



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 12:57 PM UTC

PDB ID : 9PBF / pdb_00009pbf
EMDB ID : EMD-71478
Title : 21bin20S complex (NSF-alphaSNAP-2:1 syntaxin-1a:SNAP-25), non-hydrolyzing, class 10
Authors : White, K.I.; Brunger, A.T.
Deposited on : 2025-06-26
Resolution : 4.01 Å(reported)
Based on initial model : 6MDM

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:

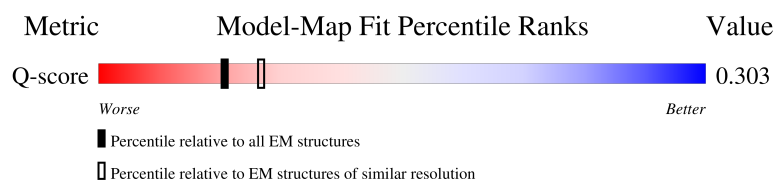
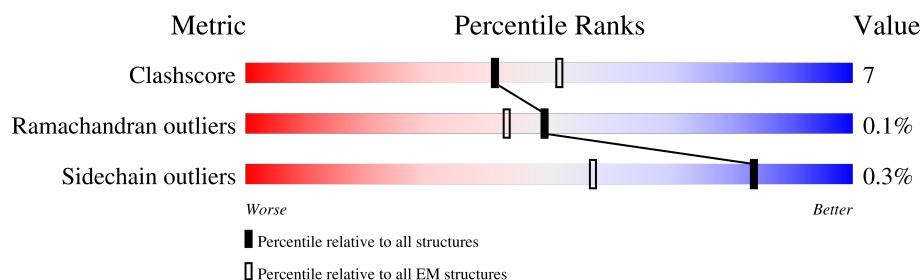
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 4.01 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	6765 (3.51 - 4.51)

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	G	267	
1	I	267	
2	J	296	
2	K	296	

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Mol	Chain	Length	Quality of chain
2	L	296	
3	A	747	
3	B	747	
3	C	747	
3	D	747	
3	E	747	
3	F	747	
4	H	222	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 87349 atoms, of which 43910 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 Syntaxin-1A.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	G	87	Total	C	H	N	O	S	0	0
			1375	430	683	116	140	6		
1	I	63	Total	C	H	N	O	S	0	0
			1023	320	506	89	103	5		

- Molecule 2 is a protein called Alpha-soluble NSF attachment protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	J	287	Total	C	H	N	O	S	0	0
			4467	1424	2212	375	438	18		
2	K	276	Total	C	H	N	O	S	0	0
			4320	1373	2143	363	423	18		
2	L	275	Total	C	H	N	O	S	0	0
			4306	1368	2137	362	421	18		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	0	GLY	-	expression tag	UNP P54921
K	0	GLY	-	expression tag	UNP P54921
L	0	GLY	-	expression tag	UNP P54921

- Molecule 3 is a protein called Vesicle-fusing ATPase.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	725	Total	C	H	N	O	S	7	0
			11577	3616	5854	1001	1075	31		
3	F	708	Total	C	H	N	O	S	5	0
			11281	3530	5709	971	1042	29		
3	A	725	Total	C	H	N	O	S	6	0
			11546	3604	5842	995	1074	31		
3	B	717	Total	C	H	N	O	S	7	0
			11455	3573	5799	994	1059	30		

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Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	725	Total	C	H	N	O	S	8	0
			11610	3620	5879	1005	1076	30		
3	E	725	Total	C	H	N	O	S	3	0
			11510	3597	5823	992	1068	30		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P18708
C	-1	ALA	-	expression tag	UNP P18708
C	0	HIS	-	expression tag	UNP P18708
F	-2	GLY	-	expression tag	UNP P18708
F	-1	ALA	-	expression tag	UNP P18708
F	0	HIS	-	expression tag	UNP P18708
A	-2	GLY	-	expression tag	UNP P18708
A	-1	ALA	-	expression tag	UNP P18708
A	0	HIS	-	expression tag	UNP P18708
B	-2	GLY	-	expression tag	UNP P18708
B	-1	ALA	-	expression tag	UNP P18708
B	0	HIS	-	expression tag	UNP P18708
D	-2	GLY	-	expression tag	UNP P18708
D	-1	ALA	-	expression tag	UNP P18708
D	0	HIS	-	expression tag	UNP P18708
E	-2	GLY	-	expression tag	UNP P18708
E	-1	ALA	-	expression tag	UNP P18708
E	0	HIS	-	expression tag	UNP P18708

- Molecule 4 is a protein called Synaptosomal-associated protein 25.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	H	153	Total	C	H	N	O	S	0	0
			2410	721	1191	228	259	11		

There are 20 discrepancies between the modelled and reference sequences:

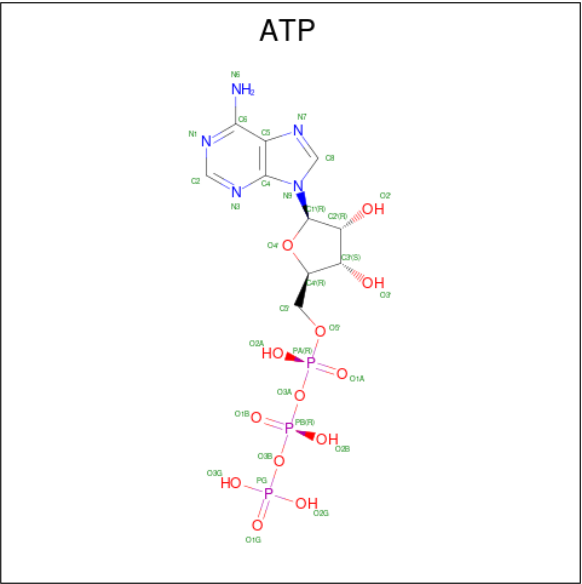
Chain	Residue	Modelled	Actual	Comment	Reference
H	-15	MET	-	expression tag	UNP P60881
H	-14	GLY	-	expression tag	UNP P60881
H	-13	SER	-	expression tag	UNP P60881
H	-12	SER	-	expression tag	UNP P60881
H	-11	HIS	-	expression tag	UNP P60881
H	-10	HIS	-	expression tag	UNP P60881

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	HIS	-	expression tag	UNP P60881
H	-8	HIS	-	expression tag	UNP P60881
H	-7	HIS	-	expression tag	UNP P60881
H	-6	HIS	-	expression tag	UNP P60881
H	-5	SER	-	expression tag	UNP P60881
H	-4	GLN	-	expression tag	UNP P60881
H	-3	ASP	-	expression tag	UNP P60881
H	-2	PRO	-	expression tag	UNP P60881
H	-1	ASN	-	expression tag	UNP P60881
H	0	SER	-	expression tag	UNP P60881
H	85	ALA	CYS	conflict	UNP P60881
H	88	ALA	CYS	conflict	UNP P60881
H	90	ALA	CYS	conflict	UNP P60881
H	92	ALA	CYS	conflict	UNP P60881

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



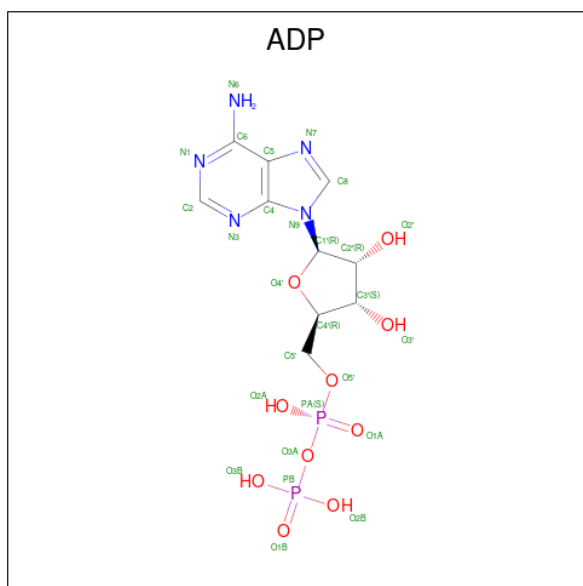
Mol	Chain	Residues	Atoms						AltConf
5	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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Mol	Chain	Residues	Atoms						AltConf
5	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

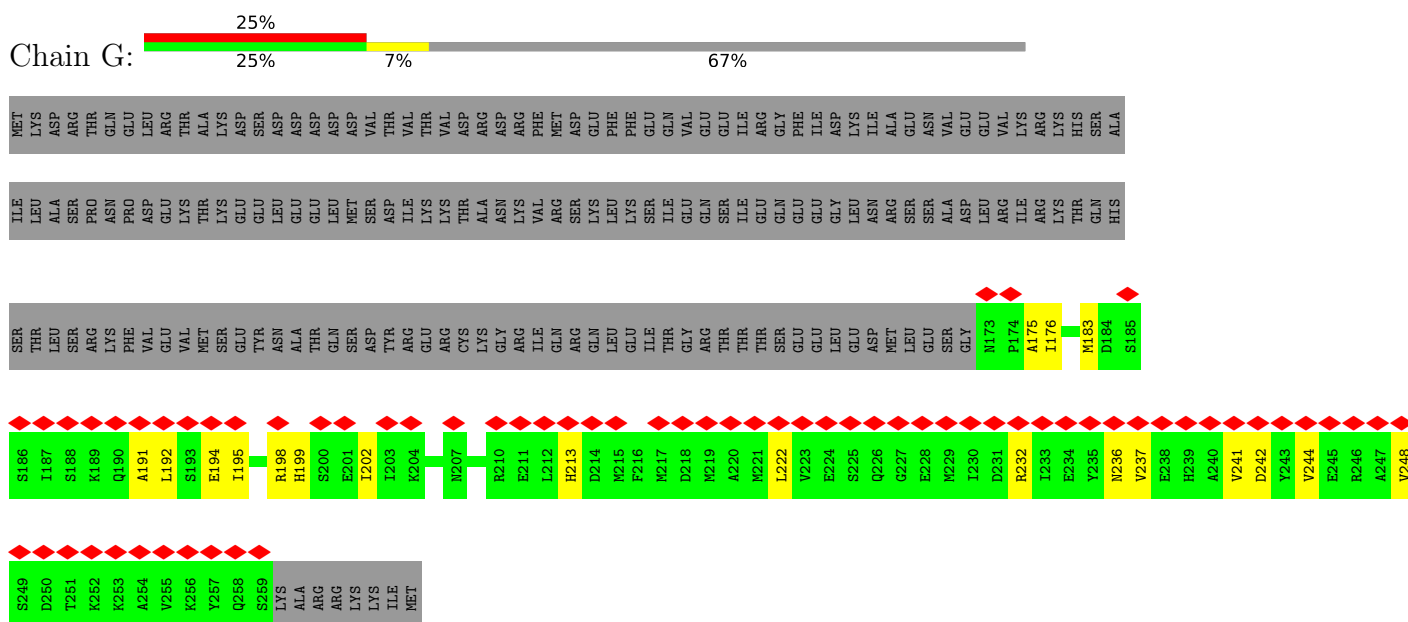


Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

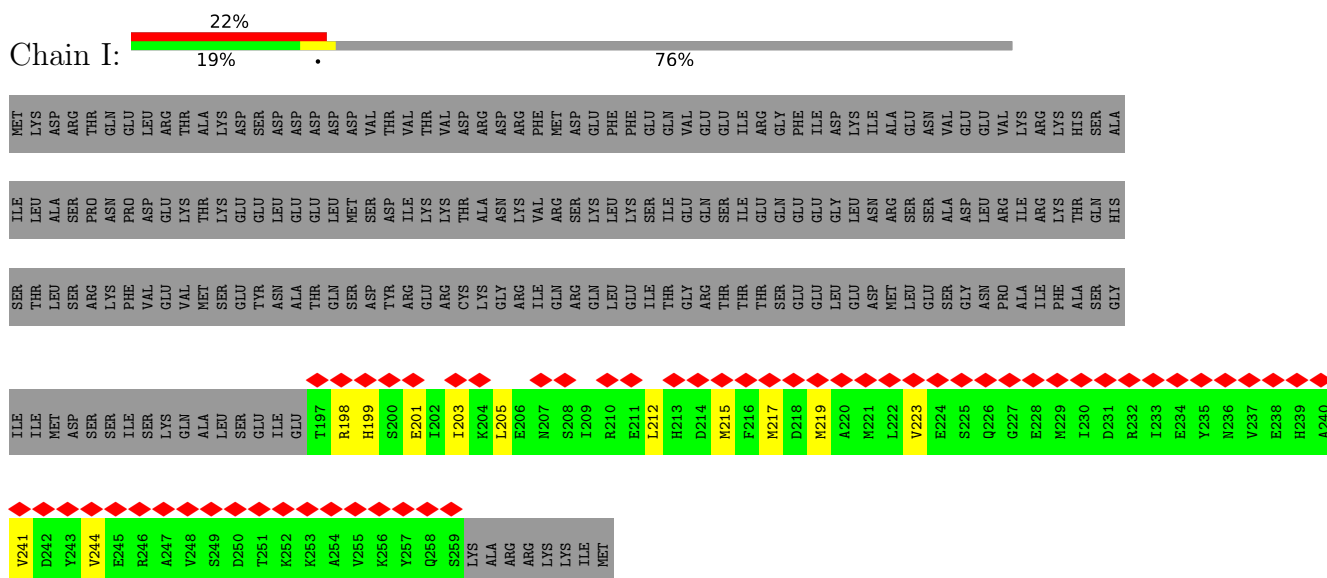
3 Residue-property plots

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

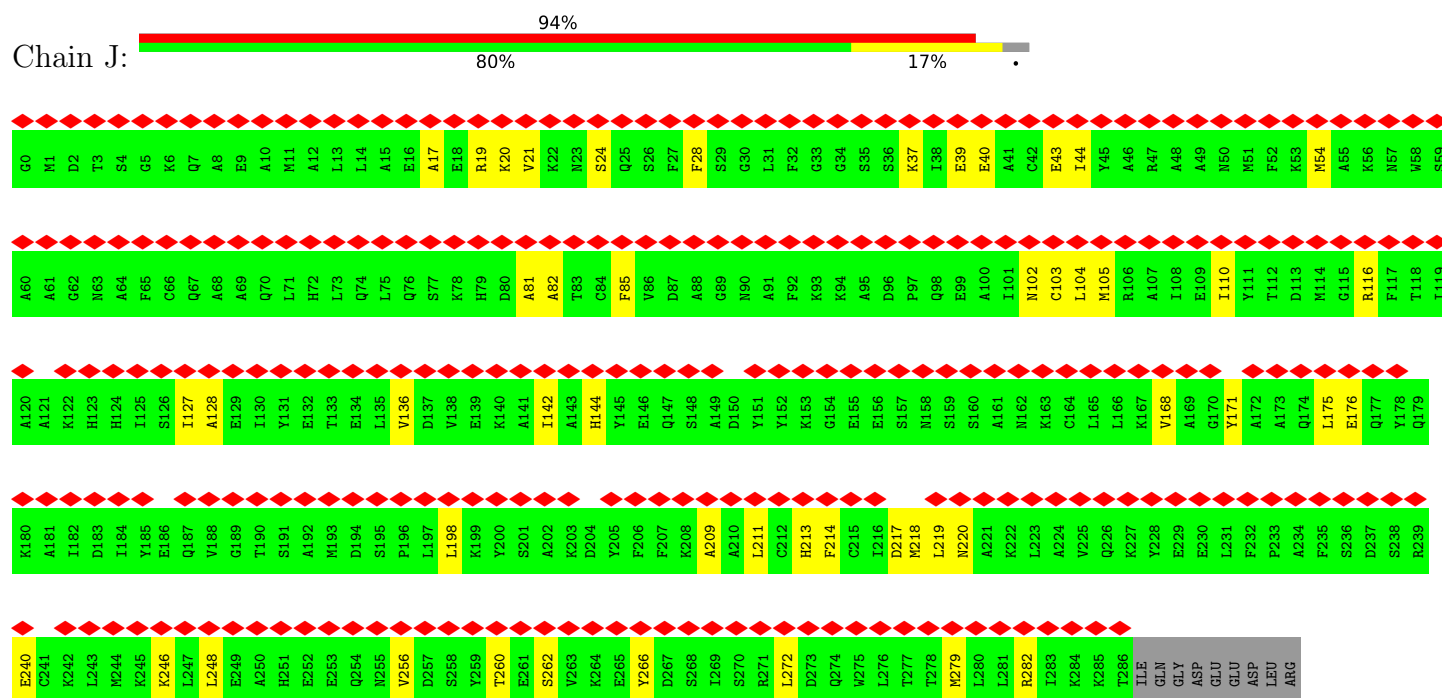
• Molecule 1: Syntaxin-1A

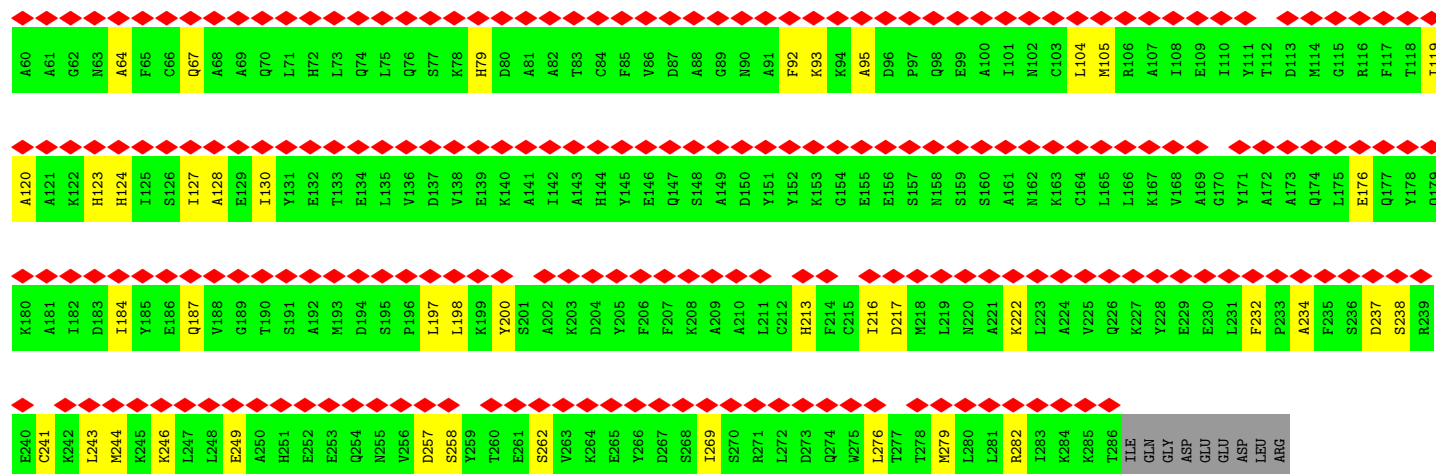


• Molecule 1: Syntaxin-1A

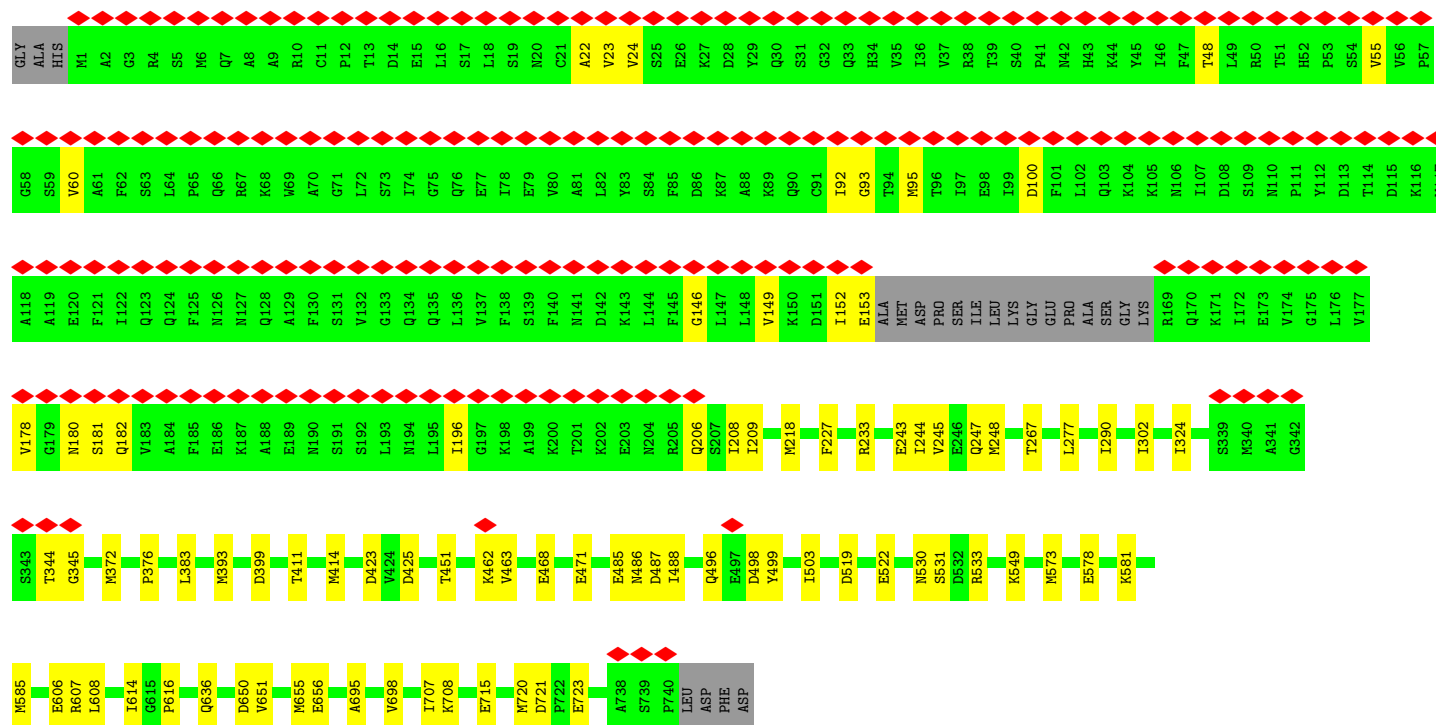
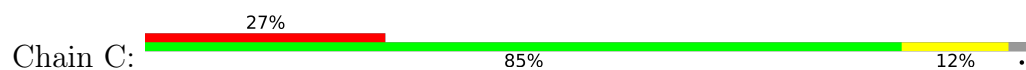


