



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:07 AM UTC

PDB ID : 7NJQ / pdb_00007njq
EMDB ID : EMD-12407
Title : Mycobacterium smegmatis ATP synthase state 3a
Authors : Montgomery, M.G.; Petri, J.; Spikes, T.E.; Walker, J.E.
Deposited on : 2021-02-17
Resolution : 2.67 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

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:

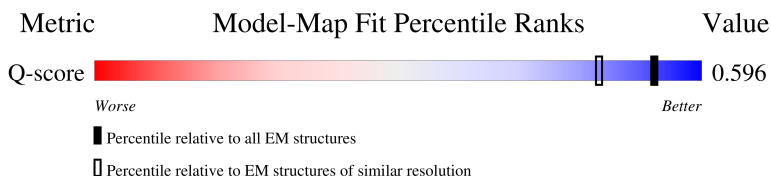
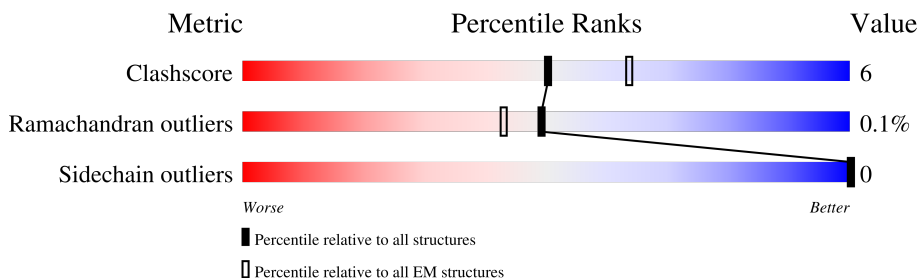
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.67 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.



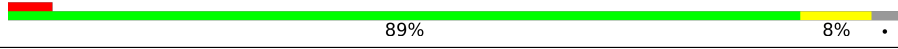
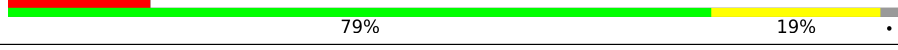
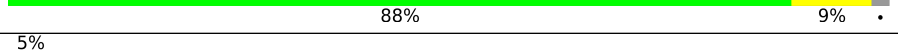
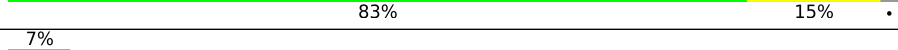
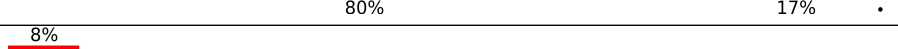
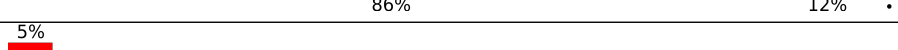
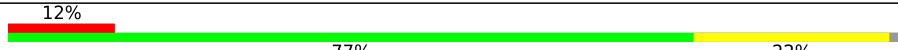
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9182 (2.17 - 3.17)

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

Mol	Chain	Length	Quality of chain
1	A	548	84% 10% 6% 5%
1	B	548	81% 11% 8% 5%
1	C	548	85% 10% 5% 5%
2	D	475	88% 10% .

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Mol	Chain	Length	Quality of chain
2	E	475	
2	F	475	
3	G	307	
4	H	121	
5	L	86	
5	M	86	
5	N	86	
5	O	86	
5	P	86	
5	Q	86	
5	R	86	
5	S	86	
5	T	86	
6	a	252	
7	b	180	
8	d	445	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 74741 atoms, of which 37429 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 ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	517	Total	C	H	N	O	S	0	0
			7808	2451	3904	674	769	10		
1	B	504	Total	C	H	N	O	S	0	0
			7618	2389	3814	658	747	10		
1	C	521	Total	C	H	N	O	S	3	0
			7941	2493	3979	685	774	10		

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	467	Total	C	H	N	O	S	2	0
			7143	2259	3562	615	694	13		
2	E	464	Total	C	H	N	O	S	0	0
			7087	2243	3533	609	689	13		
2	F	468	Total	C	H	N	O	S	0	0
			7144	2260	3564	614	693	13		

- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	297	Total	C	H	N	O	S	0	0
			4567	1418	2290	412	441	6		

- Molecule 4 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	H	118	Total	C	H	N	O	S	0	0
			1802	565	891	161	184	1		

- Molecule 5 is a protein called ATP synthase subunit c.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	L	84	Total	C	H	N	O	S	0	0
			1192	387	603	96	104	2		
5	M	85	Total	C	H	N	O	S	0	0
			1204	391	607	97	107	2		
5	N	84	Total	C	H	N	O	S	0	0
			1192	387	603	96	104	2		
5	O	84	Total	C	H	N	O	S	0	0
			1192	387	603	96	104	2		
5	P	84	Total	C	H	N	O	S	0	0
			1192	387	603	96	104	2		
5	Q	84	Total	C	H	N	O	S	0	0
			1192	387	603	96	104	2		
5	R	85	Total	C	H	N	O	S	0	0
			1204	391	607	97	107	2		
5	S	85	Total	C	H	N	O	S	0	0
			1204	391	607	97	107	2		
5	T	85	Total	C	H	N	O	S	0	0
			1204	391	607	97	107	2		

- Molecule 6 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	a	238	Total	C	H	N	O	S	0	0
			3767	1252	1916	292	301	6		

- Molecule 7 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	b	144	Total	C	H	N	O	S	0	0
			2161	664	1090	193	212	2		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	171	HIS	-	expression tag	UNP A0R204
b	172	HIS	-	expression tag	UNP A0R204
b	173	HIS	-	expression tag	UNP A0R204
b	174	HIS	-	expression tag	UNP A0R204
b	175	HIS	-	expression tag	UNP A0R204
b	176	HIS	-	expression tag	UNP A0R204
b	177	HIS	-	expression tag	UNP A0R204
b	178	HIS	-	expression tag	UNP A0R204
b	179	HIS	-	expression tag	UNP A0R204

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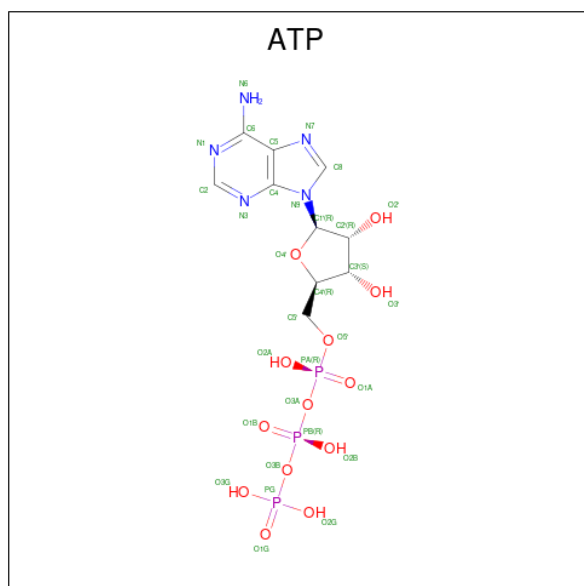
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Chain	Residue	Modelled	Actual	Comment	Reference
b	180	HIS	-	expression tag	UNP A0R204

- Molecule 8 is a protein called ATP synthase subunit b-delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	d	438	Total	C	H	N	O	S	0	0
			6656	2034	3371	597	649	5		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

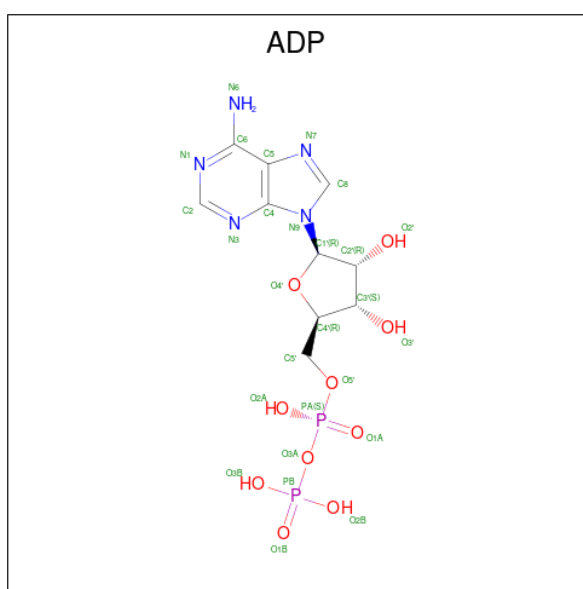
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
10	B	1	Total	Mg	0
			1	1	
10	C	1	Total	Mg	0
			1	1	
10	D	1	Total	Mg	0
			1	1	
10	F	1	Total	Mg	0
			1	1	

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms						AltConf
11	D	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
11	E	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	A	3	Total	O	0
			3	3	
12	B	3	Total	O	0
			3	3	
12	C	3	Total	O	0
			3	3	

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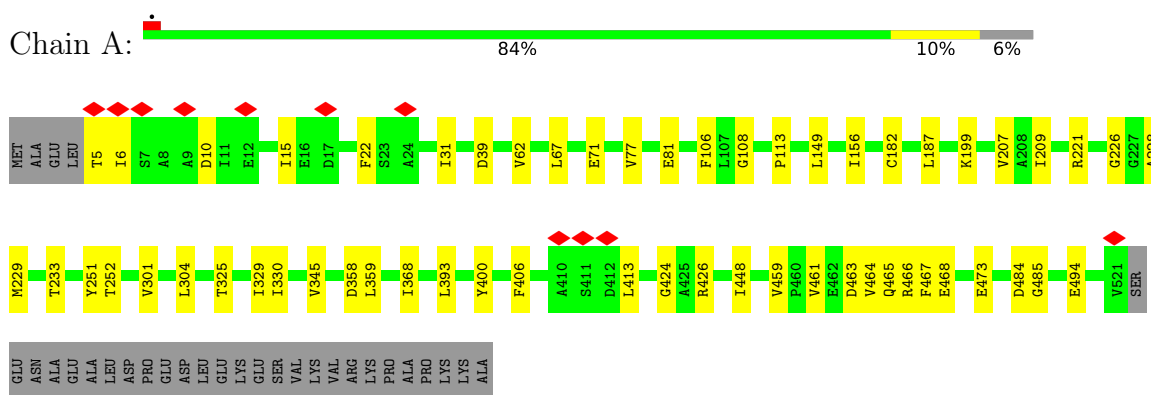
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Mol	Chain	Residues	Atoms		AltConf
12	D	4	Total	O	0
			4	4	
12	F	3	Total	O	0
			3	3	

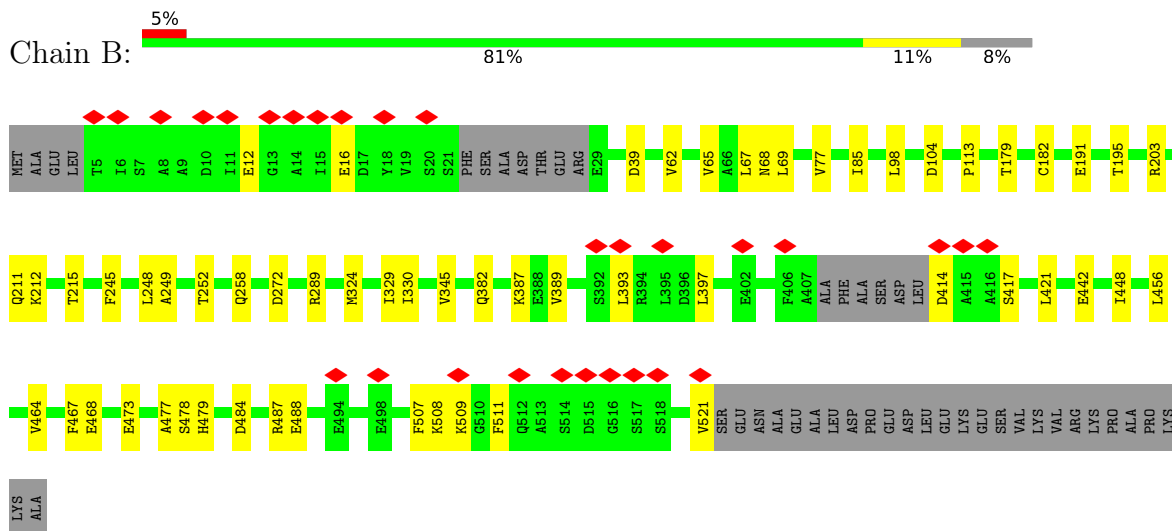
3 Residue-property plots

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.

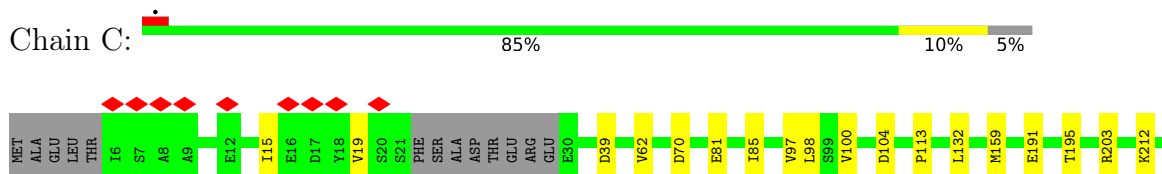
- Molecule 1: ATP synthase subunit alpha

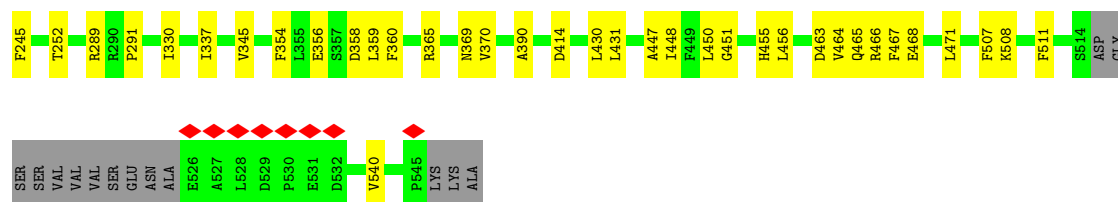


- Molecule 1: ATP synthase subunit alpha



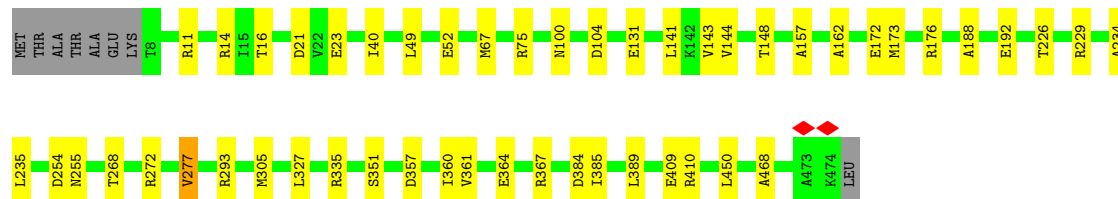
- Molecule 1: ATP synthase subunit alpha





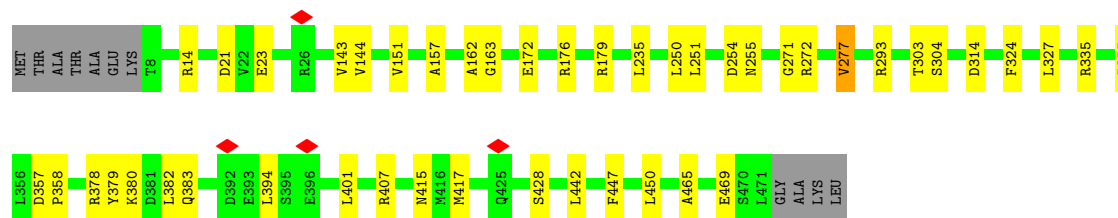
• Molecule 2: ATP synthase subunit beta

Chain D: 88% 10% .



