



## Full wwPDB EM Validation Report ⓘ

May 18, 2025 – 03:16 PM EDT

PDB ID : 6AP1 / pdb\_00006ap1  
EMDB ID : EMD-8887  
Title : Vps4p-Vta1p complex with peptide binding to the central pore of Vps4p  
Authors : Han, H.; Monroe, N.; Shen, P.; Sundquist, W.I.; Hill, C.P.  
Deposited on : 2017-08-16  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

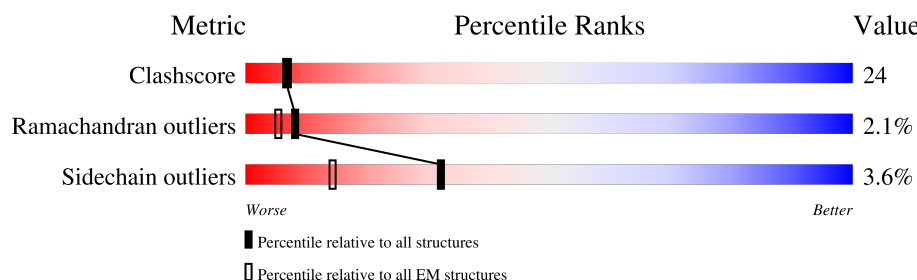
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	519	<div> <div>33%</div> <div>48%</div> <div>10%</div> <div>39%</div> </div>
1	B	519	<div> <div>18%</div> <div>50%</div> <div>11%</div> <div>38%</div> </div>
1	C	519	<div> <div>18%</div> <div>50%</div> <div>10%</div> <div>38%</div> </div>
1	D	519	<div> <div>23%</div> <div>51%</div> <div>9%</div> <div>38%</div> </div>
1	E	519	<div> <div>41%</div> <div>45%</div> <div>12%</div> <div>41%</div> </div>
1	F	519	<div> <div>59%</div> <div>34%</div> <div>22%</div> <div>41%</div> </div>
2	G	10	<div> <div>60%</div> <div>90%</div> <div>10%</div> </div>
3	H	330	<div> <div>13%</div> <div>8%</div> <div>87%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	330	<div><div><div></div><div></div><div></div></div><div>13% 7% 5% .</div><div>87%</div></div>
3	J	330	<div><div><div></div><div></div><div></div></div><div>13% . 8% .</div><div>87%</div></div>
3	K	330	<div><div><div></div><div></div><div></div></div><div>13% 7% . .</div><div>87%</div></div>
3	L	330	<div><div><div></div><div></div><div></div></div><div>13% . 7% .</div><div>87%</div></div>
3	M	330	<div><div><div></div><div></div><div></div></div><div>13% 7% 5% .</div><div>87%</div></div>
3	N	330	<div><div><div></div><div></div><div></div></div><div>13% . 8% .</div><div>87%</div></div>
3	O	330	<div><div><div></div><div></div><div></div></div><div>13% 7% 5% .</div><div>87%</div></div>
3	P	330	<div><div><div></div><div></div><div></div></div><div>13% . 7% .</div><div>87%</div></div>
3	Q	330	<div><div><div></div><div></div><div></div></div><div>13% 7% 5% .</div><div>87%</div></div>
3	R	330	<div><div><div></div><div></div><div></div></div><div>13% . 8% .</div><div>87%</div></div>
3	S	330	<div><div><div></div><div></div><div></div></div><div>13% 7% . .</div><div>87%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18838 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 Vacuolar protein sorting-associated protein 4, Protein hcp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	314	Total	C	N	O	S	0	0
			2427	1530	414	474	9		
1	B	322	Total	C	N	O	S	0	0
			2491	1568	427	487	9		
1	C	322	Total	C	N	O	S	0	0
			2491	1568	427	487	9		
1	D	322	Total	C	N	O	S	0	0
			2491	1568	427	487	9		
1	E	304	Total	C	N	O	S	0	0
			2360	1489	401	461	9		
1	F	308	Total	C	N	O	S	0	0
			2387	1507	405	466	9		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	GLY	-	expression tag	UNP P52917
A	438	GLY	-	linker	UNP P52917
A	439	GLY	-	linker	UNP P52917
A	440	GLY	-	linker	UNP P52917
A	441	GLY	-	linker	UNP P52917
A	442	SER	-	linker	UNP P52917
A	443	GLY	-	linker	UNP P52917
A	444	GLY	-	linker	UNP P52917
A	445	GLY	-	linker	UNP P52917
A	446	GLY	-	linker	UNP P52917
A	447	SER	-	linker	UNP P52917
A	448	GLY	-	linker	UNP P52917
A	449	GLY	-	linker	UNP P52917
A	450	GLY	-	linker	UNP P52917
A	451	GLY	-	linker	UNP P52917
A	452	SER	-	linker	UNP P52917
A	453	GLY	-	linker	UNP P52917
A	454	GLY	-	linker	UNP P52917

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Chain	Residue	Modelled	Actual	Comment	Reference
A	455	GLY	-	linker	UNP P52917
A	618	GLY	-	expression tag	UNP Q9I747
B	100	GLY	-	expression tag	UNP P52917
B	438	GLY	-	linker	UNP P52917
B	439	GLY	-	linker	UNP P52917
B	440	GLY	-	linker	UNP P52917
B	441	GLY	-	linker	UNP P52917
B	442	SER	-	linker	UNP P52917
B	443	GLY	-	linker	UNP P52917
B	444	GLY	-	linker	UNP P52917
B	445	GLY	-	linker	UNP P52917
B	446	GLY	-	linker	UNP P52917
B	447	SER	-	linker	UNP P52917
B	448	GLY	-	linker	UNP P52917
B	449	GLY	-	linker	UNP P52917
B	450	GLY	-	linker	UNP P52917
B	451	GLY	-	linker	UNP P52917
B	452	SER	-	linker	UNP P52917
B	453	GLY	-	linker	UNP P52917
B	454	GLY	-	linker	UNP P52917
B	455	GLY	-	linker	UNP P52917
B	618	GLY	-	expression tag	UNP Q9I747
C	100	GLY	-	expression tag	UNP P52917
C	438	GLY	-	linker	UNP P52917
C	439	GLY	-	linker	UNP P52917
C	440	GLY	-	linker	UNP P52917
C	441	GLY	-	linker	UNP P52917
C	442	SER	-	linker	UNP P52917
C	443	GLY	-	linker	UNP P52917
C	444	GLY	-	linker	UNP P52917
C	445	GLY	-	linker	UNP P52917
C	446	GLY	-	linker	UNP P52917
C	447	SER	-	linker	UNP P52917
C	448	GLY	-	linker	UNP P52917
C	449	GLY	-	linker	UNP P52917
C	450	GLY	-	linker	UNP P52917
C	451	GLY	-	linker	UNP P52917
C	452	SER	-	linker	UNP P52917
C	453	GLY	-	linker	UNP P52917
C	454	GLY	-	linker	UNP P52917
C	455	GLY	-	linker	UNP P52917
C	618	GLY	-	expression tag	UNP Q9I747

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Chain	Residue	Modelled	Actual	Comment	Reference
D	100	GLY	-	expression tag	UNP P52917
D	438	GLY	-	linker	UNP P52917
D	439	GLY	-	linker	UNP P52917
D	440	GLY	-	linker	UNP P52917
D	441	GLY	-	linker	UNP P52917
D	442	SER	-	linker	UNP P52917
D	443	GLY	-	linker	UNP P52917
D	444	GLY	-	linker	UNP P52917
D	445	GLY	-	linker	UNP P52917
D	446	GLY	-	linker	UNP P52917
D	447	SER	-	linker	UNP P52917
D	448	GLY	-	linker	UNP P52917
D	449	GLY	-	linker	UNP P52917
D	450	GLY	-	linker	UNP P52917
D	451	GLY	-	linker	UNP P52917
D	452	SER	-	linker	UNP P52917
D	453	GLY	-	linker	UNP P52917
D	454	GLY	-	linker	UNP P52917
D	455	GLY	-	linker	UNP P52917
D	618	GLY	-	expression tag	UNP Q9I747
E	100	GLY	-	expression tag	UNP P52917
E	438	GLY	-	linker	UNP P52917
E	439	GLY	-	linker	UNP P52917
E	440	GLY	-	linker	UNP P52917
E	441	GLY	-	linker	UNP P52917
E	442	SER	-	linker	UNP P52917
E	443	GLY	-	linker	UNP P52917
E	444	GLY	-	linker	UNP P52917
E	445	GLY	-	linker	UNP P52917
E	446	GLY	-	linker	UNP P52917
E	447	SER	-	linker	UNP P52917
E	448	GLY	-	linker	UNP P52917
E	449	GLY	-	linker	UNP P52917
E	450	GLY	-	linker	UNP P52917
E	451	GLY	-	linker	UNP P52917
E	452	SER	-	linker	UNP P52917
E	453	GLY	-	linker	UNP P52917
E	454	GLY	-	linker	UNP P52917
E	455	GLY	-	linker	UNP P52917
E	618	GLY	-	expression tag	UNP Q9I747
F	100	GLY	-	expression tag	UNP P52917
F	438	GLY	-	linker	UNP P52917

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Chain	Residue	Modelled	Actual	Comment	Reference
F	439	GLY	-	linker	UNP P52917
F	440	GLY	-	linker	UNP P52917
F	441	GLY	-	linker	UNP P52917
F	442	SER	-	linker	UNP P52917
F	443	GLY	-	linker	UNP P52917
F	444	GLY	-	linker	UNP P52917
F	445	GLY	-	linker	UNP P52917
F	446	GLY	-	linker	UNP P52917
F	447	SER	-	linker	UNP P52917
F	448	GLY	-	linker	UNP P52917
F	449	GLY	-	linker	UNP P52917
F	450	GLY	-	linker	UNP P52917
F	451	GLY	-	linker	UNP P52917
F	452	SER	-	linker	UNP P52917
F	453	GLY	-	linker	UNP P52917
F	454	GLY	-	linker	UNP P52917
F	455	GLY	-	linker	UNP P52917
F	618	GLY	-	expression tag	UNP Q9I747

- Molecule 2 is a protein called ACE-ASP-GLU-ILE-VAL-ASN-LYS-VAL-LEU-NH2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	10	Total	C	N	O	1	1
			68	43	11	14		

- Molecule 3 is a protein called Vacuolar protein sorting-associated protein VTA1.

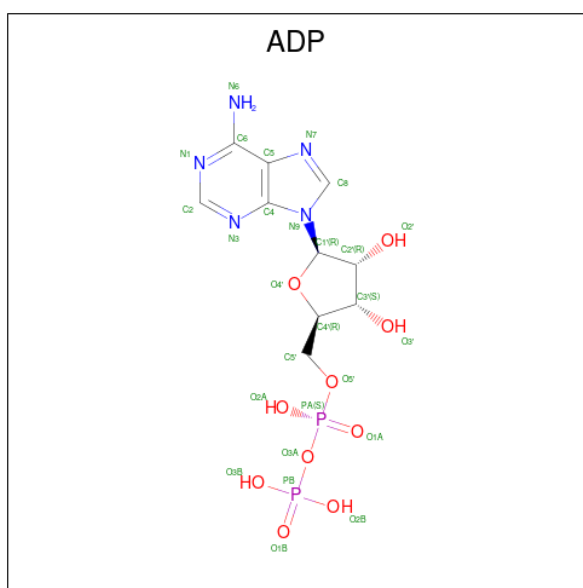
Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	42	Total	C	N	O	0	0
			331	209	54	68		
3	I	42	Total	C	N	O	0	0
			331	209	54	68		
3	J	42	Total	C	N	O	0	0
			331	209	54	68		
3	K	42	Total	C	N	O	0	0
			331	209	54	68		
3	L	42	Total	C	N	O	0	0
			331	209	54	68		
3	M	42	Total	C	N	O	0	0
			331	209	54	68		
3	N	42	Total	C	N	O	0	0
			331	209	54	68		

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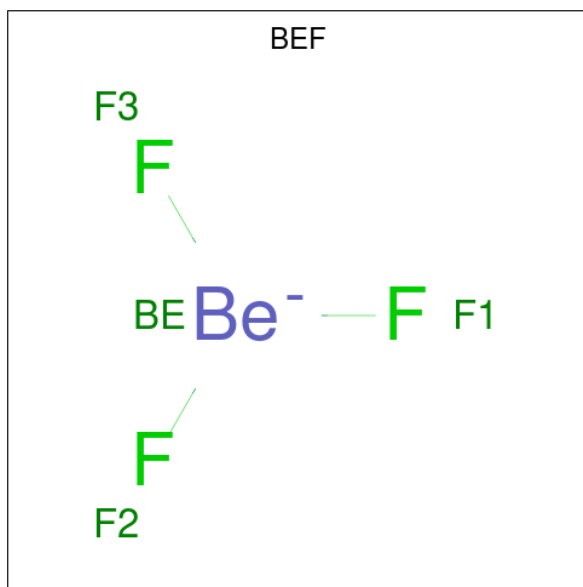
Mol	Chain	Residues	Atoms				AltConf	Trace
3	O	42	Total	C	N	O	0	0
			331	209	54	68		
3	P	42	Total	C	N	O	0	0
			331	209	54	68		
3	Q	42	Total	C	N	O	0	0
			331	209	54	68		
3	R	42	Total	C	N	O	0	0
			331	209	54	68		
3	S	42	Total	C	N	O	0	0
			331	209	54	68		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula:  $BeF_3$ ).

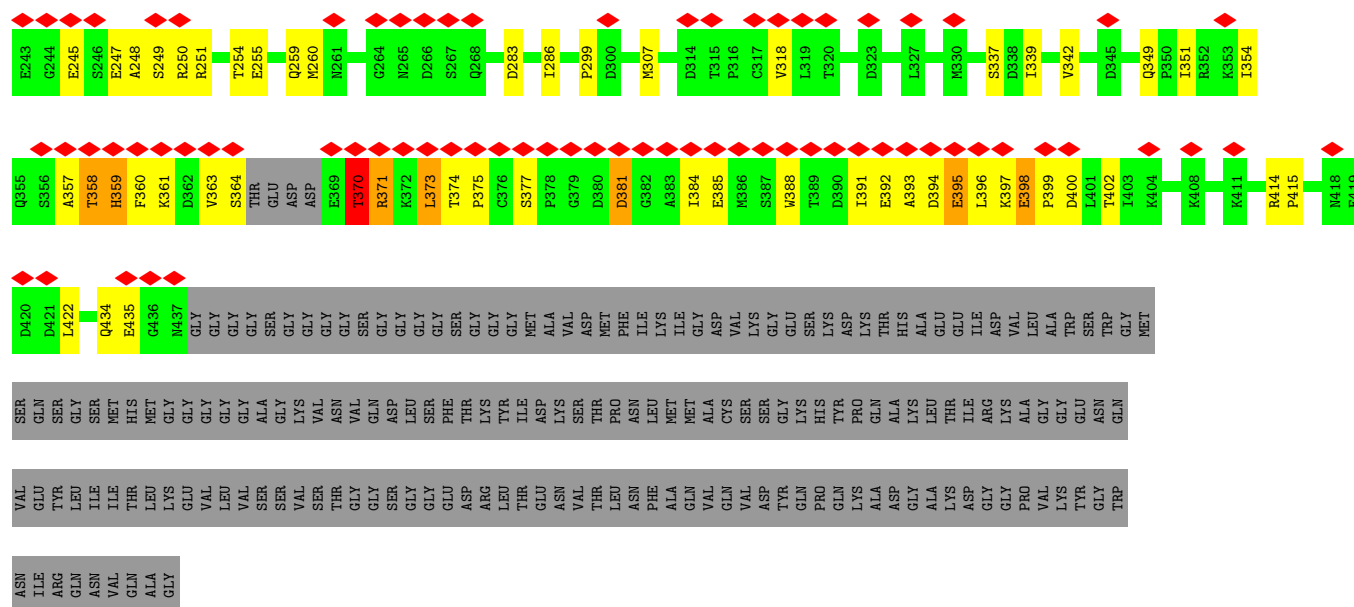


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Be	F	0
			4	1	3	
5	B	1	Total	Be	F	0
			4	1	3	
5	C	1	Total	Be	F	0
			4	1	3	

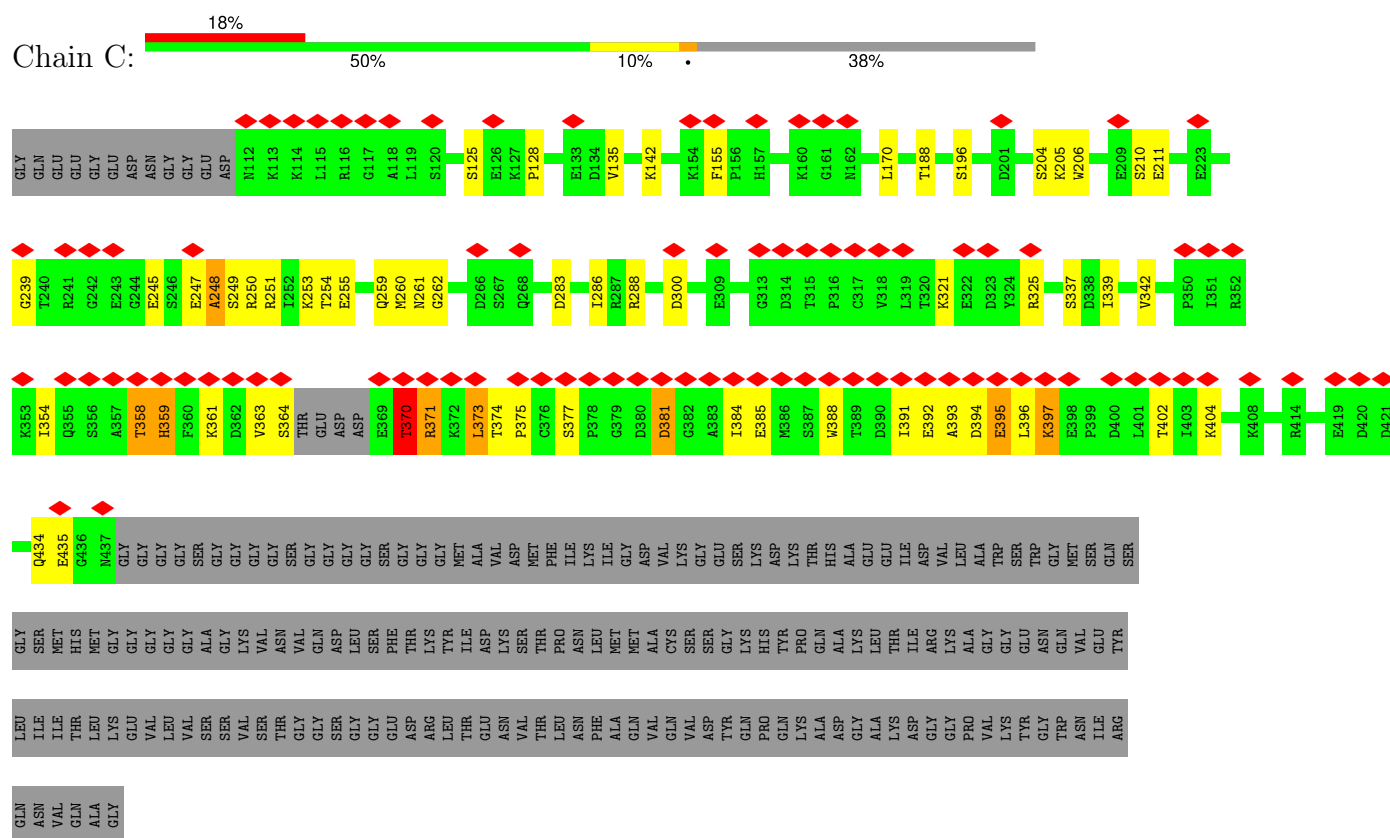
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	
6	B	1	Total	Mg	0
			1	1	
6	C	1	Total	Mg	0
			1	1	
6	D	1	Total	Mg	0
			1	1	