- Molecule 2: Alpha-soluble NSF attachment protein

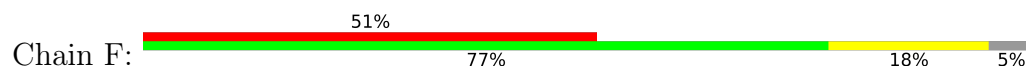


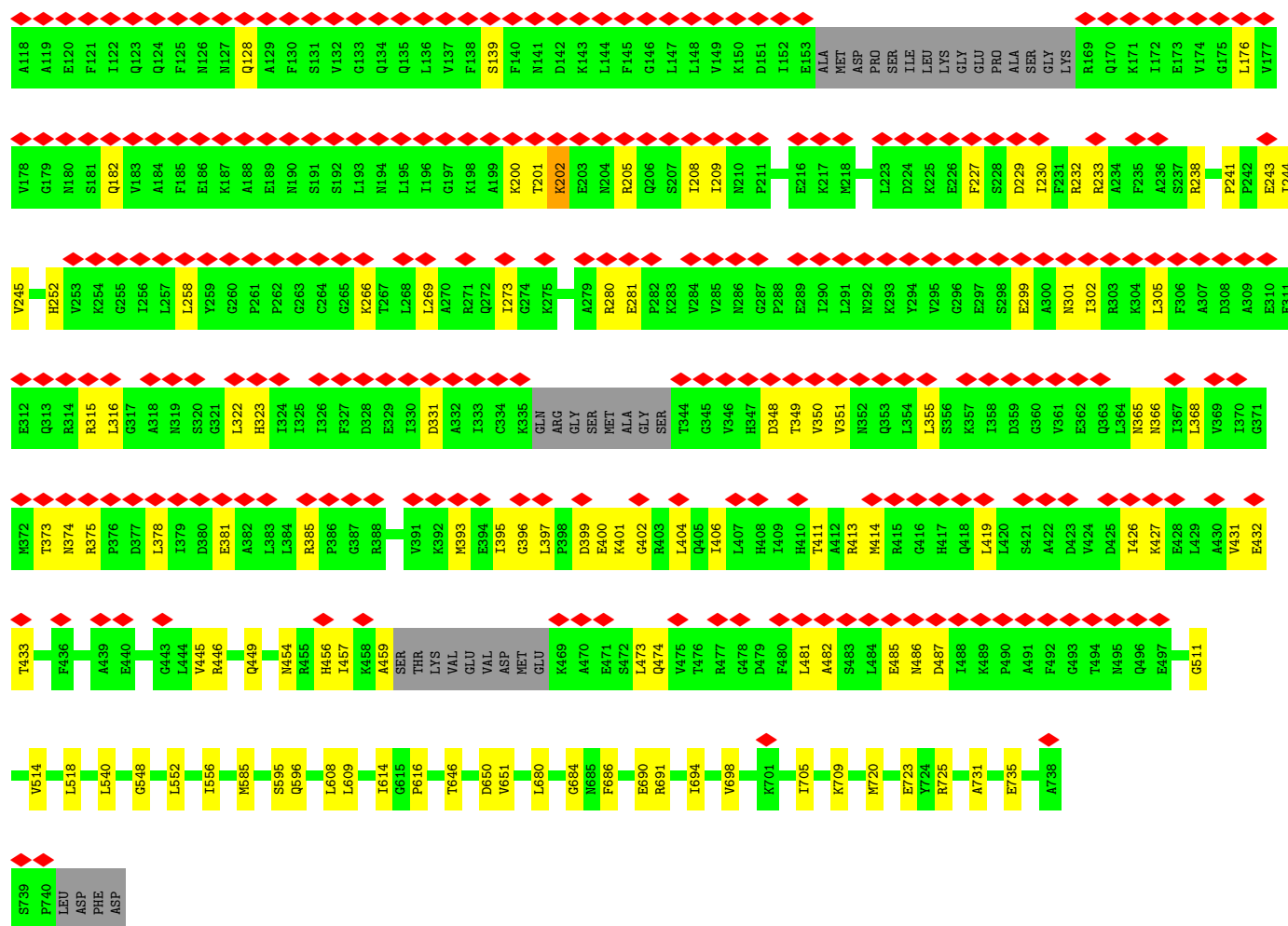


• Molecule 3: Vesicle-fusing ATPase

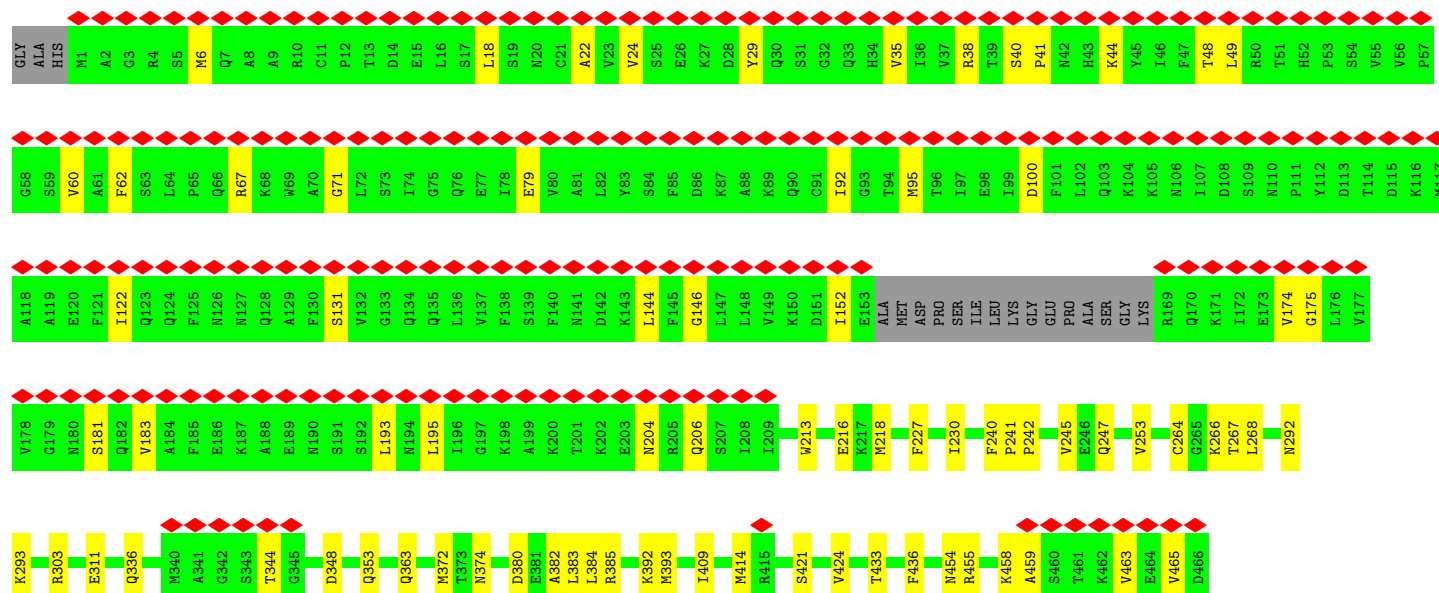
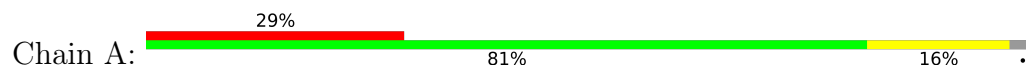


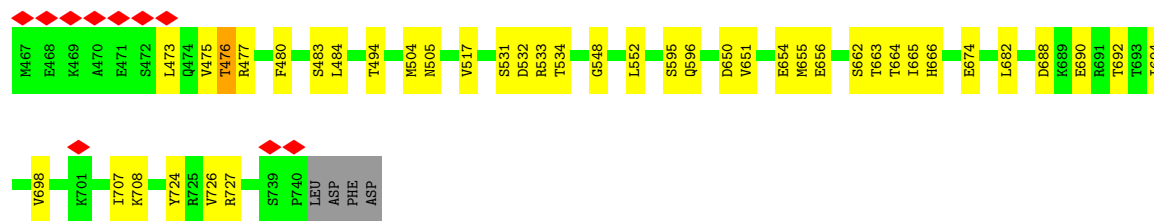
• Molecule 3: Vesicle-fusing ATPase



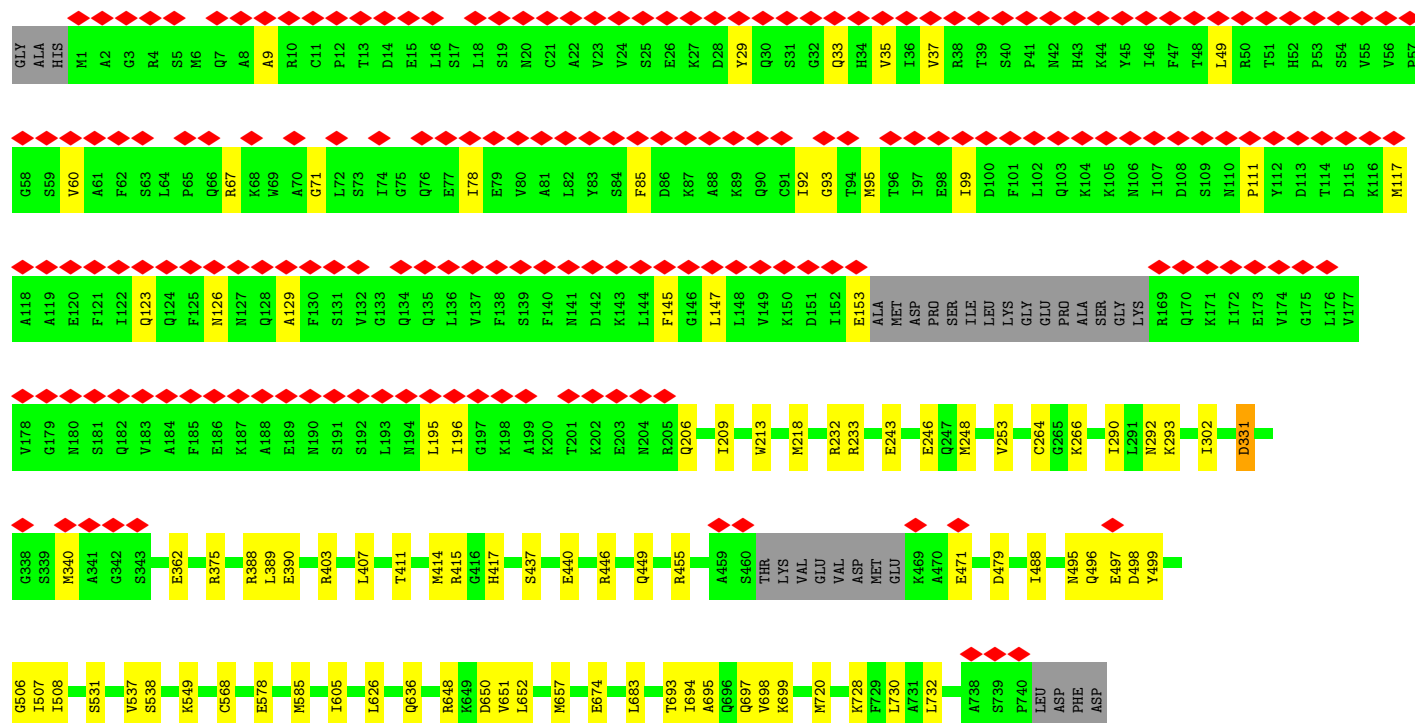
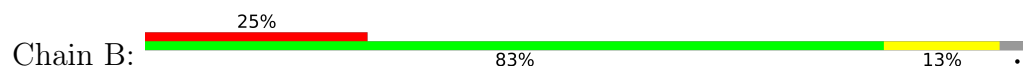


• Molecule 3: Vesicle-fusing ATPase

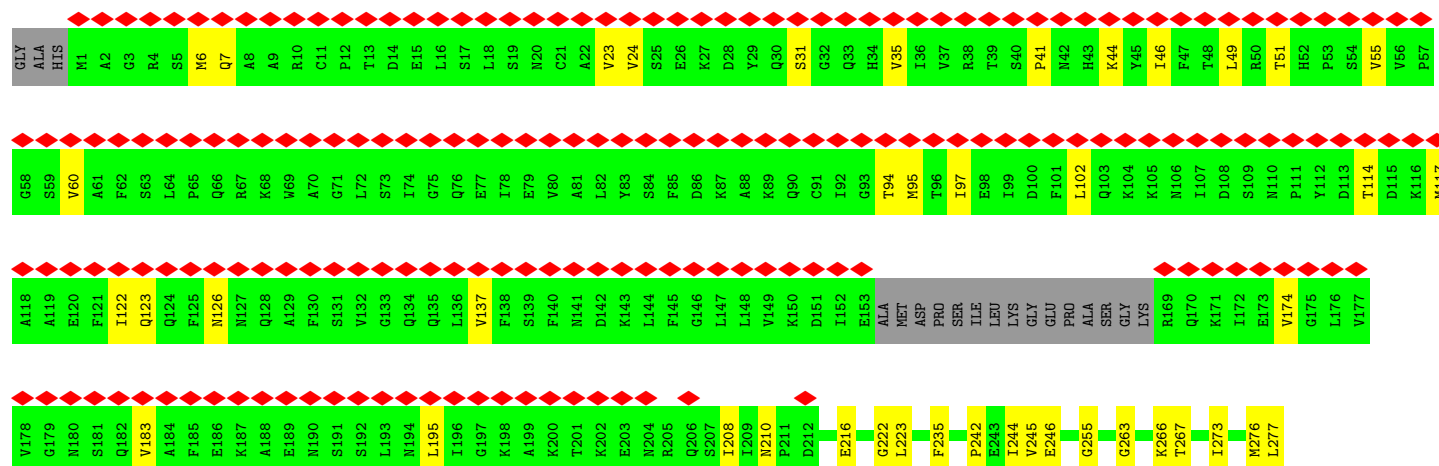
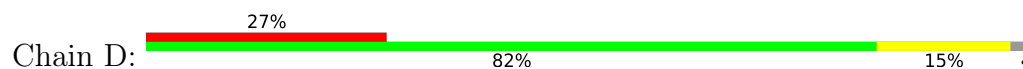


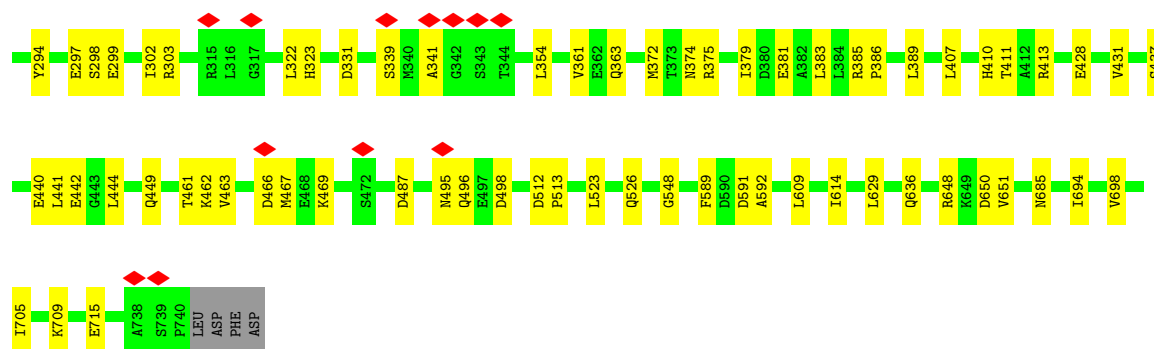


• Molecule 3: Vesicle-fusing ATPase

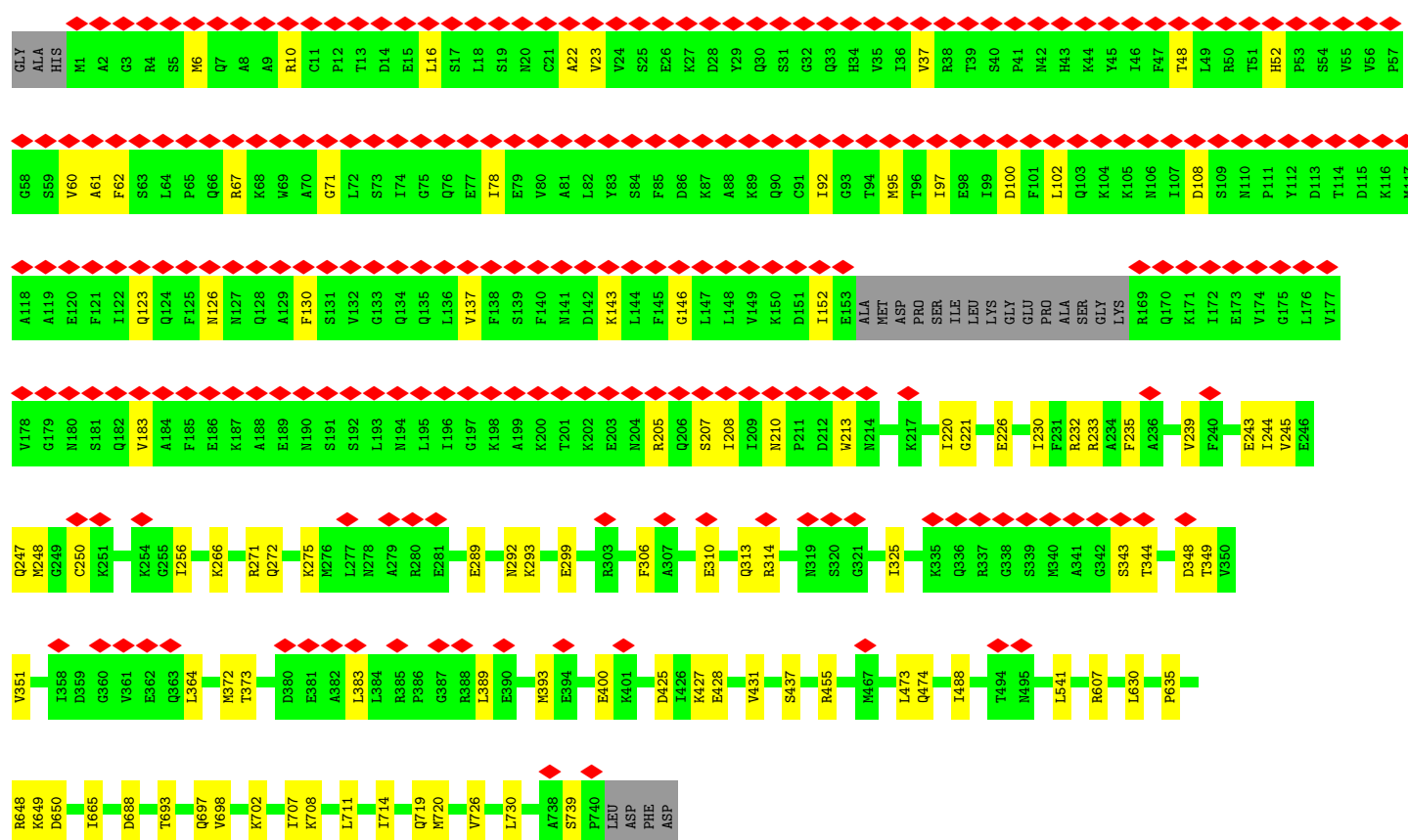
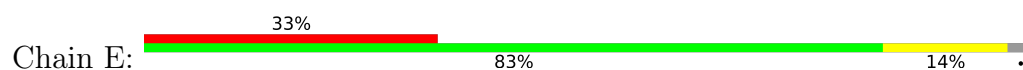


• Molecule 3: Vesicle-fusing ATPase

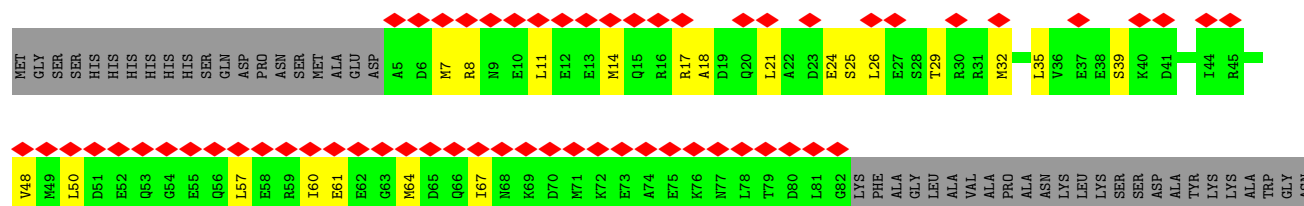


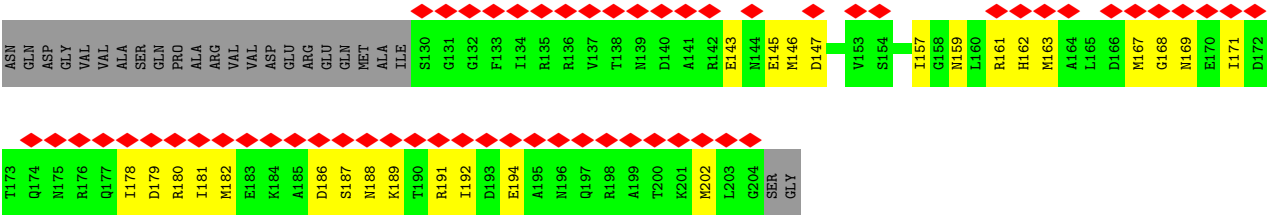


• Molecule 3: Vesicle-fusing ATPase



• Molecule 4: Synaptosomal-associated protein 25





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42789	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	31.560, 36.760, 35.480	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.083	Depositor
Minimum map value	-1.073	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	322.224, 322.224, 322.224	wwPDB
Map dimensions	294, 294, 294	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.096, 1.096, 1.096	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	G	0.16	0/700	0.32	0/939
1	I	0.14	0/523	0.29	0/700
2	J	0.10	0/2295	0.26	0/3084
2	K	0.14	0/2213	0.25	0/2975
2	L	0.10	0/2205	0.26	0/2963
3	A	0.22	0/5792	0.42	0/7802
3	B	0.20	0/5743	0.35	0/7733
3	C	0.22	1/5813 (0.0%)	0.35	0/7832
3	D	0.11	0/5819	0.27	0/7836
3	E	0.21	0/5777	0.41	0/7784
3	F	0.16	0/5669	0.33	0/7638
4	H	0.13	0/1219	0.34	0/1622
All	All	0.18	1/43768 (0.0%)	0.34	0/58908

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	423	ASP	C-N	-5.93	1.27	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	692	683	682	25	0
1	I	517	506	505	12	0
2	J	2255	2212	2212	39	0
2	K	2177	2143	2142	20	0
2	L	2169	2137	2136	32	0
3	A	5704	5842	5837	91	0
3	B	5656	5799	5792	71	0
3	C	5723	5854	5848	64	0
3	D	5731	5879	5874	82	0
3	E	5687	5823	5821	76	0
3	F	5572	5709	5696	87	0
4	H	1219	1191	1190	49	0
5	A	31	12	12	1	0
5	B	62	24	24	4	0
5	C	62	24	24	1	0
5	D	62	24	24	2	0
5	E	62	24	24	1	0
5	F	31	12	12	0	0
6	A	27	12	12	2	0
All	All	43439	43910	43867	599	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 7.