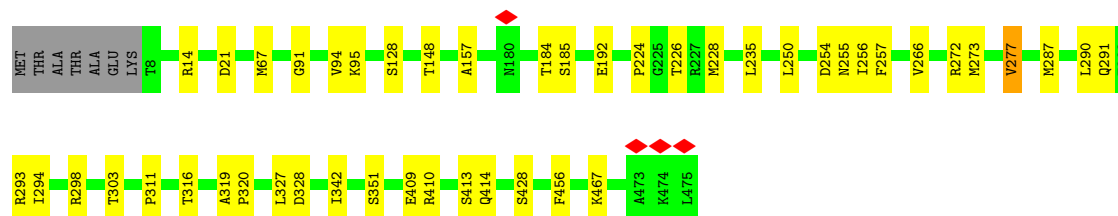
• Molecule 2: ATP synthase subunit beta

Chain E: 88% 9% .



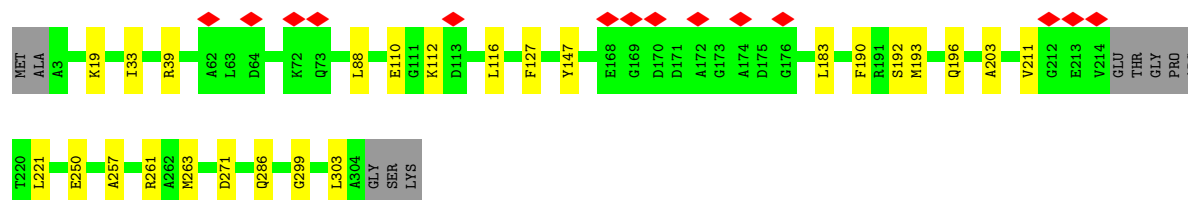
• Molecule 2: ATP synthase subunit beta

Chain F: 89% 10% .

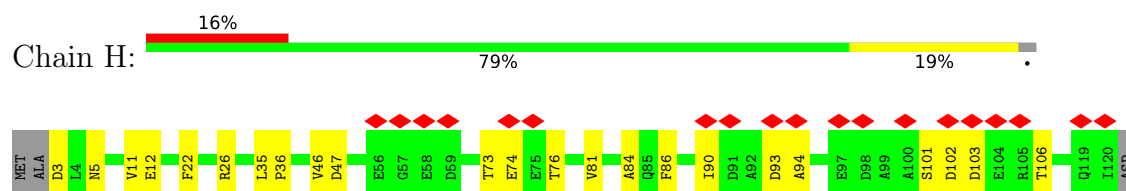


• Molecule 3: ATP synthase gamma chain

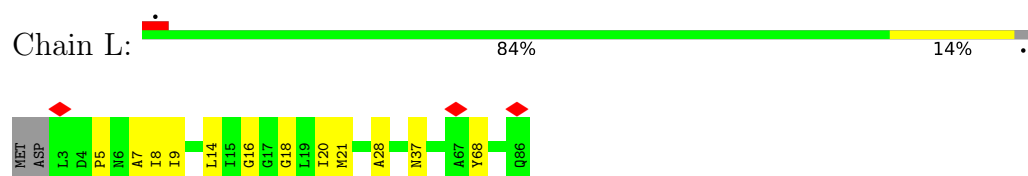
Chain G: 5% 89% 8% .



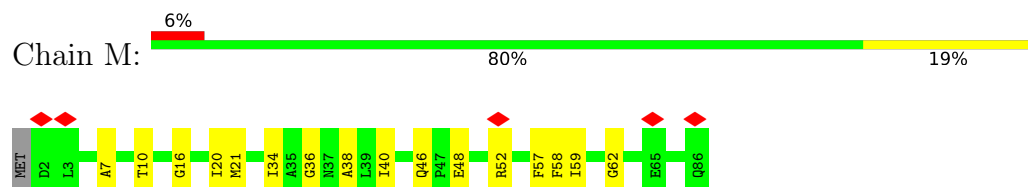
- Molecule 4: ATP synthase epsilon chain



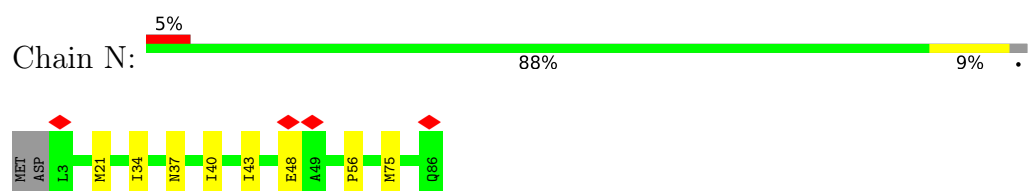
- Molecule 5: ATP synthase subunit c



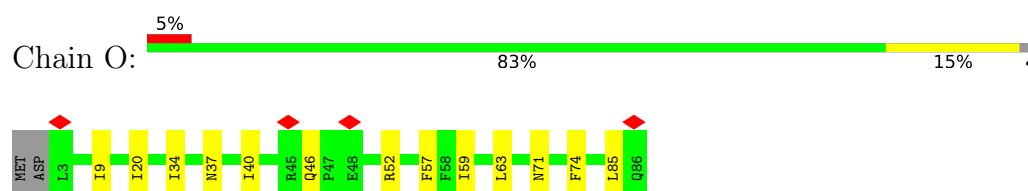
- Molecule 5: ATP synthase subunit c



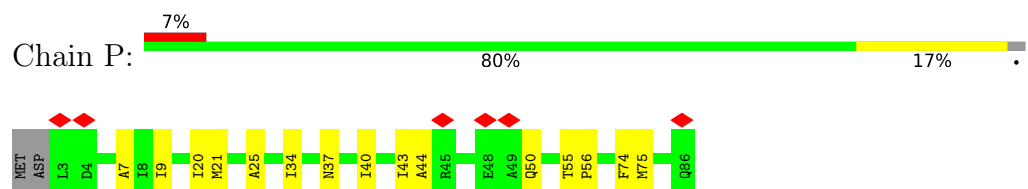
- Molecule 5: ATP synthase subunit c



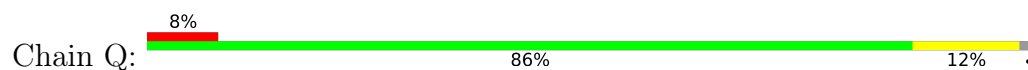
- Molecule 5: ATP synthase subunit c

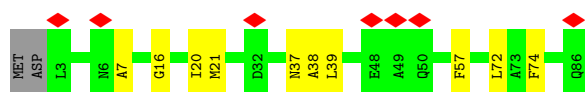


- Molecule 5: ATP synthase subunit c

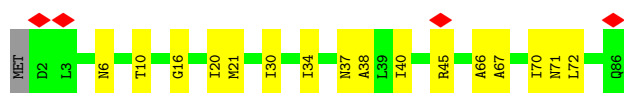
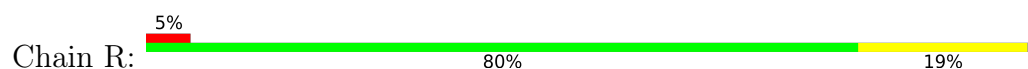


- Molecule 5: ATP synthase subunit c

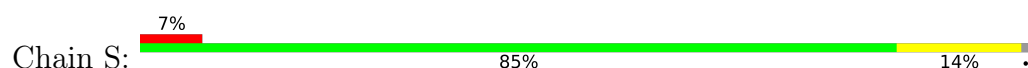




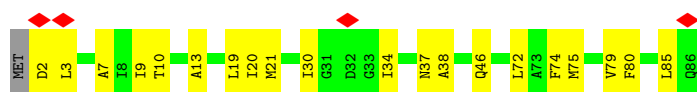
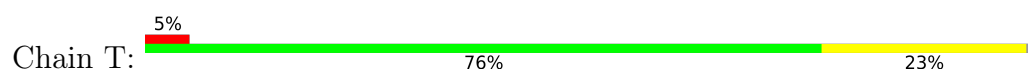
- Molecule 5: ATP synthase subunit c



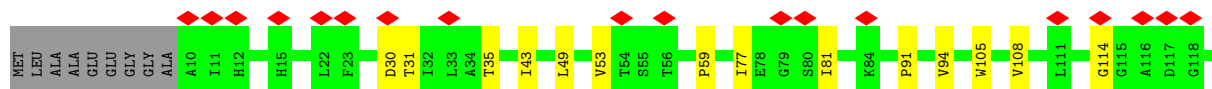
- Molecule 5: ATP synthase subunit c



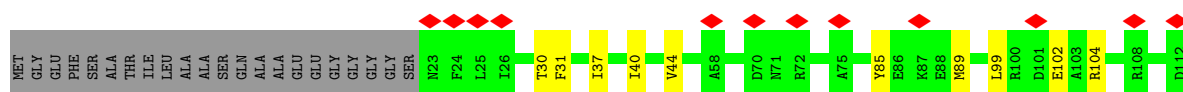
- Molecule 5: ATP synthase subunit c



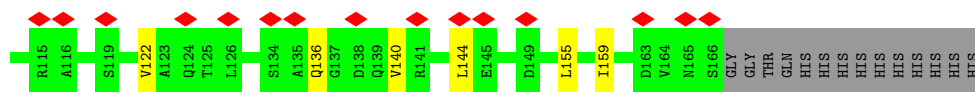
- Molecule 6: ATP synthase subunit a

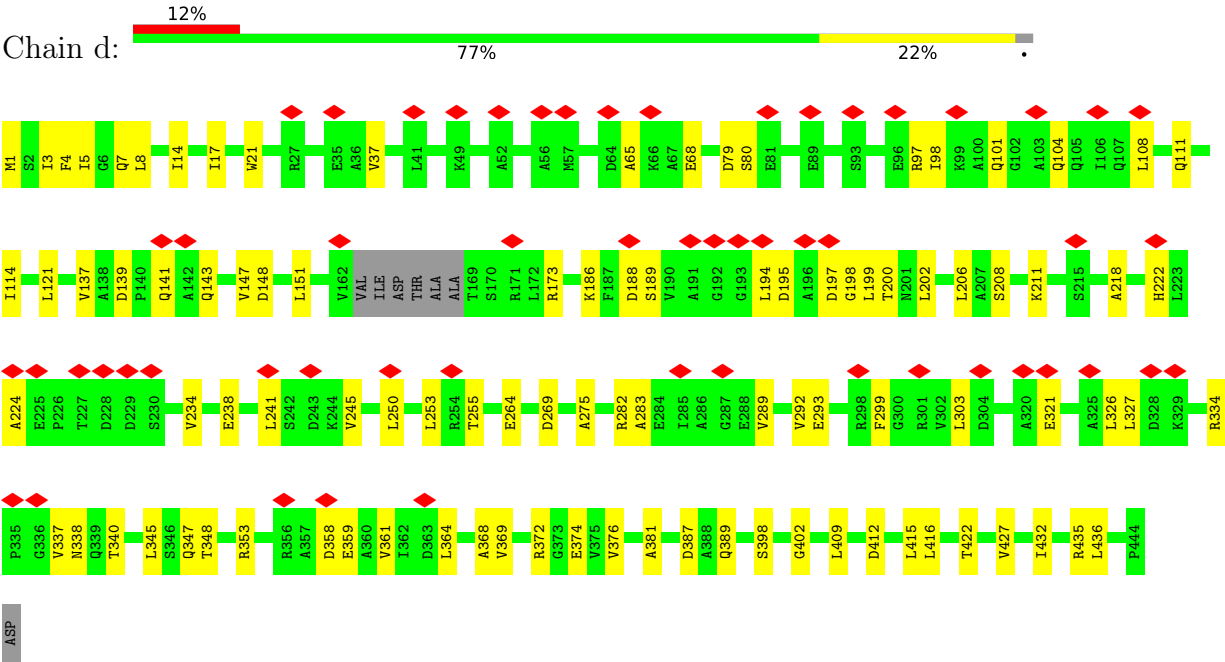


- Molecule 7: ATP synthase subunit b



- Molecule 8: ATP synthase subunit b-delta





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19516	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.86	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	415.0, 415.0, 415.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.19	0/3964	0.28	0/5368
1	B	0.18	0/3860	0.28	0/5224
1	C	0.18	0/4034	0.27	0/5458
2	D	0.18	0/3651	0.27	0/4950
2	E	0.17	0/3619	0.27	0/4908
2	F	0.19	0/3645	0.28	0/4942
3	G	0.16	0/2306	0.27	0/3117
4	H	0.13	0/922	0.27	0/1252
5	L	0.19	0/600	0.43	0/814
5	M	0.20	0/608	0.34	0/825
5	N	0.17	0/600	0.30	0/814
5	O	0.17	0/600	0.29	0/814
5	P	0.18	0/600	0.29	0/814
5	Q	0.17	0/600	0.28	0/814
5	R	0.17	0/608	0.30	0/825
5	S	0.18	0/608	0.30	0/825
5	T	0.17	0/608	0.27	0/825
6	a	0.14	0/1905	0.28	0/2602
7	b	0.14	0/1080	0.31	0/1459
8	d	0.13	0/3314	0.27	0/4488
All	All	0.17	0/37732	0.28	0/51138

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3904	3904	3904	40	0
1	B	3804	3814	3814	37	0
1	C	3962	3979	3967	35	0
2	D	3581	3562	3556	38	0
2	E	3554	3533	3533	32	0
2	F	3580	3564	3564	30	0
3	G	2277	2290	2290	21	0
4	H	911	891	891	17	0
5	L	589	603	603	21	0
5	M	597	607	607	22	0
5	N	589	603	603	10	0
5	O	589	603	603	12	0
5	P	589	603	603	17	0
5	Q	589	603	603	12	0
5	R	597	607	607	18	0
5	S	597	607	607	16	0
5	T	597	607	607	25	0
6	a	1851	1916	1916	27	0
7	b	1071	1090	1090	21	0
8	d	3285	3371	3371	77	0
9	A	31	12	12	0	0
9	B	31	12	12	0	0
9	C	31	12	12	0	0
9	F	31	12	12	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
10	F	1	0	0	0	0
11	D	27	12	12	1	0
11	E	27	12	12	1	0
12	A	3	0	0	0	0
12	B	3	0	0	1	0
12	C	3	0	0	0	0
12	D	4	0	0	2	0
12	F	3	0	0	1	0
All	All	37312	37429	37411	421	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 6.