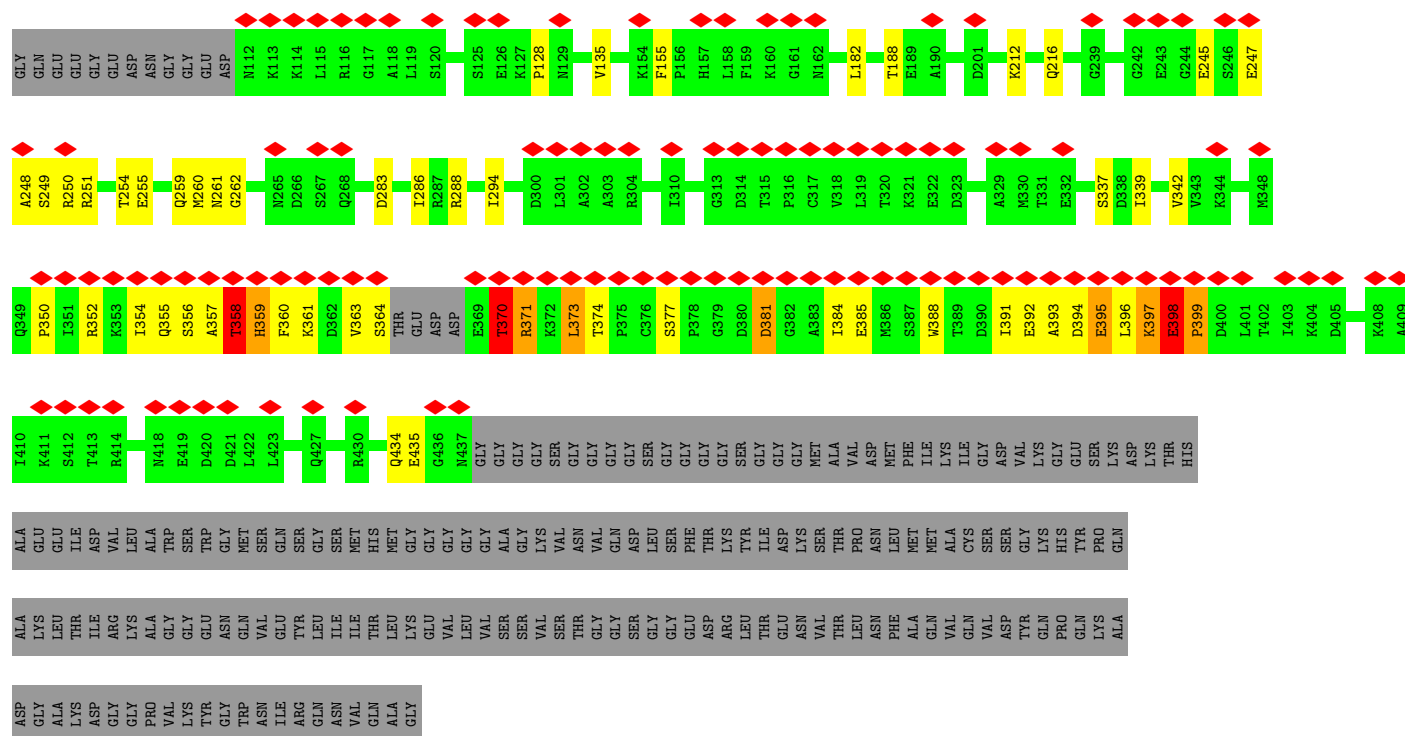


- Molecule 1: Vacuolar protein sorting-associated protein 4,Protein hcp1

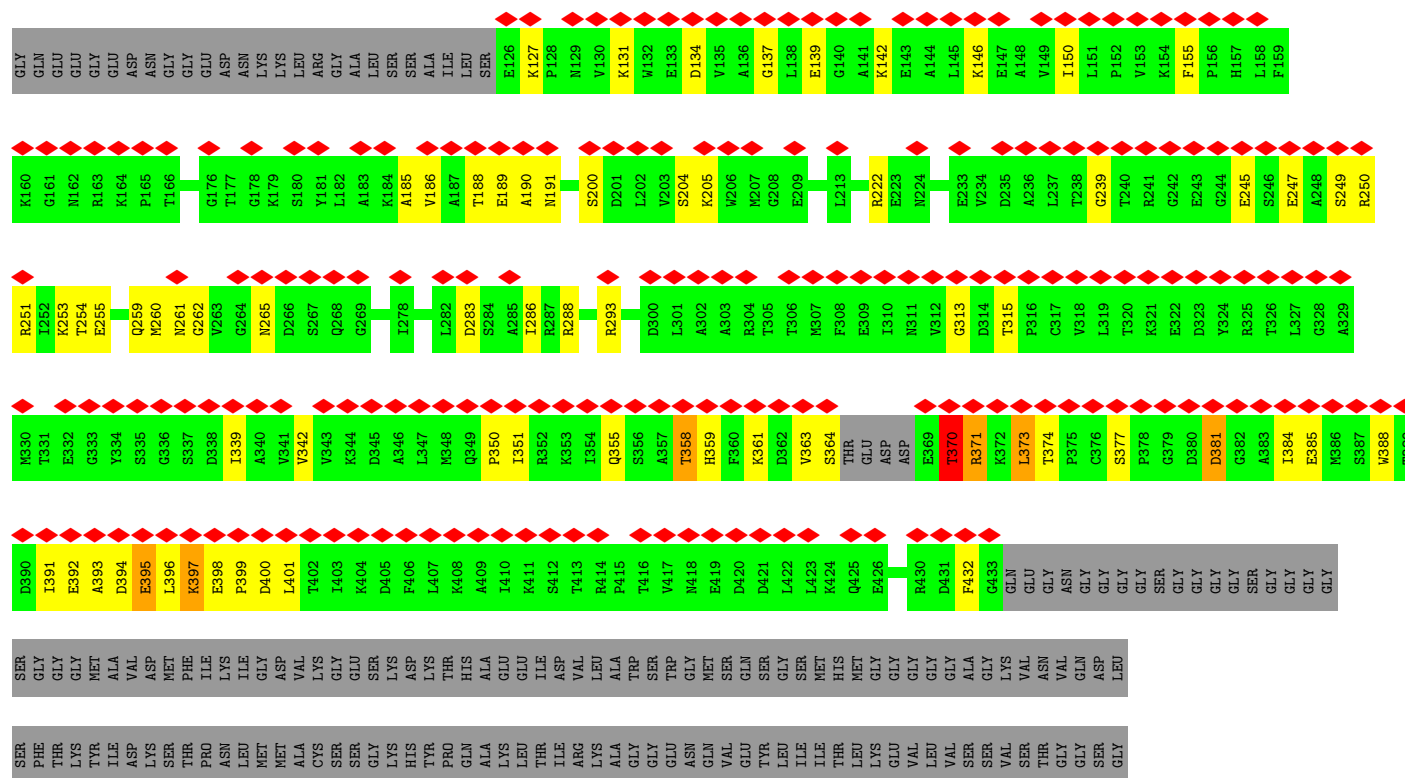
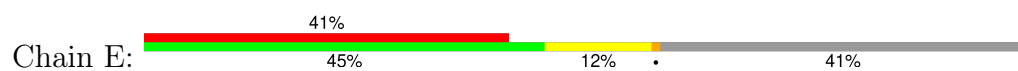


- Molecule 1: Vacuolar protein sorting-associated protein 4,Protein hcp1

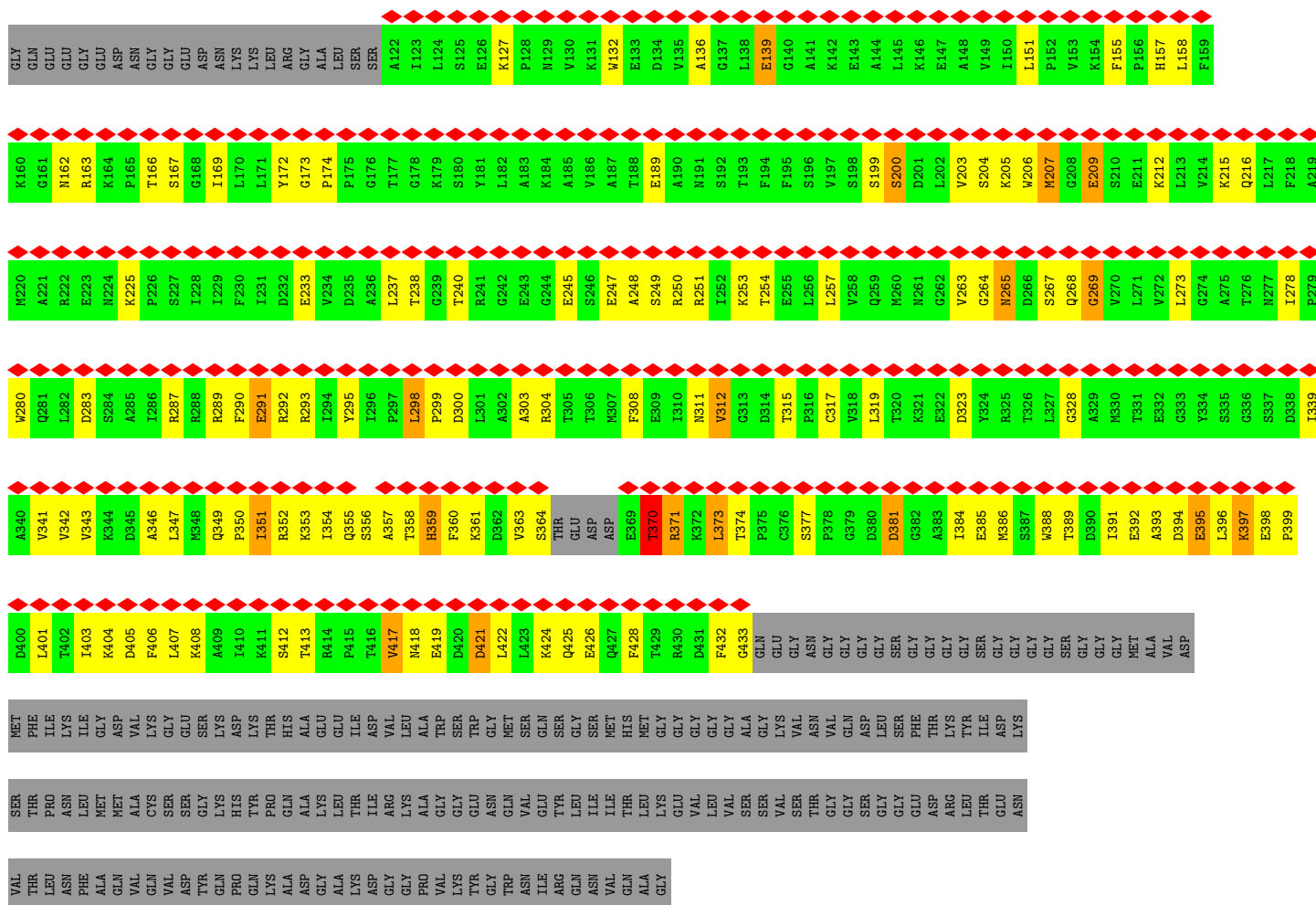
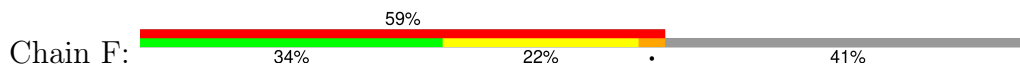




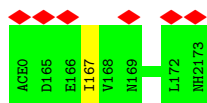
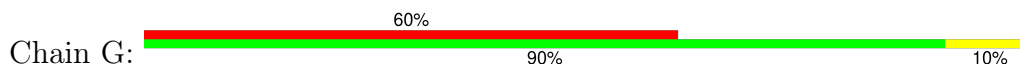
● Molecule 1: Vacuolar protein sorting-associated protein 4, Protein hcp1



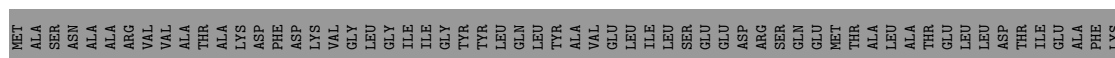
- Molecule 1: Vacuolar protein sorting-associated protein 4, Protein hcp1



- Molecule 2: ACE-ASP-GLU-ILE-VAL-ASN-LYS-VAL-LEU-NH<sub>2</sub>

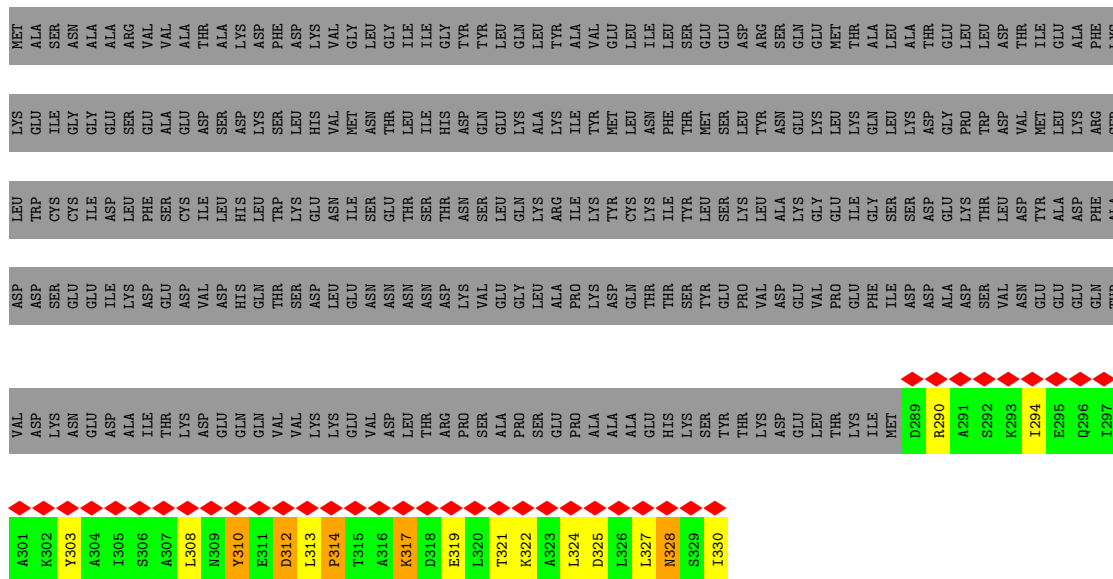


- Molecule 3: Vacuolar protein sorting-associated protein VTA1

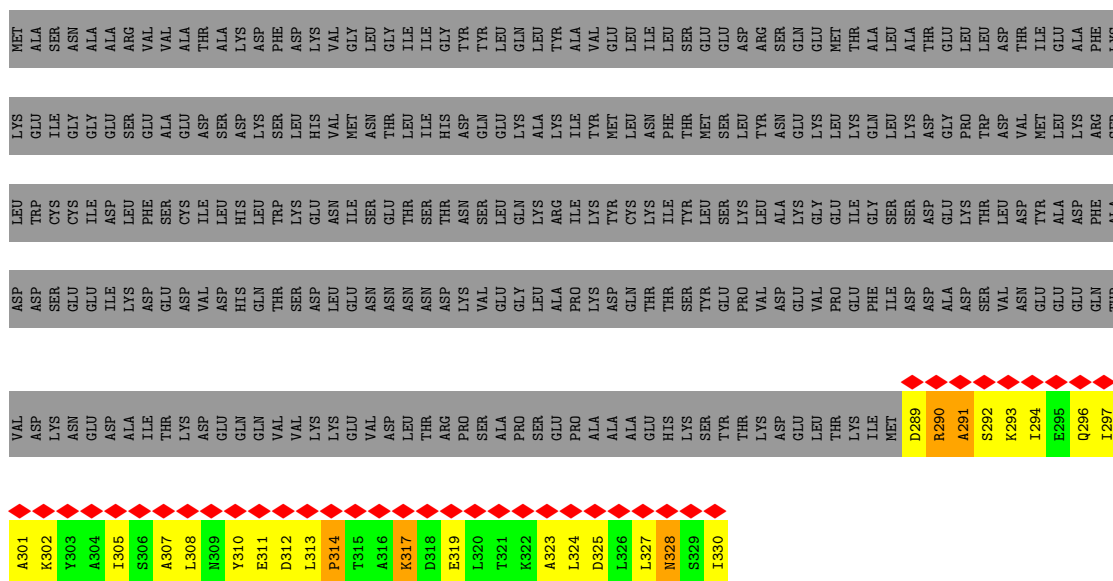




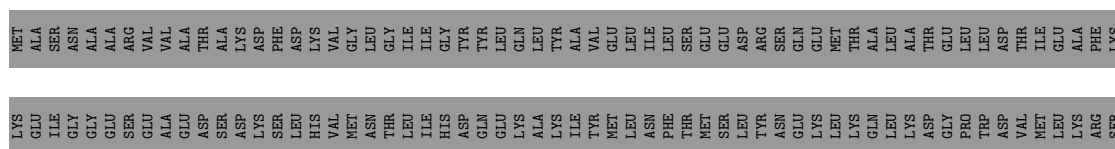
- Molecule 3: Vacuolar protein sorting-associated protein VTA1



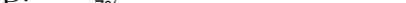
- Molecule 3: Vacuolar protein sorting-associated protein VTA1



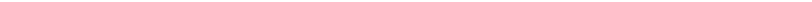
- Molecule 3: Vacuolar protein sorting-associated protein VTA1



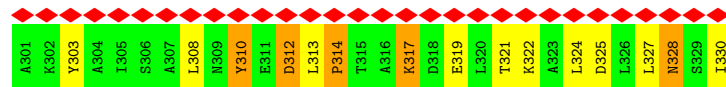
A301	K302	Y303	A304	S306	A307	L308	N309	Y310	E311	D312	L313	P314	T315	A316	K317	D318	E319	L320	T321	K322	A323	L324	D325	L326	L327	N328	S329	T330
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Chain P:  13% 7% 87%

A301	K302	Y303	A304	I305	S306	A307	L308	N309	Y310	E311	D312	L313	P314	T315	A316	K317	D318	E319	L320	T321	K322	A323	L324	D325	L326	L327	N328	S329	I330
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Chain Q:  13% 7% 5% 87%

VAL	ASP	LVS	ASN	GLU	ASP	ASP	ALA	ILE	THR	LVS	LVS	GLU	GLN	GLN	VAL	VAL	LVS	LVS	GLU	VAL	ASP	LEU	THR	ARG	PRO	ALA	SER	ALA	PRO	GLU	PRO	ALA	ALA	ALA	GLU	HIS	LVS	SER	SER	TYR	THR	THR	ILE	ILE	MET	D289	R290	A291	S292	K293	I294	E295	Q296	I297	Q298	K299	I300
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82225	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.55	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.388	Depositor
Minimum map value	-0.195	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0749	Depositor
Map size (Å)	280.6016, 280.6016, 280.6016	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0961, 1.0961, 1.0961	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BEF, ACE, ADP, NH2

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	0.70	0/2468	0.90	2/3334 (0.1%)
1	B	0.77	0/2532	0.88	4/3418 (0.1%)
1	C	0.78	0/2532	0.93	6/3418 (0.2%)
1	D	0.75	0/2532	0.89	5/3418 (0.1%)
1	E	0.71	0/2401	0.91	2/3244 (0.1%)
1	F	0.77	0/2428	1.00	7/3281 (0.2%)
2	G	0.92	0/64	0.97	0/86
3	H	0.71	0/333	1.19	5/447 (1.1%)
3	I	0.71	0/333	1.13	4/447 (0.9%)
3	J	0.72	0/333	1.19	5/447 (1.1%)
3	K	0.70	0/333	1.13	4/447 (0.9%)
3	L	0.71	0/333	1.19	5/447 (1.1%)
3	M	0.72	0/333	1.13	4/447 (0.9%)
3	N	0.72	0/333	1.19	5/447 (1.1%)
3	O	0.71	0/333	1.13	4/447 (0.9%)
3	P	0.71	0/333	1.19	5/447 (1.1%)
3	Q	0.71	0/333	1.13	4/447 (0.9%)
3	R	0.71	0/333	1.20	5/447 (1.1%)
3	S	0.71	0/333	1.13	4/447 (0.9%)
All	All	0.74	0/18953	0.98	80/25563 (0.3%)

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	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	298	LEU	CA-C-N	8.25	130.15	119.84
1	F	298	LEU	C-N-CA	8.25	130.15	119.84
1	D	398	GLU	CA-C-N	8.11	129.97	119.84
1	D	398	GLU	C-N-CA	8.11	129.97	119.84
1	F	269	GLY	N-CA-C	7.78	126.06	115.32
1	B	358	THR	N-CA-C	-7.34	98.58	109.15
3	H	291	ALA	N-CA-C	-7.28	103.33	111.71
3	J	291	ALA	N-CA-C	-7.22	103.41	111.71
3	R	291	ALA	N-CA-C	-7.20	103.43	111.71
3	N	291	ALA	N-CA-C	-7.19	103.44	111.71
3	L	291	ALA	N-CA-C	-7.16	103.48	111.71
3	P	291	ALA	N-CA-C	-7.14	103.50	111.71
3	Q	328	ASN	N-CA-C	-6.71	105.25	113.50
3	M	328	ASN	N-CA-C	-6.69	105.27	113.50
3	O	328	ASN	N-CA-C	-6.64	105.33	113.50
3	K	328	ASN	N-CA-C	-6.64	105.34	113.50
3	S	328	ASN	N-CA-C	-6.62	105.36	113.50
3	I	328	ASN	N-CA-C	-6.61	105.37	113.50
3	R	328	ASN	N-CA-C	-6.60	105.38	113.50
1	C	358	THR	N-CA-C	-6.58	99.67	109.15
3	P	328	ASN	N-CA-C	-6.56	105.44	113.50
3	H	328	ASN	N-CA-C	-6.54	105.45	113.50
3	J	328	ASN	N-CA-C	-6.51	105.49	113.50
3	N	328	ASN	N-CA-C	-6.51	105.49	113.50
3	L	328	ASN	N-CA-C	-6.50	105.50	113.50
1	F	264	GLY	N-CA-C	6.46	120.30	112.49
3	N	297	ILE	N-CA-C	-6.38	104.53	110.53
3	R	297	ILE	N-CA-C	-6.33	104.58	110.53
3	L	297	ILE	N-CA-C	-6.32	104.59	110.53
3	H	297	ILE	N-CA-C	-6.26	104.65	110.53
3	J	297	ILE	N-CA-C	-6.24	104.66	110.53
3	P	297	ILE	N-CA-C	-6.22	104.68	110.53
3	M	303	TYR	CA-C-N	6.11	128.79	120.54
3	M	303	TYR	C-N-CA	6.11	128.79	120.54
3	I	303	TYR	CA-C-N	6.06	128.72	120.54
3	I	303	TYR	C-N-CA	6.06	128.72	120.54
3	S	303	TYR	CA-C-N	6.02	128.67	120.54
3	S	303	TYR	C-N-CA	6.02	128.67	120.54
3	O	303	TYR	CA-C-N	6.00	128.64	120.54
3	O	303	TYR	C-N-CA	6.00	128.64	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	303	TYR	CA-C-N	6.00	128.64	120.54
3	Q	303	TYR	C-N-CA	6.00	128.64	120.54
3	K	303	TYR	CA-C-N	5.95	128.57	120.54
3	K	303	TYR	C-N-CA	5.95	128.57	120.54
1	F	356	SER	N-CA-C	5.93	118.58	108.02
1	D	358	THR	N-CA-C	-5.92	98.26	108.56
1	A	248	ALA	CA-C-N	-5.86	110.56	120.58
1	A	248	ALA	C-N-CA	-5.86	110.56	120.58
1	F	265	ASN	N-CA-C	-5.84	104.91	111.28
1	B	349	GLN	N-CA-C	5.73	122.46	109.81
1	C	170	LEU	CA-C-N	-5.42	115.51	123.00
1	C	170	LEU	C-N-CA	-5.42	115.51	123.00
1	C	260	MET	CA-C-N	-5.37	113.89	122.17
1	C	260	MET	C-N-CA	-5.37	113.89	122.17
1	E	260	MET	CA-C-N	-5.36	113.92	122.17
1	E	260	MET	C-N-CA	-5.36	113.92	122.17
3	L	302	LYS	N-CA-C	-5.36	104.33	111.24
1	D	260	MET	CA-C-N	-5.35	113.93	122.17
1	D	260	MET	C-N-CA	-5.35	113.93	122.17
1	B	260	MET	CA-C-N	-5.33	113.97	122.17
1	B	260	MET	C-N-CA	-5.33	113.97	122.17
3	R	302	LYS	N-CA-C	-5.31	104.39	111.24
3	P	302	LYS	N-CA-C	-5.30	104.40	111.24
3	H	302	LYS	N-CA-C	-5.30	104.40	111.24
3	H	310	TYR	N-CA-C	-5.27	104.59	112.54
1	F	421	ASP	CB-CA-C	-5.25	101.92	110.85
3	J	302	LYS	N-CA-C	-5.25	104.47	111.24
3	K	310	TYR	N-CA-C	-5.25	104.62	112.54
3	R	310	TYR	N-CA-C	-5.25	104.62	112.54
3	I	310	TYR	N-CA-C	-5.21	104.67	112.54
3	N	302	LYS	N-CA-C	-5.20	104.53	111.24
3	P	310	TYR	N-CA-C	-5.19	104.70	112.54
3	Q	310	TYR	N-CA-C	-5.18	104.71	112.54
3	L	310	TYR	N-CA-C	-5.18	104.72	112.54
3	J	310	TYR	N-CA-C	-5.17	104.73	112.54
3	S	310	TYR	N-CA-C	-5.16	104.75	112.54
3	O	310	TYR	N-CA-C	-5.15	104.76	112.54
3	M	310	TYR	N-CA-C	-5.14	104.77	112.54
3	N	310	TYR	N-CA-C	-5.13	104.80	112.54
1	C	248	ALA	O-C-N	5.07	127.30	122.07

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	GLY	Peptide
1	B	205	LYS	Peptide
1	C	125	SER	Mainchain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2427	0	2449	109	0
1	B	2491	0	2516	71	0
1	C	2491	0	2516	85	0
1	D	2491	0	2516	78	0
1	E	2360	0	2377	124	0
1	F	2387	0	2409	343	0
2	G	68	0	71	1	0
3	H	331	0	344	35	0
3	I	331	0	344	19	0
3	J	331	0	344	34	0
3	K	331	0	344	23	0
3	L	331	0	344	33	0
3	M	331	0	344	22	0
3	N	331	0	344	36	0
3	O	331	0	344	20	0
3	P	331	0	344	32	0
3	Q	331	0	344	19	0
3	R	331	0	344	36	0
3	S	331	0	344	30	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	0	0
4	E	27	0	12	0	0
5	A	4	0	0	1	0
5	B	4	0	0	1	0
5	C	4	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	18838	0	19042	919	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 24.