All (599) 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)
3:D:6:MET:HE3	3:D:60:VAL:HG23	1.43	1.01
3:F:23:VAL:HG12	3:F:55:VAL:HG21	1.60	0.84
3:D:299:GLU:N	3:D:299:GLU:OE1	2.14	0.80
3:B:652:LEU:HD12	3:B:657:MET:HE2	1.63	0.80
3:E:248:MET:HE3	3:E:248:MET:O	1.82	0.80
3:B:495:ASN:OD1	3:B:496:GLN:N	2.16	0.79
3:A:363:GLN:N	3:A:363:GLN:OE1	2.15	0.79
2:L:105:MET:HE1	2:L:127:ILE:HD12	1.64	0.77
3:D:117:MET:HE1	3:D:195:LEU:HD22	1.67	0.77
3:B:636:GLN:N	3:B:636:GLN:OE1	2.18	0.76
3:C:585:MET:HE2	3:C:608:LEU:HD21	1.65	0.76
3:C:344:THR:HG22	3:C:345:GLY:H	1.50	0.76
1:I:212:LEU:HD23	1:I:215:MET:HE3	1.67	0.75
3:B:549:LYS:N	5:B:802:ATP:O1B	2.22	0.73
3:E:702:LYS:NZ	3:E:739:SER:O	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:375:ARG:HD2	3:F:378:LEU:HD22	1.69	0.72
3:B:331:ASP:OD2	3:B:375:ARG:NH2	2.22	0.72
3:C:248:MET:HE1	3:D:449:GLN:HG3	1.72	0.72
3:F:41:PRO:O	3:F:44:LYS:NZ	2.23	0.72
3:F:205:ARG:NH2	3:F:243:GLU:OE2	2.22	0.72
3:A:292:ASN:OD1	3:A:293:LYS:N	2.23	0.71
2:J:240:GLU:OE1	2:J:240:GLU:N	2.24	0.71
3:D:266:LYS:NZ	3:D:374:ASN:OD1	2.23	0.71
3:A:62:PHE:O	3:A:67:ARG:NH1	2.24	0.71
3:B:674:GLU:N	3:B:674:GLU:OE1	2.24	0.71
2:J:176:GLU:OE2	2:J:282:ARG:NH2	2.24	0.70
3:A:421:SER:HB2	3:A:475:VAL:HG23	1.73	0.70
3:D:383:LEU:HD23	3:D:383:LEU:O	1.90	0.70
3:E:108:ASP:OD2	3:E:143:LYS:NZ	2.25	0.70
3:C:578:GLU:N	3:C:578:GLU:OE1	2.24	0.70
2:J:142:ILE:HD11	2:J:171:TYR:HB2	1.74	0.69
2:K:90:ASN:OD1	2:K:91:ALA:N	2.24	0.69
3:C:290:ILE:HD13	3:C:302:ILE:HD11	1.73	0.69
3:F:690:GLU:N	3:F:690:GLU:OE1	2.25	0.69
3:C:24:VAL:HG12	3:C:60:VAL:HG22	1.75	0.69
3:B:650:ASP:OD1	3:B:651:VAL:N	2.26	0.69
3:D:331:ASP:OD2	3:D:375[A]:ARG:NH2	2.26	0.69
3:B:206:GLN:OE1	3:B:206:GLN:N	2.25	0.69
3:C:498:ASP:OD1	3:C:499:TYR:N	2.25	0.69
3:D:216:GLU:N	3:D:216:GLU:OE1	2.27	0.68
3:B:92:ILE:HD13	3:B:95:MET:HE3	1.76	0.67
2:J:218:MET:HE2	2:J:218:MET:N	2.09	0.67
3:F:269:LEU:O	3:F:273:ILE:HD12	1.94	0.67
3:A:694:ILE:O	3:A:698:VAL:HG12	1.93	0.67
3:E:400:GLU:N	3:E:400:GLU:OE1	2.27	0.67
4:H:143:GLU:N	4:H:143:GLU:OE1	2.27	0.67
3:C:247:GLN:O	3:D:413:ARG:NH2	2.27	0.67
3:A:674:GLU:N	3:A:674:GLU:OE1	2.26	0.67
3:D:24:VAL:HG12	3:D:60:VAL:HG22	1.75	0.66
3:B:414:MET:SD	3:B:449:GLN:NE2	2.67	0.66
1:G:192:LEU:HD11	4:H:18:ALA:HB2	1.77	0.66
4:H:145:GLU:N	4:H:145:GLU:OE1	2.27	0.66
3:C:233:ARG:NH1	3:D:487:ASP:OD1	2.28	0.66
3:A:380:ASP:OD1	3:A:382:ALA:N	2.27	0.66
3:B:243:GLU:OE1	3:B:243:GLU:N	2.28	0.66
3:E:383:LEU:CD2	3:E:389:LEU:HD12	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:230:ILE:HD13	3:A:393:MET:HG3	1.76	0.66
3:F:445:VAL:HG12	3:F:449:GLN:HE21	1.62	0.65
3:F:35:VAL:HG13	3:F:49:LEU:HD11	1.79	0.65
2:K:54:MET:O	2:K:56:LYS:NZ	2.29	0.65
3:B:693:THR:HG22	3:B:697:GLN:OE1	1.96	0.65
3:E:123:GLN:O	3:E:126:ASN:ND2	2.29	0.65
3:F:266:LYS:HG2	3:F:395:ILE:HG21	1.79	0.65
3:A:656:GLU:OE1	3:B:648:ARG:NH1	2.30	0.65
3:B:123:GLN:O	3:B:126:ASN:ND2	2.29	0.65
3:F:269:LEU:CD1	3:F:395:ILE:HD12	2.28	0.64
3:A:303:ARG:NH1	3:A:353:GLN:OE1	2.30	0.64
3:A:35:VAL:HG13	3:A:49:LEU:HD11	1.79	0.64
3:B:578:GLU:N	3:B:578:GLU:OE1	2.31	0.64
3:D:235:PHE:HE2	3:D:273:ILE:HD11	1.61	0.64
1:G:192:LEU:HD11	4:H:18:ALA:CB	2.28	0.64
3:F:114:THR:HG21	3:F:200:LYS:HG3	1.79	0.64
4:H:167:MET:O	4:H:171:ILE:HD12	1.97	0.64
3:B:388:ARG:O	3:B:389:LEU:HD12	1.97	0.63
3:E:22:ALA:N	3:E:48:THR:O	2.30	0.63
3:D:302:ILE:HD11	3:D:354:LEU:HD13	1.80	0.63
2:J:17:ALA:HB2	2:J:44:ILE:HG22	1.80	0.63
3:F:404:LEU:CD1	3:F:426:ILE:HG22	2.27	0.63
3:B:411:THR:O	3:B:415[A]:ARG:NH1	2.31	0.63
3:C:208:ILE:HG22	3:C:208:ILE:O	1.99	0.63
3:D:591:ASP:OD1	3:D:592:ALA:N	2.32	0.63
3:B:495:ASN:OD1	3:B:497:GLU:N	2.32	0.63
3:D:235:PHE:CE2	3:D:273:ILE:HD11	2.33	0.63
3:E:100:ASP:O	3:E:146:GLY:N	2.31	0.63
2:J:102:ASN:OD1	2:J:103:CYS:N	2.32	0.63
3:E:95:MET:HE1	3:E:130:PHE:HB3	1.81	0.62
3:C:383:LEU:HD23	3:C:383:LEU:O	1.99	0.62
3:F:686:PHE:O	3:F:691:ARG:NE	2.31	0.62
3:B:605:ILE:HD11	3:B:626:LEU:HD21	1.81	0.62
3:D:526[A]:GLN:NE2	3:E:719:GLN:OE1	2.32	0.62
3:D:636:GLN:N	3:D:636:GLN:OE1	2.33	0.62
3:C:451:THR:OG1	3:B:232:ARG:NH1	2.33	0.61
3:A:548:GLY:N	5:A:801:ATP:O2B	2.32	0.61
3:D:95:MET:HE2	3:D:97:ILE:HD11	1.81	0.61
3:D:381:GLU:OE1	3:D:381:GLU:N	2.28	0.61
2:J:104:LEU:HB3	2:J:127:ILE:HD11	1.81	0.61
3:E:266:LYS:N	5:E:802:ATP:O2B	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:720:MET:HE3	3:C:721:ASP:H	1.64	0.61
3:F:609:LEU:HD12	3:F:609:LEU:O	2.01	0.61
3:F:694:ILE:O	3:F:698:VAL:HG22	2.00	0.61
3:F:348:ASP:OD1	3:F:349:THR:N	2.33	0.61
3:C:723:GLU:N	3:C:723:GLU:OE1	2.30	0.61
3:D:117:MET:HE1	3:D:195:LEU:CD2	2.31	0.61
1:I:219:MET:HA	1:I:219:MET:HE3	1.83	0.61
3:E:473:LEU:O	3:E:473:LEU:HD23	2.01	0.61
3:C:471:GLU:N	3:C:471:GLU:OE1	2.34	0.61
3:C:290:ILE:CD1	3:C:302:ILE:HD11	2.30	0.60
3:F:511:GLY:O	3:F:514:VAL:HG22	2.00	0.60
3:E:698:VAL:HG23	3:E:698:VAL:O	2.02	0.60
3:D:339:SER:O	3:D:341:ALA:N	2.34	0.60
3:F:35:VAL:CG1	3:F:49:LEU:HD11	2.32	0.59
3:A:22:ALA:N	3:A:48:THR:O	2.34	0.59
2:L:197:LEU:HD23	2:L:198:LEU:HB2	1.84	0.59
3:C:636:GLN:OE1	3:C:636:GLN:N	2.36	0.59
3:F:46:ILE:HG21	3:F:85:PHE:CZ	2.37	0.59
2:K:276:LEU:O	2:K:280:LEU:HD23	2.02	0.59
3:D:428:GLU:O	3:D:431:VAL:HG12	2.03	0.59
3:E:230:ILE:HD13	3:E:393:MET:HE2	1.83	0.59
2:J:17:ALA:HB2	2:J:44:ILE:CG2	2.33	0.59
3:D:407:LEU:HD21	3:D:441:LEU:HD22	1.83	0.59
2:J:219:LEU:HD12	2:J:220:ASN:N	2.17	0.59
3:A:662:SER:O	3:A:663:THR:OG1	2.18	0.59
3:D:650:ASP:OD1	3:D:651:VAL:N	2.36	0.59
3:F:375:ARG:HG3	3:F:375:ARG:O	2.02	0.59
3:B:340:MET:O	3:B:340:MET:HE3	2.03	0.59
3:F:46:ILE:HG21	3:F:85:PHE:HZ	1.68	0.58
3:C:503:ILE:HG22	3:C:503:ILE:O	2.04	0.58
3:F:402:GLY:O	3:F:406:ILE:HD12	2.04	0.58
3:F:229:ASP:O	3:F:233:ARG:N	2.37	0.58
3:E:455:ARG:NH2	3:E:474:GLN:O	2.36	0.58
3:D:123:GLN:O	3:D:126:ASN:ND2	2.36	0.58
2:J:246:LYS:NZ	2:J:262:SER:OG	2.33	0.58
3:C:650:ASP:OD1	3:C:651:VAL:N	2.37	0.58
3:F:114:THR:HG21	3:F:200:LYS:CG	2.34	0.58
3:F:540:LEU:HD11	3:F:646:THR:HG22	1.86	0.58
3:B:93:GLY:N	3:B:153:GLU:O	2.34	0.58
3:B:292:ASN:OD1	3:B:293:LYS:N	2.37	0.58
2:J:266:TYR:CE2	2:J:272:LEU:HD21	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:46:ILE:HD12	3:D:174:VAL:HG21	1.87	0.57
3:D:705:ILE:HD11	3:D:709:LYS:HG2	1.84	0.57
2:J:105:MET:CE	2:J:127:ILE:HD13	2.34	0.57
3:C:695:ALA:HA	3:C:698:VAL:HG12	1.87	0.57
3:F:238:ARG:NH1	3:F:365:ASN:O	2.35	0.57
3:B:264:CYS:N	5:B:801:ATP:O1B	2.37	0.57
3:F:723:GLU:N	3:F:723:GLU:OE1	2.36	0.57
3:D:495:ASN:N	3:D:498:ASP:OD2	2.35	0.57
2:J:266:TYR:CD2	2:J:272:LEU:HD21	2.39	0.57
3:C:22:ALA:N	3:C:48:THR:O	2.38	0.57
3:A:414:MET:HE2	3:A:414:MET:N	2.20	0.57
3:B:33:GLN:HB2	3:B:49:LEU:HD12	1.87	0.57
3:B:455:ARG:NH2	3:B:479:ASP:OD2	2.38	0.57
2:J:39:GLU:O	2:J:43:GLU:OE1	2.22	0.56
3:C:344:THR:HG22	3:C:345:GLY:N	2.20	0.56
3:E:213:TRP:NE1	3:E:275:LYS:O	2.39	0.56
3:E:95:MET:HE1	3:E:130:PHE:CB	2.35	0.56
3:B:290:ILE:CD1	3:B:302:ILE:HD11	2.36	0.56
1:G:241:VAL:HB	4:H:67:ILE:HD11	1.86	0.56
3:C:95:MET:HE1	3:C:181:SER:HB3	1.86	0.56
3:A:532:ASP:OD1	3:A:533:ARG:N	2.38	0.56
3:F:432:GLU:OE2	3:F:433:THR:HG23	2.05	0.56
3:A:663:THR:HG22	3:A:664:THR:H	1.71	0.56
3:C:93:GLY:N	3:C:153:GLU:O	2.38	0.56
3:C:95:MET:HE3	3:C:182:GLN:O	2.06	0.56
3:B:9:ALA:N	3:B:60:VAL:O	2.39	0.56
3:F:548:GLY:O	3:F:552:LEU:HD13	2.05	0.55
3:E:630:LEU:O	3:E:630:LEU:HD23	2.06	0.55
3:F:411:THR:HG22	3:F:411:THR:O	2.05	0.55
3:E:693:THR:O	3:E:697:GLN:OE1	2.25	0.55
3:F:23:VAL:HG12	3:F:55:VAL:CG2	2.33	0.55
3:D:235:PHE:CE1	3:D:277:LEU:HD21	2.41	0.55
3:E:230:ILE:CD1	3:E:393:MET:HE2	2.37	0.55
2:J:21:VAL:O	2:J:24:SER:OG	2.25	0.55
3:D:242:PRO:O	3:D:245:VAL:N	2.40	0.55
3:D:589:PHE:HD2	3:D:629:LEU:HD13	1.71	0.55
4:H:17:ARG:O	4:H:21:LEU:HD23	2.05	0.55
3:E:427:LYS:O	3:E:431:VAL:HG23	2.07	0.55
3:A:459:ALA:O	3:A:463:VAL:HB	2.07	0.54
3:E:226:GLU:OE1	3:E:226:GLU:N	2.40	0.54
3:E:97:ILE:HD12	3:E:183:VAL:CG1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:235:PHE:O	3:E:239:VAL:HG23	2.07	0.54
3:C:462:LYS:NZ	3:B:213:TRP:O	2.35	0.54
3:F:22:ALA:N	3:F:48:THR:O	2.40	0.54
3:D:496:GLN:N	3:D:496:GLN:OE1	2.40	0.54
3:F:614:ILE:O	3:F:616:PRO:HA	2.08	0.54
3:A:253:VAL:HG22	3:B:446:ARG:NH1	2.23	0.54
2:K:39:GLU:O	2:K:42:CYS:N	2.41	0.54
3:D:222:GLY:C	3:D:223:LEU:HD22	2.33	0.54
3:E:425:ASP:OD2	3:E:428:GLU:N	2.37	0.54
2:L:64:ALA:O	2:L:67:GLN:NE2	2.40	0.54
3:A:383:LEU:C	3:A:384:LEU:HD12	2.33	0.54
3:A:455:ARG:HH12	3:A:476:THR:HG21	1.73	0.54
3:B:694:ILE:HG22	3:B:730:LEU:HD21	1.90	0.54
1:I:198:ARG:NH1	1:I:201:GLU:OE2	2.41	0.54
1:G:213:HIS:NE2	4:H:39:SER:OG	2.39	0.54
2:K:16:GLU:OE2	2:K:19:ARG:NH2	2.41	0.53
1:G:244:VAL:O	1:G:248:VAL:HG23	2.07	0.53
1:I:212:LEU:HD23	1:I:215:MET:CE	2.37	0.53
3:B:37:VAL:HG13	3:B:78:ILE:HD12	1.89	0.53
3:A:688:ASP:O	3:A:692:THR:HG23	2.09	0.53
4:H:202:MET:HE2	4:H:202:MET:HA	1.91	0.53
3:C:487:ASP:OD2	3:B:233:ARG:NH1	2.41	0.53
3:E:648:ARG:O	3:E:649:LYS:C	2.52	0.53
3:C:277:LEU:HD12	3:C:324:ILE:HD11	1.91	0.52
4:H:26:LEU:HD23	4:H:146:MET:HE3	1.91	0.52
2:J:105:MET:HE3	2:J:127:ILE:HD13	1.91	0.52
3:A:24:VAL:HG11	3:A:49:LEU:HD22	1.90	0.52
3:A:698:VAL:HG22	3:A:698:VAL:O	2.08	0.52
2:L:243:LEU:O	2:L:246:LYS:HG2	2.10	0.52
3:E:313:GLN:OE1	3:E:314:ARG:NH1	2.42	0.52
3:C:614:ILE:O	3:C:616:PRO:HA	2.09	0.52
3:E:243:GLU:OE1	3:E:243:GLU:N	2.41	0.52
3:A:242:PRO:HA	3:A:245:VAL:HG12	1.91	0.52
3:B:35:VAL:HG21	3:B:49:LEU:HD21	1.91	0.52
3:D:222:GLY:O	3:D:223:LEU:HD22	2.10	0.52
2:K:284:LYS:O	2:K:287:ILE:HG22	2.10	0.52
1:G:237:VAL:HG11	4:H:60:ILE:HD11	1.92	0.52
1:I:212:LEU:HD21	4:H:161:ARG:HA	1.92	0.52
3:C:720:MET:HE3	3:C:721:ASP:N	2.25	0.52
3:A:266:LYS:N	6:A:802:ADP:O1B	2.43	0.52
3:B:99:ILE:HD11	3:B:145:PHE:CG	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:205:ARG:HG3	3:E:208:ILE:HD13	1.91	0.52
2:K:79:HIS:O	2:K:83:THR:HG23	2.10	0.52
3:B:266:LYS:N	5:B:801:ATP:O2B	2.38	0.51
3:B:699:LYS:O	3:B:699:LYS:NZ	2.18	0.51
3:E:393:MET:SD	3:E:393:MET:N	2.83	0.51
3:B:67:ARG:O	3:B:71:GLY:N	2.44	0.51
2:J:217:ASP:C	2:J:218:MET:HE2	2.36	0.51
4:H:29:THR:HG21	4:H:146:MET:SD	2.50	0.51
3:A:38:ARG:O	3:A:79:GLU:HB2	2.11	0.51
3:B:506:GLY:O	3:B:507:ILE:HD13	2.10	0.51
2:L:213:HIS:O	2:L:216:ILE:HG22	2.10	0.51
1:G:241:VAL:CB	4:H:67:ILE:HD11	2.40	0.51
3:F:331:ASP:OD1	3:F:373:THR:HG23	2.10	0.51
3:E:208:ILE:HG22	3:E:210:ASN:H	1.75	0.51
3:D:23:VAL:HG12	3:D:55:VAL:HG21	1.93	0.51
3:F:323:HIS:O	3:F:368:LEU:N	2.42	0.51
3:B:111:PRO:HB3	3:B:196:ILE:HD12	1.93	0.51
3:B:508:ILE:HD13	3:B:683:LEU:HD21	1.92	0.51
3:B:498:ASP:OD1	3:B:499:TYR:N	2.44	0.51
3:A:92:ILE:HD11	3:A:175:GLY:C	2.36	0.50
2:J:209:ALA:O	2:J:213:HIS:N	2.40	0.50
3:B:537:VAL:HG12	3:B:538:SER:N	2.26	0.50
3:E:16:LEU:HD11	3:E:52:HIS:CD2	2.45	0.50
3:B:35:VAL:HG11	3:B:49:LEU:HD11	1.94	0.50
3:D:469:LYS:O	3:D:469:LYS:NZ	2.35	0.50
3:A:100:ASP:O	3:A:146:GLY:N	2.45	0.50
3:D:294:TYR:OH	4:H:8:ARG:NE	2.44	0.50
1:G:199:HIS:O	1:G:199:HIS:CD2	2.65	0.50
3:D:267:THR:HA	3:D:372:MET:HE1	1.93	0.50
1:G:175:ALA:C	1:G:176:ILE:HD12	2.37	0.50
3:F:404:LEU:HD11	3:F:426:ILE:HG22	1.93	0.50
2:J:142:ILE:HD11	2:J:171:TYR:CB	2.39	0.50
3:C:267:THR:HA	3:C:372:MET:HE1	1.92	0.50
3:F:201:THR:O	3:F:202:LYS:HB2	2.11	0.50
3:F:232:ARG:NH1	3:A:454:ASN:HB2	2.27	0.50
3:A:663:THR:HG22	3:A:664:THR:N	2.26	0.50
3:D:244:ILE:HD12	3:D:244:ILE:H	1.76	0.50
3:D:41:PRO:O	3:D:44:LYS:NZ	2.45	0.49
4:H:186:ASP:OD1	2:L:79:HIS:NE2	2.45	0.49
4:H:189:LYS:O	4:H:192:ILE:HG22	2.12	0.49
3:E:306:PHE:HE1	3:E:325:ILE:HD13	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:269:LEU:HD13	3:F:395:ILE:HD12	1.95	0.49
3:A:92:ILE:HD13	3:A:152:ILE:HG23	1.94	0.49
3:B:35:VAL:CG1	3:B:49:LEU:HD11	2.43	0.49
3:D:208:ILE:HG22	3:D:208:ILE:O	2.12	0.49
3:C:411:THR:HG22	3:C:411:THR:O	2.13	0.49
3:F:67:ARG:O	3:F:71:GLY:N	2.46	0.49
3:D:298:SER:OG	3:D:299:GLU:OE1	2.27	0.49
3:E:95:MET:HE3	3:E:152:ILE:HG12	1.94	0.49
2:J:211:LEU:HD22	2:J:279:MET:HE2	1.93	0.49
3:B:694:ILE:O	3:B:698:VAL:HG12	2.12	0.49
1:I:203:ILE:HG23	2:L:269:ILE:HD13	1.93	0.49
3:A:38:ARG:HG3	3:A:44:LYS:HD3	1.95	0.49
3:B:437:SER:N	3:B:440:GLU:OE1	2.41	0.49
3:F:413:ARG:HG3	3:F:414:MET:HE2	1.93	0.49
3:A:268:LEU:HD23	3:A:268:LEU:C	2.37	0.49
3:A:384:LEU:HD23	3:A:392:LYS:NZ	2.27	0.49
1:G:191:ALA:O	1:G:194:GLU:HG3	2.13	0.49
3:F:404:LEU:HD12	3:F:426:ILE:HG22	1.94	0.48
2:L:119:ILE:O	2:L:123:HIS:ND1	2.46	0.48
3:E:344:THR:HG22	3:E:344:THR:O	2.13	0.48
3:F:680:LEU:O	3:F:684:GLY:N	2.42	0.48
2:J:256:VAL:O	2:J:260:THR:HG23	2.13	0.48
3:A:18:LEU:HD22	3:A:144:LEU:HD22	1.94	0.48
3:C:393:MET:HE3	3:C:393:MET:HA	1.96	0.48
3:A:29:TYR:HB3	3:A:49:LEU:HD13	1.94	0.48
3:A:267:THR:HA	3:A:372:MET:HE1	1.93	0.48
2:L:104:LEU:HD13	2:L:127:ILE:HG22	1.95	0.48
2:L:120:ALA:O	2:L:124:HIS:ND1	2.47	0.48
3:B:233:ARG:O	3:B:253:VAL:HG21	2.14	0.48
3:D:242:PRO:O	3:D:246:GLU:OE1	2.31	0.48
3:C:92:ILE:CG2	3:C:95:MET:HE2	2.44	0.48
2:J:171:TYR:O	2:J:175:LEU:HD13	2.14	0.48
3:F:322:LEU:HD11	3:F:368:LEU:HG	1.96	0.48
2:K:244:MET:HE2	2:K:247:LEU:HD12	1.96	0.48
3:F:95:MET:HE3	3:F:182:GLN:O	2.14	0.48
3:A:216:GLU:OE1	3:A:409:ILE:HD11	2.14	0.48
3:A:682:LEU:HD23	3:A:682:LEU:O	2.14	0.48
3:C:196:ILE:HG13	3:C:196:ILE:O	2.14	0.47
3:A:690:GLU:HG2	3:A:726:VAL:HG21	1.94	0.47
3:D:385:ARG:NH1	3:D:386:PRO:O	2.47	0.47
4:H:11:LEU:O	4:H:14:MET:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:222:LYS:NZ	2:L:249:GLU:OE2	2.46	0.47
2:J:40:GLU:CD	2:J:44:ILE:HD11	2.39	0.47
3:C:149:VAL:HG11	3:C:152:ILE:HD11	1.95	0.47
3:A:95:MET:HE1	3:A:181:SER:HB2	1.96	0.47
3:A:227:PHE:O	3:A:230:ILE:HG22	2.14	0.47