All (421) 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:B:211:GLN:OE1	12:B:701:HOH:O	1.90	0.90
2:E:162:ALA:O	2:E:335:ARG:NH2	2.09	0.86
5:M:58:PHE:CE2	6:a:239:LEU:HD21	2.17	0.80
2:F:14:ARG:NH1	2:F:21:ASP:OD2	2.16	0.78
5:M:52:ARG:NH1	5:N:43:ILE:O	2.16	0.78
2:D:364:GLU:OE2	2:D:367:ARG:NH1	2.17	0.77
5:O:52:ARG:NH1	5:P:43:ILE:O	2.17	0.77
8:d:269:ASP:OD1	8:d:353:ARG:NH2	2.18	0.76
1:B:382:GLN:O	1:B:387:LYS:NZ	2.19	0.76
1:B:104:ASP:OD1	1:B:203:ARG:NH1	2.19	0.75
4:H:26:ARG:NH2	5:M:46:GLN:OE1	2.19	0.75
3:G:110:GLU:OE1	3:G:112:LYS:NZ	2.20	0.75
2:D:148:THR:HG21	2:D:351:SER:HB3	1.69	0.74
1:C:356:GLU:OE2	1:C:369:ASN:ND2	2.21	0.73
3:G:190:PHE:N	3:G:250:GLU:OE2	2.20	0.73
1:A:463:ASP:OD1	1:A:466:ARG:NH2	2.22	0.72
2:F:128:SER:O	2:F:298:ARG:NH2	2.24	0.71
3:G:192:SER:O	3:G:196:GLN:NE2	2.23	0.71
8:d:283:ALA:HB2	8:d:340:THR:HG21	1.73	0.70
8:d:358:ASP:OD1	8:d:359:GLU:N	2.24	0.70
8:d:4:PHE:O	8:d:8:LEU:HD23	1.92	0.69
4:H:26:ARG:NH2	5:M:48:GLU:OE2	2.25	0.69
2:D:192:GLU:OE1	12:D:701:HOH:O	2.11	0.69
2:E:157:ALA:HB2	2:E:327:LEU:HD13	1.75	0.69
8:d:17:ILE:HD12	8:d:21:TRP:CE3	2.28	0.69
2:E:415:ASN:OD1	2:E:428:SER:OG	2.10	0.68
2:F:192:GLU:OE1	12:F:701:HOH:O	2.10	0.68
4:H:93:ASP:OD1	4:H:94:ALA:N	2.27	0.68
8:d:148:ASP:OD1	8:d:389:GLN:NE2	2.26	0.67
2:D:409:GLU:OE2	2:D:410:ARG:NH1	2.28	0.67
1:C:39:ASP:OD1	2:F:272:ARG:NH1	2.28	0.66
2:D:277:VAL:HG12	2:D:277:VAL:O	1.95	0.65
2:E:23:GLU:OE1	8:d:173:ARG:NH2	2.29	0.65
8:d:299:PHE:O	8:d:303:LEU:HD23	1.97	0.64
6:a:207:PRO:O	6:a:211:GLN:N	2.30	0.64
2:E:235:LEU:HD21	2:E:293:ARG:HB2	1.79	0.64
5:P:9:ILE:HD11	5:Q:7:ALA:HA	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:d:197:ASP:OD1	8:d:198:GLY:N	2.30	0.64
1:B:39:ASP:OD2	2:E:272:ARG:NE	2.29	0.64
5:O:9:ILE:HD11	5:P:7:ALA:HA	1.80	0.64
5:R:66:ALA:O	5:R:70:ILE:HD12	1.98	0.64
7:b:159:ILE:O	8:d:435:ARG:NH2	2.31	0.64
1:C:212:LYS:NZ	2:F:328:ASP:OD1	2.30	0.64
5:M:36:GLY:O	5:M:40:ILE:HD12	1.98	0.64
5:N:48:GLU:N	5:N:48:GLU:OE1	2.31	0.63
1:C:358:ASP:OD1	1:C:359:LEU:N	2.32	0.63
2:D:389:LEU:HD12	3:G:88:LEU:HD11	1.81	0.63
2:E:14:ARG:NH1	2:E:21:ASP:OD2	2.32	0.62
5:L:14:LEU:HD23	5:T:13:ALA:HA	1.80	0.62
2:E:324:PHE:CD1	2:E:327:LEU:HD12	2.35	0.62
5:O:46:GLN:NE2	5:P:44:ALA:O	2.33	0.62
5:S:46:GLN:OE1	5:S:52:ARG:NH2	2.33	0.62
2:D:384:ASP:OD1	2:D:385:ILE:N	2.33	0.61
2:F:456:PHE:O	2:F:467:LYS:NZ	2.33	0.61
5:S:74:PHE:CD1	5:T:75:MET:HE1	2.36	0.61
1:A:358:ASP:OD1	1:A:359:LEU:N	2.33	0.61
1:C:159:MET:HE1	1:C:370:VAL:HG22	1.83	0.61
1:C:159:MET:HE2	1:C:431:LEU:HD13	1.83	0.61
8:d:188:ASP:OD1	8:d:189:SER:N	2.33	0.61
1:B:65:VAL:HG13	1:B:67:LEU:CD1	2.31	0.61
8:d:197:ASP:O	8:d:200:THR:OG1	2.18	0.60
1:B:508:LYS:HB3	1:B:521:VAL:HG22	1.84	0.60
5:L:9:ILE:HD12	5:M:10:THR:CG2	2.31	0.60
2:D:11:ARG:NH1	2:D:23:GLU:OE1	2.34	0.60
2:F:157:ALA:HB3	2:F:327:LEU:HD13	1.84	0.60
5:L:7:ALA:HA	5:T:9:ILE:HD11	1.84	0.60
8:d:195:ASP:O	8:d:199:LEU:HD13	2.02	0.60
11:D:600:ADP:O3B	12:D:702:HOH:O	2.17	0.59
8:d:234:VAL:O	8:d:238:GLU:OE1	2.19	0.59
1:B:212:LYS:O	1:B:215:THR:OG1	2.19	0.59
5:L:20:ILE:HD13	5:M:21:MET:HB2	1.84	0.59
5:M:58:PHE:CZ	6:a:239:LEU:HD11	2.38	0.59
5:P:20:ILE:HD13	5:Q:21:MET:HB2	1.84	0.58
8:d:147:VAL:O	8:d:151:LEU:HD23	2.02	0.58
2:D:14:ARG:NE	2:D:21:ASP:OD2	2.36	0.58
2:D:389:LEU:CD1	3:G:88:LEU:HD11	2.33	0.58
8:d:412:ASP:HB3	8:d:415:LEU:HD23	1.85	0.58
4:H:73:THR:HG22	4:H:74:GLU:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:VAL:HG12	1:B:448:ILE:HG22	1.86	0.58
5:O:59:ILE:O	5:O:63:LEU:HD23	2.03	0.58
1:A:22:PHE:HE2	7:b:159:ILE:HG22	1.69	0.57
2:F:148:THR:HG21	2:F:351:SER:HB3	1.86	0.57
6:a:114:GLY:HA2	8:d:3:ILE:HD11	1.85	0.57
1:A:113:PRO:O	1:A:252:THR:OG1	2.17	0.57
1:C:291:PRO:CG	2:D:268:THR:HG22	2.35	0.57
8:d:241:LEU:HD12	8:d:241:LEU:O	2.04	0.57
3:G:263:MET:HA	3:G:263:MET:HE2	1.86	0.57
8:d:398:SER:O	8:d:402:GLY:N	2.38	0.57
7:b:144:LEU:HD13	8:d:121:LEU:HD12	1.88	0.56
1:B:417:SER:O	1:B:421:LEU:HD23	2.05	0.56
1:C:455:HIS:O	1:C:508:LYS:NZ	2.38	0.56
1:A:22:PHE:CE2	7:b:159:ILE:HG22	2.41	0.56
2:E:172:GLU:OE2	2:E:176:ARG:NE	2.39	0.56
5:R:21:MET:HE1	5:R:72:LEU:HA	1.88	0.56
1:A:494:GLU:OE1	1:A:494:GLU:N	2.38	0.55
1:B:65:VAL:HG13	1:B:67:LEU:HD11	1.89	0.55
2:D:450:LEU:HD22	2:D:468:ALA:HB1	1.87	0.55
5:M:59:ILE:HD11	6:a:166:HIS:HB2	1.89	0.55
7:b:155:LEU:O	7:b:159:ILE:HG23	2.07	0.55
6:a:49:LEU:O	6:a:53:VAL:HG13	2.06	0.55
8:d:186:LYS:NZ	8:d:255:THR:OG1	2.39	0.55
8:d:338:ASN:OD1	8:d:340:THR:N	2.40	0.55
8:d:202:LEU:HD23	8:d:206:LEU:HD12	1.89	0.54
2:D:268:THR:HG23	3:G:303:LEU:HD21	1.88	0.54
6:a:195:ALA:O	6:a:199:LEU:HD23	2.07	0.54
2:F:250:LEU:HD23	2:F:303:THR:HB	1.89	0.54
1:B:39:ASP:OD1	2:E:272:ARG:NH2	2.41	0.54
1:A:426:ARG:NH2	1:A:459:VAL:O	2.41	0.53
5:R:16:GLY:O	5:R:20:ILE:HG12	2.08	0.53
6:a:142:PHE:HA	6:a:145:TYR:CE1	2.44	0.53
8:d:17:ILE:HD12	8:d:21:TRP:CZ3	2.44	0.53
1:B:509:LYS:CE	1:B:521:VAL:HG21	2.39	0.53
4:H:5:ASN:HB2	4:H:76:THR:HG22	1.91	0.53
1:B:179:THR:OG1	1:B:272:ASP:OD2	2.27	0.53
5:O:74:PHE:CD1	5:P:75:MET:HE1	2.42	0.53
2:F:228:MET:SD	2:F:266:VAL:HG21	2.48	0.53
1:B:98:LEU:HD21	1:B:248:LEU:HD11	1.91	0.53
6:a:43:ILE:HD12	7:b:44:VAL:HG21	1.91	0.53
2:D:52:GLU:OE2	2:D:229:ARG:NE	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:PHE:O	1:C:365:ARG:NE	2.42	0.52
5:L:16:GLY:O	5:L:20:ILE:HG12	2.10	0.52
7:b:85:TYR:HD2	8:d:65:ALA:HB2	1.74	0.52
2:E:378:ARG:HH12	2:E:382:LEU:HD21	1.73	0.52
8:d:326:LEU:HD23	8:d:326:LEU:C	2.33	0.52
2:E:179:ARG:NH1	2:E:417:MET:SD	2.82	0.52
2:E:250:LEU:HD12	2:E:303:THR:O	2.10	0.52
2:E:379:TYR:CZ	2:E:383:GLN:NE2	2.77	0.52
2:F:67:MET:O	2:F:226:THR:OG1	2.27	0.52
5:M:58:PHE:HE2	6:a:239:LEU:HD21	1.68	0.52
5:T:21:MET:HE1	5:T:72:LEU:HA	1.92	0.52
1:C:70:ASP:O	2:D:75:ARG:NH1	2.41	0.52
2:E:407:ARG:NH2	2:E:450:LEU:O	2.40	0.52
1:A:15:ILE:HG13	8:d:121:LEU:HD22	1.91	0.51
1:A:156:ILE:HD11	1:A:368:ILE:HD11	1.92	0.51
5:L:9:ILE:HD12	5:M:10:THR:HG23	1.91	0.51
5:M:58:PHE:CE2	6:a:239:LEU:HD11	2.45	0.51
2:D:172:GLU:OE2	2:D:176:ARG:NE	2.43	0.51
3:G:221:LEU:HD11	5:R:45:ARG:HG2	1.93	0.51
1:A:67:LEU:HD13	1:A:77:VAL:HG23	1.92	0.51
5:Q:16:GLY:O	5:Q:20:ILE:HG12	2.10	0.51
1:A:39:ASP:OD1	2:D:272:ARG:NH2	2.44	0.51
2:D:141:LEU:HD12	2:D:173:MET:CE	2.41	0.50
1:C:62:VAL:HG11	1:C:85:ILE:HD11	1.93	0.50
7:b:159:ILE:HD12	8:d:436:LEU:HD22	1.93	0.50
8:d:334:ARG:O	8:d:337:VAL:HG12	2.12	0.50
1:A:473:GLU:OE1	7:b:104:ARG:NH2	2.44	0.50
1:B:414:ASP:OD2	1:B:417:SER:N	2.42	0.50
1:C:291:PRO:HG2	2:D:268:THR:HG22	1.93	0.50
5:L:21:MET:HE2	5:T:20:ILE:HD12	1.92	0.50
8:d:104:GLN:O	8:d:108:LEU:HD23	2.11	0.50
8:d:137:VAL:HG22	8:d:143:GLN:OE1	2.11	0.50
5:M:57:PHE:HA	5:N:40:ILE:HD11	1.94	0.50
2:F:256:ILE:HD11	2:F:290:LEU:HD21	1.94	0.50
3:G:147:TYR:CD1	4:H:11:VAL:HG11	2.47	0.50
3:G:88:LEU:HD12	3:G:263:MET:HE1	1.94	0.49
5:M:16:GLY:O	5:M:20:ILE:HG12	2.12	0.49
5:R:20:ILE:HD13	5:S:21:MET:HB3	1.94	0.49
5:T:9:ILE:HG21	5:T:85:LEU:HD12	1.95	0.49
5:P:43:ILE:HD12	5:P:50:GLN:CG	2.42	0.49
2:E:379:TYR:CE1	2:E:383:GLN:NE2	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:NH2	2:D:131:GLU:OE2	2.44	0.49
2:F:316:THR:O	2:F:316:THR:HG22	2.13	0.49
5:L:21:MET:HE3	5:T:20:ILE:HG23	1.94	0.49
5:P:74:PHE:HE2	5:Q:72:LEU:HD11	1.78	0.49
5:R:38:ALA:HB2	5:S:37:ASN:OD1	2.12	0.49
2:D:357:ASP:O	2:D:361:VAL:HG22	2.13	0.49
2:D:141:LEU:HD12	2:D:173:MET:HE1	1.95	0.49
5:Q:20:ILE:HD13	5:R:21:MET:HB2	1.95	0.49
8:d:289:VAL:HG11	8:d:372:ARG:NH1	2.27	0.49
8:d:218:ALA:O	8:d:222:HIS:ND1	2.40	0.48
1:B:509:LYS:HE2	1:B:521:VAL:HG21	1.94	0.48
5:L:9:ILE:HD11	5:M:7:ALA:HA	1.95	0.48
1:A:71:GLU:OE1	2:E:14:ARG:NE	2.46	0.48
1:A:108:GLY:HA2	1:A:229:MET:HE3	1.95	0.48
5:M:38:ALA:HB2	5:N:37:ASN:OD1	2.12	0.48
8:d:381:ALA:HB3	8:d:409:LEU:HD11	1.95	0.48
1:C:113:PRO:O	1:C:252:THR:OG1	2.29	0.48
1:C:330:ILE:HD11	1:C:345:VAL:HG21	1.96	0.48
2:E:465:ALA:O	2:E:469:GLU:OE1	2.32	0.48
3:G:299:GLY:O	3:G:303:LEU:HD23	2.13	0.48
1:C:97:VAL:HG12	1:C:98:LEU:N	2.29	0.48
2:E:277:VAL:HG12	2:E:277:VAL:O	2.13	0.48
5:Q:57:PHE:N	5:R:40:ILE:HD11	2.29	0.48
8:d:7:GLN:NE2	8:d:8:LEU:HD22	2.29	0.47
8:d:372:ARG:HB2	8:d:374:GLU:OE1	2.14	0.47
1:A:106:PHE:O	1:A:233:THR:OG1	2.20	0.47
2:E:163:GLY:N	11:E:600:ADP:O2B	2.41	0.47
2:F:409:GLU:OE2	2:F:410:ARG:NH1	2.48	0.47
3:G:39:ARG:NH2	4:H:12:GLU:OE1	2.48	0.47
4:H:3:ASP:N	4:H:3:ASP:OD1	2.45	0.47
8:d:208:SER:O	8:d:211:LYS:HG3	2.15	0.47
1:A:149:LEU:HD22	1:A:325:THR:HG21	1.96	0.47
1:A:187:LEU:HD23	1:A:228:ALA:HB2	1.96	0.47
1:C:15:ILE:O	1:C:19:VAL:HG23	2.15	0.47
1:C:507:PHE:O	1:C:511:PHE:N	2.47	0.47
2:F:235:LEU:HD21	2:F:293:ARG:CB	2.45	0.47
5:M:34:ILE:HG22	5:N:37:ASN:HB2	1.96	0.47
6:a:77:ILE:O	6:a:81:ILE:N	2.41	0.47
7:b:85:TYR:O	7:b:89:MET:HG2	2.14	0.47
1:B:289:ARG:NH1	2:E:271:GLY:O	2.41	0.47
2:F:277:VAL:HG12	2:F:277:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:9:ILE:HG21	5:O:85:LEU:HA	1.96	0.47
1:B:62:VAL:HG11	1:B:85:ILE:HD11	1.97	0.47
1:B:478:SER:OG	1:B:479:HIS:ND1	2.43	0.47
2:D:162:ALA:O	2:D:335:ARG:NH2	2.46	0.47
2:E:380:LYS:HA	2:E:383:GLN:HG2	1.96	0.47
8:d:202:LEU:CD2	8:d:206:LEU:HD12	2.45	0.47
1:C:104:ASP:OD1	1:C:203:ARG:NH1	2.46	0.47
8:d:289:VAL:O	8:d:292:VAL:HG22	2.15	0.47
2:D:357:ASP:OD1	2:D:360:ILE:HD13	2.15	0.47
2:E:378:ARG:NH1	2:E:382:LEU:HD21	2.30	0.47
4:H:101:SER:OG	4:H:102:ASP:N	2.48	0.47
7:b:85:TYR:CD2	8:d:65:ALA:HB2	2.50	0.47
8:d:97:ARG:O	8:d:101:GLN:OE1	2.32	0.47
8:d:194:LEU:HD23	8:d:199:LEU:HD12	1.96	0.47
8:d:293:GLU:OE1	8:d:369:VAL:HG13	2.15	0.47
5:P:43:ILE:HD12	5:P:50:GLN:HG2	1.97	0.47
3:G:88:LEU:HD12	3:G:263:MET:CE	2.45	0.46
5:L:18:GLY:HA2	5:T:20:ILE:HD11	1.97	0.46
5:L:37:ASN:HB2	5:T:34:ILE:HG22	1.97	0.46
5:P:20:ILE:CD1	5:Q:21:MET:HB2	2.45	0.46
5:Q:38:ALA:HB2	5:R:37:ASN:OD1	2.14	0.46
6:a:91:PRO:HA	6:a:94:VAL:HG12	1.96	0.46
1:C:451:GLY:HA2	1:C:456:LEU:HD12	1.97	0.46
5:P:34:ILE:HG22	5:Q:37:ASN:HB2	1.96	0.46
5:S:20:ILE:HG12	5:T:21:MET:HB2	1.96	0.46
2:D:235:LEU:HD21	2:D:293:ARG:HB3	1.98	0.46
8:d:5:ILE:HD12	8:d:5:ILE:H	1.80	0.46
8:d:14:ILE:O	8:d:17:ILE:HG22	2.16	0.46
5:P:55:THR:HB	5:P:56:PRO:HD3	1.97	0.46
5:L:5:PRO:O	5:L:8:ILE:HG22	2.16	0.46
5:S:30:ILE:HB	5:T:30:ILE:HD13	1.98	0.46
5:S:34:ILE:HG22	5:T:37:ASN:HB2	1.97	0.46
2:F:224:PRO:HB2	2:F:266:VAL:HG23	1.97	0.46
5:M:62:GLY:O	6:a:177:GLU:OE2	2.34	0.46
2:E:314:ASP:OD2	3:G:286:GLN:NE2	2.43	0.46
5:L:14:LEU:HD23	5:T:13:ALA:CA	2.44	0.46
5:R:66:ALA:O	5:R:67:ALA:C	2.58	0.46
6:a:125:LYS:NZ	6:a:129:SER:OG	2.41	0.46
8:d:282:ARG:NH1	8:d:340:THR:HG23	2.31	0.46
8:d:345:LEU:HD13	8:d:361:VAL:HG22	1.97	0.46
5:O:57:PHE:HA	5:P:40:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:GLU:O	1:B:195:THR:HG23	2.16	0.45
1:C:113:PRO:HG2	1:C:245:PHE:HB3	1.97	0.45
2:F:95:LYS:HD3	2:F:184:THR:HG23	1.98	0.45
1:B:113:PRO:HG2	1:B:245:PHE:HB3	1.98	0.45
1:C:159:MET:HE1	1:C:370:VAL:CG2	2.45	0.45
8:d:1:MET:O	8:d:5:ILE:HD12	2.15	0.45
8:d:348:THR:HG21	8:d:364:LEU:HD11	1.98	0.45
1:A:393:LEU:HD11	1:A:448:ILE:HD12	1.99	0.45
1:C:430:LEU:HD21	1:C:447:ALA:O	2.16	0.45
2:E:378:ARG:HG2	2:E:401:LEU:CD2	2.45	0.45
8:d:4:PHE:CZ	8:d:8:LEU:HD21	2.51	0.45
1:B:68:ASN:C	1:B:69:LEU:HD12	2.41	0.45
2:D:173:MET:HG3	2:D:305:MET:SD	2.57	0.45
5:S:26:ILE:O	5:S:30:ILE:HG12	2.17	0.45
1:A:187:LEU:HD22	1:A:226:GLY:HA3	1.99	0.45
2:D:235:LEU:HD21	2:D:293:ARG:CB	2.46	0.45
2:E:151:VAL:HG22	2:E:355:ILE:HG21	1.97	0.45
3:G:183:LEU:O	3:G:203:ALA:N	2.50	0.45
5:Q:20:ILE:CD1	5:R:21:MET:HB2	2.47	0.45
2:F:414:GLN:NE2	2:F:428:SER:O	2.49	0.45
5:S:9:ILE:HD11	5:T:7:ALA:HA	1.97	0.45
1:A:330:ILE:HD11	1:A:345:VAL:HG21	1.98	0.44
2:F:342:ILE:HG23	2:F:413:SER:HB3	1.99	0.44
4:H:22:PHE:HD1	4:H:35:LEU:HD12	1.82	0.44
6:a:130:ASP:OD1	6:a:132:ASN:ND2	2.50	0.44
2:D:254:ASP:HA	2:D:255:ASN:HA	1.81	0.44
6:a:185:LEU:HD22	6:a:233:PHE:CE1	2.52	0.44
8:d:293:GLU:OE2	8:d:368:ALA:HB1	2.17	0.44
4:H:73:THR:HG22	4:H:74:GLU:N	2.29	0.44
1:A:6:ILE:HG23	8:d:114:ILE:HG12	1.99	0.44
5:L:21:MET:HE2	5:T:20:ILE:CD1	2.48	0.44
5:R:30:ILE:HB	5:S:30:ILE:CD1	2.48	0.44
1:A:182:CYS:SG	1:A:329:ILE:HD11	2.58	0.44
2:F:91:GLY:O	2:F:94:VAL:HG22	2.17	0.44
1:A:251:TYR:OH	1:A:304:LEU:HD12	2.18	0.44
4:H:86:PHE:O	4:H:90:ILE:HD12	2.18	0.44
6:a:150:ILE:O	6:a:154:GLY:N	2.51	0.44
8:d:4:PHE:CE1	8:d:8:LEU:HD21	2.53	0.44
1:A:426:ARG:NH1	1:A:461:VAL:HG23	2.33	0.44
1:B:473:GLU:O	1:B:477:ALA:N	2.48	0.44
5:R:67:ALA:O	5:R:71:ASN:OD1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:71:ASN:ND2	5:S:21:MET:SD	2.91	0.44
8:d:321:GLU:OE1	8:d:321:GLU:N	2.47	0.44
1:C:289:ARG:HA	2:F:273:MET:SD	2.58	0.44
2:D:16:THR:HG23	2:D:16:THR:O	2.17	0.44
2:E:382:LEU:HD22	2:E:394:LEU:HD11	1.99	0.44
4:H:81:VAL:HG21	4:H:84:ALA:HB2	2.00	0.44
4:H:103:ASP:HB3	4:H:106:THR:HG22	2.00	0.44
8:d:79:ASP:OD1	8:d:80:SER:N	2.51	0.44
1:C:466:ARG:O	1:C:467:PHE:C	2.61	0.43
2:D:277:VAL:O	2:D:277:VAL:CG1	2.65	0.43
6:a:156:VAL:O	6:a:160:ILE:HD12	2.18	0.43
2:D:67:MET:O	2:D:226:THR:OG1	2.36	0.43
5:M:20:ILE:CD1	5:N:21:MET:HB2	2.48	0.43
5:O:20:ILE:HG12	5:P:21:MET:HB2	1.99	0.43
5:O:71:ASN:ND2	5:P:25:ALA:HB2	2.33	0.43
1:C:337:ILE:HG21	1:C:354[A]:PHE:CE1	2.53	0.43
2:D:357:ASP:OD1	2:D:357:ASP:N	2.52	0.43
3:G:116:LEU:HD21	3:G:127:PHE:CD2	2.53	0.43
5:O:34:ILE:HG22	5:P:37:ASN:HB2	2.00	0.43
8:d:327:LEU:HD21	8:d:345:LEU:HG	1.99	0.43
1:B:12:GLU:O	1:B:16:GLU:OE2	2.37	0.43
1:C:191:GLU:O	1:C:195:THR:HG23	2.19	0.43
5:S:30:ILE:HG21	5:T:30:ILE:CD1	2.48	0.43
6:a:187:LEU:O	6:a:188:ARG:C	2.62	0.43
7:b:122:VAL:HG21	8:d:98:ILE:HG22	2.00	0.43
8:d:353:ARG:O	8:d:353:ARG:HG2	2.18	0.43
1:A:464:VAL:O	1:A:465:GLN:C	2.62	0.43
5:L:20:ILE:CD1	5:M:21:MET:HB2	2.47	0.43
1:B:484:ASP:O	1:B:488:GLU:OE1	2.37	0.42
1:B:507:PHE:O	1:B:511:PHE:N	2.44	0.42
1:C:81:GLU:OE1	1:C:81:GLU:N	2.52	0.42
3:G:33:ILE:HD11	3:G:257:ALA:HA	2.00	0.42
8:d:137:VAL:HG22	8:d:137:VAL:O	2.19	0.42
8:d:275:ALA:HB1	8:d:347:GLN:OE1	2.19	0.42
1:A:5:THR:HG23	7:b:136:GLN:HE22	1.83	0.42
1:B:467:PHE:O	1:B:468:GLU:C	2.62	0.42
2:D:157:ALA:HB2	2:D:327:LEU:HD11	2.01	0.42
2:F:184:THR:HG22	2:F:185:SER:N	2.34	0.42
1:A:400:TYR:HB2	1:A:424:GLY:HA3	2.01	0.42
7:b:37:ILE:O	7:b:40:ILE:HG12	2.19	0.42
4:H:46:VAL:HG22	4:H:47:ASP:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:d:137:VAL:HG21	8:d:416:LEU:O	2.19	0.42
1:A:467:PHE:O	1:A:468:GLU:C	2.62	0.42
2:F:157:ALA:HB2	2:F:327:LEU:HD22	2.00	0.42
5:M:20:ILE:HD13	5:N:21:MET:HB2	2.02	0.42
5:S:9:ILE:HD12	5:T:10:THR:OG1	2.18	0.42
2:E:357:ASP:OD1	2:E:358:PRO:HD2	2.19	0.42
2:F:319:ALA:HB3	2:F:320:PRO:CD	2.50	0.42
4:H:35:LEU:HD13	5:T:46:GLN:NE2	2.34	0.42
5:Q:74:PHE:CZ	5:R:72:LEU:HD11	2.54	0.42
8:d:194:LEU:CD2	8:d:202:LEU:HD13	2.49	0.42
8:d:432:ILE:O	8:d:436:LEU:HD23	2.20	0.42
1:A:207:VAL:HG12	1:A:209:ILE:HD11	2.01	0.42
1:A:484:ASP:O	1:A:485:GLY:C	2.63	0.42
1:A:10:ASP:OD1	1:A:10:ASP:N	2.46	0.42
1:A:199:LYS:N	1:A:199:LYS:CD	2.83	0.42
1:A:466:ARG:O	1:A:467:PHE:C	2.62	0.42
2:F:235:LEU:HD13	2:F:294:ILE:HG12	2.02	0.42
3:G:196:GLN:OE1	3:G:261:ARG:NH2	2.43	0.42
5:M:36:GLY:O	5:M:40:ILE:CD1	2.66	0.42
6:a:43:ILE:CD1	7:b:44:VAL:HG21	2.49	0.42
1:C:467:PHE:O	1:C:468:GLU:C	2.62	0.41
2:E:143:VAL:HG13	2:E:144:VAL:N	2.35	0.41
5:S:19:LEU:HD13	5:T:19:LEU:HG	2.02	0.41
6:a:219:LYS:HB2	8:d:14:ILE:HD11	2.00	0.41
2:E:442:LEU:HD23	2:E:447:PHE:HD2	1.84	0.41
5:L:37:ASN:OD1	5:T:38:ALA:HB2	2.20	0.41
8:d:358:ASP:OD1	8:d:358:ASP:C	2.62	0.41
1:A:62:VAL:HG22	1:A:81:GLU:CG	2.51	0.41
1:B:67:LEU:HD13	1:B:77:VAL:HG23	2.03	0.41
7:b:89:MET:SD	8:d:68:GLU:CD	3.04	0.41
1:C:414:ASP:OD1	1:C:414:ASP:N	2.51	0.41
2:F:257:PHE:CZ	2:F:311:PRO:HG3	2.55	0.41
6:a:59:PRO:CD	8:d:37:VAL:HG11	2.51	0.41
8:d:108:LEU:HD13	8:d:111:GLN:HE21	1.86	0.41
1:B:113:PRO:HG3	1:B:249:ALA:HB2	2.03	0.41
1:C:100:VAL:HG13	1:C:132:LEU:HD21	2.02	0.41
3:G:33:ILE:HG21	3:G:193:MET:HE1	2.01	0.41
5:L:5:PRO:O	5:L:9:ILE:HG12	2.19	0.41
6:a:222:ASP:O	6:a:222:ASP:OD2	2.38	0.41
5:N:21:MET:HG2	5:N:75:MET:HG3	2.02	0.41
5:P:56:PRO:HB3	5:Q:39:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:2:ASP:C	5:T:3:LEU:HD12	2.45	0.41
1:B:456:LEU:CD2	1:B:464:VAL:HG13	2.50	0.41
6:a:35:THR:HG22	7:b:37:ILE:HG21	2.03	0.41
1:B:393:LEU:HD23	1:B:393:LEU:C	2.46	0.41
1:C:390:ALA:HB2	1:C:448:ILE:HG21	2.03	0.41
2:E:254:ASP:HA	2:E:255:ASN:HA	1.83	0.41
7:b:30:THR:O	7:b:31:PHE:C	2.63	0.41
8:d:289:VAL:O	8:d:293:GLU:HG2	2.21	0.41
1:A:221:ARG:NH1	2:D:131:GLU:OE2	2.49	0.41
1:B:113:PRO:O	1:B:252:THR:OG1	2.27	0.41
1:B:442:GLU:OE2	1:B:487:ARG:NH2	2.54	0.41
1:C:450:LEU:HD11	1:C:471:LEU:HD22	2.02	0.41
2:D:188:ALA:HB2	2:D:234:ALA:CB	2.50	0.41
2:E:251:LEU:O	2:E:304:SER:HA	2.21	0.41
2:F:254:ASP:HA	2:F:255:ASN:HA	1.89	0.41
2:F:287:MET:HE3	2:F:291:GLN:CG	2.50	0.41
4:H:35:LEU:HB3	4:H:36:PRO:HD2	2.03	0.41
5:L:21:MET:HE1	5:T:74:PHE:HB2	2.02	0.41
5:L:21:MET:HE1	5:T:74:PHE:CB	2.51	0.41
5:N:34:ILE:HG22	5:O:37:ASN:HB2	2.01	0.41
7:b:144:LEU:C	7:b:144:LEU:HD12	2.46	0.41
8:d:224:ALA:HB1	8:d:264:GLU:HA	2.02	0.41
1:A:31:ILE:HD13	8:d:427:VAL:CG1	2.51	0.41
1:B:258:GLN:HG3	1:B:324:MET:HE1	2.03	0.41
1:B:330:ILE:HD11	1:B:345:VAL:HG21	2.03	0.41
1:C:464:VAL:O	1:C:465:GLN:C	2.62	0.41
2:D:40:ILE:HD11	2:D:49:LEU:HD11	2.03	0.41
5:R:6:ASN:O	5:R:10:THR:HG23	2.21	0.41
5:R:34:ILE:HG22	5:S:37:ASN:HB2	2.01	0.41
7:b:136:GLN:O	7:b:140:VAL:HG23	2.21	0.41
5:R:21:MET:CE	5:R:72:LEU:HA	2.51	0.40
8:d:422:THR:O	8:d:422:THR:HG23	2.20	0.40
1:B:393:LEU:HD21	1:B:397:LEU:HD12	2.02	0.40
1:C:540:VAL:O	3:G:211:VAL:HG22	2.21	0.40
2:D:100:ASN:OD1	2:D:104:ASP:N	2.52	0.40
8:d:139:ASP:OD1	8:d:141:GLN:N	2.41	0.40
8:d:245:VAL:HG23	8:d:250:LEU:CD2	2.51	0.40
1:A:301:VAL:O	1:A:304:LEU:HB3	2.21	0.40
6:a:105:TRP:O	6:a:108:VAL:HG12	2.21	0.40
8:d:206:LEU:HD23	8:d:253:LEU:HD21	2.04	0.40
8:d:376:VAL:O	8:d:376:VAL:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:d:387:ASP:OD1	8:d:387:ASP:N	2.53	0.40
1:A:463:ASP:O	1:A:464:VAL:C	2.65	0.40
1:B:182:CYS:SG	1:B:329:ILE:HD11	2.61	0.40
1:C:463:ASP:O	1:C:464:VAL:C	2.64	0.40
3:G:19:LYS:NZ	3:G:271:ASP:OD1	2.47	0.40
5:L:21:MET:CE	5:T:20:ILE:HD12	2.52	0.40
5:L:28:ALA:HB2	5:L:68:TYR:HB2	2.03	0.40
6:a:30:ASP:OD1	6:a:31:THR:N	2.54	0.40
7:b:99:LEU:O	7:b:102:GLU:HG3	2.22	0.40
1:A:406:PHE:HB3	1:A:413:LEU:HD21	2.04	0.40
2:D:143:VAL:HG13	2:D:144:VAL:N	2.37	0.40
2:F:235:LEU:HD21	2:F:293:ARG:HB3	2.03	0.40
5:N:56:PRO:HG2	5:O:40:ILE:HD13	2.02	0.40
5:S:21:MET:HE1	5:S:72:LEU:CD1	2.52	0.40
5:T:79:VAL:HG23	5:T:80:PHE:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	515/548 (94%)	506 (98%)	9 (2%)	0	100	100
1	B	498/548 (91%)	485 (97%)	13 (3%)	0	100	100
1	C	518/548 (94%)	504 (97%)	14 (3%)	0	100	100
2	D	467/475 (98%)	456 (98%)	10 (2%)	1 (0%)	43	65
2	E	462/475 (97%)	453 (98%)	8 (2%)	1 (0%)	43	65
2	F	466/475 (98%)	457 (98%)	8 (2%)	1 (0%)	43	65
3	G	293/307 (95%)	290 (99%)	3 (1%)	0	100	100
4	H	116/121 (96%)	111 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	L	82/86 (95%)	79 (96%)	3 (4%)	0	100	100
5	M	83/86 (96%)	80 (96%)	3 (4%)	0	100	100
5	N	82/86 (95%)	82 (100%)	0	0	100	100
5	O	82/86 (95%)	80 (98%)	2 (2%)	0	100	100
5	P	82/86 (95%)	80 (98%)	2 (2%)	0	100	100
5	Q	82/86 (95%)	80 (98%)	2 (2%)	0	100	100
5	R	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
5	S	83/86 (96%)	81 (98%)	2 (2%)	0	100	100
5	T	83/86 (96%)	83 (100%)	0	0	100	100
6	a	236/252 (94%)	231 (98%)	5 (2%)	0	100	100
7	b	142/180 (79%)	137 (96%)	5 (4%)	0	100	100
8	d	434/445 (98%)	425 (98%)	9 (2%)	0	100	100
All	All	4889/5148 (95%)	4782 (98%)	104 (2%)	3 (0%)	49	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	277	VAL
2	F	277	VAL
2	D	277	VAL