All (919) 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:F:172:TYR:CZ	1:F:428:PHE:CD2	1.78	1.63
1:F:172:TYR:CZ	1:F:428:PHE:HD2	0.93	1.57
1:F:295:TYR:CE1	1:F:425:GLN:HB3	1.37	1.54
1:F:199:SER:HB3	1:F:237:LEU:CG	1.39	1.53
1:E:388:TRP:CZ3	1:F:151:LEU:CD1	1.90	1.52
1:A:325:ARG:CZ	3:S:310:TYR:HB3	1.37	1.51
1:F:172:TYR:CE1	1:F:428:PHE:CD2	2.01	1.48
1:E:388:TRP:CE3	1:F:151:LEU:HD13	1.46	1.46
1:E:355:GLN:CG	1:F:151:LEU:HD22	1.45	1.43
1:F:295:TYR:CE1	1:F:425:GLN:CB	2.00	1.43
1:F:323:ASP:CB	1:F:403:ILE:HD12	1.46	1.42
1:E:355:GLN:NE2	1:F:151:LEU:HD21	1.29	1.41
1:F:172:TYR:CE1	1:F:428:PHE:CE2	2.13	1.35
1:B:354:ILE:CD1	1:B:396:LEU:HD11	1.54	1.35
1:E:388:TRP:CZ3	1:F:151:LEU:HD12	1.52	1.34
1:A:151:LEU:HD21	1:F:355:GLN:CD	1.52	1.33
1:A:151:LEU:HD21	1:F:355:GLN:NE2	1.41	1.33
1:E:388:TRP:CE3	1:F:151:LEU:CD1	2.06	1.33
1:E:355:GLN:HG2	1:F:151:LEU:CD2	1.59	1.33
1:A:241:ARG:NE	1:F:205:LYS:CA	1.87	1.32
1:B:354:ILE:HD11	1:B:396:LEU:CD1	1.60	1.31
1:F:317:CYS:CB	1:F:401:LEU:HD23	1.60	1.31
1:E:388:TRP:CH2	1:F:151:LEU:HB2	1.66	1.30
1:A:163:ARG:CZ	1:F:351:ILE:HD11	1.60	1.29
1:F:350:PRO:O	1:F:399:PRO:HD2	1.20	1.29
1:F:173:GLY:HA2	1:F:425:GLN:CD	1.59	1.28
1:A:151:LEU:CD2	1:F:355:GLN:CD	2.10	1.24
1:F:199:SER:CB	1:F:237:LEU:HG	1.68	1.22
1:F:350:PRO:HB3	1:F:399:PRO:O	1.31	1.22
1:E:388:TRP:CZ2	1:F:151:LEU:HB2	1.76	1.20
1:E:388:TRP:CZ3	1:F:151:LEU:HD13	1.60	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:295:TYR:CD1	1:F:425:GLN:HB3	1.75	1.20
1:F:173:GLY:HA2	1:F:425:GLN:NE2	1.57	1.19
1:D:358:THR:O	1:D:359:HIS:CD2	1.95	1.19
1:E:355:GLN:HA	1:E:388:TRP:CD1	1.78	1.18
1:F:358:THR:HA	1:F:386:MET:O	1.39	1.18
1:A:241:ARG:HE	1:F:205:LYS:CA	1.47	1.18
1:E:355:GLN:NE2	1:F:151:LEU:CD2	2.07	1.18
1:E:388:TRP:CD2	1:F:151:LEU:HD13	1.79	1.18
1:F:353:LYS:HB2	1:F:399:PRO:CG	1.74	1.17
1:F:317:CYS:HB3	1:F:401:LEU:CD2	1.73	1.17
1:A:325:ARG:CZ	3:S:310:TYR:CB	2.23	1.17
1:F:323:ASP:HB3	1:F:403:ILE:HD12	1.16	1.16
1:E:351:ILE:HD11	1:F:163:ARG:HD3	1.28	1.14
1:F:319:LEU:HD21	1:F:403:ILE:HA	1.30	1.13
1:E:351:ILE:HD11	1:F:163:ARG:CD	1.77	1.13
1:A:151:LEU:CD2	1:F:355:GLN:NE2	2.10	1.13
1:F:354:ILE:HG22	1:F:396:LEU:CD2	1.80	1.11
1:E:355:GLN:CG	1:F:151:LEU:CD2	2.21	1.11
1:F:358:THR:O	1:F:360:PHE:CD1	2.04	1.11
1:F:350:PRO:O	1:F:399:PRO:CD	1.99	1.10
1:C:374:THR:HB	1:C:397:LYS:HG3	1.30	1.09
1:F:173:GLY:CA	1:F:425:GLN:NE2	2.15	1.09
1:F:354:ILE:HG13	1:F:399:PRO:HD3	1.10	1.09
1:F:293:ARG:HG2	1:F:428:PHE:HZ	1.11	1.08
1:E:355:GLN:HE21	1:F:151:LEU:CD2	1.64	1.08
1:E:388:TRP:CH2	1:F:151:LEU:CB	2.37	1.07
1:F:293:ARG:HG2	1:F:428:PHE:CZ	1.89	1.07
1:F:354:ILE:HG13	1:F:399:PRO:CD	1.85	1.07
1:F:319:LEU:CD2	1:F:403:ILE:HB	1.84	1.06
1:A:373:LEU:HD12	1:A:391:ILE:HD13	1.38	1.06
1:F:203:VAL:HG23	1:F:237:LEU:HD23	1.38	1.06
1:F:293:ARG:HB3	1:F:428:PHE:CE2	1.91	1.05
1:F:293:ARG:HB3	1:F:428:PHE:HE2	1.18	1.05
1:F:354:ILE:CG2	1:F:396:LEU:HG	1.86	1.05
1:A:241:ARG:HG3	1:F:204:SER:O	1.54	1.05
1:A:242:GLY:HA2	1:F:207:MET:HE3	1.39	1.05
1:F:358:THR:HG23	1:F:359:HIS:H	0.97	1.05
1:F:373:LEU:HD12	1:F:391:ILE:HD13	1.38	1.05
1:F:358:THR:CA	1:F:386:MET:O	2.05	1.05
1:F:354:ILE:CG1	1:F:399:PRO:HD3	1.88	1.03
1:A:325:ARG:NH1	3:S:310:TYR:O	1.90	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:LEU:HD12	1:B:391:ILE:HD13	1.38	1.03
1:F:354:ILE:HG22	1:F:396:LEU:HD21	1.05	1.03
1:C:373:LEU:HD12	1:C:391:ILE:HD13	1.38	1.02
1:D:373:LEU:HD12	1:D:391:ILE:CD1	1.89	1.02
1:C:373:LEU:HD12	1:C:391:ILE:CD1	1.89	1.02
1:D:358:THR:O	1:D:359:HIS:CG	2.13	1.02
1:F:354:ILE:CG2	1:F:396:LEU:CG	2.37	1.02
1:A:373:LEU:HD12	1:A:391:ILE:CD1	1.89	1.02
1:F:373:LEU:HD12	1:F:391:ILE:CD1	1.89	1.02
1:D:373:LEU:HD12	1:D:391:ILE:HD13	1.38	1.02
1:A:163:ARG:CZ	1:F:351:ILE:CD1	2.37	1.01
1:E:373:LEU:HD12	1:E:391:ILE:CD1	1.89	1.01
1:F:172:TYR:CE2	1:F:428:PHE:CD2	2.47	1.01
1:F:295:TYR:HE1	1:F:425:GLN:CG	1.73	1.01
1:E:373:LEU:HD12	1:E:391:ILE:HD13	1.38	1.01
1:F:172:TYR:CE2	1:F:428:PHE:HB3	1.95	1.01
1:A:361:LYS:HD2	1:A:381:ASP:O	1.61	1.00
1:B:373:LEU:HD12	1:B:391:ILE:CD1	1.89	1.00
1:F:323:ASP:CA	1:F:403:ILE:HD12	1.91	1.00
1:B:361:LYS:HD2	1:B:381:ASP:O	1.61	1.00
1:F:361:LYS:HD2	1:F:381:ASP:O	1.61	1.00
1:F:173:GLY:C	1:F:425:GLN:NE2	2.20	1.00
1:A:325:ARG:NE	3:S:310:TYR:HB3	1.76	1.00
1:A:241:ARG:NE	1:F:205:LYS:HA	0.99	0.99
1:D:361:LYS:HD2	1:D:381:ASP:O	1.61	0.99
1:F:350:PRO:C	1:F:399:PRO:HD2	1.87	0.99
1:F:203:VAL:HG23	1:F:237:LEU:CD2	1.92	0.99
1:C:361:LYS:HD2	1:C:381:ASP:O	1.61	0.99
1:E:361:LYS:HD2	1:E:381:ASP:O	1.61	0.99
1:F:353:LYS:HB2	1:F:399:PRO:HG2	1.03	0.99
1:F:358:THR:O	1:F:360:PHE:HD1	1.39	0.98
1:F:354:ILE:CG2	1:F:396:LEU:CD2	2.41	0.98
1:E:355:GLN:CD	1:F:151:LEU:CD2	2.37	0.98
1:F:354:ILE:CG2	1:F:396:LEU:HD21	1.92	0.97
1:C:377:SER:OG	3:L:307:ALA:HA	1.65	0.97
1:F:293:ARG:HD3	1:F:432:PHE:HB3	1.44	0.97
1:B:377:SER:OG	3:J:307:ALA:HA	1.64	0.97
1:F:377:SER:OG	3:R:307:ALA:HA	1.64	0.97
1:F:203:VAL:CG2	1:F:237:LEU:HD23	1.95	0.97
1:A:377:SER:OG	3:H:307:ALA:HA	1.64	0.96
1:F:323:ASP:CB	1:F:403:ILE:CD1	2.41	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:TYR:OH	1:F:428:PHE:HD2	1.47	0.96
1:E:377:SER:OG	3:P:307:ALA:HA	1.64	0.96
1:D:377:SER:OG	3:N:307:ALA:HA	1.64	0.96
1:F:199:SER:CB	1:F:237:LEU:CG	2.33	0.96
1:F:295:TYR:CE1	1:F:425:GLN:CG	2.48	0.95
1:F:199:SER:HB3	1:F:237:LEU:CD1	1.96	0.94
1:F:353:LYS:CB	1:F:399:PRO:HG2	1.94	0.94
1:F:358:THR:HG23	1:F:359:HIS:N	1.63	0.94
1:E:388:TRP:CH2	1:F:151:LEU:CD1	2.50	0.94
1:F:319:LEU:HD23	1:F:403:ILE:HB	1.47	0.94
1:F:174:PRO:HB2	1:F:417:VAL:HG11	1.50	0.94
1:F:238:THR:HA	1:F:253:LYS:HD3	1.49	0.93
1:F:172:TYR:CE1	1:F:428:PHE:HE2	1.83	0.93
1:F:323:ASP:HB3	1:F:403:ILE:CD1	1.98	0.93
1:A:163:ARG:NH2	1:F:351:ILE:HD11	1.83	0.92
1:E:351:ILE:O	1:E:355:GLN:OE1	1.87	0.92
1:F:247:GLU:O	1:F:251:ARG:HB2	1.69	0.92
1:E:398:GLU:OE1	1:F:163:ARG:NH1	2.03	0.92
1:F:174:PRO:HD3	1:F:421:ASP:OD2	1.70	0.92
1:F:173:GLY:C	1:F:425:GLN:HE22	1.77	0.92
1:B:245:GLU:O	1:B:249:SER:HB3	1.69	0.91
1:F:323:ASP:CG	1:F:403:ILE:HD12	1.96	0.90
1:F:357:ALA:O	1:F:360:PHE:HE1	1.54	0.90
1:A:325:ARG:NH1	3:S:310:TYR:HB3	1.84	0.90
1:F:245:GLU:O	1:F:249:SER:HB3	1.69	0.90
1:F:354:ILE:HG23	1:F:396:LEU:HG	1.53	0.90
1:A:154:LYS:NZ	1:F:388:TRP:CZ3	2.39	0.89
1:E:388:TRP:CH2	1:F:151:LEU:HD13	2.06	0.89
1:F:350:PRO:CB	1:F:399:PRO:O	2.20	0.88
1:F:319:LEU:CD2	1:F:403:ILE:CA	2.51	0.88
1:F:354:ILE:HG23	1:F:396:LEU:CG	2.04	0.88
1:E:355:GLN:CA	1:E:388:TRP:CD1	2.56	0.88
1:F:199:SER:CB	1:F:237:LEU:CD1	2.51	0.88
1:F:319:LEU:CD2	1:F:403:ILE:HA	2.03	0.88
1:F:319:LEU:CD2	1:F:403:ILE:CB	2.51	0.88
1:C:245:GLU:O	1:C:249:SER:HB3	1.74	0.87
1:C:374:THR:HB	1:C:397:LYS:CG	2.03	0.87
1:F:319:LEU:HD21	1:F:403:ILE:CA	2.04	0.87
1:A:163:ARG:NH1	1:F:351:ILE:HD11	1.89	0.86
1:D:358:THR:HG22	1:D:359:HIS:CD2	2.10	0.86
1:E:186:VAL:O	1:E:190:ALA:HB2	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:THR:CB	1:C:397:LYS:HG3	2.06	0.86
1:E:355:GLN:HA	1:E:388:TRP:HD1	1.35	0.85
1:F:172:TYR:CD1	1:F:428:PHE:CE2	2.63	0.85
3:L:311:GLU:CD	3:M:290:ARG:HH12	1.84	0.85
1:A:154:LYS:HD3	1:F:388:TRP:HZ3	1.39	0.85
3:P:311:GLU:CD	3:Q:290:ARG:HH12	1.84	0.85
3:H:311:GLU:CD	3:I:290:ARG:HH12	1.85	0.85
1:E:351:ILE:HD11	1:F:163:ARG:CG	2.07	0.85
1:F:295:TYR:CZ	1:F:425:GLN:CB	2.60	0.84
3:J:311:GLU:CD	3:K:290:ARG:HH12	1.85	0.84
3:N:311:GLU:CD	3:O:290:ARG:HH12	1.85	0.84
1:E:351:ILE:CD1	1:F:163:ARG:HD3	2.05	0.84
1:F:355:GLN:O	1:F:388:TRP:CD1	2.29	0.84
3:R:311:GLU:CD	3:S:290:ARG:HH12	1.84	0.84
1:F:173:GLY:CA	1:F:425:GLN:HE22	1.85	0.83
1:F:295:TYR:CE1	1:F:425:GLN:HB2	2.13	0.83
1:E:355:GLN:CD	1:F:151:LEU:HD21	2.02	0.83
1:F:250:ARG:O	1:F:254:THR:OG1	1.95	0.83
1:E:358:THR:HG23	1:E:359:HIS:CD2	2.14	0.83
1:F:357:ALA:HB3	1:F:360:PHE:CZ	2.14	0.83
1:A:242:GLY:CA	1:F:207:MET:HE3	2.09	0.82
1:D:245:GLU:O	1:D:249:SER:HB3	1.80	0.81
1:B:358:THR:O	1:B:359:HIS:HB2	1.79	0.81
1:F:374:THR:HB	1:F:397:LYS:HB3	1.62	0.81
1:E:313:GLY:HA3	1:F:162:ASN:HD21	1.45	0.81
1:F:295:TYR:CZ	1:F:425:GLN:HB2	2.14	0.81
1:F:358:THR:CG2	1:F:359:HIS:N	2.39	0.80
1:F:317:CYS:HB3	1:F:401:LEU:HD23	0.83	0.80
1:E:388:TRP:HZ3	1:F:151:LEU:HD12	1.45	0.79
1:F:199:SER:HB3	1:F:237:LEU:HG	0.81	0.79
1:E:398:GLU:OE1	1:F:163:ARG:CZ	2.30	0.79
1:D:358:THR:O	1:D:359:HIS:CB	2.29	0.79
1:F:323:ASP:CG	1:F:403:ILE:CD1	2.55	0.79
1:F:199:SER:HB3	1:F:237:LEU:CD2	2.13	0.79
1:F:199:SER:CB	1:F:237:LEU:HD11	2.13	0.78
1:F:357:ALA:O	1:F:360:PHE:CE1	2.36	0.78
1:F:238:THR:O	1:F:283:ASP:HB2	1.83	0.78
1:A:151:LEU:HD22	1:F:355:GLN:CD	2.09	0.78
1:C:354:ILE:HD13	1:C:375:PRO:CG	2.13	0.78
1:F:172:TYR:HE2	1:F:428:PHE:HB3	1.49	0.78
1:F:319:LEU:HD22	1:F:403:ILE:HB	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:TRP:CE2	1:F:151:LEU:HD13	2.18	0.77
3:J:291:ALA:HA	3:J:294:ILE:HD11	1.66	0.77
1:F:173:GLY:HA2	1:F:425:GLN:OE1	1.84	0.77
1:A:358:THR:HG22	1:A:359:HIS:CD2	2.18	0.77
3:J:289:ASP:O	3:J:290:ARG:HB3	1.84	0.77
3:P:289:ASP:O	3:P:290:ARG:HB3	1.84	0.77
3:R:291:ALA:HA	3:R:294:ILE:HD11	1.67	0.77
3:L:291:ALA:HA	3:L:294:ILE:HD11	1.67	0.77
1:E:361:LYS:CD	1:E:381:ASP:O	2.33	0.77
3:N:308:LEU:HD12	3:O:298:GLN:HG3	1.67	0.77
3:P:308:LEU:HD12	3:Q:298:GLN:HG3	1.67	0.77
1:C:361:LYS:CD	1:C:381:ASP:O	2.33	0.77
3:L:308:LEU:HD12	3:M:298:GLN:HG3	1.67	0.77
3:P:291:ALA:HA	3:P:294:ILE:HD11	1.66	0.77
3:H:289:ASP:O	3:H:290:ARG:HB3	1.84	0.76
3:R:289:ASP:O	3:R:290:ARG:HB3	1.84	0.76
1:F:319:LEU:HD23	1:F:403:ILE:CB	2.14	0.76
3:N:289:ASP:O	3:N:290:ARG:HB3	1.84	0.76
3:N:291:ALA:HA	3:N:294:ILE:HD11	1.66	0.76
1:A:154:LYS:HD3	1:F:388:TRP:CZ3	2.20	0.76
1:A:361:LYS:CD	1:A:381:ASP:O	2.33	0.76
1:D:361:LYS:CD	1:D:381:ASP:O	2.33	0.76
1:F:361:LYS:CD	1:F:381:ASP:O	2.33	0.76
1:A:241:ARG:CZ	1:F:205:LYS:C	2.54	0.75
3:L:289:ASP:O	3:L:290:ARG:HB3	1.84	0.75
3:H:308:LEU:HD12	3:I:298:GLN:HG3	1.68	0.75
3:J:308:LEU:HD12	3:K:298:GLN:HG3	1.67	0.75
1:F:353:LYS:CB	1:F:399:PRO:CG	2.59	0.75
3:R:308:LEU:HD12	3:S:298:GLN:HG3	1.67	0.75
1:D:358:THR:O	1:D:359:HIS:HD2	1.69	0.75
1:C:388:TRP:CH2	1:D:155:PHE:CE2	2.74	0.75
1:F:317:CYS:CB	1:F:401:LEU:CD2	2.45	0.74
3:H:291:ALA:HA	3:H:294:ILE:HD11	1.67	0.74
1:B:354:ILE:HD11	1:B:396:LEU:HD11	0.78	0.74
1:A:241:ARG:NE	1:F:205:LYS:C	2.44	0.74
1:C:321:LYS:HD3	3:K:310:TYR:HD1	1.52	0.74
1:F:354:ILE:HG23	1:F:396:LEU:CD1	2.17	0.74
1:F:354:ILE:HG21	1:F:396:LEU:HG	1.69	0.73
1:B:361:LYS:CD	1:B:381:ASP:O	2.33	0.73
1:F:174:PRO:HB2	1:F:417:VAL:CG1	2.19	0.72
1:F:172:TYR:OH	1:F:428:PHE:CD2	2.29	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:TRP:HH2	1:C:155:PHE:CE2	2.08	0.72
1:B:388:TRP:CH2	1:C:155:PHE:CE2	2.78	0.72
1:E:355:GLN:HB3	1:E:388:TRP:NE1	2.05	0.72
1:C:388:TRP:HH2	1:D:155:PHE:CE2	2.08	0.71
1:F:323:ASP:OD1	1:F:403:ILE:HD13	1.89	0.71
1:B:358:THR:O	1:B:359:HIS:CB	2.37	0.71
1:F:172:TYR:CZ	1:F:428:PHE:CG	2.73	0.71
1:E:394:ASP:O	1:E:396:LEU:N	2.23	0.71
1:F:172:TYR:CE2	1:F:428:PHE:CB	2.71	0.71
1:A:358:THR:O	1:A:359:HIS:CD2	2.44	0.71
1:F:317:CYS:HA	1:F:401:LEU:HB3	1.72	0.71
1:F:346:ALA:CB	1:F:406:PHE:CD1	2.74	0.71
1:B:394:ASP:O	1:B:396:LEU:N	2.24	0.71
1:F:240:THR:HA	1:F:283:ASP:OD1	1.90	0.71
1:F:394:ASP:O	1:F:396:LEU:N	2.24	0.70
1:C:394:ASP:O	1:C:396:LEU:N	2.24	0.70
1:F:349:GLN:OE1	1:F:352:ARG:HD2	1.92	0.70
1:F:358:THR:O	1:F:360:PHE:CE1	2.44	0.70
1:A:394:ASP:O	1:A:396:LEU:N	2.23	0.70
1:D:358:THR:HG21	3:N:303:TYR:CE1	2.25	0.70
1:F:373:LEU:CD1	1:F:391:ILE:HD13	2.20	0.70
1:E:388:TRP:CH2	1:F:151:LEU:CA	2.73	0.70
1:F:174:PRO:CD	1:F:421:ASP:OD2	2.39	0.70
1:C:404:LYS:NZ	3:M:291:ALA:HB1	2.06	0.70
1:A:163:ARG:NH2	1:F:351:ILE:CD1	2.54	0.70
1:D:388:TRP:HZ3	1:E:155:PHE:CZ	2.08	0.70
1:B:373:LEU:CD1	1:B:391:ILE:CD1	2.69	0.70
1:A:241:ARG:CZ	1:F:205:LYS:O	2.40	0.70
1:A:373:LEU:CD1	1:A:391:ILE:CD1	2.69	0.70
1:F:199:SER:OG	1:F:237:LEU:CD1	2.41	0.69
1:B:373:LEU:CD1	1:B:391:ILE:HD13	2.20	0.69
1:F:357:ALA:C	1:F:360:PHE:HE1	2.00	0.69
1:A:154:LYS:CD	1:F:388:TRP:HZ3	2.05	0.69
1:A:325:ARG:NH2	3:S:310:TYR:CB	2.55	0.69
1:D:394:ASP:O	1:D:396:LEU:N	2.24	0.69
1:F:238:THR:C	1:F:283:ASP:HB2	2.17	0.69
1:A:358:THR:O	1:A:359:HIS:CB	2.41	0.69
1:A:373:LEU:CD1	1:A:391:ILE:HD13	2.20	0.69
1:F:346:ALA:HB3	1:F:406:PHE:CE1	2.28	0.69
1:F:358:THR:C	1:F:386:MET:O	2.36	0.68
1:C:373:LEU:CD1	1:C:391:ILE:HD13	2.20	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:247:GLU:OE1	1:F:251:ARG:NH1	2.26	0.68
1:A:151:LEU:CD2	1:F:355:GLN:OE1	2.40	0.68
1:F:263:VAL:HG12	1:F:267:SER:CB	2.23	0.68
1:C:358:THR:O	1:C:359:HIS:CB	2.42	0.68
1:F:354:ILE:HG12	1:F:397:LYS:O	1.93	0.68
1:F:404:LYS:HE2	3:R:311:GLU:CD	2.18	0.68
1:F:350:PRO:HB3	1:F:399:PRO:C	2.18	0.68
1:F:172:TYR:CD1	1:F:428:PHE:CD2	2.79	0.67
1:E:373:LEU:CD1	1:E:391:ILE:HD13	2.20	0.67
1:B:354:ILE:CG1	1:B:396:LEU:HD11	2.22	0.67
1:F:263:VAL:HG12	1:F:267:SER:HB2	1.76	0.67
3:N:308:LEU:HD12	3:O:298:GLN:CG	2.25	0.67
1:A:374:THR:HB	1:A:397:LYS:HB3	1.76	0.67
1:C:373:LEU:CD1	1:C:391:ILE:CD1	2.70	0.67
1:F:373:LEU:CD1	1:F:391:ILE:CD1	2.69	0.67
1:F:298:LEU:HD21	1:F:417:VAL:HG21	1.77	0.67
3:J:308:LEU:HD13	3:K:294:ILE:HG23	1.77	0.67
1:E:373:LEU:CD1	1:E:391:ILE:CD1	2.69	0.67
3:R:308:LEU:HD13	3:S:294:ILE:HG23	1.77	0.67
1:C:358:THR:O	1:C:359:HIS:CD2	2.48	0.66
1:F:293:ARG:CG	1:F:428:PHE:CZ	2.73	0.66
3:L:308:LEU:HD12	3:M:298:GLN:CG	2.25	0.66
3:P:308:LEU:HD12	3:Q:298:GLN:CG	2.25	0.66
1:D:373:LEU:CD1	1:D:391:ILE:HD13	2.20	0.66
3:H:308:LEU:HD12	3:I:298:GLN:CG	2.25	0.66
1:F:172:TYR:CE2	1:F:428:PHE:CG	2.83	0.66
3:J:308:LEU:HD12	3:K:298:GLN:CG	2.25	0.66
1:F:317:CYS:CB	1:F:401:LEU:HB3	2.25	0.66
1:F:355:GLN:O	1:F:388:TRP:CG	2.49	0.66
1:C:358:THR:O	1:C:359:HIS:HB2	1.96	0.66
3:L:291:ALA:HA	3:L:294:ILE:CD1	2.26	0.66
3:N:308:LEU:HD13	3:O:294:ILE:HG23	1.78	0.66
1:A:151:LEU:HD23	1:F:355:GLN:NE2	2.10	0.66
1:E:388:TRP:CH2	1:F:151:LEU:HA	2.31	0.66
1:D:373:LEU:CD1	1:D:391:ILE:CD1	2.70	0.66
1:A:358:THR:O	1:A:359:HIS:HB2	1.96	0.66