3:B:720:MET:HE2	3:B:728:LYS:HD2	1.94	0.47
3:D:122:ILE:HD11	3:D:183:VAL:HG23	1.95	0.47
2:L:16:GLU:O	2:L:19:ARG:HG3	2.14	0.47
1:G:199:HIS:CE1	4:H:25:SER:HB2	2.50	0.47
2:J:198:LEU:HD23	4:H:48:VAL:HG12	1.96	0.47
3:F:731:ALA:O	3:F:735:GLU:OE1	2.31	0.47
3:A:655:MET:HE2	3:A:655:MET:N	2.29	0.47
3:A:384:LEU:HD23	3:A:392:LYS:HZ1	1.78	0.47
3:F:457:ILE:HG23	3:F:459:ALA:H	1.79	0.47
3:F:481:LEU:O	3:F:485:GLU:CD	2.57	0.47
3:E:62:PHE:O	3:E:67:ARG:NH1	2.48	0.47
3:E:299:GLU:N	3:E:299:GLU:OE1	2.47	0.47
2:K:239:ARG:NH1	2:K:269:ILE:HG21	2.30	0.47
3:F:208:ILE:HG22	3:F:209:ILE:HG12	1.95	0.47
3:F:456:HIS:NE2	3:F:473:LEU:HD13	2.30	0.47
3:A:213:TRP:CG	3:A:213:TRP:O	2.68	0.47
3:D:694:ILE:O	3:D:698:VAL:HG22	2.15	0.47
4:H:61:GLU:OE2	4:H:180:ARG:NH1	2.43	0.47
1:I:217:MET:HE3	2:L:200:TYR:HB2	1.97	0.47
3:C:656:GLU:OE2	3:D:648:ARG:NH1	2.48	0.47
3:A:122:ILE:HD11	3:A:183:VAL:HG23	1.96	0.47
3:A:242:PRO:O	3:A:245:VAL:HG12	2.15	0.47
3:F:393:MET:HG2	3:F:395:ILE:HD11	1.95	0.47
3:A:67:ARG:O	3:A:71:GLY:N	2.48	0.47
3:B:568:CYS:SG	3:B:585:MET:HE1	2.54	0.47
3:E:67:ARG:O	3:E:71:GLY:N	2.47	0.47
2:L:19:ARG:NH2	2:L:23:ASN:OD1	2.48	0.47
2:L:93:LYS:HE2	2:L:130:ILE:HD13	1.96	0.47
3:A:374[B]:ASN:OD1	3:A:374[B]:ASN:N	2.47	0.47
3:B:388:ARG:C	3:B:389:LEU:HD12	2.40	0.47
4:H:57:LEU:HA	4:H:60:ILE:HG22	1.97	0.47
3:F:241:PRO:HD2	3:F:244:ILE:HD12	1.97	0.46
3:B:213:TRP:NE1	3:B:218:MET:SD	2.82	0.46
2:J:136:VAL:HG12	2:J:136:VAL:O	2.15	0.46
3:F:473:LEU:HD12	3:F:474:GLN:N	2.30	0.46
3:A:311:GLU:C	3:A:311:GLU:OE2	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:162:HIS:O	4:H:163:MET:C	2.56	0.46
3:A:650:ASP:OD1	3:A:651:VAL:N	2.45	0.46
3:D:35:VAL:HG11	3:D:49:LEU:HD11	1.97	0.46
3:E:383:LEU:HD21	3:E:389:LEU:HD12	1.95	0.46
3:A:383:LEU:HD23	3:A:383:LEU:O	2.14	0.46
3:A:385:ARG:NH2	5:B:801:ATP:O3G	2.46	0.46
3:B:99:ILE:HD12	3:B:147:LEU:HD21	1.97	0.46
3:B:246:GLU:C	3:B:246:GLU:OE2	2.58	0.46
3:D:102:LEU:HD22	3:D:137:VAL:CG2	2.45	0.46
3:E:6:MET:HE2	3:E:60:VAL:HG23	1.97	0.46
3:C:496:GLN:OE1	3:C:496:GLN:N	2.48	0.46
3:B:362:GLU:OE1	3:B:362:GLU:N	2.39	0.46
3:D:303[B]:ARG:NH2	3:E:289:GLU:OE1	2.48	0.46
3:D:609:LEU:HD12	3:D:609:LEU:O	2.16	0.46
2:K:257:ASP:OD1	2:K:258:SER:N	2.49	0.46
2:L:105:MET:HE1	2:L:127:ILE:CD1	2.39	0.46
3:D:6:MET:SD	3:D:7:GLN:N	2.88	0.46
3:C:585:MET:CE	3:C:608:LEU:HD21	2.39	0.46
3:F:201:THR:O	3:F:202:LYS:CB	2.63	0.46
3:E:37:VAL:HG13	3:E:78:ILE:HD12	1.97	0.46
4:H:167:MET:O	4:H:168:GLY:C	2.58	0.46
3:A:433:THR:HG22	3:A:436:PHE:CE1	2.50	0.46
3:D:361:VAL:O	3:D:363:GLN:NE2	2.46	0.46
3:E:97:ILE:HD12	3:E:183:VAL:HG11	1.98	0.46
2:K:244:MET:CE	2:K:247:LEU:HD12	2.45	0.46
1:G:222:LEU:HD22	1:I:223:VAL:HG11	1.98	0.46
1:G:242:ASP:OD2	2:J:116:ARG:NE	2.49	0.46
2:J:40:GLU:OE1	2:J:44:ILE:HD11	2.16	0.46
3:F:351:VAL:O	3:F:355:LEU:HD13	2.15	0.46
3:A:268:LEU:HD23	3:A:268:LEU:O	2.15	0.46
3:C:24:VAL:CG1	3:C:60:VAL:HG22	2.45	0.46
3:A:35:VAL:CG1	3:A:49:LEU:HD11	2.45	0.46
3:A:655:MET:HE2	3:A:655:MET:HA	1.98	0.46
3:D:97:ILE:HD12	3:D:183:VAL:HG13	1.98	0.46
2:K:90:ASN:OD1	2:K:90:ASN:C	2.59	0.46
2:L:197:LEU:HD23	2:L:198:LEU:N	2.30	0.46
3:F:301:ASN:O	3:F:305:LEU:HG	2.15	0.45
3:D:210:ASN:ND2	3:D:276:MET:O	2.49	0.45
3:E:372:MET:O	3:E:373:THR:HG23	2.15	0.45
2:L:56:LYS:CG	2:L:56:LYS:O	2.63	0.45
1:G:183:MET:HE1	3:E:344:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:410:HIS:ND1	3:D:442:GLU:OE1	2.50	0.45
3:E:726:VAL:O	3:E:730:LEU:HD23	2.16	0.45
4:H:64:MET:HE3	4:H:67:ILE:HB	1.98	0.45
2:K:39:GLU:O	2:K:43:GLU:OE1	2.34	0.45
2:L:257:ASP:OD1	2:L:258:SER:N	2.48	0.45
3:D:263:GLY:N	5:D:802:ATP:O2B	2.43	0.45
1:I:205:LEU:HD11	4:H:157:ILE:HD13	1.97	0.45
3:E:207:SER:C	3:E:208:ILE:HD12	2.42	0.45
3:A:682:LEU:HD23	3:A:682:LEU:C	2.41	0.45
3:A:724:TYR:HB3	3:A:727:ARG:HD3	1.99	0.45
2:K:98:GLN:OE1	2:K:102:ASN:ND2	2.48	0.45
3:A:595:SER:OG	3:A:596:GLN:N	2.50	0.45
3:E:310:GLU:OE2	3:E:364:LEU:HD22	2.16	0.45
2:J:104:LEU:CB	2:J:127:ILE:HD11	2.45	0.45
3:A:264:CYS:N	6:A:802:ADP:O2B	2.49	0.45
3:A:504[A]:MET:O	3:A:505:ASN:ND2	2.50	0.45
3:E:383:LEU:HD22	3:E:389:LEU:HD12	1.95	0.45
3:D:437:SER:O	3:D:440:GLU:N	2.50	0.45
3:E:720:MET:HE3	3:E:720:MET:HA	1.99	0.45
3:F:128:GLN:C	3:F:176:LEU:HD12	2.41	0.45
3:B:253:VAL:HG22	3:B:390:GLU:OE2	2.17	0.45
3:D:548:GLY:N	5:D:801:ATP:O2B	2.50	0.45
1:G:241:VAL:HA	4:H:67:ILE:HD11	1.99	0.44
3:C:519:ASP:O	3:C:522:GLU:HG3	2.17	0.44
3:F:650:ASP:OD1	3:F:651:VAL:N	2.49	0.44
3:A:424:VAL:HG22	3:A:477:ARG:CA	2.47	0.44
3:C:549:LYS:N	5:C:801:ATP:O1B	2.50	0.44
3:B:495:ASN:OD1	3:B:495:ASN:C	2.60	0.44
3:D:297:GLU:N	3:D:297:GLU:CD	2.75	0.44
1:G:237:VAL:HG11	4:H:60:ILE:CD1	2.47	0.44
3:A:655:MET:HE2	3:A:655:MET:CA	2.47	0.44
2:L:176:GLU:OE2	2:L:282:ARG:NH1	2.51	0.44
3:C:655:MET:SD	3:D:614:ILE:HD12	2.58	0.44
3:E:344:THR:O	3:E:344:THR:CG2	2.66	0.44
3:D:428:GLU:HA	3:D:431:VAL:HG12	1.98	0.44
4:H:50:LEU:HD13	4:H:171:ILE:HD11	1.99	0.44
4:H:143:GLU:O	4:H:146:MET:HB2	2.18	0.44
3:F:8:ALA:CB	3:F:72:LEU:HD21	2.47	0.44
3:A:35:VAL:CG2	3:A:49:LEU:HD21	2.47	0.44
3:D:255:GLY:HA3	3:D:389:LEU:HD23	1.99	0.44
3:F:128:GLN:O	3:F:176:LEU:HD12	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:381:GLU:OE2	3:F:385:ARG:NH1	2.50	0.44
3:D:114:THR:HA	3:D:117:MET:HG2	2.00	0.44
3:E:97:ILE:HD12	3:E:183:VAL:HG13	1.99	0.44
3:E:348:ASP:OD1	3:E:349:THR:N	2.51	0.44
2:L:216:ILE:HG23	2:L:217:ASP:OD1	2.17	0.44
3:A:531:SER:OG	3:A:534:THR:OG1	2.24	0.44
3:A:665:ILE:HG22	3:A:666:HIS:N	2.32	0.44
3:E:102:LEU:HD13	3:E:137:VAL:HG22	2.00	0.44
2:L:16:GLU:HA	2:L:19:ARG:HG2	2.00	0.44
3:E:23:VAL:HB	3:E:61:ALA:HB3	2.00	0.44
3:C:244:ILE:H	3:C:244:ILE:HD12	1.83	0.43
3:C:399:ASP:OD1	3:C:399:ASP:N	2.50	0.43
3:F:323:HIS:N	3:F:366:ASN:O	2.46	0.43
3:F:419:LEU:HD11	3:E:247:GLN:HG2	2.00	0.43
3:A:517:VAL:HG11	3:A:552:LEU:HD23	1.99	0.43
3:E:292:ASN:OD1	3:E:293:LYS:N	2.51	0.43
2:J:19:ARG:HD2	2:J:20:LYS:N	2.34	0.43
3:A:218:MET:O	3:A:218:MET:HG3	2.18	0.43
3:D:102:LEU:HD22	3:D:137:VAL:HG22	2.00	0.43
4:H:179:ASP:O	4:H:182:MET:HB3	2.18	0.43
3:B:403:ARG:O	3:B:407:LEU:HD23	2.18	0.43
2:L:237:ASP:OD1	2:L:238:SER:N	2.51	0.43
3:C:92:ILE:HG22	3:C:95:MET:HE2	1.99	0.43
3:F:446:ARG:NH1	3:E:250:CYS:SG	2.91	0.43
3:F:705:ILE:HD11	3:F:709:LYS:HG2	2.01	0.43
3:A:414:MET:HE2	3:A:414:MET:CA	2.49	0.43
3:B:29:TYR:CB	3:B:49:LEU:HD13	2.48	0.43
3:B:471:GLU:OE1	3:B:471:GLU:N	2.50	0.43
3:E:16:LEU:HD13	3:E:23:VAL:HG13	2.01	0.43
4:H:159:ASN:HB3	4:H:163:MET:HE1	2.00	0.43
4:H:178:ILE:O	4:H:181:ILE:HG12	2.19	0.43
3:F:299:GLU:OE1	3:F:299:GLU:N	2.52	0.43
3:D:411:THR:O	3:D:411:THR:HG22	2.18	0.43
4:H:181:ILE:O	4:H:182:MET:C	2.61	0.43
3:F:518:LEU:HD23	3:F:556:ILE:HD11	1.99	0.43
3:D:466:ASP:O	3:D:467:MET:HB3	2.19	0.43
3:E:541:LEU:HD23	3:E:665:ILE:HB	2.01	0.43
4:H:168:GLY:O	4:H:169:ASN:C	2.60	0.43
2:K:10:ALA:O	2:K:14:LEU:HD13	2.17	0.43
3:E:220:ILE:HG22	3:E:221:GLY:N	2.34	0.43
3:C:245:VAL:HA	3:C:248:MET:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:414:MET:CG	3:B:248:MET:HE1	2.49	0.43
3:C:533:ARG:NH1	3:D:685:ASN:OD1	2.44	0.43
3:F:18:LEU:HD13	3:F:139:SER:HB2	2.00	0.43
3:F:227:PHE:HA	3:F:230:ILE:HD12	2.01	0.43
3:D:467:MET:O	3:D:467:MET:SD	2.77	0.43
3:F:427:LYS:O	3:F:431:VAL:HG23	2.17	0.43
3:A:204:ASN:OD1	3:A:206:GLN:NE2	2.51	0.43
3:D:31:SER:OG	3:D:51:THR:OG1	2.32	0.43
4:H:159:ASN:O	4:H:163:MET:HE2	2.18	0.43
1:G:213:HIS:CE1	4:H:35:LEU:HB3	2.54	0.43
1:I:199:HIS:O	1:I:203:ILE:HD12	2.17	0.43
3:A:24:VAL:CG1	3:A:49:LEU:HD22	2.48	0.43
3:A:193:LEU:HD21	3:A:195:LEU:HD21	2.00	0.43
3:A:433:THR:HG22	3:A:436:PHE:CD1	2.54	0.43
3:B:605:ILE:HD11	3:B:626:LEU:CD2	2.47	0.43
3:B:695:ALA:HA	3:B:698:VAL:HG12	1.99	0.43
3:B:728:LYS:O	3:B:732:LEU:HD13	2.18	0.43
3:D:322:LEU:HD12	3:D:323:HIS:H	1.83	0.43
3:E:343:SER:O	3:E:344:THR:HB	2.19	0.43
4:H:145:GLU:HG2	4:H:146:MET:HE2	2.00	0.43
2:K:80:ASP:OD1	2:K:81:ALA:N	2.52	0.43
3:A:380:ASP:O	3:A:384:LEU:HD13	2.19	0.42
2:J:82:ALA:HB2	2:J:110:ILE:HG21	2.00	0.42
3:A:95:MET:HE1	3:A:181:SER:CB	2.49	0.42
2:L:92:PHE:O	2:L:95:ALA:N	2.49	0.42
1:G:241:VAL:CA	4:H:67:ILE:HD11	2.49	0.42
2:J:81:ALA:O	2:J:85:PHE:CD2	2.72	0.42
3:C:531:SER:OG	3:D:715:GLU:OE2	2.36	0.42
3:F:454:ASN:O	3:F:457:ILE:HG22	2.19	0.42
3:A:18:LEU:CD2	3:A:144:LEU:HD22	2.50	0.42
3:E:688:ASP:OD1	3:E:688:ASP:N	2.51	0.42
4:H:187:SER:O	4:H:188:ASN:C	2.62	0.42
4:H:191:ARG:O	4:H:194:GLU:HG3	2.19	0.42
2:L:232:PHE:CE1	2:L:234:ALA:HB3	2.55	0.42
1:G:195:ILE:HA	1:G:198:ARG:HG2	2.01	0.42
3:F:29:TYR:CB	3:F:49:LEU:HD13	2.49	0.42
3:A:424:VAL:HG22	3:A:477:ARG:CB	2.49	0.42
1:I:241:VAL:HA	1:I:244:VAL:HG12	2.01	0.42
3:C:485:GLU:OE1	3:C:486:ASN:OD1	2.37	0.42
3:C:707:ILE:HG23	3:C:708:LYS:N	2.35	0.42
3:B:117:MET:SD	3:B:195:LEU:HD22	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:128:ALA:HB2	2:J:144:HIS:HB2	2.02	0.42
3:A:242:PRO:HA	3:A:245:VAL:CG1	2.49	0.42
3:B:85:PHE:HZ	3:B:129:ALA:HB2	1.84	0.42
3:E:232:ARG:HE	3:E:233:ARG:HG2	1.83	0.42
2:K:75:LEU:HD12	2:K:75:LEU:O	2.20	0.42
2:L:6:LYS:NZ	2:L:51:MET:HE1	2.34	0.42
1:G:202:ILE:HG23	4:H:32:MET:HE1	2.00	0.42
3:F:302:ILE:HD11	3:F:350:VAL:HG13	2.02	0.42
3:F:585:MET:HE1	3:F:608:LEU:HD21	2.01	0.42
2:J:40:GLU:OE2	2:J:44:ILE:HD11	2.20	0.42
3:C:243:GLU:N	3:C:243:GLU:OE1	2.53	0.42
3:C:715:GLU:OE1	3:B:531:SER:OG	2.31	0.42
3:A:654:GLU:C	3:A:655:MET:HE2	2.45	0.42
3:D:512:ASP:N	3:D:513:PRO:CD	2.83	0.42
3:E:711:LEU:O	3:E:714:ILE:HG22	2.19	0.42
3:A:424:VAL:HG22	3:A:477:ARG:HB2	2.01	0.42
3:A:463:VAL:HG12	3:A:465:VAL:HG23	2.02	0.42
4:H:159:ASN:C	4:H:163:MET:HE2	2.45	0.42
3:C:100:ASP:O	3:C:146:GLY:N	2.46	0.41
3:F:37:VAL:HG22	3:F:80:VAL:HG22	2.01	0.41
3:F:280:ARG:NH1	3:F:281:GLU:O	2.47	0.41
3:F:396:GLY:C	3:F:397:LEU:HD12	2.45	0.41
3:A:240:PHE:CG	3:A:241:PRO:HD2	2.55	0.41
2:L:184:ILE:HD13	2:L:187:GLN:NE2	2.35	0.41
2:J:279:MET:SD	2:J:279:MET:C	3.03	0.41
3:C:178:VAL:HG23	3:C:180:ASN:OD1	2.20	0.41
3:F:258:LEU:HD22	3:F:395:ILE:HD11	2.01	0.41
3:A:247:GLN:OE1	3:B:417:HIS:ND1	2.53	0.41
3:D:24:VAL:CG1	3:D:60:VAL:HG22	2.45	0.41
3:D:97:ILE:HD12	3:D:183:VAL:CG1	2.50	0.41
3:D:379:ILE:HD12	3:D:379:ILE:H	1.85	0.41
3:E:92:ILE:HD13	3:E:95:MET:SD	2.60	0.41
1:G:192:LEU:O	1:G:195:ILE:HG22	2.21	0.41
3:A:253:VAL:HG22	3:B:446:ARG:HH12	1.82	0.41
3:E:102:LEU:HD22	3:E:137:VAL:CG2	2.49	0.41
3:E:348:ASP:HA	3:E:351:VAL:HG12	2.02	0.41
2:K:3:THR:HG23	2:K:4:SER:N	2.34	0.41
2:L:246:LYS:HE3	2:L:262:SER:HB3	2.01	0.41
3:C:206:GLN:OE1	3:C:206:GLN:N	2.54	0.41
3:C:463:VAL:HG21	3:B:209:ILE:HG21	2.02	0.41
3:A:131:SER:OG	3:A:174:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:214:PHE:O	2:J:218:MET:HE1	2.21	0.41
3:F:720:MET:O	3:F:725:ARG:NE	2.39	0.41
3:E:244:ILE:HG23	3:E:245:VAL:N	2.36	0.41
1:G:222:LEU:HD22	1:I:223:VAL:CG1	2.50	0.41
3:C:606:GLU:HG2	3:C:607:ARG:N	2.36	0.41
3:F:269:LEU:O	3:F:273:ILE:CD1	2.68	0.41
3:F:482:ALA:O	3:F:486:ASN:OD1	2.39	0.41
3:B:498:ASP:OD1	3:B:499:TYR:CD1	2.74	0.41
4:H:7:MET:SD	4:H:8:ARG:HG2	2.60	0.41
2:L:198:LEU:O	2:L:198:LEU:HG	2.21	0.41
2:J:28:PHE:HB2	2:J:37:LYS:HE3	2.02	0.41
3:E:649:LYS:O	3:E:650:ASP:C	2.63	0.41
2:L:127:ILE:HG13	2:L:128:ALA:N	2.36	0.41
2:J:214:PHE:HE1	2:J:248:LEU:HD21	1.86	0.41
3:C:573:MET:HE3	3:C:581:LYS:HG2	2.03	0.41
3:A:6:MET:HE3	3:A:60:VAL:HG23	2.01	0.41
3:C:23:VAL:HG12	3:C:55:VAL:HG21	2.02	0.41
3:F:245:VAL:HG21	3:F:252:HIS:CE1	2.56	0.41
3:F:595:SER:OG	3:F:596:GLN:N	2.54	0.41
3:A:40:SER:HB3	3:A:41:PRO:HD2	2.02	0.41
3:D:94:THR:HG22	3:D:95:MET:N	2.36	0.41
3:E:271:ARG:HG3	3:E:272:GLN:N	2.35	0.41
3:E:707:ILE:HG23	3:E:708:LYS:N	2.35	0.41
3:D:461:THR:HG23	3:D:462:LYS:N	2.36	0.41
3:E:230:ILE:CD1	3:E:256:ILE:HD11	2.51	0.41
2:L:241:CYS:HA	2:L:244:MET:HE3	2.03	0.41
3:F:457:ILE:HD11	3:E:239:VAL:HG11	2.02	0.40
3:E:10:ARG:O	3:E:61:ALA:HB1	2.20	0.40
2:K:100:ALA:O	2:K:104:LEU:HD13	2.21	0.40
2:J:54:MET:HE2	2:J:54:MET:HA	2.03	0.40
3:F:40:SER:HB3	3:F:41:PRO:HD2	2.03	0.40
3:F:315:ARG:HG3	3:F:316:LEU:HG	2.03	0.40
3:A:707:ILE:HG23	3:A:708:LYS:N	2.36	0.40
2:J:142:ILE:HD12	2:J:168:VAL:HG13	2.03	0.40
3:F:373:THR:HG22	3:F:374:ASN:N	2.36	0.40
3:E:607:ARG:HA	3:E:607:ARG:NE	2.35	0.40
4:H:11:LEU:HD22	4:H:14:MET:HE2	2.03	0.40
4:H:186:ASP:O	4:H:187:SER:C	2.64	0.40
2:K:6:LYS:HD2	2:K:51:MET:SD	2.60	0.40
1:G:199:HIS:CE1	4:H:24:GLU:OE2	2.74	0.40
3:C:468:GLU:OE1	3:C:468:GLU:N	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:276:LEU:O	2:L:279:MET:HG2	2.21	0.40
1:G:213:HIS:CE1	4:H:39:SER:OG	2.74	0.40
1:G:232:ARG:O	1:G:236:ASN:ND2	2.41	0.40
3:C:209:ILE:HG21	3:D:463:VAL:HG21	2.04	0.40
3:C:218:MET:HE1	3:C:227:PHE:CZ	2.56	0.40
3:A:494:THR:O	3:A:494:THR:HG23	2.22	0.40
3:D:114:THR:HA	3:D:117:MET:CG	2.51	0.40
3:D:444:LEU:HD23	3:D:444:LEU:C	2.46	0.40
3:D:523:LEU:C	3:D:523:LEU:HD23	2.46	0.40
4:H:146:MET:O	4:H:147:ASP:C	2.65	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	G	85/267 (32%)	82 (96%)	3 (4%)	0	100	100
1	I	61/267 (23%)	61 (100%)	0	0	100	100
2	J	285/296 (96%)	280 (98%)	5 (2%)	0	100	100
2	K	272/296 (92%)	269 (99%)	3 (1%)	0	100	100
2	L	271/296 (92%)	263 (97%)	8 (3%)	0	100	100
3	A	727/747 (97%)	708 (97%)	19 (3%)	0	100	100
3	B	718/747 (96%)	695 (97%)	22 (3%)	1 (0%)	48	81
3	C	728/747 (98%)	706 (97%)	21 (3%)	1 (0%)	48	81
3	D	729/747 (98%)	708 (97%)	21 (3%)	0	100	100
3	E	724/747 (97%)	693 (96%)	29 (4%)	2 (0%)	36	70
3	F	705/747 (94%)	687 (97%)	15 (2%)	3 (0%)	30	65
4	H	149/222 (67%)	139 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5454/6126 (89%)	5291 (97%)	156 (3%)	7 (0%)	49 81