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	415/441 (94%)	415 (100%)	0	100	100
1	B	405/441 (92%)	405 (100%)	0	100	100
1	C	422/441 (96%)	422 (100%)	0	100	100
2	D	383/388 (99%)	383 (100%)	0	100	100
2	E	381/388 (98%)	381 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	383/388 (99%)	383 (100%)	0	100	100
3	G	231/238 (97%)	231 (100%)	0	100	100
4	H	94/96 (98%)	94 (100%)	0	100	100
5	L	54/56 (96%)	54 (100%)	0	100	100
5	M	55/56 (98%)	55 (100%)	0	100	100
5	N	54/56 (96%)	54 (100%)	0	100	100
5	O	54/56 (96%)	54 (100%)	0	100	100
5	P	54/56 (96%)	54 (100%)	0	100	100
5	Q	54/56 (96%)	54 (100%)	0	100	100
5	R	55/56 (98%)	55 (100%)	0	100	100
5	S	55/56 (98%)	55 (100%)	0	100	100
5	T	55/56 (98%)	55 (100%)	0	100	100
6	a	191/200 (96%)	191 (100%)	0	100	100
7	b	110/134 (82%)	110 (100%)	0	100	100
8	d	342/347 (99%)	342 (100%)	0	100	100
All	All	3847/4006 (96%)	3847 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	305	HIS
1	A	352	GLN
1	A	420	GLN
1	A	465	GLN
1	A	474	HIS
1	B	258	GLN
1	B	335	ASN
1	C	200	GLN
1	C	505	ASN
2	E	97	HIS
2	E	208	ASN
2	F	421	GLN
3	G	288	GLN
4	H	38	HIS