1:F:358:THR:CG2	1:F:359:HIS:H	1.83	0.66
1:F:359:HIS:CE1	1:F:385:GLU:HB2	2.31	0.66
3:N:291:ALA:HA	3:N:294:ILE:CD1	2.26	0.66
1:A:151:LEU:HD21	1:F:355:GLN:CG	2.26	0.65
3:R:308:LEU:HD12	3:S:298:GLN:CG	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:323:ASP:OD1	1:F:403:ILE:CD1	2.44	0.65
1:F:174:PRO:N	1:F:425:GLN:NE2	2.44	0.65
1:B:245:GLU:O	1:B:249:SER:CB	2.44	0.65
1:C:359:HIS:CE1	1:C:385:GLU:HB2	2.31	0.65
1:D:337:SER:OG	1:E:288:ARG:NH1	2.30	0.65
3:L:308:LEU:HD13	3:M:294:ILE:HG23	1.77	0.65
1:A:359:HIS:CE1	1:A:385:GLU:HB2	2.32	0.65
1:B:359:HIS:CE1	1:B:385:GLU:HB2	2.31	0.65
1:E:359:HIS:CE1	1:E:385:GLU:HB2	2.32	0.65
1:F:293:ARG:CB	1:F:428:PHE:CE2	2.73	0.65
1:D:359:HIS:CE1	1:D:385:GLU:HB2	2.31	0.65
3:P:291:ALA:HA	3:P:294:ILE:CD1	2.26	0.65
1:F:199:SER:O	1:F:237:LEU:HD21	1.96	0.65
1:F:405:ASP:O	1:F:408:LYS:HB3	1.97	0.65
3:H:291:ALA:HA	3:H:294:ILE:CD1	2.26	0.65
3:P:308:LEU:HD13	3:Q:294:ILE:HG23	1.77	0.65
3:R:291:ALA:HA	3:R:294:ILE:CD1	2.26	0.65
1:B:248:ALA:HB1	1:C:251:ARG:HH22	1.62	0.64
1:E:396:LEU:CD2	1:F:158:LEU:HD11	2.27	0.64
1:F:250:ARG:O	1:F:254:THR:CB	2.45	0.64
3:H:308:LEU:HD13	3:I:294:ILE:HG23	1.78	0.64
1:F:354:ILE:HG23	1:F:396:LEU:HD11	1.79	0.64
1:F:323:ASP:HA	1:F:403:ILE:HD12	1.74	0.64
1:F:397:LYS:HA	1:F:397:LYS:HZ2	1.61	0.64
1:F:357:ALA:C	1:F:360:PHE:CE1	2.75	0.64
3:J:291:ALA:HA	3:J:294:ILE:CD1	2.26	0.64
1:A:388:TRP:CH2	1:B:155:PHE:CE2	2.86	0.64
1:F:295:TYR:HE1	1:F:425:GLN:CD	2.05	0.64
1:E:245:GLU:O	1:E:249:SER:HB3	1.98	0.64
1:F:167:SER:OG	1:F:263:VAL:HG21	1.98	0.64
1:D:354:ILE:HD13	1:D:396:LEU:HD11	1.80	0.63
1:E:127:LYS:NZ	1:E:188:THR:O	2.29	0.63
1:F:323:ASP:HA	1:F:403:ILE:CD1	2.28	0.63
1:F:394:ASP:C	1:F:396:LEU:H	2.07	0.63
1:A:151:LEU:HD22	1:F:355:GLN:OE1	1.98	0.63
1:A:281:GLN:OE1	1:B:250:ARG:NH2	2.31	0.63
1:F:404:LYS:NZ	3:R:311:GLU:OE1	2.31	0.63
1:A:357:ALA:HB1	1:A:360:PHE:CE1	2.34	0.63
1:A:325:ARG:NH2	3:S:310:TYR:HB2	2.13	0.62
1:D:388:TRP:CZ3	1:E:155:PHE:CE2	2.87	0.62
1:E:247:GLU:HG2	1:E:251:ARG:HD2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ASP:OD1	1:A:400:ASP:N	2.25	0.62
1:F:169:ILE:HB	1:F:273:LEU:HD23	1.80	0.62
1:F:358:THR:O	1:F:359:HIS:C	2.41	0.62
1:E:388:TRP:CZ2	1:F:151:LEU:HD13	2.35	0.62
1:E:377:SER:OG	3:P:307:ALA:CA	2.46	0.62
1:E:398:GLU:CD	1:F:163:ARG:HH22	2.07	0.62
1:C:354:ILE:HD13	1:C:375:PRO:HG3	1.80	0.62
1:A:154:LYS:NZ	1:F:389:THR:HG22	2.15	0.62
1:A:377:SER:OG	3:H:307:ALA:CA	2.46	0.61
1:E:394:ASP:C	1:E:396:LEU:H	2.07	0.61
1:D:377:SER:OG	3:N:307:ALA:CA	2.46	0.61
1:C:394:ASP:C	1:C:396:LEU:H	2.08	0.61
1:F:319:LEU:HD23	1:F:403:ILE:CA	2.30	0.61
1:C:321:LYS:HD3	3:K:310:TYR:CD1	2.36	0.61
1:B:394:ASP:C	1:B:396:LEU:H	2.08	0.61
1:E:398:GLU:OE1	1:F:163:ARG:NH2	2.32	0.61
1:F:317:CYS:HB2	1:F:401:LEU:CG	2.30	0.61
1:A:394:ASP:C	1:A:396:LEU:H	2.08	0.61
1:E:247:GLU:O	1:E:251:ARG:HB2	2.01	0.61
1:C:388:TRP:HH2	1:D:155:PHE:HE2	1.47	0.60
1:A:241:ARG:NE	1:F:205:LYS:O	2.34	0.60
1:A:358:THR:HG22	1:A:358:THR:O	2.00	0.60
1:A:358:THR:O	1:A:359:HIS:CG	2.55	0.60
3:N:290:ARG:O	3:N:294:ILE:HG12	2.02	0.60
1:F:323:ASP:CA	1:F:403:ILE:CD1	2.74	0.60
1:E:355:GLN:HG2	1:F:151:LEU:HD22	0.65	0.60
1:A:388:TRP:CZ3	1:B:155:PHE:CZ	2.89	0.60
1:C:388:TRP:HZ3	1:D:155:PHE:CZ	2.20	0.60
3:R:290:ARG:O	3:R:294:ILE:HG12	2.02	0.60
1:D:358:THR:O	1:D:358:THR:HG22	2.01	0.59
3:J:290:ARG:O	3:J:294:ILE:HG12	2.02	0.59
1:F:346:ALA:HB3	1:F:406:PHE:CD1	2.37	0.59
1:F:317:CYS:CA	1:F:401:LEU:HB3	2.32	0.59
1:F:418:ASN:OD1	1:F:419:GLU:N	2.35	0.59
3:L:290:ARG:O	3:L:294:ILE:HG12	2.02	0.59
1:C:388:TRP:CZ3	1:D:155:PHE:CZ	2.89	0.59
1:D:394:ASP:C	1:D:396:LEU:H	2.08	0.59
1:F:199:SER:OG	1:F:237:LEU:HD11	2.00	0.59
1:A:388:TRP:HZ3	1:B:155:PHE:CZ	2.20	0.59
3:H:290:ARG:O	3:H:294:ILE:HG12	2.01	0.59
1:A:373:LEU:HD12	1:A:391:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:290:ARG:O	3:P:294:ILE:HG12	2.02	0.59
1:E:355:GLN:CB	1:E:388:TRP:NE1	2.66	0.59
1:F:173:GLY:CA	1:F:425:GLN:CD	2.52	0.58
1:F:203:VAL:CG2	1:F:237:LEU:CD2	2.68	0.58
1:D:128:PRO:O	1:D:188:THR:OG1	2.20	0.58
1:F:350:PRO:CA	1:F:399:PRO:HD2	2.32	0.58
1:F:377:SER:OG	3:R:307:ALA:CA	2.46	0.58
1:B:358:THR:O	1:B:358:THR:HG23	2.03	0.58
1:D:358:THR:O	1:D:359:HIS:HB2	2.03	0.58
3:R:298:GLN:HG3	3:S:308:LEU:HD12	1.86	0.58
1:F:373:LEU:HD12	1:F:391:ILE:HD11	1.84	0.58
3:N:298:GLN:HG3	3:O:308:LEU:HD12	1.86	0.58
1:C:358:THR:O	1:C:358:THR:HG23	2.02	0.58
1:E:351:ILE:CD1	1:F:163:ARG:CG	2.79	0.58
3:J:298:GLN:HG3	3:K:308:LEU:HD12	1.86	0.58
1:D:388:TRP:CH2	1:E:155:PHE:HE2	2.22	0.58
1:A:241:ARG:HD2	1:F:205:LYS:O	2.04	0.58
1:C:128:PRO:O	1:C:188:THR:OG1	2.22	0.58
1:E:204:SER:OG	1:E:205:LYS:N	2.37	0.58
1:E:396:LEU:HD23	1:F:158:LEU:HD11	1.86	0.58
1:E:222:ARG:NE	1:E:265:ASN:O	2.37	0.57
1:F:317:CYS:CB	1:F:401:LEU:CG	2.82	0.57
3:N:300:LEU:HD12	3:N:323:ALA:CA	2.34	0.57
1:B:373:LEU:HD12	1:B:391:ILE:HD11	1.84	0.57
1:D:388:TRP:CZ3	1:E:155:PHE:CZ	2.91	0.57
3:H:298:GLN:HG3	3:I:308:LEU:HD12	1.86	0.57
3:H:300:LEU:HD12	3:H:323:ALA:CA	2.35	0.57
1:C:247:GLU:O	1:C:251:ARG:HB2	2.03	0.57
1:C:354:ILE:HD13	1:C:375:PRO:HG2	1.87	0.57
1:F:308:PHE:O	1:F:312:VAL:HG13	2.05	0.57
1:F:300:ASP:OD1	1:F:303:ALA:HB3	2.05	0.57
1:E:355:GLN:CB	1:E:388:TRP:CD1	2.88	0.57
1:F:404:LYS:HA	1:F:407:LEU:HD12	1.86	0.57
3:P:300:LEU:HD12	3:P:323:ALA:CA	2.34	0.57
3:R:300:LEU:HD12	3:R:323:ALA:CA	2.35	0.57
1:D:352:ARG:O	1:D:356:SER:HB3	2.05	0.57
3:L:298:GLN:HG3	3:M:308:LEU:HD12	1.86	0.57
1:E:373:LEU:HD11	1:E:391:ILE:HG12	1.87	0.57
1:C:404:LYS:HZ3	3:M:291:ALA:HB1	1.68	0.57
3:P:298:GLN:HG3	3:Q:308:LEU:HD12	1.86	0.57
1:C:358:THR:O	1:C:359:HIS:CG	2.58	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:ALA:O	1:E:189:GLU:HB2	2.04	0.57
1:B:373:LEU:HD11	1:B:391:ILE:HG12	1.87	0.56
1:E:351:ILE:HG23	1:E:355:GLN:HE22	1.69	0.56
4:C:701:ADP:O3B	5:C:702:BEF:F2	2.13	0.56
1:E:388:TRP:HH2	1:F:151:LEU:CA	2.18	0.56
1:F:373:LEU:HD11	1:F:391:ILE:HG12	1.87	0.56
3:J:300:LEU:HD12	3:J:323:ALA:CA	2.35	0.56
1:A:154:LYS:CE	1:F:388:TRP:HZ3	2.18	0.56
1:C:373:LEU:HD11	1:C:391:ILE:HG12	1.87	0.56
1:F:203:VAL:HG21	1:F:237:LEU:HD23	1.87	0.56
3:L:300:LEU:HD12	3:L:323:ALA:CA	2.34	0.56
1:A:227:SER:H	1:A:269:GLY:HA2	1.71	0.56
1:A:285:ALA:HB2	1:F:205:LYS:CE	2.36	0.56
1:A:373:LEU:HD11	1:A:391:ILE:HG12	1.87	0.55
1:E:358:THR:HG23	1:E:359:HIS:HD2	1.66	0.55
1:E:373:LEU:HD12	1:E:391:ILE:HD11	1.84	0.55
1:A:154:LYS:CE	1:F:388:TRP:CZ3	2.89	0.55
1:C:377:SER:OG	3:L:307:ALA:CA	2.46	0.55
1:D:373:LEU:HD11	1:D:391:ILE:HG12	1.87	0.55
1:E:313:GLY:HA3	1:F:162:ASN:ND2	2.19	0.55
1:B:377:SER:OG	3:J:307:ALA:CA	2.46	0.55
1:C:373:LEU:HD12	1:C:391:ILE:HD11	1.84	0.55
1:E:255:GLU:OE2	1:E:259:GLN:NE2	2.40	0.55
1:F:295:TYR:CE1	1:F:425:GLN:HG3	2.40	0.55
1:D:393:ALA:O	1:D:394:ASP:CG	2.50	0.54
1:D:373:LEU:HD12	1:D:391:ILE:HD11	1.84	0.54
1:E:131:LYS:N	1:E:134:ASP:OD2	2.41	0.54
1:F:280:TRP:CH2	1:F:424:LYS:HD3	2.43	0.54
1:A:128:PRO:O	1:A:188:THR:OG1	2.25	0.54
1:C:393:ALA:O	1:C:394:ASP:CG	2.51	0.54
1:D:245:GLU:O	1:D:249:SER:CB	2.53	0.54
1:F:349:GLN:OE1	1:F:352:ARG:NH1	2.39	0.54
3:J:290:ARG:HG3	3:J:291:ALA:N	2.22	0.54
1:B:255:GLU:O	1:B:259:GLN:HB2	2.08	0.54
1:B:388:TRP:CZ3	1:C:155:PHE:CZ	2.95	0.54
1:C:248:ALA:HB1	1:D:251:ARG:HH22	1.72	0.54
1:D:377:SER:HG	3:N:307:ALA:HA	1.71	0.54
3:H:290:ARG:HG3	3:H:291:ALA:N	2.22	0.54
1:C:255:GLU:O	1:C:259:GLN:HB2	2.08	0.54
1:C:325:ARG:HH22	3:K:312:ASP:HB2	1.72	0.54
1:D:255:GLU:O	1:D:259:GLN:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:TRP:CE3	1:F:151:LEU:HD11	2.32	0.54
1:E:392:GLU:HB2	1:E:395:GLU:CD	2.33	0.54
1:F:304:ARG:NH1	1:F:328:GLY:O	2.40	0.54
1:E:255:GLU:O	1:E:259:GLN:HB2	2.08	0.54
3:P:290:ARG:HG3	3:P:291:ALA:N	2.22	0.54
1:B:392:GLU:HB2	1:B:395:GLU:CD	2.33	0.54
1:F:392:GLU:HB2	1:F:395:GLU:CD	2.33	0.54
3:L:290:ARG:HG3	3:L:291:ALA:N	2.22	0.54
1:A:393:ALA:O	1:A:394:ASP:CG	2.51	0.54
1:B:255:GLU:OE2	1:B:259:GLN:NE2	2.40	0.54
1:B:393:ALA:O	1:B:394:ASP:CG	2.50	0.54
1:F:174:PRO:CG	1:F:421:ASP:OD2	2.56	0.54
1:F:393:ALA:O	1:F:394:ASP:CG	2.50	0.54
3:R:290:ARG:HG3	3:R:291:ALA:N	2.22	0.54
1:D:358:THR:C	1:D:359:HIS:CG	2.84	0.53
1:F:353:LYS:HB2	1:F:399:PRO:HG3	1.82	0.53
1:C:392:GLU:HB2	1:C:395:GLU:CD	2.33	0.53
1:D:255:GLU:OE2	1:D:259:GLN:NE2	2.40	0.53
1:F:300:ASP:OD1	1:F:303:ALA:CB	2.56	0.53
1:A:392:GLU:HB2	1:A:395:GLU:CD	2.33	0.53
1:E:388:TRP:HH2	1:F:151:LEU:HA	1.72	0.53
1:E:293:ARG:NH2	1:E:432:PHE:O	2.41	0.53
1:C:354:ILE:HD12	1:C:396:LEU:HD11	1.91	0.53
1:D:392:GLU:HB2	1:D:395:GLU:CD	2.33	0.53
1:F:295:TYR:HE1	1:F:425:GLN:HG3	1.65	0.53
1:A:116:ARG:HA	1:A:220:MET:HE1	1.91	0.53
1:E:355:GLN:HE21	1:F:151:LEU:HD21	0.67	0.53
1:F:323:ASP:HB3	1:F:403:ILE:CG1	2.39	0.53
1:A:353:LYS:O	1:A:375:PRO:HG2	2.08	0.53
1:D:135:VAL:HG11	1:D:182:LEU:HD13	1.90	0.53
3:N:290:ARG:HG3	3:N:291:ALA:N	2.22	0.53
1:B:393:ALA:O	1:B:394:ASP:OD1	2.27	0.52
1:E:393:ALA:O	1:E:394:ASP:CG	2.51	0.52
1:B:337:SER:OG	1:C:288:ARG:NH1	2.42	0.52
1:C:393:ALA:O	1:C:394:ASP:OD1	2.27	0.52
1:E:397:LYS:O	1:E:397:LYS:HG3	2.09	0.52
1:F:342:VAL:HG12	1:F:413:THR:HB	1.91	0.52
1:F:393:ALA:O	1:F:394:ASP:OD1	2.27	0.52
1:A:241:ARG:CD	1:F:205:LYS:O	2.57	0.52
1:A:244:GLY:C	1:A:250:ARG:HH12	2.16	0.52
1:B:388:TRP:HH2	1:C:155:PHE:HE2	1.54	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:293:LYS:HZ2	3:H:330:ILE:HD13	1.74	0.52
1:A:388:TRP:HH2	1:B:155:PHE:CE2	2.26	0.52
1:F:245:GLU:O	1:F:249:SER:CB	2.51	0.52
1:F:166:THR:HG23	1:F:291:GLU:CD	2.34	0.52
1:F:339:ILE:HA	1:F:342:VAL:HG22	1.91	0.52
1:F:293:ARG:HD3	1:F:432:PHE:CB	2.29	0.52
3:N:330:ILE:HG22	3:N:330:ILE:OXT	2.09	0.52
3:Q:330:ILE:OXT	3:Q:330:ILE:HG22	2.10	0.52
1:E:146:LYS:O	1:E:150:ILE:HB	2.09	0.52
3:L:293:LYS:HZ2	3:L:330:ILE:HD13	1.74	0.52
3:N:293:LYS:HZ2	3:N:330:ILE:HD13	1.75	0.52
1:C:255:GLU:OE2	1:C:259:GLN:NE2	2.40	0.52
1:E:393:ALA:O	1:E:394:ASP:OD1	2.27	0.52
3:R:330:ILE:HG22	3:R:330:ILE:OXT	2.09	0.52
3:J:293:LYS:HZ2	3:J:330:ILE:HD13	1.74	0.52
4:B:701:ADP:O3B	5:B:702:BEF:F2	2.17	0.52
1:D:393:ALA:O	1:D:394:ASP:OD1	2.27	0.52
1:F:350:PRO:HA	1:F:399:PRO:CG	2.39	0.52
3:H:330:ILE:HG22	3:H:330:ILE:OXT	2.10	0.52
1:F:238:THR:HB	1:F:283:ASP:HB3	1.91	0.51
3:M:325:ASP:HA	3:M:328:ASN:HD22	1.76	0.51
1:E:200:SER:OG	1:F:250:ARG:HD2	2.11	0.51
1:E:351:ILE:CG1	1:F:163:ARG:HD3	2.40	0.51
1:F:317:CYS:HB2	1:F:401:LEU:HG	1.91	0.51
3:J:325:ASP:HA	3:J:328:ASN:HD22	1.75	0.51
3:Q:325:ASP:HA	3:Q:328:ASN:HD22	1.75	0.51
1:A:325:ARG:HH22	3:S:312:ASP:HB2	1.75	0.51
1:B:204:SER:HB3	1:B:209:GLU:HB2	1.92	0.51
1:C:397:LYS:HD2	1:C:397:LYS:C	2.35	0.51
3:H:325:ASP:HA	3:H:328:ASN:HD22	1.75	0.51
3:P:330:ILE:HG22	3:P:330:ILE:OXT	2.10	0.51
1:A:393:ALA:O	1:A:394:ASP:OD1	2.27	0.51
1:E:351:ILE:HD11	1:F:163:ARG:HG3	1.87	0.51
1:A:154:LYS:CD	1:F:388:TRP:CZ3	2.89	0.51
3:P:325:ASP:HA	3:P:328:ASN:HD22	1.75	0.51
3:R:325:ASP:HA	3:R:328:ASN:HD22	1.75	0.51
3:S:325:ASP:HA	3:S:328:ASN:HD22	1.75	0.51
1:B:354:ILE:HD13	1:B:396:LEU:HD21	1.93	0.51
3:I:325:ASP:HA	3:I:328:ASN:HD22	1.75	0.51
3:I:330:ILE:HG22	3:I:330:ILE:OXT	2.10	0.51
3:J:330:ILE:HG22	3:J:330:ILE:OXT	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:330:ILE:HG22	3:K:330:ILE:OXT	2.09	0.51
1:A:325:ARG:NE	3:S:310:TYR:CB	2.59	0.51
3:P:289:ASP:HA	3:P:292:SER:OG	2.11	0.51
3:L:325:ASP:HA	3:L:328:ASN:HD22	1.75	0.51
3:P:293:LYS:HZ2	3:P:330:ILE:HD13	1.76	0.51
1:F:350:PRO:HA	1:F:399:PRO:HB2	1.92	0.50
3:M:330:ILE:HG22	3:M:330:ILE:OXT	2.10	0.50
3:O:325:ASP:HA	3:O:328:ASN:HD22	1.75	0.50
3:L:330:ILE:OXT	3:L:330:ILE:HG22	2.10	0.50
1:C:211:GLU:OE1	1:C:251:ARG:HB3	2.12	0.50
1:D:250:ARG:O	1:D:254:THR:CB	2.60	0.50
3:N:325:ASP:HA	3:N:328:ASN:HD22	1.75	0.50
3:R:293:LYS:HZ2	3:R:330:ILE:HD13	1.74	0.50
3:K:325:ASP:HA	3:K:328:ASN:HD22	1.75	0.50
1:A:325:ARG:NH2	3:S:312:ASP:HB2	2.26	0.50
1:B:128:PRO:O	1:B:188:THR:OG1	2.28	0.50
1:E:398:GLU:CD	1:F:163:ARG:NH2	2.69	0.50
1:A:285:ALA:HB2	1:F:205:LYS:HE3	1.93	0.50
1:F:207:MET:SD	1:F:248:ALA:HB2	2.52	0.50
3:R:289:ASP:HA	3:R:292:SER:OG	2.12	0.50
3:O:330:ILE:HG22	3:O:330:ILE:OXT	2.10	0.50
1:B:250:ARG:O	1:B:254:THR:CB	2.60	0.50
1:E:127:LYS:HZ3	1:E:191:ASN:H	1.60	0.50
1:E:250:ARG:O	1:E:254:THR:CB	2.60	0.50
3:S:330:ILE:HG22	3:S:330:ILE:OXT	2.10	0.50
1:F:323:ASP:CG	1:F:403:ILE:HG21	2.36	0.50
3:H:289:ASP:HA	3:H:292:SER:OG	2.12	0.50
1:D:354:ILE:HG22	1:D:388:TRP:HB3	1.94	0.49
1:F:290:PHE:O	1:F:291:GLU:C	2.55	0.49
3:N:289:ASP:HA	3:N:292:SER:OG	2.11	0.49
3:L:289:ASP:HA	3:L:292:SER:OG	2.12	0.49
1:B:250:ARG:O	1:B:254:THR:HB	2.13	0.49
1:B:388:TRP:HZ3	1:C:155:PHE:CZ	2.30	0.49
1:B:400:ASP:OD1	1:B:400:ASP:N	2.42	0.49
1:C:250:ARG:O	1:C:254:THR:HB	2.13	0.49
1:C:397:LYS:C	1:C:397:LYS:CD	2.85	0.49
1:E:388:TRP:CH2	1:F:151:LEU:CG	2.95	0.49
1:F:350:PRO:O	1:F:354:ILE:HG13	2.11	0.49
1:D:250:ARG:O	1:D:254:THR:HB	2.12	0.49
1:B:247:GLU:O	1:B:251:ARG:HB2	2.13	0.49
1:C:250:ARG:O	1:C:254:THR:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:ILE:HA	1:D:434:GLN:HB3	1.95	0.49
3:J:327:LEU:HD12	3:J:327:LEU:O	2.13	0.49
1:E:239:GLY:H	1:E:253:LYS:HE2	1.77	0.49
1:E:400:ASP:CG	1:E:401:LEU:H	2.21	0.49
3:K:327:LEU:HD12	3:K:327:LEU:O	2.13	0.49
1:C:321:LYS:HD3	3:K:310:TYR:HA	1.95	0.49
1:F:404:LYS:O	1:F:407:LEU:HB2	2.12	0.48
3:H:313:LEU:N	3:H:314:PRO:CD	2.76	0.48
3:J:313:LEU:N	3:J:314:PRO:CD	2.76	0.48
3:P:313:LEU:N	3:P:314:PRO:CD	2.76	0.48
3:S:313:LEU:N	3:S:314:PRO:CD	2.76	0.48
1:D:388:TRP:CH2	1:E:155:PHE:CE2	3.01	0.48
1:E:250:ARG:O	1:E:254:THR:HB	2.12	0.48
1:F:395:GLU:O	1:F:395:GLU:HG3	2.13	0.48
3:I:327:LEU:O	3:I:327:LEU:HD12	2.13	0.48
3:L:311:GLU:CD	3:M:290:ARG:NH1	2.64	0.48
3:Q:327:LEU:HD12	3:Q:327:LEU:O	2.13	0.48
1:F:293:ARG:NH1	1:F:432:PHE:CD1	2.81	0.48
3:L:327:LEU:HD12	3:L:327:LEU:O	2.13	0.48
3:O:313:LEU:N	3:O:314:PRO:CD	2.76	0.48
3:P:327:LEU:HD12	3:P:327:LEU:O	2.13	0.48
1:A:357:ALA:CB	1:A:360:PHE:CE1	2.96	0.48
3:R:313:LEU:N	3:R:314:PRO:CD	2.76	0.48
1:E:355:GLN:HB3	1:E:388:TRP:HE1	1.75	0.48