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	202	LYS
3	F	487	ASP
3	F	399	ASP
3	C	488	ILE
3	E	488	ILE
3	B	488	ILE
3	E	635	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	G	78/245 (32%)	78 (100%)	0	100 100
1	I	58/245 (24%)	58 (100%)	0	100 100
2	J	235/243 (97%)	235 (100%)	0	100 100
2	K	227/243 (93%)	227 (100%)	0	100 100
2	L	226/243 (93%)	226 (100%)	0	100 100
3	A	628/638 (98%)	619 (99%)	9 (1%)	59 71
3	B	621/638 (97%)	620 (100%)	1 (0%)	87 87
3	C	629/638 (99%)	625 (99%)	4 (1%)	78 81
3	D	630/638 (99%)	630 (100%)	0	100 100
3	E	625/638 (98%)	624 (100%)	1 (0%)	87 87
3	F	613/638 (96%)	611 (100%)	2 (0%)	86 85
4	H	133/187 (71%)	133 (100%)	0	100 100
All	All	4703/5234 (90%)	4686 (100%)	17 (0%)	84 84

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	376	PRO
3	C	425	ASP
3	C	530[A]	ASN
3	C	530[B]	ASN
3	F	400	GLU
3	F	401	LYS
3	A	336	GLN
3	A	344	THR
3	A	348	ASP
3	A	458	LYS
3	A	473	LEU
3	A	476	THR
3	A	480	PHE
3	A	483	SER
3	A	484	LEU
3	B	331	ASP
3	E	437	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	199	HIS
1	G	226	GLN
2	J	123	HIS
3	C	76	GLN
3	C	103	GLN
3	C	286	ASN
3	C	719	GLN
3	F	123	GLN
3	F	252	HIS
3	F	353	GLN
3	F	486	ASN
3	F	505	ASN
3	A	110	ASN
3	A	123	GLN
3	A	135	GLN
3	A	272	GLN
3	A	408	HIS
3	B	20	ASN
3	B	123	GLN
3	B	374	ASN
3	D	110	ASN
3	D	123	GLN

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Mol	Chain	Res	Type
3	E	66	GLN
3	E	128	GLN
3	E	323	HIS
3	E	353	GLN
3	E	408	HIS
3	E	435	ASN
3	E	666	HIS
2	K	162	ASN
2	K	177	GLN
2	K	226	GLN
2	K	251	HIS
2	L	220	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 [i](#)

11 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	ATP	D	802	-	32,33,33	0.39	0	48,52,52	0.74	0
5	ATP	E	802	-	32,33,33	0.30	0	48,52,52	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ADP	A	802	-	28,29,29	1.36	5 (17%)	43,45,45	1.91	10 (23%)
5	ATP	B	801	-	32,33,33	0.38	0	48,52,52	0.75	0
5	ATP	E	801	-	32,33,33	0.54	0	48,52,52	0.61	0
5	ATP	C	801	-	32,33,33	0.46	0	48,52,52	0.75	1 (2%)
5	ATP	A	801	-	32,33,33	0.39	0	48,52,52	0.75	0
5	ATP	D	801	-	32,33,33	0.34	0	48,52,52	0.74	0
5	ATP	B	802	-	32,33,33	0.40	0	48,52,52	0.77	1 (2%)
5	ATP	F	1100	-	32,33,33	0.50	0	48,52,52	0.68	0
5	ATP	C	802	-	32,33,33	0.58	0	48,52,52	0.65	0

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	ATP	D	802	-	-	4/22/38/38	0/3/3/3
5	ATP	E	802	-	-	7/22/38/38	0/3/3/3
6	ADP	A	802	-	-	2/16/32/32	0/3/3/3
5	ATP	B	801	-	-	5/22/38/38	0/3/3/3
5	ATP	E	801	-	-	5/22/38/38	0/3/3/3
5	ATP	C	801	-	-	3/22/38/38	0/3/3/3
5	ATP	A	801	-	-	2/22/38/38	0/3/3/3
5	ATP	D	801	-	-	4/22/38/38	0/3/3/3
5	ATP	B	802	-	-	5/22/38/38	0/3/3/3
5	ATP	F	1100	-	-	2/22/38/38	0/3/3/3
5	ATP	C	802	-	-	6/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	802	ADP	C5-C4	4.36	1.46	1.39
6	A	802	ADP	C5-C6	2.51	1.48	1.41
6	A	802	ADP	C5-N7	-2.49	1.34	1.39
6	A	802	ADP	C8-N7	2.23	1.36	1.31
6	A	802	ADP	C4-N9	-2.03	1.33	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	802	ADP	C5-C4-N3	-5.83	118.69	126.72
6	A	802	ADP	N3-C4-N9	4.68	135.12	127.17
6	A	802	ADP	C2-N3-C4	3.80	121.12	111.83
6	A	802	ADP	N3-C2-N1	-3.61	123.11	128.58
6	A	802	ADP	C4-C5-N7	-3.52	106.55	110.58
6	A	802	ADP	C4-N9-C8	3.04	108.93	105.74
6	A	802	ADP	C5-N7-C8	2.75	107.77	103.45
6	A	802	ADP	N9-C8-N7	-2.38	110.56	113.94
6	A	802	ADP	C3'-C2'-C1'	2.35	105.91	101.46
5	C	801	ATP	O3'-C3'-C4'	-2.06	105.18	111.08
6	A	802	ADP	C6-C5-N7	2.04	136.03	132.09
5	B	802	ATP	O3'-C3'-C4'	-2.03	105.26	111.08

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	802	ATP	C5'-O5'-PA-O2A
5	C	802	ATP	C5'-O5'-PA-O3A
5	A	801	ATP	O4'-C1'-N9-C4
5	B	801	ATP	C5'-O5'-PA-O1A
5	B	802	ATP	C5'-O5'-PA-O1A
5	B	802	ATP	C5'-O5'-PA-O3A
5	B	802	ATP	O4'-C1'-N9-C8
5	B	802	ATP	O4'-C1'-N9-C4
5	E	802	ATP	PB-O3B-PG-O2G
5	E	802	ATP	PB-O3B-PG-O3G
5	E	802	ATP	C5'-O5'-PA-O2A
5	E	802	ATP	O4'-C4'-C5'-O5'
6	A	802	ADP	C5'-O5'-PA-O3A
5	D	801	ATP	C3'-C4'-C5'-O5'
5	D	802	ATP	O4'-C4'-C5'-O5'
5	D	802	ATP	C3'-C4'-C5'-O5'
5	A	801	ATP	O4'-C1'-N9-C8
5	D	801	ATP	O4'-C4'-C5'-O5'
5	D	801	ATP	O4'-C1'-N9-C4
5	E	802	ATP	C3'-C4'-C5'-O5'
5	D	801	ATP	O4'-C1'-N9-C8
5	C	802	ATP	O4'-C4'-C5'-O5'
5	B	801	ATP	PB-O3B-PG-O1G
5	C	801	ATP	O4'-C1'-N9-C4
5	C	801	ATP	O4'-C1'-N9-C8
5	B	802	ATP	PG-O3B-PB-O2B

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Mol	Chain	Res	Type	Atoms
5	D	802	ATP	PG-O3B-PB-O2B
5	B	801	ATP	C5'-O5'-PA-O3A
5	E	802	ATP	C5'-O5'-PA-O3A
6	A	802	ADP	C5'-O5'-PA-O1A
5	E	801	ATP	C4'-C5'-O5'-PA
5	E	802	ATP	C4'-C5'-O5'-PA
5	E	801	ATP	O4'-C4'-C5'-O5'
5	F	1100	ATP	O4'-C1'-N9-C4
5	F	1100	ATP	O4'-C1'-N9-C8
5	E	801	ATP	O4'-C1'-N9-C8
5	B	801	ATP	PG-O3B-PB-O3A
5	E	801	ATP	O4'-C1'-N9-C4
5	B	801	ATP	PG-O3B-PB-O1B
5	D	802	ATP	PG-O3B-PB-O1B
5	E	801	ATP	PB-O3A-PA-O2A
5	C	802	ATP	C2'-C1'-N9-C8
5	C	802	ATP	C3'-C4'-C5'-O5'
5	C	801	ATP	PG-O3B-PB-O1B
5	C	802	ATP	PB-O3A-PA-O2A

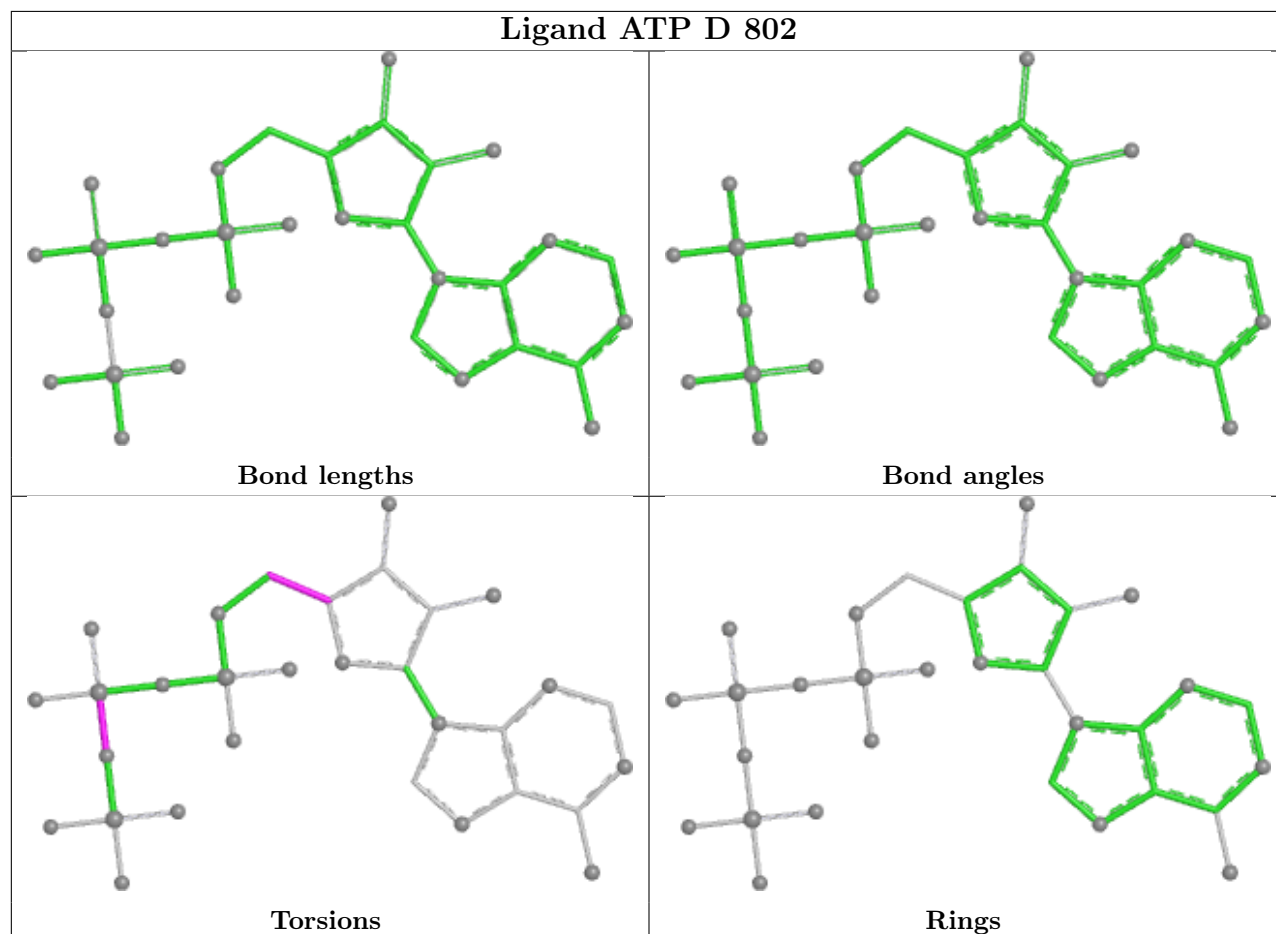
There are no ring outliers.

8 monomers are involved in 11 short contacts:

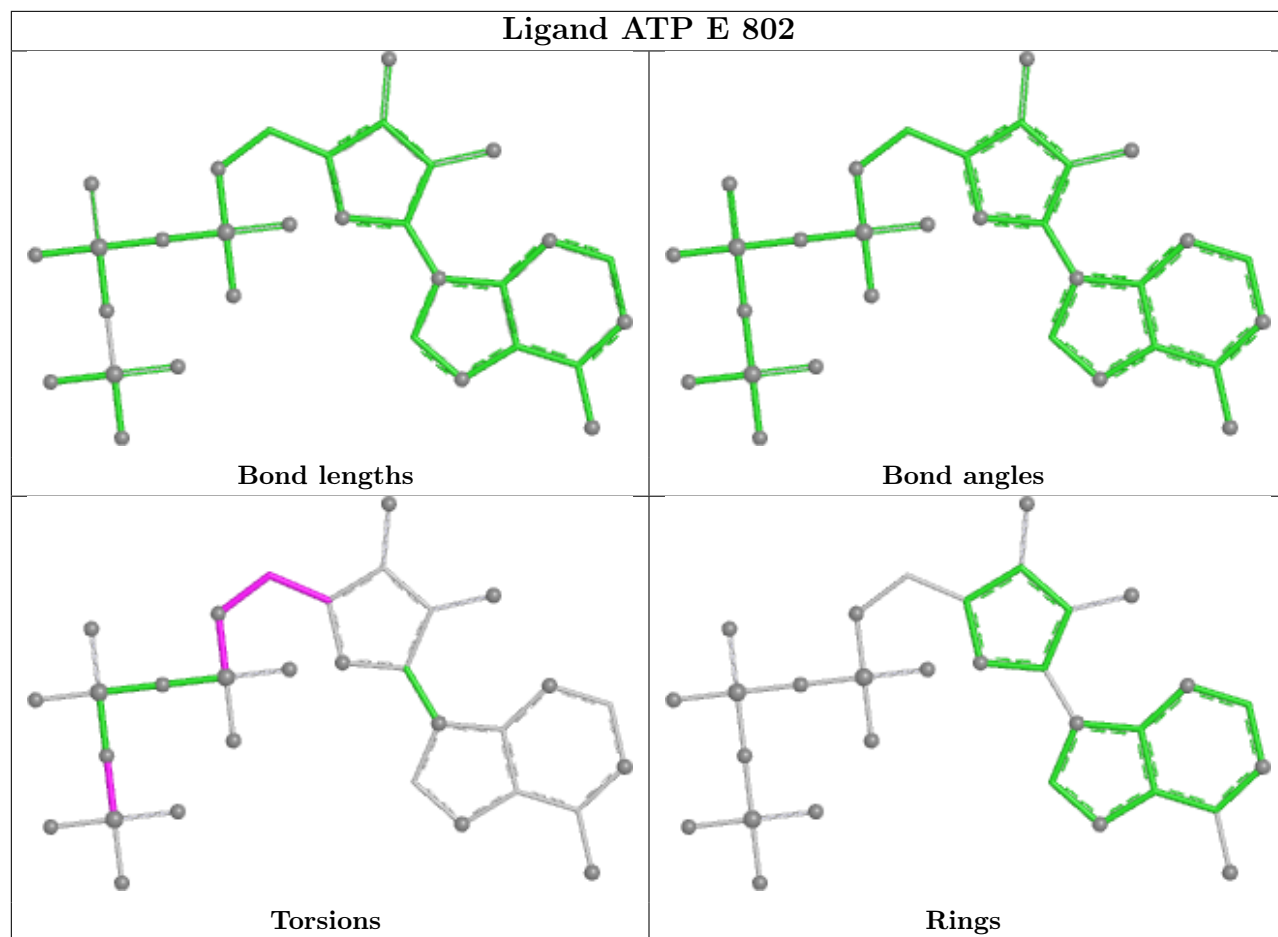
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	802	ATP	1	0
5	E	802	ATP	1	0
6	A	802	ADP	2	0
5	B	801	ATP	3	0
5	C	801	ATP	1	0
5	A	801	ATP	1	0
5	D	801	ATP	1	0
5	B	802	ATP	1	0

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

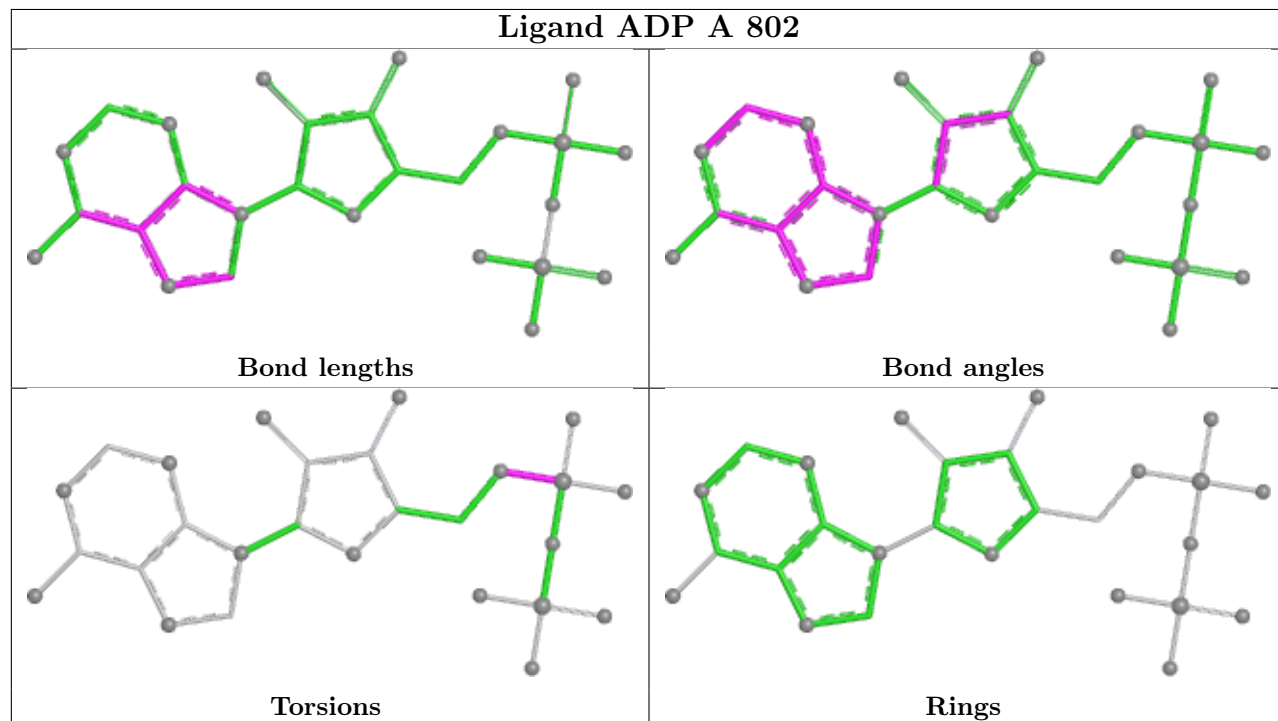
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

