



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 02:56 AM UTC

PDB ID : 6YO0 / pdb_00006yo0
EMDB ID : EMD-10862
Title : Cryo-EM structure of Tetrahymena thermophila mitochondrial ATP synthase
- F1/peripheral stalk
Authors : Kock Flygaard, R.; Muhleip, A.; Amunts, A.
Deposited on : 2020-04-14
Resolution : 2.90 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

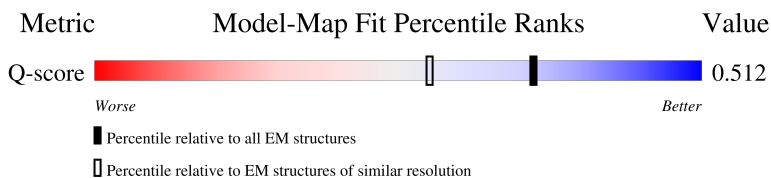
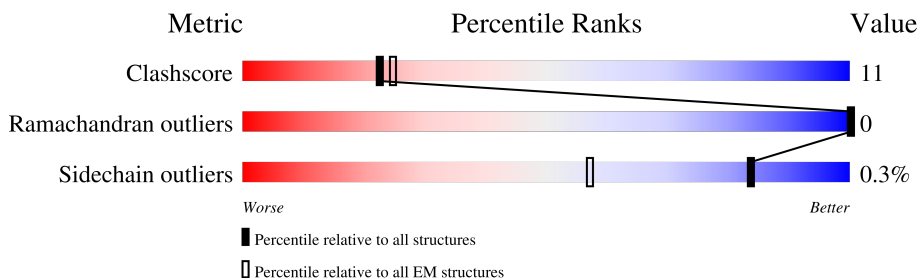
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



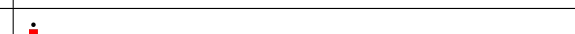
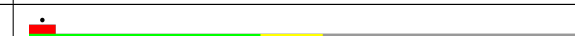
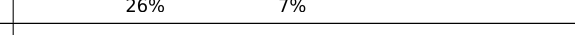
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	G1	219	
2	g1	299	
3	A1	546	
3	B1	546	

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Mol	Chain	Length	Quality of chain
3	C1	546	 71%22%6%
4	D1	497	 70%24%5%
4	E1	497	 73%22%5%
4	F1	497	 69%26%6%
5	il	108	 26%7%67%
6	s	145	 9%12%79%
7	b	381	 11%40%14%46%
8	d	234	 10%30%14%56%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 55840 atoms, of which 28162 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 Oligomycin sensitivity-conferring protein (OSCP).

Mol	Chain	Residues	Atoms						AltConf	Trace
1	G1	188	Total	C	H	N	O	S	0	0
			3000	942	1515	252	287	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	g1	90	Total	C	H	N	O	S	0	0
			1420	419	743	123	128	7		

- Molecule 3 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C1	513	Total	C	H	N	O	S	0	0
			7980	2481	4058	685	739	17		
3	B1	511	Total	C	H	N	O	S	0	0
			7934	2469	4030	681	737	17		
3	A1	512	Total	C	H	N	O	S	0	0
			7946	2472	4037	682	738	17		

- Molecule 4 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D1	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
4	F1	469	Total	C	H	N	O	S	0	0
			7112	2237	3567	610	687	11		
4	E1	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		

- Molecule 5 is a protein called Inhibitor of F1 (IF1).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	i1	36	Total	C	H	N	O	S	0	0
			638	197	320	58	62	1		

- Molecule 6 is a protein called ATPTT13.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	s	31	Total	C	H	N	O	S	0	0
			486	152	245	42	45	2		