3:S:327:LEU:O	3:S:327:LEU:HD12	2.13	0.48
3:I:313:LEU:N	3:I:314:PRO:CD	2.76	0.48
3:K:313:LEU:N	3:K:314:PRO:CD	2.76	0.48
1:A:401:LEU:HD13	1:A:406:PHE:CE2	2.49	0.48
1:C:397:LYS:HG3	1:C:397:LYS:O	2.14	0.48
1:C:395:GLU:O	1:C:395:GLU:HG3	2.14	0.48
1:E:395:GLU:HG3	1:E:395:GLU:O	2.14	0.48
3:J:289:ASP:HA	3:J:292:SER:OG	2.12	0.48
3:N:313:LEU:N	3:N:314:PRO:CD	2.76	0.48
3:N:327:LEU:O	3:N:327:LEU:HD12	2.13	0.48
1:C:325:ARG:NH2	3:K:312:ASP:HB2	2.28	0.48
3:M:327:LEU:HD12	3:M:327:LEU:O	2.13	0.48
1:F:257:LEU:HD23	1:F:289:ARG:HG3	1.95	0.47
3:N:296:GLN:HE21	3:N:300:LEU:HG	1.79	0.47
3:O:327:LEU:HD12	3:O:327:LEU:O	2.13	0.47
1:C:300:ASP:OD1	1:C:300:ASP:N	2.43	0.47
1:F:166:THR:HG23	1:F:291:GLU:OE1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206:TRP:O	1:F:209:GLU:HG2	2.14	0.47
3:L:313:LEU:N	3:L:314:PRO:CD	2.76	0.47
1:A:395:GLU:O	1:A:395:GLU:HG3	2.14	0.47
1:C:261:ASN:ND2	1:C:288:ARG:HH22	2.11	0.47
1:D:395:GLU:O	1:D:395:GLU:HG3	2.14	0.47
1:F:351:ILE:O	1:F:355:GLN:HG3	2.14	0.47
3:M:313:LEU:N	3:M:314:PRO:CD	2.76	0.47
3:Q:313:LEU:N	3:Q:314:PRO:CD	2.76	0.47
3:H:327:LEU:HD12	3:H:327:LEU:O	2.13	0.47
1:D:248:ALA:HB1	1:E:251:ARG:HH22	1.78	0.47
3:R:327:LEU:HD12	3:R:327:LEU:O	2.13	0.47
1:D:394:ASP:OD1	1:D:395:GLU:N	2.48	0.47
3:H:296:GLN:HE21	3:H:300:LEU:HG	1.79	0.47
1:A:349:GLN:OE1	1:A:352:ARG:NH1	2.46	0.47
1:E:139:GLU:HA	1:E:142:LYS:HD2	1.96	0.47
1:F:311:ASN:HB3	1:F:343:VAL:HG11	1.97	0.47
1:F:394:ASP:OD1	1:F:395:GLU:N	2.48	0.47
3:J:296:GLN:HE21	3:J:300:LEU:HG	1.79	0.47
3:N:311:GLU:CD	3:O:290:ARG:NH1	2.64	0.47
3:P:296:GLN:HE21	3:P:300:LEU:HG	1.79	0.47
1:C:394:ASP:OD1	1:C:395:GLU:N	2.48	0.47
1:D:397:LYS:HD2	1:D:397:LYS:HA	1.31	0.47
1:E:186:VAL:O	1:E:190:ALA:CB	2.55	0.47
3:R:296:GLN:HE21	3:R:300:LEU:HG	1.79	0.47
4:A:701:ADP:O1B	5:A:702:BEF:F2	2.22	0.47
1:B:394:ASP:OD1	1:B:395:GLU:N	2.48	0.47
1:B:395:GLU:O	1:B:395:GLU:HG3	2.14	0.47
1:C:404:LYS:HZ2	3:M:291:ALA:HB1	1.77	0.47
1:A:242:GLY:HA2	1:F:207:MET:CE	2.28	0.46
1:D:357:ALA:HB3	1:D:360:PHE:CE1	2.50	0.46
3:K:324:LEU:O	3:K:328:ASN:ND2	2.49	0.46
1:F:249:SER:HA	1:F:253:LYS:HE3	1.97	0.46
3:P:328:ASN:OD1	3:Q:317:LYS:HE3	2.16	0.46
1:A:394:ASP:OD1	1:A:395:GLU:N	2.48	0.46
1:F:317:CYS:CB	1:F:401:LEU:CB	2.93	0.46
3:O:324:LEU:O	3:O:328:ASN:ND2	2.49	0.46
3:R:311:GLU:OE1	3:S:290:ARG:NH1	2.49	0.46
3:R:317:LYS:HE3	3:S:328:ASN:OD1	2.16	0.46
1:E:394:ASP:HA	1:F:157:HIS:CE1	2.49	0.46
3:N:328:ASN:OD1	3:O:317:LYS:HE3	2.16	0.46
3:P:324:LEU:O	3:P:328:ASN:ND2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ALA:CB	1:F:205:LYS:CE	2.94	0.46
1:D:212:LYS:O	1:D:216:GLN:HB2	2.16	0.46
1:F:139:GLU:H	1:F:139:GLU:HG2	1.45	0.46
3:H:311:GLU:CD	3:I:290:ARG:NH1	2.64	0.46
3:N:324:LEU:O	3:N:328:ASN:ND2	2.49	0.46
3:P:311:GLU:OE1	3:Q:290:ARG:NH1	2.49	0.46
1:D:374:THR:CB	1:D:397:LYS:O	2.64	0.46
3:J:317:LYS:HE3	3:K:328:ASN:OD1	2.16	0.46
3:L:317:LYS:HE3	3:M:328:ASN:OD1	2.16	0.46
3:N:311:GLU:OE1	3:O:290:ARG:NH1	2.49	0.46
3:N:317:LYS:HE3	3:O:328:ASN:OD1	2.16	0.46
3:P:317:LYS:HE3	3:Q:328:ASN:OD1	2.16	0.46
1:F:225:LYS:HD3	1:F:269:GLY:HA3	1.98	0.46
3:H:328:ASN:OD1	3:I:317:LYS:HE3	2.16	0.46
3:J:324:LEU:O	3:J:328:ASN:ND2	2.48	0.46
3:L:296:GLN:HE21	3:L:300:LEU:HG	1.80	0.46
3:R:324:LEU:O	3:R:328:ASN:ND2	2.49	0.46
1:E:351:ILE:CD1	1:F:163:ARG:HG3	2.45	0.46
1:E:358:THR:O	1:E:359:HIS:HB2	2.16	0.46
1:E:394:ASP:OD1	1:E:395:GLU:N	2.48	0.46
1:F:174:PRO:N	1:F:425:GLN:HE21	2.14	0.46
3:L:311:GLU:OE1	3:M:290:ARG:NH1	2.49	0.46
3:L:324:LEU:O	3:L:328:ASN:ND2	2.48	0.46
1:E:350:PRO:HB3	1:E:399:PRO:HB2	1.98	0.46
3:H:311:GLU:OE1	3:I:290:ARG:NH1	2.49	0.46
3:H:317:LYS:HE3	3:I:328:ASN:OD1	2.16	0.46
3:I:324:LEU:O	3:I:328:ASN:ND2	2.49	0.46
3:J:328:ASN:OD1	3:K:317:LYS:HE3	2.16	0.46
3:P:311:GLU:CD	3:Q:290:ARG:NH1	2.64	0.46
1:A:397:LYS:C	1:A:397:LYS:CD	2.88	0.46
1:F:295:TYR:CE1	1:F:425:GLN:CD	2.89	0.45
1:F:298:LEU:CD2	1:F:417:VAL:HG21	2.45	0.45
1:F:136:ALA:HB1	1:F:303:ALA:HB1	1.98	0.45
1:F:315:THR:HG21	1:F:347:LEU:HD22	1.98	0.45
3:P:301:ALA:O	3:P:305:ILE:HG13	2.16	0.45
1:F:212:LYS:HE3	1:F:216:GLN:HE21	1.81	0.45
3:L:328:ASN:OD1	3:M:317:LYS:HE3	2.16	0.45
1:B:414:ARG:HD3	1:B:415:PRO:HD2	1.99	0.45
1:E:127:LYS:HG2	1:E:188:THR:HA	1.98	0.45
1:F:250:ARG:O	1:F:254:THR:HB	2.15	0.45
3:H:324:LEU:O	3:H:328:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:301:ALA:O	3:L:305:ILE:HG13	2.16	0.45
3:N:301:ALA:O	3:N:305:ILE:HG13	2.16	0.45
3:R:328:ASN:OD1	3:S:317:LYS:HE3	2.16	0.45
3:S:324:LEU:O	3:S:328:ASN:ND2	2.49	0.45
1:A:370:THR:O	1:A:371:ARG:O	2.35	0.45
3:J:311:GLU:CD	3:K:290:ARG:NH1	2.64	0.45
3:J:311:GLU:OE1	3:K:290:ARG:NH1	2.49	0.45
3:M:324:LEU:O	3:M:328:ASN:ND2	2.49	0.45
3:Q:324:LEU:O	3:Q:328:ASN:ND2	2.49	0.45
3:R:301:ALA:O	3:R:305:ILE:HG13	2.16	0.45
1:E:374:THR:HB	1:E:397:LYS:HG2	1.97	0.45
1:F:263:VAL:CG1	1:F:267:SER:HB2	2.46	0.45
1:F:172:TYR:HE1	1:F:428:PHE:CE2	2.14	0.45
1:F:199:SER:CA	1:F:237:LEU:HD21	2.47	0.45
1:A:163:ARG:HD3	1:F:351:ILE:HG12	1.99	0.45
1:F:357:ALA:HB3	1:F:360:PHE:CE1	2.51	0.45
1:C:239:GLY:H	1:C:253:LYS:CE	2.30	0.45
1:D:247:GLU:O	1:D:251:ARG:HB2	2.17	0.45
3:J:301:ALA:O	3:J:305:ILE:HG13	2.16	0.45
1:C:135:VAL:HB	1:C:142:LYS:HE2	1.99	0.44
1:C:206:TRP:HZ3	2:G:167:ILE:HB	1.82	0.44
1:C:245:GLU:O	1:C:249:SER:CB	2.57	0.44
1:C:370:THR:O	1:C:371:ARG:O	2.35	0.44
1:D:355:GLN:HA	1:D:388:TRP:CD1	2.51	0.44
1:E:250:ARG:O	1:E:254:THR:OG1	2.34	0.44
1:E:370:THR:O	1:E:371:ARG:O	2.35	0.44
3:J:300:LEU:HD12	3:J:323:ALA:HA	1.99	0.44
1:C:388:TRP:CZ3	1:D:155:PHE:CE2	3.04	0.44
1:D:388:TRP:HZ3	1:E:155:PHE:HZ	1.60	0.44
3:H:301:ALA:O	3:H:305:ILE:HG13	2.16	0.44
1:F:394:ASP:C	1:F:396:LEU:N	2.75	0.44
1:A:334:TYR:CE1	1:A:415:PRO:HG3	2.52	0.44
1:B:370:THR:O	1:B:371:ARG:O	2.35	0.44
3:P:300:LEU:HD12	3:P:323:ALA:HA	1.99	0.44
3:P:308:LEU:CD1	3:Q:298:GLN:HG3	2.44	0.44
3:R:300:LEU:HD12	3:R:323:ALA:HA	1.99	0.44
1:F:353:LYS:CB	1:F:399:PRO:HG3	2.41	0.44
1:A:194:PHE:HD1	1:A:228:ILE:HG23	1.83	0.44
1:B:388:TRP:CH2	1:C:155:PHE:CZ	3.05	0.44
1:C:337:SER:OG	1:D:288:ARG:NH1	2.50	0.44
1:D:370:THR:O	1:D:371:ARG:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:354:ILE:CG2	1:F:396:LEU:HD11	2.46	0.44
1:F:363:VAL:O	1:F:364:SER:HB3	2.18	0.44
1:B:250:ARG:O	1:B:254:THR:OG1	2.34	0.44
1:D:350:PRO:HB3	1:D:399:PRO:HB2	2.00	0.44
1:F:370:THR:O	1:F:371:ARG:O	2.35	0.43
1:A:363:VAL:O	1:A:364:SER:HB3	2.18	0.43
1:B:351:ILE:HA	1:B:354:ILE:HG22	2.00	0.43
1:B:363:VAL:O	1:B:364:SER:HB3	2.18	0.43
1:F:354:ILE:CG2	1:F:396:LEU:CD1	2.87	0.43
1:A:210:SER:OG	1:A:247:GLU:OE2	2.22	0.43
1:A:375:PRO:HD2	1:A:399:PRO:HG3	2.01	0.43
1:A:388:TRP:HH2	1:B:155:PHE:HE2	1.63	0.43
1:C:261:ASN:OD1	1:C:262:GLY:N	2.51	0.43
1:D:363:VAL:O	1:D:364:SER:HB3	2.18	0.43
1:F:351:ILE:CD1	1:F:398:GLU:OE1	2.66	0.43
1:A:358:THR:HG22	1:A:359:HIS:HD2	1.75	0.43
1:D:373:LEU:CD1	1:D:391:ILE:HG12	2.48	0.43
1:D:434:GLN:HG3	1:D:435:GLU:H	1.84	0.43
1:E:373:LEU:CD1	1:E:391:ILE:HG12	2.49	0.43
1:B:373:LEU:CD1	1:B:391:ILE:HG12	2.49	0.43
1:C:239:GLY:H	1:C:253:LYS:HE2	1.83	0.43
1:D:355:GLN:HA	1:D:388:TRP:HD1	1.84	0.43
1:B:357:ALA:CB	1:B:375:PRO:HB3	2.49	0.43
1:B:434:GLN:HG3	1:B:435:GLU:H	1.84	0.43
1:E:247:GLU:HG2	1:E:251:ARG:NH1	2.34	0.43
1:F:346:ALA:CB	1:F:406:PHE:CE1	2.96	0.43
1:F:351:ILE:HD11	1:F:398:GLU:OE1	2.18	0.43
1:F:373:LEU:CD1	1:F:391:ILE:HG12	2.49	0.43
3:H:300:LEU:HD12	3:H:323:ALA:HA	1.99	0.43
3:N:300:LEU:HD12	3:N:323:ALA:HA	1.99	0.43
1:A:358:THR:HG21	3:H:303:TYR:CE1	2.53	0.43
1:C:210:SER:OG	1:C:247:GLU:OE2	2.36	0.43
1:C:363:VAL:O	1:C:364:SER:HB3	2.18	0.43
1:D:374:THR:OG1	1:D:397:LYS:O	2.33	0.43
1:E:363:VAL:O	1:E:364:SER:HB3	2.18	0.43
1:F:132:TRP:CE2	1:F:189:GLU:HG3	2.53	0.43
1:F:292:ARG:HH21	1:F:433:GLY:C	2.27	0.43
1:A:398:GLU:H	1:A:398:GLU:HG3	1.59	0.43
3:L:300:LEU:HD12	3:L:323:ALA:HA	1.99	0.43
1:C:196:SER:O	1:C:196:SER:OG	2.35	0.43
1:C:283:ASP:HB3	1:C:286:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:GLN:HG3	1:C:435:GLU:H	1.84	0.42
1:F:354:ILE:CG1	1:F:399:PRO:CD	2.69	0.42
1:D:283:ASP:HB3	1:D:286:ILE:HD12	2.01	0.42
1:F:238:THR:O	1:F:283:ASP:CB	2.63	0.42
3:L:317:LYS:N	3:M:327:LEU:HD21	2.35	0.42
3:R:317:LYS:N	3:S:327:LEU:HD21	2.35	0.42
1:A:283:ASP:HB3	1:A:286:ILE:HD12	2.01	0.42
1:D:398:GLU:HA	1:D:399:PRO:HD3	1.79	0.42
1:F:265:ASN:N	1:F:265:ASN:HD22	2.17	0.42
1:F:350:PRO:HA	1:F:399:PRO:CB	2.49	0.42
1:F:422:LEU:O	1:F:426:GLU:HG3	2.19	0.42
3:R:327:LEU:HD21	3:S:317:LYS:N	2.35	0.42
3:J:317:LYS:N	3:K:327:LEU:HD21	2.35	0.42
1:B:224:ASN:O	1:B:227:SER:OG	2.37	0.42
1:B:283:ASP:HB3	1:B:286:ILE:HD12	2.01	0.42
1:B:374:THR:HB	1:B:397:LYS:HB3	2.00	0.42
1:F:238:THR:HB	1:F:283:ASP:CB	2.50	0.42
3:H:327:LEU:HD21	3:I:317:LYS:N	2.35	0.42
3:N:300:LEU:HD12	3:N:323:ALA:N	2.35	0.42
3:P:300:LEU:HD12	3:P:323:ALA:N	2.35	0.42
1:A:249:SER:HB3	1:A:250:ARG:NH1	2.34	0.42
1:B:318:VAL:HG11	1:B:402:THR:HG23	2.00	0.42
1:B:357:ALA:HB2	1:B:375:PRO:HB3	2.02	0.42
1:F:173:GLY:CA	1:F:425:GLN:OE1	2.62	0.42
1:F:174:PRO:HD3	1:F:425:GLN:HG3	2.02	0.42
3:N:317:LYS:N	3:O:327:LEU:HD21	2.35	0.42
3:N:327:LEU:HD21	3:O:317:LYS:N	2.35	0.42
3:R:300:LEU:HD12	3:R:323:ALA:N	2.35	0.42
1:B:218:PHE:CD2	1:B:259:GLN:HG3	2.54	0.42
1:D:354:ILE:CD1	1:D:396:LEU:HD11	2.49	0.42
1:E:359:HIS:HA	1:E:384:ILE:O	2.20	0.42
1:E:396:LEU:HD21	1:F:158:LEU:HD11	1.99	0.42
3:J:308:LEU:CD1	3:K:298:GLN:HG3	2.44	0.42
3:N:308:LEU:CD1	3:O:298:GLN:HG3	2.44	0.42
1:B:398:GLU:HA	1:B:399:PRO:HD3	1.96	0.42
3:H:317:LYS:N	3:I:327:LEU:HD21	2.35	0.42
3:L:327:LEU:HD21	3:M:317:LYS:N	2.35	0.42
3:P:317:LYS:N	3:Q:327:LEU:HD21	2.35	0.42
1:E:315:THR:OG1	1:F:162:ASN:HB2	2.20	0.42
3:R:311:GLU:CD	3:S:290:ARG:NH1	2.64	0.42
1:B:359:HIS:HA	1:B:384:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:ASN:OD1	1:D:262:GLY:N	2.51	0.41
1:E:283:ASP:HB3	1:E:286:ILE:HD12	2.01	0.41
1:E:374:THR:HB	1:E:397:LYS:HB3	2.02	0.41
3:H:300:LEU:HD12	3:H:323:ALA:N	2.35	0.41
3:J:330:ILE:OXT	3:J:330:ILE:CG2	2.68	0.41
3:R:330:ILE:OXT	3:R:330:ILE:CG2	2.68	0.41
1:C:204:SER:OG	1:C:205:LYS:N	2.52	0.41
3:N:321:THR:O	3:N:322:LYS:C	2.64	0.41
3:S:330:ILE:OXT	3:S:330:ILE:CG2	2.69	0.41
1:F:317:CYS:HB2	1:F:401:LEU:HB3	2.01	0.41
3:K:321:THR:O	3:K:322:LYS:C	2.64	0.41
1:B:299:PRO:HG3	1:B:307:MET:HE1	2.02	0.41
1:C:339:ILE:HA	1:C:342:VAL:HG22	2.03	0.41
1:D:250:ARG:O	1:D:254:THR:OG1	2.34	0.41
1:E:339:ILE:HA	1:E:342:VAL:HG22	2.03	0.41
3:J:327:LEU:HD21	3:K:317:LYS:N	2.35	0.41
1:A:373:LEU:CD1	1:A:391:ILE:HG12	2.49	0.41
1:C:402:THR:HG22	1:C:404:LYS:H	1.84	0.41
1:D:359:HIS:HA	1:D:384:ILE:O	2.20	0.41
3:H:305:ILE:HD13	3:I:302:LYS:HG3	2.03	0.41
3:J:321:THR:O	3:J:322:LYS:C	2.64	0.41
3:L:305:ILE:HD13	3:M:302:LYS:HG3	2.03	0.41
1:F:350:PRO:HA	1:F:399:PRO:HG2	2.01	0.41
3:H:330:ILE:OXT	3:H:330:ILE:CG2	2.68	0.41
3:P:330:ILE:OXT	3:P:330:ILE:CG2	2.68	0.41
1:B:422:LEU:HD23	1:B:422:LEU:HA	1.89	0.41
1:D:339:ILE:HA	1:D:342:VAL:HG22	2.03	0.41
3:M:330:ILE:OXT	3:M:330:ILE:CG2	2.68	0.41
1:A:228:ILE:HD12	1:A:271:LEU:HD23	2.02	0.41
1:A:385:GLU:OE2	3:H:303:TYR:OH	2.30	0.41
1:F:172:TYR:CZ	1:F:428:PHE:HB3	2.50	0.41
1:F:225:LYS:NZ	1:F:268:GLN:O	2.43	0.41
1:F:287:ARG:HG2	1:F:293:ARG:NH2	2.36	0.41
3:I:330:ILE:OXT	3:I:330:ILE:CG2	2.68	0.41
3:P:327:LEU:HD21	3:Q:317:LYS:N	2.35	0.41
1:A:205:LYS:HD3	1:B:206:TRP:HB3	2.02	0.41
1:B:339:ILE:HA	1:B:342:VAL:HG22	2.03	0.41
1:C:373:LEU:CD1	1:C:391:ILE:HG12	2.49	0.41
1:E:261:ASN:OD1	1:E:262:GLY:N	2.51	0.41
1:F:155:PHE:HB3	1:F:158:LEU:HD23	2.02	0.41
1:F:200:SER:HB3	1:F:233:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:300:LEU:HD12	3:L:323:ALA:N	2.35	0.41
3:O:330:ILE:OXT	3:O:330:ILE:CG2	2.69	0.41
3:Q:330:ILE:OXT	3:Q:330:ILE:CG2	2.68	0.41
3:R:321:THR:O	3:R:322:LYS:C	2.64	0.41
3:S:321:THR:O	3:S:322:LYS:C	2.64	0.41
1:B:357:ALA:HB3	1:B:360:PHE:CZ	2.55	0.40
1:C:359:HIS:HA	1:C:384:ILE:O	2.20	0.40
1:F:359:HIS:HA	1:F:384:ILE:O	2.20	0.40
3:J:291:ALA:C	3:J:294:ILE:HG12	2.46	0.40
3:J:300:LEU:HD12	3:J:323:ALA:N	2.35	0.40
3:O:321:THR:O	3:O:322:LYS:C	2.64	0.40
1:D:398:GLU:H	1:D:398:GLU:HG2	1.73	0.40
3:N:305:ILE:HD13	3:O:302:LYS:HG3	2.03	0.40
3:R:308:LEU:CD1	3:S:298:GLN:HG3	2.44	0.40
1:A:359:HIS:HA	1:A:384:ILE:O	2.20	0.40
1:F:172:TYR:OH	1:F:428:PHE:C	2.64	0.40
3:N:291:ALA:C	3:N:294:ILE:HG12	2.47	0.40
1:A:339:ILE:HA	1:A:342:VAL:HG22	2.03	0.40
1:C:388:TRP:CH2	1:D:155:PHE:CZ	3.08	0.40
1:E:137:GLY:O	1:E:142:LYS:HE3	2.21	0.40
3:H:321:THR:O	3:H:322:LYS:C	2.64	0.40
3:I:321:THR:O	3:I:322:LYS:C	2.64	0.40
3:L:330:ILE:OXT	3:L:330:ILE:CG2	2.69	0.40
1:A:325:ARG:NH1	3:S:310:TYR:CB	2.64	0.40
3:L:308:LEU:CD1	3:M:298:GLN:HG3	2.44	0.40
3:Q:321:THR:O	3:Q:322:LYS:C	2.64	0.40
3:R:291:ALA:C	3:R:294:ILE:HG12	2.47	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	310/519 (60%)	274 (88%)	31 (10%)	5 (2%)	8	37
1	B	318/519 (61%)	284 (89%)	29 (9%)	5 (2%)	8	37
1	C	318/519 (61%)	280 (88%)	33 (10%)	5 (2%)	8	37
1	D	318/519 (61%)	279 (88%)	33 (10%)	6 (2%)	6	34
1	E	300/519 (58%)	260 (87%)	36 (12%)	4 (1%)	10	41
1	F	304/519 (59%)	277 (91%)	20 (7%)	7 (2%)	5	29
2	G	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
3	H	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	1	13
3	I	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	4	28
3	J	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	1	13
3	K	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	4	28
3	L	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	1	13
3	M	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	4	28
3	N	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	1	13
3	O	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	4	28
3	P	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	1	13
3	Q	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	4	28
3	R	40/330 (12%)	31 (78%)	7 (18%)	2 (5%)	1	13
3	S	40/330 (12%)	34 (85%)	5 (12%)	1 (2%)	4	28
All	All	2356/7084 (33%)	2050 (87%)	256 (11%)	50 (2%)	8	31