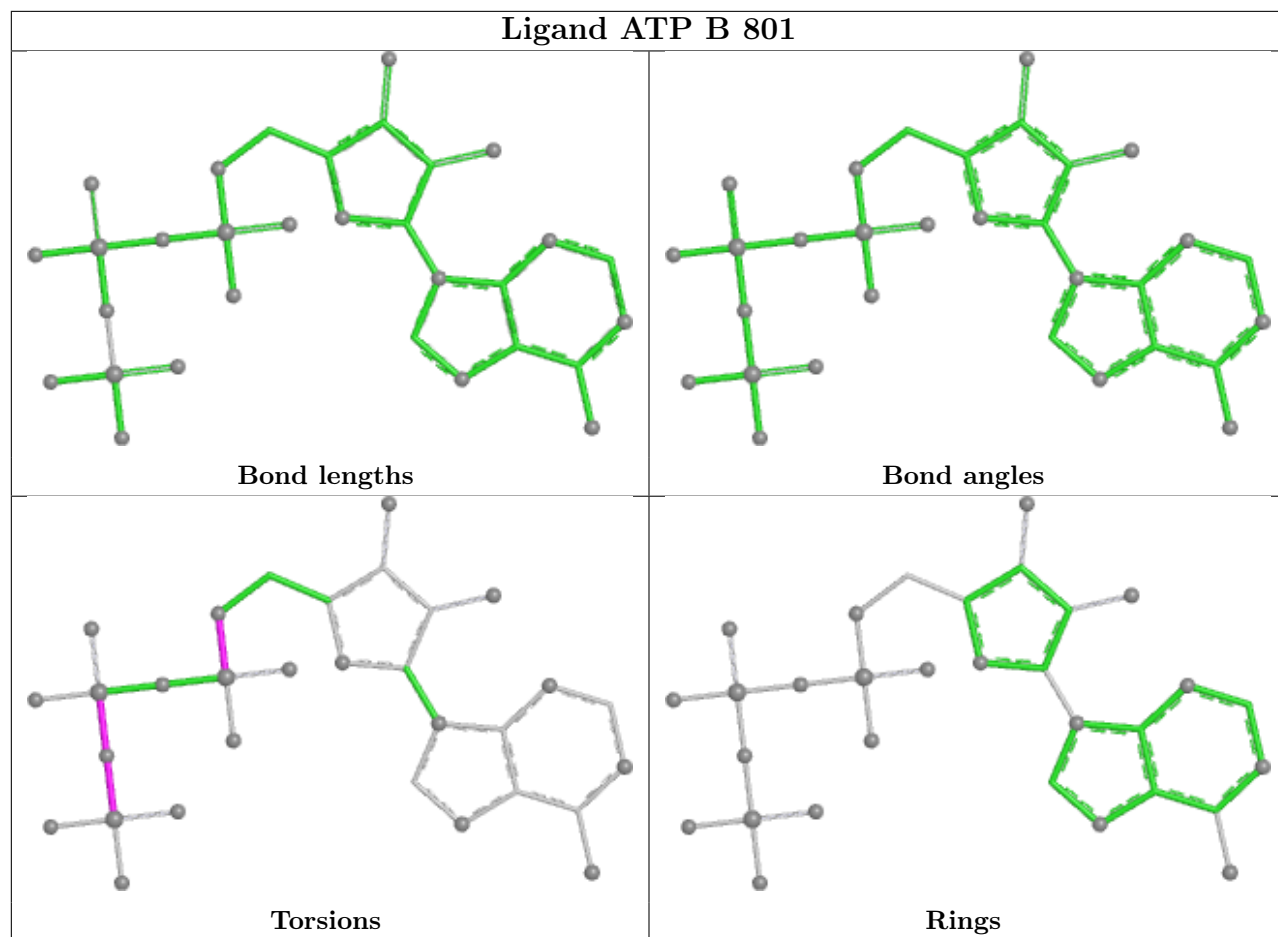


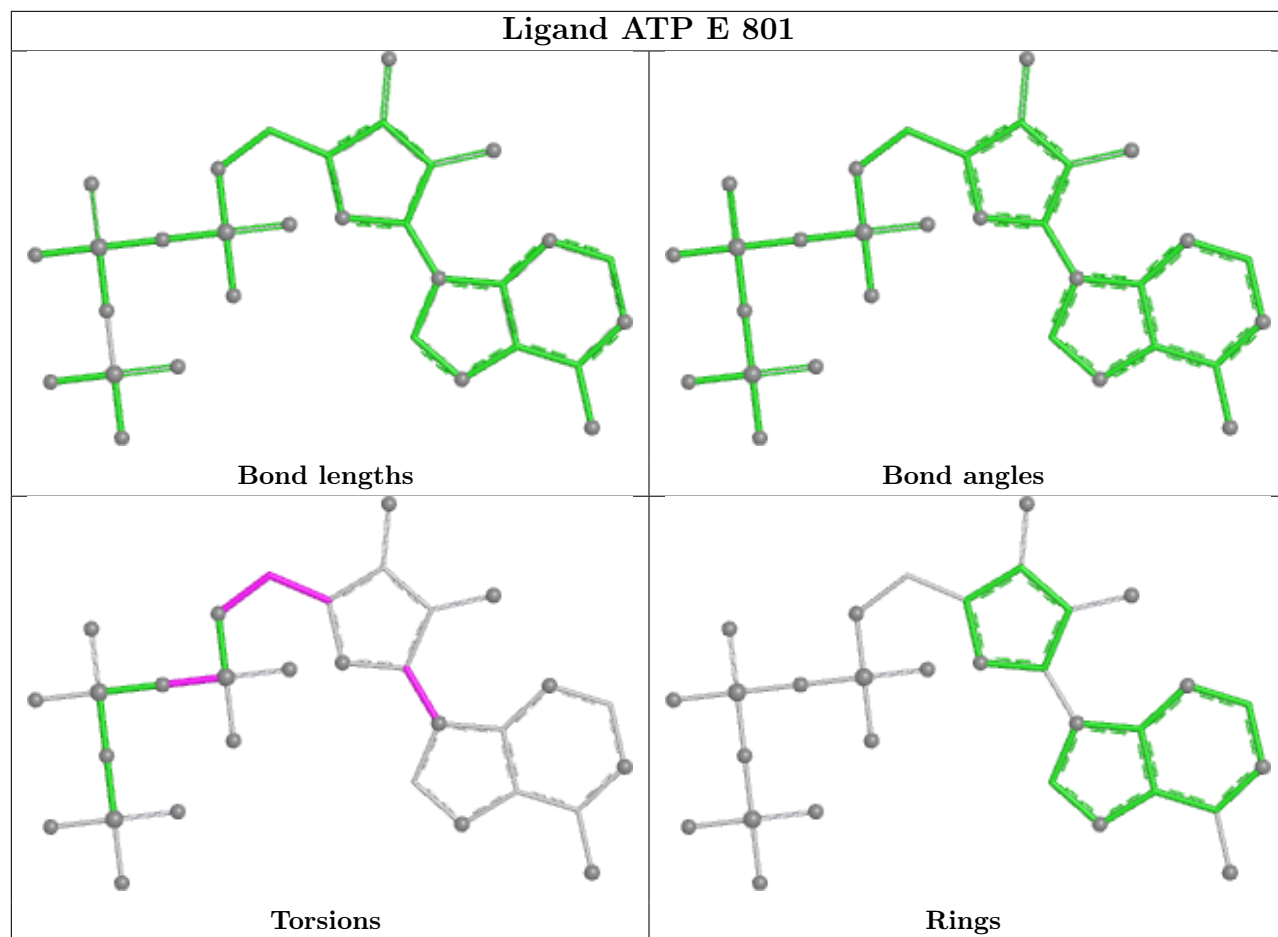
Ligand ATP E 802

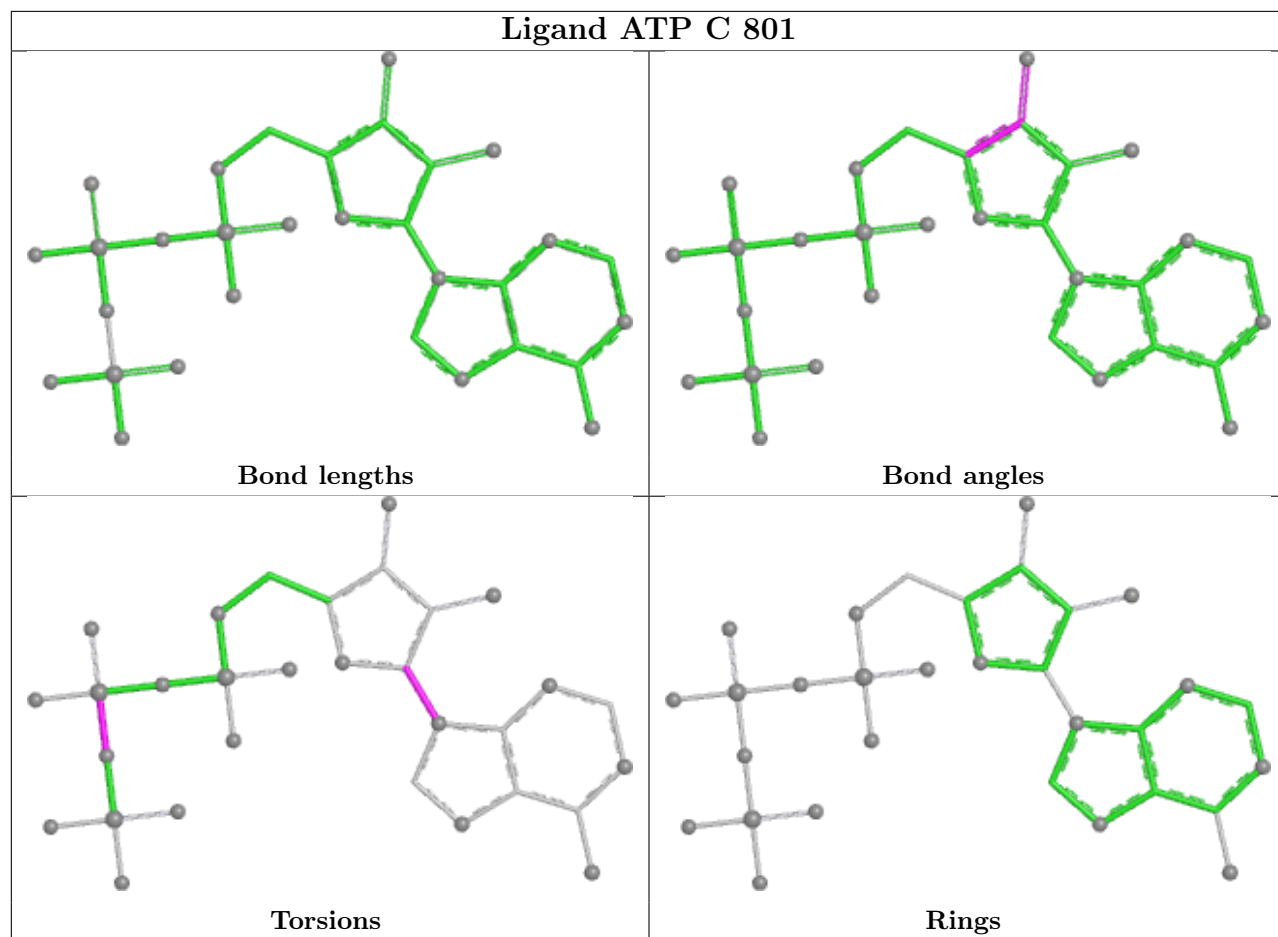


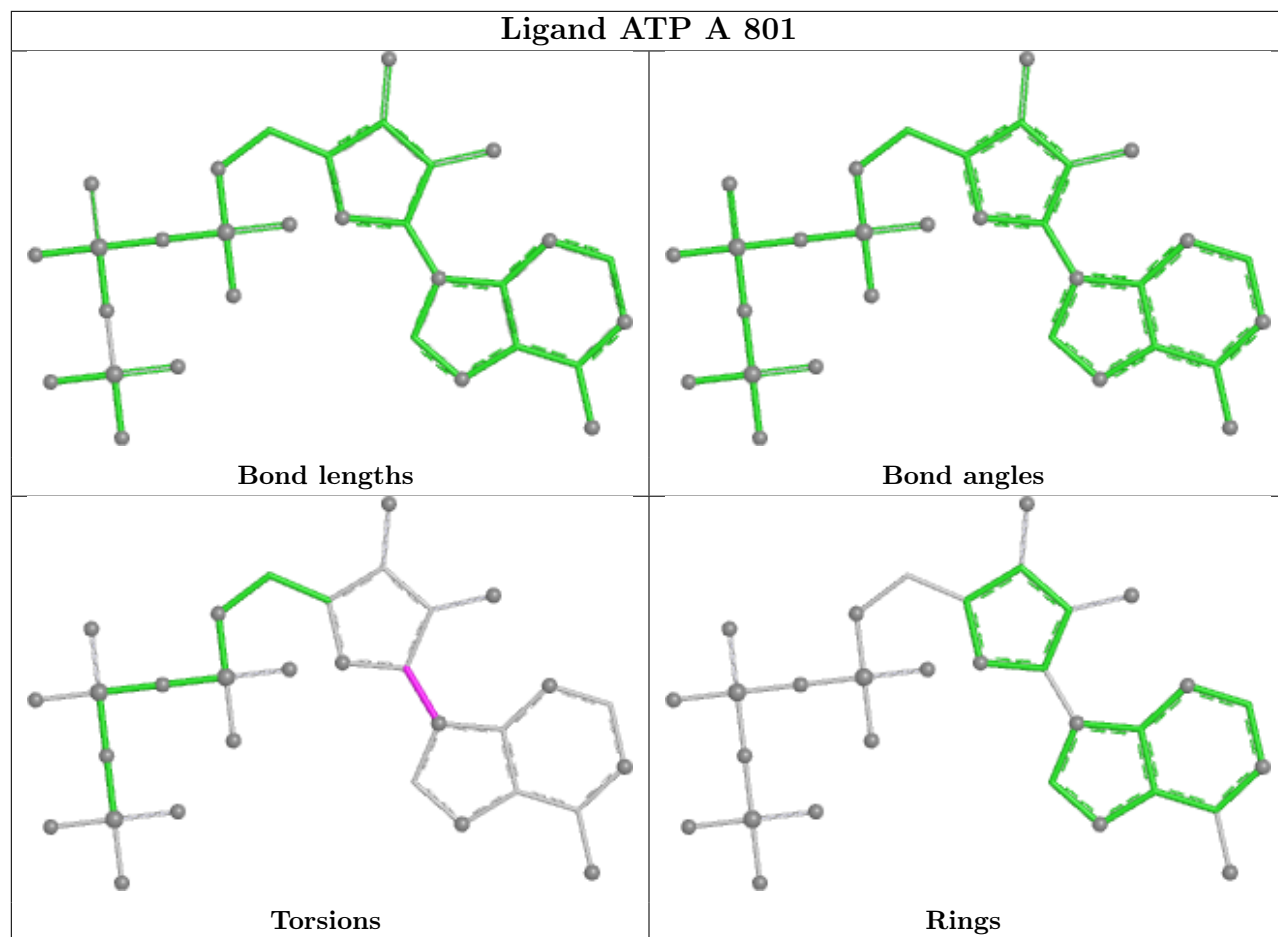
Ligand ADP A 802

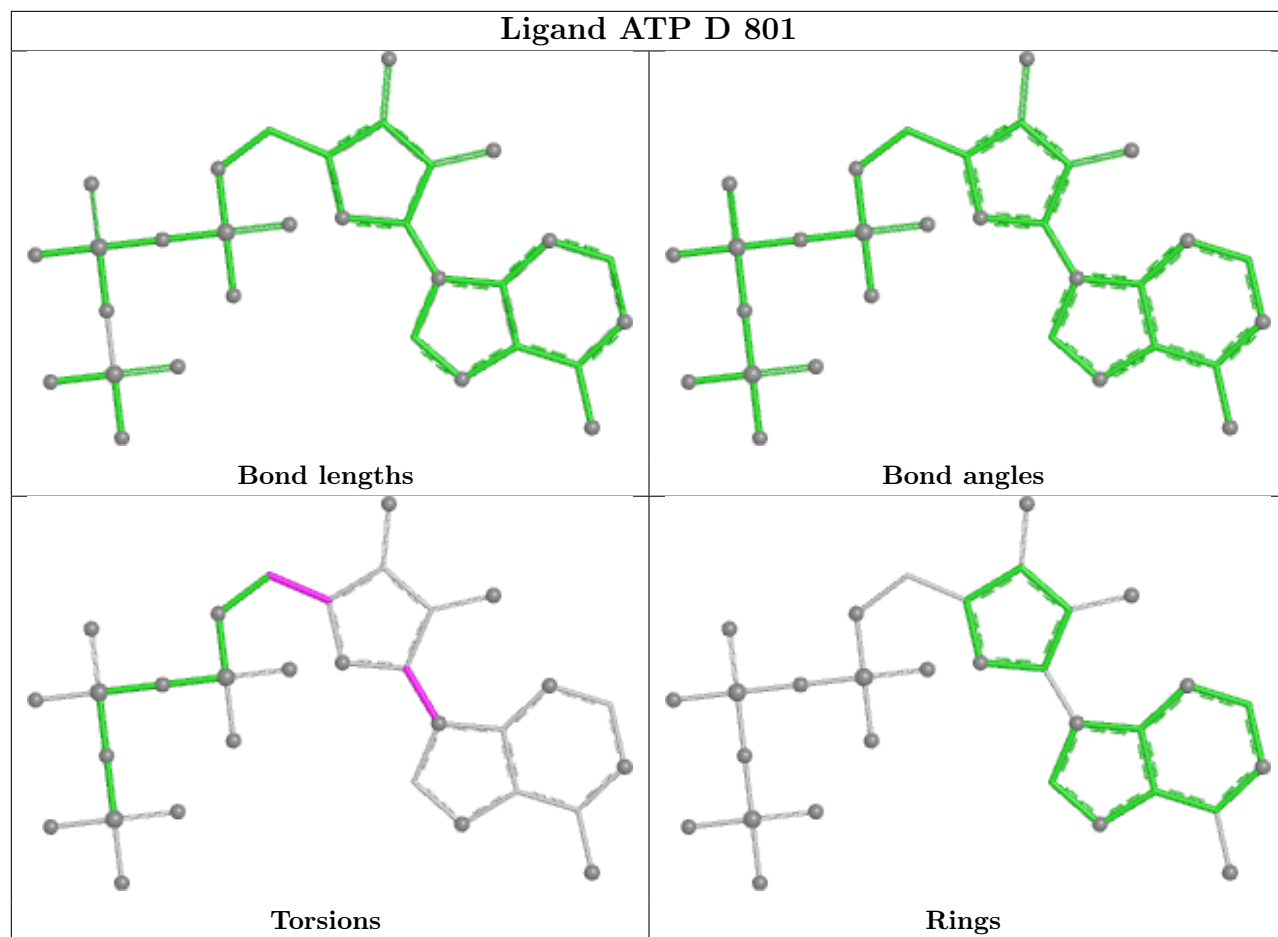


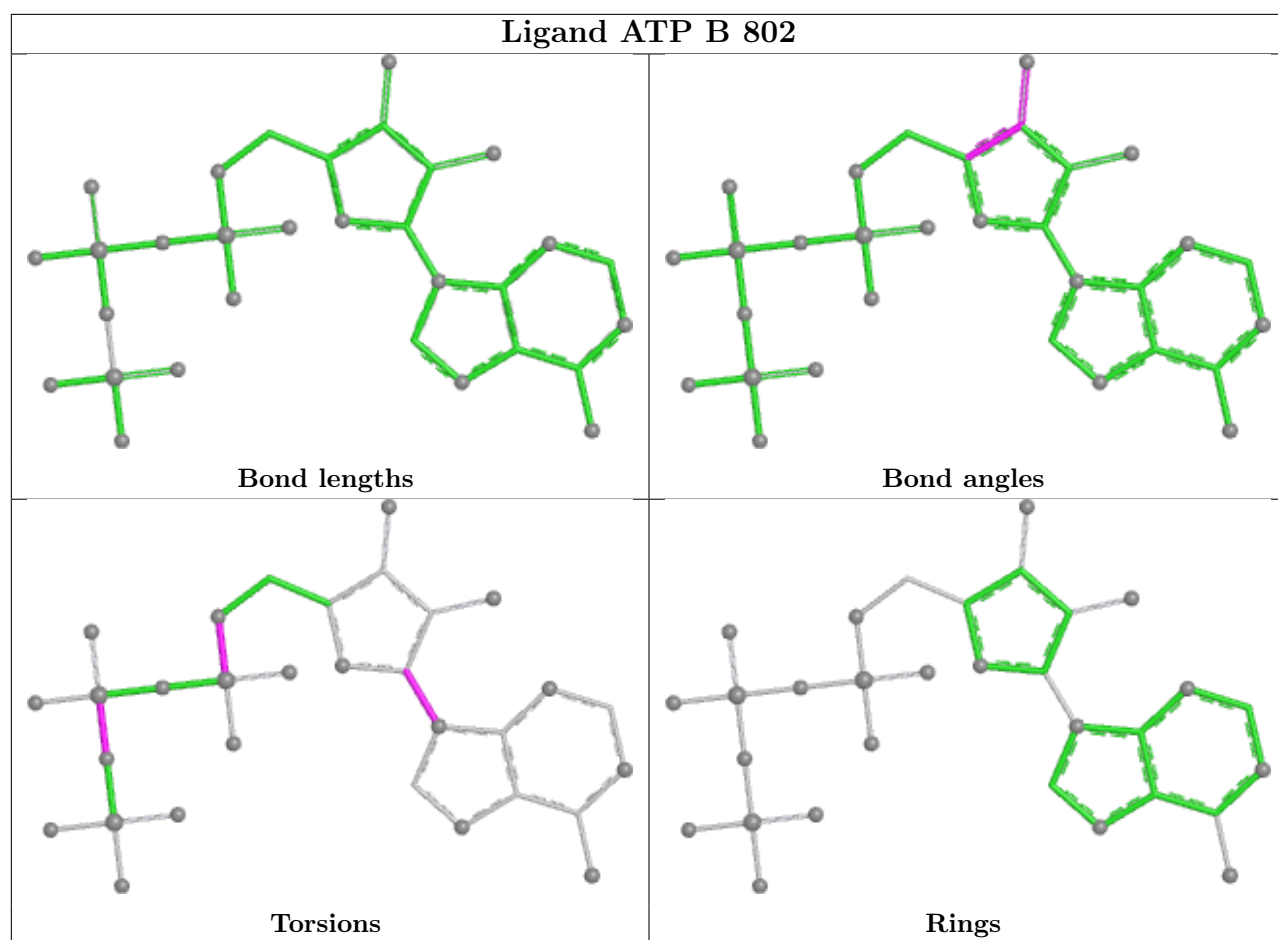


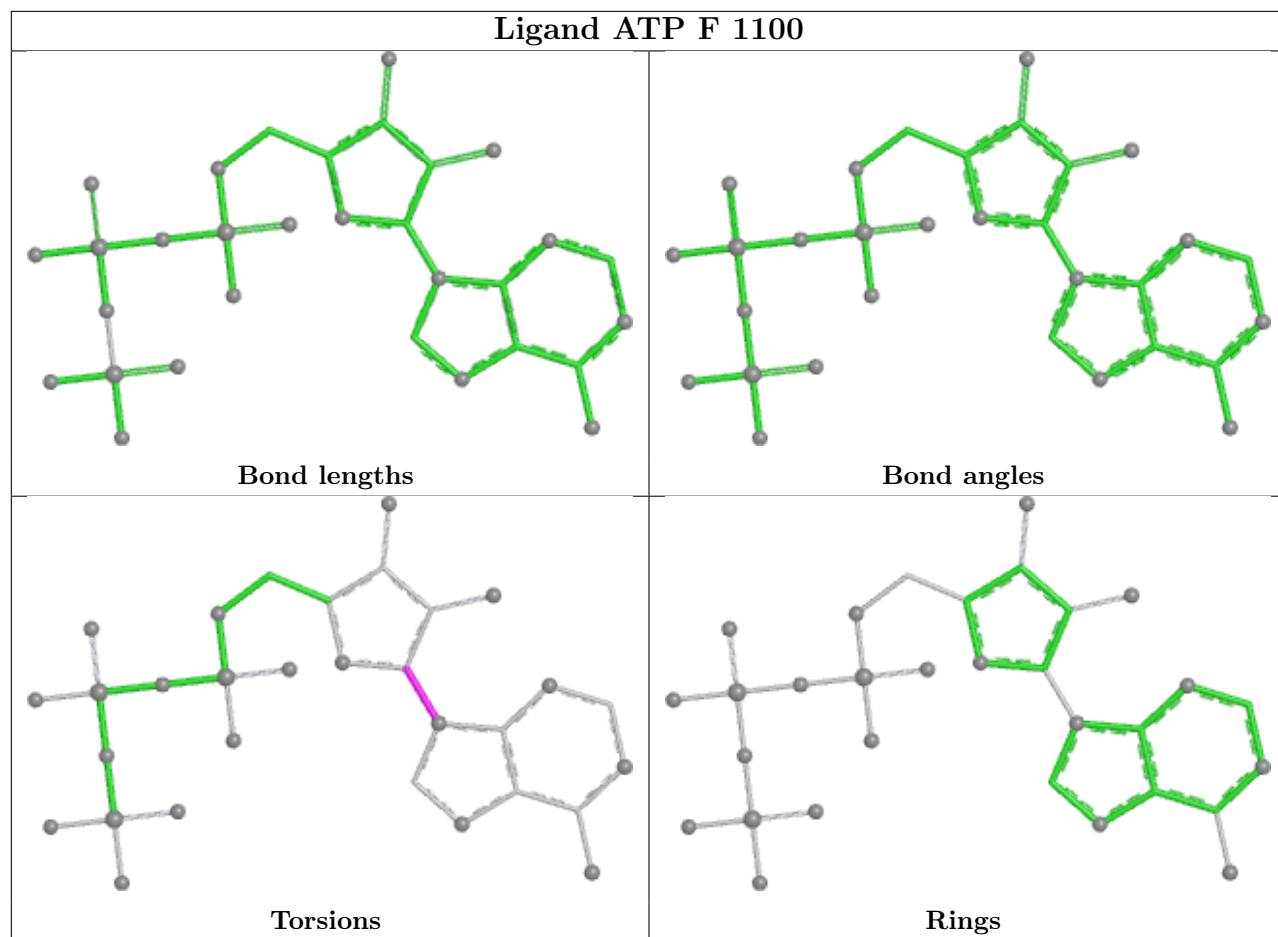


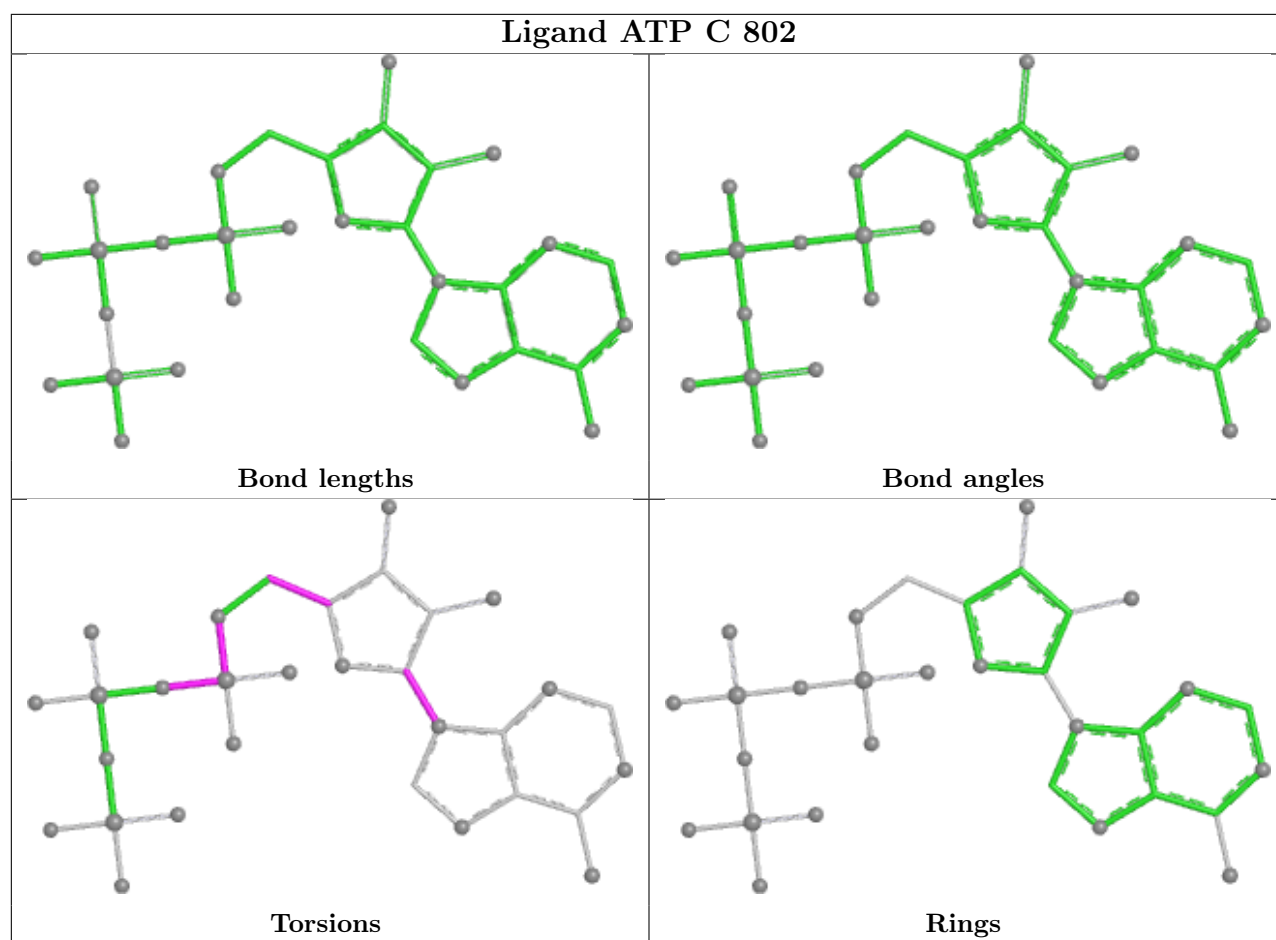












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

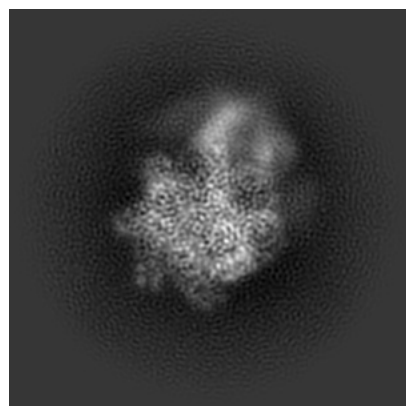
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71478. These allow visual inspection of the internal detail of the map and identification of artifacts.

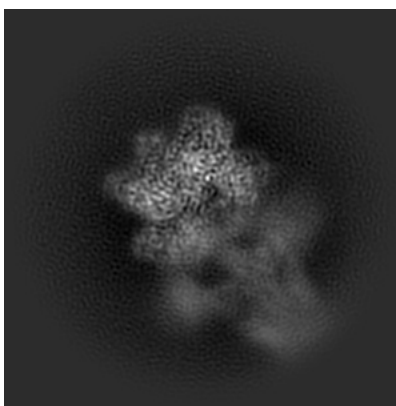
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

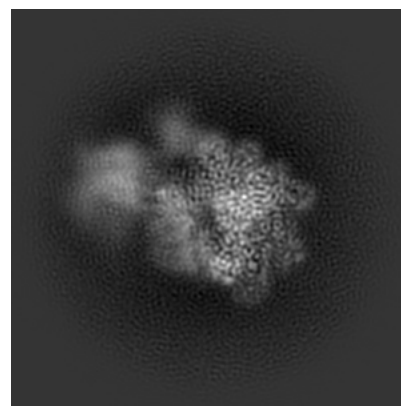
6.1.1 Primary map



X

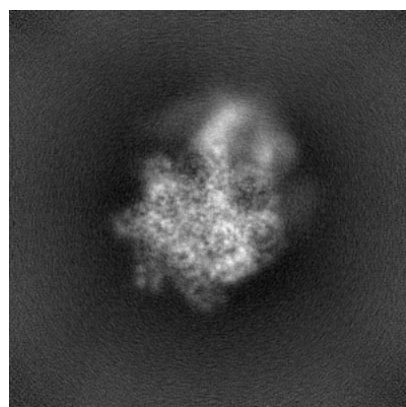


Y

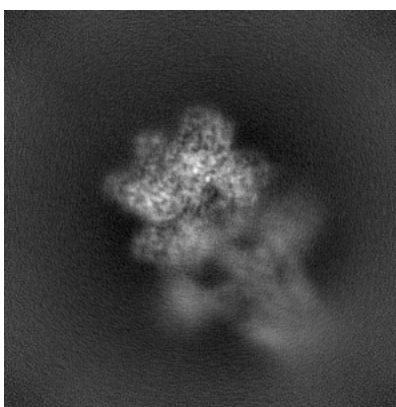


Z

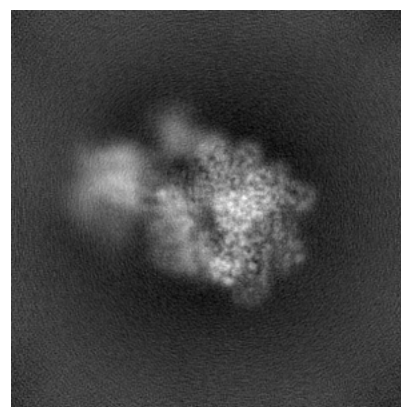
6.1.2 Raw map



X



Y

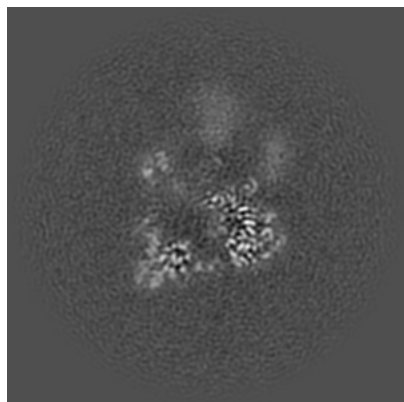


Z

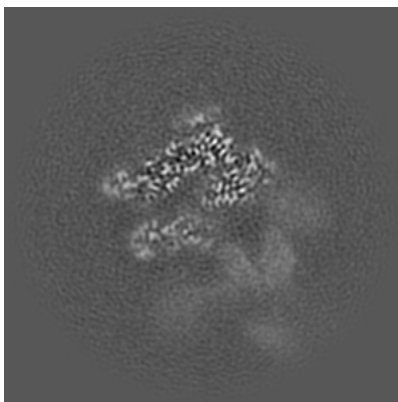
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

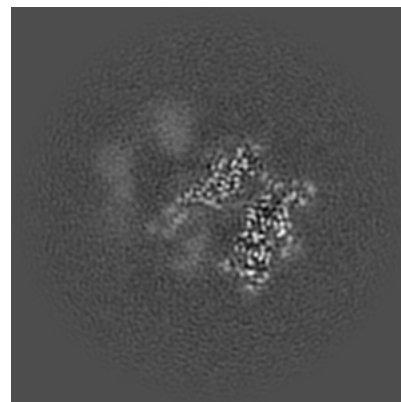
6.2.1 Primary map



X Index: 147