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Mol	Chain	Res	Type
5	N	71	ASN
5	R	71	ASN
5	T	46	GLN
7	b	95	GLN
7	b	136	GLN
8	d	58	HIS
8	d	111	GLN
8	d	112	GLN
8	d	201	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](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	$\# Z > 2$
9	ATP	B	600	10	32,33,33	0.49	0	48,52,52	0.69	1 (2%)
11	ADP	D	600	10	28,29,29	1.35	5 (17%)	43,45,45	1.87	10 (23%)
9	ATP	C	600	10	32,33,33	0.49	0	48,52,52	0.67	0
9	ATP	A	600	10	32,33,33	0.53	0	48,52,52	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ATP	F	600	10	32,33,33	0.68	2 (6%)	48,52,52	0.69	0
11	ADP	E	600	-	28,29,29	1.38	4 (14%)	43,45,45	1.91	10 (23%)

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
9	ATP	B	600	10	-	1/22/38/38	0/3/3/3
11	ADP	D	600	10	-	6/16/32/32	0/3/3/3
9	ATP	C	600	10	-	1/22/38/38	0/3/3/3
9	ATP	A	600	10	-	0/22/38/38	0/3/3/3
9	ATP	F	600	10	-	2/22/38/38	0/3/3/3
11	ADP	E	600	-	-	1/16/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E	600	ADP	C5-C4	4.51	1.47	1.39
11	D	600	ADP	C5-C4	4.31	1.46	1.39
11	E	600	ADP	C5-C6	2.62	1.48	1.41
9	F	600	ATP	PB-O3B	-2.60	1.56	1.59
11	D	600	ADP	C5-N7	-2.54	1.34	1.39
11	E	600	ADP	C5-N7	-2.49	1.34	1.39
11	D	600	ADP	C5-C6	2.36	1.47	1.41
11	E	600	ADP	C8-N7	2.23	1.36	1.31
11	D	600	ADP	C8-N7	2.06	1.35	1.31
11	D	600	ADP	C4-N9	-2.05	1.33	1.37
9	F	600	ATP	PA-O3A	-2.04	1.57	1.59

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	600	ADP	C5-C4-N3	-5.96	118.52	126.72
11	D	600	ADP	C5-C4-N3	-5.78	118.75	126.72
11	D	600	ADP	N3-C4-N9	4.87	135.45	127.17
11	E	600	ADP	N3-C4-N9	4.79	135.31	127.17
11	E	600	ADP	C2-N3-C4	3.89	121.34	111.83
11	D	600	ADP	C2-N3-C4	3.82	121.15	111.83
11	D	600	ADP	N3-C2-N1	-3.74	122.92	128.58

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	600	ADP	N3-C2-N1	-3.69	122.99	128.58
11	E	600	ADP	C4-C5-N7	-3.34	106.76	110.58
11	D	600	ADP	C4-C5-N7	-3.21	106.92	110.58
11	D	600	ADP	C4-N9-C8	3.20	109.10	105.74
11	E	600	ADP	C4-N9-C8	2.69	108.56	105.74
11	E	600	ADP	C5-N7-C8	2.64	107.60	103.45
11	D	600	ADP	C5-N7-C8	2.61	107.55	103.45
11	E	600	ADP	C3'-C2'-C1'	2.56	106.31	101.46
11	D	600	ADP	C2'-C1'-N9	-2.54	106.99	113.30
11	D	600	ADP	N9-C8-N7	-2.32	110.64	113.94
11	E	600	ADP	N9-C8-N7	-2.13	110.91	113.94
9	B	600	ATP	O3'-C3'-C2'	-2.12	105.03	111.82
11	D	600	ADP	C2-N1-C6	2.10	122.18	118.73
11	E	600	ADP	C2-N1-C6	2.02	122.05	118.73

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	600	ADP	C5'-O5'-PA-O2A
11	D	600	ADP	C5'-O5'-PA-O3A
9	F	600	ATP	PA-O3A-PB-O1B
11	D	600	ADP	PB-O3A-PA-O1A
9	B	600	ATP	C5'-O5'-PA-O1A
9	C	600	ATP	C5'-O5'-PA-O1A
11	D	600	ADP	C5'-O5'-PA-O1A
11	D	600	ADP	O4'-C4'-C5'-O5'
9	F	600	ATP	PA-O3A-PB-O2B
11	D	600	ADP	C3'-C4'-C5'-O5'
11	E	600	ADP	PB-O3A-PA-O2A