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	HIS
1	A	371	ARG
1	A	395	GLU
1	B	371	ARG
1	B	395	GLU
1	C	371	ARG
1	C	395	GLU
1	D	359	HIS
1	D	371	ARG
1	D	395	GLU
1	E	371	ARG
1	E	395	GLU

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Mol	Chain	Res	Type
1	F	299	PRO
1	F	371	ARG
1	F	395	GLU
1	C	359	HIS
1	F	207	MET
3	H	312	ASP
3	I	312	ASP
3	J	312	ASP
3	K	312	ASP
3	L	312	ASP
3	M	312	ASP
3	N	312	ASP
3	O	312	ASP
3	P	312	ASP
3	Q	312	ASP
3	R	312	ASP
3	S	312	ASP
1	A	381	ASP
1	B	359	HIS
1	B	381	ASP
1	C	381	ASP
1	D	381	ASP
1	E	381	ASP
1	F	381	ASP
3	H	290	ARG
3	J	290	ARG
3	L	290	ARG
3	N	290	ARG
3	P	290	ARG
3	R	290	ARG
1	F	359	HIS
1	A	370	THR
1	B	370	THR
1	C	370	THR
1	D	370	THR
1	E	370	THR
1	F	370	THR
1	D	399	PRO

### 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	266/418 (64%)	258 (97%)	8 (3%)	36	66
1	B	273/418 (65%)	270 (99%)	3 (1%)	70	86
1	C	273/418 (65%)	270 (99%)	3 (1%)	70	86
1	D	273/418 (65%)	268 (98%)	5 (2%)	54	77
1	E	259/418 (62%)	255 (98%)	4 (2%)	60	81
1	F	262/418 (63%)	247 (94%)	15 (6%)	17	50
2	G	8/8 (100%)	8 (100%)	0	100	100
3	H	36/294 (12%)	33 (92%)	3 (8%)	9	35
3	I	36/294 (12%)	33 (92%)	3 (8%)	9	35
3	J	36/294 (12%)	33 (92%)	3 (8%)	9	35
3	K	36/294 (12%)	33 (92%)	3 (8%)	9	35
3	L	36/294 (12%)	33 (92%)	3 (8%)	9	35
3	M	36/294 (12%)	33 (92%)	3 (8%)	9	35
3	N	36/294 (12%)	33 (92%)	3 (8%)	9	35
3	O	36/294 (12%)	33 (92%)	3 (8%)	9	35
3	P	36/294 (12%)	33 (92%)	3 (8%)	9	35
3	Q	36/294 (12%)	33 (92%)	3 (8%)	9	35
3	R	36/294 (12%)	33 (92%)	3 (8%)	9	35
3	S	36/294 (12%)	33 (92%)	3 (8%)	9	35
All	All	2046/6044 (34%)	1972 (96%)	74 (4%)	32	62

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	356	SER
1	A	358	THR
1	A	370	THR
1	A	373	LEU

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Mol	Chain	Res	Type
1	A	397	LYS
1	A	398	GLU
1	A	400	ASP
1	A	401	LEU
1	B	370	THR
1	B	373	LEU
1	B	398	GLU
1	C	370	THR
1	C	373	LEU
1	C	397	LYS
1	D	358	THR
1	D	370	THR
1	D	373	LEU
1	D	397	LYS
1	D	398	GLU
1	E	358	THR
1	E	370	THR
1	E	373	LEU
1	E	397	LYS
1	F	127	LYS
1	F	139	GLU
1	F	200	SER
1	F	209	GLU
1	F	215	LYS
1	F	278	ILE
1	F	291	GLU
1	F	312	VAL
1	F	341	VAL
1	F	351	ILE
1	F	370	THR
1	F	373	LEU
1	F	397	LYS
1	F	412	SER
1	F	417	VAL
3	H	314	PRO
3	H	317	LYS
3	H	319	GLU
3	I	314	PRO
3	I	317	LYS
3	I	319	GLU
3	J	314	PRO
3	J	317	LYS

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Mol	Chain	Res	Type
3	J	319	GLU
3	K	314	PRO
3	K	317	LYS
3	K	319	GLU
3	L	314	PRO
3	L	317	LYS
3	L	319	GLU
3	M	314	PRO
3	M	317	LYS
3	M	319	GLU
3	N	314	PRO
3	N	317	LYS
3	N	319	GLU
3	O	314	PRO
3	O	317	LYS
3	O	319	GLU
3	P	314	PRO
3	P	317	LYS
3	P	319	GLU
3	Q	314	PRO
3	Q	317	LYS
3	Q	319	GLU
3	R	314	PRO
3	R	317	LYS
3	R	319	GLU
3	S	314	PRO
3	S	317	LYS
3	S	319	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	GLN
1	A	359	HIS
1	C	311	ASN
1	C	349	GLN
1	C	359	HIS
1	C	434	GLN
1	D	216	GLN
1	D	359	HIS
1	D	434	GLN
1	E	349	GLN

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Mol	Chain	Res	Type
1	F	157	HIS
1	F	162	ASN
1	F	191	ASN
1	F	216	GLN
1	F	265	ASN
1	F	355	GLN
1	F	425	GLN
1	F	427	GLN
3	H	296	GLN
3	H	328	ASN
3	I	298	GLN
3	I	328	ASN
3	J	296	GLN
3	K	298	GLN
3	K	328	ASN
3	L	296	GLN
3	M	298	GLN
3	M	328	ASN
3	N	296	GLN
3	O	298	GLN
3	O	328	ASN
3	P	296	GLN
3	Q	298	GLN
3	Q	328	ASN
3	R	296	GLN
3	S	298	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	BEF	A	702	4	0,3,3	-	-	-		
5	BEF	C	702	4	0,3,3	-	-	-		
4	ADP	A	701	5,6	24,29,29	1.67	4 (16%)	29,45,45	1.73	7 (24%)
4	ADP	D	701	6	24,29,29	1.01	0	29,45,45	1.62	6 (20%)
4	ADP	C	701	5,6	24,29,29	2.02	5 (20%)	29,45,45	2.11	11 (37%)
5	BEF	B	702	4	0,3,3	-	-	-		
4	ADP	B	701	5,6	24,29,29	1.97	6 (25%)	29,45,45	1.84	8 (27%)
4	ADP	E	701	-	24,29,29	0.89	0	29,45,45	1.28	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	701	5,6	-	6/12/32/32	0/3/3/3
4	ADP	D	701	6	-	1/12/32/32	0/3/3/3
4	ADP	C	701	5,6	-	2/12/32/32	0/3/3/3
4	ADP	B	701	5,6	-	4/12/32/32	0/3/3/3
4	ADP	E	701	-	-	3/12/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	701	ADP	PA-O3A	-6.64	1.52	1.59
4	B	701	ADP	PA-O3A	-6.62	1.52	1.59
4	A	701	ADP	PA-O3A	-5.15	1.53	1.59
4	C	701	ADP	C8-N7	-3.12	1.29	1.34
4	C	701	ADP	C1'-N9	-3.09	1.42	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	ADP	C8-N7	-2.81	1.29	1.34
4	B	701	ADP	PA-O2A	-2.60	1.43	1.55
4	A	701	ADP	C8-N7	-2.60	1.30	1.34
4	A	701	ADP	C1'-N9	-2.55	1.43	1.49
4	A	701	ADP	PB-O2B	-2.34	1.46	1.54
4	C	701	ADP	PA-O2A	-2.30	1.44	1.55
4	B	701	ADP	PB-O2B	-2.29	1.46	1.54
4	C	701	ADP	PB-O2B	-2.27	1.46	1.54
4	B	701	ADP	C1'-N9	-2.16	1.44	1.49
4	B	701	ADP	C4-N3	-2.15	1.32	1.35

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	701	ADP	C4'-O4'-C1'	-4.90	105.44	109.92
4	C	701	ADP	O4'-C1'-N9	-4.87	102.28	108.75
4	B	701	ADP	O3B-PB-O1B	-4.23	94.35	110.83
4	B	701	ADP	O4'-C1'-N9	-4.22	103.15	108.75
4	E	701	ADP	N3-C2-N1	-4.13	123.07	128.67
4	A	701	ADP	C2'-C3'-C4'	-4.02	94.84	102.61
4	D	701	ADP	N3-C2-N1	-3.69	123.66	128.67
4	C	701	ADP	O2B-PB-O3A	3.60	116.71	104.64
4	A	701	ADP	O3B-PB-O1B	-3.58	96.89	110.83
4	C	701	ADP	C4-C5-N7	3.40	112.93	109.34
4	A	701	ADP	C4'-O4'-C1'	-3.38	106.83	109.92
4	C	701	ADP	O3B-PB-O1B	-3.27	98.10	110.83
4	B	701	ADP	O2B-PB-O3A	3.26	115.57	104.64
4	D	701	ADP	C4'-O4'-C1'	3.25	112.90	109.92
4	A	701	ADP	O2B-PB-O3A	3.02	114.76	104.64
4	B	701	ADP	C4-C5-N7	2.92	112.42	109.34
4	E	701	ADP	C4-C5-N7	-2.90	106.27	109.34
4	D	701	ADP	O3'-C3'-C4'	-2.74	103.20	111.08
4	A	701	ADP	C5-C6-N6	2.71	124.45	120.31
4	B	701	ADP	O3B-PB-O3A	2.69	113.66	104.64
4	D	701	ADP	O3'-C3'-C2'	-2.68	103.23	111.82
4	D	701	ADP	O3B-PB-O2B	2.50	117.18	107.80
4	C	701	ADP	O4'-C4'-C3'	-2.46	100.27	105.15
4	B	701	ADP	O2'-C2'-C3'	-2.38	104.18	111.82
4	A	701	ADP	O5'-PA-O1A	2.25	117.85	108.94
4	B	701	ADP	O3'-C3'-C2'	-2.24	104.64	111.82
4	C	701	ADP	O2A-PA-O5'	2.19	117.50	107.57
4	C	701	ADP	C2'-C3'-C4'	-2.12	98.51	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	701	ADP	O2'-C2'-C3'	-2.12	105.01	111.82
4	C	701	ADP	O3B-PB-O3A	2.10	111.66	104.64
4	A	701	ADP	O4'-C4'-C3'	-2.03	101.12	105.15
4	B	701	ADP	O2A-PA-O5'	2.03	116.76	107.57
4	C	701	ADP	O3B-PB-O2B	2.01	115.34	107.80
4	D	701	ADP	O2A-PA-O1A	2.01	121.79	112.44