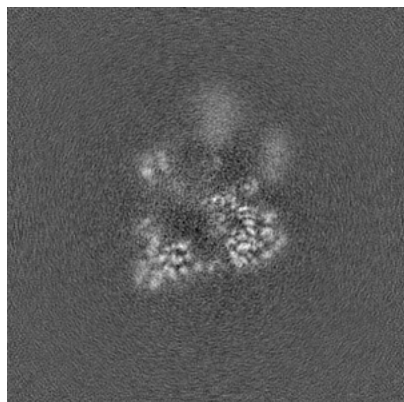


Y Index: 147

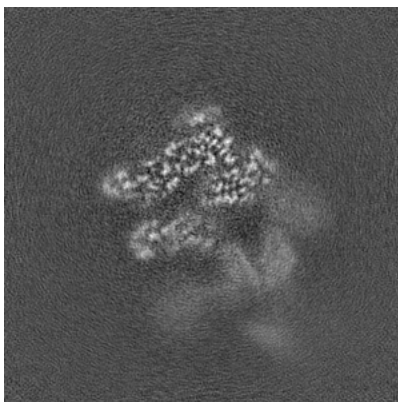


Z Index: 147

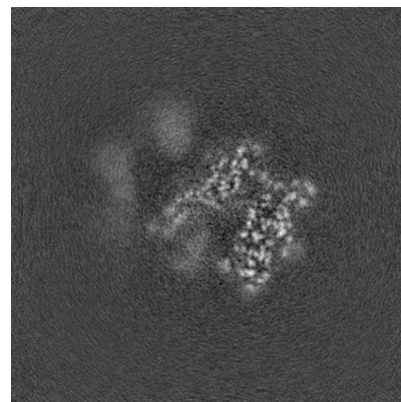
6.2.2 Raw map



X Index: 147



Y Index: 147

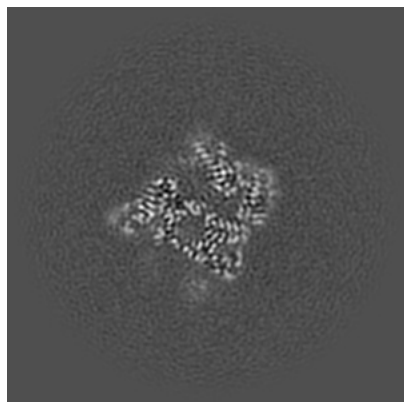


Z Index: 147

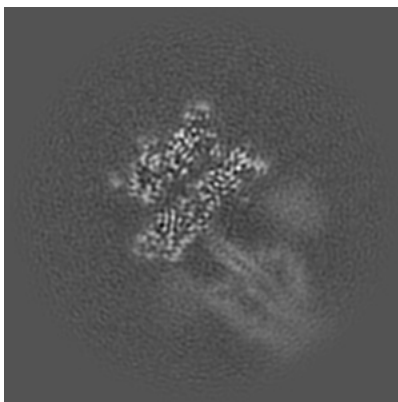
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

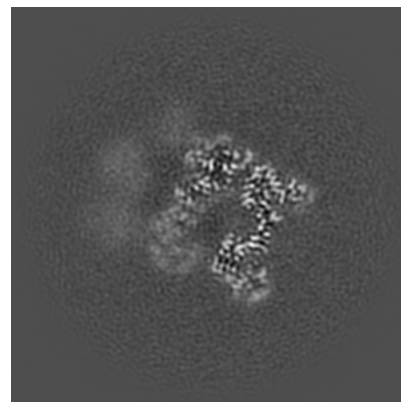
6.3.1 Primary map



X Index: 175

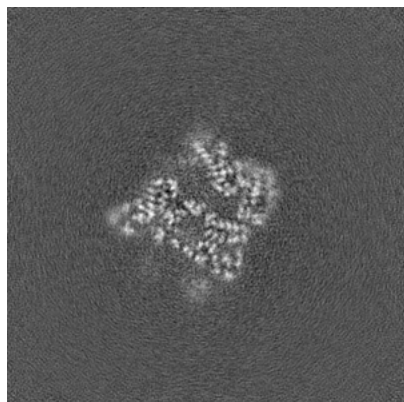


Y Index: 159

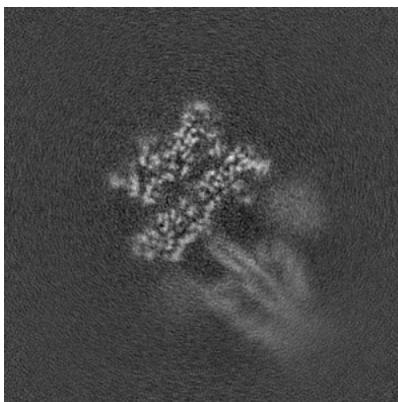


Z Index: 135

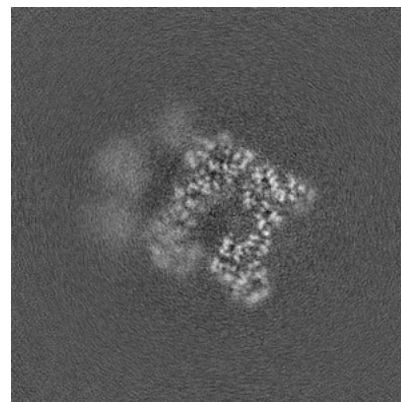
6.3.2 Raw map



X Index: 175



Y Index: 158

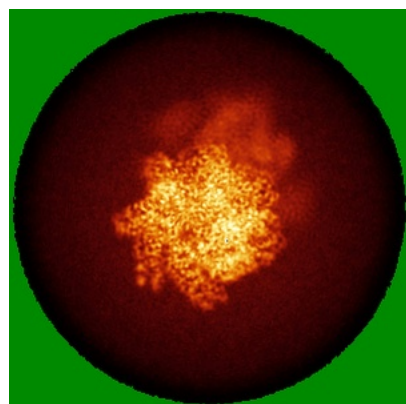


Z Index: 136

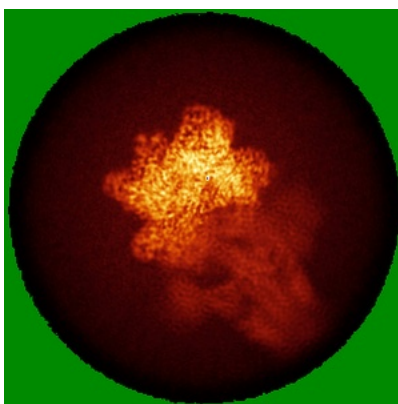
The images above show the largest variance slices of the map in three orthogonal directions.

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

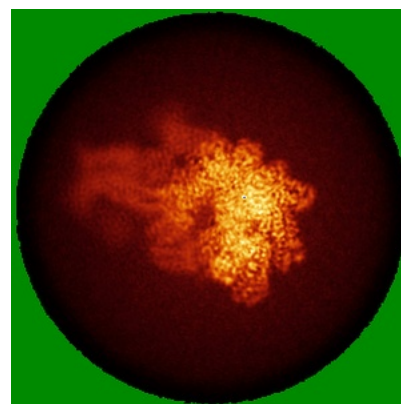
6.4.1 Primary map



X

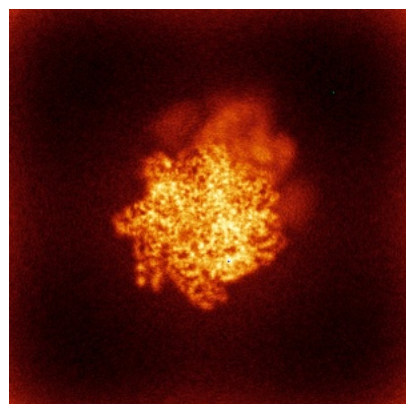


Y

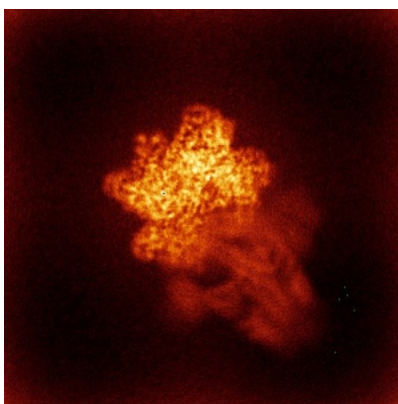


Z

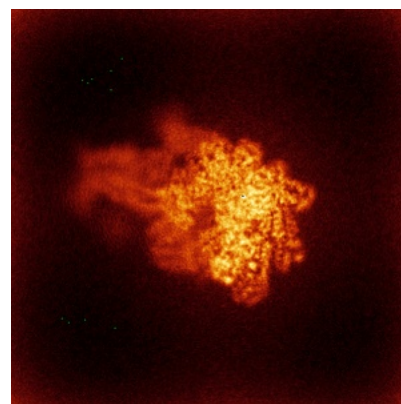
6.4.2 Raw map



X



Y

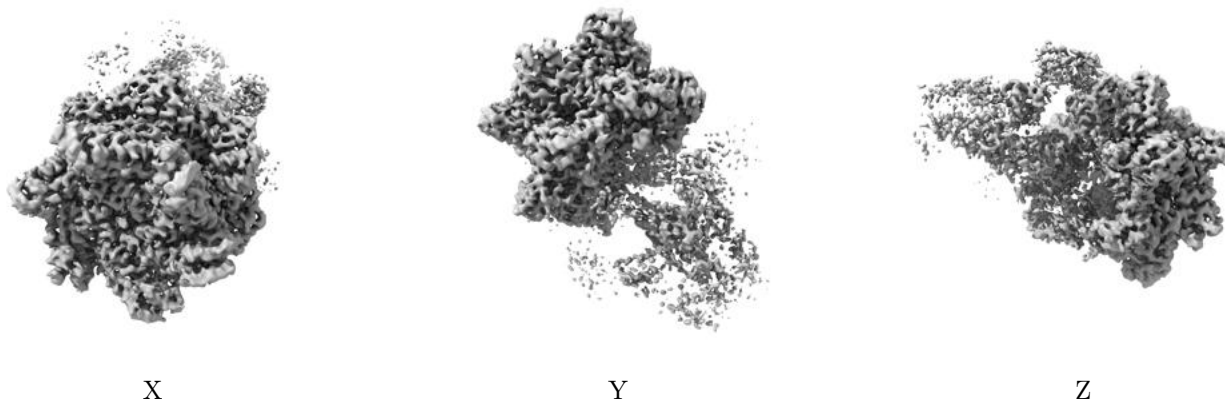


Z

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.

