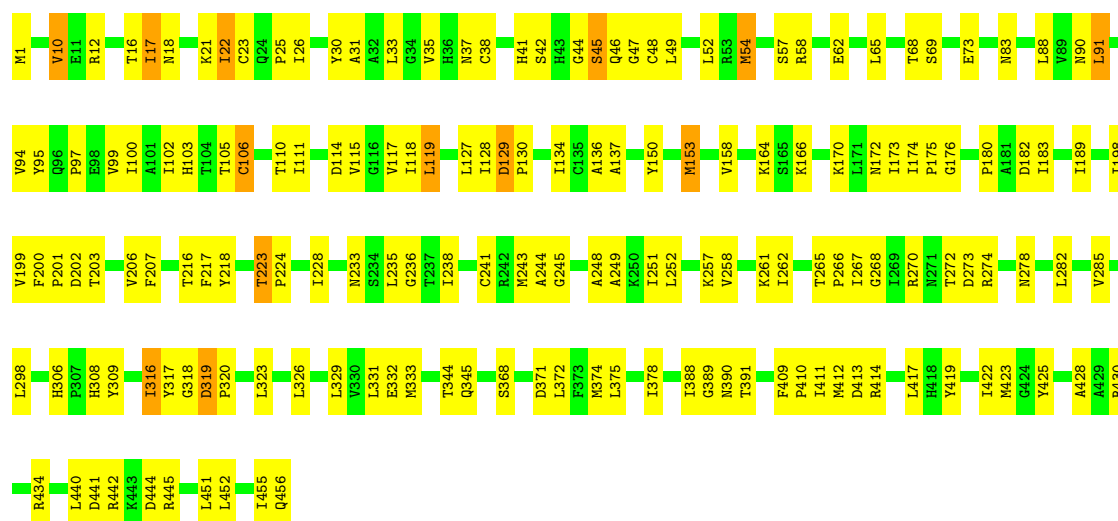
Chain X: 71% 27% .





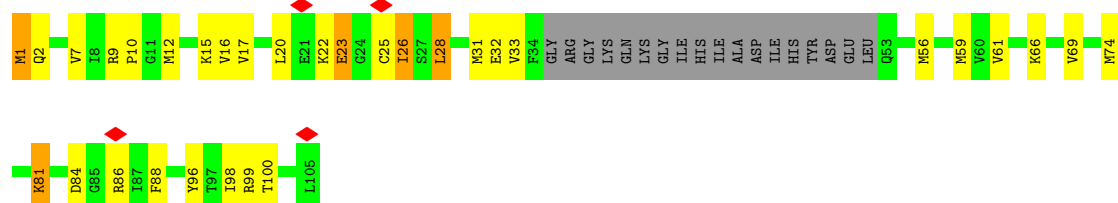
• Molecule 2: Nitrogenase molybdenum-iron protein beta chain

Chain N: 63% 34% .



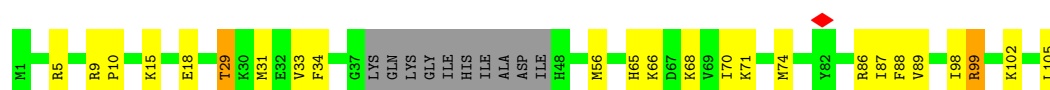
• Molecule 3: P-II family nitrogen regulatory protein

Chain H: 51% 27% 5% 17%

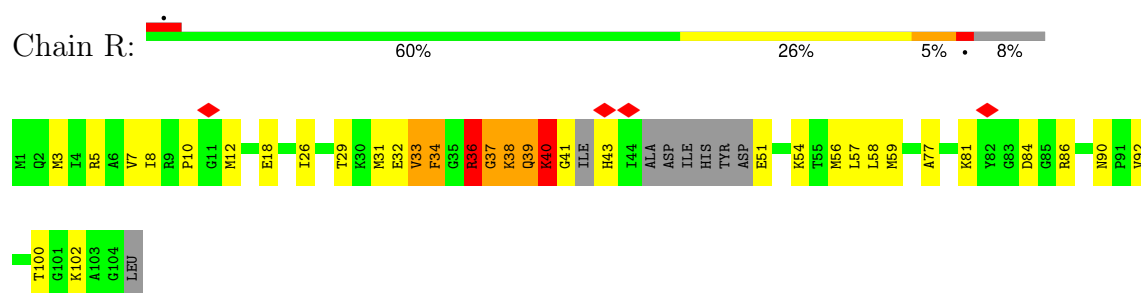


• Molecule 3: P-II family nitrogen regulatory protein

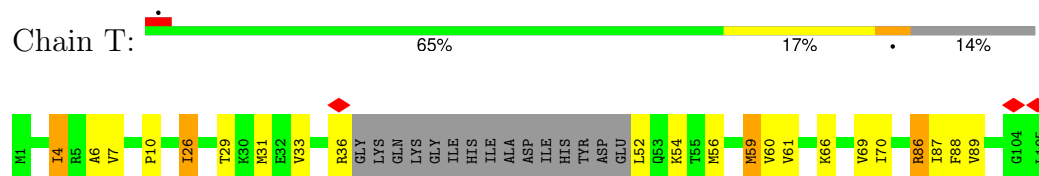
Chain J: 68% 21% 10%



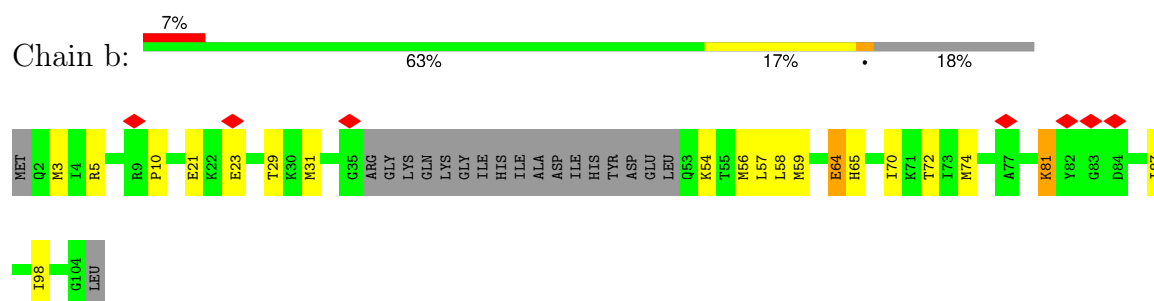
• Molecule 3: P-II family nitrogen regulatory protein



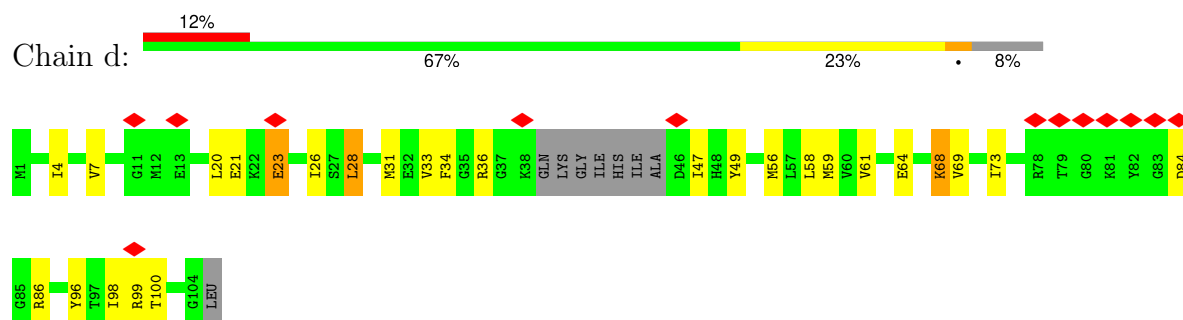
- Molecule 3: P-II family nitrogen regulatory protein



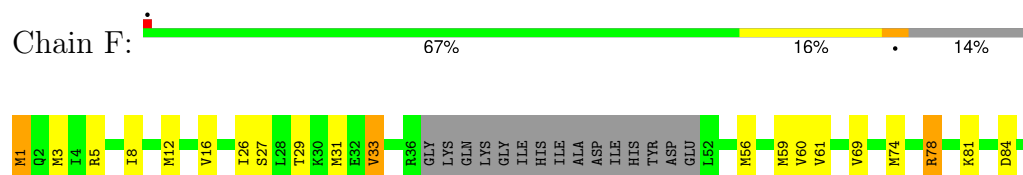
- Molecule 3: P-II family nitrogen regulatory protein



- Molecule 3: P-II family nitrogen regulatory protein

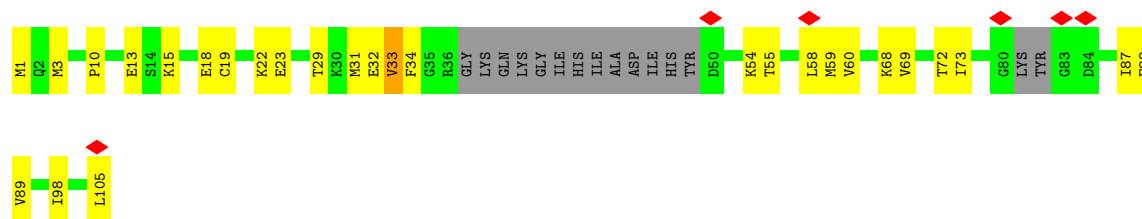


- Molecule 3: P-II family nitrogen regulatory protein

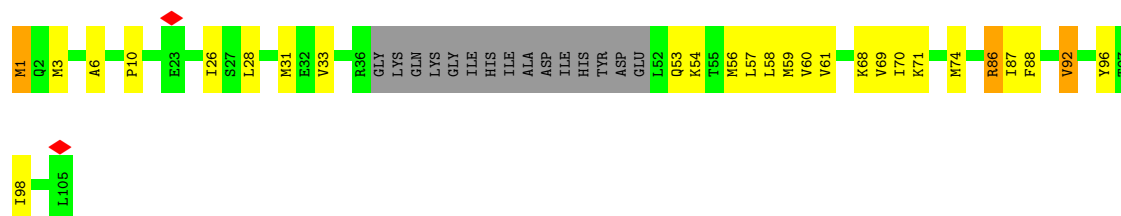


- Molecule 3: P-II family nitrogen regulatory protein

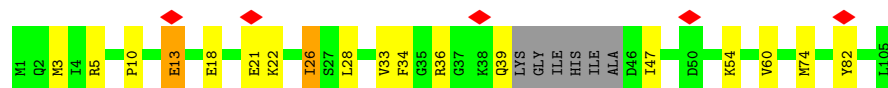
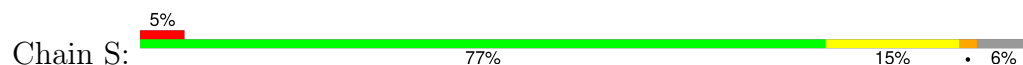




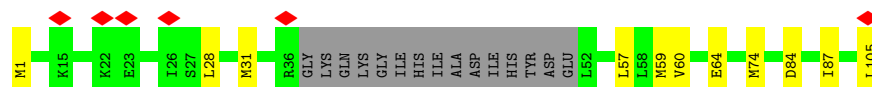
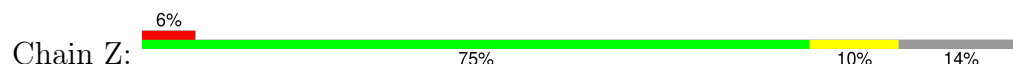
- Molecule 3: P-II family nitrogen regulatory protein



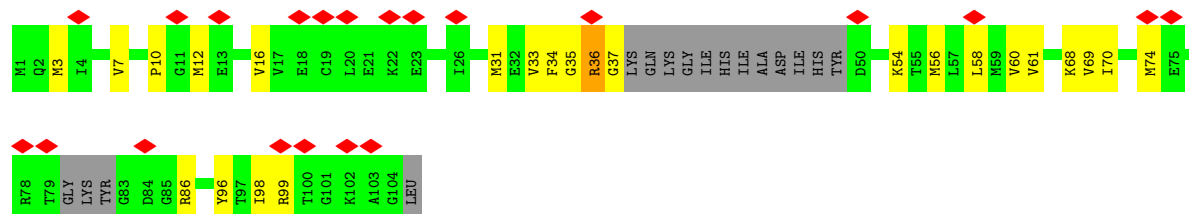
- Molecule 3: P-II family nitrogen regulatory protein



- Molecule 3: P-II family nitrogen regulatory protein

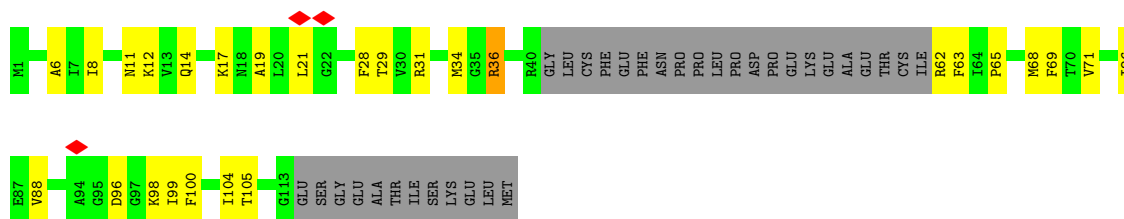


- Molecule 3: P-II family nitrogen regulatory protein

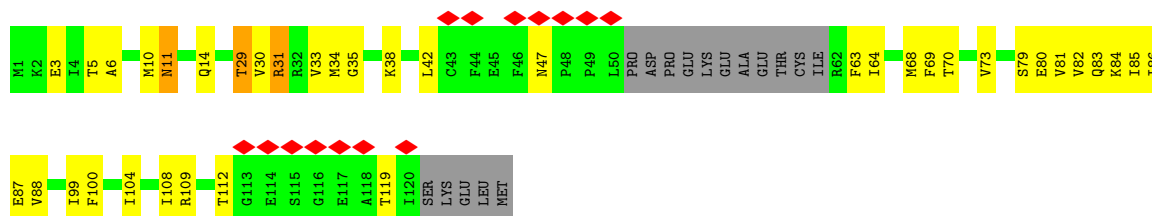


- Molecule 4: P-II family nitrogen regulatory protein

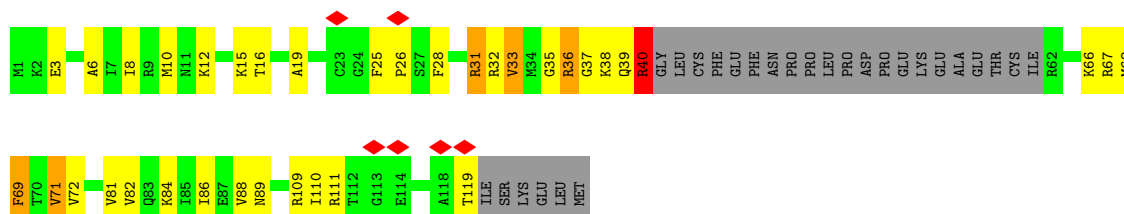




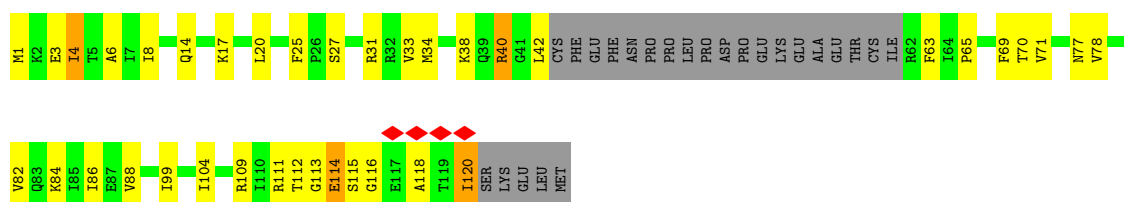
- Molecule 4: P-II family nitrogen regulatory protein



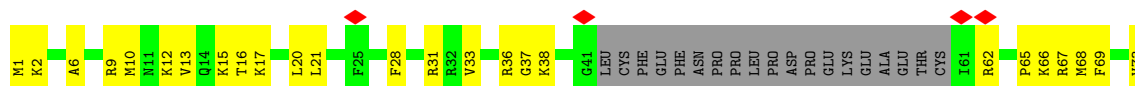
- Molecule 4: P-II family nitrogen regulatory protein

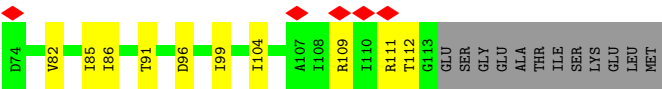


- Molecule 4: P-II family nitrogen regulatory protein

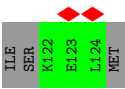
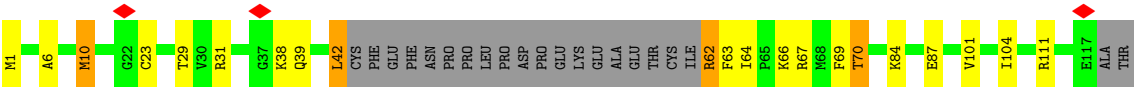


- Molecule 4: P-II family nitrogen regulatory protein





• Molecule 4: P-II family nitrogen regulatory protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68595	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	150000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.770	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.0142	Depositor
Map size ($\text{\AA}$)	371.19998, 371.19998, 371.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.928, 0.928, 0.928	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HCA, ICS, CLF

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	0.34	2/4030 (0.0%)	0.72	20/5433 (0.4%)
1	C	0.24	0/4228	0.57	9/5698 (0.2%)
1	K	0.28	1/4136 (0.0%)	0.47	3/5572 (0.1%)
1	L	0.22	0/4224	0.47	10/5694 (0.2%)
1	U	0.23	0/4159	0.48	3/5606 (0.1%)
1	V	0.20	0/4142	0.47	4/5582 (0.1%)
2	B	0.25	0/3548	0.56	4/4819 (0.1%)
2	D	0.22	0/3537	0.43	1/4804 (0.0%)
2	M	0.33	1/3537 (0.0%)	0.55	14/4804 (0.3%)
2	N	0.21	0/3537	0.41	0/4804
2	W	0.20	0/3537	0.37	1/4804 (0.0%)
2	X	0.24	0/3537	0.54	9/4804 (0.2%)
3	F	0.13	0/709	0.34	0/942
3	H	0.29	0/686	0.47	1/912 (0.1%)
3	I	0.10	0/703	0.34	0/933
3	J	0.14	0/754	0.42	0/1003
3	P	0.11	0/709	0.32	0/942
3	R	0.27	0/762	0.71	3/1010 (0.3%)
3	S	0.11	0/788	0.34	0/1048
3	T	0.13	0/709	0.40	0/942
3	Z	0.09	0/709	0.22	0/942
3	b	0.10	0/673	0.31	0/896
3	c	0.11	0/694	0.37	0/922
3	d	0.27	0/770	0.45	1/1025 (0.1%)
4	E	0.14	0/871	0.41	0/1166
4	G	0.11	0/728	0.32	0/971
4	O	0.26	0/788	0.40	0/1052
4	Q	0.24	0/768	0.53	3/1025 (0.3%)
4	Y	0.10	0/793	0.29	0/1055
4	a	0.14	0/740	0.40	0/987
All	All	0.24	4/59506 (0.0%)	0.49	86/80197 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	1
1	K	0	1
1	L	0	1
1	U	0	4
2	M	0	1
3	J	0	1
3	R	0	1
4	Q	0	1
All	All	0	14

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	25	PRO	C-O	-12.66	1.07	1.24
1	K	348	ALA	C-O	-8.85	1.13	1.23
1	A	351	SER	C-O	-6.80	1.15	1.23
1	A	58	CYS	N-CA	5.13	1.51	1.45

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	48	CYS	CB-CA-C	-19.90	80.32	110.96
1	A	352	ARG	N-CA-CB	14.64	133.43	110.73
1	C	267	CYS	CB-CA-C	-12.56	90.21	111.31
1	C	149	CYS	CB-CA-C	-12.36	85.82	110.17
1	K	348	ALA	CA-C-O	-11.47	107.16	121.50
2	M	25	PRO	CA-C-O	-10.75	101.04	120.60
1	C	267	CYS	CA-CB-SG	-10.37	90.56	114.40
2	X	215	HIS	CA-CB-CG	-9.84	103.97	113.80
1	A	352	ARG	N-CA-C	-9.49	100.64	112.88
1	A	58	CYS	CA-CB-SG	9.30	135.80	114.40
1	V	149	CYS	CA-C-N	-9.01	109.75	121.91
1	V	149	CYS	C-N-CA	-9.01	109.75	121.91
1	L	84	CYS	CA-CB-SG	-8.94	93.83	114.40
2	M	24	GLN	N-CA-C	-8.11	101.64	113.16
2	X	218	TYR	CB-CA-C	8.06	119.81	108.76
1	A	351	SER	CA-C-N	-7.98	110.16	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	SER	C-N-CA	-7.98	110.16	122.60
2	M	25	PRO	N-CA-C	7.94	128.82	112.47
1	A	352	ARG	CA-C-N	-7.90	104.73	121.80
1	A	352	ARG	C-N-CA	-7.90	104.73	121.80
1	C	84	CYS	CA-CB-SG	-7.79	96.48	114.40
1	A	58	CYS	CA-C-N	7.75	131.00	120.38
1	A	58	CYS	C-N-CA	7.75	131.00	120.38
2	M	47	GLY	CA-C-N	-7.58	110.13	120.44
2	M	47	GLY	C-N-CA	-7.58	110.13	120.44
1	C	267	CYS	CA-C-N	-7.26	111.06	120.65
1	C	267	CYS	C-N-CA	-7.26	111.06	120.65
3	R	34	PHE	CA-C-N	-7.26	116.57	122.16
3	R	34	PHE	C-N-CA	-7.26	116.57	122.16
2	W	48	CYS	N-CA-CB	-7.25	99.50	110.01
1	L	149	CYS	CB-CA-C	-6.99	100.77	113.49
1	A	181	TYR	N-CA-C	-6.96	103.77	111.36
1	U	84	CYS	CA-CB-SG	-6.94	98.43	114.40
1	C	92	ARG	CB-CG-CD	-6.93	95.35	111.30
1	V	58	CYS	CA-CB-SG	6.90	130.27	114.40
1	L	266	LEU	CA-C-N	-6.85	113.31	122.42
1	L	266	LEU	C-N-CA	-6.85	113.31	122.42
1	A	150	PRO	N-CA-C	-6.78	103.65	113.75
1	A	352	ARG	CB-CA-C	-6.77	99.28	110.72
3	R	40	LYS	N-CA-C	-6.76	102.05	111.52
2	M	23	CYS	CB-CA-C	-6.76	95.66	109.65
2	M	48	CYS	CA-C-N	-6.73	111.16	120.38
2	M	48	CYS	C-N-CA	-6.73	111.16	120.38
2	X	106	CYS	CB-CA-C	-6.72	100.28	110.90
2	X	218	TYR	N-CA-CB	-6.55	96.90	110.45
1	K	266	LEU	CA-C-N	-6.47	112.35	121.99
1	K	266	LEU	C-N-CA	-6.47	112.35	121.99
1	A	180	GLY	CA-C-N	-6.44	111.15	120.29
1	A	180	GLY	C-N-CA	-6.44	111.15	120.29
4	Q	36	ARG	O-C-N	-6.43	116.06	123.33
2	M	48	CYS	CA-CB-SG	-6.42	99.63	114.40
2	M	26	ILE	N-CA-C	-6.30	104.35	110.72
1	V	267	CYS	CB-CA-C	-6.25	99.65	109.84
1	A	83	GLY	CA-C-N	-6.19	112.39	120.44
1	A	83	GLY	C-N-CA	-6.19	112.39	120.44
1	L	151	VAL	N-CA-C	-6.14	107.87	113.71
1	A	485	HIS	CA-CB-CG	5.96	119.76	113.80
1	L	267	CYS	CA-CB-SG	-5.87	100.89	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	48	CYS	CA-CB-SG	-5.75	101.18	114.40
1	L	84	CYS	CA-C-N	-5.75	112.58	120.28
1	L	84	CYS	C-N-CA	-5.75	112.58	120.28
1	U	83	GLY	CA-C-N	-5.55	112.41	120.29
1	U	83	GLY	C-N-CA	-5.55	112.41	120.29
1	L	83	GLY	CA-C-N	-5.54	112.42	120.29
1	L	83	GLY	C-N-CA	-5.54	112.42	120.29
2	M	105	THR	CA-C-N	-5.54	111.11	120.58
2	M	105	THR	C-N-CA	-5.54	111.11	120.58
4	Q	36	ARG	CA-C-N	-5.51	114.82	122.86
4	Q	36	ARG	C-N-CA	-5.51	114.82	122.86
2	M	106	CYS	CA-C-N	-5.50	113.50	120.60
2	M	106	CYS	C-N-CA	-5.50	113.50	120.60
2	X	47	GLY	CA-C-N	-5.41	113.08	120.44
2	X	47	GLY	C-N-CA	-5.41	113.08	120.44
2	B	105	THR	CA-C-N	-5.41	111.68	120.71
2	B	105	THR	C-N-CA	-5.41	111.68	120.71
1	A	58	CYS	CA-C-O	-5.38	114.94	121.28
2	D	230	ASP	CA-CB-CG	5.21	117.81	112.60
2	B	453	GLU	N-CA-C	-5.21	105.81	113.72
3	d	23	GLU	N-CA-C	-5.20	106.99	113.38
1	A	192	ILE	N-CA-C	-5.19	104.71	110.62
1	C	266	LEU	CA-C-N	-5.17	115.67	122.85
1	C	266	LEU	C-N-CA	-5.17	115.67	122.85
3	H	26	ILE	CA-C-O	-5.13	114.36	120.78
1	A	191	HIS	N-CA-C	-5.04	106.82	113.12
2	X	48	CYS	CA-C-N	-5.03	113.54	120.28
2	X	48	CYS	C-N-CA	-5.03	113.54	120.28

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	ARG	Sidechain
1	A	352	ARG	Sidechain
1	A	92	ARG	Sidechain
1	C	92	ARG	Sidechain
3	J	99	ARG	Peptide
1	K	352	ARG	Sidechain
1	L	352	ARG	Sidechain
2	M	25	PRO	Mainchain
4	Q	40	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	R	36	ARG	Sidechain
1	U	177	ARG	Sidechain
1	U	352	ARG	Sidechain
1	U	92	ARG	Sidechain
1	U	93	ARG	Sidechain

5.2 Too-close contacts

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	3944	0	3895	147	0
1	C	4137	0	4073	154	0
1	K	4049	0	3992	113	0
1	L	4133	0	4071	148	0
1	U	4070	0	4005	130	0
1	V	4054	0	3995	119	0
2	B	3474	0	3488	102	0
2	D	3467	0	3481	123	0
2	M	3467	0	3480	116	0
2	N	3467	0	3480	122	0
2	W	3467	0	3481	111	0
2	X	3467	0	3479	98	0
3	F	704	0	745	17	0
3	H	681	0	718	23	0
3	I	700	0	732	22	0
3	J	747	0	774	20	0
3	P	704	0	745	21	0
3	R	757	0	797	32	0
3	S	781	0	810	11	0
3	T	704	0	745	17	0
3	Z	704	0	745	9	0
3	b	668	0	698	17	0
3	c	691	0	721	18	0
3	d	763	0	791	15	0
4	E	858	0	897	29	0
4	G	723	0	771	18	0
4	O	783	0	828	29	0
4	Q	763	0	803	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Y	789	0	834	16	0
4	a	735	0	785	25	0
5	A	15	0	0	6	0
5	D	15	0	0	9	0
5	L	15	0	0	6	0
5	M	15	0	0	7	0
5	V	15	0	0	9	0
5	W	15	0	0	11	0
6	A	18	0	0	13	0
6	C	18	0	0	11	0
6	K	18	0	0	7	0
6	L	18	0	0	6	0
6	U	18	0	0	11	0
6	V	18	0	0	16	0
7	A	14	0	7	1	0
7	D	14	0	6	0	0
7	K	14	0	6	0	0
7	L	14	0	6	1	0
7	U	14	0	5	0	0
7	V	14	0	6	1	0
All	All	58733	0	58895	1678	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 14.