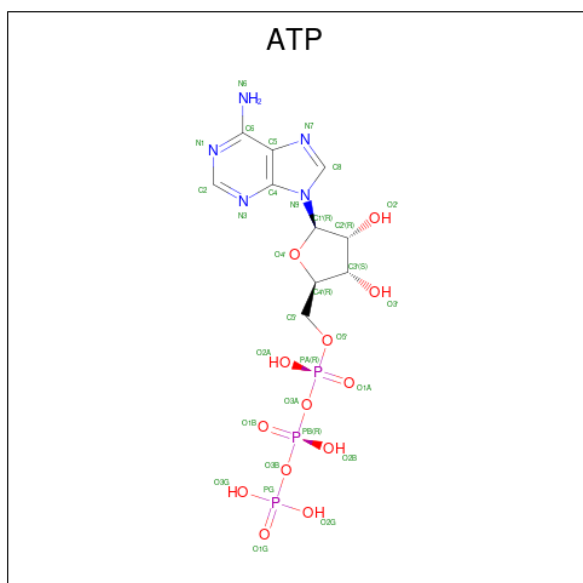
- Molecule 7 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	b	205	Total	C	H	N	O	S	0	0
			3227	999	1626	281	319	2		

- Molecule 8 is a protein called subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	d	103	Total	C	H	N	O	S	0	0
			1615	508	799	135	172	1		

- 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	C1	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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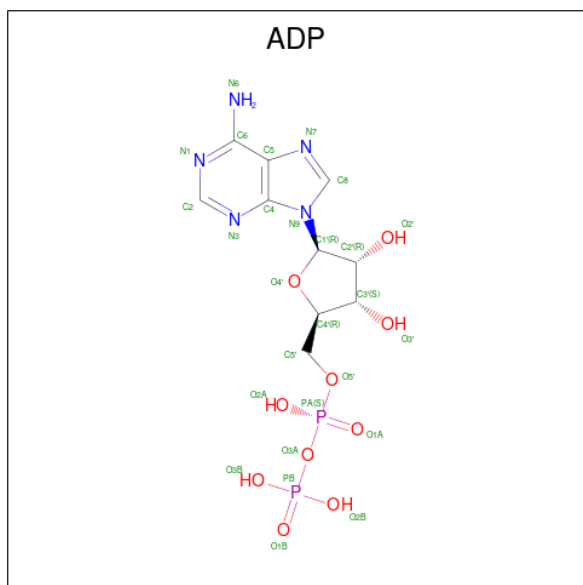
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Mol	Chain	Residues	Atoms					AltConf	
9	B1	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
9	A1	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

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

Mol	Chain	Residues	Atoms		AltConf
10	C1	1	Total	Mg	0
			1	1	
10	D1	1	Total	Mg	0
			1	1	
10	B1	1	Total	Mg	0
			1	1	
10	A1	1	Total	Mg	0
			1	1	
10	E1	1	Total	Mg	0
			1	1	

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

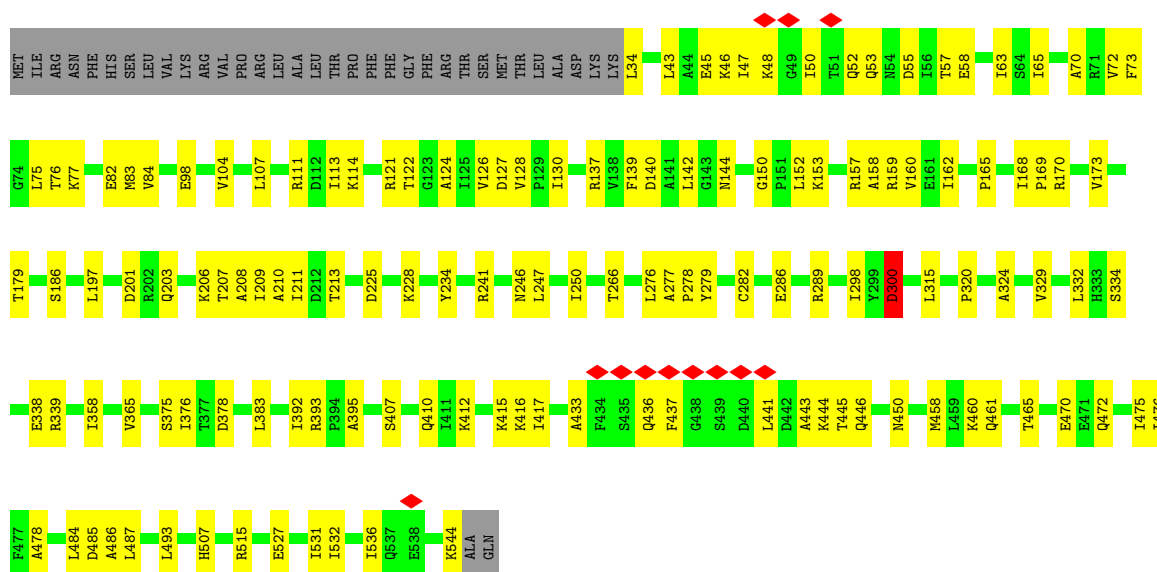


Mol	Chain	Residues	Atoms						AltConf
11	D1	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
11	E1	1	Total 39	C 10	H 12	N 5	O 10	P 2	0