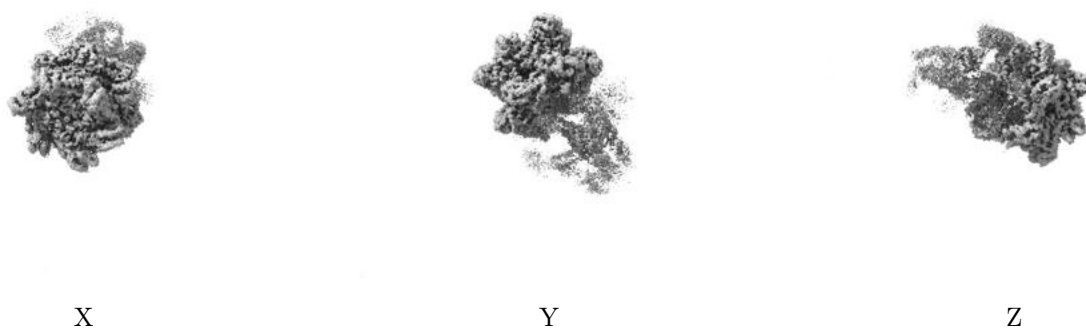
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

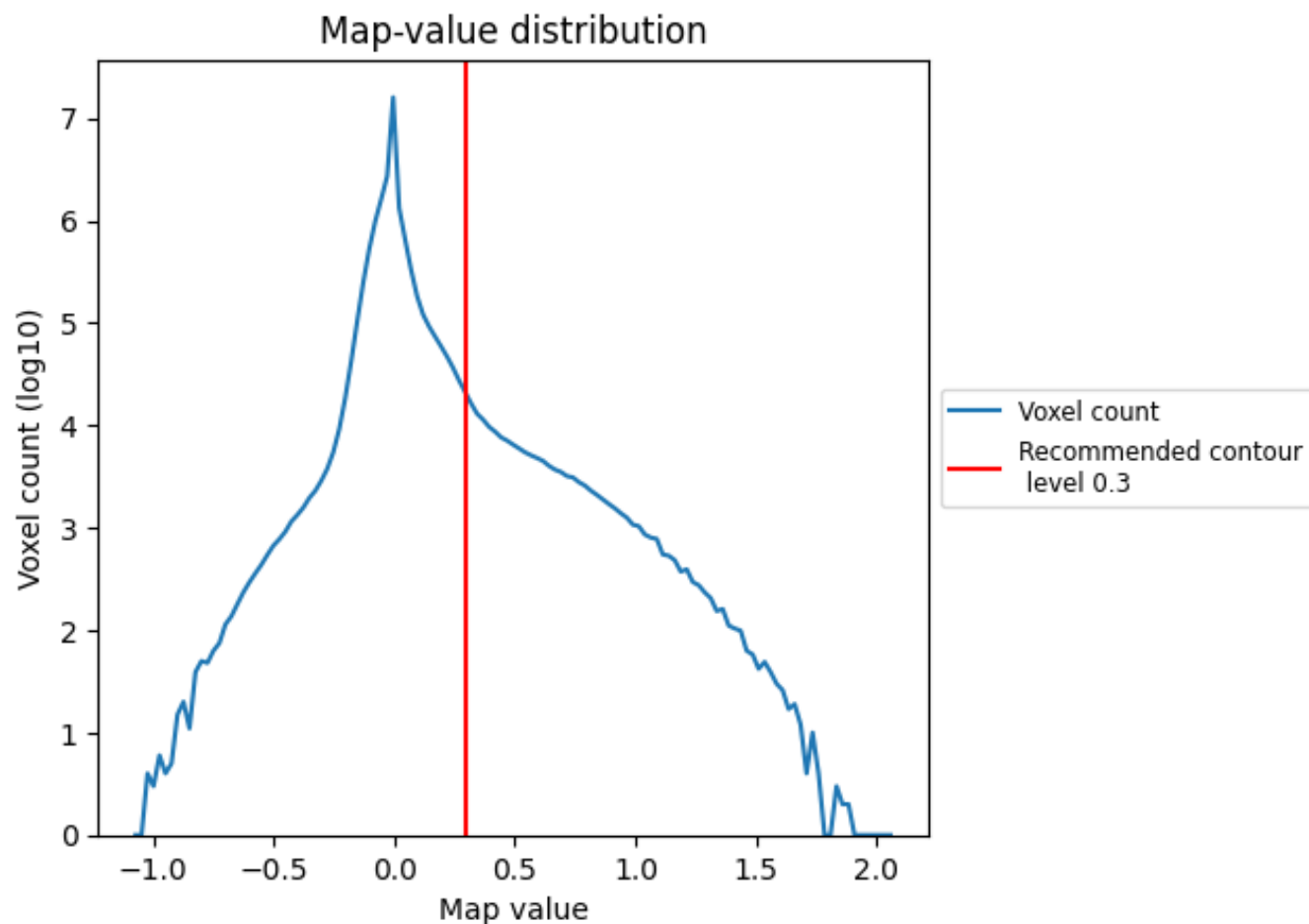
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

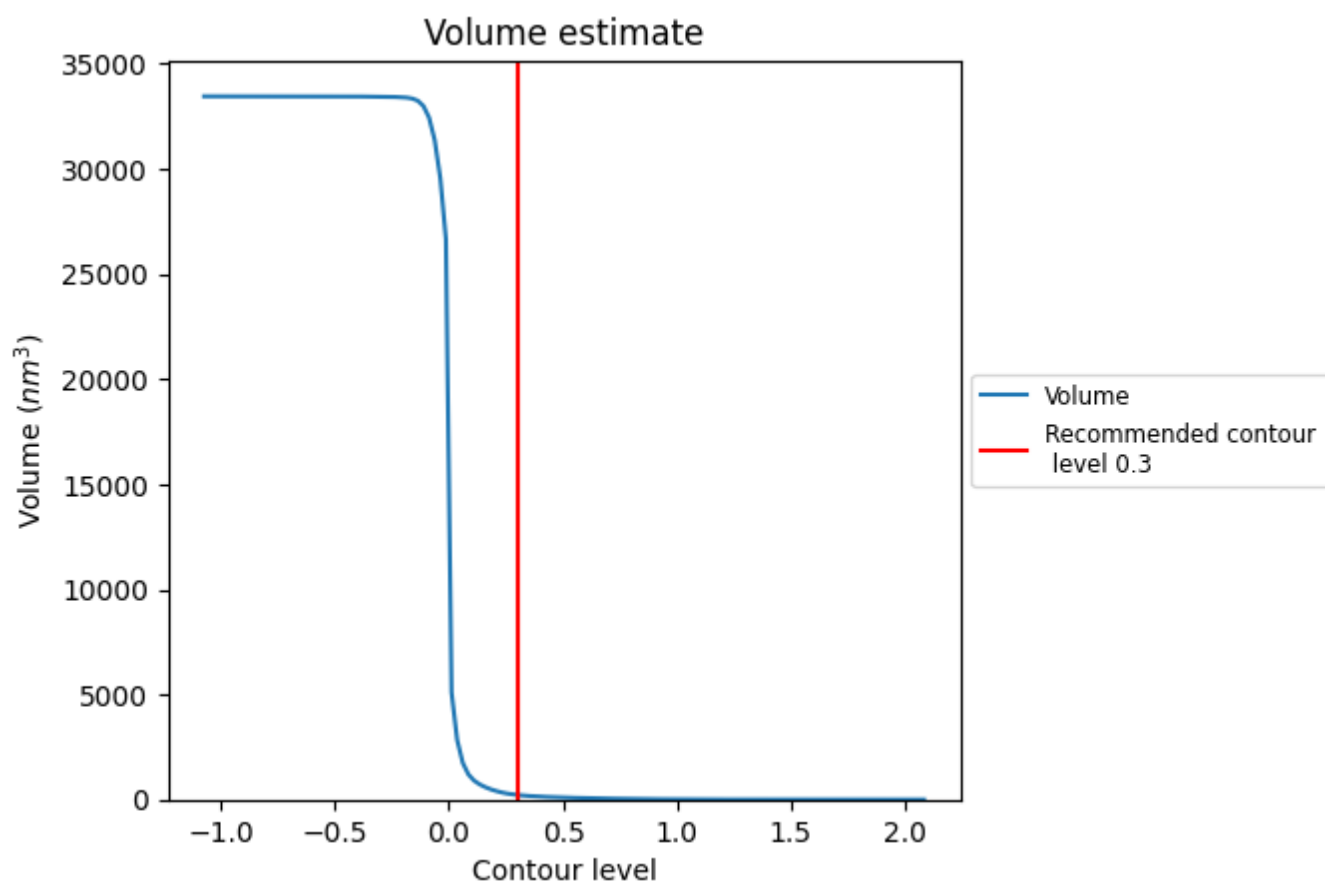
This section contains the results of statistical analysis of the map.

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.

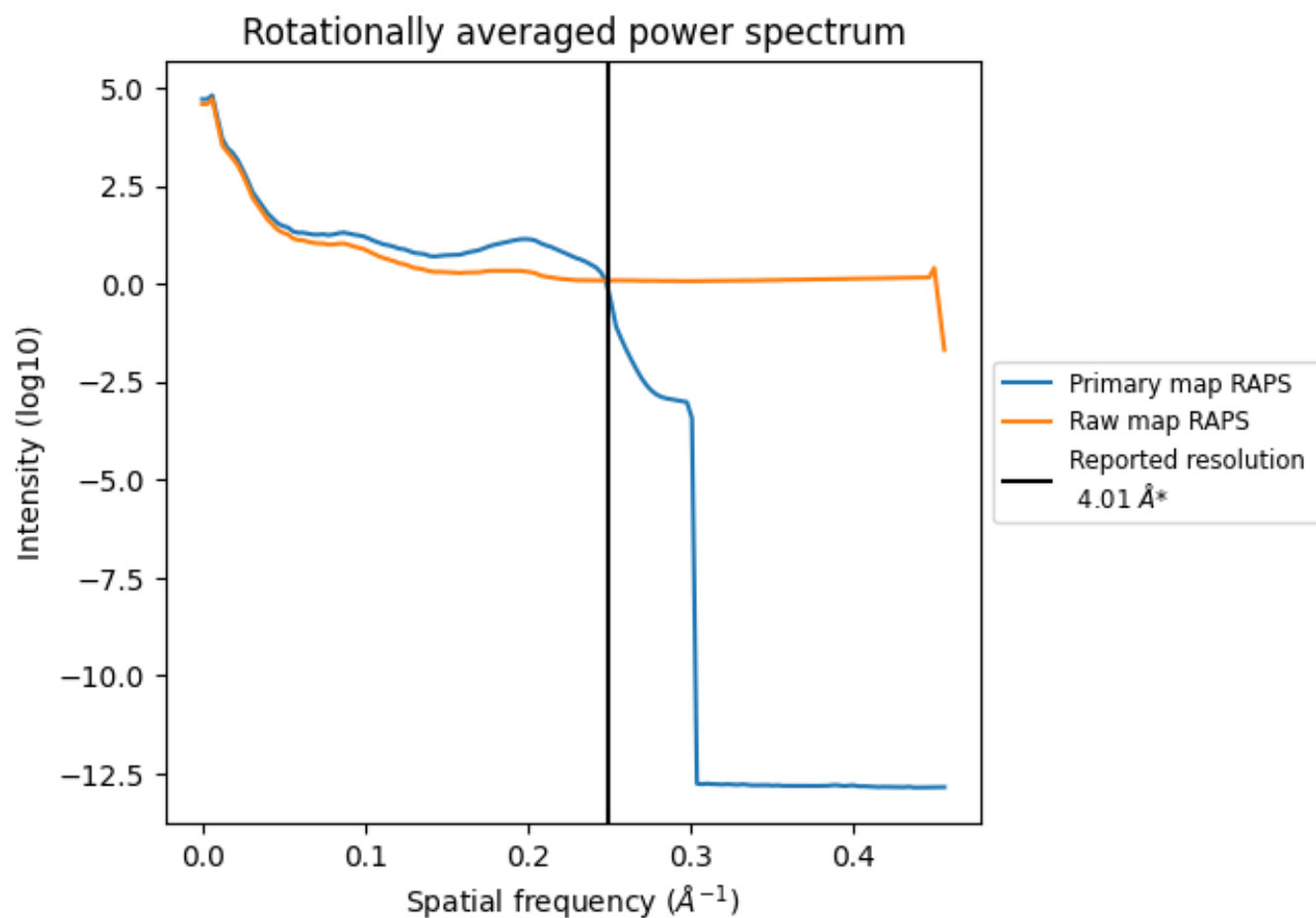
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 219 nm³; this corresponds to an approximate mass of 198 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 ⓘ

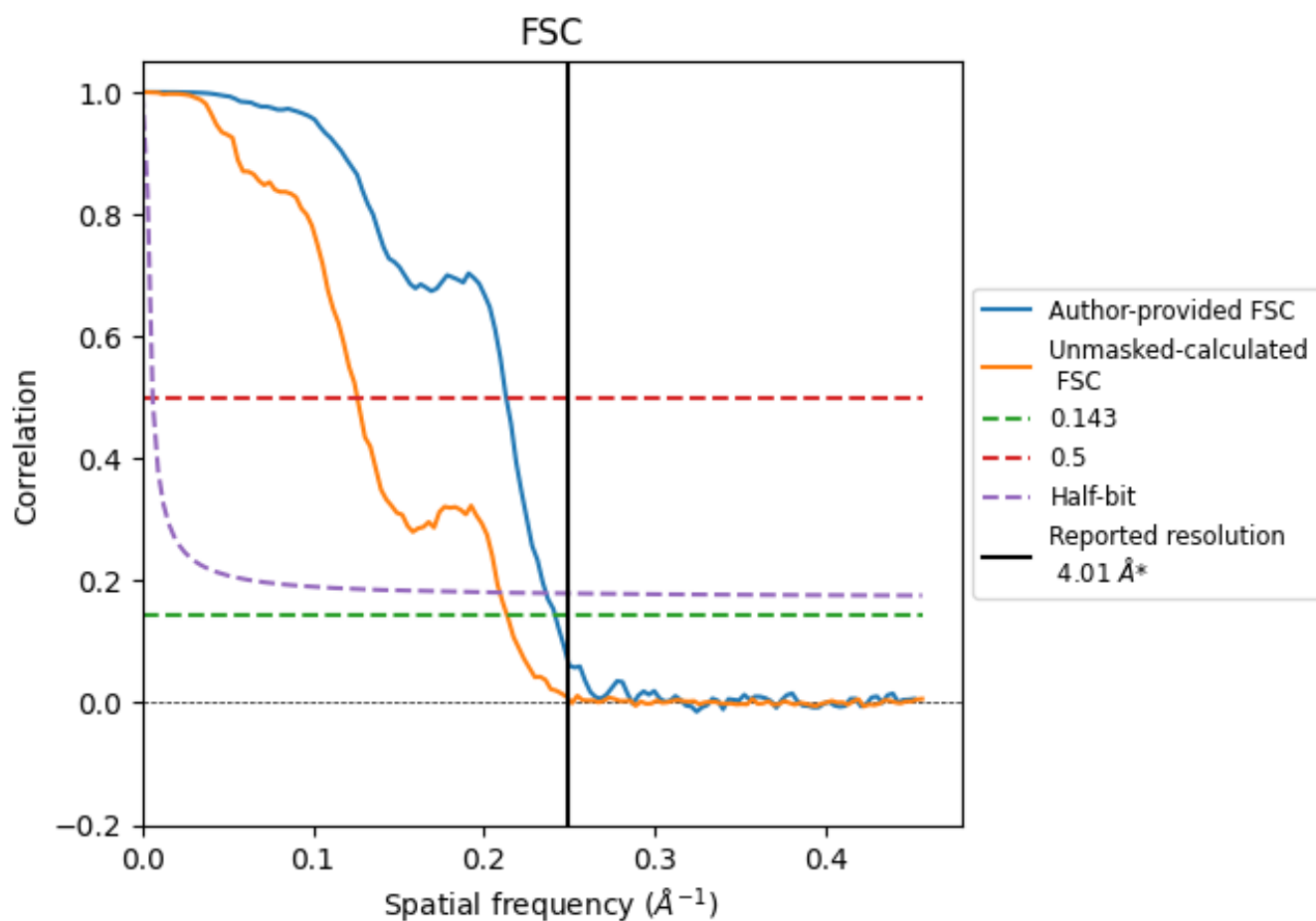


*Reported resolution corresponds to spatial frequency of 0.249 Å⁻¹

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 0.249 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

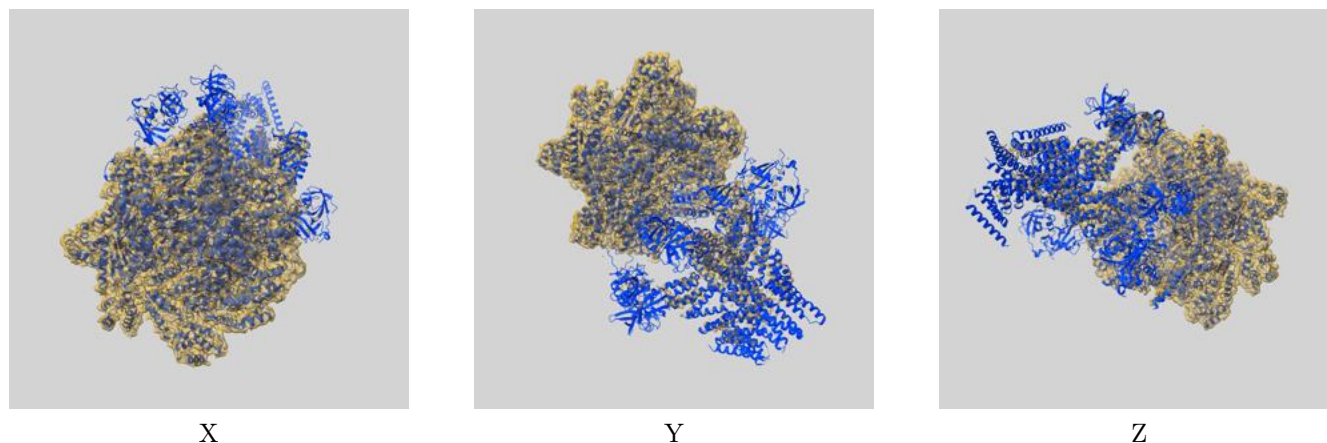
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.01	-	-
Author-provided FSC curve	4.14	4.70	4.23
Unmasked-calculated*	4.68	7.95	4.78

*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 4.68 differs from the reported value 4.01 by more than 10 %

9 Map-model fit [i](#)

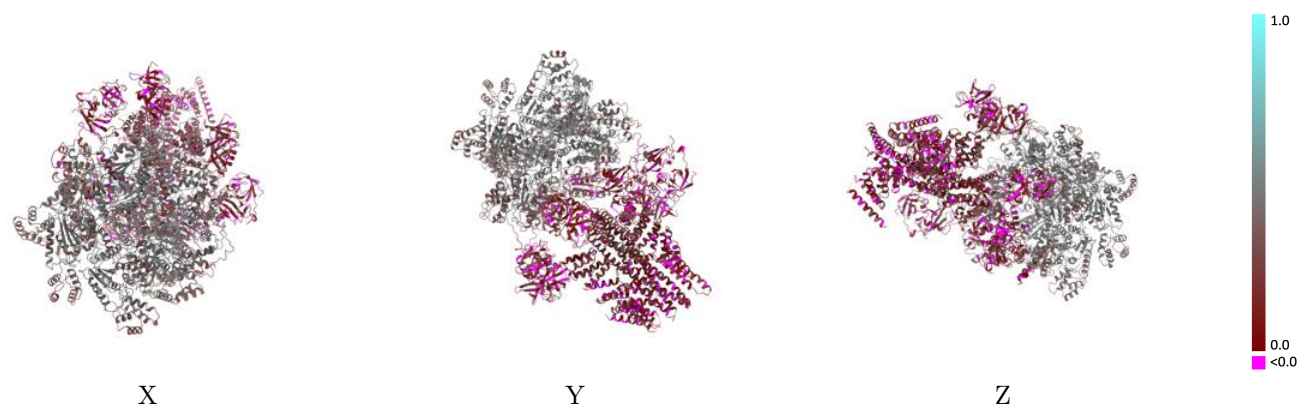
This section contains information regarding the fit between EMDB map EMD-71478 and PDB model 9PBF. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



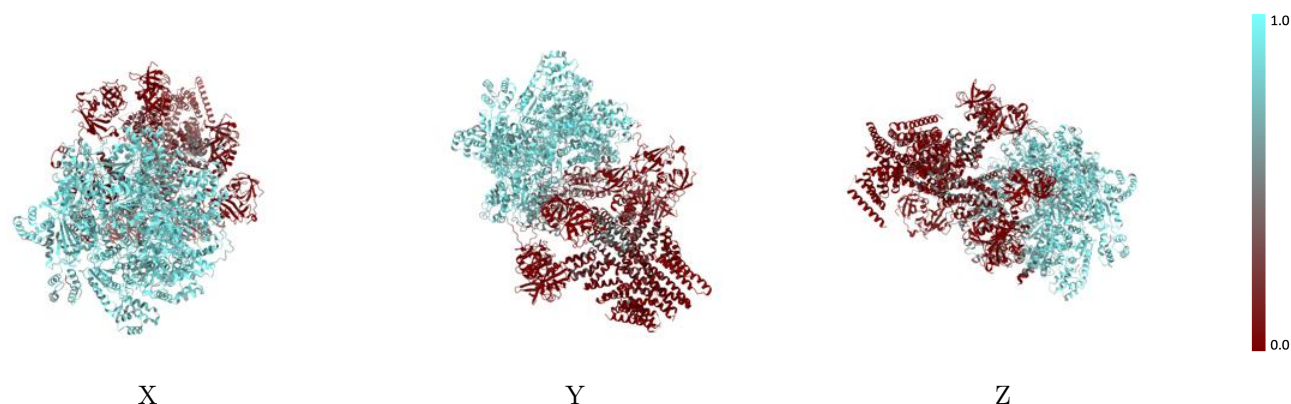
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



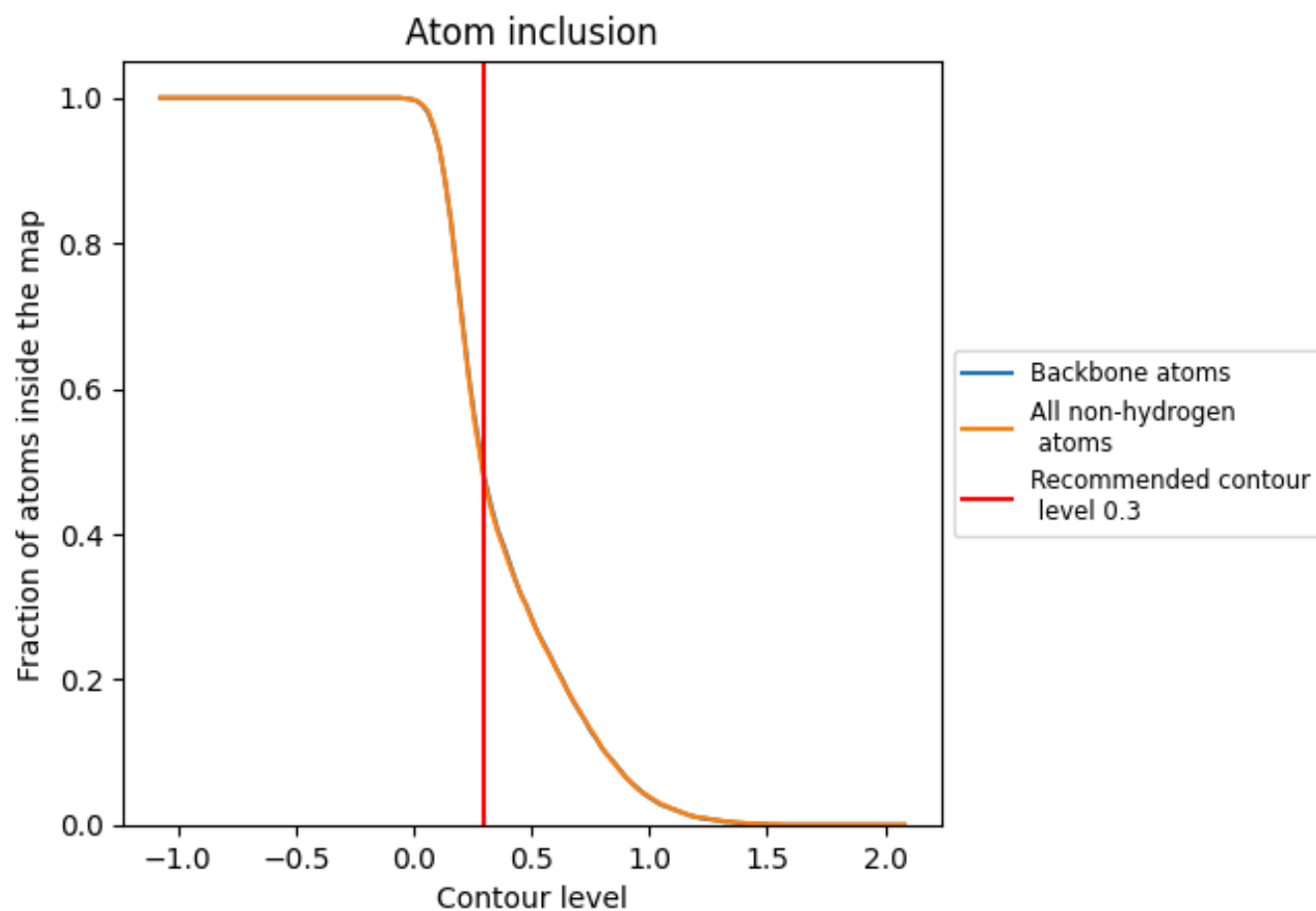
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 47% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4730	0.3030
A	0.6020	0.3560
B	0.6550	0.3800
C	0.6320	0.3660
D	0.6190	0.3530
E	0.5310	0.3220
F	0.3970	0.2620
G	0.2280	0.1920
H	0.2130	0.1850
I	0.1170	0.1510
J	0.0900	0.1580
K	0.1480	0.1800
L	0.0570	0.1260

1.0

0.0

<0.0