All (1678) 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:K:81:PRO:HB2	5:M:501:CLF:S2A	1.59	1.43
1:U:350:GLY:HA3	6:U:601:ICS:S4A	1.88	1.14
1:K:81:PRO:CB	5:M:501:CLF:S2A	2.35	1.14
1:C:81:PRO:HG2	5:D:601:CLF:S2B	1.91	1.11
1:A:149:CYS:SG	5:A:601:CLF:S3B	2.49	1.10
1:V:149:CYS:N	5:V:601:CLF:S2A	2.29	1.06
2:D:45:SER:CB	5:D:601:CLF:S2A	2.45	1.04
2:B:23:CYS:SG	2:B:25:PRO:HD2	2.00	1.02
2:D:45:SER:HB2	5:D:601:CLF:S2A	2.00	1.00
2:D:172:ASN:HD21	2:D:230:ASP:HB3	1.22	1.00
1:A:352:ARG:HB2	6:A:602:ICS:S5A	2.08	0.93
1:C:81:PRO:CG	5:D:601:CLF:S2B	2.57	0.93
1:K:268:HIS:O	1:K:272:ASN:HB3	1.69	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:352:ARG:HB2	6:V:602:ICS:S3A	2.09	0.91
1:V:66:VAL:HG11	6:V:602:ICS:S2B	2.11	0.90
1:L:386:ILE:HG13	1:L:387:PRO:HD3	1.54	0.89
2:N:23:CYS:HB3	2:N:25:PRO:HD2	1.54	0.89
3:c:36:ARG:HD3	3:c:37:GLY:H	1.38	0.88
1:K:148:THR:HG23	5:M:501:CLF:S3B	2.14	0.88
2:D:230:ASP:OD2	2:D:252:LEU:HD11	1.73	0.88
5:W:601:CLF:S2B	1:U:180:GLY:HA3	2.16	0.86
1:V:349:GLY:HA2	1:V:373:GLN:HB3	1.56	0.86
1:K:148:THR:HG22	1:K:150:PRO:HD2	1.58	0.84
1:A:81:PRO:HD2	1:A:148:THR:HG21	1.58	0.84
2:W:23:CYS:SG	2:W:25:PRO:HD2	2.17	0.84
1:V:58:CYS:HB2	2:X:47:GLY:HA3	1.59	0.84
1:C:219:GLY:HA3	1:C:267:CYS:HB2	1.59	0.83
1:C:219:GLY:CA	1:C:267:CYS:HB2	2.09	0.81
1:V:58:CYS:SG	1:V:180:GLY:HA3	2.20	0.81
1:K:28:ARG:HH12	3:I:22:LYS:HG3	1.42	0.81
2:N:46:GLN:HA	2:N:69:SER:HB2	1.62	0.81
4:a:1:MET:HE3	4:a:2:LYS:H	1.44	0.81
1:C:92:ARG:CD	1:C:223:ILE:HD11	2.10	0.81
1:V:92:ARG:NH2	6:V:602:ICS:S5A	2.54	0.80
1:A:349:GLY:HA3	6:A:602:ICS:S4B	2.22	0.80
2:D:45:SER:HB3	5:D:601:CLF:S2A	2.22	0.80
1:K:350:GLY:N	6:K:601:ICS:S5A	2.55	0.79
2:N:175:PRO:HD2	2:N:201:PRO:HG2	1.64	0.79
1:A:485:HIS:HA	6:A:602:ICS:S3B	2.23	0.79
2:D:165:SER:H	2:D:232:ALA:HB2	1.47	0.79
1:C:92:ARG:HD2	1:C:223:ILE:HD11	1.63	0.78
3:H:61:VAL:HG11	3:H:69:VAL:HG21	1.63	0.78
2:W:48:CYS:HA	5:W:601:CLF:S4A	2.24	0.78
1:U:198:MET:HE2	1:U:198:MET:HA	1.66	0.77
2:W:85:LYS:HD3	2:W:118:ILE:HD11	1.66	0.77
2:B:266:PRO:HG2	2:B:423:MET:HG3	1.66	0.77
5:V:601:CLF:S4A	2:X:45:SER:HB2	2.24	0.77
1:K:221:TYR:HE2	6:K:601:ICS:S1A	2.08	0.76
1:A:148:THR:HG23	5:A:601:CLF:S4B	2.26	0.76
2:B:126:GLU:HB3	3:b:81:LYS:HB3	1.68	0.76
1:A:150:PRO:O	1:A:154:ILE:HG23	1.85	0.76
1:V:221:TYR:HE2	6:V:602:ICS:S2A	2.09	0.76
1:V:350:GLY:N	6:V:602:ICS:S1B	2.59	0.76
1:C:56:ARG:HD3	1:C:185:SER:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:220:GLU:HG2	1:K:227:LEU:HD13	1.68	0.75
2:D:213:LYS:H	2:D:213:LYS:HD3	1.52	0.75
1:V:81:PRO:HB2	5:V:601:CLF:S3B	2.25	0.75
3:d:59:MET:HE1	3:d:69:VAL:HG11	1.67	0.75
1:C:347:TYR:HB3	1:C:466:SER:HB2	1.69	0.75
4:E:5:THR:HB	4:E:100:PHE:HB2	1.68	0.75
1:K:15:ILE:HG12	1:K:454:PHE:HB3	1.68	0.74
1:V:92:ARG:NH2	6:V:602:ICS:S3B	2.59	0.74
4:a:17:LYS:HG2	4:a:28:PHE:HZ	1.52	0.74
1:K:348:ALA:HB2	1:K:484:ILE:HG21	1.69	0.74
1:L:27:ARG:HH22	1:L:451:GLU:HG2	1.51	0.74
2:W:309:TYR:HE2	2:W:333:MET:HG2	1.52	0.74
4:E:6:ALA:HB3	4:E:69:PHE:HB2	1.69	0.74
1:V:485:HIS:HA	6:V:602:ICS:S4B	2.28	0.74
3:J:70:ILE:HG22	3:J:74:MET:HE3	1.69	0.74
1:V:494:THR:H	1:V:498:GLY:HA3	1.53	0.73
1:A:149:CYS:SG	1:A:150:PRO:HD3	2.27	0.73
1:L:368:VAL:HG23	1:L:369:VAL:HG23	1.70	0.73
2:D:294:GLU:HB3	2:D:425:TYR:HD2	1.53	0.73
1:C:450:HIS:HB2	2:D:95:TYR:HE1	1.53	0.73
1:K:60:PHE:HE2	1:K:84:CYS:HB3	1.54	0.73
1:L:350:GLY:HA2	1:L:372:TYR:CE2	2.23	0.73
3:T:26:ILE:HG23	4:Q:38:LYS:HA	1.70	0.72
4:O:6:ALA:HB3	4:O:69:PHE:HB2	1.71	0.72
1:V:198:MET:HE1	1:V:277:MET:HG2	1.71	0.72
2:D:243:MET:HE2	2:D:320:PRO:HG2	1.72	0.72
1:U:485:HIS:HA	6:U:601:ICS:S3B	2.29	0.72
1:A:207:ILE:HG22	1:A:256:GLN:HB3	1.70	0.71
2:N:200:PHE:HB2	2:N:228:ILE:HG12	1.72	0.71
1:C:81:PRO:HB2	5:D:601:CLF:S2B	2.31	0.71
1:V:58:CYS:HB3	5:V:601:CLF:S3A	2.30	0.71
1:L:450:HIS:HB2	2:N:95:TYR:HE1	1.55	0.71
1:C:339:LEU:HD21	1:C:510:ILE:HG21	1.71	0.70
1:U:427:LEU:HG	1:U:428:MET:HE2	1.73	0.70
1:U:221:TYR:CE2	6:U:601:ICS:S1A	2.85	0.70
4:Y:62:ARG:HE	4:Y:63:PHE:H	1.36	0.70
2:B:119:LEU:HD22	2:B:134:ILE:HD11	1.73	0.70
1:K:60:PHE:CE2	1:K:84:CYS:HB3	2.26	0.70
2:X:23:CYS:SG	2:X:25:PRO:HD2	2.32	0.70
3:R:7:VAL:HG22	3:R:56:MET:HE1	1.73	0.70
1:A:386:ILE:HG23	1:A:387:PRO:HD3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:THR:O	1:C:321:ILE:HG12	1.92	0.69
2:D:172:ASN:ND2	2:D:230:ASP:HB3	2.03	0.69
2:N:266:PRO:HD2	2:N:423:MET:HE3	1.74	0.69
1:A:262:LEU:HD21	1:A:264:ILE:HG23	1.74	0.69
1:C:350:GLY:N	6:C:601:ICS:S3A	2.58	0.69
4:a:6:ALA:HB3	4:a:69:PHE:HB2	1.73	0.69
1:C:369:VAL:HG13	1:C:442:ILE:HB	1.73	0.69
2:X:42:SER:HB2	2:X:49:LEU:HD12	1.74	0.69
1:U:52:ILE:HG13	1:U:448:ASN:HD22	1.57	0.69
2:D:243:MET:HE1	2:D:344:THR:HG21	1.74	0.69
2:M:324:SER:HA	2:M:353:ILE:HD11	1.75	0.69
1:C:211:THR:HG23	1:C:213:PHE:H	1.58	0.69
1:V:325:LYS:HG3	1:V:496:PHE:HE2	1.57	0.69
2:W:37:ASN:HA	2:W:218:TYR:HD2	1.57	0.69
2:D:175:PRO:HD2	2:D:201:PRO:HD2	1.75	0.69
3:T:31:MET:HE1	4:Q:31:ARG:HD2	1.75	0.69
4:Q:82:VAL:O	4:Q:86:ILE:HG12	1.93	0.69
4:Y:10:MET:HG2	4:Y:67:ARG:HD3	1.74	0.68
2:W:29:VAL:HG11	2:W:52:LEU:HD21	1.75	0.68
2:B:182:ASP:HB3	2:B:423:MET:SD	2.32	0.68
1:K:354:HIS:HB2	1:K:433:LEU:HD13	1.73	0.68
1:U:221:TYR:HE2	6:U:601:ICS:S1A	2.16	0.68
4:O:99:ILE:HB	3:P:96:TYR:HB2	1.75	0.68
1:A:476:LYS:HD3	2:B:211:LEU:HD12	1.76	0.68
1:C:143:ILE:HB	1:C:173:VAL:HG12	1.75	0.68
1:C:483:GLN:HB2	1:C:488:ASP:H	1.58	0.68
1:V:374:PHE:CZ	6:V:602:ICS:S2B	2.87	0.68
1:C:294:THR:HG23	1:C:499:VAL:HG11	1.74	0.68
1:U:135:VAL:HG22	1:U:171:ILE:HD11	1.75	0.68
1:A:81:PRO:HG2	5:A:601:CLF:S4A	2.34	0.67
2:W:280:ALA:HB2	2:W:287:ILE:HD11	1.76	0.67
2:W:443:LYS:HG2	2:W:455:ILE:HD12	1.77	0.67
1:V:53:LEU:HD21	2:X:66:ALA:H	1.58	0.67
1:V:58:CYS:SG	1:V:180:GLY:CA	2.82	0.67
2:X:390:ASN:HB3	2:X:410:PRO:HD2	1.77	0.67
3:I:33:VAL:HG22	3:I:54:LYS:HB2	1.76	0.67
2:W:106:CYS:SG	5:W:601:CLF:S1	2.86	0.67
1:L:221:TYR:HE2	6:L:602:ICS:S1A	2.17	0.67
2:B:452:LEU:HG	2:D:394:LYS:HD2	1.77	0.67
1:C:41:HIS:HB3	1:C:377:ARG:HH22	1.60	0.67
2:N:236:GLY:HA3	2:N:282:LEU:HD23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:83:GLN:HA	4:E:86:ILE:HG12	1.77	0.66
2:W:212:THR:HG22	2:W:214:GLU:H	1.60	0.66
1:L:15:ILE:HD12	1:L:454:PHE:HB3	1.78	0.66
1:A:58:CYS:SG	2:B:47:GLY:HA3	2.34	0.66
3:F:26:ILE:HG23	3:F:59:MET:HE2	1.77	0.66
1:A:368:VAL:HG12	1:A:369:VAL:HG23	1.76	0.66
1:A:485:HIS:CE1	6:A:602:ICS:S4B	2.87	0.66
3:T:26:ILE:CG2	4:Q:38:LYS:HA	2.25	0.66
1:A:349:GLY:HA2	1:A:373:GLN:HB2	1.78	0.66
1:C:66:VAL:HG23	1:C:67:VAL:HG23	1.77	0.66
2:X:84:LEU:HD23	2:X:118:ILE:HG21	1.78	0.66
1:A:58:CYS:SG	2:B:45:SER:HB2	2.36	0.66
2:X:39:MET:HB3	2:X:100:ILE:HG22	1.78	0.66
1:L:276:ARG:O	1:L:280:GLU:HG2	1.95	0.66
1:U:211:THR:HG22	1:U:213:PHE:H	1.60	0.66
1:L:116:GLU:HA	1:L:119:ILE:HG22	1.78	0.66
1:K:81:PRO:CG	5:M:501:CLF:S2A	2.84	0.65
2:N:103:HIS:HB3	2:N:153:MET:HE1	1.77	0.65
1:V:313:LEU:O	1:V:317:THR:HG23	1.95	0.65
2:B:310:HIS:HB3	1:C:508:MET:HE2	1.77	0.65
2:M:126:GLU:HB2	3:H:81:LYS:HE3	1.79	0.65
1:C:264:ILE:HG21	1:C:304:MET:HE3	1.78	0.65
1:L:431:GLU:HG3	1:L:435:PRO:HG2	1.78	0.65
1:L:140:PRO:HG2	1:L:143:ILE:HD11	1.79	0.65
1:U:336:ARG:HH21	1:U:364:GLY:HA3	1.60	0.65
1:U:368:VAL:HG12	1:U:369:VAL:HG23	1.78	0.65
3:I:3:MET:HB2	3:I:60:VAL:HG22	1.79	0.65
3:c:12:MET:HE1	3:c:16:VAL:HG13	1.78	0.65
1:A:351:SER:HA	1:A:372:TYR:HE1	1.62	0.65
1:V:221:TYR:CE2	6:V:602:ICS:S2A	2.90	0.65
2:D:35:VAL:HA	2:D:223:THR:HG23	1.78	0.65
1:K:53:LEU:HB2	2:M:95:TYR:HE2	1.61	0.65
1:V:276:ARG:HD3	1:V:383:ARG:HH12	1.61	0.65
2:W:65:LEU:HD12	1:U:53:LEU:HD21	1.79	0.65
2:X:294:GLU:HB3	2:X:425:TYR:HD2	1.61	0.65
3:R:29:THR:HB	3:R:58:LEU:HB3	1.78	0.65
3:R:31:MET:HE2	3:R:56:MET:HG3	1.78	0.65
4:E:29:THR:HG23	4:E:70:THR:HB	1.78	0.65
1:A:422:LYS:HA	1:A:427:LEU:HB3	1.79	0.65
2:M:353:ILE:HG22	2:M:366:ILE:HD13	1.79	0.65
2:N:390:ASN:HD22	2:N:410:PRO:HG2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:THR:HG22	1:A:150:PRO:HD2	1.79	0.64
2:M:37:ASN:HB2	2:M:98:GLU:HB2	1.78	0.64
1:L:386:ILE:HA	1:L:389:ILE:HG13	1.79	0.64
1:U:275:ASN:HA	1:U:278:MET:HG2	1.79	0.64
1:C:81:PRO:CB	5:D:601:CLF:S2B	2.85	0.64
2:D:390:ASN:HB3	2:D:410:PRO:HD2	1.80	0.64
3:T:61:VAL:HG11	3:T:69:VAL:HG21	1.78	0.64
1:L:58:CYS:SG	2:N:47:GLY:HA3	2.37	0.64
2:M:243:MET:HE2	2:M:320:PRO:HG3	1.79	0.64
2:M:268:GLY:HA2	2:M:329:LEU:HD13	1.80	0.64
5:L:603:CLF:S2B	2:N:106:CYS:SG	2.96	0.64
1:L:450:HIS:HB2	2:N:95:TYR:CE1	2.33	0.64
4:Y:6:ALA:HB3	4:Y:69:PHE:HB2	1.80	0.64
1:V:349:GLY:H	1:V:485:HIS:CE1	2.15	0.64
2:W:37:ASN:HA	2:W:218:TYR:CD2	2.33	0.64
2:X:39:MET:HE1	2:X:95:TYR:HB2	1.78	0.64
3:F:3:MET:HA	3:F:60:VAL:HA	1.79	0.64
2:D:323:LEU:HD12	2:D:340:VAL:HG13	1.80	0.64
2:M:67:THR:HG21	2:M:91:LEU:HD11	1.79	0.64
1:U:237:ILE:HG12	1:U:320:VAL:HG21	1.80	0.64
1:A:370:ALA:HB3	1:A:437:MET:HE1	1.79	0.64
2:N:316:ILE:HG23	2:N:388:ILE:HB	1.79	0.64
2:M:406:ARG:NH2	2:M:414:ARG:HE	1.95	0.63
2:M:59:HIS:CD2	2:M:60:TYR:HD1	2.16	0.63
1:V:58:CYS:CB	5:V:601:CLF:S3A	2.85	0.63
1:C:227:LEU:O	1:C:231:LYS:HB3	1.98	0.63
1:L:221:TYR:CE2	6:L:602:ICS:S1A	2.90	0.63
2:N:37:ASN:HD22	2:N:218:TYR:HD2	1.44	0.63
2:D:391:THR:HG21	2:D:413:ASP:H	1.63	0.63
3:d:36:ARG:HG2	3:d:49:TYR:HD2	1.64	0.63
4:G:17:LYS:O	4:G:21:LEU:HD12	1.98	0.63
4:Q:32:ARG:HG2	4:Q:67:ARG:HH12	1.63	0.63
1:A:292:ILE:HD12	1:A:355:HIS:HB3	1.80	0.63
1:C:15:ILE:HG12	1:C:454:PHE:HB3	1.79	0.63
3:J:86:ARG:HH11	4:E:119:THR:HG22	1.63	0.63
2:D:102:ILE:HD11	2:D:134:ILE:HD11	1.80	0.63
4:E:33:VAL:HG11	4:E:68:MET:HE3	1.81	0.63
2:W:21:LYS:HD2	1:U:82:ILE:HG21	1.81	0.63
4:Q:37:GLY:H	4:Q:40:ARG:HB2	1.63	0.63
2:M:266:PRO:HG2	2:M:423:MET:HE3	1.81	0.62
2:W:330:VAL:HG13	2:W:335:MET:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:4:ILE:HD12	4:O:71:VAL:HG13	1.81	0.62
1:A:346:ILE:HD13	1:A:465:CYS:HB2	1.80	0.62
1:C:350:GLY:HA3	6:C:601:ICS:S1A	2.39	0.62
1:A:16:LEU:HA	1:A:19:LEU:HD12	1.81	0.62
2:D:84:LEU:HD23	2:D:118:ILE:HG21	1.81	0.62
2:W:95:TYR:HE1	1:U:450:HIS:HB2	1.64	0.62
5:L:603:CLF:S4B	2:N:106:CYS:SG	2.98	0.62
4:Q:26:PRO:HB2	3:S:39:GLN:HA	1.82	0.62
4:O:115:SER:H	4:O:118:ALA:HB3	1.63	0.62
1:A:294:THR:HG23	1:A:499:VAL:HG21	1.81	0.62
2:B:170:LYS:HD3	2:B:198:ILE:HG13	1.82	0.62
1:C:352:ARG:HB2	6:C:601:ICS:S3A	2.40	0.62
1:K:53:LEU:HD11	2:M:65:LEU:HD22	1.80	0.62
2:M:1:MET:HE1	2:N:452:LEU:HD23	1.82	0.62
1:U:150:PRO:O	1:U:154:ILE:HG22	1.99	0.62
1:A:369:VAL:HG22	1:A:442:ILE:HB	1.82	0.62
1:C:471:LYS:HD2	1:C:483:GLN:HG3	1.82	0.62
1:A:216:ASN:HD21	1:A:257:ALA:HB1	1.64	0.62
1:C:190:HIS:HE1	6:C:601:ICS:S2B	2.22	0.62
1:L:290:ASN:HD21	1:L:355:HIS:HA	1.64	0.62
1:K:120:VAL:HG23	4:Q:67:ARG:HD3	1.82	0.61
3:H:2:GLN:HG3	3:H:66:LYS:HE2	1.82	0.61
1:L:351:SER:H	1:L:372:TYR:HE2	1.48	0.61
1:L:482:ARG:NH1	1:L:505:ASP:HB3	2.15	0.61
2:N:88:LEU:HD22	2:N:127:LEU:HD21	1.82	0.61
4:E:83:GLN:O	4:E:87:GLU:HG3	2.01	0.61
2:D:255:ARG:HG3	2:D:256:TYR:CD1	2.34	0.61
2:W:93:THR:HG21	1:U:20:PRO:HG3	1.82	0.61
2:B:276:ILE:HD12	2:B:291:LEU:HD13	1.81	0.61
1:C:66:VAL:HG11	6:C:601:ICS:S2B	2.40	0.61
2:D:230:ASP:HA	2:D:233:ASN:HB3	1.82	0.61
1:K:190:HIS:NE2	6:K:601:ICS:S3A	2.73	0.61
3:R:38:LYS:H	3:R:51:GLU:HA	1.65	0.61
1:L:339:LEU:HD11	1:L:510:ILE:HD12	1.82	0.61
1:L:289:VAL:HG21	1:L:304:MET:HE2	1.82	0.61
2:M:23:CYS:HB3	2:M:25:PRO:HD2	1.83	0.61
1:U:502:PHE:O	1:U:506:ILE:HG22	2.00	0.61
1:C:267:CYS:HB3	1:C:270:SER:HB3	1.83	0.61
1:C:450:HIS:HB2	2:D:95:TYR:CE1	2.34	0.61
1:K:483:GLN:HB2	1:K:488:ASP:H	1.65	0.61
2:W:26:ILE:HD11	2:W:56:LEU:HG	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:317:TYR:HE2	2:W:387:LEU:HD22	1.66	0.61
1:V:120:VAL:HA	4:Y:67:ARG:NH2	2.15	0.61
3:H:98:ILE:HG22	4:G:96:ASP:HB3	1.83	0.61
3:c:33:VAL:HG11	3:c:56:MET:HE3	1.83	0.61
1:A:58:CYS:HB2	5:A:601:CLF:S2B	2.40	0.61
2:B:39:MET:HE2	2:B:91:LEU:HD11	1.81	0.61
2:B:268:GLY:HA2	2:B:329:LEU:HD13	1.81	0.61
3:T:4:ILE:HB	3:T:59:MET:HG2	1.83	0.61
3:d:21:GLU:HG3	3:d:28:LEU:HD21	1.80	0.61
2:B:309:TYR:HB2	2:B:335:MET:HE3	1.82	0.60
2:W:269:ILE:HG23	2:W:295:ARG:HE	1.66	0.60
1:C:295:LYS:HE2	1:C:358:ASN:HB2	1.83	0.60
1:A:81:PRO:HD3	1:A:150:PRO:HG2	1.82	0.60
2:B:341:LEU:HD13	2:B:375:LEU:HB2	1.81	0.60
2:M:314:VAL:HG12	2:M:386:LEU:HB3	1.83	0.60
2:M:406:ARG:HB3	2:M:411:ILE:HD12	1.81	0.60
1:L:68:PHE:HD2	1:L:144:THR:HG21	1.67	0.60
1:C:221:TYR:CE2	6:C:601:ICS:S2A	2.95	0.60
2:W:48:CYS:CB	5:W:601:CLF:S4A	2.90	0.60
2:X:49:LEU:HD13	2:X:68:THR:HB	1.84	0.60
4:a:82:VAL:O	4:a:86:ILE:HG12	2.02	0.60
1:K:331:GLU:HB3	1:K:500:LEU:HD21	1.84	0.60
1:L:137:ILE:HG12	2:N:10:VAL:HG11	1.84	0.60
1:L:464:PHE:HD2	1:L:474:ALA:HB2	1.66	0.60
1:U:374:PHE:CZ	6:U:601:ICS:S3A	2.95	0.60
1:A:84:CYS:N	5:A:601:CLF:S4A	2.75	0.60
1:U:202:ILE:HD11	1:U:245:LEU:HD21	1.82	0.60
4:Q:3:GLU:HA	4:Q:72:VAL:HA	1.84	0.60
1:C:92:ARG:HD2	1:C:223:ILE:CD1	2.32	0.60
2:W:173:ILE:HD11	2:W:190:LEU:HD22	1.82	0.60
3:d:99:ARG:HE	3:d:100:THR:HG23	1.67	0.60
4:O:114:GLU:HG3	4:O:118:ALA:HB1	1.82	0.60
1:K:28:ARG:NH1	3:I:22:LYS:HG3	2.16	0.60
1:K:351:SER:O	1:K:355:HIS:CE1	2.55	0.60
2:N:390:ASN:HB3	2:N:410:PRO:HD2	1.84	0.60
1:C:133:GLU:O	1:C:137:ILE:HG22	2.02	0.59
1:V:201:LEU:HD13	1:V:254:ILE:HG21	1.84	0.59
2:W:44:GLY:HA2	2:W:71:PHE:HD2	1.67	0.59
2:W:333:MET:HE2	2:W:335:MET:HE2	1.84	0.59
1:U:12:VAL:HA	1:U:15:ILE:HD12	1.84	0.59
3:I:59:MET:HE1	3:I:69:VAL:HG11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ALA:HB1	1:A:151:VAL:CG2	2.32	0.59
2:D:317:TYR:CE1	2:D:389:GLY:HA3	2.37	0.59
3:d:84:ASP:HB2	4:Y:111:ARG:HB2	1.84	0.59
4:a:13:VAL:HG21	4:a:67:ARG:HD2	1.84	0.59
1:V:198:MET:HG3	1:V:202:ILE:HD11	1.84	0.59
3:c:35:GLY:HA3	3:c:54:LYS:HD2	1.85	0.59
2:N:243:MET:HE1	2:N:344:THR:HG21	1.84	0.59
1:C:92:ARG:HD3	1:C:223:ILE:HD11	1.84	0.59
2:D:413:ASP:OD1	2:D:414:ARG:HD3	2.02	0.59
3:J:66:LYS:O	3:J:70:ILE:HG12	2.03	0.59
3:J:70:ILE:O	3:J:74:MET:HG2	2.02	0.59
3:P:28:LEU:HD21	3:P:57:LEU:HD22	1.85	0.59
1:A:143:ILE:HB	1:A:173:VAL:HG12	1.84	0.59
1:A:349:GLY:HA2	1:A:373:GLN:CB	2.33	0.59
1:K:522:TRP:HZ3	2:N:273:ASP:HB2	1.68	0.59
2:M:33:LEU:HD13	2:M:207:PHE:HZ	1.67	0.59
3:R:86:ARG:NH1	4:O:27:SER:HB2	2.18	0.59
1:L:217:ILE:HG12	1:L:264:ILE:HD11	1.83	0.59
1:A:193:ALA:O	1:A:194:SER:C	2.44	0.59
2:M:48:CYS:O	2:M:49:LEU:C	2.45	0.59
1:A:374:PHE:HE1	6:A:602:ICS:S3A	2.25	0.59
3:d:96:TYR:HB2	3:Z:87:ILE:HB	1.85	0.59
4:a:1:MET:HE3	4:a:2:LYS:N	2.17	0.59
2:M:386:LEU:HD11	2:M:405:VAL:HG23	1.85	0.59
4:O:109:ARG:HD2	4:O:114:GLU:HB2	1.84	0.59
1:K:81:PRO:HG2	5:M:501:CLF:S2A	2.42	0.58
2:W:323:LEU:HD12	2:W:342:THR:HB	1.85	0.58
3:b:3:MET:HE2	3:b:3:MET:HA	1.85	0.58
1:K:159:GLU:O	1:K:163:ARG:HG3	2.02	0.58
1:K:292:ILE:HG21	1:K:356:TYR:CD1	2.38	0.58
2:M:180:PRO:HB3	2:M:203:THR:HG22	1.85	0.58
1:U:483:GLN:HB2	1:U:488:ASP:H	1.69	0.58
2:B:92:THR:HG21	2:B:128:ILE:HB	1.84	0.58
2:B:94:VAL:HG13	2:B:95:TYR:CD2	2.39	0.58
1:K:149:CYS:HA	1:K:179:GLU:HG3	1.85	0.58
2:M:59:HIS:ND1	2:M:410:PRO:HA	2.19	0.58
1:V:418:ILE:HG23	1:V:428:MET:HE1	1.85	0.58
2:W:45:SER:HB3	2:W:48:CYS:SG	2.43	0.58
1:L:298:GLU:HA	1:L:321:ILE:HD11	1.84	0.58
2:W:48:CYS:CA	5:W:601:CLF:S4A	2.89	0.58
2:W:175:PRO:HG3	2:W:183:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:268:HIS:O	1:L:272:ASN:HB2	2.02	0.58
1:C:78:VAL:HG21	1:C:85:ALA:HB2	1.85	0.58
2:M:24:GLN:HG2	2:M:139:THR:HB	1.85	0.58
2:M:357:ILE:HD12	2:M:366:ILE:HD11	1.85	0.58
1:V:143:ILE:HD11	1:V:171:ILE:HD12	1.86	0.58
3:I:13:GLU:HG2	3:I:55:THR:HG21	1.85	0.58
2:M:12:ARG:HH21	2:M:17:ILE:HD12	1.69	0.58
1:V:201:LEU:HD21	1:V:251:PHE:HB2	1.86	0.58
1:C:506:ILE:O	1:C:510:ILE:HG22	2.04	0.57
2:D:54:MET:HE3	2:D:58:ARG:HH12	1.69	0.57
1:K:459:LEU:O	1:K:461:PRO:HD3	2.04	0.57
2:X:167:PRO:HG2	2:N:224:PRO:HB2	1.85	0.57
3:T:66:LYS:O	3:T:70:ILE:HD12	2.04	0.57
1:L:92:ARG:HD3	1:L:94:ASN:HB3	1.86	0.57
2:N:164:LYS:HA	2:N:233:ASN:HD21	1.68	0.57
2:W:211:LEU:HG	1:U:518:ILE:HD11	1.86	0.57
2:N:31:ALA:HB2	2:N:150:TYR:HD1	1.69	0.57
2:N:391:THR:HG21	2:N:413:ASP:H	1.69	0.57
1:C:345:PHE:CE1	1:C:369:VAL:HB	2.39	0.57
2:M:45:SER:HB2	5:M:501:CLF:S2B	2.44	0.57
1:V:374:PHE:HZ	6:V:602:ICS:S2B	2.27	0.57
3:R:40:LYS:O	3:R:43:HIS:N	2.37	0.57
1:L:467:GLY:HA2	1:L:485:HIS:HD2	1.69	0.57
3:R:86:ARG:HH12	4:O:27:SER:HB2	1.69	0.57
1:L:292:ILE:HD12	1:L:355:HIS:HB3	1.85	0.57
1:A:349:GLY:CA	6:A:602:ICS:S4B	2.92	0.57
1:A:433:LEU:HD21	1:A:437:MET:HE2	1.86	0.57
2:W:106:CYS:SG	5:W:601:CLF:S3A	3.02	0.57
2:B:301:MET:HG3	2:D:416:ASN:ND2	2.19	0.57
5:V:601:CLF:S4A	2:X:45:SER:CB	2.92	0.57
1:L:239:TYR:HE1	1:L:313:LEU:HD11	1.70	0.57
2:M:454:THR:HB	1:L:93:ARG:NH1	2.20	0.57
1:L:251:PHE:HA	1:L:254:ILE:HG22	1.87	0.57
4:Q:8:ILE:HD13	4:Q:16:THR:HG21	1.87	0.57
4:a:12:LYS:O	4:a:16:THR:HG23	2.04	0.57
1:C:135:VAL:HG22	1:C:171:ILE:HD11	1.86	0.57
2:M:240:LEU:HD13	2:M:423:MET:HE1	1.85	0.57
1:K:127:LEU:HD23	1:K:161:VAL:HG21	1.87	0.57
2:X:123:SER:O	2:X:126:GLU:HB3	2.05	0.57
3:R:100:THR:HG23	3:R:102:LYS:H	1.69	0.57
1:L:444:VAL:HG21	1:L:447:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:LEU:HD23	2:B:118:ILE:HG21	1.86	0.56
1:C:53:LEU:HB2	2:D:95:TYR:HE2	1.70	0.56
2:D:200:PHE:HE1	2:D:228:ILE:HA	1.70	0.56
1:V:327:LYS:HD2	1:V:328:TYR:CZ	2.40	0.56
2:X:174:ILE:HG21	2:X:245:GLY:HA3	1.87	0.56
1:C:48:VAL:HG21	1:C:54:THR:HG21	1.87	0.56
1:L:258:HIS:HB2	1:L:282:TYR:CD2	2.39	0.56
1:L:331:GLU:HB3	1:L:500:LEU:HD11	1.86	0.56
1:A:80:GLY:HA3	1:A:148:THR:HB	1.87	0.56
1:C:92:ARG:NE	1:C:94:ASN:OD1	2.39	0.56
2:D:386:LEU:HD21	2:D:435:ILE:HG12	1.88	0.56
1:K:160:SER:O	1:K:164:GLU:HG2	2.05	0.56
1:V:58:CYS:SG	2:X:45:SER:HB3	2.46	0.56
1:L:242:ILE:HD11	1:L:260:ALA:HB2	1.86	0.56
2:N:170:LYS:HD3	2:N:198:ILE:HD11	1.87	0.56
1:U:352:ARG:HB2	6:U:601:ICS:S5A	2.45	0.56
2:B:58:ARG:HD3	2:D:455:ILE:HD12	1.86	0.56
2:M:430:ARG:HE	2:M:434:ARG:HH21	1.53	0.56
3:d:31:MET:HB2	3:d:56:MET:HB3	1.86	0.56
1:U:218:PHE:HB3	1:U:271:ILE:HG21	1.87	0.56
4:Q:19:ALA:HB1	4:Q:84:LYS:HG2	1.88	0.56
1:C:148:THR:O	1:C:151:VAL:HG12	2.05	0.56
1:C:218:PHE:CD1	1:C:245:LEU:HB2	2.41	0.56
1:K:93:ARG:HD2	1:K:489:TYR:HD1	1.71	0.56
3:I:60:VAL:HG12	3:I:105:LEU:HD11	1.87	0.56
1:C:68:PHE:HE1	1:C:197:LEU:HD13	1.70	0.56
1:C:347:TYR:HE2	1:C:447:LEU:HB3	1.70	0.56
1:K:427:LEU:HD21	1:K:428:MET:HE2	1.88	0.56
2:M:391:THR:HG21	2:M:412:MET:HG3	1.88	0.56
1:V:60:PHE:HA	1:V:178:CYS:HB2	1.88	0.56
2:X:287:ILE:H	2:X:287:ILE:HD12	1.71	0.56
3:R:38:LYS:H	3:R:51:GLU:CA	2.19	0.56
4:G:105:THR:HB	3:I:89:VAL:HG23	1.88	0.56
1:A:31:ILE:HB	1:A:444:VAL:HG23	1.86	0.56
2:X:208:ASP:HB2	2:X:419:TYR:CE1	2.41	0.56
1:L:218:PHE:HE1	1:L:245:LEU:HD13	1.71	0.56
1:L:482:ARG:HH12	1:L:505:ASP:HB3	1.71	0.56
1:C:258:HIS:HD2	1:C:259:GLN:OE1	1.88	0.56
2:D:391:THR:HG23	2:D:411:ILE:HA	1.86	0.56
3:H:7:VAL:HG22	3:H:56:MET:HB2	1.87	0.56
2:W:317:TYR:OH	2:W:393:GLY:HA3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:232:ALA:HB1	2:X:256:TYR:CD2	2.41	0.56
3:H:16:VAL:O	3:H:20:LEU:HG	2.06	0.56
4:Q:111:ARG:HD3	3:S:82:TYR:HA	1.86	0.56
1:C:49:ILE:HD12	1:C:50:PRO:HD2	1.88	0.55
2:W:51:TYR:HB3	1:U:87:PHE:HD2	1.72	0.55
2:N:111:ILE:O	4:O:65:PRO:HG3	2.06	0.55
1:U:154:ILE:HG23	1:U:155:GLY:N	2.21	0.55
4:O:86:ILE:HD13	3:P:98:ILE:HG23	1.87	0.55
2:B:59:HIS:HD2	2:B:411:ILE:H	1.54	0.55
2:D:49:LEU:HD23	2:D:68:THR:HB	1.87	0.55
1:K:31:ILE:HG12	1:K:444:VAL:HG12	1.89	0.55
2:X:119:LEU:HD12	2:X:134:ILE:HG21	1.88	0.55
1:L:213:PHE:HA	1:L:308:PHE:HE2	1.71	0.55
4:Q:19:ALA:HB2	4:Q:88:VAL:HG11	1.88	0.55
2:X:453:GLU:HG3	2:X:456:GLN:HB3	1.87	0.55
3:H:31:MET:HE2	3:I:31:MET:HG3	1.88	0.55
1:L:86:TYR:CD2	2:N:22:ILE:HG13	2.42	0.55
1:L:122:GLY:HA2	1:L:154:ILE:HD13	1.89	0.55
1:L:188:ALA:O	1:L:192:ILE:HG22	2.07	0.55
1:U:197:LEU:HD11	1:U:245:LEU:HD23	1.87	0.55
1:U:258:HIS:HD2	1:U:259:GLN:HG3	1.72	0.55
1:U:269:ARG:HD3	1:U:376:HIS:H	1.71	0.55
1:K:75:VAL:HG13	1:K:143:ILE:HG23	1.88	0.55
2:M:269:ILE:HB	2:M:332:GLU:OE2	2.07	0.55
1:U:349:GLY:O	6:U:601:ICS:S5A	2.64	0.55
1:A:80:GLY:HA2	1:A:114:MET:HG3	1.88	0.55
2:M:24:GLN:HG3	2:M:149:GLY:CA	2.36	0.55
2:W:333:MET:SD	2:W:432:VAL:HG22	2.46	0.55
3:b:57:LEU:HB3	3:b:59:MET:HE1	1.89	0.55
2:N:268:GLY:O	2:N:272:THR:HG22	2.07	0.55
4:a:1:MET:HB3	4:a:104:ILE:HB	1.89	0.55
1:A:352:ARG:CB	6:A:602:ICS:S5A	2.89	0.55
1:A:369:VAL:HG11	1:A:455:LEU:HD13	1.88	0.55
1:C:313:LEU:O	1:C:317:THR:HG23	2.06	0.55
1:L:92:ARG:NH2	6:L:602:ICS:S2B	2.80	0.55
1:L:265:LEU:HD21	1:L:268:HIS:HA	1.87	0.55
1:L:269:ARG:HH22	1:L:379:ASP:HB2	1.71	0.55
1:L:312:GLU:HA	1:L:315:ARG:HG2	1.87	0.55
1:K:221:TYR:CE2	6:K:601:ICS:S1A	2.96	0.55
3:P:28:LEU:HA	3:P:59:MET:HB3	1.88	0.55
2:D:54:MET:HE3	2:D:58:ARG:HH22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:TYR:CD2	2:D:207:PHE:HD2	2.25	0.55
3:J:29:THR:HG23	3:F:33:VAL:HG13	1.89	0.55
2:B:324:SER:HA	2:B:353:ILE:HD11	1.89	0.55
1:C:27:ARG:HH11	1:C:27:ARG:HA	1.70	0.55
1:V:82:ILE:HG21	2:X:21:LYS:HG3	1.89	0.55
1:V:342:LYS:HB2	1:V:365:MET:HG2	1.88	0.55
2:N:128:ILE:HG22	2:N:130:PRO:HD2	1.88	0.55
1:C:66:VAL:HA	1:C:92:ARG:NH1	2.22	0.55
1:C:83:GLY:HA3	2:D:23:CYS:SG	2.47	0.55
1:C:268:HIS:O	1:C:272:ASN:HB3	2.07	0.55
2:M:59:HIS:CD2	2:M:60:TYR:CD1	2.94	0.55
1:U:60:PHE:HA	1:U:63:THR:HG22	1.89	0.55
1:U:217:ILE:HD13	1:U:264:ILE:HD11	1.88	0.55
1:V:350:GLY:HA3	6:V:602:ICS:S3A	2.47	0.54
3:c:70:ILE:HG22	3:c:74:MET:HE2	1.89	0.54
1:A:477:ILE:HA	2:B:215[B]:HIS:CD2	2.41	0.54
1:C:267:CYS:O	1:C:268:HIS:C	2.47	0.54
2:W:45:SER:OG	5:W:601:CLF:S2B	2.45	0.54
4:G:6:ALA:HB3	4:G:69:PHE:HB2	1.89	0.54
2:B:43:HIS:CD2	2:B:84:LEU:HD13	2.43	0.54
2:D:180:PRO:HG3	2:D:203:THR:HG22	1.89	0.54
1:V:267:CYS:SG	1:V:270:SER:HB2	2.47	0.54
2:X:94:VAL:HG13	2:X:95:TYR:CD1	2.42	0.54
1:U:75:VAL:HG13	1:U:143:ILE:HG23	1.89	0.54
1:A:306:GLU:HG3	1:A:425:ILE:HG12	1.90	0.54
2:D:88:LEU:HA	2:D:91:LEU:HD23	1.88	0.54
1:L:467:GLY:HA2	1:L:485:HIS:CD2	2.41	0.54
1:C:518:ILE:HD11	2:D:211:LEU:O	2.07	0.54
1:K:207:ILE:HG12	1:K:256:GLN:HB3	1.89	0.54
3:J:33:VAL:HG12	4:E:31:ARG:HD2	1.89	0.54
2:N:199:VAL:O	2:N:202:ASP:HB2	2.07	0.54
3:H:33:VAL:HG12	3:I:31:MET:HB2	1.90	0.54
2:N:200:PHE:HA	2:N:223:THR:HG21	1.90	0.54
3:c:7:VAL:HG22	3:c:56:MET:HE2	1.89	0.54
1:V:135:VAL:HG22	1:V:171:ILE:HD11	1.90	0.54
1:L:198:MET:HE2	1:L:277:MET:HE2	1.90	0.54
1:C:267:CYS:CB	1:C:270:SER:HB3	2.38	0.54
3:R:56:MET:HE2	3:R:56:MET:HA	1.89	0.54
3:d:33:VAL:HG23	4:Y:31:ARG:HB2	1.89	0.54
1:L:86:TYR:HD2	2:N:22:ILE:HG13	1.72	0.54
2:B:198:ILE:HD13	2:B:227:ASP:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:377:GLN:HB3	2:B:381:ARG:HH21	1.73	0.54
1:K:226:ASP:OD1	1:K:494:THR:HG21	2.08	0.54
1:V:350:GLY:HA3	6:V:602:ICS:S1A	2.48	0.54
1:L:148:THR:HG22	1:L:149:CYS:H	1.72	0.54
1:U:66:VAL:HG13	6:U:601:ICS:S1A	2.48	0.54
2:M:206:VAL:HG23	2:M:219:PRO:HG2	1.90	0.53
2:W:240:LEU:HD22	2:W:266:PRO:HG3	1.90	0.53
3:F:61:VAL:HG11	3:F:69:VAL:HG21	1.90	0.53
1:A:489:TYR:CG	2:D:456:GLN:HA	2.43	0.53
2:N:267:ILE:HG21	2:N:326:LEU:HD23	1.90	0.53
1:U:154:ILE:HG23	1:U:155:GLY:H	1.72	0.53
2:B:28:ALA:HB1	2:B:153:MET:HE3	1.91	0.53
4:O:1:MET:HE2	4:O:1:MET:N	2.24	0.53
1:A:81:PRO:HD2	1:A:148:THR:CG2	2.33	0.53
1:A:103:ASP:HB3	1:A:105:TYR:HE1	1.73	0.53
1:C:108:TYR:HE1	2:D:2:LEU:HD22	1.72	0.53
1:C:127:LEU:HD23	1:C:161:VAL:HG11	1.90	0.53
2:D:42:SER:HB2	2:D:49:LEU:HD22	1.89	0.53
1:K:33:VAL:HG22	1:K:442:ILE:HG12	1.90	0.53
1:K:231:LYS:O	1:K:235:GLU:HG3	2.08	0.53
3:b:23:GLU:HG3	3:b:72:THR:HG21	1.91	0.53
2:N:54:MET:HE3	2:N:58:ARG:HH22	1.72	0.53
4:a:85:ILE:HG21	4:a:99:ILE:HD11	1.90	0.53
1:A:149:CYS:O	1:A:150:PRO:C	2.50	0.53
1:C:292:ILE:HD13	1:C:355:HIS:HB3	1.89	0.53
2:M:23:CYS:HB3	2:M:25:PRO:CD	2.39	0.53
2:M:42:SER:HB2	2:M:49:LEU:HD13	1.90	0.53
1:V:258:HIS:HB2	1:V:282:TYR:HD2	1.73	0.53
1:U:127:LEU:HD11	1:U:145:ILE:HD12	1.90	0.53
4:O:84:LYS:O	4:O:88:VAL:HG23	2.09	0.53
2:B:243:MET:HE1	2:B:346:ASN:HB3	1.89	0.53
1:K:120:VAL:HG11	3:S:34:PHE:CG	2.44	0.53
1:K:187:SER:HB2	1:K:269:ARG:HH21	1.73	0.53
2:X:217:PHE:HB3	2:X:218:TYR:CD1	2.43	0.53
1:L:482:ARG:HD3	1:L:509:ALA:HB2	1.90	0.53
1:U:289:VAL:HB	1:U:300:SER:HB3	1.91	0.53
1:A:351:SER:HA	1:A:372:TYR:CE1	2.44	0.53
1:A:372:TYR:HD2	1:A:380:TYR:CZ	2.27	0.53
2:B:49:LEU:HD11	2:B:66:ALA:HB1	1.91	0.53
2:D:225:ILE:HD12	2:D:228:ILE:HD12	1.91	0.53
2:M:168:ASN:ND2	2:M:230:ASP:HB3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:190:HIS:CE1	6:K:601:ICS:S3A	3.02	0.53
1:K:218:PHE:HB3	1:K:271:ILE:HG21	1.90	0.53
2:M:17:ILE:HD12	2:M:17:ILE:H	1.74	0.53
1:L:66:VAL:HG11	6:L:602:ICS:S3A	2.48	0.53
1:L:350:GLY:HA2	1:L:372:TYR:CD2	2.43	0.53
4:G:36:ARG:HB3	4:G:63:PHE:HA	1.91	0.53
4:Q:6:ALA:HB3	4:Q:69:PHE:HB2	1.91	0.53
1:K:265:LEU:HD13	1:K:275:ASN:HD22	1.72	0.52
2:W:330:VAL:HG22	2:W:335:MET:HE3	1.90	0.52
5:W:601:CLF:S2A	1:U:83:GLY:HA3	2.49	0.52
1:U:219:GLY:HA3	1:U:267:CYS:H	1.74	0.52
1:U:266:LEU:HD22	1:U:291:TYR:CE2	2.44	0.52
2:B:129:ASP:HB3	2:B:132:ILE:HG12	1.92	0.52
1:C:245:LEU:HD11	1:C:254:ILE:HG23	1.90	0.52
1:C:305:ALA:HB2	1:C:317:THR:HG21	1.90	0.52
2:D:294:GLU:HB3	2:D:425:TYR:CD2	2.40	0.52
4:E:3:GLU:HG2	4:E:104:ILE:HD11	1.91	0.52
1:A:331:GLU:HB3	1:A:500:LEU:HD21	1.91	0.52
2:D:173:ILE:HD13	2:D:238:ILE:HB	1.92	0.52
3:P:31:MET:HG2	3:P:56:MET:HB3	1.91	0.52
4:a:37:GLY:O	4:a:38:LYS:HG2	2.10	0.52
1:A:274:THR:O	1:A:278:MET:HG2	2.09	0.52
2:W:114:ASP:HB3	2:W:117:VAL:HG22	1.92	0.52
2:N:268:GLY:HA2	2:N:329:LEU:HD13	1.92	0.52
1:C:422:LYS:HA	1:C:427:LEU:HB3	1.92	0.52
2:M:23:CYS:SG	2:M:141:SER:OG	2.68	0.52
1:V:191:HIS:NE2	1:V:273:TYR:HE2	2.06	0.52
2:X:200:PHE:CG	2:X:201:PRO:HD3	2.44	0.52
1:L:51:GLY:HA2	2:N:68:THR:H	1.74	0.52
3:H:23:GLU:HA	3:H:26:ILE:HD11	1.91	0.52
1:L:339:LEU:HG	1:L:365:MET:HE3	1.90	0.52
2:N:16:THR:HG23	2:N:371:ASP:HB3	1.90	0.52
2:D:119:LEU:HA	2:D:122:VAL:HG12	1.90	0.52
2:M:49:LEU:HD22	2:M:68:THR:HB	1.92	0.52
2:W:42:SER:HB2	2:W:49:LEU:HD13	1.91	0.52
2:N:37:ASN:ND2	2:N:218:TYR:HD2	2.07	0.52
2:N:62:GLU:HG3	2:N:207:PHE:O	2.10	0.52
4:Y:62:ARG:NE	4:Y:63:PHE:H	2.07	0.52
1:A:266:LEU:HG	1:A:355:HIS:HE1	1.74	0.52
1:A:447:LEU:HB3	1:A:452:THR:HG23	1.91	0.52
2:M:168:ASN:HD22	2:M:230:ASP:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:125:GLU:HG2	3:F:81:LYS:HD3	1.91	0.52
2:N:12:ARG:HH22	2:N:374:MET:HE2	1.74	0.52
1:U:506:ILE:O	1:U:510:ILE:HG22	2.10	0.52
1:A:350:GLY:HA3	6:A:602:ICS:S4A	2.50	0.52
1:C:299:LYS:O	1:C:303:LYS:HG3	2.10	0.52
1:V:120:VAL:HG21	3:d:34:PHE:CE1	2.45	0.52
2:W:205:ASP:HB3	2:W:221:GLY:HA3	1.91	0.52
3:H:98:ILE:HD13	4:G:86:ILE:HD13	1.92	0.52
1:A:178:CYS:O	1:A:179:GLU:C	2.53	0.52
1:C:66:VAL:HA	1:C:92:ARG:CZ	2.39	0.52
2:W:376:HIS:HE1	2:W:400:GLU:OE2	1.93	0.52
3:J:74:MET:HE1	4:E:108:ILE:HG21	1.90	0.52
1:L:262:LEU:HD11	1:L:287:LEU:HD22	1.92	0.52
2:N:95:TYR:O	2:N:97:PRO:HD3	2.10	0.52
1:V:149:CYS:SG	1:V:150:PRO:HD3	2.50	0.51
1:V:351:SER:HA	1:V:372:TYR:CZ	2.45	0.51
1:L:78:VAL:HG21	1:L:85:ALA:HB2	1.92	0.51
1:L:265:LEU:HD22	1:L:275:ASN:HD21	1.75	0.51
4:Q:32:ARG:HG2	4:Q:67:ARG:NH1	2.24	0.51
2:B:376:HIS:O	2:B:380:LYS:HG2	2.10	0.51
2:D:200:PHE:O	2:D:223:THR:HG21	2.10	0.51
1:K:63:THR:HG21	1:K:178:CYS:CB	2.40	0.51
2:X:247:ALA:HA	2:X:250:LYS:HE2	1.92	0.51
3:T:6:ALA:HB2	3:T:87:ILE:HG23	1.92	0.51
2:N:100:ILE:HB	2:N:134:ILE:HG12	1.91	0.51
2:B:30:TYR:CZ	2:B:203:THR:HG21	2.45	0.51
2:B:106:CYS:O	2:B:107:VAL:C	2.52	0.51
2:B:379:ILE:HD11	2:B:387:LEU:HD21	1.90	0.51
2:M:317:TYR:CE1	2:M:389:GLY:HA3	2.45	0.51
3:R:10:PRO:HD3	3:R:54:LYS:HA	1.91	0.51
1:L:471:LYS:HD2	1:L:483:GLN:HG2	1.92	0.51
4:G:104:ILE:HD12	3:I:88:PHE:HB3	1.91	0.51
1:A:130:ALA:O	1:A:134:VAL:HG12	2.10	0.51
1:U:92:ARG:NH2	6:U:601:ICS:S2B	2.84	0.51
4:a:12:LYS:HD3	4:a:15:LYS:NZ	2.26	0.51
1:C:331:GLU:HB3	1:C:500:LEU:HD21	1.92	0.51
2:M:315:ALA:HB3	2:M:387:LEU:HD22	1.92	0.51
2:W:182:ASP:HB3	2:W:423:MET:HE2	1.91	0.51
2:X:199:VAL:O	2:X:202:ASP:HB2	2.10	0.51
1:L:92:ARG:HB2	7:L:601:HCA:H51	1.91	0.51
1:V:350:GLY:CA	6:V:602:ICS:S1A	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:23:CYS:O	2:W:26:ILE:HG22	2.11	0.51
2:N:391:THR:HG23	2:N:411:ILE:HA	1.93	0.51
1:A:371:GLY:HA3	1:A:444:VAL:HG12	1.93	0.51
1:C:374:PHE:CZ	6:C:601:ICS:S1B	3.04	0.51
2:D:49:LEU:HD11	2:D:66:ALA:HB3	1.92	0.51
1:V:183:GLY:HA3	1:V:188:ALA:HB2	1.93	0.51
2:W:240:LEU:HD13	2:W:423:MET:HE1	1.91	0.51
3:T:33:VAL:HG23	3:T:54:LYS:HB2	1.92	0.51
1:U:356:TYR:HD1	1:U:359:LEU:HD23	1.75	0.51
3:P:53:GLN:O	3:P:54:LYS:HD3	2.10	0.51
4:a:111:ARG:HH21	4:a:112:THR:HG22	1.75	0.51
1:A:8:LYS:HG3	1:A:33:VAL:HG11	1.92	0.51
1:C:427:LEU:HG	1:C:428:MET:HE2	1.92	0.51
2:M:154:VAL:O	2:M:158:VAL:HG23	2.11	0.51
2:W:1:MET:HB2	2:X:449:ASP:OD1	2.10	0.51
4:G:34:MET:HG2	4:G:65:PRO:HA	1.92	0.51
3:c:10:PRO:HD3	3:c:54:LYS:HA	1.92	0.51
1:A:103:ASP:HB3	1:A:105:TYR:CE1	2.46	0.51
1:K:70:PRO:HG3	1:K:94:ASN:HD22	1.76	0.51
2:W:452:LEU:HD22	2:X:1:MET:HE1	1.92	0.51
2:X:379:ILE:HD12	2:X:384:VAL:HB	1.93	0.51
1:L:63:THR:HG22	1:L:193:ALA:HB2	1.93	0.51
3:S:36:ARG:O	3:S:36:ARG:HD3	2.11	0.51
2:D:236:GLY:HA3	2:D:282:LEU:HD22	1.93	0.51
2:M:59:HIS:CD2	2:M:59:HIS:C	2.89	0.51
3:T:86:ARG:HB2	3:T:88:PHE:CE1	2.46	0.51
3:b:5:ARG:HG2	3:b:56:MET:HE3	1.92	0.51
1:L:383:ARG:HH12	1:L:386:ILE:HG21	1.75	0.51
1:U:168:GLU:HG3	1:U:169:HIS:ND1	2.26	0.51
1:A:267:CYS:SG	1:A:270:SER:HB3	2.51	0.50
1:K:150:PRO:O	1:K:154:ILE:HG23	2.10	0.50
1:K:312:GLU:HG3	1:K:315:ARG:HH21	1.75	0.50
1:V:281:LYS:HG3	1:V:282:TYR:CD1	2.45	0.50
2:W:110:THR:HG23	1:U:119:ILE:HD11	1.93	0.50
4:a:109:ARG:HD2	4:a:112:THR:HG23	1.93	0.50
1:V:438:LYS:HD2	1:V:439:ASP:H	1.75	0.50
2:W:51:TYR:HB3	1:U:87:PHE:CD2	2.45	0.50
4:a:31:ARG:HG3	4:a:68:MET:HG3	1.93	0.50
3:b:64:GLU:HG3	3:b:65:HIS:ND1	2.26	0.50
4:O:3:GLU:HB3	4:O:104:ILE:HD11	1.93	0.50
4:Y:62:ARG:HH21	4:Y:63:PHE:HD2	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ILE:HA	1:A:255:SER:HA	1.92	0.50
1:A:237:ILE:HG12	1:A:320:VAL:HG21	1.93	0.50
2:M:237:THR:HG21	2:M:252:LEU:HD13	1.92	0.50
1:U:20:PRO:HD2	1:U:23:ALA:HB3	1.93	0.50
1:V:149:CYS:HB3	5:V:601:CLF:S2A	2.52	0.50
2:N:26:ILE:HA	2:N:52:LEU:HG	1.94	0.50
2:N:41:HIS:CE1	2:N:91:LEU:HD22	2.46	0.50
2:N:182:ASP:HB3	2:N:423:MET:SD	2.51	0.50
2:N:317:TYR:CE2	2:N:389:GLY:HA3	2.47	0.50
1:U:273:TYR:O	1:U:277:MET:HG2	2.11	0.50
1:K:349:GLY:N	6:K:601:ICS:S5A	2.84	0.50
2:M:99:VAL:HG21	2:M:225:ILE:HD13	1.92	0.50
1:L:339:LEU:HD21	1:L:506:ILE:HG22	1.92	0.50
4:E:82:VAL:O	4:E:86:ILE:HG12	2.12	0.50
2:W:297:ARG:HG2	2:X:419:TYR:CE1	2.46	0.50
1:L:110:VAL:HG22	2:N:17:ILE:HG23	1.94	0.50
2:B:23:CYS:O	2:B:26:ILE:HG22	2.12	0.50
1:C:147:ALA:HB1	1:C:151:VAL:HG11	1.92	0.50
2:M:106:CYS:O	2:M:107:VAL:C	2.55	0.50
1:V:354:HIS:CD2	1:V:436:GLU:HG3	2.46	0.50
1:A:191:HIS:O	1:A:192:ILE:C	2.54	0.50
2:B:43:HIS:HD2	2:B:84:LEU:HD13	1.77	0.50
2:M:272:THR:O	2:M:276:ILE:HG12	2.12	0.50
1:V:149:CYS:CB	5:V:601:CLF:S2A	3.00	0.50
1:L:158:ILE:HD11	1:L:177:ARG:NE	2.26	0.50
4:Q:35:GLY:HA3	4:Q:66:LYS:NZ	2.26	0.50
2:M:289:PRO:O	2:M:292:GLU:HG3	2.11	0.49
1:V:289:VAL:HB	1:V:300:SER:HB2	1.94	0.49
2:W:48:CYS:HB3	5:W:601:CLF:S4A	2.52	0.49
2:W:317:TYR:CE1	2:W:389:GLY:HA3	2.47	0.49
2:X:200:PHE:CD2	2:X:201:PRO:HD3	2.47	0.49
3:J:5:ARG:HB3	3:J:56:MET:HE2	1.94	0.49
3:R:92:VAL:HG21	3:P:88:PHE:HB3	1.94	0.49
3:T:10:PRO:HD3	3:T:54:LYS:HA	1.94	0.49
5:L:603:CLF:S3A	2:N:45:SER:HB3	2.52	0.49
2:N:200:PHE:CG	2:N:201:PRO:HD3	2.47	0.49
4:Q:25:PHE:HD2	4:Q:81:VAL:HG11	1.78	0.49
1:C:216:ASN:O	1:C:264:ILE:HG12	2.11	0.49
2:X:118:ILE:HG22	2:X:119:LEU:HD22	1.93	0.49
1:U:250:SER:O	1:U:254:ILE:HG12	2.13	0.49
2:B:166:LYS:HG2	2:M:230:ASP:OD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:MET:HG3	2:D:416:ASN:HD21	1.77	0.49
1:K:198:MET:HG3	1:K:277:MET:HG3	1.93	0.49
2:M:172:ASN:HB2	2:M:237:THR:HG22	1.93	0.49
2:M:184:ARG:HH21	2:M:204:THR:HB	1.76	0.49
1:V:71:ILE:HG21	1:V:74:MET:HE3	1.94	0.49
1:U:310:ASP:HB2	1:U:313:LEU:HB2	1.93	0.49
2:M:259:PRO:HB2	2:M:282:LEU:HD11	1.93	0.49
2:W:60:TYR:HD2	2:W:207:PHE:CG	2.31	0.49
2:W:173:ILE:HB	2:W:199:VAL:HG12	1.93	0.49
2:W:175:PRO:HA	2:W:240:LEU:HD12	1.93	0.49
1:L:19:LEU:HB3	1:L:23:ALA:HB3	1.94	0.49
1:C:237:ILE:HD11	1:C:320:VAL:HG11	1.94	0.49
2:D:200:PHE:CE2	2:D:230:ASP:OD2	2.65	0.49
1:K:135:VAL:HG21	1:K:169:HIS:CD2	2.48	0.49
1:L:349:GLY:HA3	6:L:602:ICS:S4B	2.51	0.49
2:N:308:HIS:ND1	2:N:440:LEU:HD11	2.28	0.49
2:M:314:VAL:HG21	2:M:330:VAL:HG11	1.95	0.49
1:L:56:ARG:HB3	2:N:46:GLN:NE2	2.28	0.49
1:A:472:TYR:CE2	2:B:61:ARG:HA	2.47	0.49
2:M:171:LEU:HD12	2:M:283:ALA:HB2	1.94	0.49
2:W:5:THR:HG21	2:W:376:HIS:CD2	2.47	0.49
3:R:31:MET:HE1	4:O:31:ARG:NH2	2.27	0.49
1:A:110:VAL:HG13	2:B:15:ILE:HG23	1.94	0.49
1:V:305:ALA:HB2	1:V:317:THR:HG21	1.94	0.49
2:W:341:LEU:HD13	2:W:375:LEU:HB2	1.95	0.49
3:b:87:ILE:HB	3:c:96:TYR:HB2	1.95	0.49
1:U:119:ILE:HD12	1:U:154:ILE:HG13	1.95	0.49
4:G:34:MET:HE3	4:G:63:PHE:HB2	1.94	0.49
2:D:106:CYS:SG	2:D:107:VAL:N	2.86	0.49
1:L:299:LYS:HG2	1:L:303:LYS:HE3	1.94	0.49
1:U:68:PHE:C	1:U:76:HIS:HE1	2.21	0.49
4:G:19:ALA:HB2	4:G:88:VAL:HG11	1.94	0.49
4:O:84:LYS:HA	4:O:84:LYS:HD3	1.57	0.49
1:C:154:ILE:O	4:E:11:ASN:HA	2.13	0.49
3:J:33:VAL:HG12	4:E:31:ARG:HH11	1.77	0.49
3:R:33:VAL:HG21	3:R:56:MET:HE3	1.94	0.49
1:A:144:THR:HG22	1:A:174:ILE:HB	1.95	0.48
1:V:47:LYS:HE2	1:V:47:LYS:HB2	1.58	0.48
2:W:141:SER:OG	5:W:601:CLF:S2A	2.71	0.48
2:X:317:TYR:CE2	2:X:389:GLY:HA3	2.48	0.48
2:X:378:ILE:HG12	2:X:381:ARG:NH2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:20:LEU:HD21	3:d:73:ILE:HG13	1.94	0.48
2:N:22:ILE:HG22	2:N:23:CYS:N	2.28	0.48
1:A:63:THR:HG23	1:A:189:GLY:HA2	1.95	0.48
1:A:349:GLY:N	6:A:602:ICS:S4B	2.86	0.48
2:X:391:THR:HG21	2:X:413:ASP:H	1.79	0.48
1:L:55:ASN:OD1	1:L:469:LYS:HD2	2.13	0.48
1:L:290:ASN:ND2	1:L:355:HIS:HA	2.28	0.48
3:P:10:PRO:HG2	3:P:53:GLN:HG2	1.95	0.48
1:C:108:TYR:CE1	2:D:2:LEU:HD22	2.48	0.48
1:K:158:ILE:HA	1:K:161:VAL:HG22	1.95	0.48
2:W:386:LEU:HD21	2:W:435:ILE:HG12	1.95	0.48
2:X:90:ASN:O	2:X:94:VAL:HG12	2.13	0.48
1:L:42:ILE:HD11	1:L:445:ASP:HB2	1.95	0.48
4:G:28:PHE:HB3	4:G:71:VAL:HB	1.95	0.48
2:B:147:ILE:HD11	2:B:319:ASP:OD2	2.14	0.48
1:V:120:VAL:HA	4:Y:67:ARG:HH22	1.78	0.48
2:N:65:LEU:HD22	2:N:217:PHE:CE1	2.48	0.48
1:A:143:ILE:HG13	1:A:171:ILE:HD11	1.94	0.48
1:L:48:VAL:HG11	1:L:54:THR:HG21	1.95	0.48
2:N:174:ILE:HG21	2:N:245:GLY:HA3	1.96	0.48
2:N:374:MET:O	2:N:378:ILE:HG13	2.12	0.48
1:U:15:ILE:HG12	1:U:454:PHE:HB3	1.95	0.48
4:Q:33:VAL:HG21	4:Q:68:MET:HB3	1.95	0.48
3:Z:28:LEU:HD11	3:Z:57:LEU:HB3	1.95	0.48
1:K:59:ALA:O	1:K:63:THR:HG22	2.14	0.48
2:M:12:ARG:HH21	2:M:17:ILE:CD1	2.27	0.48
2:M:267:ILE:HD13	2:M:423:MET:HA	1.94	0.48
1:V:127:LEU:HD22	1:V:161:VAL:HG11	1.95	0.48
1:V:374:PHE:CZ	6:V:602:ICS:S1B	3.07	0.48
1:U:174:ILE:HG23	1:U:200:HIS:HB3	1.95	0.48
1:A:348:ALA:HB1	6:A:602:ICS:S5A	2.53	0.48
2:B:87:ALA:O	2:B:91:LEU:HB2	2.13	0.48
2:M:33:LEU:HD13	2:M:207:PHE:CZ	2.48	0.48
1:L:27:ARG:HH21	1:L:31:ILE:HD11	1.78	0.48
1:U:233:ILE:O	1:U:237:ILE:HG13	2.14	0.48
3:P:70:ILE:O	3:P:74:MET:HE2	2.14	0.48
1:A:53:LEU:H	2:B:67:THR:HG23	1.79	0.48
1:A:75:VAL:HG13	1:A:143:ILE:HG23	1.95	0.48
1:C:77:LEU:HD11	1:C:112:THR:HG23	1.96	0.48
1:C:271:ILE:HG22	1:C:271:ILE:O	2.14	0.48
1:C:437:MET:SD	1:C:441:THR:HG21	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:63:THR:HG21	1:K:178:CYS:HB2	1.95	0.48
2:X:341:LEU:HG	2:X:367:ILE:HD11	1.96	0.48
4:E:85:ILE:HG21	4:E:99:ILE:HD11	1.96	0.48
1:A:138:PHE:HZ	2:B:17:ILE:HD13	1.79	0.48
5:A:601:CLF:S2A	2:B:106:CYS:SG	3.12	0.48
2:M:127:LEU:O	2:M:127:LEU:HD12	2.14	0.48
2:M:175:PRO:HA	2:M:240:LEU:HD12	1.94	0.48
2:M:331:LEU:HD11	2:M:357:ILE:HA	1.95	0.48
1:V:251:PHE:HA	1:V:254:ILE:HB	1.95	0.48
1:L:77:LEU:HD13	1:L:110:VAL:HG12	1.95	0.48
2:N:31:ALA:HB2	2:N:150:TYR:CD1	2.48	0.48
1:U:166:GLU:HG3	1:U:172:LYS:HA	1.95	0.48
1:U:203:GLY:HA2	1:U:258:HIS:CE1	2.48	0.48
4:G:98:LYS:HE3	4:G:100:PHE:HZ	1.78	0.48
1:A:184:VAL:O	2:B:46:GLN:NE2	2.46	0.48
1:A:383:ARG:HG3	1:A:430:TYR:HB3	1.94	0.48
2:B:267:ILE:HG12	2:B:423:MET:HB3	1.95	0.48
2:D:175:PRO:HA	2:D:240:LEU:HD23	1.95	0.48
2:M:164:LYS:HE3	2:M:164:LYS:HB3	1.68	0.48
2:M:241:CYS:HB2	2:M:244:ALA:HB3	1.96	0.48
1:L:149:CYS:HB2	1:L:150:PRO:HD3	1.96	0.48
1:L:218:PHE:HD1	1:L:245:LEU:HB2	1.79	0.48
2:N:119:LEU:HD11	2:N:134:ILE:HG21	1.96	0.48
3:I:15:LYS:O	3:I:18:GLU:HG2	2.13	0.48
1:A:83:GLY:O	1:A:84:CYS:C	2.51	0.47
1:A:268:HIS:O	1:A:272:ASN:HB3	2.14	0.47
2:B:39:MET:HE2	2:B:91:LEU:HD21	1.96	0.47
1:C:80:GLY:HA3	1:C:148:THR:OG1	2.14	0.47
1:K:131:ILE:O	1:K:135:VAL:HG13	2.13	0.47
2:M:109:GLU:HG3	2:M:140:PRO:HA	1.95	0.47
2:M:270:ARG:HG3	2:M:332:GLU:OE1	2.14	0.47
1:V:93:ARG:HH22	1:V:489:TYR:HD1	1.62	0.47
1:V:274:THR:O	1:V:278:MET:HG3	2.14	0.47
2:W:289:PRO:O	2:W:292:GLU:HG3	2.14	0.47
3:H:32:GLU:O	3:I:31:MET:HG2	2.13	0.47
2:B:137:ALA:HB2	2:B:156:SER:HB3	1.96	0.47
2:B:161:PHE:CD2	2:B:225:ILE:HD11	2.49	0.47
2:B:410:PRO:O	2:B:411:ILE:HD13	2.13	0.47
1:C:92:ARG:NH2	6:C:601:ICS:S3B	2.83	0.47
2:D:226:GLY:HA3	2:N:166:LYS:HA	1.95	0.47
1:V:197:LEU:HD21	1:V:245:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:37:ASN:HA	2:X:218:TYR:CD2	2.48	0.47
2:X:208:ASP:HB2	2:X:419:TYR:CZ	2.49	0.47
3:R:36:ARG:O	3:R:37:GLY:C	2.56	0.47
3:I:23:GLU:HB3	3:I:68:LYS:HD3	1.96	0.47
3:Z:28:LEU:HD13	3:Z:59:MET:SD	2.53	0.47
2:B:175:PRO:HG3	2:B:183:ILE:HD11	1.96	0.47
1:K:198:MET:HG2	1:K:277:MET:HE2	1.96	0.47
2:M:267:ILE:HG21	2:M:326:LEU:HD12	1.95	0.47
3:J:9:ARG:HG2	3:J:10:PRO:HD2	1.96	0.47
4:E:85:ILE:HA	4:E:88:VAL:HG22	1.96	0.47
1:A:139:ASN:N	1:A:140:PRO:HD3	2.29	0.47
1:C:116:GLU:O	1:C:119:ILE:HG22	2.14	0.47
1:V:265:LEU:HG	1:V:275:ASN:HD22	1.78	0.47
2:X:374:MET:O	2:X:378:ILE:HG13	2.14	0.47
2:D:92:THR:HA	2:D:97:PRO:HD3	1.97	0.47
2:D:170:LYS:HB2	2:D:233:ASN:OD1	2.14	0.47
1:K:344:ALA:HB3	1:K:367:VAL:HA	1.97	0.47
1:U:137:ILE:HG22	1:U:138:PHE:HD1	1.79	0.47
4:E:109:ARG:HG2	4:E:112:THR:H	1.79	0.47
1:A:187:SER:O	1:A:188:ALA:C	2.54	0.47