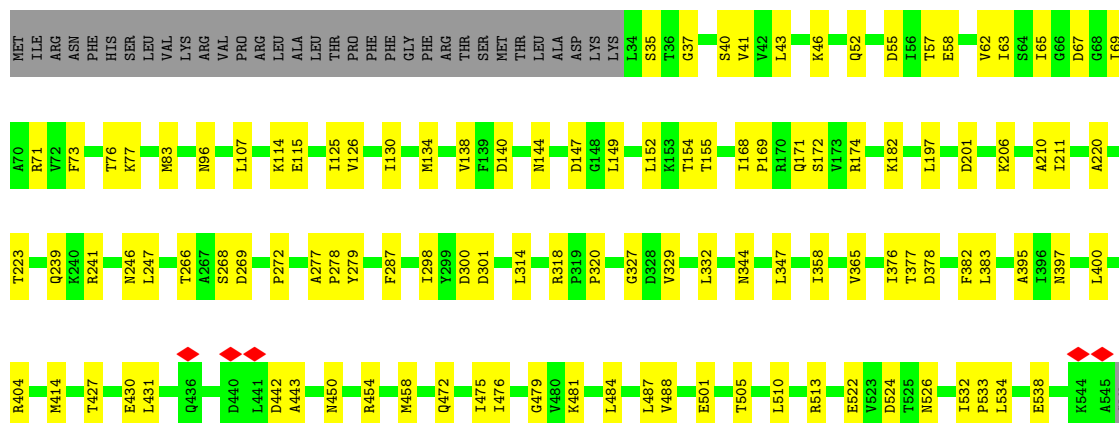
• Molecule 3: ATP synthase subunit alpha

Chain B1: 69% 25% 6%



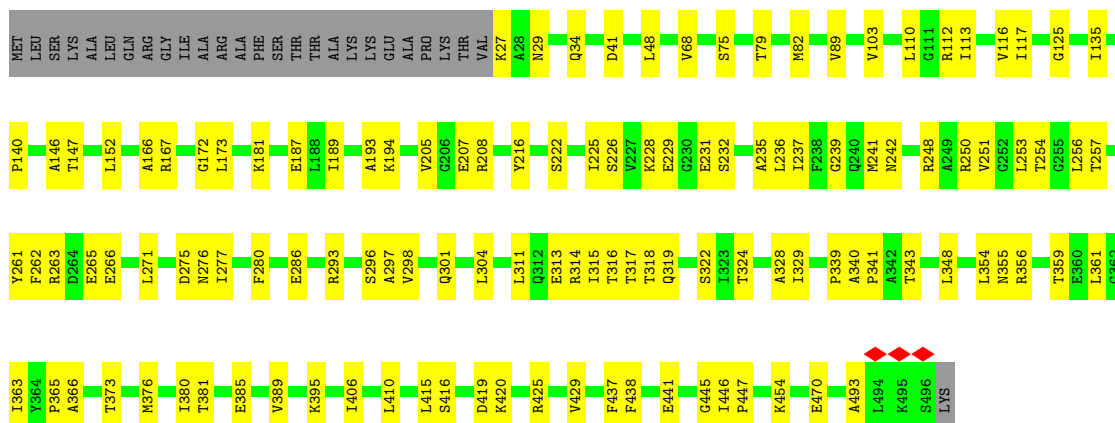
• Molecule 3: ATP synthase subunit alpha