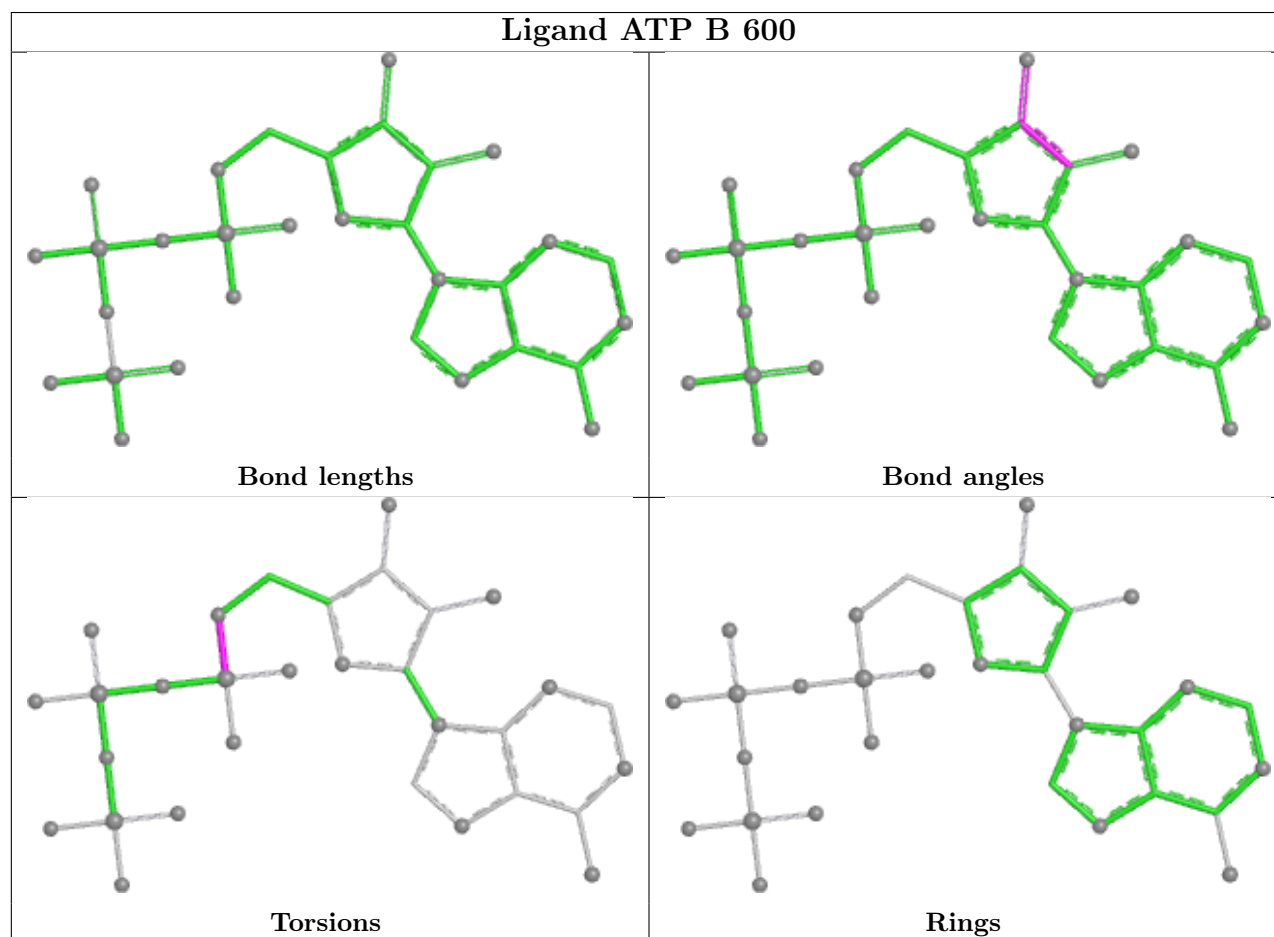
There are no ring outliers.

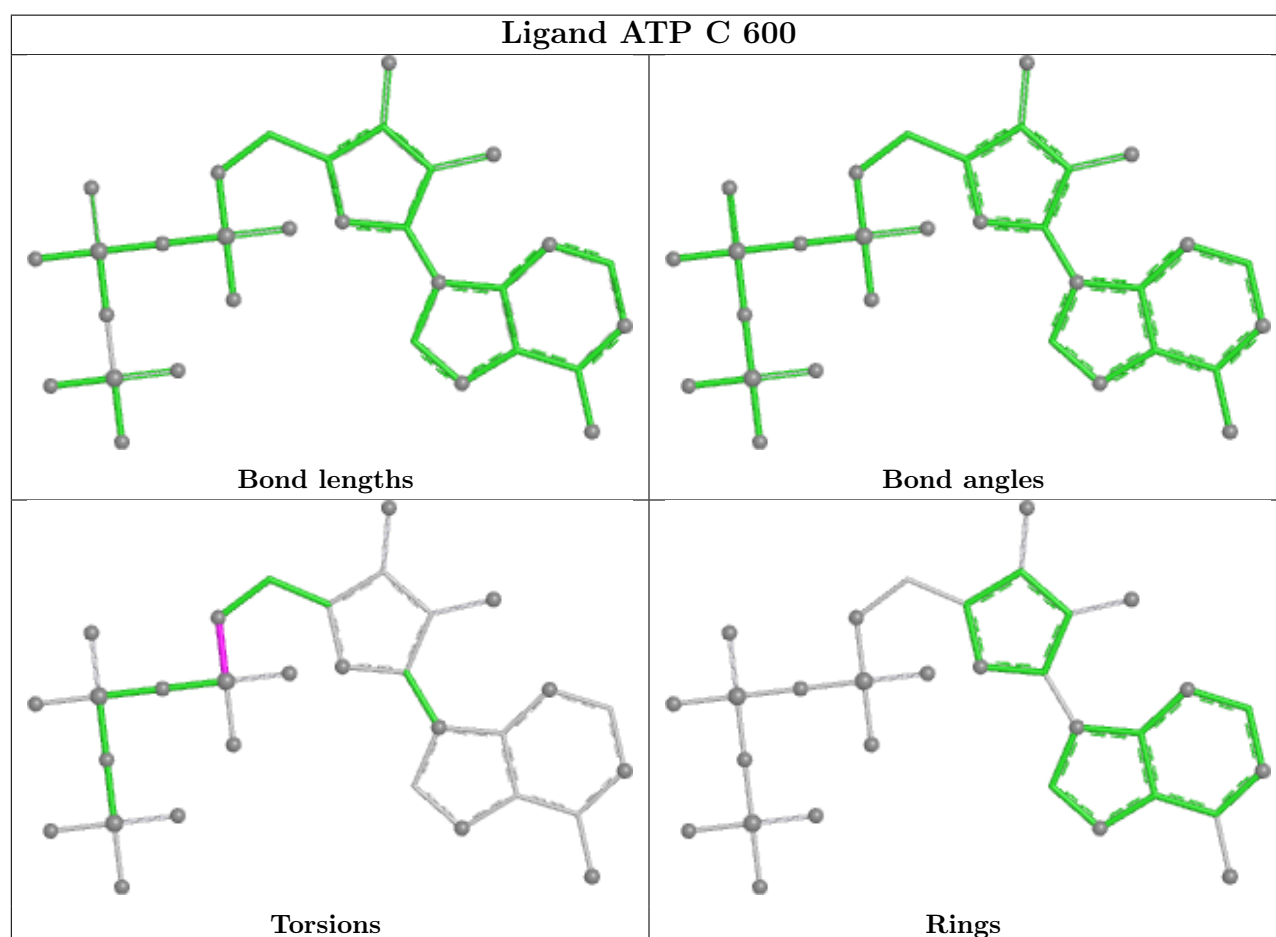
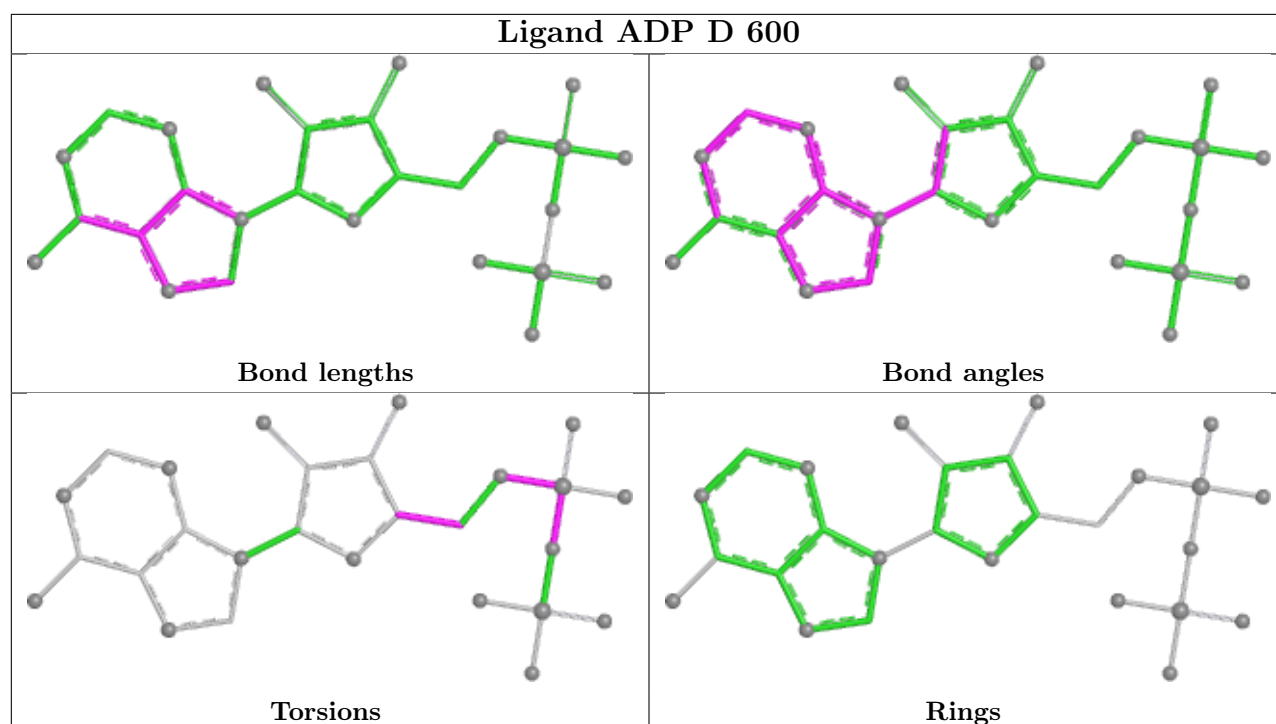
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	600	ADP	1	0
11	E	600	ADP	1	0

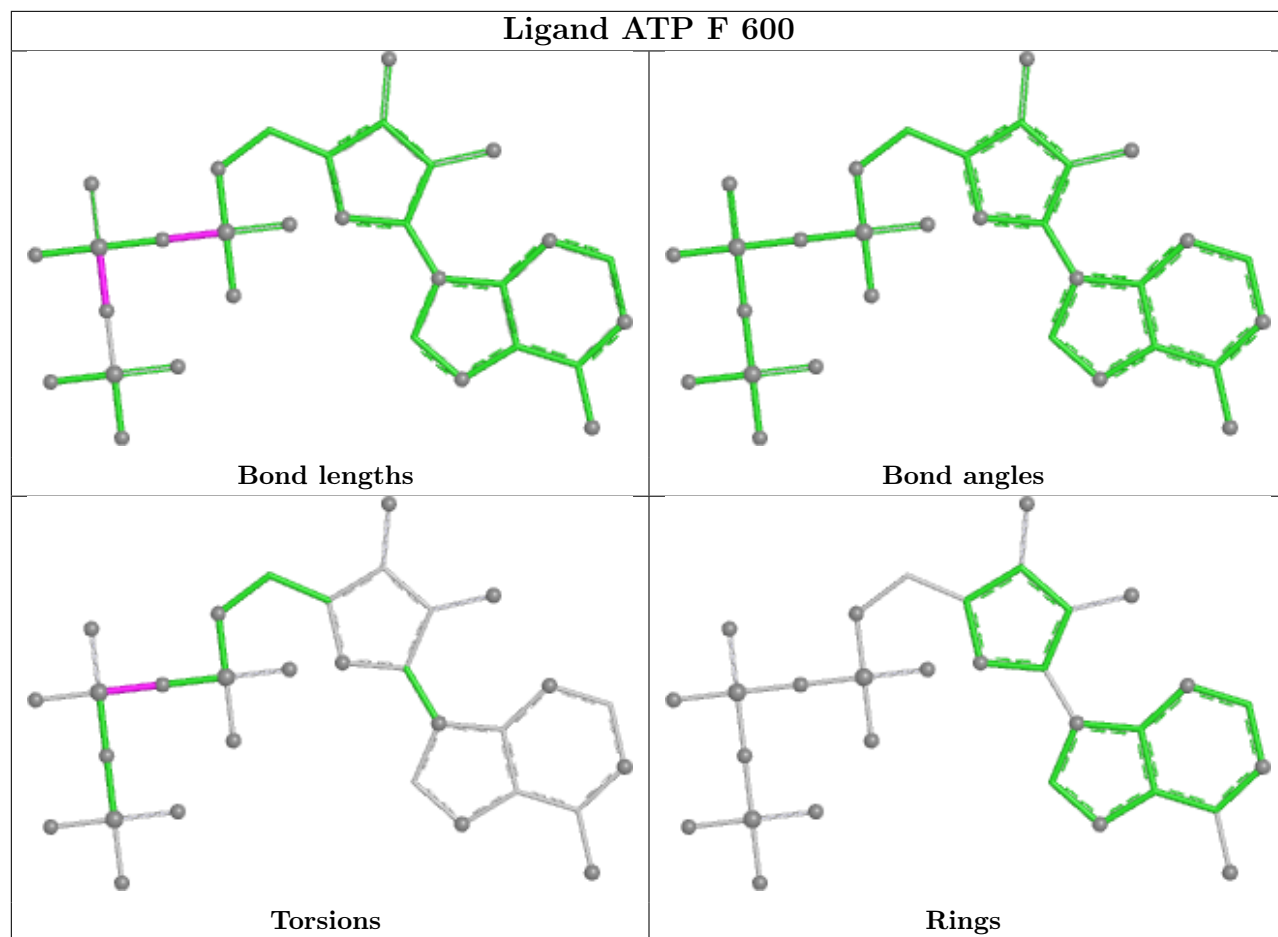
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

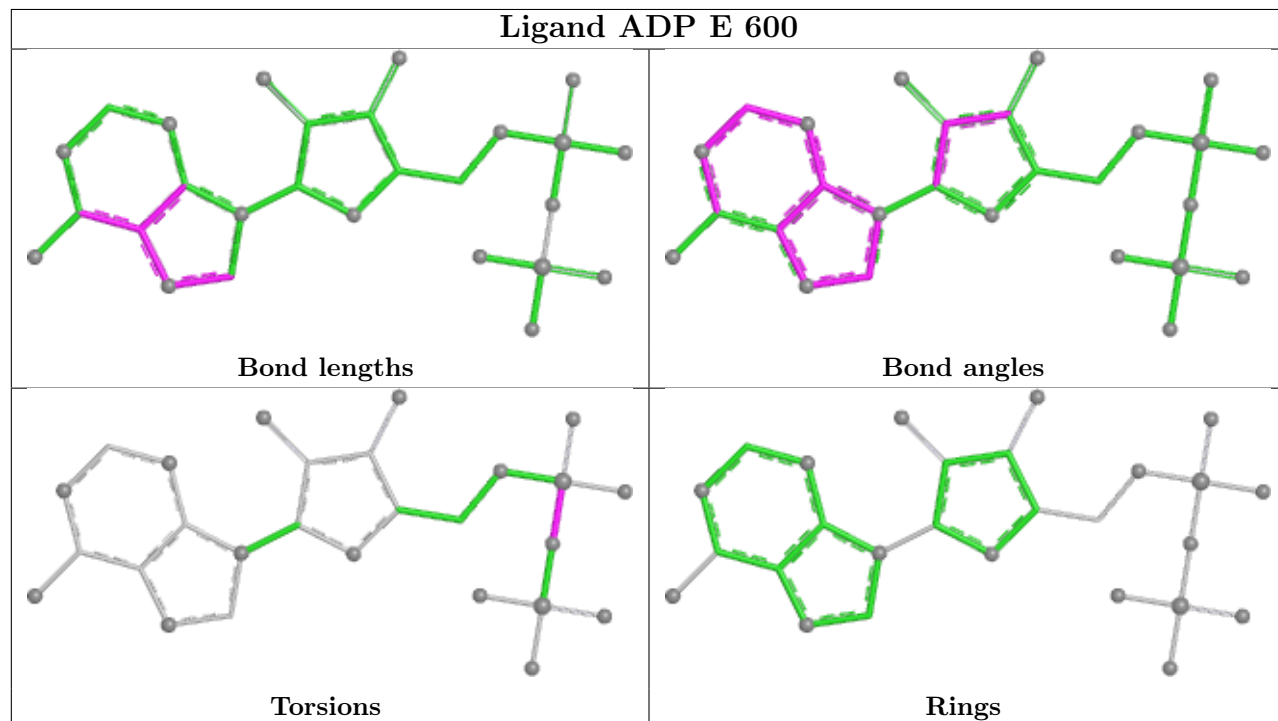




Ligand ATP F 600



Ligand ADP E 600



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.