2:B:85:LYS:HE2	2:B:85:LYS:HB2	1.76	0.47
1:C:183:GLY:HA3	1:C:188:ALA:HB2	1.95	0.47
2:D:182:ASP:HB3	2:D:423:MET:SD	2.54	0.47
1:V:72:LYS:HD2	1:V:96:ALA:HB1	1.95	0.47
1:L:127:LEU:HD23	1:L:161:VAL:HG11	1.97	0.47
1:L:215:ILE:HD11	1:L:241:ILE:HG13	1.97	0.47
1:A:220:GLU:OE2	1:A:226:ASP:HB2	2.15	0.47
1:A:350:GLY:CA	6:A:602:ICS:S4A	3.02	0.47
2:B:241:CYS:HB3	2:B:321:ASP:OD2	2.14	0.47
2:D:213:LYS:HD3	2:D:213:LYS:N	2.27	0.47
1:K:67:VAL:HG23	1:K:246:THR:HG21	1.97	0.47
2:M:1:MET:HE3	2:M:395:PHE:HA	1.96	0.47
7:V:603:HCA:H21	7:V:603:HCA:H52	1.65	0.47
2:W:242:ARG:HE	2:W:243:MET:HE3	1.80	0.47
5:W:601:CLF:S2A	1:U:81:PRO:HB2	2.54	0.47
2:X:397:SER:HA	2:X:402:VAL:HG23	1.96	0.47
3:H:86:ARG:HD3	3:H:88:PHE:HZ	1.79	0.47
3:d:7:VAL:HG23	3:d:86:ARG:H	1.80	0.47
1:L:117:THR:O	1:L:121:PHE:HB2	2.14	0.47
1:L:328:TYR:O	1:L:332:ILE:HG22	2.14	0.47
4:E:33:VAL:HG12	3:F:31:MET:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:34:MET:HE2	4:O:63:PHE:HB3	1.97	0.47
3:P:71:LYS:HE3	3:P:71:LYS:HB3	1.73	0.47
4:a:10:MET:HG2	4:a:65:PRO:O	2.14	0.47
1:A:18:VAL:HG23	2:B:94:VAL:HG23	1.97	0.47
1:A:97:LYS:HG2	1:A:98:ALA:H	1.80	0.47
1:A:448:ASN:HD21	1:A:451:GLU:HG3	1.80	0.47
1:C:327:LYS:HG2	1:C:328:TYR:CD1	2.49	0.47
1:V:163:ARG:NH1	1:V:163:ARG:HB2	2.30	0.47
1:V:217:ILE:HG13	1:V:264:ILE:HD11	1.97	0.47
2:W:120:GLU:OE1	2:W:120:GLU:HA	2.14	0.47
3:R:38:LYS:HA	3:R:51:GLU:N	2.29	0.47
1:L:281:LYS:HD3	1:L:282:TYR:HE1	1.80	0.47
2:N:26:ILE:HD11	2:N:409:PHE:CZ	2.50	0.47
2:N:35:VAL:HB	2:N:38:CYS:HB2	1.97	0.47
3:I:29:THR:HB	3:I:58:LEU:HB3	1.96	0.47
1:A:47:LYS:HA	1:A:184:VAL:HG11	1.97	0.47
1:A:414:ASN:O	1:A:418:ILE:HG13	2.15	0.47
2:W:442:ARG:HA	2:W:442:ARG:HH11	1.80	0.47
1:L:287:LEU:HB3	1:L:427:LEU:HD12	1.96	0.47
1:L:307:PHE:HD1	1:L:308:PHE:HD1	1.63	0.47
1:U:245:LEU:HA	1:U:246:THR:HA	1.50	0.47
4:Q:28:PHE:HB3	4:Q:71:VAL:HB	1.96	0.47
4:O:25:PHE:HE1	4:O:120:ILE:HB	1.80	0.47
2:B:440:LEU:HD22	2:B:455:ILE:HG22	1.97	0.47
1:C:137:ILE:HD11	2:D:373:PHE:CZ	2.49	0.47
1:C:270:SER:O	1:C:271:ILE:HD13	2.15	0.47
1:C:438:LYS:HD2	1:C:439:ASP:H	1.80	0.47
1:K:473:TRP:O	1:K:477:ILE:HG12	2.15	0.47
2:M:173:ILE:HD13	2:M:238:ILE:HB	1.95	0.47
2:M:317:TYR:OH	2:M:393:GLY:HA3	2.14	0.47
1:V:198:MET:HA	1:V:202:ILE:HG12	1.96	0.47
3:J:99:ARG:HD3	3:F:78:ARG:HB3	1.97	0.47
2:N:440:LEU:HG	2:N:456:GLN:NE2	2.30	0.47
1:U:84:CYS:O	1:U:88:THR:HG22	2.15	0.47
2:B:301:MET:HE3	2:B:429:ALA:HB1	1.97	0.46
1:K:77:LEU:HD13	1:K:110:VAL:HG12	1.97	0.46
1:K:296:GLY:HA2	1:K:299:LYS:HE2	1.97	0.46
1:K:303:LYS:HD2	1:K:425:ILE:HA	1.96	0.46
2:W:190:LEU:HD23	2:W:197:SER:HB3	1.97	0.46
2:X:206:VAL:HG22	2:X:219:PRO:HB2	1.96	0.46
3:b:70:ILE:O	3:b:74:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:98:ILE:HB	3:Z:84:ASP:HB3	1.96	0.46
1:L:122:GLY:HA3	4:O:14:GLN:OE1	2.15	0.46
1:L:265:LEU:HD22	1:L:275:ASN:ND2	2.30	0.46
1:U:154:ILE:HA	4:a:10:MET:CE	2.45	0.46
1:A:120:VAL:HG21	3:I:34:PHE:CD2	2.51	0.46
1:A:217:ILE:HG13	1:A:264:ILE:HD11	1.97	0.46
1:A:363:LEU:HD11	1:A:503:ALA:HB2	1.97	0.46
1:C:347:TYR:CE2	1:C:447:LEU:HB3	2.49	0.46
2:M:17:ILE:HG22	2:M:18:ASN:OD1	2.15	0.46
2:M:295:ARG:HD2	2:M:425:TYR:OH	2.14	0.46
1:V:202:ILE:HA	1:V:255:SER:HA	1.97	0.46
2:W:5:THR:HG21	2:W:376:HIS:NE2	2.30	0.46
3:R:36:ARG:HH22	3:R:86:ARG:HH21	1.63	0.46
1:L:149:CYS:SG	1:L:180:GLY:HA3	2.54	0.46
1:L:201:LEU:HD13	1:L:254:ILE:HG21	1.97	0.46
2:N:42:SER:HA	2:N:103:HIS:CE1	2.50	0.46
2:N:249:ALA:HB3	2:N:262:ILE:HD11	1.95	0.46
1:A:342:LYS:HB2	1:A:365:MET:HB3	1.98	0.46
1:C:349:GLY:HA3	6:C:601:ICS:S1B	2.55	0.46
1:K:245:LEU:HA	1:K:246:THR:HA	1.48	0.46
1:V:74:MET:HE2	1:V:251:PHE:HB3	1.97	0.46
2:W:29:VAL:HG22	2:W:40:PRO:HB2	1.96	0.46
1:L:66:VAL:HG12	1:L:92:ARG:NH2	2.30	0.46
2:N:298:LEU:HD23	2:N:425:TYR:HD1	1.79	0.46
2:N:411:ILE:HD13	2:N:417:LEU:HD23	1.97	0.46
3:P:86:ARG:HG3	3:P:88:PHE:CZ	2.51	0.46
1:A:218:PHE:HB3	1:A:271:ILE:HG21	1.98	0.46
1:C:81:PRO:HD3	1:C:150:PRO:HG2	1.97	0.46
1:C:327:LYS:HG2	1:C:328:TYR:HD1	1.81	0.46
1:C:431:GLU:HB2	1:C:435:PRO:HG2	1.98	0.46
2:X:243:MET:HE1	2:X:346:ASN:ND2	2.30	0.46
1:U:198:MET:HG2	1:U:277:MET:SD	2.55	0.46
1:C:21:GLU:HG3	3:R:26:ILE:HG12	1.96	0.46
1:C:215:ILE:HG13	1:C:241:ILE:HD13	1.97	0.46
1:C:457:LYS:HE2	2:D:215:HIS:CD2	2.50	0.46
2:M:267:ILE:HD11	2:M:423:MET:HG2	1.97	0.46
2:X:249:ALA:HB1	2:X:260:ALA:HB1	1.98	0.46
3:T:4:ILE:HD13	3:T:89:VAL:HG22	1.96	0.46
1:L:58:CYS:O	1:L:61:ALA:HB3	2.15	0.46
2:N:298:LEU:HD21	2:N:428:ALA:HB3	1.97	0.46
3:S:10:PRO:HD3	3:S:54:LYS:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ALA:O	1:A:191:HIS:N	2.45	0.46
2:D:155:LYS:HE2	2:D:247:ALA:HB1	1.98	0.46
2:D:166:LYS:H	2:D:232:ALA:HB1	1.81	0.46
2:M:182:ASP:HB3	2:M:423:MET:SD	2.56	0.46
1:V:114:MET:HA	1:V:118:ASP:OD2	2.15	0.46
2:X:79:GLY:H	4:Y:42:LEU:HD21	1.80	0.46
2:X:85:LYS:O	2:X:89:VAL:HG13	2.16	0.46
1:L:56:ARG:HD3	1:L:185:SER:HB2	1.98	0.46
1:L:207:ILE:HA	1:L:256:GLN:NE2	2.31	0.46
1:U:153:LEU:HA	1:U:153:LEU:HD23	1.76	0.46
1:U:467:GLY:HA2	1:U:485:HIS:CD2	2.51	0.46
2:B:407:VAL:HB	2:B:422:ILE:HD12	1.97	0.46
1:C:219:GLY:HA2	1:C:267:CYS:HB2	1.96	0.46
1:K:261:LYS:HB2	1:K:308:PHE:HZ	1.81	0.46
2:W:417:LEU:HD12	2:W:417:LEU:HA	1.79	0.46
2:X:323:LEU:HD12	2:X:340:VAL:HG13	1.98	0.46
2:N:114:ASP:O	2:N:117:VAL:HG22	2.16	0.46
2:N:241:CYS:HB2	2:N:244:ALA:HB3	1.98	0.46
4:Y:23:CYS:SG	4:Y:84:LYS:HG3	2.56	0.46
1:A:374:PHE:CE1	6:A:602:ICS:S3A	3.08	0.46
7:A:603:HCA:H22	2:B:54:MET:SD	2.56	0.46
2:D:26:ILE:HD11	2:D:409:PHE:CZ	2.50	0.46
2:M:41:HIS:HB3	2:M:102:ILE:HG22	1.98	0.46
2:M:316:ILE:HG23	2:M:388:ILE:HB	1.97	0.46
1:V:131:ILE:HA	1:V:131:ILE:HD12	1.80	0.46
2:W:146:HIS:CE1	2:W:147:ILE:HG12	2.51	0.46
1:U:346:ILE:HG12	1:U:465:CYS:HB2	1.96	0.46
1:K:148:THR:O	1:K:149:CYS:C	2.59	0.46
1:K:251:PHE:C	1:K:251:PHE:CD1	2.93	0.46
2:W:30:TYR:CZ	2:W:203:THR:HG21	2.51	0.46
2:X:456:GLN:HA	1:U:489:TYR:CG	2.50	0.46
3:T:36:ARG:HH12	3:S:26:ILE:HG22	1.81	0.46
3:d:4:ILE:HB	3:d:59:MET:HE2	1.98	0.46
1:L:264:ILE:HG22	1:L:287:LEU:HD21	1.98	0.46
2:D:49:LEU:O	2:D:49:LEU:HD12	2.15	0.46
2:D:225:ILE:HD12	2:D:225:ILE:HA	1.80	0.46
2:W:91:LEU:HD12	2:W:95:TYR:HB2	1.97	0.46
2:W:251:ILE:HD12	2:W:251:ILE:HA	1.81	0.46
2:X:314:VAL:HG21	2:X:330:VAL:HG11	1.98	0.46
1:L:485:HIS:HA	6:L:602:ICS:S3B	2.57	0.46
1:U:274:THR:O	1:U:278:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:374:PHE:HZ	6:U:601:ICS:S3A	2.39	0.46
4:E:34:MET:HE2	4:E:63:PHE:HB3	1.98	0.46
4:O:1:MET:SD	4:O:116:GLY:HA2	2.56	0.46
2:B:319:ASP:O	2:B:323:LEU:HB2	2.16	0.45
1:C:135:VAL:HG21	1:C:169:HIS:HD2	1.80	0.45
1:C:207:ILE:HD11	1:C:259:GLN:O	2.16	0.45
1:C:476:LYS:HD3	2:D:211:LEU:HD12	1.98	0.45
1:K:267:CYS:SG	1:K:270:SER:HB3	2.56	0.45
3:H:59:MET:HE3	3:H:61:VAL:HG12	1.98	0.45
2:N:309:TYR:CZ	2:N:333:MET:HE3	2.50	0.45
3:c:3:MET:HG2	3:c:60:VAL:HG22	1.98	0.45
2:B:37:ASN:HA	2:B:218:TYR:CD2	2.51	0.45
1:C:241:ILE:HD13	1:C:241:ILE:HA	1.85	0.45
1:K:87:PHE:CG	2:M:51:TYR:HB3	2.52	0.45
2:W:390:ASN:HD22	2:W:410:PRO:HD2	1.80	0.45
2:X:391:THR:HG21	2:X:412:MET:H	1.80	0.45
1:L:11:ILE:O	1:L:15:ILE:HG12	2.16	0.45
2:N:22:ILE:HG21	2:N:26:ILE:HG21	1.98	0.45
2:N:102:ILE:HB	2:N:136:ALA:HA	1.98	0.45
1:U:268:HIS:CD2	1:U:430:TYR:HD2	2.35	0.45
3:F:59:MET:HG3	3:F:60:VAL:N	2.30	0.45
4:Q:36:ARG:HD2	4:Q:37:GLY:N	2.31	0.45
1:A:147:ALA:HB1	1:A:151:VAL:HG21	1.97	0.45
1:C:287:LEU:HD21	1:C:307:PHE:HB2	1.97	0.45
2:D:397:SER:HB2	2:D:402:VAL:O	2.16	0.45
2:N:323:LEU:HA	2:N:323:LEU:HD13	1.74	0.45
1:U:216:ASN:HB3	1:U:218:PHE:HE1	1.81	0.45
2:D:106:CYS:SG	5:D:601:CLF:S1	3.09	0.45
2:D:274:ARG:HH22	2:D:278:ASN:HB3	1.82	0.45
2:D:413:ASP:OD1	2:D:413:ASP:C	2.59	0.45
2:W:109:GLU:HG3	2:W:140:PRO:HA	1.99	0.45
2:W:302:MET:HE1	2:W:332:GLU:HG2	1.99	0.45
3:H:74:MET:HE3	3:H:74:MET:O	2.17	0.45
4:G:62:ARG:HD3	4:G:62:ARG:HA	1.71	0.45
1:A:69:GLY:HA2	1:A:76:HIS:NE2	2.31	0.45
1:A:275:ASN:ND2	1:A:286:TRP:CD2	2.83	0.45
1:A:352:ARG:NH1	6:A:602:ICS:S3B	2.84	0.45
2:B:289:PRO:O	2:B:292:GLU:HG3	2.16	0.45
1:C:52:ILE:HG13	1:C:52:ILE:O	2.17	0.45
1:C:346:ILE:O	1:C:370:ALA:HA	2.16	0.45
3:J:68:LYS:HE3	3:J:68:LYS:HB3	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:98:ILE:HG13	3:F:84:ASP:HB3	1.97	0.45
1:L:79:HIS:HA	1:L:112:THR:HG23	1.97	0.45
1:A:158:ILE:HD11	1:A:177:ARG:HG2	1.97	0.45
1:K:351:SER:N	1:K:372:TYR:CE1	2.85	0.45
1:K:472:TYR:HE2	2:M:61:ARG:HA	1.81	0.45
2:W:353:ILE:HG21	2:W:366:ILE:HD13	1.98	0.45
3:J:15:LYS:HE2	3:J:15:LYS:HB3	1.75	0.45
2:B:419:TYR:HE2	2:D:297:ARG:HG2	1.82	0.45
1:C:465:CYS:HA	1:C:482:ARG:O	2.17	0.45
2:M:158:VAL:HG11	2:M:252:LEU:HG	1.98	0.45
2:M:184:ARG:NH2	2:M:204:THR:HB	2.31	0.45
3:H:28:LEU:H	3:H:28:LEU:HG	1.62	0.45
3:b:81:LYS:H	3:b:81:LYS:HG2	1.49	0.45
2:N:44:GLY:HA3	2:N:105:THR:OG1	2.17	0.45
1:U:63:THR:HG21	1:U:178:CYS:SG	2.57	0.45
3:I:73:ILE:HG21	3:I:87:ILE:HD11	1.98	0.45
3:Z:60:VAL:HG12	3:Z:105:LEU:HD11	1.97	0.45
1:A:73:ASP:OD1	1:A:73:ASP:C	2.60	0.45
1:C:482:ARG:HD3	1:C:488:ASP:HB2	1.98	0.45
1:V:93:ARG:HG2	1:V:224:GLY:H	1.82	0.45
1:L:119:ILE:HD11	2:N:110:THR:OG1	2.16	0.45
2:N:137:ALA:HB3	2:N:153:MET:HE2	1.99	0.45
2:N:372:LEU:HD13	2:N:375:LEU:HD23	1.98	0.45
1:U:49:ILE:HD12	1:U:49:ILE:H	1.82	0.45
1:U:290:ASN:HD21	1:U:358:ASN:HD21	1.65	0.45
1:A:422:LYS:HG3	1:A:427:LEU:O	2.16	0.45
1:K:258:HIS:CE1	1:K:259:GLN:HG3	2.52	0.45
2:M:429:ALA:O	2:M:432:VAL:HG12	2.17	0.45
1:V:468:ILE:HG12	2:X:58:ARG:HG3	1.97	0.45
2:X:114:ASP:O	2:X:117:VAL:HG22	2.17	0.45
3:R:40:LYS:O	3:R:41:GLY:C	2.60	0.45
2:N:30:TYR:CE1	2:N:203:THR:HG21	2.52	0.45
4:E:38:LYS:HE2	3:F:26:ILE:HD12	1.98	0.45
4:Q:84:LYS:HE2	4:Q:84:LYS:HB2	1.83	0.45
2:B:302:MET:HE3	2:B:333:MET:HA	1.99	0.45
2:D:168:ASN:HD21	2:D:233:ASN:ND2	2.15	0.45
2:D:390:ASN:HD22	2:D:410:PRO:HG2	1.80	0.45
2:D:391:THR:HG22	2:D:406:ARG:NH1	2.32	0.45
1:V:218:PHE:HB3	1:V:271:ILE:HG21	1.99	0.45
2:X:175:PRO:HG2	2:X:201:PRO:O	2.16	0.45
3:H:96:TYR:HB2	4:G:99:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:87:ILE:C	3:J:88:PHE:HD1	2.25	0.45
1:L:245:LEU:HA	1:L:246:THR:HA	1.52	0.45
4:O:33:VAL:HG12	3:P:31:MET:HB2	1.98	0.45
4:Y:31:ARG:HD2	3:Z:31:MET:SD	2.56	0.45
1:C:55:ASN:HB3	1:C:469:LYS:HD2	1.99	0.44
2:D:317:TYR:C	2:D:323:LEU:HD21	2.41	0.44
2:M:333:MET:HE3	2:M:333:MET:HB2	1.87	0.44
2:W:81:ALA:O	2:W:85:LYS:HG2	2.17	0.44
3:b:98:ILE:HG22	4:a:96:ASP:HB3	1.98	0.44
1:L:60:PHE:HB3	5:L:603:CLF:S2A	2.56	0.44
2:D:128:ILE:HA	2:D:128:ILE:HD13	1.74	0.44
1:K:50:PRO:O	2:M:87:ALA:HA	2.18	0.44
1:K:82:ILE:HD12	1:K:111:CYS:SG	2.57	0.44
1:K:250:SER:H	1:K:253:LYS:NZ	2.15	0.44
1:K:295:LYS:HG2	1:K:299:LYS:HZ3	1.82	0.44
1:K:316:LYS:HA	1:K:316:LYS:HD2	1.63	0.44
1:V:354:HIS:HD2	1:V:436:GLU:HG3	1.82	0.44
2:W:154:VAL:O	2:W:158:VAL:HG12	2.16	0.44
2:X:442:ARG:CZ	2:X:445:ARG:HH21	2.29	0.44
3:H:9:ARG:HD3	3:H:12:MET:HE3	1.99	0.44
3:J:86:ARG:HG2	3:J:88:PHE:HE1	1.81	0.44
3:R:12:MET:HE1	3:R:77:ALA:HA	1.98	0.44
3:R:31:MET:HB2	3:R:56:MET:HB2	1.98	0.44
3:d:68:LYS:HD3	3:d:69:VAL:N	2.32	0.44
1:L:352:ARG:HD3	1:L:484:ILE:HG12	1.99	0.44
4:E:38:LYS:HA	4:E:38:LYS:HD3	1.83	0.44
3:c:31:MET:SD	3:c:58:LEU:HB2	2.58	0.44
1:A:78:VAL:HG11	1:A:85:ALA:HB2	1.99	0.44
1:A:108:TYR:CE2	1:A:138:PHE:HE2	2.36	0.44
2:B:300:ASP:HB2	2:D:211:LEU:HB2	1.99	0.44
1:C:157:ASP:O	1:C:161:VAL:HG23	2.17	0.44
1:C:374:PHE:HZ	6:C:601:ICS:S1B	2.39	0.44
1:K:233:ILE:O	1:K:237:ILE:HG22	2.17	0.44
2:M:82:ALA:O	2:M:86:GLU:HG3	2.16	0.44
2:M:90:ASN:O	2:M:94:VAL:HG12	2.17	0.44
2:M:164:LYS:HG2	2:M:232:ALA:HB1	2.00	0.44
2:X:59:HIS:C	2:X:59:HIS:CD2	2.95	0.44
1:L:349:GLY:H	1:L:485:HIS:HE1	1.66	0.44
2:N:413:ASP:C	2:N:413:ASP:OD1	2.60	0.44
1:A:58:CYS:SG	2:B:47:GLY:CA	3.05	0.44
1:A:172:LYS:HD3	1:A:251:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:VAL:C	1:A:174:ILE:HD13	2.42	0.44
1:C:119:ILE:HG12	2:D:142:TYR:CE2	2.52	0.44
1:C:427:LEU:HG	1:C:428:MET:CE	2.47	0.44
2:D:243:MET:HE3	2:D:243:MET:HB3	1.85	0.44
1:K:357:ILE:HG21	1:K:436:GLU:HB3	2.00	0.44
2:M:323:LEU:HD12	2:M:323:LEU:HA	1.76	0.44
1:V:17:LYS:HD2	3:J:18:GLU:HG3	1.98	0.44
1:V:346:ILE:O	1:V:370:ALA:HA	2.18	0.44
3:R:3:MET:HE1	3:R:90:ASN:HB2	1.99	0.44
1:L:289:VAL:HG13	1:L:300:SER:HB3	2.00	0.44
1:U:163:ARG:HH11	1:U:163:ARG:HG3	1.82	0.44
4:G:11:ASN:O	4:G:12:LYS:HD3	2.18	0.44
3:P:61:VAL:HG11	3:P:69:VAL:HG21	2.00	0.44
1:K:216:ASN:HB3	1:K:218:PHE:HE1	1.83	0.44
1:K:216:ASN:OD1	1:K:243:SER:HB3	2.17	0.44
1:V:66:VAL:HG12	1:V:92:ARG:NH2	2.32	0.44
2:N:38:CYS:SG	2:N:99:VAL:HB	2.58	0.44
1:U:223:ILE:HG13	1:U:352:ARG:HH22	1.82	0.44
3:F:1:MET:HE2	3:F:1:MET:HB3	1.80	0.44
4:Y:66:LYS:C	4:Y:67:ARG:HD2	2.41	0.44
1:A:231:LYS:HB2	1:A:231:LYS:HE2	1.71	0.44
1:A:462:ASP:HB2	1:A:510:ILE:HD11	1.99	0.44
2:B:171:LEU:HD21	2:B:238:ILE:HD11	2.00	0.44
1:C:345:PHE:HE1	1:C:369:VAL:HB	1.81	0.44
2:D:273:ASP:O	2:D:277:MET:HG3	2.18	0.44
1:K:182:ARG:HD3	1:K:397:ILE:HG21	1.99	0.44
1:K:471:LYS:HD2	1:K:483:GLN:HG2	1.99	0.44
1:V:208:LYS:HE2	1:V:208:LYS:HB2	1.65	0.44
3:R:38:LYS:HB3	3:R:39:GLN:H	1.59	0.44
3:b:29:THR:HB	3:b:58:LEU:HB3	1.98	0.44
1:L:213:PHE:HA	1:L:308:PHE:CE2	2.52	0.44
1:L:218:PHE:CD1	1:L:245:LEU:HB2	2.53	0.44
3:I:1:MET:HE2	3:I:105:LEU:HG	2.00	0.44
4:a:12:LYS:HD3	4:a:15:LYS:HZ1	1.81	0.44
2:B:250:LYS:HD2	2:B:250:LYS:HA	1.85	0.44
1:C:218:PHE:CE2	1:C:278:MET:HE1	2.53	0.44
1:K:177:ARG:HD3	1:K:177:ARG:HA	1.89	0.44
1:V:73:ASP:OD1	1:V:103:ASP:HB2	2.18	0.44
1:V:265:LEU:HG	1:V:275:ASN:ND2	2.33	0.44
2:W:132:ILE:HD13	2:W:132:ILE:HA	1.80	0.44
1:L:438:LYS:HD2	1:L:439:ASP:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:448:ASN:OD1	1:U:451:GLU:HB2	2.17	0.44
4:E:80:GLU:HA	4:E:83:GLN:OE1	2.18	0.44
1:A:60:PHE:HD1	1:A:178:CYS:SG	2.40	0.44
1:A:271:ILE:HG13	1:A:274:THR:HB	1.99	0.44
2:B:1:MET:HE3	2:D:449:ASP:OD1	2.18	0.44
2:B:406:ARG:CZ	2:B:414:ARG:HE	2.31	0.44
2:B:448:PRO:HG2	2:B:451:LEU:HG	1.99	0.44
1:C:116:GLU:HG2	3:J:34:PHE:CZ	2.53	0.44
2:D:199:VAL:O	2:D:223:THR:HB	2.17	0.44
2:M:409:PHE:HA	2:M:410:PRO:HA	1.87	0.44
2:M:452:LEU:HD23	2:M:452:LEU:HA	1.86	0.44
1:V:271:ILE:HG13	1:V:274:THR:HB	2.00	0.44
2:W:49:LEU:HD12	2:W:52:LEU:HD22	1.98	0.44
2:W:326:LEU:HD11	2:W:407:VAL:HG21	1.99	0.44
2:X:21:LYS:C	2:X:22:ILE:HD12	2.43	0.44
3:R:34:PHE:CB	1:L:120:VAL:HG11	2.48	0.44
1:A:97:LYS:HB2	1:A:228:TRP:CZ2	2.53	0.44
1:A:264:ILE:O	1:A:264:ILE:HG13	2.17	0.44
2:B:25:PRO:HB2	2:B:52:LEU:HD11	1.99	0.44
1:C:469:LYS:HB2	2:D:53:ARG:NH2	2.33	0.44
2:D:200:PHE:HE2	2:D:230:ASP:OD2	2.01	0.44
2:D:217:PHE:CD1	2:D:217:PHE:C	2.93	0.44
2:W:185:GLU:OE1	2:W:421:PRO:HG3	2.18	0.44
2:X:134:ILE:HD13	2:X:134:ILE:HA	1.88	0.44
2:X:147:ILE:HD11	2:X:319:ASP:HB3	1.99	0.44
3:R:34:PHE:HB3	1:L:120:VAL:HG11	2.00	0.44
1:L:115:LYS:HA	1:L:115:LYS:HD3	1.89	0.44
1:U:168:GLU:HG3	1:U:169:HIS:HD1	1.83	0.44
3:Z:28:LEU:HD21	3:Z:57:LEU:HD22	1.99	0.44
1:A:245:LEU:HA	1:A:246:THR:HA	1.49	0.43
2:B:270:ARG:HG3	2:B:332:GLU:OE2	2.18	0.43
2:M:58:ARG:HD3	2:N:455:ILE:HG12	1.98	0.43
1:V:107:ASN:ND2	2:X:1:MET:HG3	2.33	0.43
2:W:146:HIS:ND1	2:W:147:ILE:HG12	2.33	0.43
2:X:417:LEU:HD23	2:X:417:LEU:HA	1.79	0.43
1:L:69:GLY:HA2	1:L:76:HIS:CD2	2.53	0.43
1:L:119:ILE:HD12	1:L:154:ILE:HG21	2.00	0.43
1:L:357:ILE:HG21	1:L:436:GLU:HB3	1.99	0.43
1:U:482:ARG:HA	1:U:482:ARG:HD2	1.69	0.43
3:c:61:VAL:HG11	3:c:69:VAL:HG21	1.99	0.43
2:D:109:GLU:HG3	2:D:140:PRO:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:186:ILE:HD13	2:M:186:ILE:HA	1.83	0.43
2:W:416:ASN:OD1	2:X:305:ALA:HB2	2.19	0.43
2:X:41:HIS:HB3	2:X:102:ILE:HG22	2.00	0.43
2:X:413:ASP:OD1	2:X:414:ARG:HD3	2.18	0.43
3:H:99:ARG:HG2	3:H:100:THR:HG23	1.99	0.43
3:b:74:MET:HE1	3:c:96:TYR:HB3	2.00	0.43
3:b:81:LYS:O	3:c:99:ARG:HG3	2.18	0.43
1:A:156:ASP:HA	4:G:14:GLN:NE2	2.32	0.43
1:A:159:GLU:CD	1:A:159:GLU:H	2.25	0.43
1:A:179:GLU:H	1:A:179:GLU:HG3	1.49	0.43
1:C:79:HIS:HA	1:C:112:THR:OG1	2.18	0.43
2:D:18:ASN:HB3	2:D:372:LEU:HB2	2.00	0.43
2:M:39:MET:HE1	2:M:95:TYR:HB3	2.00	0.43
1:V:128:LYS:O	1:V:131:ILE:HG22	2.18	0.43
2:W:309:TYR:CE2	2:W:333:MET:HE3	2.53	0.43
2:N:22:ILE:HG22	2:N:23:CYS:H	1.84	0.43
1:U:172:LYS:HB2	1:U:172:LYS:HE2	1.82	0.43
4:Q:66:LYS:HE2	4:Q:66:LYS:HB2	1.63	0.43
4:O:40:ARG:HB2	4:O:40:ARG:HH11	1.83	0.43
3:Z:1:MET:HE2	3:Z:1:MET:HB3	1.83	0.43
3:c:86:ARG:HD3	3:c:86:ARG:HA	1.78	0.43
1:A:271:ILE:O	1:A:272:ASN:C	2.61	0.43
1:A:285:PRO:HG3	1:A:413:ILE:HG12	2.00	0.43
1:C:220:GLU:HG2	1:C:227:LEU:HD13	2.00	0.43
2:M:14:ALA:C	2:M:15:ILE:HD13	2.43	0.43
1:V:299:LYS:HE3	1:V:303:LYS:HE3	2.01	0.43
2:W:56:LEU:HD23	2:W:56:LEU:HA	1.77	0.43
2:N:153:MET:HE3	2:N:153:MET:HB2	1.63	0.43
2:N:217:PHE:CD1	2:N:217:PHE:C	2.96	0.43
1:U:310:ASP:HB3	1:U:312:GLU:OE1	2.19	0.43
3:P:3:MET:HE3	3:P:58:LEU:HD13	2.00	0.43
3:S:13:GLU:H	3:S:13:GLU:HG3	1.47	0.43
2:B:133:LYS:HB3	2:B:161:PHE:CZ	2.54	0.43
1:C:190:HIS:CE1	6:C:601:ICS:S2B	3.09	0.43
1:V:325:LYS:HG3	1:V:496:PHE:CE2	2.45	0.43
1:L:106:MET:HE3	1:L:106:MET:HB3	1.76	0.43
4:Q:88:VAL:HG23	4:Q:89:ASN:OD1	2.18	0.43
4:Y:1:MET:HB3	4:Y:104:ILE:HB	2.00	0.43
1:A:56:ARG:HE	1:A:446:ASP:CG	2.26	0.43
2:B:331:LEU:HD12	2:B:331:LEU:HA	1.84	0.43
2:B:452:LEU:C	2:B:454:THR:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ILE:HG22	1:C:175:PRO:HB3	2.00	0.43
1:C:218:PHE:HD1	1:C:245:LEU:HB2	1.84	0.43
1:V:227:LEU:HA	1:V:230:ILE:HG22	2.00	0.43
1:V:290:ASN:ND2	1:V:358:ASN:HD21	2.17	0.43
2:W:22:ILE:HG22	2:W:23:CYS:H	1.84	0.43
2:X:18:ASN:HB3	2:X:372:LEU:HB2	1.99	0.43
2:X:218:TYR:HA	2:X:219:PRO:HD3	1.93	0.43
2:N:319:ASP:O	2:N:323:LEU:HD23	2.18	0.43
4:a:28:PHE:HD2	3:c:36:ARG:HG2	1.83	0.43
4:Y:29:THR:HB	4:Y:70:THR:HB	2.01	0.43
2:B:386:LEU:HD12	2:B:387:LEU:N	2.34	0.43
1:C:359:LEU:HA	1:C:362:GLU:OE2	2.19	0.43
1:K:356:TYR:HH	1:K:487:TYR:HE1	1.67	0.43
1:V:93:ARG:CZ	1:V:93:ARG:HB2	2.49	0.43
1:V:307:PHE:CD1	1:V:307:PHE:C	2.96	0.43
2:W:269:ILE:HB	2:W:332:GLU:OE1	2.18	0.43
2:X:444:ASP:OD1	2:X:452:LEU:HD11	2.19	0.43
3:T:31:MET:HB3	4:Q:33:VAL:HG13	2.00	0.43
1:L:491:GLY:HA3	1:L:493:TYR:CZ	2.53	0.43
2:N:270:ARG:HG3	2:N:332:GLU:CD	2.43	0.43
2:N:274:ARG:HG2	2:N:274:ARG:HH11	1.84	0.43
4:a:17:LYS:HE2	4:a:17:LYS:HB2	1.73	0.43
1:A:190:HIS:HB3	1:A:270:SER:O	2.19	0.43
1:C:328:TYR:CE2	1:C:497:SER:HA	2.53	0.43
1:C:345:PHE:CD1	1:C:369:VAL:HB	2.54	0.43
1:K:231:LYS:N	1:K:232:PRO:HD2	2.33	0.43
1:K:472:TYR:CE2	2:M:61:ARG:HA	2.53	0.43
2:M:420:PHE:N	2:M:420:PHE:CD1	2.86	0.43
1:V:60:PHE:CD2	1:V:84:CYS:SG	3.12	0.43
2:W:217:PHE:CD1	2:W:217:PHE:C	2.97	0.43
2:X:317:TYR:HA	2:X:341:LEU:O	2.18	0.43
3:H:1:MET:HE2	3:H:1:MET:HB3	1.77	0.43
3:b:31:MET:CG	4:a:33:VAL:HG12	2.48	0.43
1:L:383:ARG:HG2	1:L:430:TYR:HB3	2.01	0.43
2:N:217:PHE:C	2:N:217:PHE:HD1	2.27	0.43
1:U:66:VAL:HA	1:U:92:ARG:NH2	2.34	0.43
1:U:333:GLU:HA	1:U:336:ARG:HG2	2.01	0.43
2:B:59:HIS:CD2	2:B:411:ILE:H	2.34	0.43
2:B:267:ILE:HG12	2:B:423:MET:CB	2.49	0.43
2:W:41:HIS:CE1	2:W:87:ALA:HB1	2.53	0.43
2:X:268:GLY:HA2	2:X:329:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:391:THR:HG23	2:X:411:ILE:HA	2.00	0.43
3:R:81:LYS:HB2	3:R:81:LYS:HE2	1.79	0.43
1:U:77:LEU:HD13	1:U:110:VAL:HG12	2.01	0.43
1:U:386:ILE:HG22	1:U:387:PRO:HD3	2.00	0.43
4:a:9:ARG:HB2	4:a:12:LYS:HG3	2.01	0.43
1:A:49:ILE:HD13	1:A:52:ILE:HD13	2.01	0.43
1:A:518:ILE:HD11	2:B:211:LEU:HD23	1.99	0.43
2:B:416:ASN:HD22	2:D:301:MET:HG2	1.84	0.43
1:C:153:LEU:HD23	1:C:153:LEU:HA	1.87	0.43
2:D:265:THR:HA	2:D:266:PRO:HD3	1.86	0.43
2:M:333:MET:SD	2:M:432:VAL:HG23	2.58	0.43
2:W:42:SER:HA	2:W:103:HIS:CE1	2.54	0.43
2:X:58:ARG:HB3	2:X:412:MET:HE3	2.00	0.43
2:X:147:ILE:HG21	2:X:243:MET:HB3	2.00	0.43
3:b:10:PRO:HD3	3:b:54:LYS:HA	2.00	0.43
1:U:177:ARG:HA	1:U:177:ARG:HD2	1.34	0.43
4:Q:15:LYS:HB3	4:Q:15:LYS:HE2	1.74	0.43
3:P:74:MET:HE3	3:P:74:MET:HB2	1.93	0.43
4:Y:1:MET:HE2	4:Y:1:MET:N	2.33	0.43
1:A:482:ARG:HD3	1:A:509:ALA:HB2	2.01	0.42
2:B:168:ASN:C	2:B:168:ASN:OD1	2.61	0.42
2:B:391:THR:HG22	2:B:410:PRO:O	2.18	0.42
1:C:92:ARG:HE	1:C:92:ARG:HB3	1.49	0.42
1:C:465:CYS:HB3	1:C:484:ILE:HD13	2.00	0.42
1:V:334:ARG:O	1:V:338:LYS:HG2	2.18	0.42
1:V:420:GLU:HG2	1:V:424:LYS:HE2	2.00	0.42
2:W:65:LEU:HD11	1:U:449:HIS:CD2	2.54	0.42
2:X:173:ILE:HD13	2:X:238:ILE:HB	2.00	0.42
1:L:113:ASP:HB3	1:L:115:LYS:NZ	2.34	0.42
1:L:293:GLY:O	1:L:297:THR:HG22	2.19	0.42
2:N:42:SER:HB2	2:N:49:LEU:HD22	2.01	0.42
2:N:173:ILE:HB	2:N:199:VAL:HG12	2.01	0.42
2:N:182:ASP:OD1	2:N:422:ILE:HG22	2.19	0.42
2:N:317:TYR:CZ	2:N:389:GLY:HA3	2.54	0.42
4:Q:110:ILE:HA	3:S:74:MET:HE1	2.00	0.42
3:S:3:MET:HE3	3:S:3:MET:HB2	1.90	0.42
1:A:354:HIS:ND1	1:A:436:GLU:HG3	2.34	0.42
1:C:140:PRO:HG2	1:C:143:ILE:HD11	2.00	0.42
1:C:273:TYR:C	1:C:273:TYR:CD1	2.96	0.42
1:V:118:ASP:OD2	1:V:126:LYS:HE3	2.19	0.42
1:V:359:LEU:HD21	1:V:502:PHE:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:463:ILE:HD13	1:V:463:ILE:HA	1.93	0.42
1:L:349:GLY:HA2	1:L:373:GLN:HB3	2.00	0.42
2:N:318:GLY:N	2:N:323:LEU:HD21	2.34	0.42
1:U:264:ILE:HA	1:U:287:LEU:O	2.20	0.42
4:O:109:ARG:HB3	4:O:114:GLU:N	2.34	0.42
1:A:215:ILE:HG22	1:A:262:LEU:HD22	2.00	0.42
2:B:452:LEU:HD12	2:B:452:LEU:HA	1.79	0.42
1:C:416:GLU:HG2	1:C:417:ARG:N	2.34	0.42
2:D:44:GLY:HA3	2:D:105:THR:OG1	2.19	0.42
2:D:59:HIS:ND1	2:D:60:TYR:CE1	2.88	0.42
1:K:211:THR:HG21	1:K:240:ARG:HE	1.85	0.42
1:K:473:TRP:NE1	1:K:477:ILE:HD11	2.35	0.42
2:M:60:TYR:HD2	2:M:207:PHE:CD2	2.37	0.42
1:V:149:CYS:CA	5:V:601:CLF:S2A	3.07	0.42
1:V:450:HIS:HB2	2:X:95:TYR:CE1	2.55	0.42
2:W:236:GLY:HA3	2:W:282:LEU:HD12	2.01	0.42
1:L:148:THR:O	1:L:151:VAL:HG12	2.19	0.42
1:L:231:LYS:HD3	1:L:241:ILE:HD13	2.00	0.42
1:U:66:VAL:HA	1:U:92:ARG:CZ	2.49	0.42
1:U:202:ILE:HD13	1:U:257:ALA:HB3	2.02	0.42
4:a:28:PHE:HE1	4:a:69:PHE:CE2	2.37	0.42
2:B:333:MET:HE1	2:B:435:ILE:HD13	2.00	0.42
1:C:245:LEU:HA	1:C:246:THR:HA	1.51	0.42
2:D:40:PRO:HG2	2:D:66:ALA:HB2	2.01	0.42
2:D:339:VAL:HG22	2:D:365:ASP:HB2	2.01	0.42
1:U:371:GLY:HA3	1:U:444:VAL:HG23	2.01	0.42
4:Q:31:ARG:HE	3:S:33:VAL:HG12	1.83	0.42
1:C:360:PHE:HB3	1:C:365:MET:HB2	2.01	0.42
2:D:43:HIS:CE1	2:D:84:LEU:HD22	2.54	0.42
2:X:35:VAL:HG11	2:X:225:ILE:HD13	2.01	0.42
2:X:48:CYS:O	2:X:49:LEU:C	2.61	0.42
1:L:339:LEU:HD12	1:L:339:LEU:HA	1.89	0.42
1:U:163:ARG:HG3	1:U:163:ARG:NH1	2.35	0.42
4:G:29:THR:HG22	4:G:31:ARG:HD2	1.99	0.42
4:E:84:LYS:HD2	4:E:84:LYS:HA	1.79	0.42
1:A:34:ARG:HD2	1:A:34:ARG:HA	1.84	0.42
2:B:308:HIS:HE1	2:B:456:GLN:O	2.03	0.42
2:W:147:ILE:HG21	2:W:243:MET:HG3	2.01	0.42
2:W:323:LEU:HD23	2:W:323:LEU:HA	1.86	0.42
2:X:155:LYS:NZ	2:X:247:ALA:HB1	2.35	0.42
1:L:300:SER:O	1:L:304:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:132:ASP:HA	1:U:169:HIS:NE2	2.34	0.42
1:U:312:GLU:OE1	1:U:312:GLU:N	2.51	0.42
3:F:5:ARG:HG3	3:F:56:MET:SD	2.60	0.42
1:A:15:ILE:HG12	1:A:451:GLU:HG2	2.02	0.42
1:A:198:MET:HE3	1:A:277:MET:HB3	2.01	0.42
2:B:287:ILE:HD13	2:B:287:ILE:N	2.34	0.42
1:C:58:CYS:SG	2:D:47:GLY:HA3	2.60	0.42
1:C:147:ALA:CB	1:C:151:VAL:HG11	2.50	0.42
1:K:48:VAL:HB	1:K:56:ARG:HD2	2.01	0.42
2:M:115:VAL:HA	2:M:118:ILE:HG22	2.01	0.42
2:M:452:LEU:C	2:M:454:THR:H	2.27	0.42
1:V:93:ARG:HG3	1:V:95:LEU:HD21	2.01	0.42
2:W:99:VAL:HG11	2:W:225:ILE:HD13	2.02	0.42
1:L:15:ILE:CD1	1:L:454:PHE:HB3	2.49	0.42
2:N:261:LYS:HD3	2:N:278:ASN:ND2	2.34	0.42
2:N:326:LEU:HD23	2:N:326:LEU:HA	1.65	0.42
2:N:442:ARG:CZ	2:N:445:ARG:HH21	2.32	0.42
4:E:79:SER:O	4:E:83:GLN:OE1	2.37	0.42
4:Q:109:ARG:HB2	4:Q:119:THR:HB	2.02	0.42
3:P:1:MET:O	3:P:92:VAL:HB	2.20	0.42
1:A:270:SER:OG	1:A:271:ILE:N	2.53	0.42
1:A:303:LYS:HB3	1:A:425:ILE:HG23	2.02	0.42
1:A:422:LYS:HE2	1:A:428:MET:HB2	2.01	0.42
2:D:166:LYS:O	2:D:232:ALA:HB1	2.18	0.42
1:K:350:GLY:HA3	6:K:601:ICS:S4A	2.60	0.42
1:V:42:ILE:HD12	1:V:42:ILE:HA	1.89	0.42
3:H:15:LYS:HE2	3:H:15:LYS:HB2	1.81	0.42
1:L:139:ASN:N	1:L:140:PRO:HD3	2.35	0.42
2:N:21:LYS:C	2:N:22:ILE:HD12	2.45	0.42
2:N:22:ILE:HD12	2:N:22:ILE:N	2.35	0.42
2:N:129:ASP:OD1	2:N:130:PRO:HD3	2.19	0.42
2:N:345:GLN:HA	2:N:368:SER:OG	2.20	0.42
2:N:413:ASP:O	2:N:414:ARG:HD3	2.18	0.42
1:U:93:ARG:H	1:U:93:ARG:HG2	1.47	0.42
1:U:424:LYS:HG3	1:U:425:ILE:HG13	2.02	0.42
1:U:434:PHE:HE1	1:U:443:VAL:HG11	1.84	0.42
3:F:27:SER:HB2	3:F:59:MET:HE1	2.01	0.42
1:C:142:ALA:C	1:C:143:ILE:HD12	2.45	0.42
2:D:306:HIS:HA	2:D:309:TYR:CE1	2.54	0.42
1:K:149:CYS:O	1:K:150:PRO:C	2.61	0.42
1:K:267:CYS:SG	1:K:270:SER:CB	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:333:GLU:O	1:K:337:GLU:HG3	2.19	0.42
2:M:91:LEU:HA	2:M:91:LEU:HD23	1.83	0.42
1:V:124:GLU:N	1:V:124:GLU:OE2	2.53	0.42
1:V:236:LYS:HA	1:V:236:LYS:HD2	1.73	0.42
1:V:350:GLY:CA	6:V:602:ICS:S3A	3.07	0.42
2:W:291:LEU:HD23	2:W:291:LEU:HA	1.89	0.42
2:X:133:LYS:HB3	2:X:161:PHE:CZ	2.55	0.42
1:L:229:GLU:HG2	1:L:492:ARG:HE	1.85	0.42
1:L:237:ILE:HD12	1:L:237:ILE:HA	1.88	0.42
1:L:413:ILE:HG13	1:L:418:ILE:HG13	2.02	0.42
1:U:120:VAL:HG21	3:c:34:PHE:CE1	2.54	0.42
4:O:109:ARG:HG2	4:O:113:GLY:N	2.35	0.42
2:B:39:MET:CE	2:B:91:LEU:HD21	2.50	0.42
2:B:150:TYR:CE1	2:B:176:GLY:HA2	2.55	0.42
1:C:483:GLN:HB2	1:C:488:ASP:N	2.30	0.42
2:D:90:ASN:O	2:D:94:VAL:HG22	2.20	0.42
2:D:339:VAL:HG11	2:D:375:LEU:HD13	2.02	0.42
1:K:405:ARG:HD3	1:K:405:ARG:HA	1.88	0.42
2:W:25:PRO:HB3	2:W:103:HIS:NE2	2.34	0.42
2:X:84:LEU:HD12	2:X:84:LEU:HA	1.82	0.42
2:X:95:TYR:CD2	2:X:217:PHE:HE2	2.38	0.42
2:X:182:ASP:HB3	2:X:423:MET:SD	2.60	0.42
3:J:98:ILE:O	3:F:74:MET:HG2	2.20	0.42
2:N:54:MET:HE3	2:N:58:ARG:HH12	1.84	0.42
1:C:317:THR:O	1:C:320:VAL:HG12	2.20	0.41
1:K:47:LYS:HA	1:K:184:VAL:HB	2.02	0.41
1:K:160:SER:HA	1:K:163:ARG:HE	1.85	0.41
1:V:242:ILE:HD13	1:V:242:ILE:HA	1.85	0.41
1:V:465:CYS:HA	1:V:482:ARG:O	2.20	0.41
2:W:87:ALA:HA	1:U:50:PRO:O	2.20	0.41
2:X:44:GLY:HA3	2:X:105:THR:OG1	2.19	0.41
2:X:409:PHE:HB3	2:X:410:PRO:HD3	2.01	0.41
3:H:9:ARG:HA	3:H:10:PRO:HD3	1.93	0.41
1:L:33:VAL:HG22	1:L:442:ILE:HD12	2.02	0.41
2:N:22:ILE:CG2	2:N:26:ILE:HG21	2.50	0.41
2:N:90:ASN:O	2:N:94:VAL:HG12	2.19	0.41
1:U:120:VAL:HA	4:a:67:ARG:NH1	2.35	0.41
2:B:109:GLU:HG3	2:B:140:PRO:HA	2.02	0.41
1:C:116:GLU:HA	1:C:119:ILE:HG22	2.03	0.41
1:C:275:ASN:HD22	1:C:286:TRP:CG	2.39	0.41
2:D:128:ILE:HG23	2:D:132:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:PHE:CB	2:D:201:PRO:HD3	2.51	0.41
2:M:306:HIS:CD2	1:L:512:SER:HB2	2.55	0.41
1:V:217:ILE:HD11	1:V:241:ILE:HD12	2.02	0.41
2:W:102:ILE:HD12	2:W:119:LEU:HD21	2.01	0.41
1:L:216:ASN:O	1:L:264:ILE:HG12	2.20	0.41
1:L:218:PHE:CG	1:L:271:ILE:HG21	2.55	0.41
1:L:367:VAL:HG11	1:L:370:ALA:HB2	2.02	0.41
1:L:371:GLY:HA3	1:L:444:VAL:HG13	2.03	0.41
1:U:83:GLY:O	1:U:84:CYS:C	2.59	0.41
1:U:304:MET:HE2	1:U:304:MET:HB3	1.79	0.41
1:U:347:TYR:CZ	1:U:447:LEU:HB2	2.55	0.41
4:O:99:ILE:HD13	4:O:99:ILE:HA	1.84	0.41
3:P:6:ALA:HB2	3:P:87:ILE:HG23	2.02	0.41
3:P:71:LYS:HA	3:P:74:MET:CE	2.50	0.41
1:A:12:VAL:O	1:A:15:ILE:HG22	2.19	0.41
1:A:500:LEU:HD23	1:A:500:LEU:HA	1.82	0.41
2:B:90:ASN:O	2:B:94:VAL:HG12	2.20	0.41
1:C:220:GLU:HG3	1:C:222:ASN:H	1.85	0.41
1:C:303:LYS:HD3	1:C:425:ILE:HB	2.00	0.41
1:C:353:SER:HB3	1:C:372:TYR:CE1	2.55	0.41
2:D:60:TYR:HA	2:D:418:HIS:CD2	2.55	0.41
2:D:252:LEU:HD23	2:D:252:LEU:HA	1.82	0.41
1:V:237:ILE:HD13	1:V:237:ILE:HA	1.84	0.41
1:V:369:VAL:HG13	1:V:442:ILE:HB	2.02	0.41
2:W:440:LEU:HD22	2:W:455:ILE:HG22	2.03	0.41
3:R:59:MET:HE2	3:R:59:MET:HB3	1.79	0.41
3:T:31:MET:CE	4:Q:31:ARG:HD2	2.49	0.41
1:L:66:VAL:HG23	1:L:67:VAL:HG23	2.00	0.41
2:N:42:SER:HB2	2:N:49:LEU:HD13	2.02	0.41
2:N:238:ILE:HD11	2:N:278:ASN:HB3	2.02	0.41
1:U:131:ILE:HD13	1:U:145:ILE:HD11	2.02	0.41
1:U:159:GLU:O	1:U:162:ALA:HB3	2.20	0.41
1:C:366:LYS:HE2	1:C:438:LYS:HE2	2.01	0.41
2:M:177:PHE:CE2	2:M:409:PHE:HD2	2.39	0.41
2:M:192:ILE:HD13	2:M:192:ILE:HA	1.97	0.41
1:L:294:THR:HB	1:L:362:GLU:OE2	2.21	0.41
2:N:150:TYR:HE2	2:N:176:GLY:C	2.29	0.41
2:N:158:VAL:HG21	2:N:248:ALA:HB1	2.02	0.41
1:U:467:GLY:HA2	1:U:485:HIS:HD2	1.84	0.41
3:F:8:ILE:HD13	3:F:16:VAL:HG11	2.03	0.41
3:P:10:PRO:HD3	3:P:54:LYS:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:MET:HE1	2:B:41:HIS:HB2	2.01	0.41
2:B:189:ILE:O	2:B:192:ILE:HG22	2.21	0.41
2:B:323:LEU:HA	2:B:323:LEU:HD12	1.87	0.41
2:D:240:LEU:HD12	2:D:240:LEU:HA	1.89	0.41
1:K:317:THR:O	1:K:321:ILE:HG12	2.21	0.41
2:M:24:GLN:HG3	2:M:149:GLY:HA2	2.02	0.41
2:M:440:LEU:HD11	2:M:455:ILE:O	2.20	0.41
1:V:74:MET:HE3	1:V:74:MET:HB2	1.75	0.41
1:V:206:ASP:OD1	1:V:206:ASP:N	2.54	0.41
2:W:95:TYR:CE2	1:U:53:LEU:HB2	2.55	0.41
2:W:309:TYR:CE2	2:W:333:MET:HG2	2.42	0.41
2:X:49:LEU:HD21	2:X:66:ALA:HB3	2.02	0.41
2:X:216:THR:O	2:X:217:PHE:C	2.63	0.41
1:L:476:LYS:HE2	1:L:476:LYS:HB2	1.84	0.41
2:N:83:ASN:HD22	2:N:83:ASN:HA	1.72	0.41
1:U:172:LYS:NZ	1:U:174:ILE:HD11	2.36	0.41
1:U:217:ILE:HG21	1:U:227:LEU:HD11	2.01	0.41
1:U:352:ARG:O	1:U:356:TYR:HD2	2.03	0.41
4:G:98:LYS:HE3	4:G:98:LYS:HB2	1.89	0.41
4:E:73:VAL:HG11	4:E:81:VAL:HG21	2.01	0.41
1:C:124:GLU:HB2	4:E:14:GLN:NE2	2.35	0.41
2:D:31:ALA:HB2	2:D:150:TYR:CD2	2.55	0.41
1:K:16:LEU:HD11	1:K:27:ARG:HB3	2.02	0.41
1:K:213:PHE:HA	1:K:308:PHE:CE2	2.55	0.41
1:K:292:ILE:HG21	1:K:356:TYR:HD1	1.81	0.41
1:V:104:ASN:OD1	1:V:104:ASN:C	2.63	0.41
1:V:245:LEU:HA	1:V:246:THR:HA	1.53	0.41
2:W:1:MET:HE2	1:U:107:ASN:HD21	1.85	0.41
2:W:14:ALA:HB1	1:U:126:LYS:HG2	2.03	0.41
2:W:33:LEU:HD23	2:W:33:LEU:HA	1.82	0.41
2:X:39:MET:HE1	2:X:95:TYR:CB	2.48	0.41
3:H:17:VAL:HG13	3:H:28:LEU:HD21	2.02	0.41
1:L:307:PHE:CE2	1:L:421:LEU:HD13	2.56	0.41
2:N:172:ASN:HB2	2:N:236:GLY:O	2.20	0.41
1:U:70:PRO:HB3	1:U:247:GLY:HA2	2.01	0.41
1:U:485:HIS:ND1	6:U:601:ICS:S4B	2.94	0.41
3:Z:28:LEU:HA	3:Z:59:MET:HB3	2.01	0.41
1:A:138:PHE:HB2	1:A:140:PRO:HD3	2.02	0.41
2:B:183:ILE:HG21	2:B:202:ASP:OD1	2.20	0.41
1:C:92:ARG:NH2	1:C:221:TYR:CD2	2.88	0.41
1:C:405:ARG:HD3	1:C:405:ARG:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:193:MET:HG2	2:X:288:PRO:HD3	2.03	0.41
3:T:88:PHE:CE1	3:S:60:VAL:HG21	2.55	0.41
1:L:148:THR:HG22	1:L:149:CYS:N	2.34	0.41
2:N:33:LEU:O	2:N:206:VAL:HG11	2.21	0.41
1:U:198:MET:HA	1:U:198:MET:CE	2.44	0.41
1:U:215:ILE:HD13	1:U:215:ILE:HA	1.88	0.41
1:U:414:ASN:HB2	1:U:416:GLU:OE1	2.20	0.41
3:I:3:MET:O	3:I:89:VAL:HA	2.21	0.41
4:O:77:ASN:OD1	4:O:77:ASN:N	2.54	0.41
1:A:67:VAL:C	1:A:70:PRO:HD2	2.46	0.41
2:B:99:VAL:HG21	2:B:225:ILE:HD13	2.02	0.41
1:C:66:VAL:HG12	1:C:92:ARG:NH2	2.35	0.41
1:C:121:PHE:HE1	4:E:30:VAL:HB	1.86	0.41
2:D:127:LEU:HD12	2:D:127:LEU:O	2.21	0.41
2:D:409:PHE:HB3	2:D:410:PRO:HD3	2.01	0.41
2:M:269:ILE:O	2:M:273:ASP:HB2	2.21	0.41
1:V:98:ALA:HB2	1:V:104:ASN:HB3	2.03	0.41
1:V:374:PHE:HZ	6:V:602:ICS:S1B	2.44	0.41
2:W:302:MET:CE	2:W:332:GLU:HG2	2.51	0.41
2:W:313:LYS:HB2	2:W:384:VAL:HA	2.03	0.41
2:X:332:GLU:HG3	1:U:517:PHE:CE2	2.56	0.41
3:b:5:ARG:HE	3:c:3:MET:HE1	1.86	0.41
3:b:21:GLU:HG3	4:a:36:ARG:HH22	1.85	0.41
3:d:64:GLU:H	3:d:64:GLU:HG2	1.66	0.41
1:L:121:PHE:CD1	4:O:17:LYS:HD3	2.56	0.41
1:L:390:LYS:HD2	1:L:390:LYS:HA	1.83	0.41
2:N:252:LEU:HD23	2:N:252:LEU:HA	1.93	0.41
1:U:7:ASP:O	1:U:11:ILE:HG12	2.21	0.41
1:U:271:ILE:HD13	1:U:271:ILE:HA	1.89	0.41
1:U:418:ILE:H	1:U:418:ILE:HG13	1.70	0.41
4:O:8:ILE:HD11	4:O:69:PHE:CE1	2.55	0.41
1:A:14:ASN:HA	1:A:17:LYS:HB2	2.01	0.41
1:A:34:ARG:NH1	1:A:437:MET:HB2	2.36	0.41
1:A:105:TYR:HE2	1:A:138:PHE:HB3	1.85	0.41
1:A:265:LEU:HD21	1:A:268:HIS:HA	2.01	0.41
2:B:17:ILE:O	2:B:371:ASP:HB2	2.21	0.41
2:B:346:ASN:C	2:B:346:ASN:OD1	2.64	0.41
1:C:106:MET:HE2	1:C:106:MET:HB3	1.97	0.41
1:C:110:VAL:HG13	2:D:17:ILE:HG12	2.03	0.41
1:C:277:MET:N	1:C:277:MET:SD	2.94	0.41
1:C:469:LYS:H	1:C:469:LYS:HG2	1.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:59:HIS:CD2	2:D:59:HIS:C	2.98	0.41
2:D:137:ALA:HB2	2:D:156:SER:HB2	2.03	0.41
1:K:153:LEU:HD21	2:M:111:ILE:HG23	2.03	0.41
1:K:160:SER:HA	1:K:163:ARG:NE	2.36	0.41
1:K:303:LYS:HB2	1:K:303:LYS:HE3	1.65	0.41
2:M:45:SER:CB	5:M:501:CLF:S2B	3.09	0.41
2:W:276:ILE:HD12	2:W:291:LEU:HD13	2.02	0.41
2:X:390:ASN:HD22	2:X:410:PRO:HG2	1.85	0.41
2:X:413:ASP:O	2:X:414:ARG:HD2	2.20	0.41
3:R:84:ASP:HB3	4:O:111:ARG:HB2	2.03	0.41
3:T:7:VAL:HG12	3:T:56:MET:HB3	2.03	0.41
3:T:26:ILE:HG22	4:Q:38:LYS:HG2	2.03	0.41
1:L:114:MET:HA	1:L:118:ASP:OD2	2.21	0.41
1:L:143:ILE:HG12	1:L:171:ILE:HD11	2.03	0.41
1:L:405:ARG:HD3	1:L:405:ARG:HA	1.79	0.41
2:N:129:ASP:OD1	2:N:129:ASP:N	2.53	0.41
2:N:243:MET:HE2	2:N:320:PRO:HG2	2.02	0.41
2:N:452:LEU:HD12	2:N:452:LEU:HA	1.67	0.41
1:U:77:LEU:HB3	1:U:145:ILE:HD13	2.03	0.41
3:I:19:CYS:HB3	3:I:72:THR:HG22	2.03	0.41
1:A:444:VAL:HG11	1:A:447:LEU:HG	2.03	0.41
1:C:518:ILE:HD12	1:C:518:ILE:HA	1.69	0.41
2:D:12:ARG:NH1	2:D:12:ARG:HB2	2.36	0.41
2:D:96:GLN:HB3	2:N:257:LYS:HE3	2.01	0.41
2:X:301:MET:HE1	2:X:429:ALA:HB1	2.02	0.41
2:X:346:ASN:OD1	2:X:346:ASN:C	2.64	0.41
1:L:81:PRO:HG2	5:L:603:CLF:S4B	2.61	0.41
2:N:180:PRO:HA	2:N:183:ILE:HD12	2.03	0.41
2:N:430:ARG:HH22	2:N:434:ARG:NH1	2.19	0.41
1:U:513:PRO:HB3	1:U:516:ARG:HH12	1.86	0.41
4:E:34:MET:CE	4:E:63:PHE:HB3	2.51	0.41
1:A:73:ASP:HB2	1:A:103:ASP:HB2	2.03	0.40
1:A:347:TYR:CD2	1:A:447:LEU:HD12	2.56	0.40
1:C:263:SER:O	1:C:286:TRP:HA	2.21	0.40
1:C:520:PRO:HA	1:C:521:PRO:HD3	1.95	0.40
2:D:48:CYS:HB3	5:D:601:CLF:S4B	2.61	0.40
2:D:99:VAL:HA	2:D:133:LYS:O	2.20	0.40
1:V:148:THR:H	1:V:151:VAL:HG21	1.85	0.40
2:W:390:ASN:OD1	2:W:390:ASN:N	2.54	0.40
2:X:366:ILE:N	2:X:366:ILE:HD12	2.36	0.40
2:N:18:ASN:HB2	2:N:372:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:192:ILE:HD12	1:U:192:ILE:HA	1.85	0.40
4:Q:12:LYS:HD3	4:Q:12:LYS:HA	1.66	0.40
3:c:68:LYS:HB2	3:c:68:LYS:HE3	1.94	0.40
1:A:172:LYS:NZ	1:A:201:LEU:HA	2.37	0.40
2:B:50:SER:O	2:B:54:MET:HB2	2.21	0.40
2:B:115:VAL:O	2:B:119:LEU:HG	2.20	0.40
2:B:405:VAL:HG13	2:B:434:ARG:HG2	2.03	0.40
1:C:359:LEU:HD12	1:C:502:PHE:CD2	2.56	0.40
2:D:61:ARG:HH21	2:D:415:ALA:HB2	1.85	0.40
2:D:418:HIS:CE1	2:D:419:TYR:CE1	3.10	0.40
1:K:357:ILE:HD13	1:K:357:ILE:HA	1.90	0.40
1:K:469:LYS:HE2	1:K:469:LYS:HB2	1.87	0.40
2:M:394:LYS:NZ	2:M:413:ASP:HB3	2.36	0.40
2:W:403:PRO:HG3	2:W:442:ARG:CZ	2.51	0.40
3:H:84:ASP:HB3	3:I:98:ILE:HB	2.03	0.40
3:R:5:ARG:HA	3:R:57:LEU:O	2.21	0.40
1:L:60:PHE:CB	5:L:603:CLF:S2A	3.09	0.40
1:L:518:ILE:H	1:L:518:ILE:HG13	1.61	0.40
3:I:10:PRO:HD3	3:I:54:LYS:HA	2.03	0.40
4:O:78:VAL:O	4:O:82:VAL:HG23	2.21	0.40
3:P:3:MET:HB2	3:P:60:VAL:HG12	2.03	0.40
1:C:464:PHE:HB3	1:C:481:SER:HB2	2.02	0.40
2:D:111:ILE:HD12	4:E:10:MET:HE1	2.02	0.40
2:D:343:GLY:O	2:D:369:GLY:HA2	2.21	0.40
1:K:17:LYS:HE2	1:K:17:LYS:HB2	1.88	0.40
1:K:20:PRO:HG3	2:M:93:THR:HG21	2.02	0.40
1:K:110:VAL:HG13	2:M:15:ILE:HG23	2.04	0.40
1:K:154:ILE:HG22	2:M:110:THR:HG21	2.04	0.40
1:K:194:SER:HB2	1:K:273:TYR:HD2	1.85	0.40
2:W:305:ALA:HB2	2:X:416:ASN:OD1	2.22	0.40
3:R:36:ARG:HH12	3:R:86:ARG:HE	1.70	0.40
1:L:74:MET:HB2	1:L:76:HIS:CE1	2.57	0.40
1:U:273:TYR:OH	1:U:400:ASP:HA	2.21	0.40
1:U:453:GLU:HA	1:U:473:TRP:HZ2	1.86	0.40
4:Q:10:MET:HA	4:Q:10:MET:HE2	2.03	0.40
1:A:15:ILE:HD11	1:A:451:GLU:O	2.21	0.40
1:A:287:LEU:HD13	1:A:425:ILE:HG22	2.04	0.40
1:C:365:MET:HE2	1:C:365:MET:HB3	1.86	0.40
2:D:230:ASP:O	2:D:231:SER:C	2.65	0.40
2:D:314:VAL:HG12	2:D:386:LEU:HB3	2.04	0.40
2:D:336:GLU:HB2	2:D:361:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:76:HIS:HD1	1:K:76:HIS:N	2.18	0.40
1:K:89:TRP:CD1	1:K:109:SER:HB2	2.56	0.40
1:V:216:ASN:O	1:V:264:ILE:HG12	2.21	0.40
1:V:310:ASP:HB3	1:V:313:LEU:HB2	2.02	0.40
2:W:217:PHE:CD1	2:W:218:TYR:HD1	2.39	0.40
2:W:241:CYS:HB2	2:W:244:ALA:HB3	2.02	0.40
2:X:122:VAL:HG13	2:X:125:GLU:HA	2.03	0.40
3:J:99:ARG:HD3	3:F:78:ARG:CB	2.52	0.40
3:R:29:THR:HG23	3:P:33:VAL:HG13	2.03	0.40
1:L:230:ILE:HD12	1:L:230:ILE:HA	1.93	0.40
2:N:115:VAL:HA	2:N:118:ILE:HG22	2.03	0.40
1:U:131:ILE:HA	1:U:134:VAL:HG12	2.02	0.40
4:E:35:GLY:HA2	3:F:29:THR:HA	2.03	0.40
1:A:63:THR:O	1:A:68:PHE:HB2	2.22	0.40
2:D:190:LEU:HD23	2:D:197:SER:HB3	2.04	0.40
2:M:60:TYR:CD2	2:M:207:PHE:CD2	3.10	0.40
2:M:140:PRO:HB2	2:M:143:VAL:HG12	2.03	0.40
2:M:203:THR:O	2:M:206:VAL:HG12	2.22	0.40
2:M:301:MET:HE2	2:N:419:TYR:CG	2.57	0.40
2:M:360:GLU:HB3	2:M:361:TYR:CD1	2.57	0.40
1:V:51:GLY:HA2	2:X:67:THR:HB	2.03	0.40
2:W:147:ILE:HG23	2:W:244:ALA:HB2	2.03	0.40
2:X:30:TYR:CE1	2:X:203:THR:HG21	2.56	0.40
3:R:36:ARG:HE	3:R:54:LYS:HD2	1.86	0.40
1:L:262:LEU:HD13	1:L:307:PHE:CE1	2.57	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	492/559 (88%)	464 (94%)	28 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	515/559 (92%)	490 (95%)	25 (5%)	0	100	100
1	K	501/559 (90%)	470 (94%)	31 (6%)	0	100	100
1	L	515/559 (92%)	490 (95%)	25 (5%)	0	100	100
1	U	505/559 (90%)	475 (94%)	30 (6%)	0	100	100
1	V	504/559 (90%)	479 (95%)	25 (5%)	0	100	100
2	B	455/456 (100%)	435 (96%)	20 (4%)	0	100	100
2	D	454/456 (100%)	417 (92%)	37 (8%)	0	100	100
2	M	454/456 (100%)	427 (94%)	27 (6%)	0	100	100
2	N	454/456 (100%)	426 (94%)	28 (6%)	0	100	100
2	W	454/456 (100%)	436 (96%)	18 (4%)	0	100	100
2	X	454/456 (100%)	424 (93%)	30 (7%)	0	100	100
3	F	86/105 (82%)	83 (96%)	3 (4%)	0	100	100
3	H	83/105 (79%)	78 (94%)	5 (6%)	0	100	100
3	I	84/105 (80%)	83 (99%)	1 (1%)	0	100	100
3	J	91/105 (87%)	88 (97%)	3 (3%)	0	100	100
3	P	86/105 (82%)	83 (96%)	3 (4%)	0	100	100
3	R	91/105 (87%)	87 (96%)	3 (3%)	1 (1%)	11	41
3	S	95/105 (90%)	90 (95%)	5 (5%)	0	100	100
3	T	86/105 (82%)	82 (95%)	3 (4%)	1 (1%)	10	40
3	Z	86/105 (82%)	86 (100%)	0	0	100	100
3	b	82/105 (78%)	78 (95%)	3 (4%)	1 (1%)	10	40
3	c	83/105 (79%)	81 (98%)	2 (2%)	0	100	100
3	d	93/105 (89%)	89 (96%)	4 (4%)	0	100	100
4	E	106/125 (85%)	101 (95%)	5 (5%)	0	100	100
4	G	88/125 (70%)	81 (92%)	7 (8%)	0	100	100
4	O	97/125 (78%)	95 (98%)	2 (2%)	0	100	100
4	Q	94/125 (75%)	86 (92%)	8 (8%)	0	100	100
4	Y	95/125 (76%)	92 (97%)	3 (3%)	0	100	100
4	a	90/125 (72%)	84 (93%)	6 (7%)	0	100	100
All	All	7373/8100 (91%)	6980 (95%)	390 (5%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	b	64	GLU
3	R	37	GLY
3	T	26	ILE