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	ADP	PA-O3A-PB-O2B
4	A	701	ADP	C5'-O5'-PA-O2A
4	A	701	ADP	C5'-O5'-PA-O3A
4	B	701	ADP	PA-O3A-PB-O2B
4	E	701	ADP	C5'-O5'-PA-O2A
4	E	701	ADP	C5'-O5'-PA-O3A
4	B	701	ADP	C3'-C4'-C5'-O5'
4	B	701	ADP	O4'-C4'-C5'-O5'
4	C	701	ADP	O4'-C4'-C5'-O5'
4	A	701	ADP	C3'-C4'-C5'-O5'
4	A	701	ADP	C5'-O5'-PA-O1A
4	C	701	ADP	C5'-O5'-PA-O3A
4	D	701	ADP	C5'-O5'-PA-O1A
4	E	701	ADP	C5'-O5'-PA-O1A
4	A	701	ADP	O4'-C4'-C5'-O5'
4	B	701	ADP	PA-O3A-PB-O1B

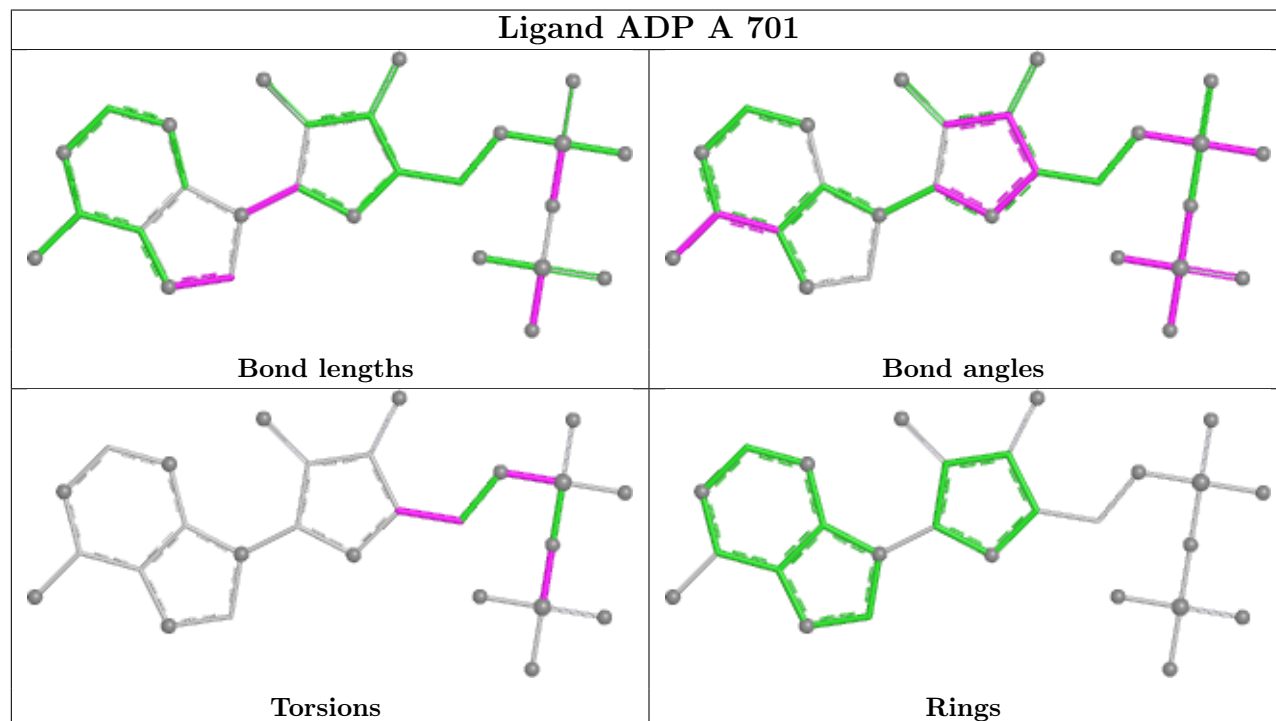
There are no ring outliers.

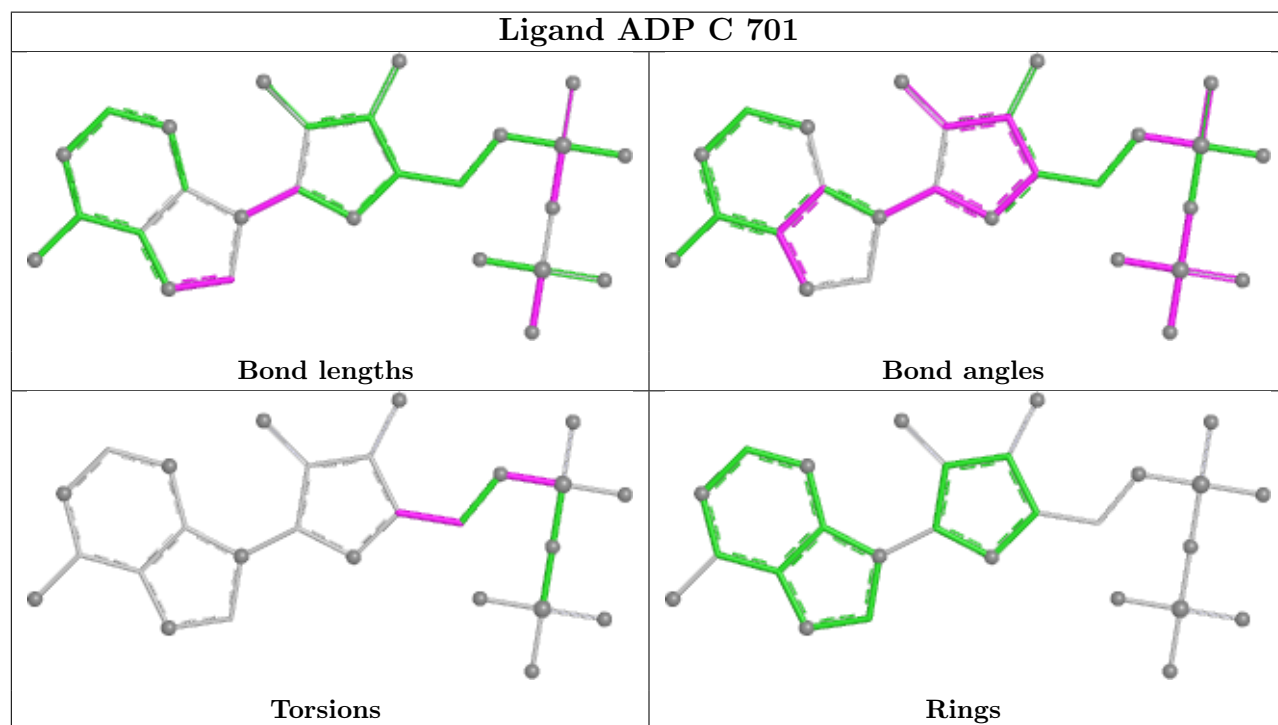
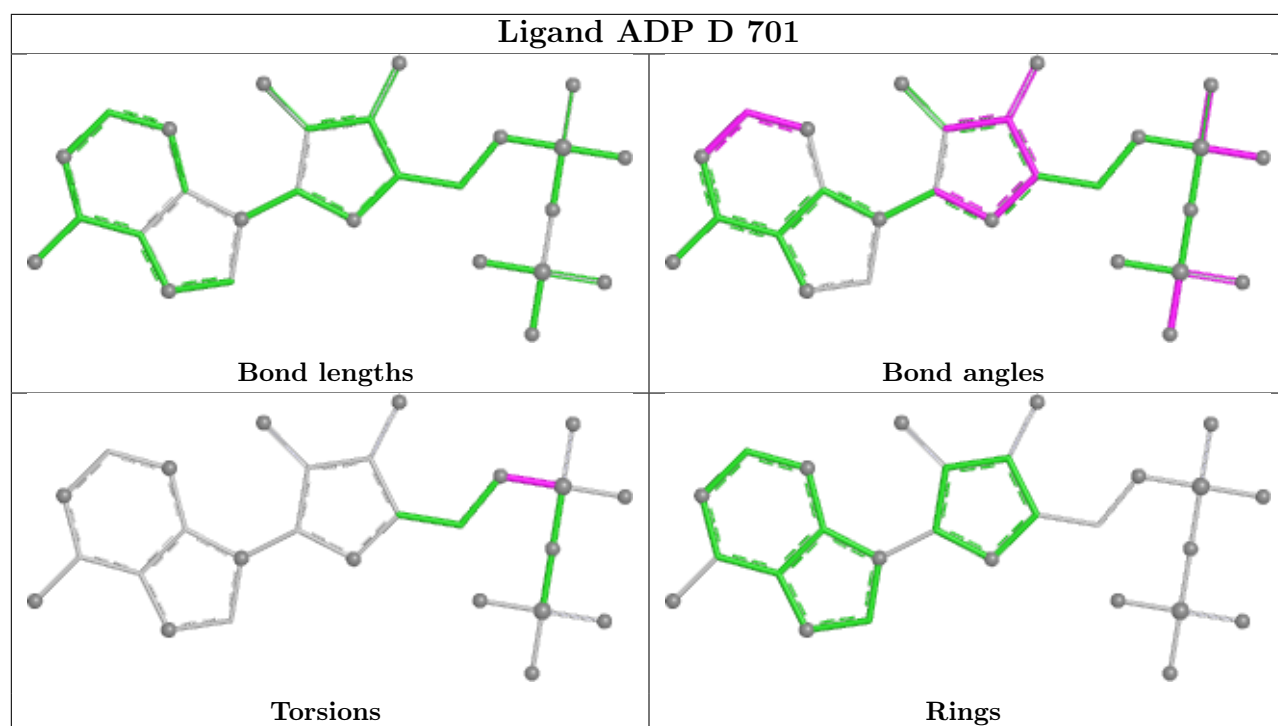
6 monomers are involved in 3 short contacts:

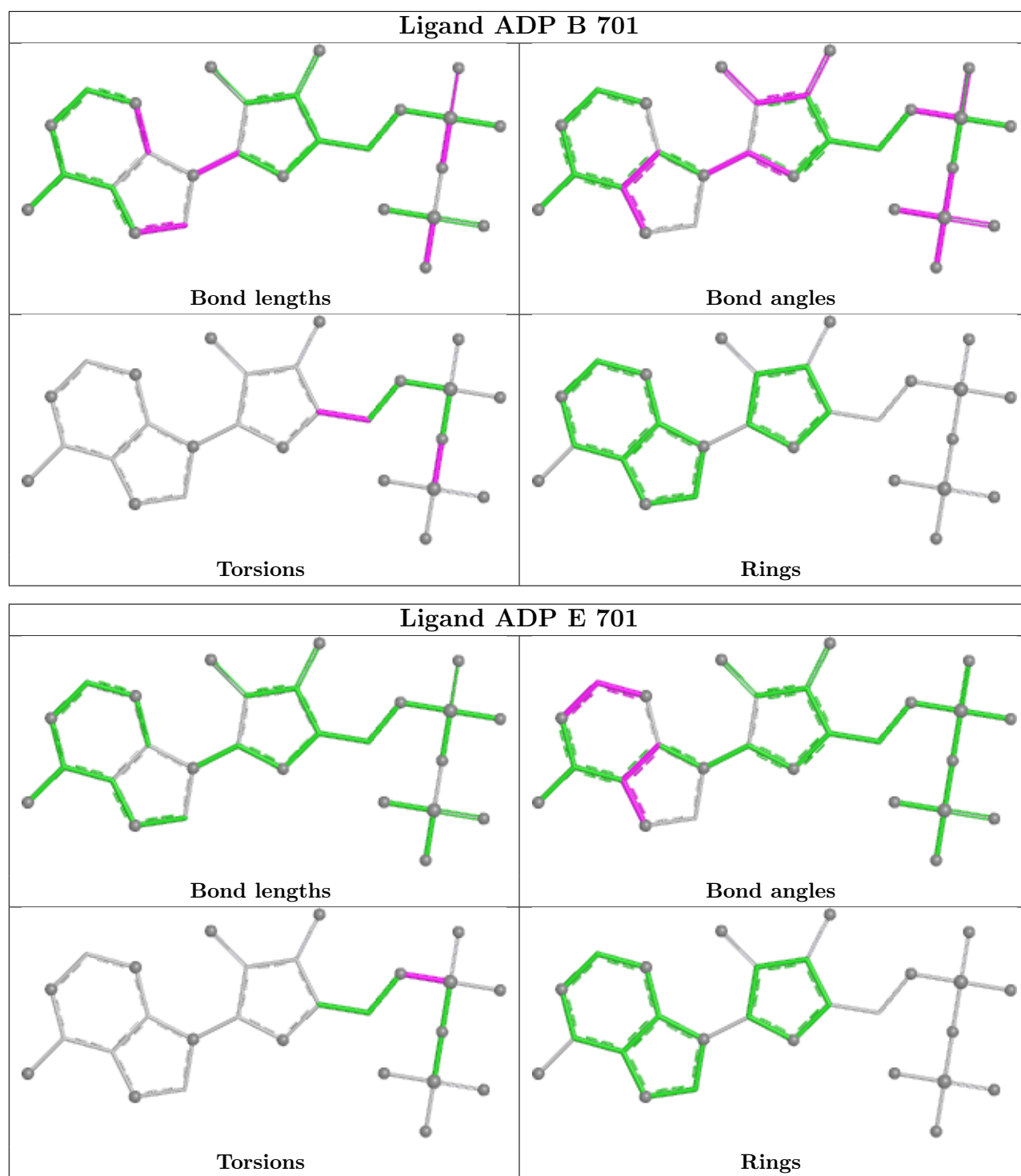
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	702	BEF	1	0
5	C	702	BEF	1	0
4	A	701	ADP	1	0
4	C	701	ADP	1	0
5	B	702	BEF	1	0
4	B	701	ADP	1	0

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

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







## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

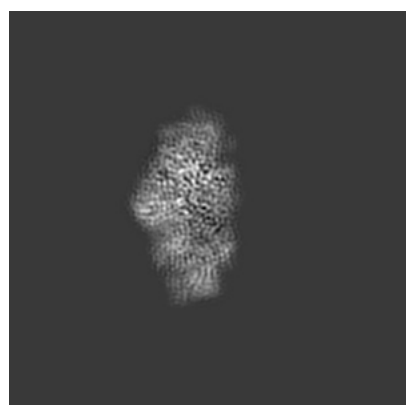
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8887. These allow visual inspection of the internal detail of the map and identification of artifacts.

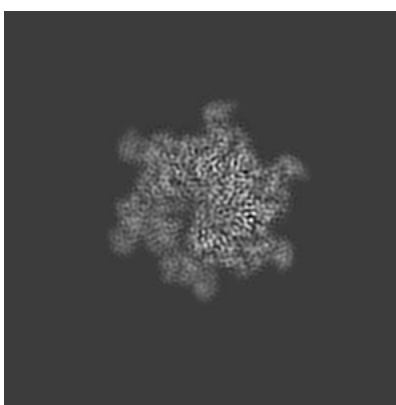
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

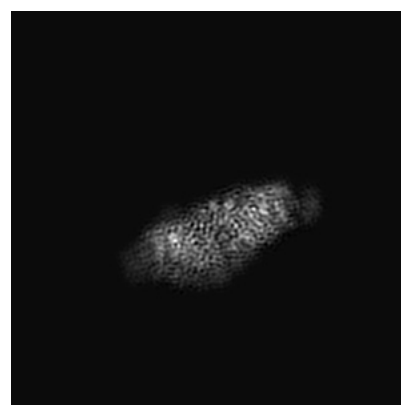
#### 6.1.1 Primary map



X



Y

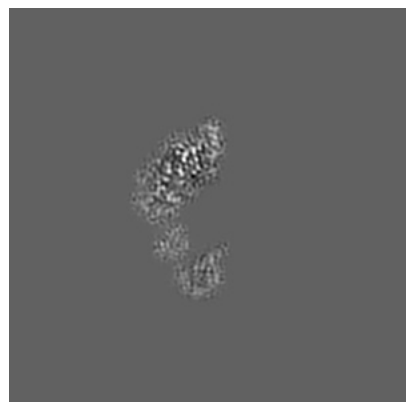


Z

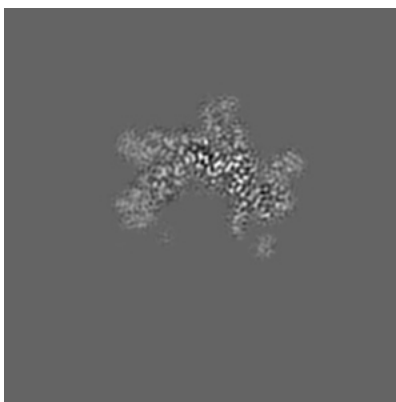
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

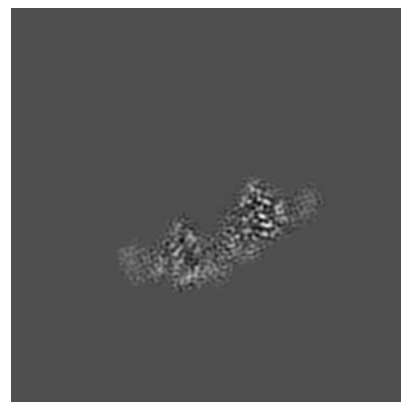
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

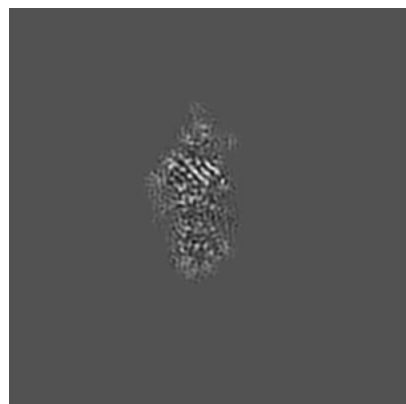


Z Index: 128

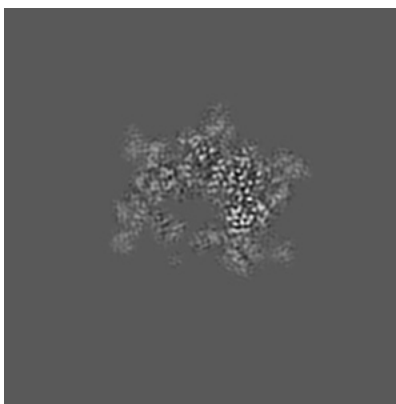
The images above show central slices of the map in three orthogonal directions.

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

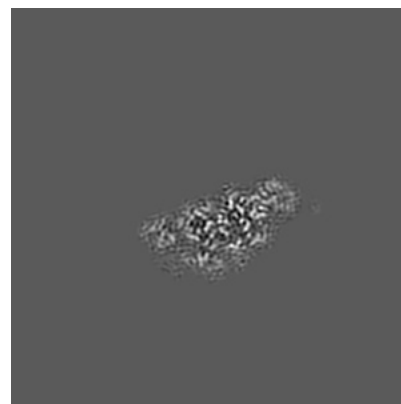
### 6.3.1 Primary map



X Index: 147



Y Index: 118

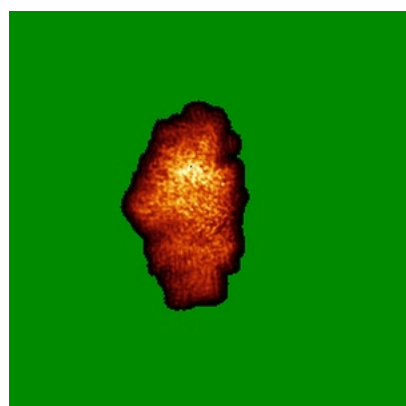


Z Index: 150

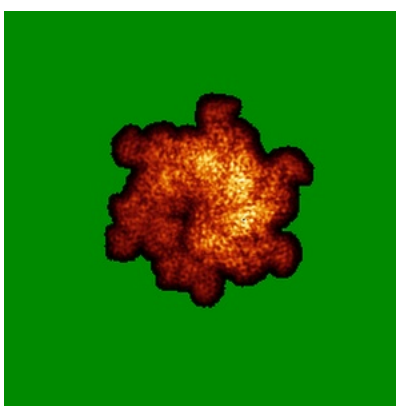
The images above show the largest variance slices of the map in three orthogonal directions.