Chain A1: 73% 20% 6%



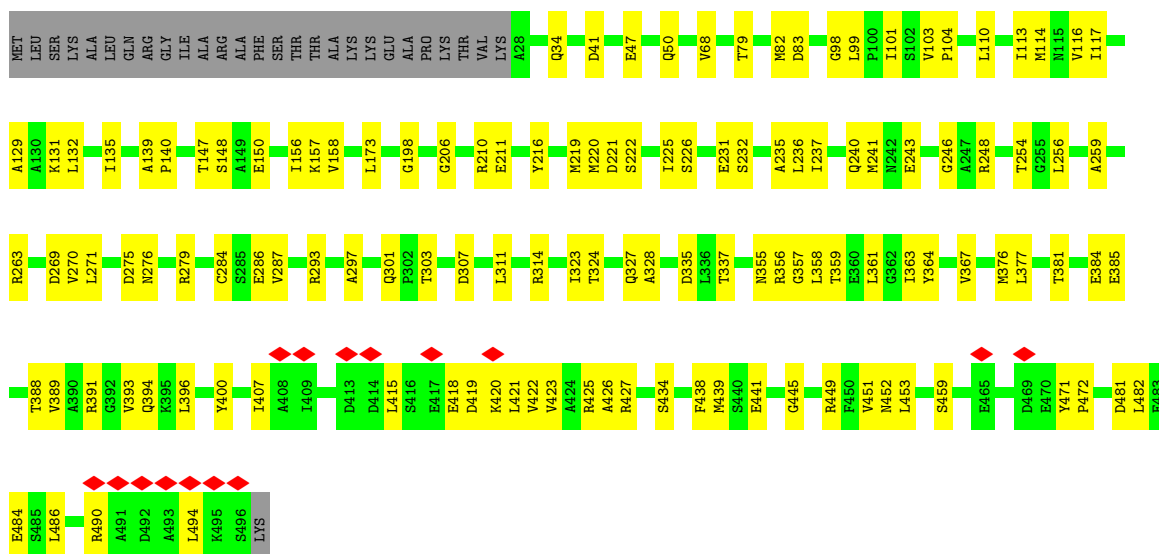
• Molecule 4: ATP synthase subunit beta

Chain D1: 



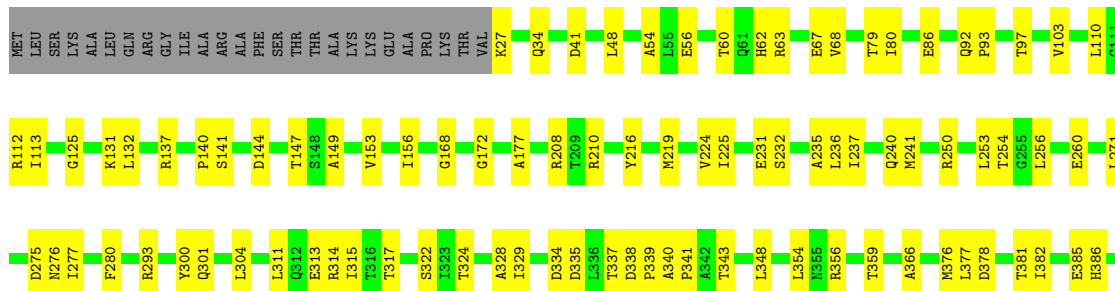
• Molecule 4: ATP synthase subunit beta

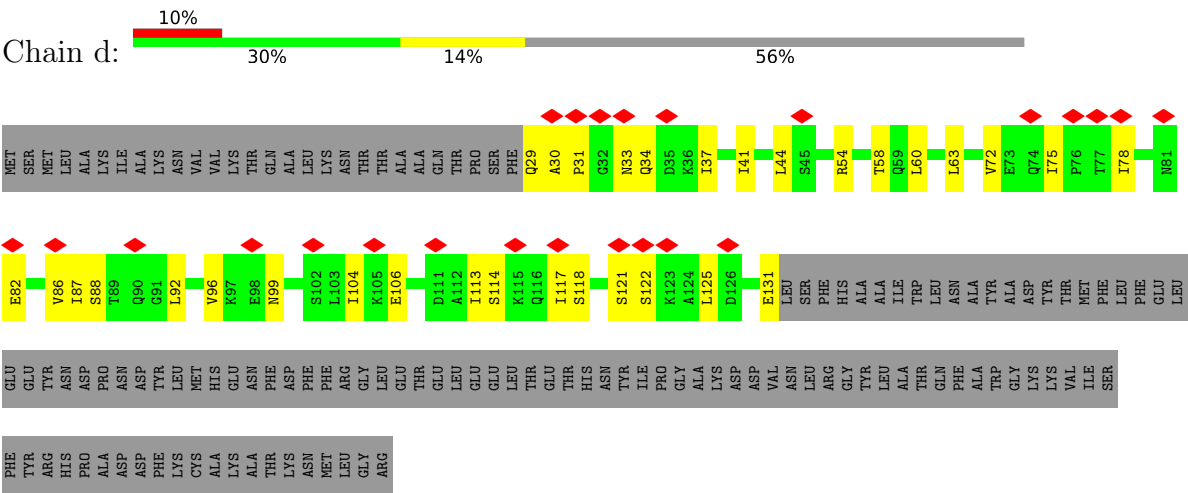
Chain F1: 