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	420/467 (90%)	395 (94%)	25 (6%)	17	43
1	C	440/467 (94%)	417 (95%)	23 (5%)	21	46
1	K	430/467 (92%)	412 (96%)	18 (4%)	26	50
1	L	439/467 (94%)	417 (95%)	22 (5%)	22	47
1	U	433/467 (93%)	401 (93%)	32 (7%)	13	38
1	V	430/467 (92%)	410 (95%)	20 (5%)	23	48
2	B	379/378 (100%)	363 (96%)	16 (4%)	26	50
2	D	378/378 (100%)	359 (95%)	19 (5%)	22	47
2	M	378/378 (100%)	352 (93%)	26 (7%)	14	40
2	N	378/378 (100%)	348 (92%)	30 (8%)	11	36
2	W	378/378 (100%)	358 (95%)	20 (5%)	20	45
2	X	378/378 (100%)	361 (96%)	17 (4%)	24	48
3	F	77/89 (86%)	73 (95%)	4 (5%)	21	46
3	H	75/89 (84%)	68 (91%)	7 (9%)	8	30
3	I	77/89 (86%)	75 (97%)	2 (3%)	40	60
3	J	81/89 (91%)	74 (91%)	7 (9%)	10	33
3	P	77/89 (86%)	72 (94%)	5 (6%)	15	42
3	R	82/89 (92%)	74 (90%)	8 (10%)	7	29
3	S	85/89 (96%)	77 (91%)	8 (9%)	8	30
3	T	77/89 (86%)	71 (92%)	6 (8%)	11	36
3	Z	77/89 (86%)	75 (97%)	2 (3%)	40	60
3	b	73/89 (82%)	72 (99%)	1 (1%)	59	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	76/89 (85%)	74 (97%)	2 (3%)	40	60
3	d	83/89 (93%)	76 (92%)	7 (8%)	10	34
4	E	95/109 (87%)	89 (94%)	6 (6%)	16	42
4	G	80/109 (73%)	77 (96%)	3 (4%)	29	53
4	O	86/109 (79%)	77 (90%)	9 (10%)	6	26
4	Q	84/109 (77%)	78 (93%)	6 (7%)	13	39
4	Y	87/109 (80%)	78 (90%)	9 (10%)	7	27
4	a	81/109 (74%)	75 (93%)	6 (7%)	13	38
All	All	6314/6792 (93%)	5948 (94%)	366 (6%)	20	44