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

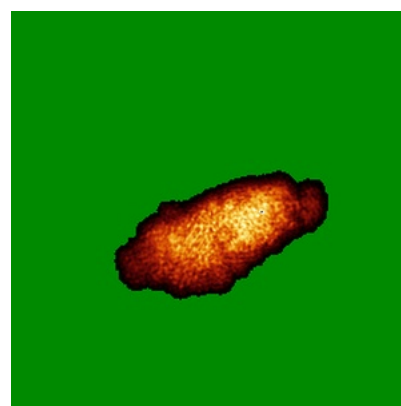
### 6.4.1 Primary map



X



Y

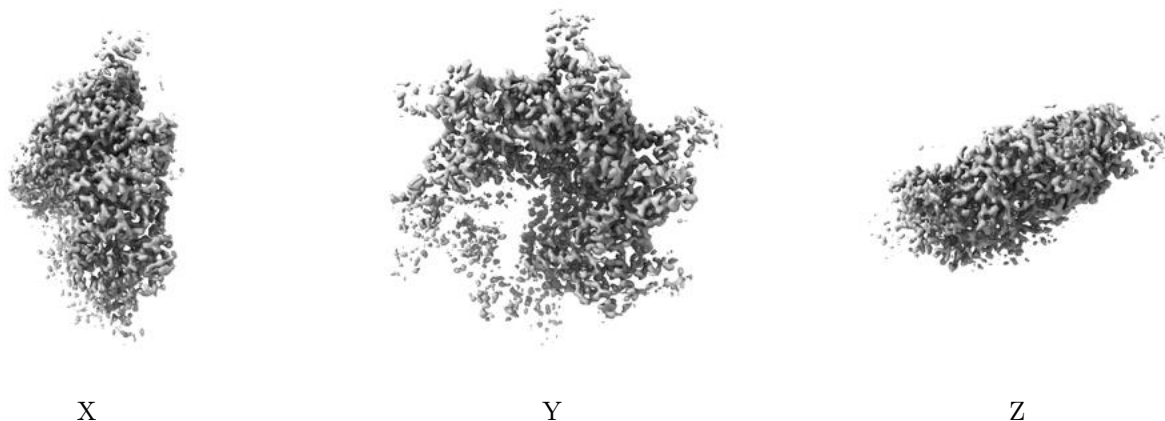


Z

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 0.0749. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

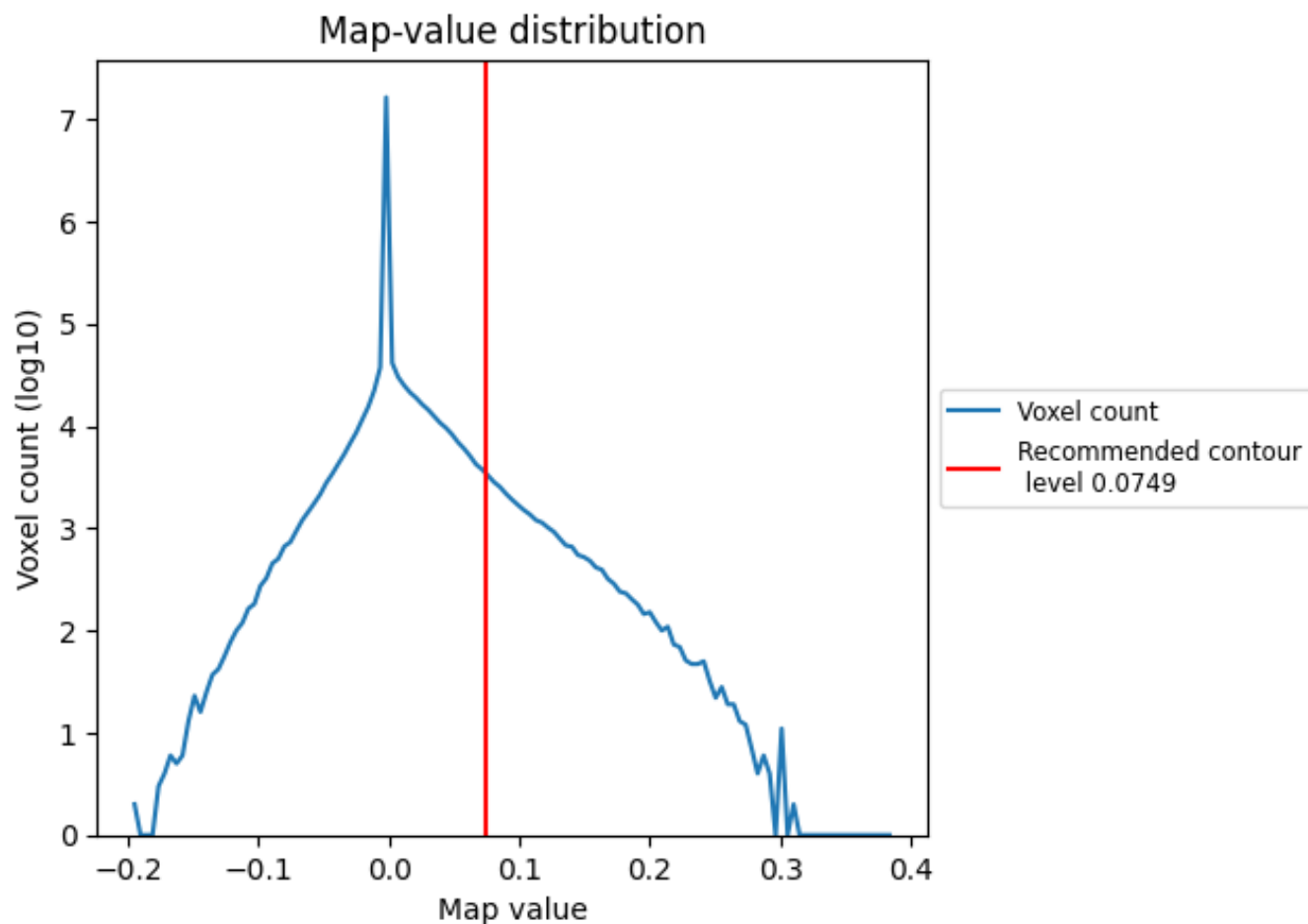
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

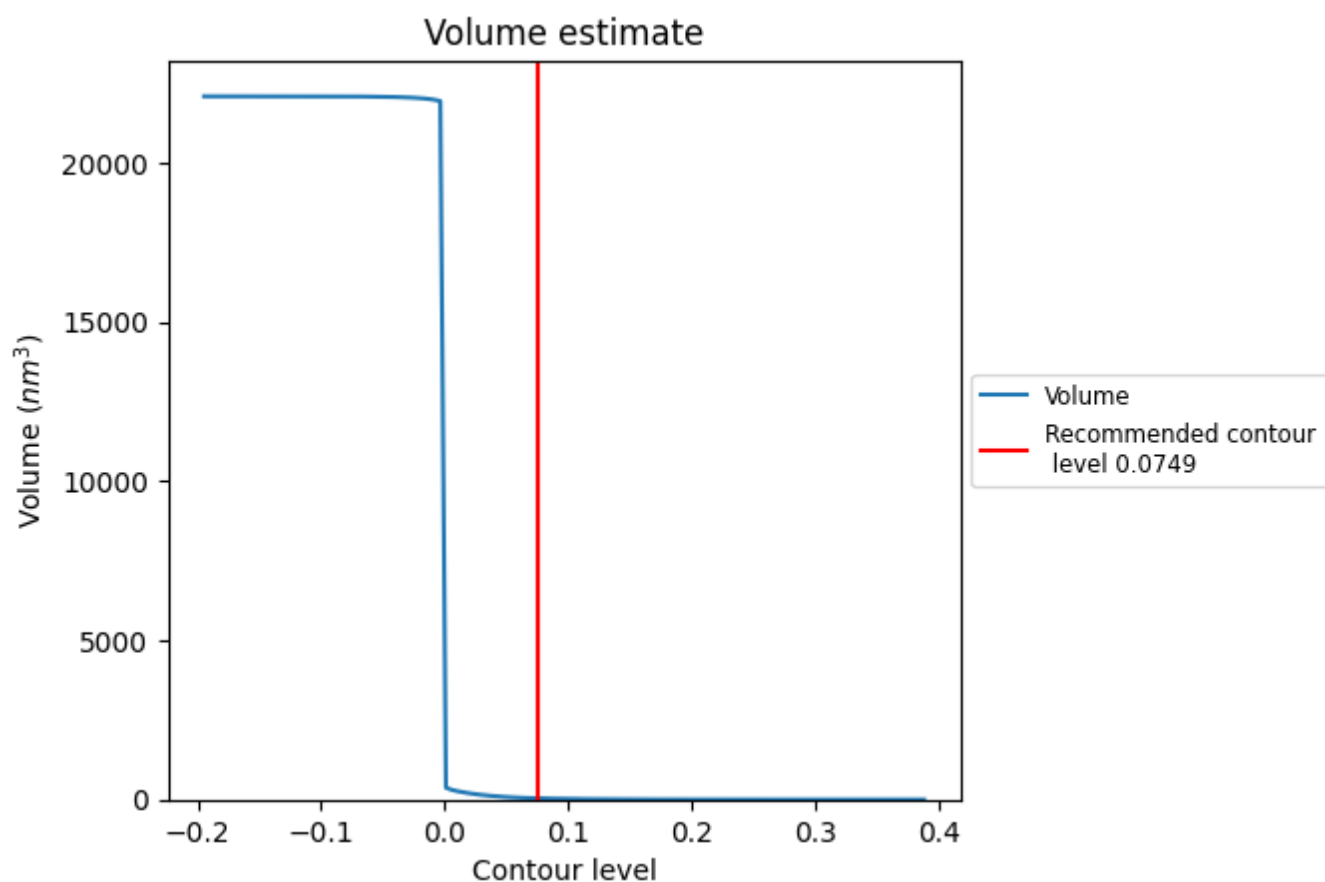
This section contains the results of statistical analysis of the map.

### 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.

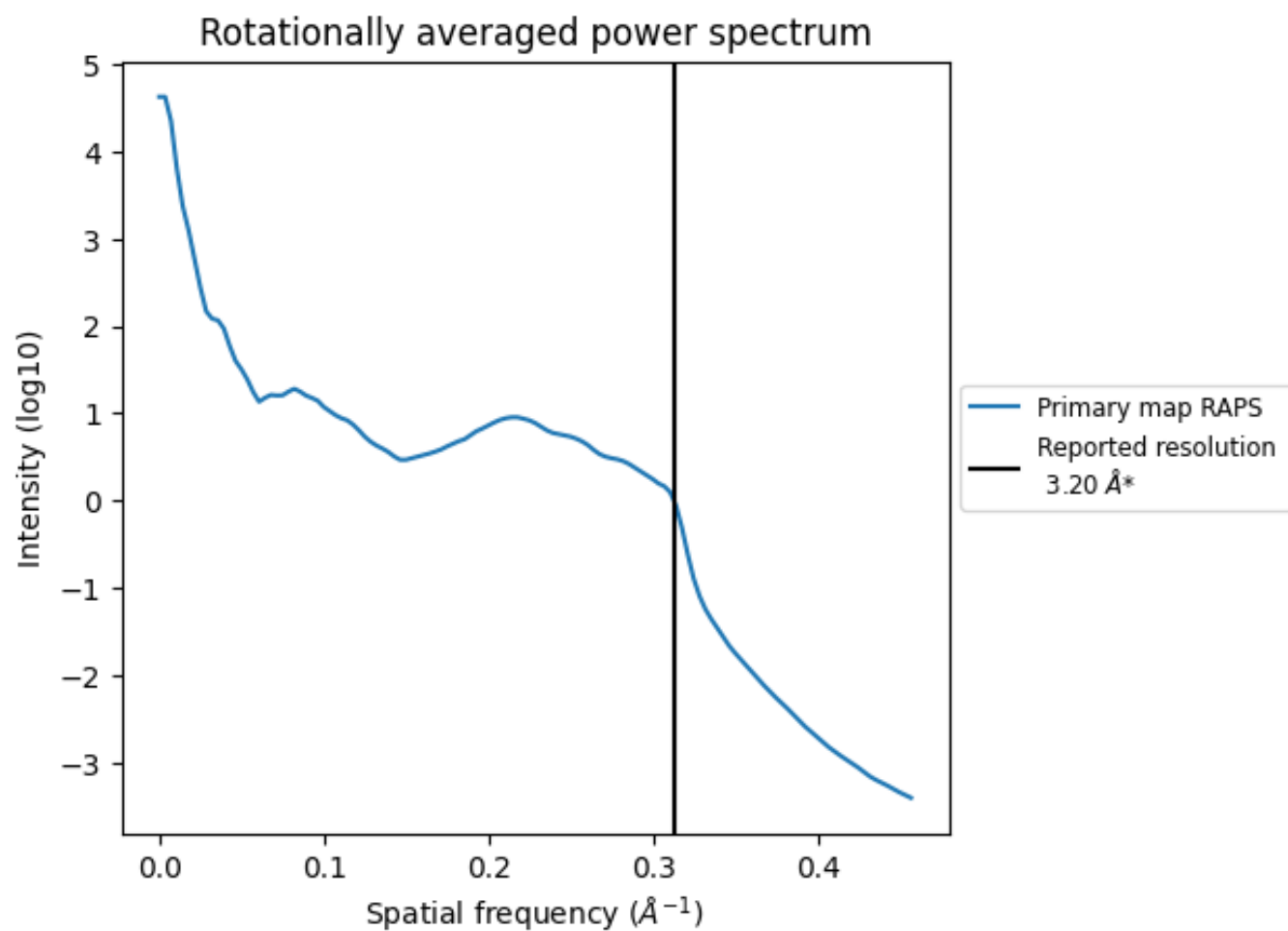
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 39 nm<sup>3</sup>; this corresponds to an approximate mass of 35 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 0.312  $\text{\AA}^{-1}$

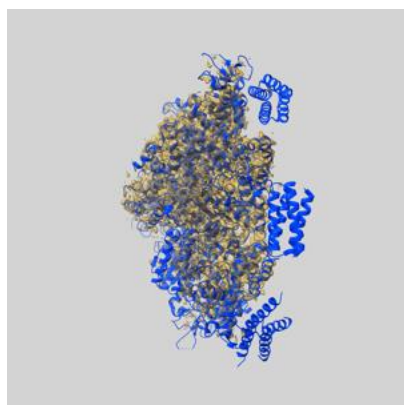
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

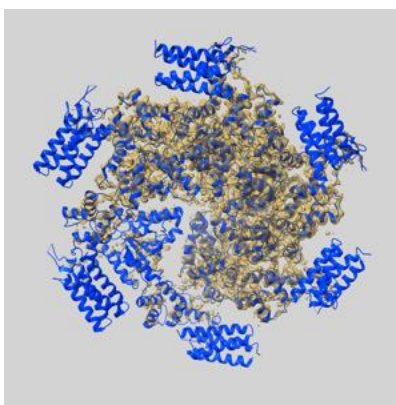
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8887 and PDB model 6AP1. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

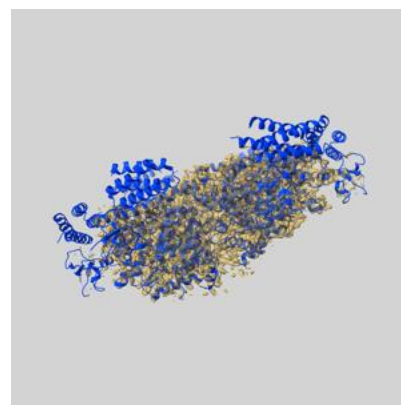
### 9.1 Map-model overlay [i](#)



X



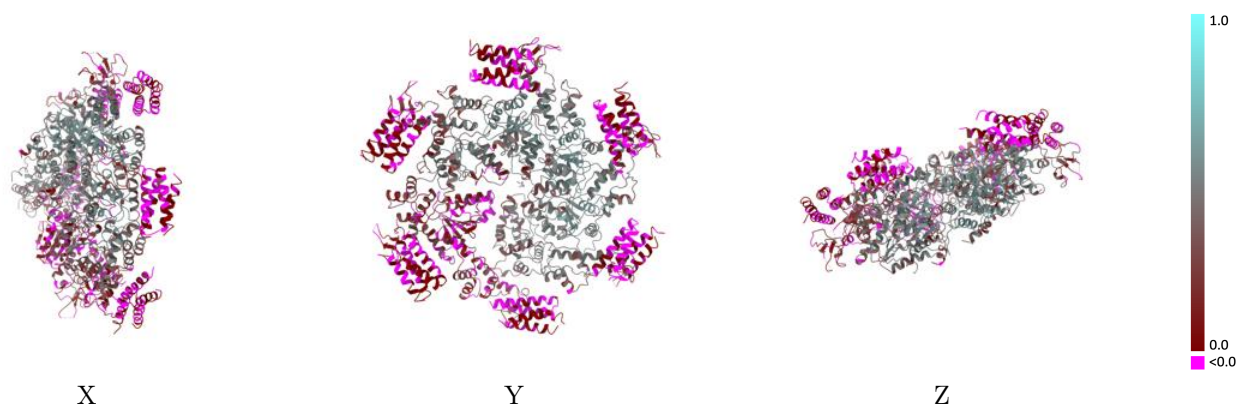
Y



Z

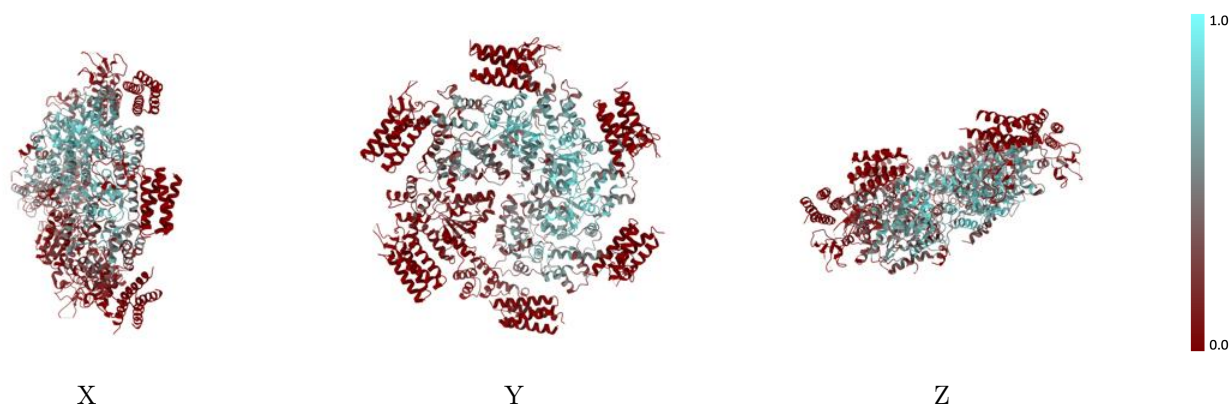
The images above show the 3D surface view of the map at the recommended contour level 0.0749 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



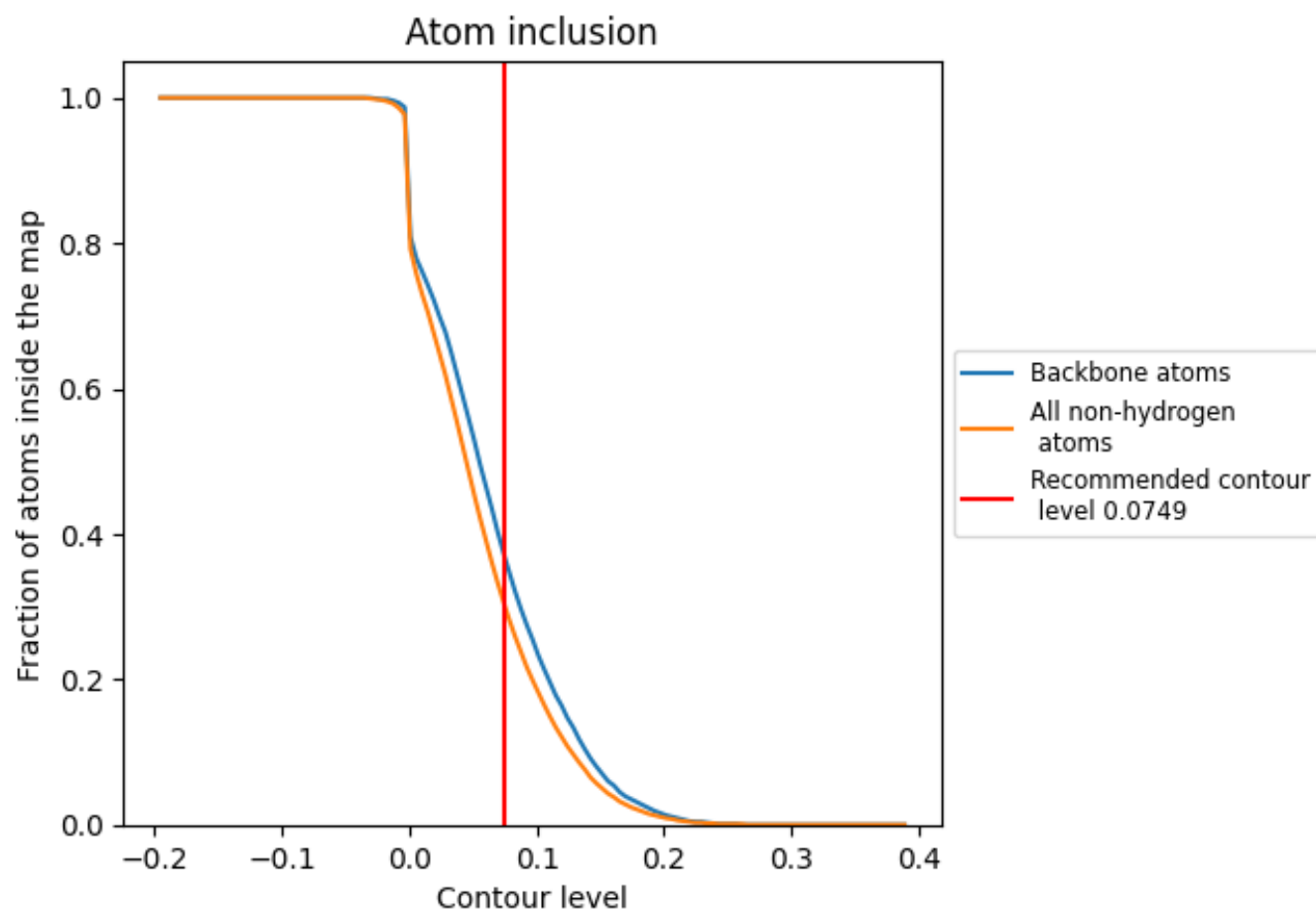
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0749).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 37% of all backbone atoms, 30% 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 (0.0749) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3020	<div></div> 0.2740
A	<div></div> 0.3750	<div></div> 0.3850
B	<div></div> 0.5540	<div></div> 0.4520
C	<div></div> 0.5630	<div></div> 0.4620
D	<div></div> 0.4950	<div></div> 0.4220
E	<div></div> 0.2640	<div></div> 0.3250
F	<div></div> 0.0250	<div></div> 0.0570
G	<div></div> 0.3430	<div></div> 0.4940
H	<div></div> 0.0000	<div></div> -0.0030
I	<div></div> 0.0030	<div></div> -0.0450
J	<div></div> 0.0000	<div></div> 0.0020
K	<div></div> 0.0000	<div></div> -0.0460
L	<div></div> 0.0000	<div></div> -0.0200
M	<div></div> 0.0000	<div></div> -0.0280
N	<div></div> 0.0000	<div></div> -0.0130
O	<div></div> 0.0000	<div></div> -0.0150
P	<div></div> 0.0000	<div></div> -0.0400
Q	<div></div> 0.0000	<div></div> -0.0400
R	<div></div> 0.0000	<div></div> -0.0290
S	<div></div> 0.0000	<div></div> -0.0310

1.0

0.0

<0.0