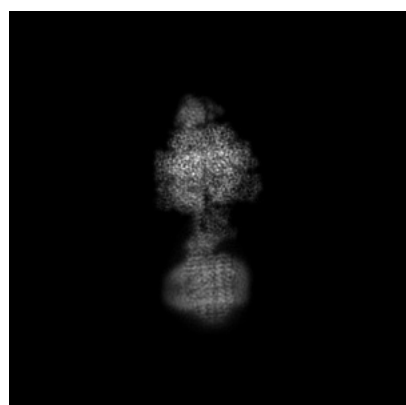
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12407. These allow visual inspection of the internal detail of the map and identification of artifacts.

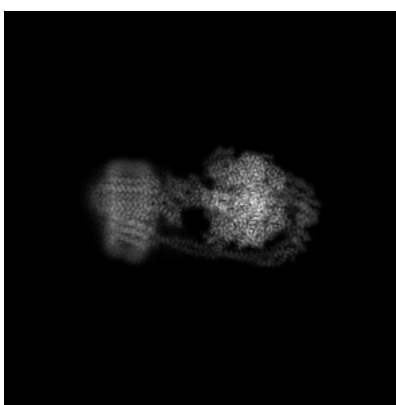
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

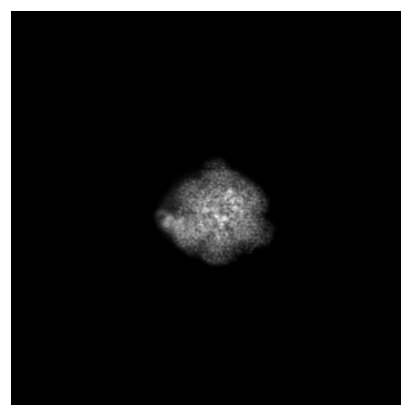
6.1.1 Primary map



X



Y

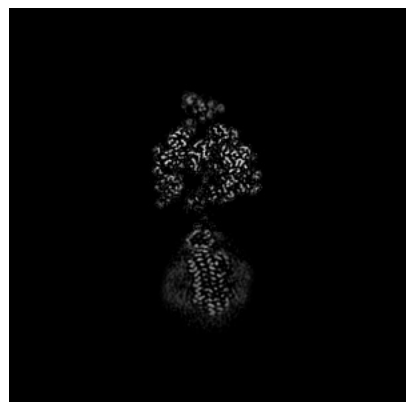


Z

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

6.2 Central slices [i](#)

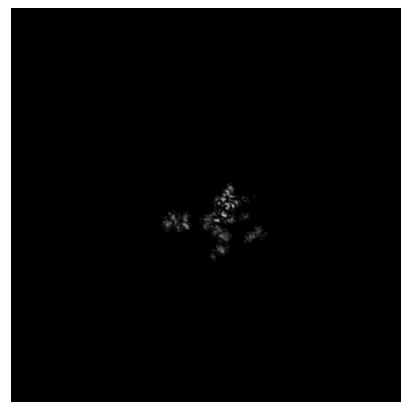
6.2.1 Primary map



X Index: 250



Y Index: 250

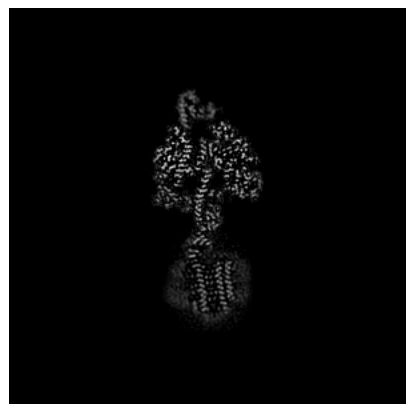


Z Index: 250

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

6.3 Largest variance slices [i](#)

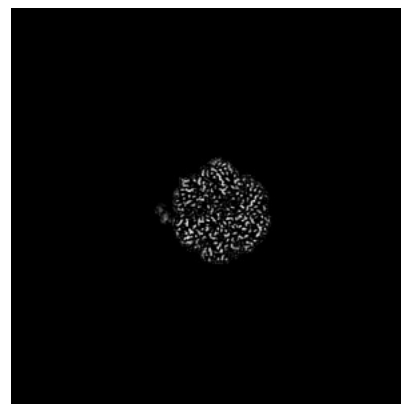
6.3.1 Primary map



X Index: 258



Y Index: 238

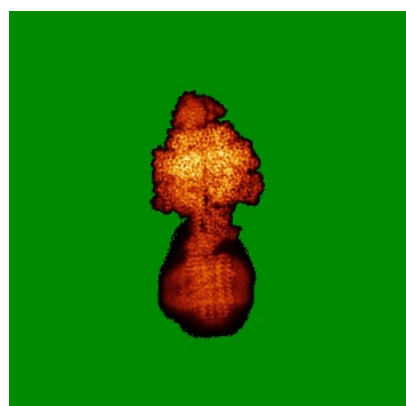


Z Index: 313

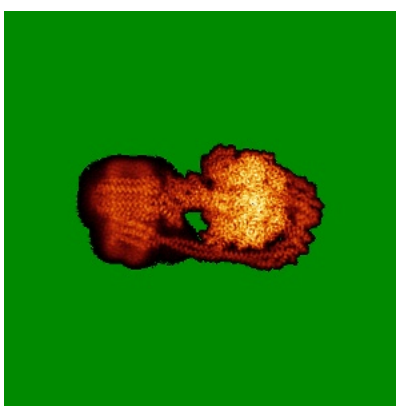
The images above show the largest variance slices of the map in three orthogonal directions.

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

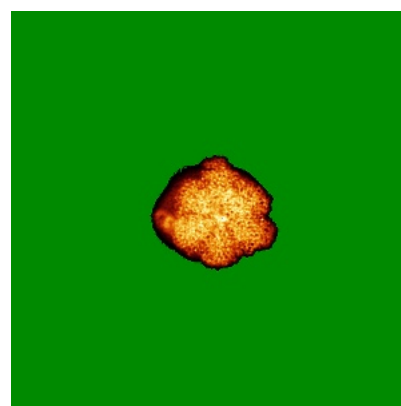
6.4.1 Primary map



X



Y



Z

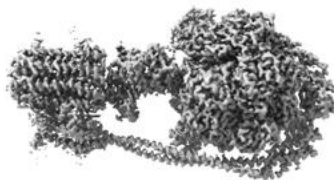
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

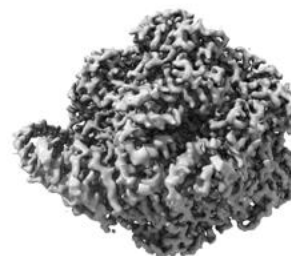
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

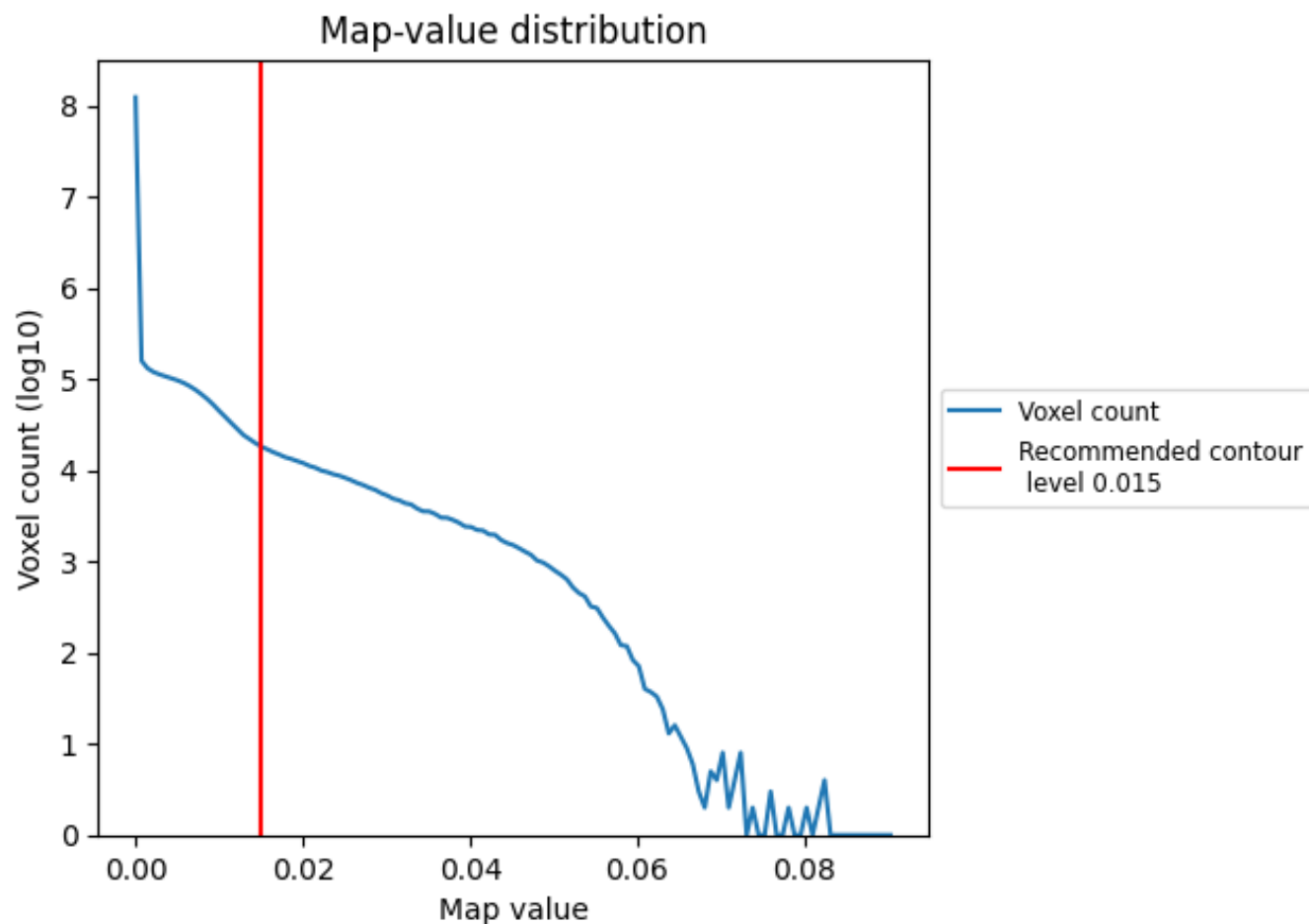
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

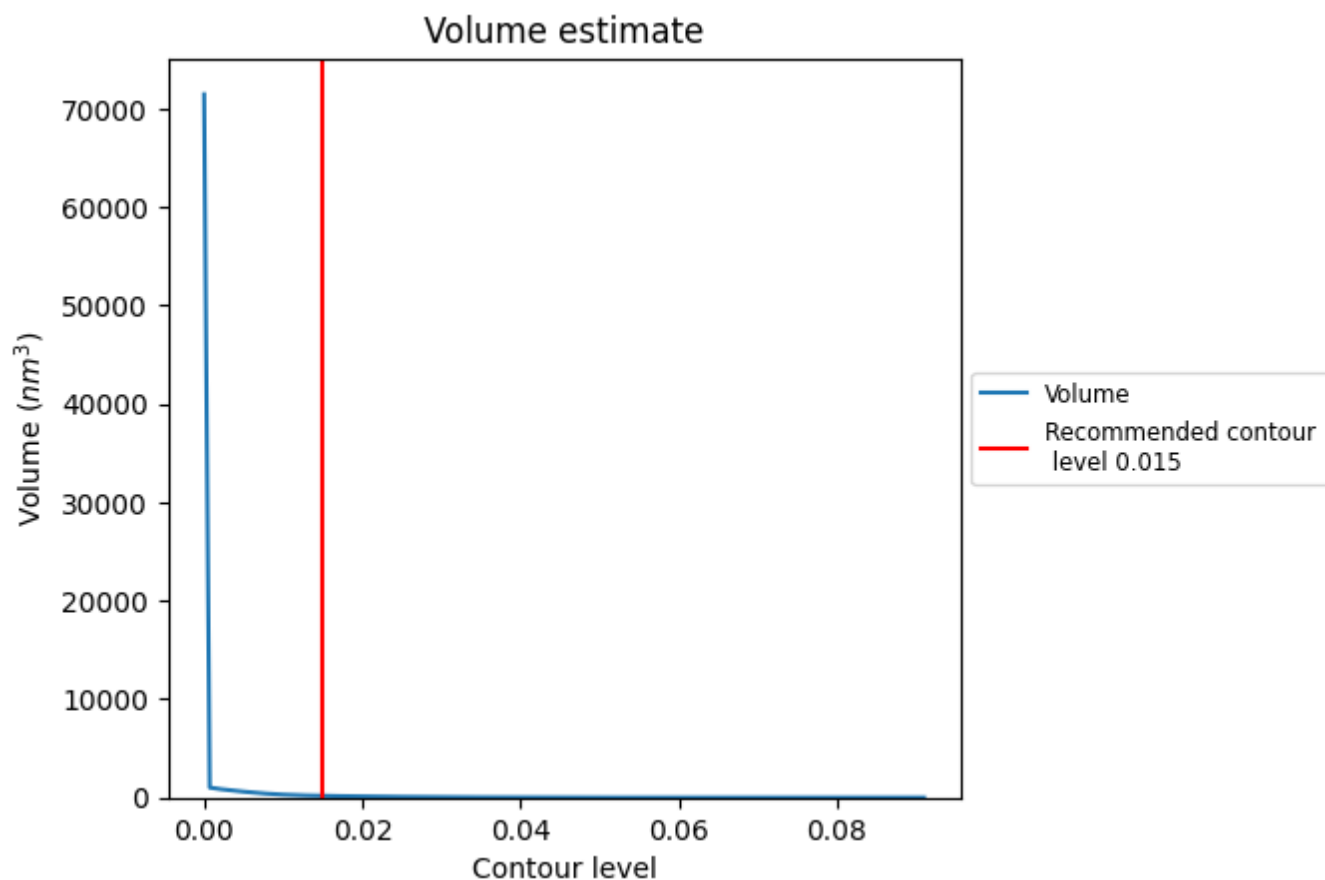
This section contains the results of statistical analysis of the map.