All (366) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	25	ARG
1	A	74	MET
1	A	92	ARG
1	A	115	LYS
1	A	125	LYS
1	A	150	PRO
1	A	151	VAL
1	A	156	ASP
1	A	177	ARG
1	A	179	GLU
1	A	182	ARG
1	A	184	VAL
1	A	213	PHE
1	A	262	LEU
1	A	274	THR
1	A	332	ILE
1	A	334	ARG
1	A	336	ARG
1	A	351	SER
1	A	352	ARG
1	A	374	PHE
1	A	386	ILE
1	A	477	ILE
1	A	508	MET
2	B	1	MET

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Mol	Chain	Res	Type
2	B	106	CYS
2	B	172	ASN
2	B	192	ILE
2	B	235	LEU
2	B	250	LYS
2	B	251	ILE
2	B	290	GLU
2	B	306	HIS
2	B	323	LEU
2	B	356	LEU
2	B	361	TYR
2	B	379	ILE
2	B	394	LYS
2	B	417	LEU
2	B	455	ILE
1	C	33	VAL
1	C	53	LEU
1	C	82	ILE
1	C	92	ARG
1	C	161	VAL
1	C	177	ARG
1	C	211	THR
1	C	227	LEU
1	C	265	LEU
1	C	267	CYS
1	C	278	MET
1	C	312	GLU
1	C	327	LYS
1	C	339	LEU
1	C	346	ILE
1	C	352	ARG
1	C	379	ASP
1	C	438	LYS
1	C	460	LYS
1	C	476	LYS
1	C	479	VAL
1	C	493	TYR
1	C	500	LEU
2	D	91	LEU
2	D	98	GLU
2	D	120	GLU
2	D	128	ILE

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Mol	Chain	Res	Type
2	D	190	LEU
2	D	200	PHE
2	D	229	GLU
2	D	230	ASP
2	D	231	SER
2	D	243	MET
2	D	262	ILE
2	D	316	ILE
2	D	319	ASP
2	D	321	ASP
2	D	323	LEU
2	D	341	LEU
2	D	374	MET
2	D	412	MET
2	D	453	GLU
1	K	53	LEU
1	K	67	VAL
1	K	116	GLU
1	K	119	ILE
1	K	149	CYS
1	K	197	LEU
1	K	216	ASN
1	K	252	HIS
1	K	254	ILE
1	K	272	ASN
1	K	303	LYS
1	K	351	SER
1	K	352	ARG
1	K	431	GLU
1	K	454	PHE
1	K	459	LEU
1	K	468	ILE
1	K	479	VAL
2	M	22	ILE
2	M	24	GLN
2	M	25	PRO
2	M	26	ILE
2	M	45	SER
2	M	46	GLN
2	M	48	CYS
2	M	69	SER
2	M	75	THR

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Mol	Chain	Res	Type
2	M	106	CYS
2	M	115	VAL
2	M	122	VAL
2	M	157	PHE
2	M	189	ILE
2	M	215	HIS
2	M	228	ILE
2	M	243	MET
2	M	281	LYS
2	M	316	ILE
2	M	323	LEU
2	M	331	LEU
2	M	339	VAL
2	M	344	THR
2	M	431	LEU
2	M	440	LEU
2	M	455	ILE
1	V	13	ASP
1	V	18	VAL
1	V	58	CYS
1	V	74	MET
1	V	77	LEU
1	V	84	CYS
1	V	143	ILE
1	V	227	LEU
1	V	265	LEU
1	V	277	MET
1	V	279	GLU
1	V	288	LYS
1	V	334	ARG
1	V	384	GLN
1	V	402	HIS
1	V	431	GLU
1	V	438	LYS
1	V	479	VAL
1	V	488	ASP
1	V	493	TYR
2	W	5	THR
2	W	15	ILE
2	W	21	LYS
2	W	29	VAL
2	W	52	LEU

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Mol	Chain	Res	Type
2	W	57	SER
2	W	67	THR
2	W	75	THR
2	W	96	GLN
2	W	99	VAL
2	W	106	CYS
2	W	155	LYS
2	W	223	THR
2	W	258	VAL
2	W	302	MET
2	W	306	HIS
2	W	316	ILE
2	W	339	VAL
2	W	366	ILE
2	W	397	SER
2	X	54	MET
2	X	77	VAL
2	X	134	ILE
2	X	199	VAL
2	X	203	THR
2	X	214	GLU
2	X	216	THR
2	X	217	PHE
2	X	220	LYS
2	X	235	LEU
2	X	333	MET
2	X	350	GLU
2	X	352	GLU
2	X	361	TYR
2	X	397	SER
2	X	416	ASN
2	X	451	LEU
3	H	1	MET
3	H	22	LYS
3	H	23	GLU
3	H	25	CYS
3	H	28	LEU
3	H	75	GLU
3	H	81	LYS
3	J	29	THR
3	J	31	MET
3	J	65	HIS

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Mol	Chain	Res	Type
3	J	71	LYS
3	J	89	VAL
3	J	102	LYS
3	J	105	LEU
3	R	8	ILE
3	R	18	GLU
3	R	32	GLU
3	R	33	VAL
3	R	36	ARG
3	R	38	LYS
3	R	39	GLN
3	R	40	LYS
3	T	4	ILE
3	T	29	THR
3	T	52	LEU
3	T	59	MET
3	T	60	VAL
3	T	86	ARG
3	b	81	LYS
3	d	23	GLU
3	d	26	ILE
3	d	28	LEU
3	d	47	ILE
3	d	58	LEU
3	d	61	VAL
3	d	68	LYS
1	L	32	VAL
1	L	53	LEU
1	L	78	VAL
1	L	106	MET
1	L	112	THR
1	L	202	ILE
1	L	215	ILE
1	L	246	THR
1	L	258	HIS
1	L	279	GLU
1	L	287	LEU
1	L	298	GLU
1	L	313	LEU
1	L	321	ILE
1	L	335	TYR
1	L	352	ARG

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Mol	Chain	Res	Type
1	L	353	SER
1	L	365	MET
1	L	386	ILE
1	L	438	LYS
1	L	493	TYR
1	L	500	LEU
2	N	1	MET
2	N	10	VAL
2	N	17	ILE
2	N	22	ILE
2	N	45	SER
2	N	48	CYS
2	N	54	MET
2	N	57	SER
2	N	73	GLU
2	N	91	LEU
2	N	106	CYS
2	N	119	LEU
2	N	129	ASP
2	N	153	MET
2	N	189	ILE
2	N	216	THR
2	N	223	THR
2	N	235	LEU
2	N	251	ILE
2	N	258	VAL
2	N	265	THR
2	N	285	VAL
2	N	306	HIS
2	N	316	ILE
2	N	319	ASP
2	N	331	LEU
2	N	412	MET
2	N	441	ASP
2	N	444	ASP
2	N	451	LEU
1	U	36	CYS
1	U	42	ILE
1	U	47	LYS
1	U	53	LEU
1	U	54	THR
1	U	88	THR

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Mol	Chain	Res	Type
1	U	92	ARG
1	U	93	ARG
1	U	94	ASN
1	U	106	MET
1	U	132	ASP
1	U	154	ILE
1	U	159	GLU
1	U	160	SER
1	U	173	VAL
1	U	177	ARG
1	U	240	ARG
1	U	242	ILE
1	U	250	SER
1	U	276	ARG
1	U	291	TYR
1	U	313	LEU
1	U	352	ARG
1	U	354	HIS
1	U	357	ILE
1	U	362	GLU
1	U	459	LEU
1	U	479	VAL
1	U	500	LEU
1	U	508	MET
1	U	517	PHE
1	U	518	ILE
4	G	8	ILE
4	G	36	ARG
4	G	68	MET
4	E	11	ASN
4	E	29	THR
4	E	31	ARG
4	E	42	LEU
4	E	47	ASN
4	E	64	ILE
3	F	1	MET
3	F	12	MET
3	F	33	VAL
3	F	78	ARG
3	I	32	GLU
3	I	33	VAL
4	Q	31	ARG

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Mol	Chain	Res	Type
4	Q	33	VAL
4	Q	39	GLN
4	Q	40	ARG
4	Q	69	PHE
4	Q	71	VAL
4	O	4	ILE
4	O	20	LEU
4	O	38	LYS
4	O	40	ARG
4	O	42	LEU
4	O	70	THR
4	O	112	THR
4	O	114	GLU
4	O	120	ILE
3	P	1	MET
3	P	26	ILE
3	P	68	LYS
3	P	86	ARG
3	P	92	VAL
3	S	5	ARG
3	S	13	GLU
3	S	18	GLU
3	S	21	GLU
3	S	22	LYS
3	S	26	ILE
3	S	28	LEU
3	S	47	ILE
4	a	20	LEU
4	a	21	LEU
4	a	62	ARG
4	a	66	LYS
4	a	73	VAL
4	a	91	THR
4	Y	10	MET
4	Y	38	LYS
4	Y	39	GLN
4	Y	42	LEU
4	Y	62	ARG
4	Y	64	ILE
4	Y	70	THR
4	Y	87	GLU
4	Y	101	VAL

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Mol	Chain	Res	Type
3	Z	64	GLU
3	Z	74	MET
3	c	36	ARG
3	c	98	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	186	GLN
1	A	190	HIS
2	B	46	GLN
2	B	172	ASN
2	B	308	HIS
1	C	9	GLN
1	C	30	HIS
1	C	79	HIS
1	C	190	HIS
1	C	216	ASN
1	C	252	HIS
1	C	258	HIS
1	C	275	ASN
1	C	414	ASN
2	D	172	ASN
2	D	310	HIS
1	K	107	ASN
1	K	449	HIS
2	M	24	GLN
2	M	46	GLN
2	M	59	HIS
2	M	306	HIS
1	V	190	HIS
1	V	252	HIS
1	V	475	GLN
2	W	41	HIS
2	W	90	ASN
2	W	346	ASN
2	W	376	HIS
2	X	284	ASN
2	X	418	HIS
3	H	2	GLN
3	H	53	GLN

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Mol	Chain	Res	Type
3	H	65	HIS
3	R	39	GLN
3	R	53	GLN
1	L	252	HIS
1	L	290	ASN
1	L	475	GLN
1	L	485	HIS
2	N	36	HIS
2	N	46	GLN
2	N	172	ASN
2	N	308	HIS
2	N	418	HIS
2	N	456	GLN
1	U	76	HIS
1	U	94	ASN
1	U	258	HIS
1	U	414	ASN
4	E	39	GLN
4	Q	14	GLN
4	Q	93	ASN
4	O	11	ASN
4	O	14	GLN
3	S	90	ASN
4	Y	77	ASN
4	Y	103	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

18 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
5	CLF	L	603	2,1	0,24,24	-	-	-		
7	HCA	L	601	6	13,13,13	1.08	0	15,18,18	1.26	2 (13%)
6	ICS	U	601	7,1	6,30,30	2.26	3 (50%)	-		
7	HCA	V	603	6	13,13,13	1.10	0	15,18,18	1.21	2 (13%)
6	ICS	C	601	7,1	6,30,30	1.93	2 (33%)	-		
6	ICS	L	602	7,1	6,30,30	2.50	2 (33%)	-		
7	HCA	D	602	6	13,13,13	1.13	0	15,18,18	1.20	2 (13%)
7	HCA	A	603	6	13,13,13	1.19	1 (7%)	15,18,18	1.40	3 (20%)
7	HCA	K	602	6	13,13,13	1.14	0	15,18,18	1.35	3 (20%)
5	CLF	D	601	2,1	0,24,24	-	-	-		
5	CLF	M	501	2,1	0,24,24	-	-	-		
5	CLF	V	601	2,1	0,24,24	-	-	-		
5	CLF	A	601	2,1	0,24,24	-	-	-		
5	CLF	W	601	2,1	0,24,24	-	-	-		
6	ICS	K	601	7,1	6,30,30	1.85	2 (33%)	-		
7	HCA	U	602	6	13,13,13	1.15	1 (7%)	15,18,18	1.24	2 (13%)
6	ICS	A	602	7,1	6,30,30	1.66	1 (16%)	-		
6	ICS	V	602	7,1	6,30,30	1.88	2 (33%)	-		

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
5	CLF	L	603	2,1	-	-	0/12/10/10
7	HCA	L	601	6	-	4/17/17/17	-
7	HCA	V	603	6	-	5/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HCA	K	602	6	-	9/17/17/17	-
7	HCA	D	602	6	-	14/17/17/17	-
7	HCA	A	603	6	-	6/17/17/17	-
5	CLF	D	601	2,1	-	-	0/12/10/10
5	CLF	M	501	2,1	-	-	0/12/10/10
5	CLF	A	601	2,1	-	-	0/12/10/10
5	CLF	V	601	2,1	-	-	0/12/10/10
5	CLF	W	601	2,1	-	-	0/12/10/10
7	HCA	U	602	6	-	13/17/17/17	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	602	ICS	S5A-FE7	-4.04	2.15	2.24
6	U	601	ICS	S5A-FE7	-3.81	2.15	2.24
6	L	602	ICS	S2B-FE6	-3.73	2.16	2.24
6	C	601	ICS	S2B-FE6	-3.38	2.16	2.24
6	K	601	ICS	S2B-FE6	-3.36	2.17	2.24
6	A	602	ICS	S2B-FE6	-3.25	2.17	2.24
6	V	602	ICS	S2B-FE2	-3.20	2.17	2.24
6	U	601	ICS	S2B-FE6	-3.02	2.17	2.24
7	A	603	HCA	C3-C7	2.32	1.55	1.53
6	K	601	ICS	S2B-FE2	-2.27	2.19	2.24
6	U	601	ICS	S2B-FE2	-2.27	2.19	2.24
7	U	602	HCA	C3-C7	2.21	1.55	1.53
6	V	602	ICS	S2B-FE6	-2.17	2.19	2.24
6	C	601	ICS	S5A-FE7	-2.03	2.20	2.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	602	HCA	O7-C3-C4	-2.96	104.15	108.88
7	L	601	HCA	O5-C7-C3	-2.57	117.11	122.09
7	A	603	HCA	O6-C7-C3	2.55	118.04	113.14
7	A	603	HCA	O5-C7-C3	-2.55	117.16	122.09
7	V	603	HCA	O5-C7-C3	-2.44	117.37	122.09
7	D	602	HCA	O5-C7-C3	-2.40	117.45	122.09
7	U	602	HCA	O7-C3-C4	-2.34	105.14	108.88
7	L	601	HCA	O6-C7-C3	2.22	117.40	113.14
7	V	603	HCA	O6-C7-C3	2.22	117.39	113.14
7	K	602	HCA	O5-C7-C3	-2.17	117.89	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	603	HCA	O7-C3-C4	-2.13	105.48	108.88
7	U	602	HCA	O5-C7-C3	-2.09	118.04	122.09
7	D	602	HCA	O6-C7-C3	2.04	117.06	113.14
7	K	602	HCA	O6-C7-C3	2.01	117.00	113.14

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	603	HCA	C2-C3-C4-C5
7	A	603	HCA	O7-C3-C4-C5
7	A	603	HCA	C3-C4-C5-C6
7	D	602	HCA	C2-C3-C4-C5
7	D	602	HCA	C7-C3-C4-C5
7	D	602	HCA	O7-C3-C4-C5
7	D	602	HCA	C4-C3-C7-O6
7	D	602	HCA	O7-C3-C7-O5
7	D	602	HCA	O7-C3-C7-O6
7	K	602	HCA	C2-C3-C4-C5
7	K	602	HCA	C7-C3-C4-C5
7	K	602	HCA	O7-C3-C4-C5
7	K	602	HCA	C2-C3-C7-O5
7	K	602	HCA	C2-C3-C7-O6
7	K	602	HCA	O7-C3-C7-O5
7	K	602	HCA	O7-C3-C7-O6
7	K	602	HCA	C3-C4-C5-C6
7	V	603	HCA	C2-C3-C4-C5
7	V	603	HCA	C7-C3-C4-C5
7	V	603	HCA	O7-C3-C4-C5
7	U	602	HCA	C2-C3-C4-C5
7	U	602	HCA	C7-C3-C4-C5
7	U	602	HCA	O7-C3-C4-C5
7	U	602	HCA	C1-C2-C3-C4
7	U	602	HCA	C1-C2-C3-C7
7	U	602	HCA	C1-C2-C3-O7
7	D	602	HCA	C2-C3-C7-O5
7	D	602	HCA	C2-C3-C7-O6
7	D	602	HCA	C3-C4-C5-C6
7	L	601	HCA	C3-C4-C5-C6
7	U	602	HCA	C3-C4-C5-C6
7	U	602	HCA	O7-C3-C7-O5
7	D	602	HCA	C4-C3-C7-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	603	HCA	C7-C3-C4-C5
7	L	601	HCA	C2-C3-C4-C5
7	U	602	HCA	C2-C3-C7-O5
7	A	603	HCA	O2-C1-C2-C3
7	D	602	HCA	C1-C2-C3-O7
7	K	602	HCA	C1-C2-C3-O7
7	A	603	HCA	O1-C1-C2-C3
7	D	602	HCA	C1-C2-C3-C4
7	U	602	HCA	C2-C3-C7-O6
7	U	602	HCA	C4-C3-C7-O5
7	U	602	HCA	C4-C3-C7-O6
7	D	602	HCA	C4-C5-C6-O4
7	D	602	HCA	C4-C5-C6-O3
7	L	601	HCA	C4-C5-C6-O3
7	L	601	HCA	C4-C5-C6-O4
7	V	603	HCA	C2-C3-C7-O5
7	V	603	HCA	C2-C3-C7-O6
7	U	602	HCA	O7-C3-C7-O6

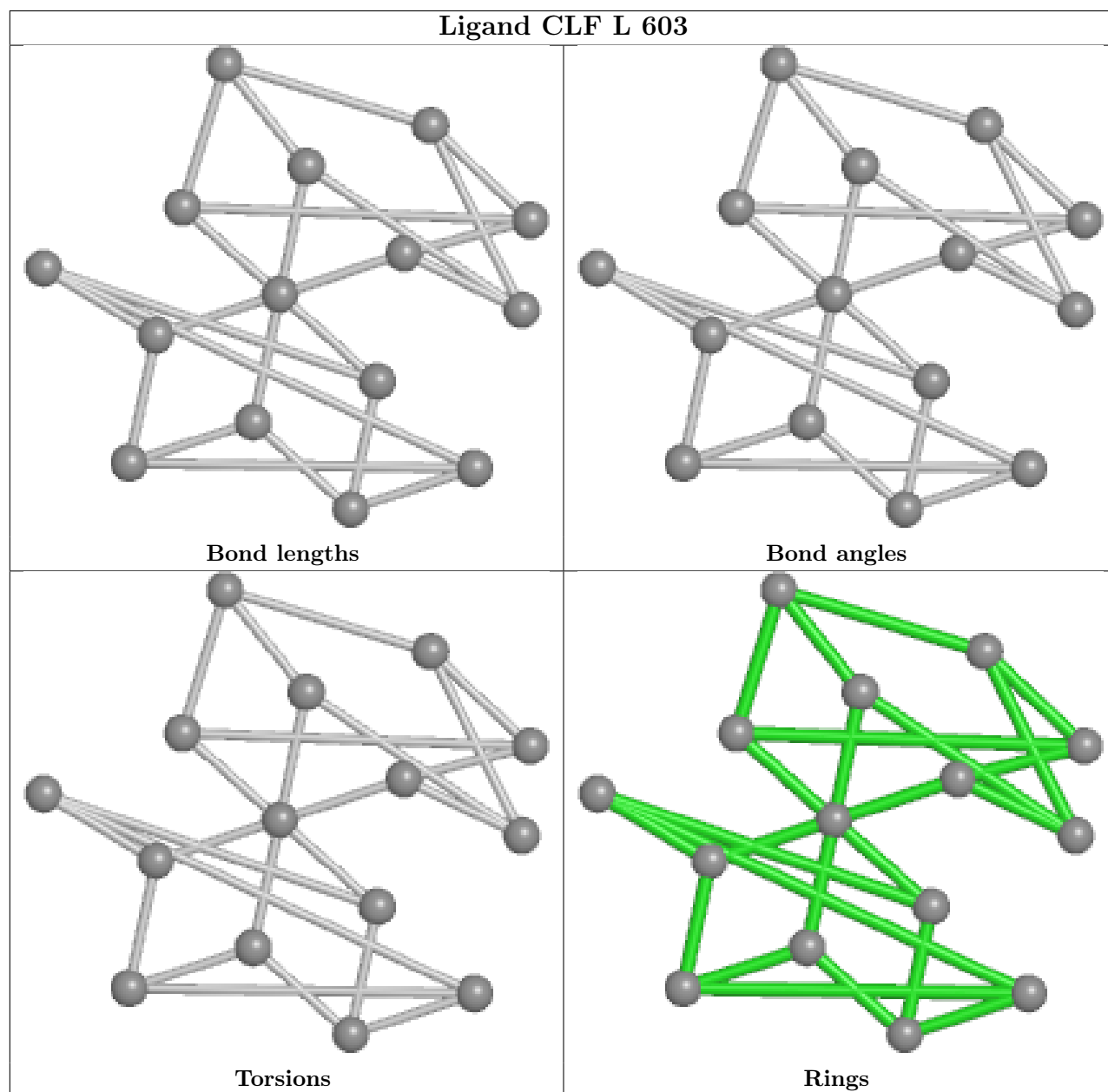
There are no ring outliers.

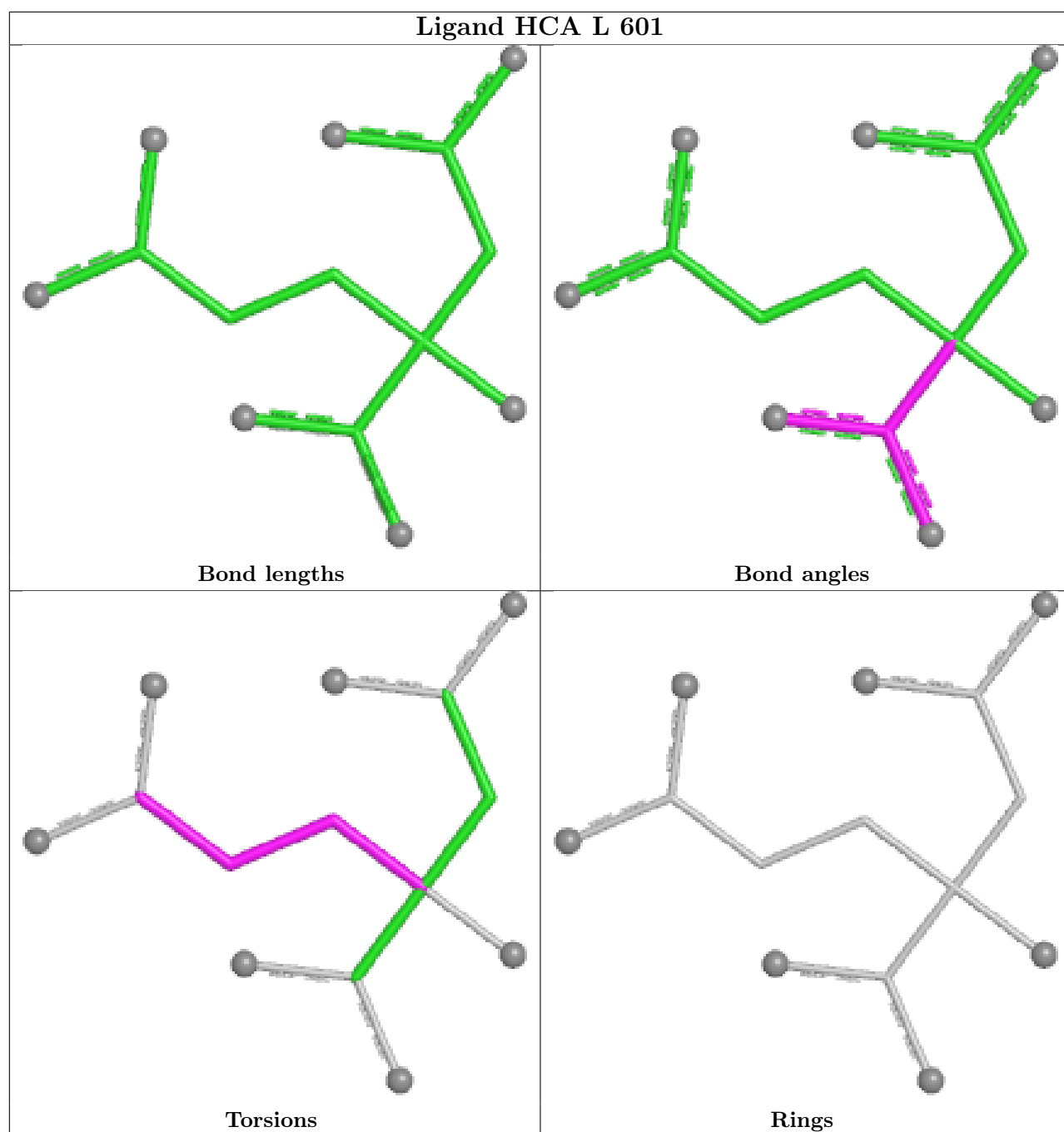
15 monomers are involved in 115 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	603	CLF	6	0
7	L	601	HCA	1	0
6	U	601	ICS	11	0
7	V	603	HCA	1	0
6	C	601	ICS	11	0
6	L	602	ICS	6	0
7	A	603	HCA	1	0
5	D	601	CLF	9	0
5	M	501	CLF	7	0
5	V	601	CLF	9	0
5	A	601	CLF	6	0
5	W	601	CLF	11	0
6	K	601	ICS	7	0
6	A	602	ICS	13	0
6	V	602	ICS	16	0

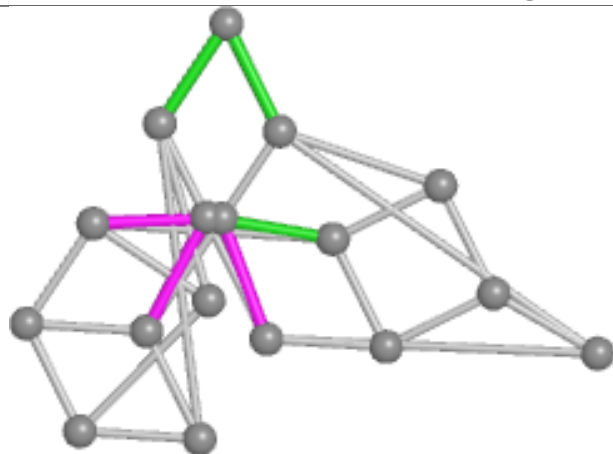
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