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.

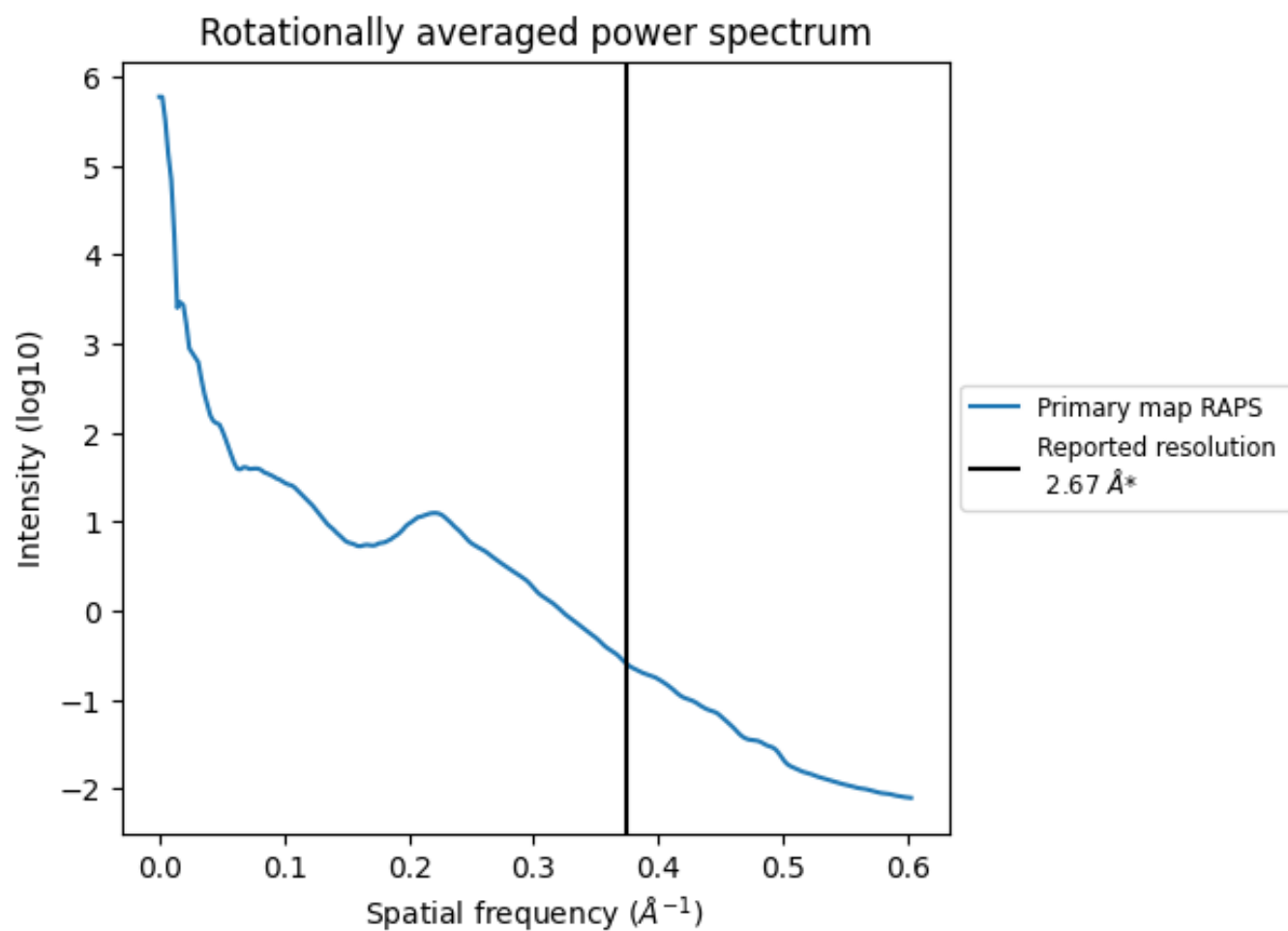
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 175 nm^3 ; this corresponds to an approximate mass of 158 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 0.375 $\text{\AA}^{-1}$

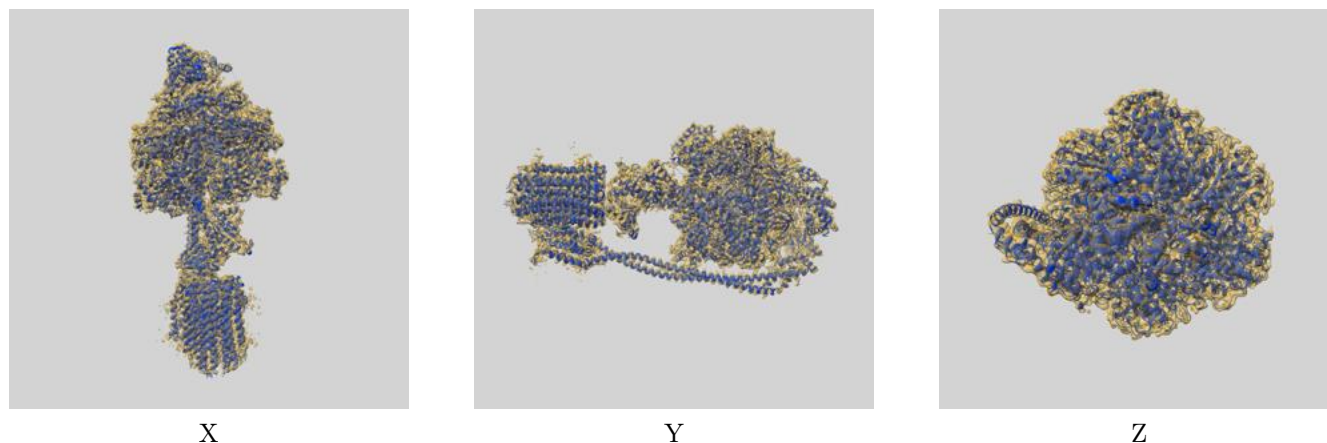
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

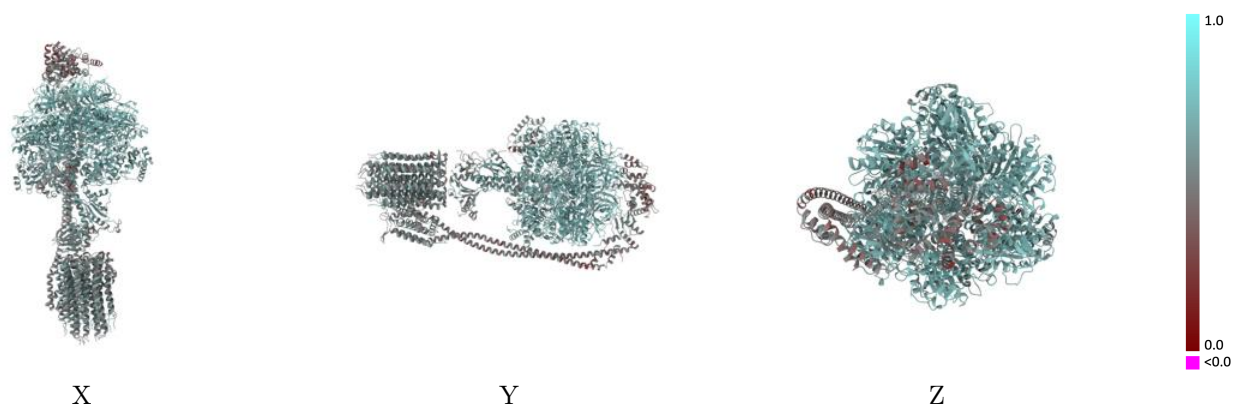
This section contains information regarding the fit between EMDB map EMD-12407 and PDB model 7NJQ. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



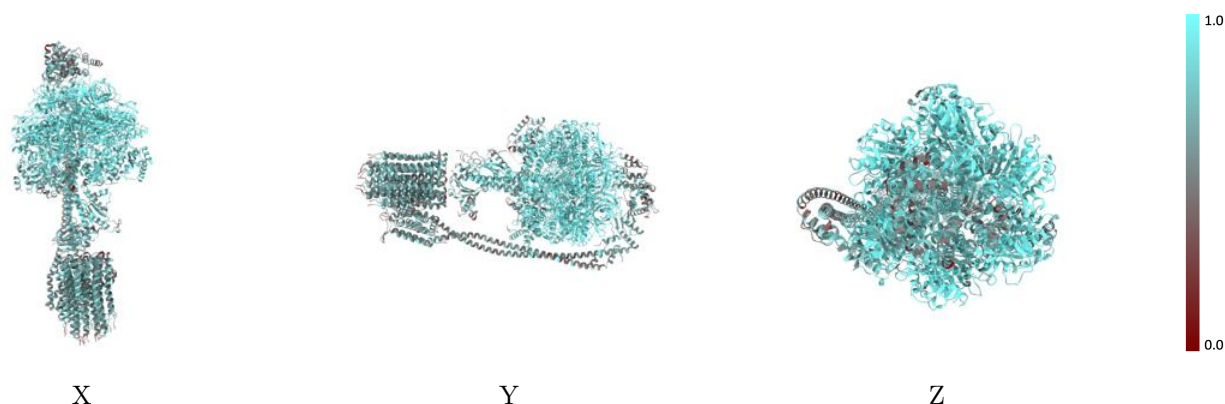
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



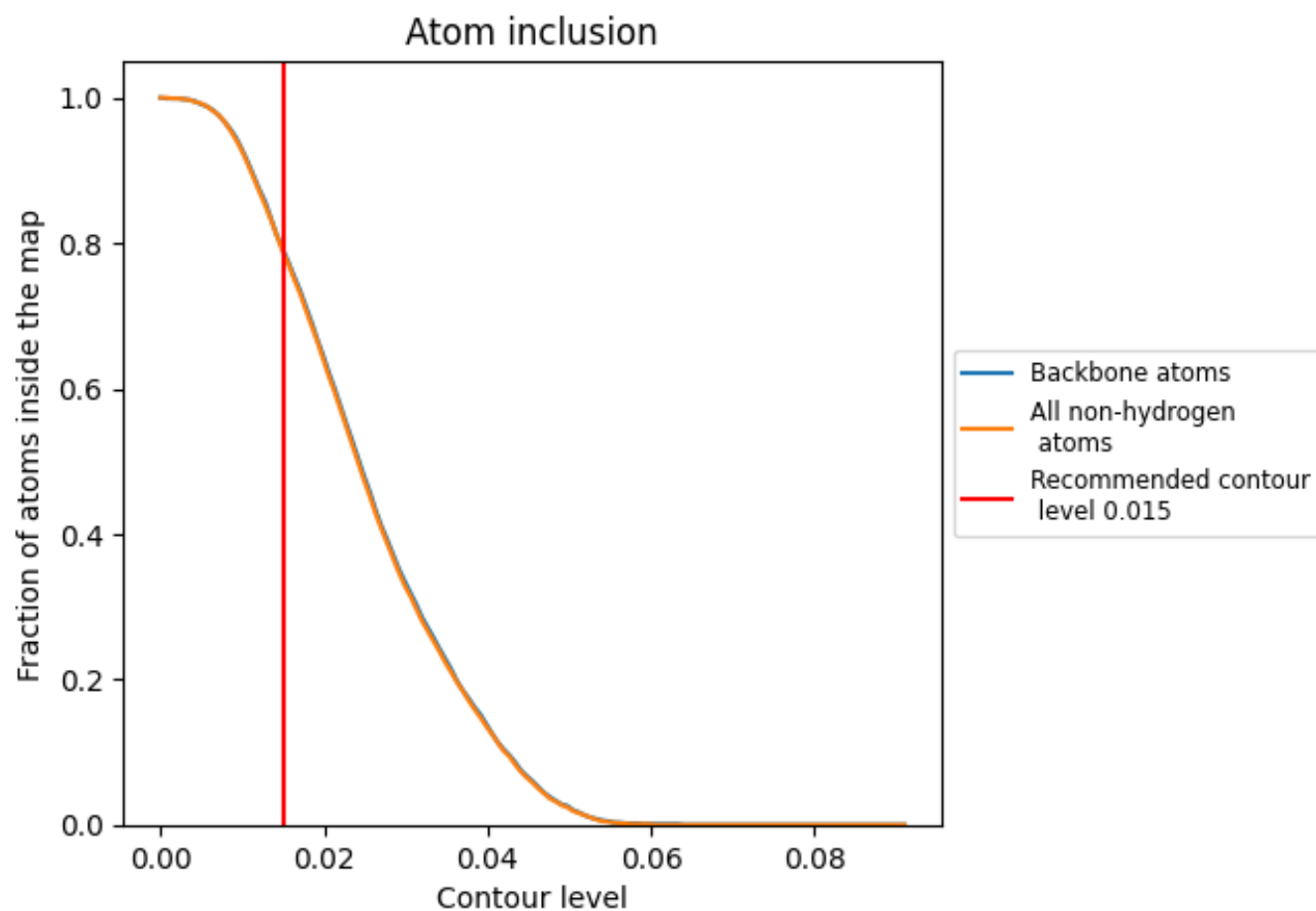
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7870	 0.5960
A	 0.8940	 0.6530
B	 0.8500	 0.6240
C	 0.8840	 0.6430
D	 0.9230	 0.6660
E	 0.8810	 0.6400
F	 0.9240	 0.6670
G	 0.7970	 0.5930
H	 0.6550	 0.5310
L	 0.6730	 0.5420
M	 0.6370	 0.5360
N	 0.6280	 0.5350
O	 0.6340	 0.5210
P	 0.6100	 0.5150
Q	 0.6230	 0.5260
R	 0.6230	 0.5260
S	 0.6220	 0.5250
T	 0.6440	 0.5400
a	 0.5960	 0.5170
b	 0.5670	 0.4590
d	 0.6120	 0.4590