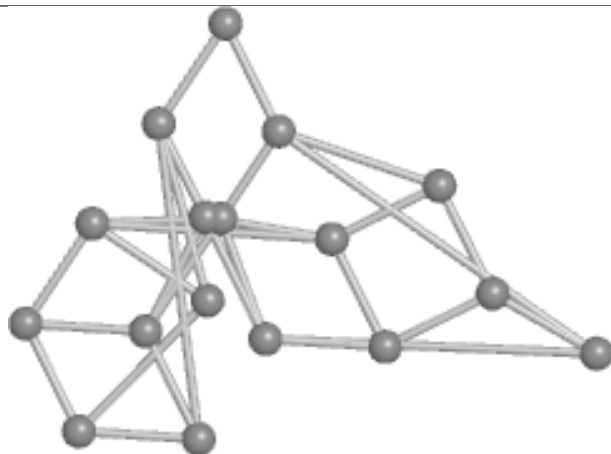




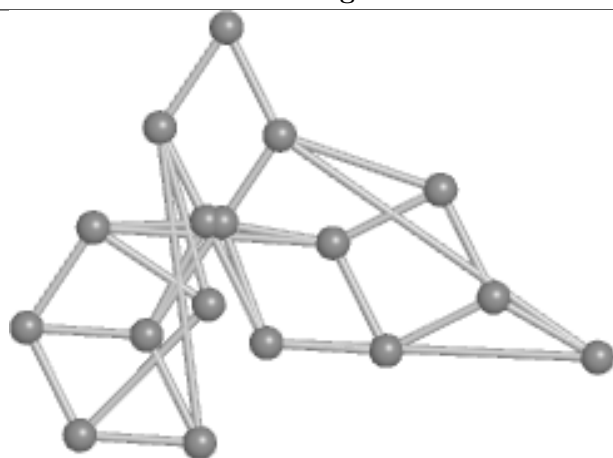
Ligand ICS U 601



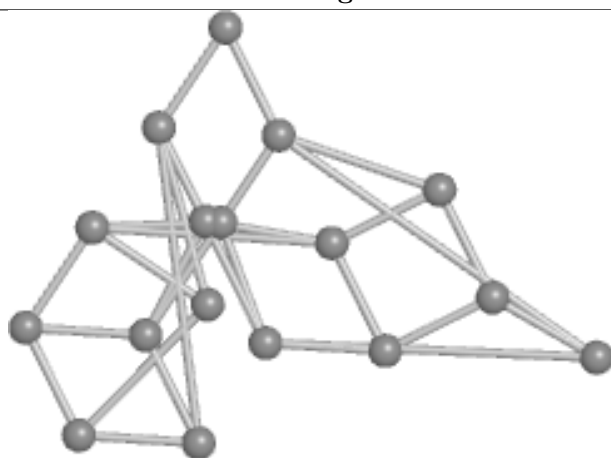
Bond lengths



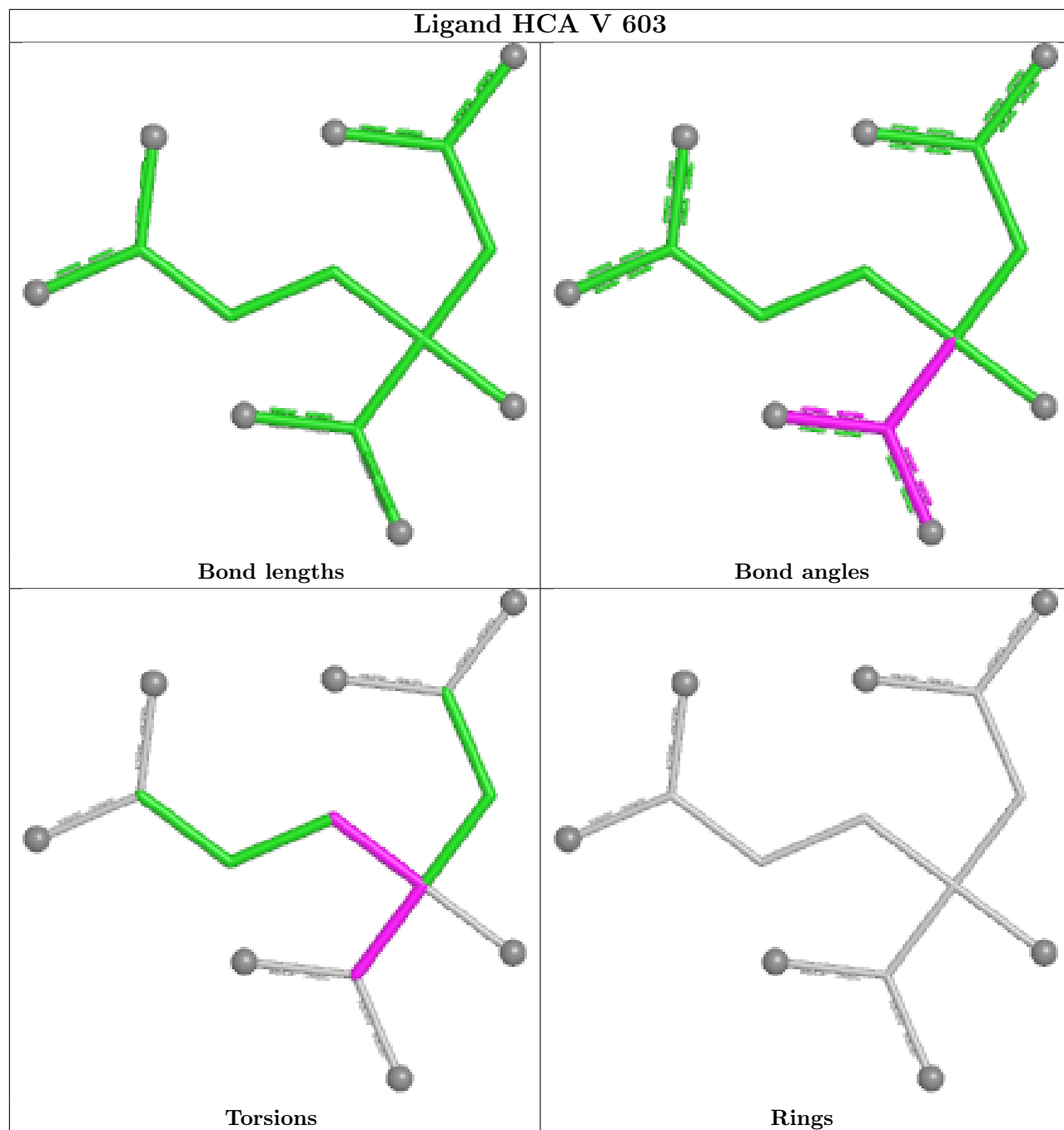
Bond angles

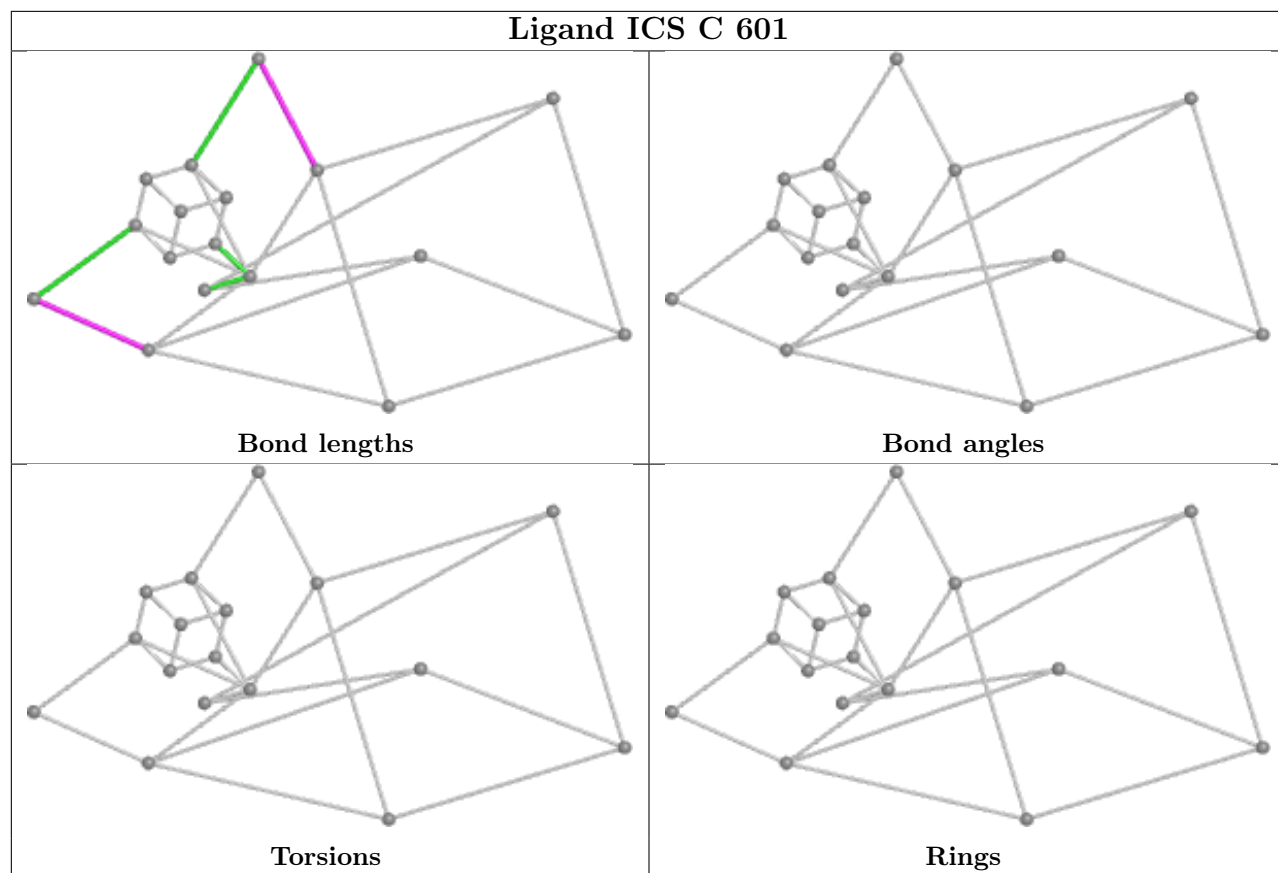


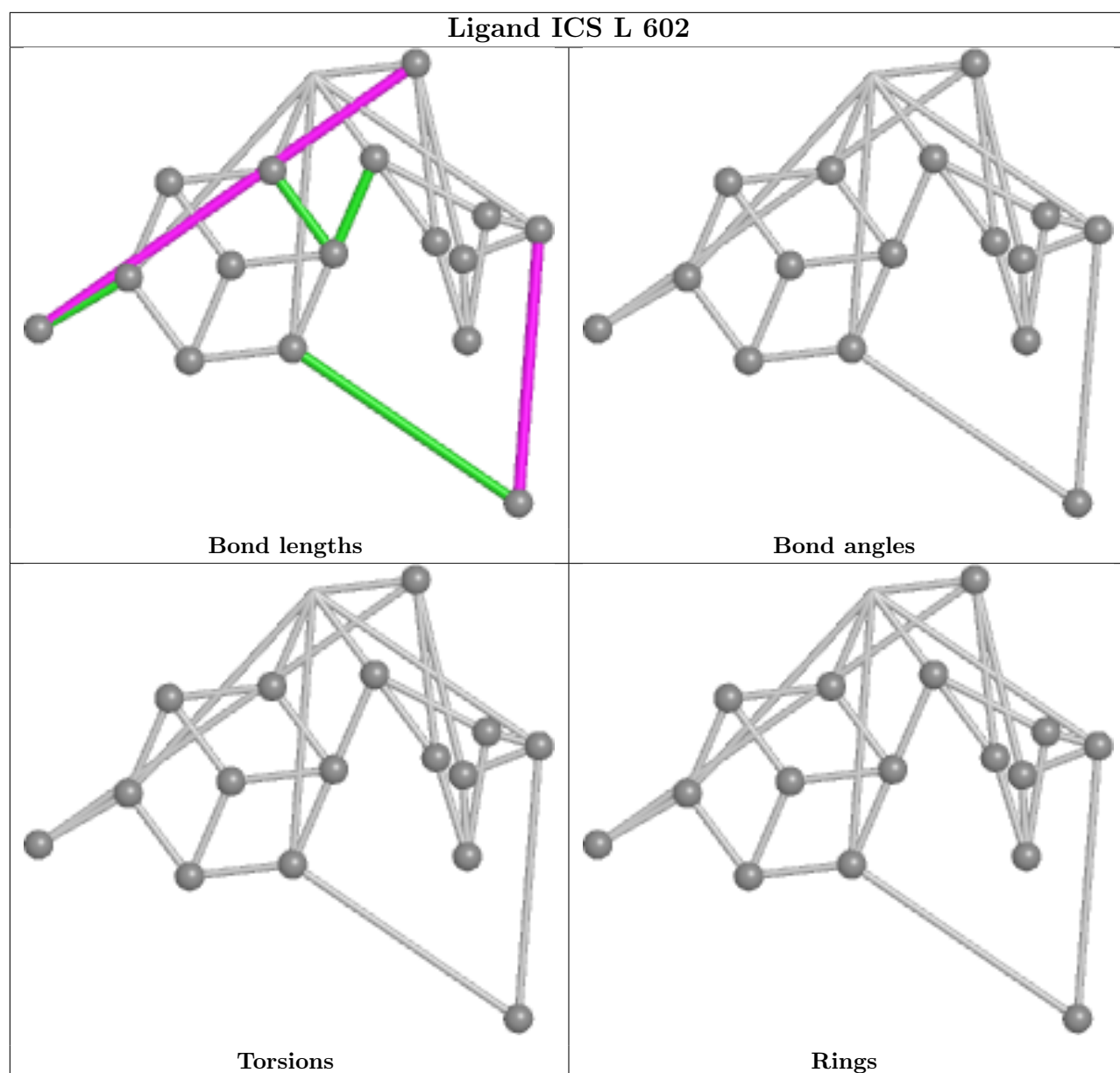
Torsions

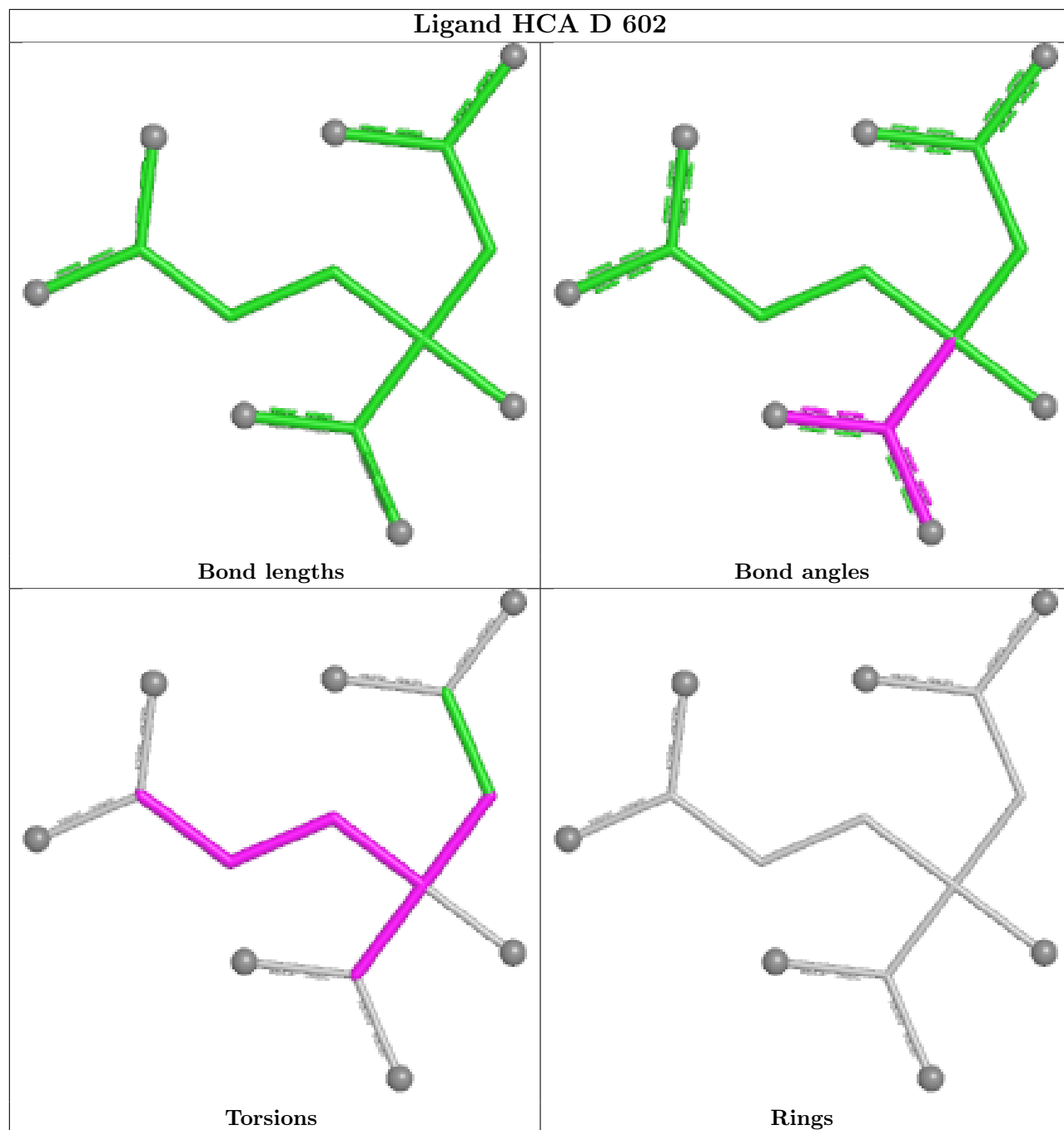


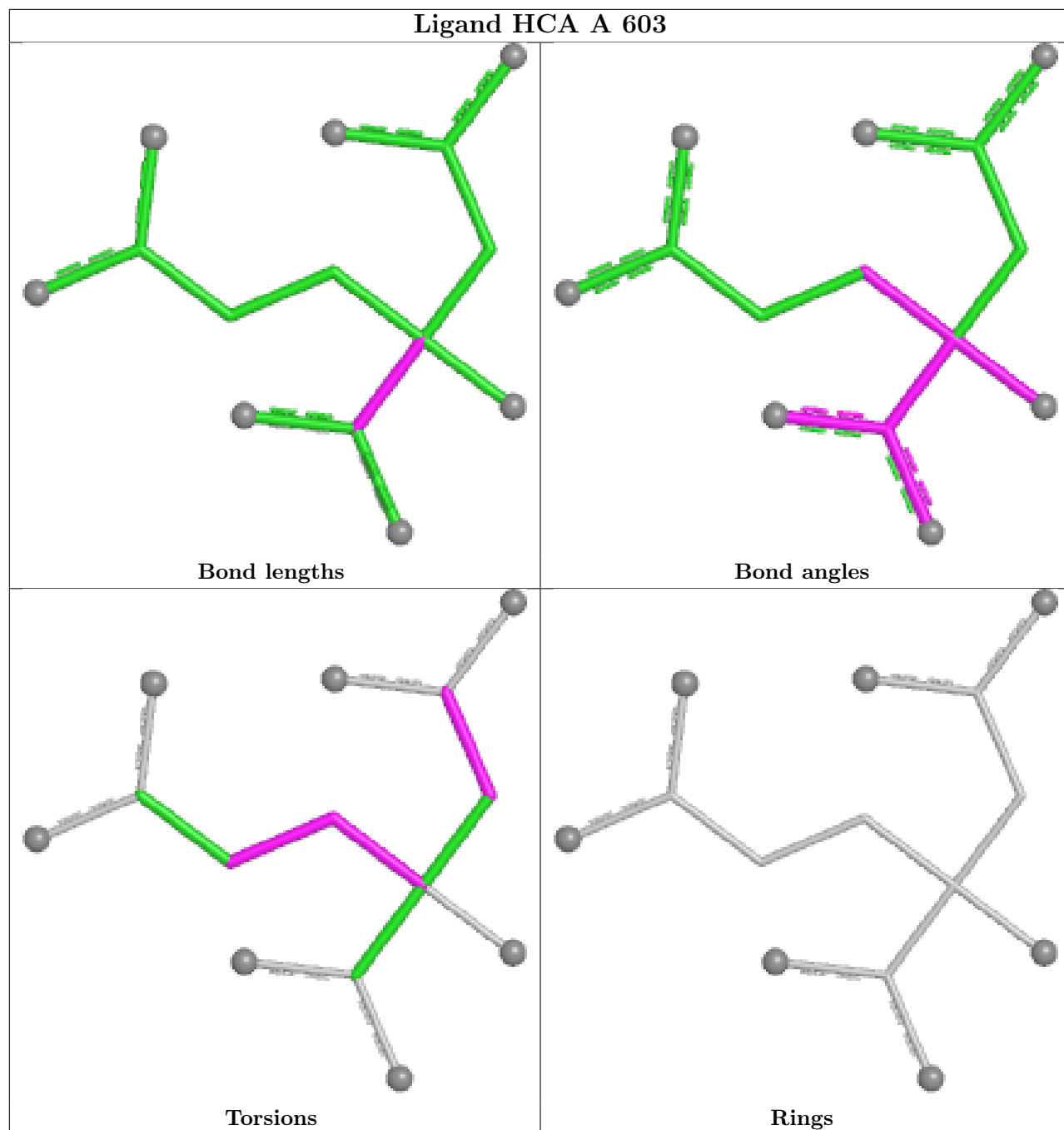
Rings

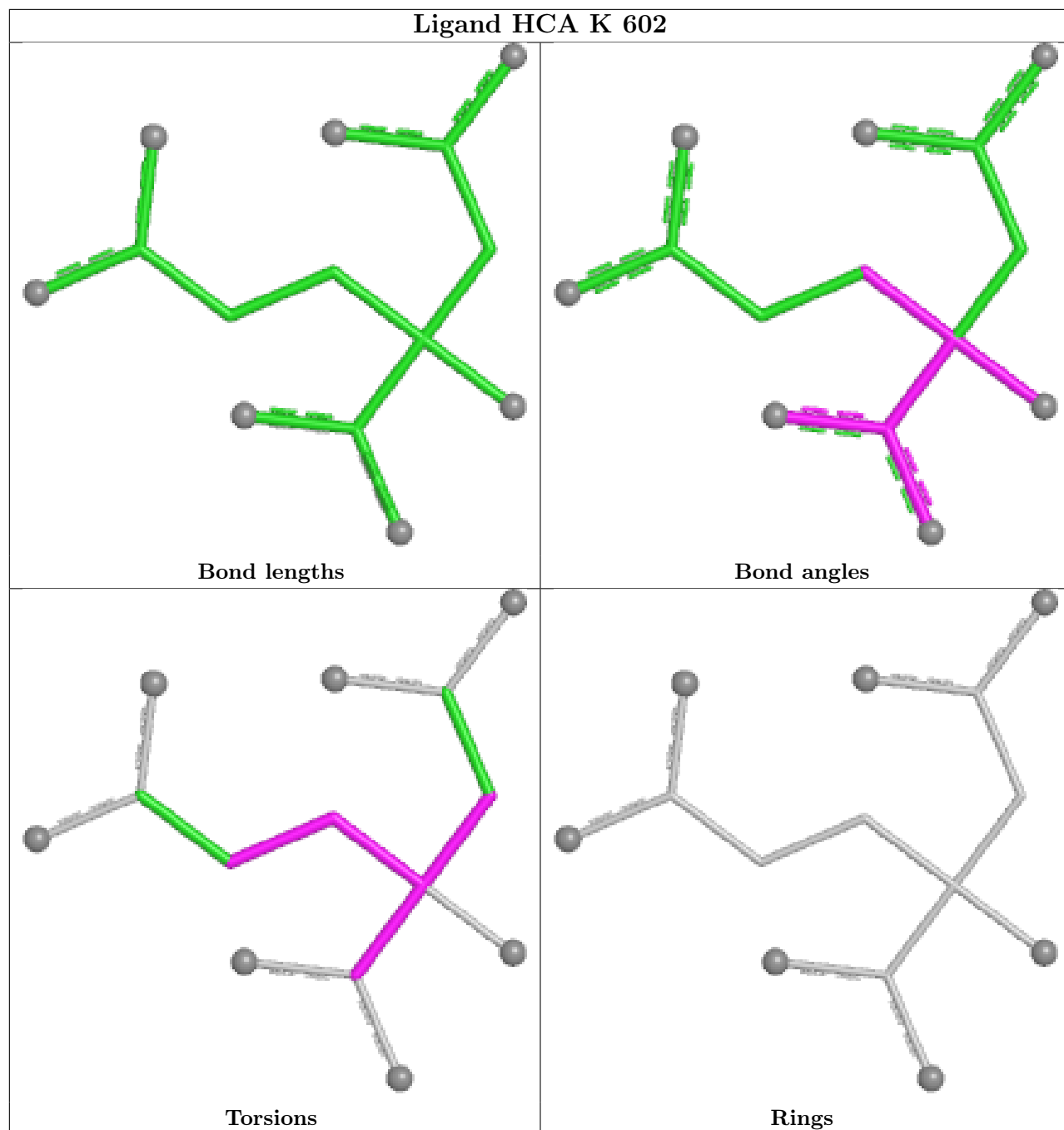




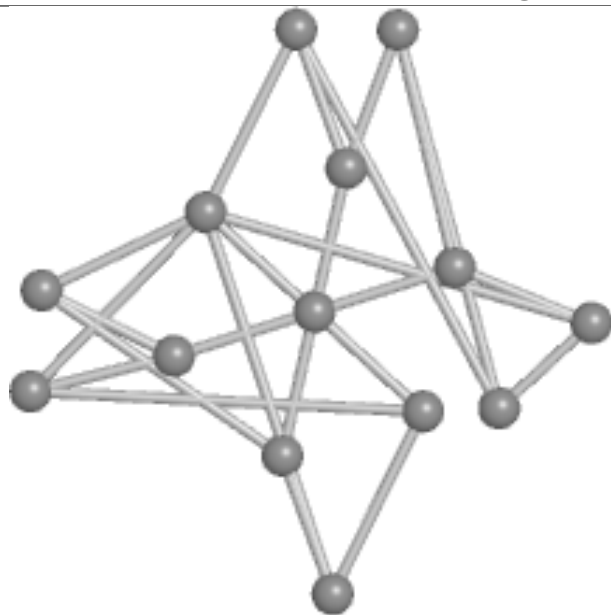




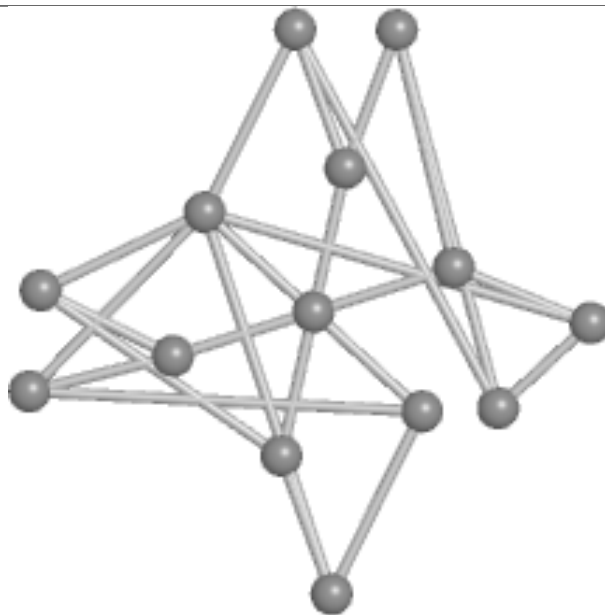




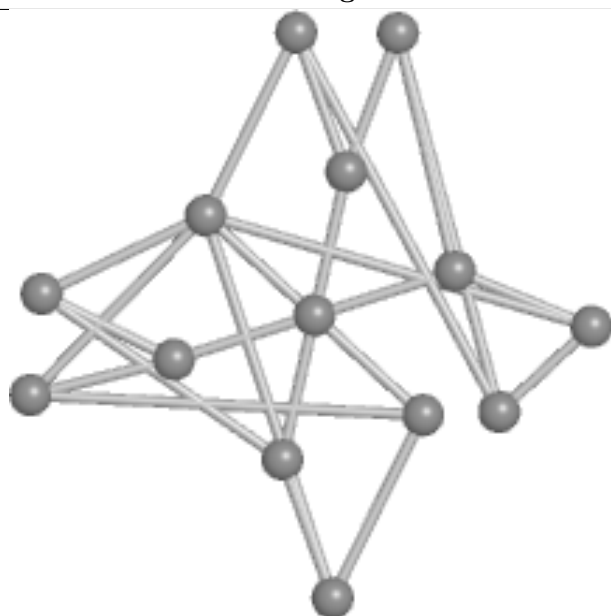
Ligand CLF D 601



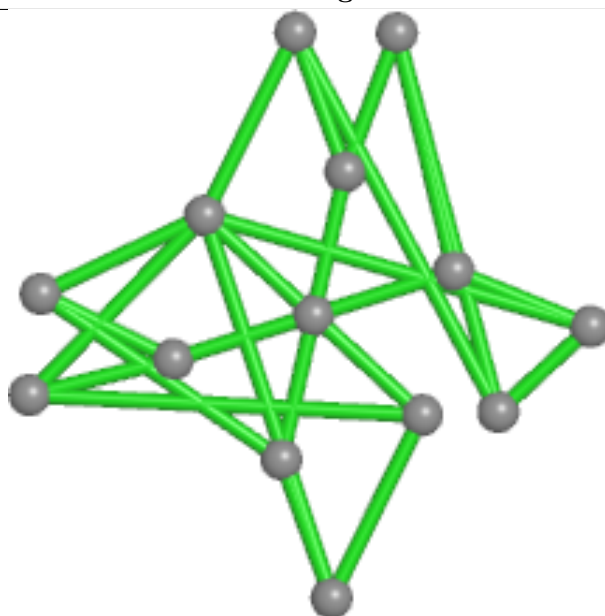
Bond lengths



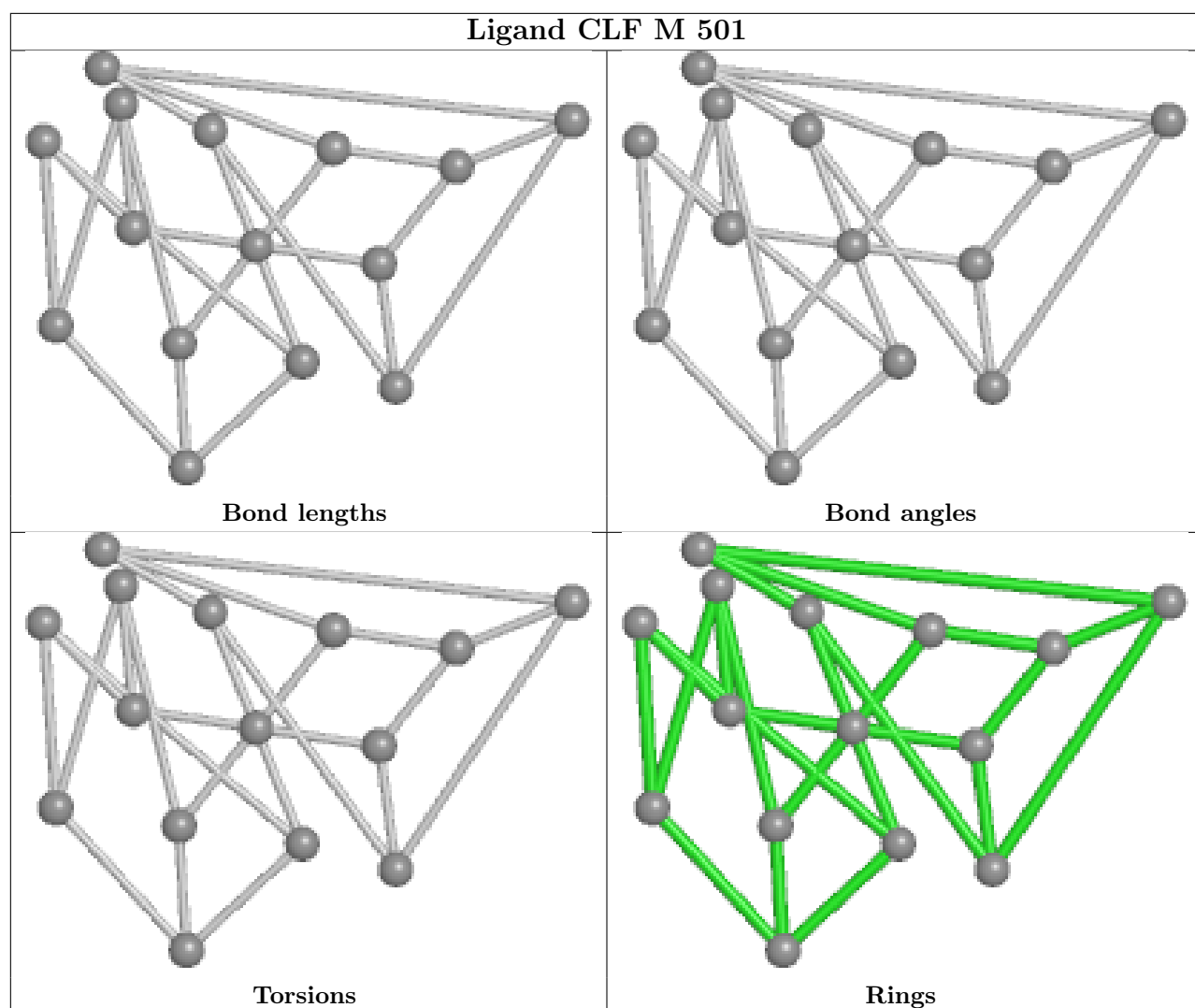
Bond angles

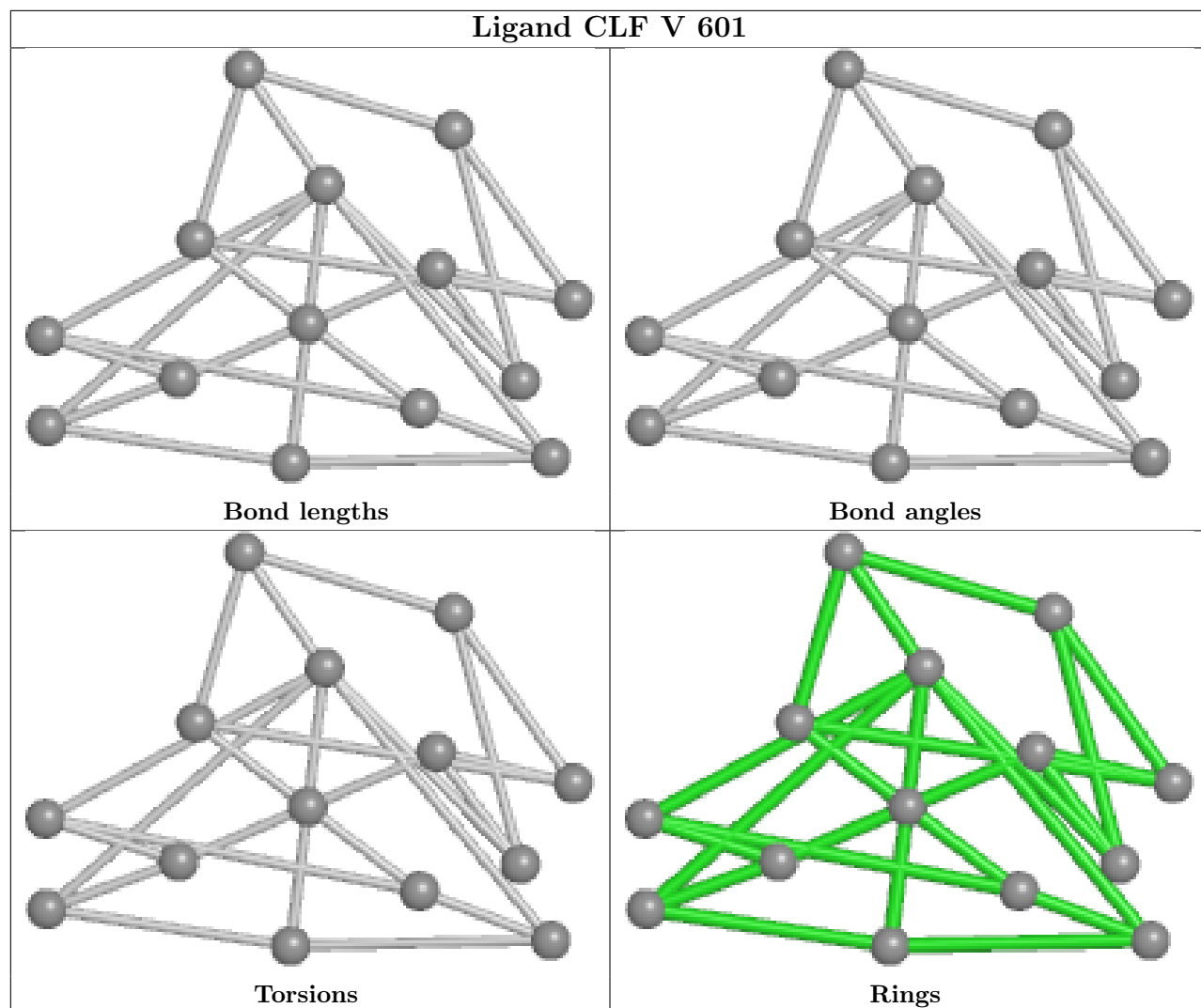


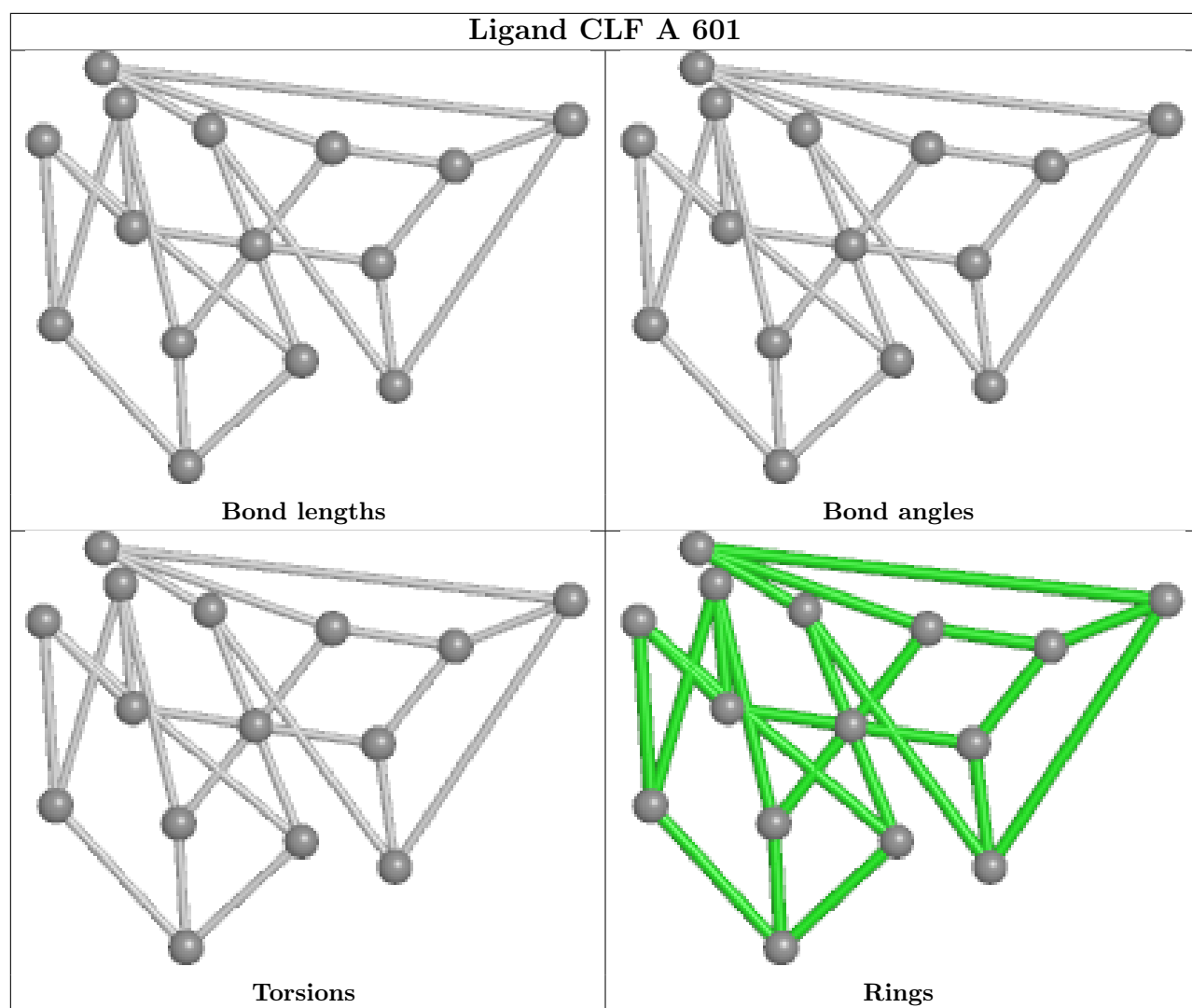
Torsions

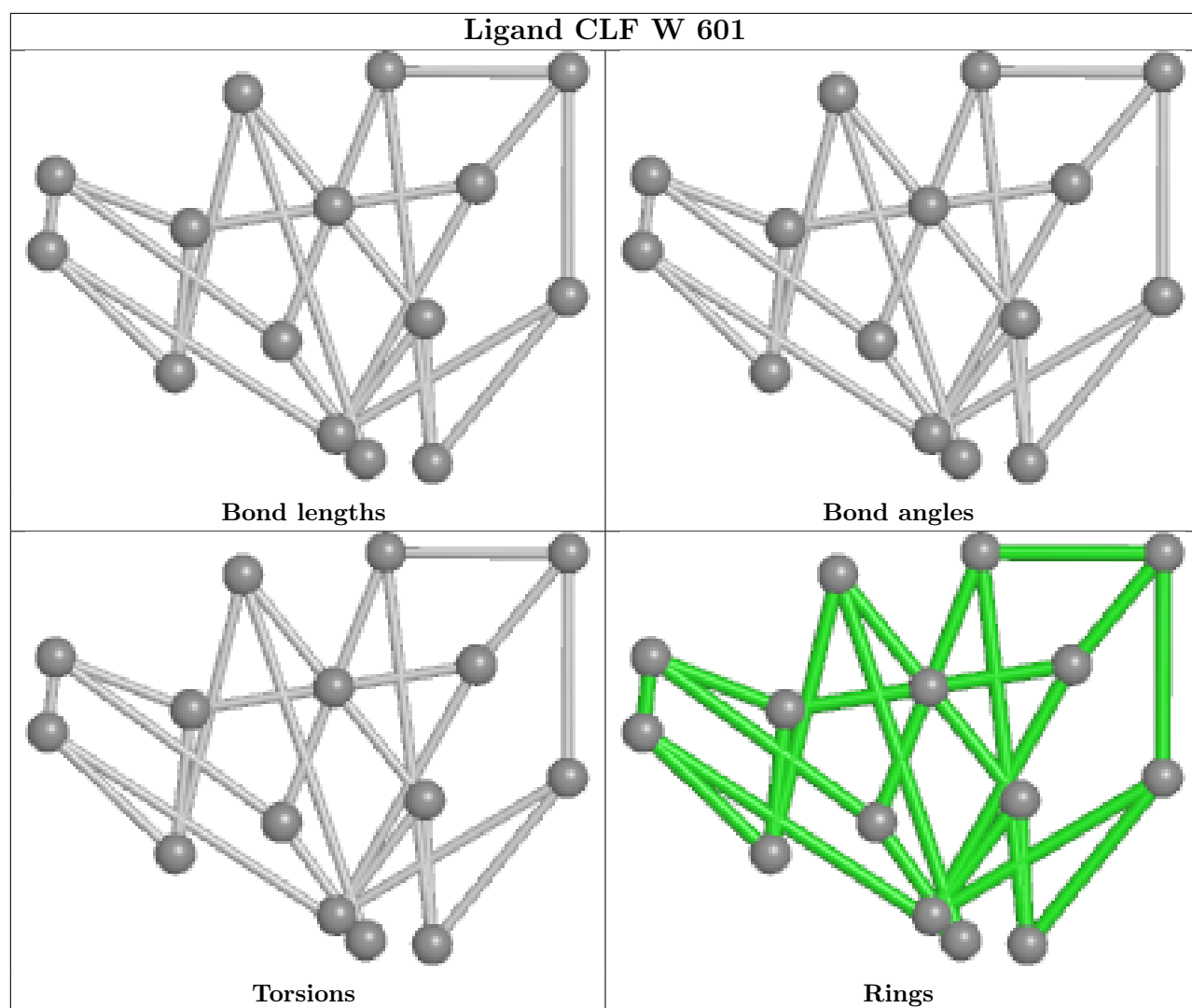


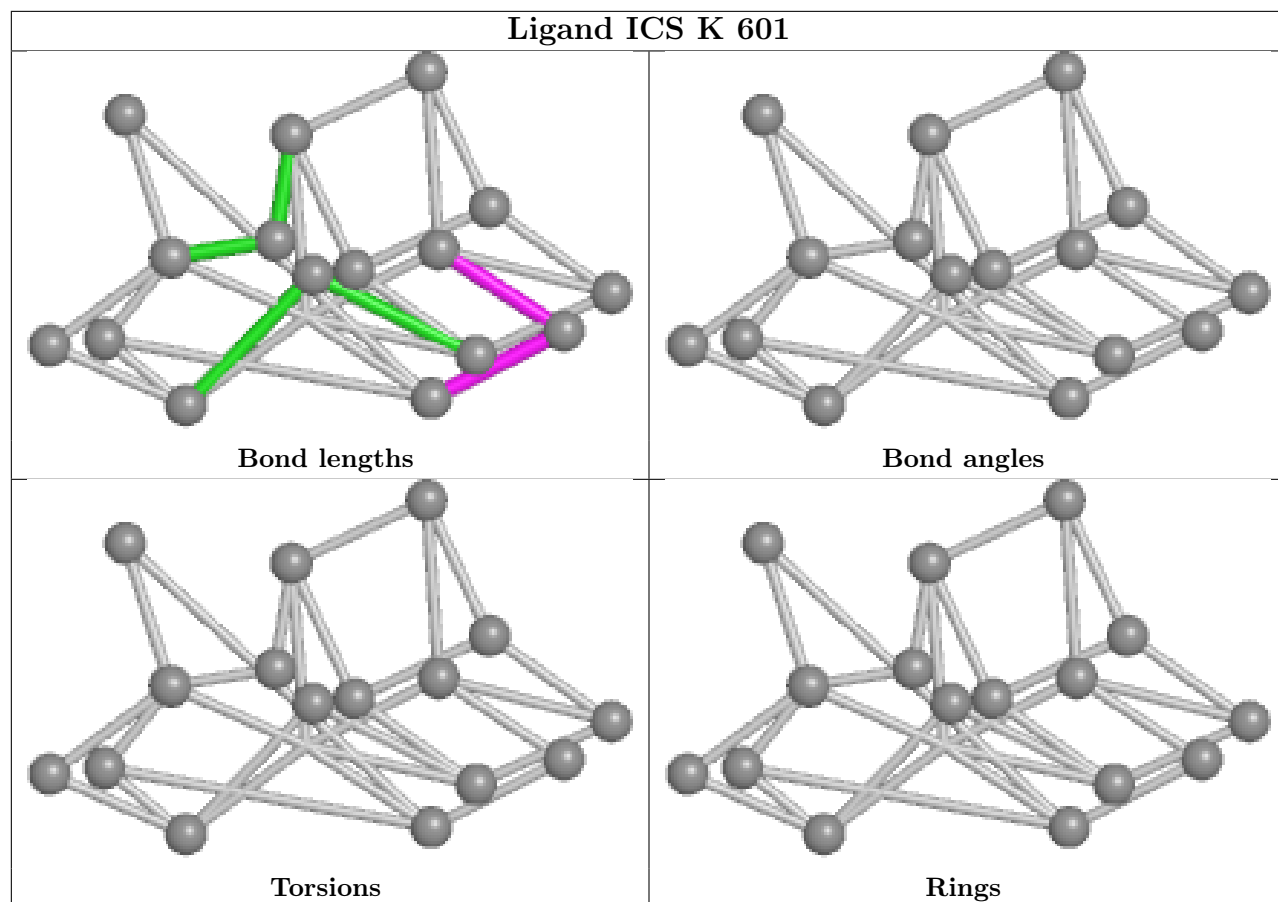
Rings

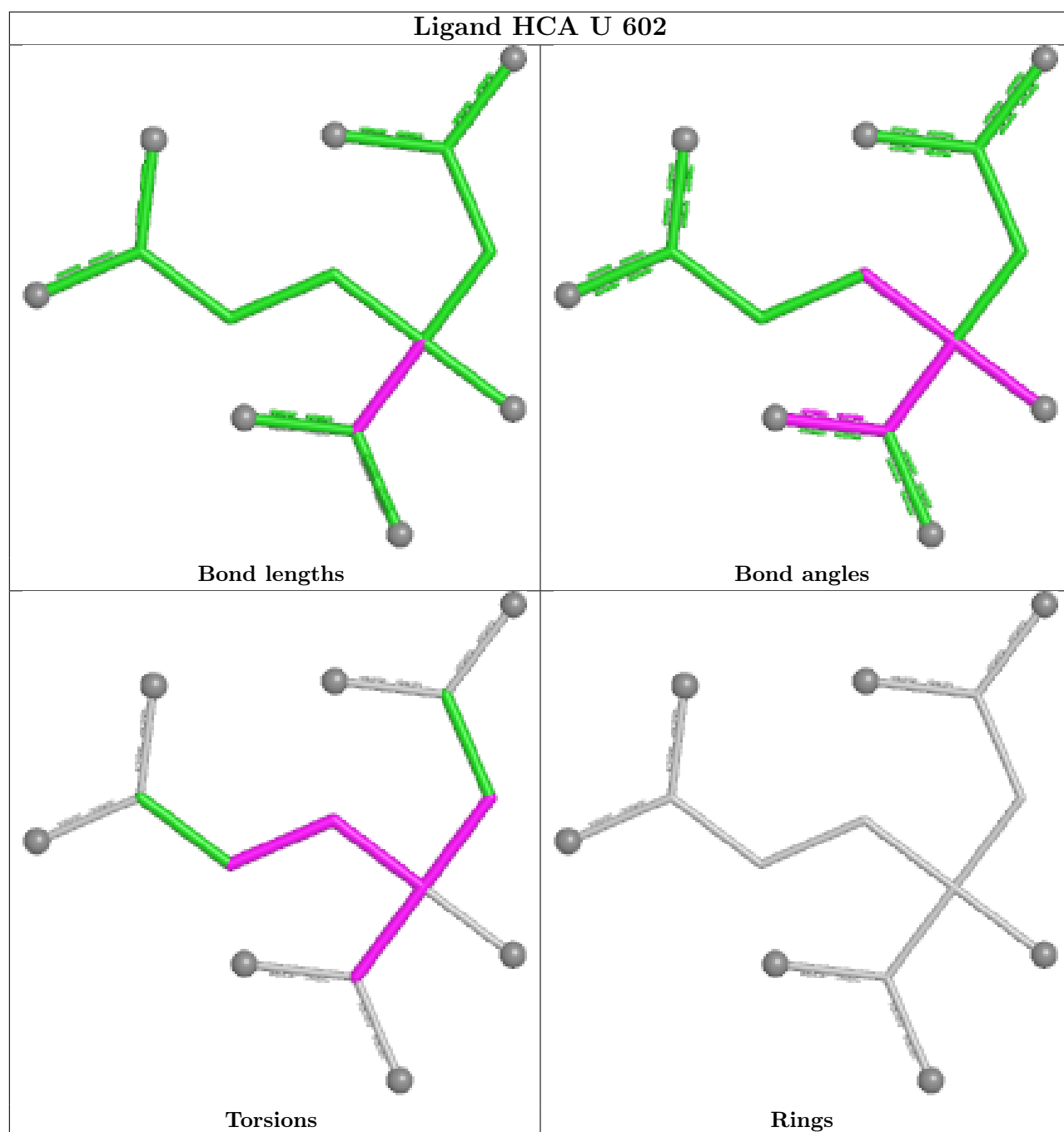


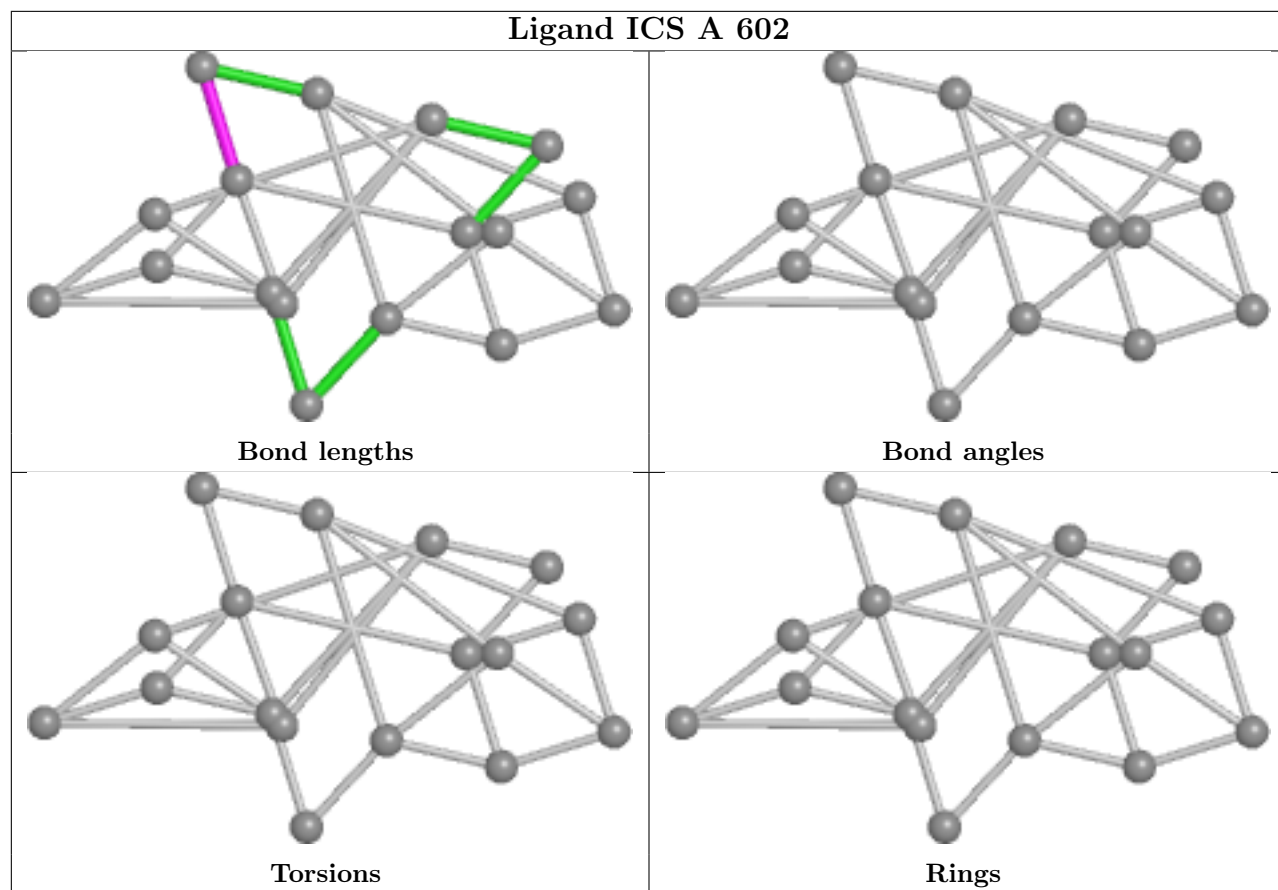


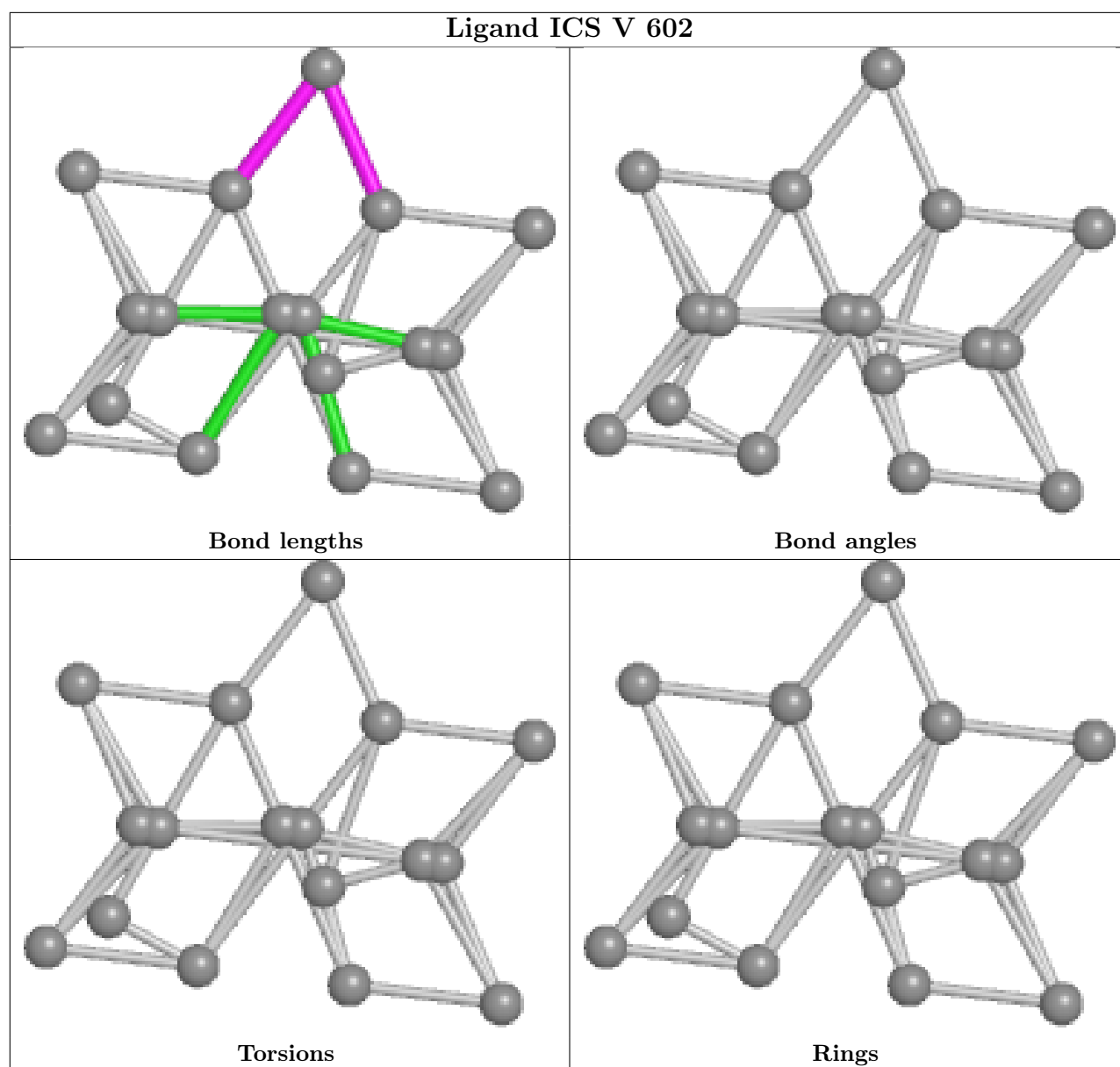












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

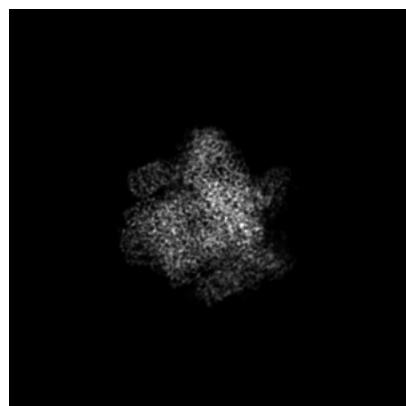
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-78079. These allow visual inspection of the internal detail of the map and identification of artifacts.

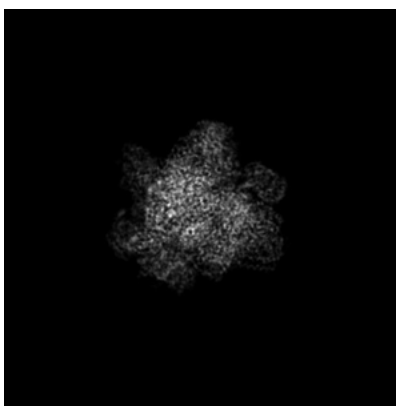
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

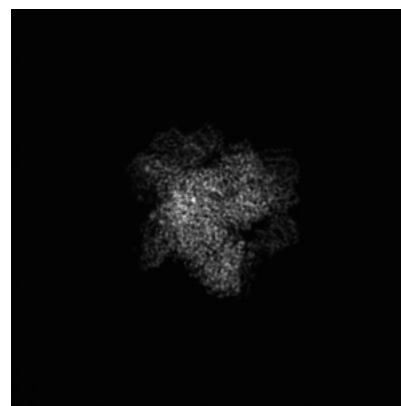
6.1.1 Primary map



X

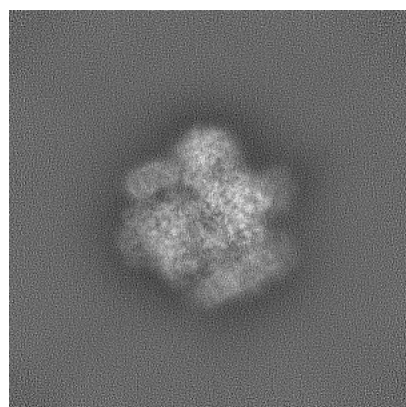


Y

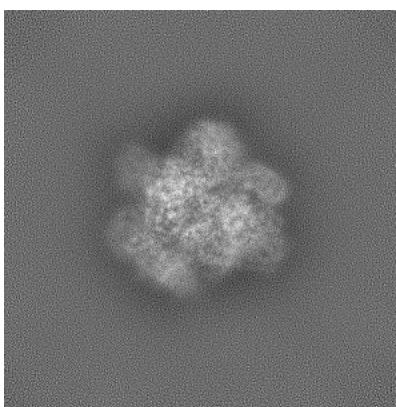


Z

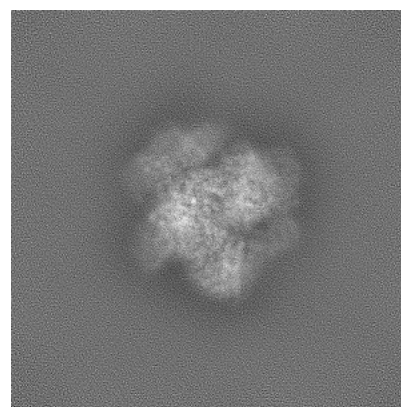
6.1.2 Raw map



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: 200

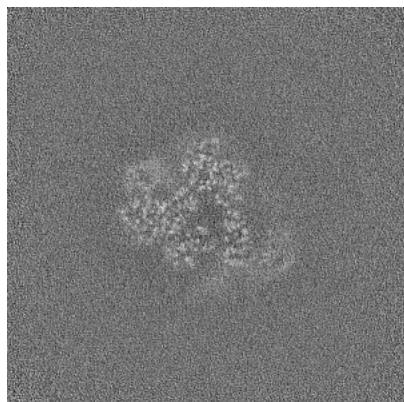


Y Index: 200

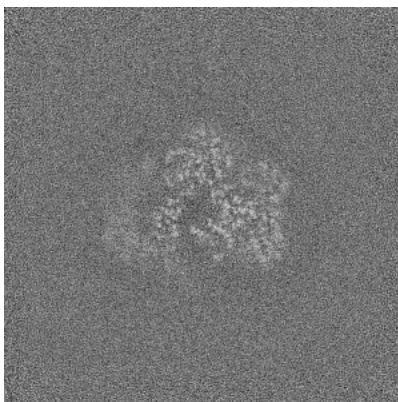


Z Index: 200

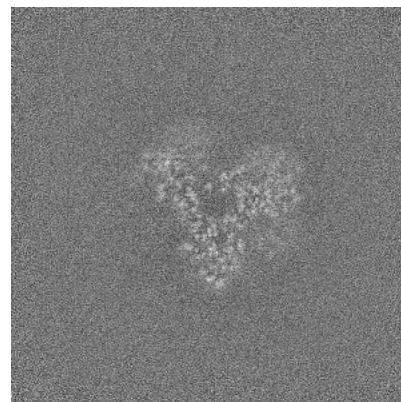
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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: 199

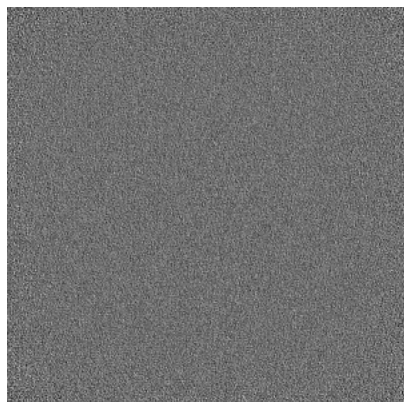


Y Index: 204

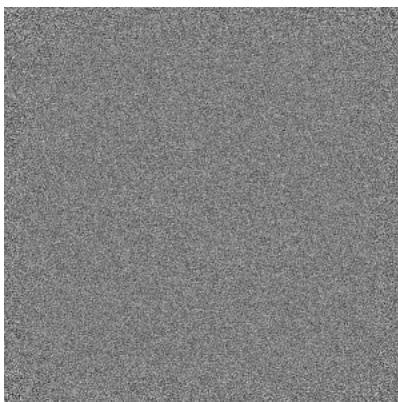


Z Index: 178

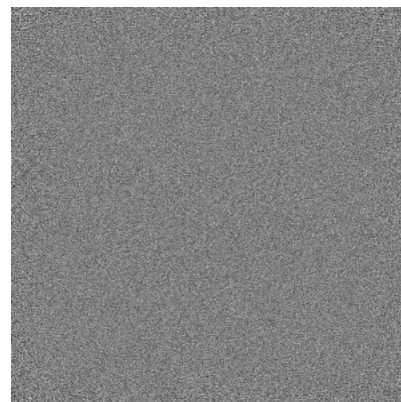
6.3.2 Raw map



X Index: 0



Y Index: 0

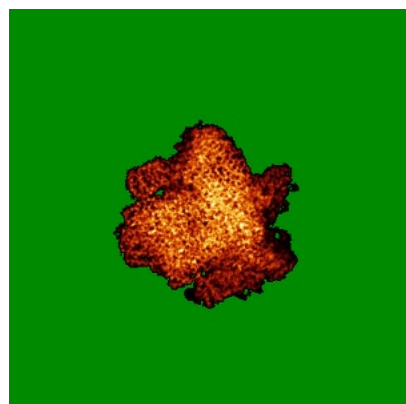


Z Index: 0

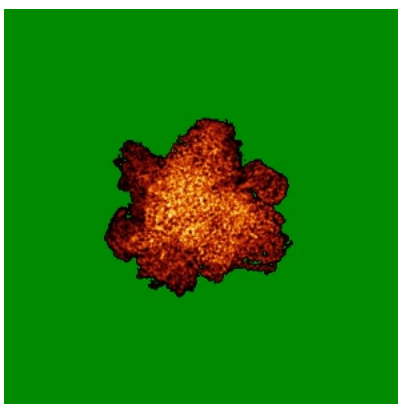
The images above show the largest variance slices of the map in three orthogonal directions.

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

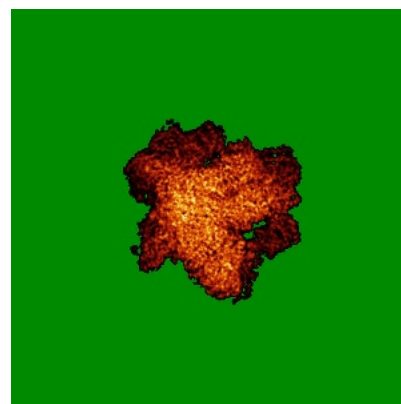
6.4.1 Primary map



X

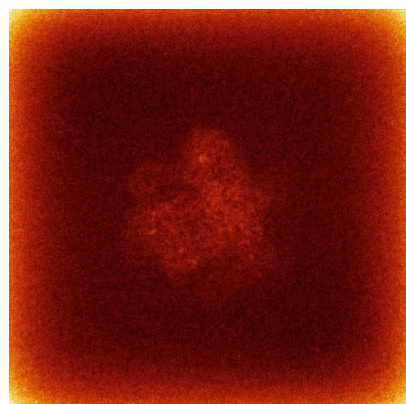


Y

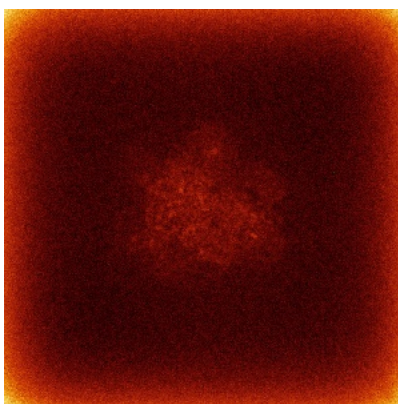


Z

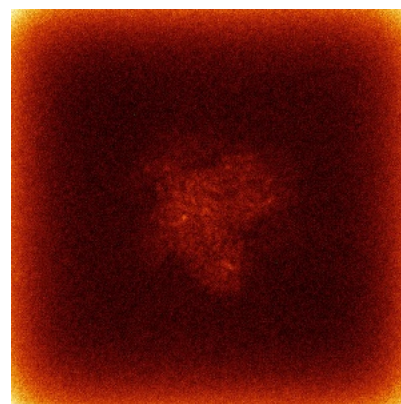
6.4.2 Raw map



X



Y

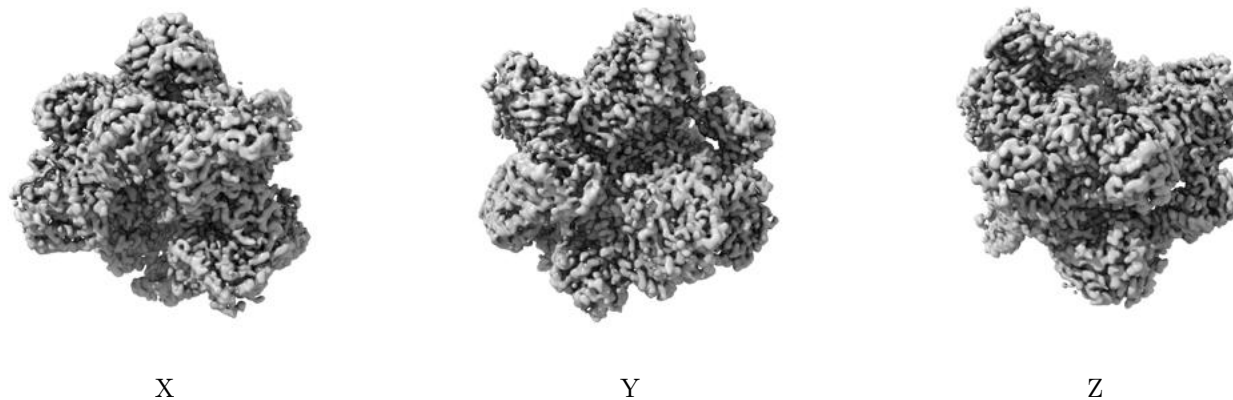


Z

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.

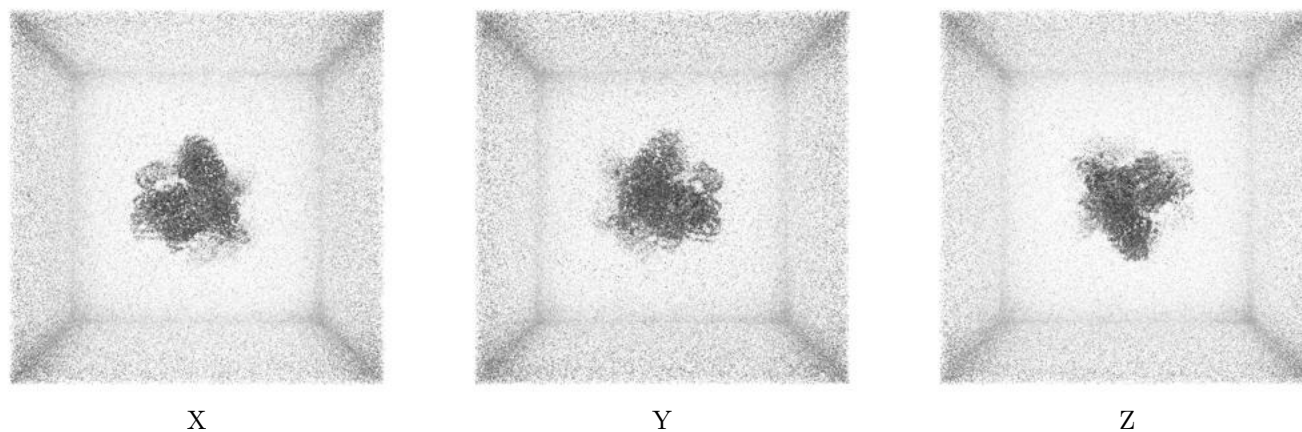
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0142. 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.

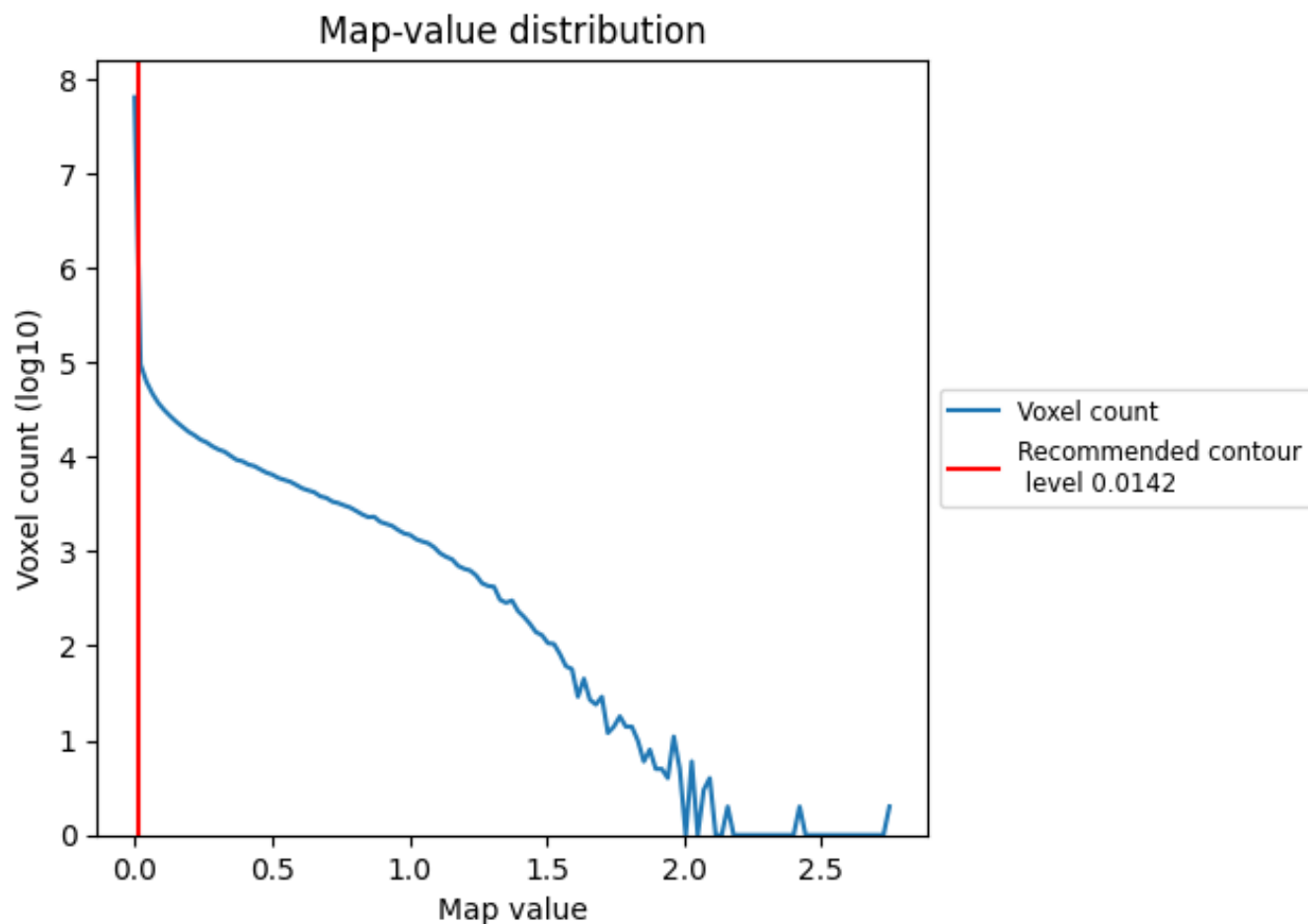
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

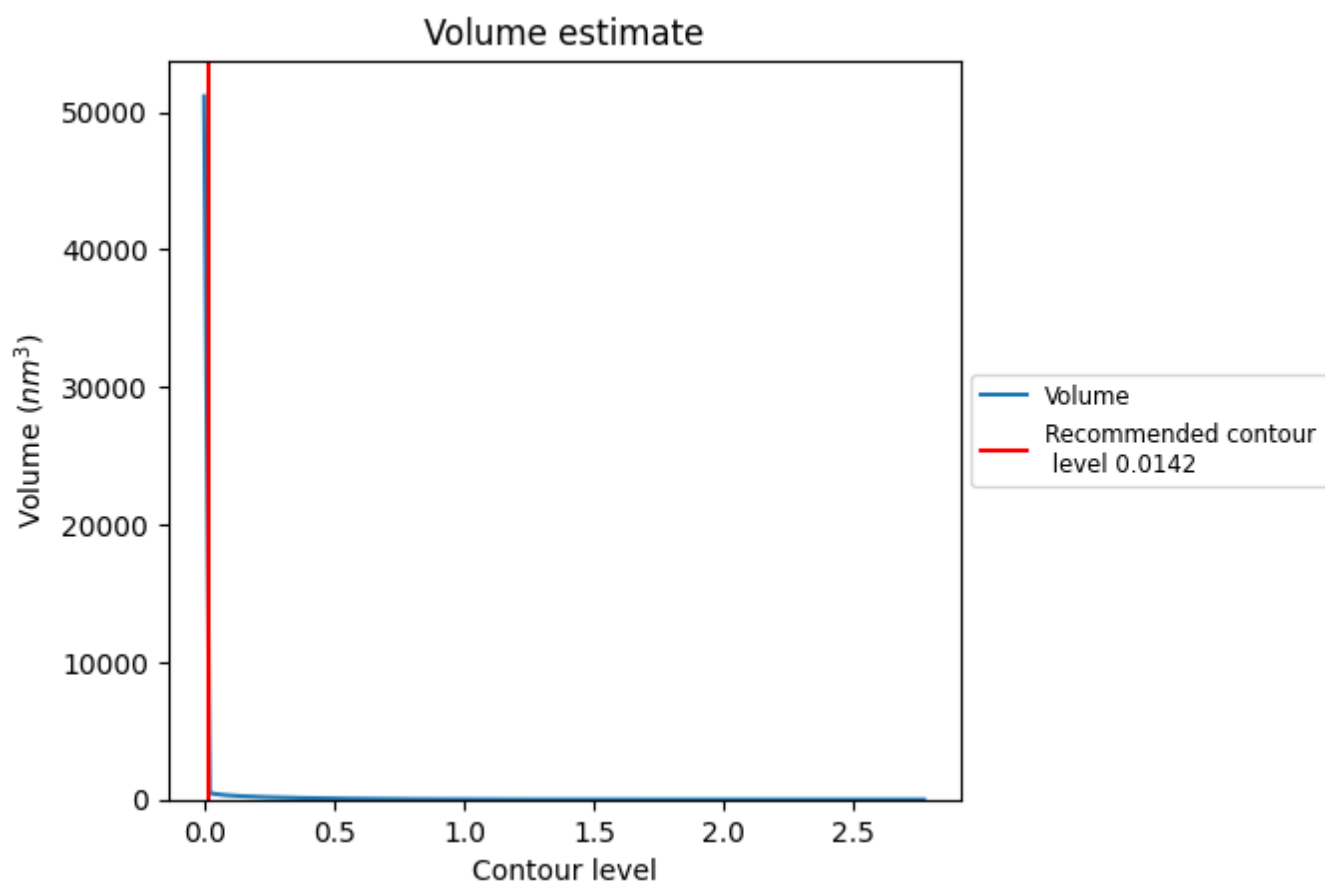
This section contains the results of statistical analysis of the map.

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.

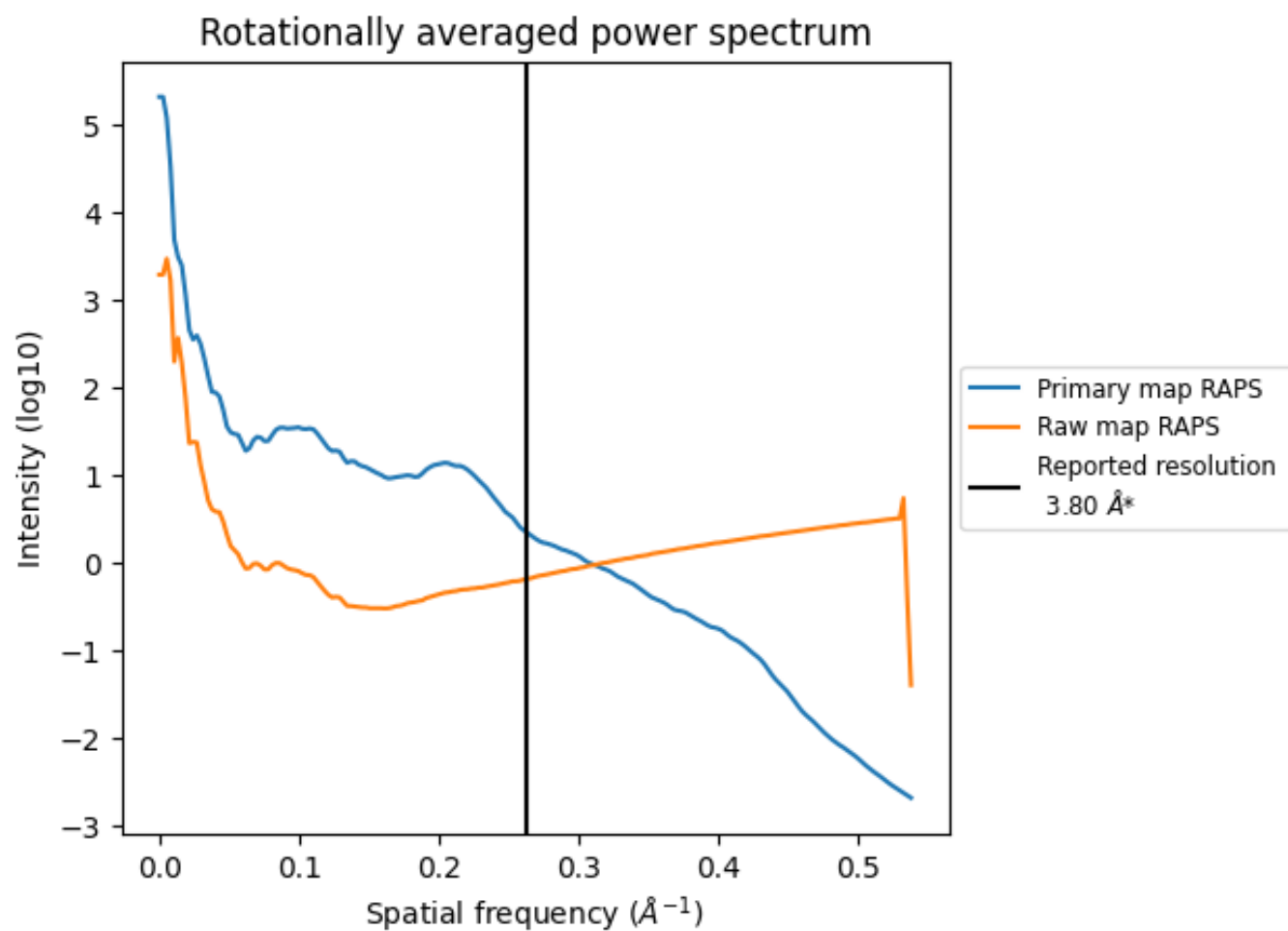
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 13898 nm³; this corresponds to an approximate mass of 12554 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 ⓘ

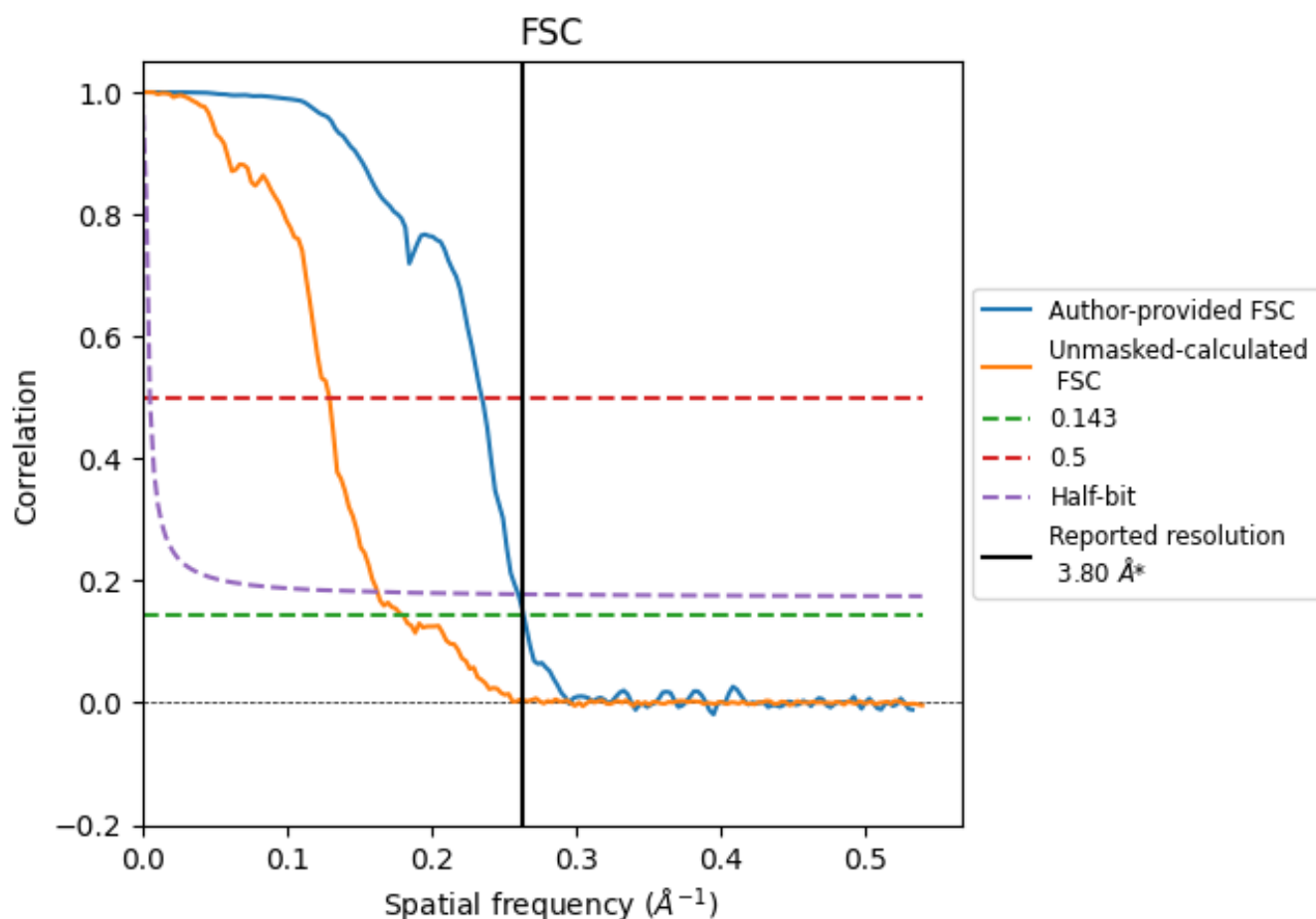


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

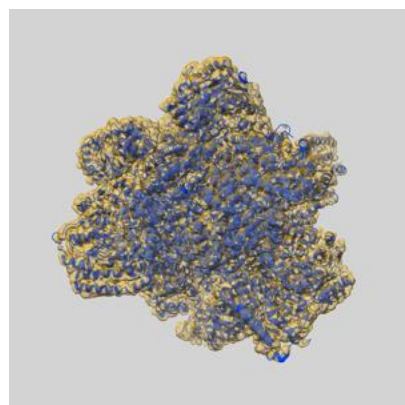
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.80	4.26	3.85
Unmasked-calculated*	5.55	7.73	6.15

*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 5.55 differs from the reported value 3.8 by more than 10 %

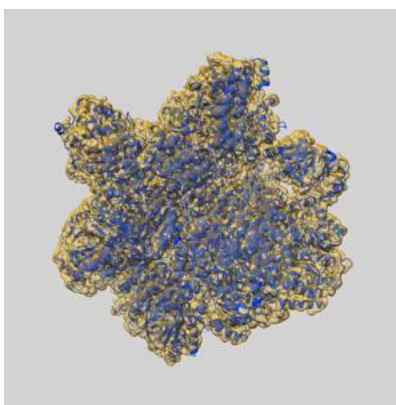
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-78079 and PDB model 37CY. Per-residue inclusion information can be found in section 3 on page 14.

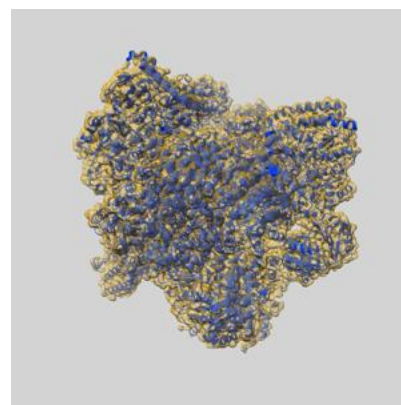
9.1 Map-model overlay [i](#)



X



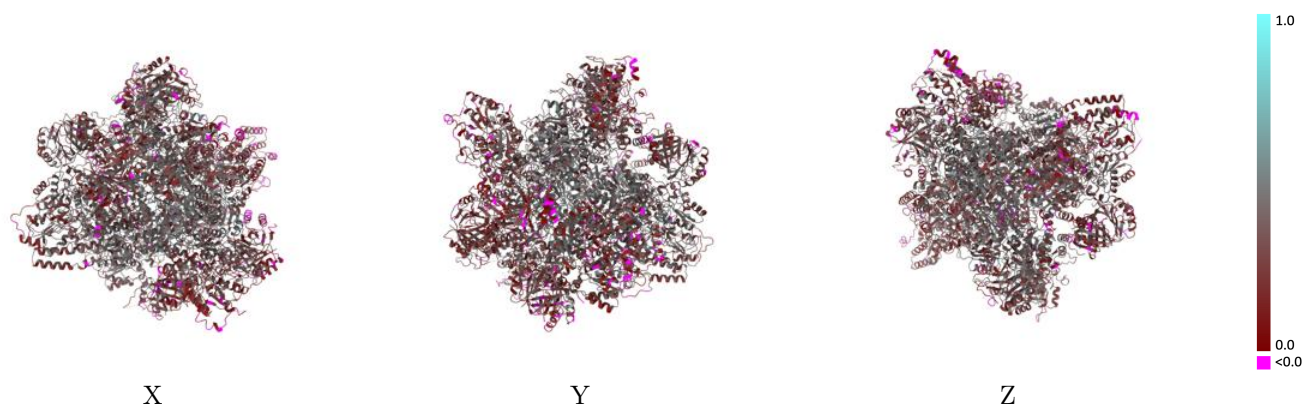
Y



Z

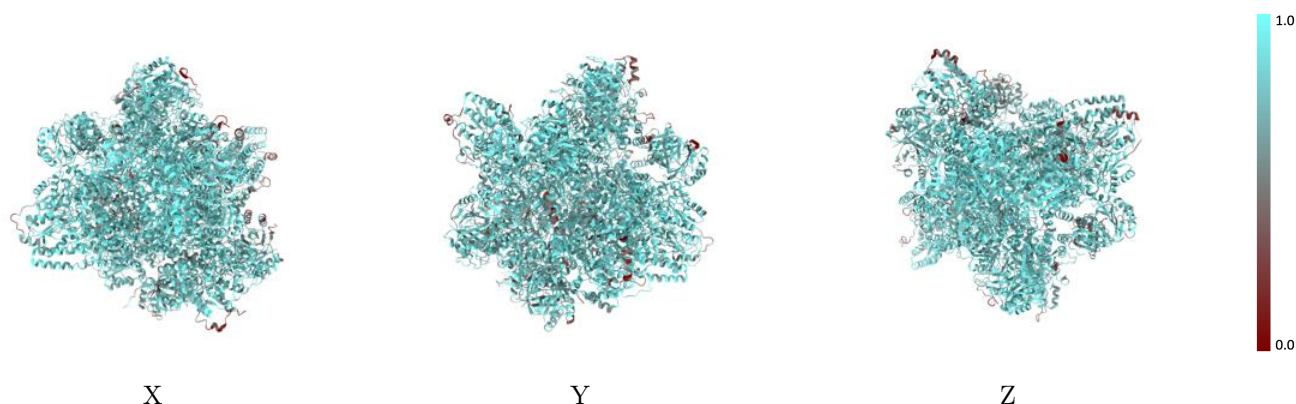
The images above show the 3D surface view of the map at the recommended contour level 0.0142 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



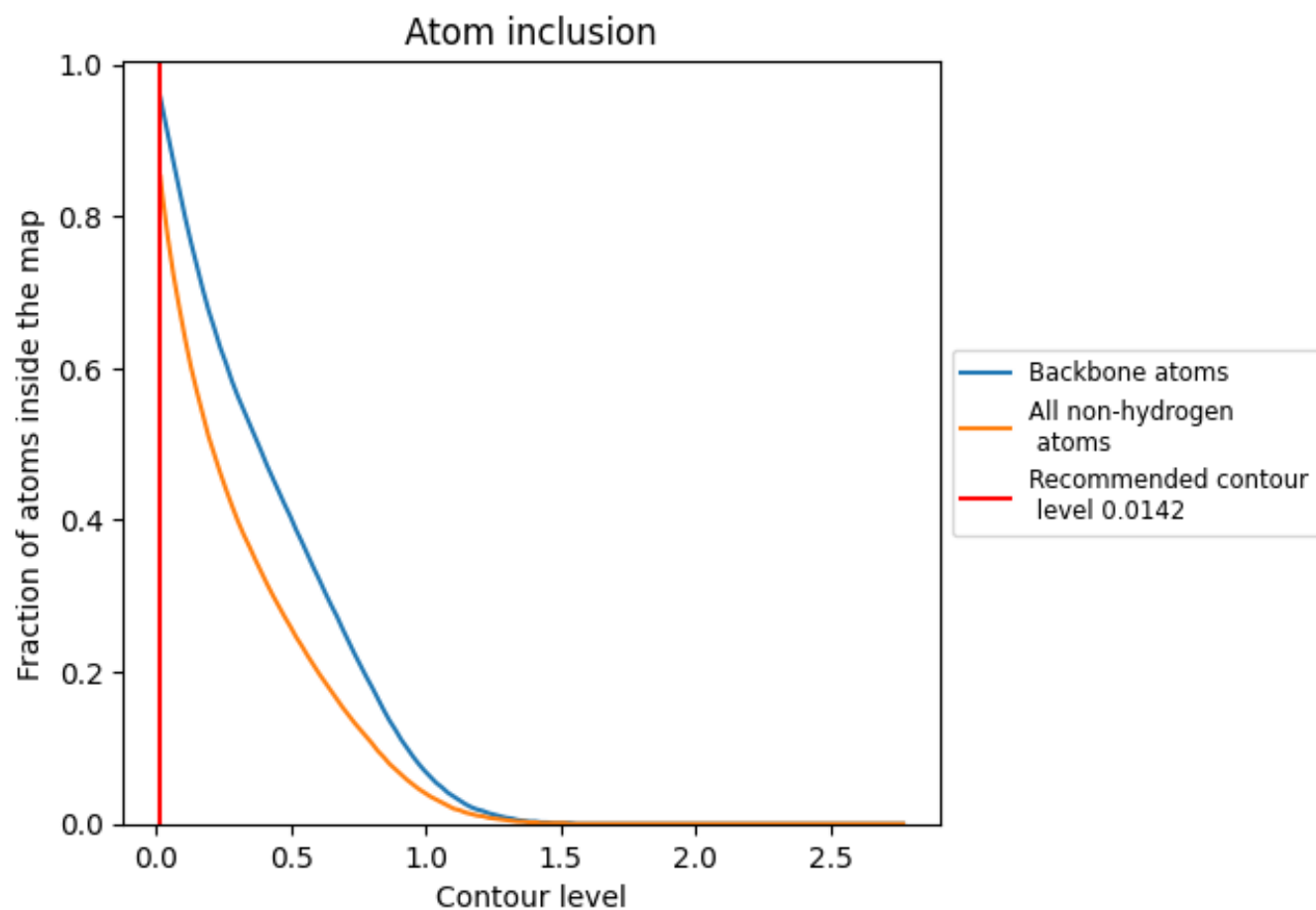
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0142).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 85% 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 (0.0142) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8520	 0.3340
A	 0.7730	 0.2630
B	 0.9320	 0.4110
C	 0.8780	 0.3550
D	 0.9470	 0.4220
E	 0.7640	 0.2800
F	 0.8220	 0.2920
G	 0.7740	 0.2430
H	 0.7580	 0.2410
I	 0.7030	 0.1900
J	 0.7920	 0.2680
K	 0.8350	 0.3060
L	 0.8810	 0.3560
M	 0.9380	 0.4190
N	 0.9480	 0.4240
O	 0.8290	 0.3200
P	 0.8230	 0.3310
Q	 0.7760	 0.2370
R	 0.7860	 0.2780
S	 0.7490	 0.2120
T	 0.7620	 0.2590
U	 0.7900	 0.2700
V	 0.8110	 0.2990
W	 0.9340	 0.4150
X	 0.9350	 0.4130
Y	 0.7730	 0.2650
Z	 0.7380	 0.2540
a	 0.7530	 0.2200
b	 0.7560	 0.2560
c	 0.5830	 0.1300
d	 0.6700	 0.2120