• Molecule 4: ATP synthase subunit beta

Chain E1: 





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61157	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 ($e^-/\text{\AA}^2$)	30.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.092	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	498.0, 498.0, 498.0	wwPDB
Map dimensions	600, 600, 600	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: MG, ADP, ATP

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	G1	0.19	0/1507	0.33	0/2027
2	g1	0.27	0/676	0.31	0/893
3	A1	0.30	0/3961	0.35	0/5346
3	B1	0.28	0/3956	0.32	0/5339
3	C1	0.30	0/3974	0.34	0/5361
4	D1	0.31	0/3613	0.34	0/4900
4	E1	0.31	0/3613	0.34	0/4900
4	F1	0.27	0/3604	0.33	0/4889
5	i1	0.24	0/321	0.36	0/425
6	s	0.13	0/243	0.32	0/326
7	b	0.15	0/1617	0.32	0/2178
8	d	0.12	0/828	0.28	0/1119
All	All	0.28	0/27913	0.33	0/37703

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B1	0	1
4	D1	0	1
4	E1	0	1
4	F1	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B1	300	ASP	Peptide
4	D1	275	ASP	Peptide
4	E1	275	ASP	Peptide
4	F1	364	TYR	Peptide

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	G1	1485	1515	1515	41	0
2	g1	677	743	743	10	0
3	A1	3909	4037	4037	84	0
3	B1	3904	4030	4029	97	0
3	C1	3922	4058	4058	86	0
4	D1	3554	3581	3581	85	0
4	E1	3554	3581	3581	79	0
4	F1	3545	3567	3567	98	0
5	i1	318	320	320	8	0
6	s	241	245	245	22	0
7	b	1601	1626	1626	46	0
8	d	816	799	799	36	0
9	A1	31	12	12	1	0
9	B1	31	12	12	4	0
9	C1	31	12	12	0	0
10	A1	1	0	0	0	0
10	B1	1	0	0	0	0
10	C1	1	0	0	0	0
10	D1	1	0	0	0	0
10	E1	1	0	0	0	0
11	D1	27	12	12	1	0
11	E1	27	12	12	0	0
All	All	27678	28162	28161	629	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 11.

All (629) 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)
8:d:41:ILE:HD13	8:d:60:LEU:HD12	1.50	0.93
4:F1:256:LEU:HD22	4:F1:311:LEU:HD12	1.51	0.92
4:D1:205:VAL:HG12	4:D1:251:VAL:HG13	1.53	0.91
4:E1:137:ARG:NH1	4:E1:260:GLU:OE1	2.04	0.90
1:G1:40:GLU:OE1	1:G1:133:LYS:NZ	2.05	0.90
3:B1:210:ALA:HB1	3:B1:298:ILE:HD13	1.52	0.89
8:d:29:GLN:O	8:d:33:ASN:ND2	2.07	0.87
3:C1:234:TYR:OH	3:C1:300:ASP:OD2	1.92	0.86
4:D1:181:LYS:NZ	11:D1:900:ADP:O2B	2.09	0.86
5:i1:30:GLU:N	5:i1:30:GLU:OE1	2.11	0.84
3:B1:234:TYR:OH	3:B1:300:ASP:OD2	1.96	0.84
3:C1:454:ARG:NH2	3:C1:487:LEU:O	2.13	0.82
3:B1:159:ARG:NH2	4:E1:86:GLU:OE1	2.13	0.81
4:E1:483:GLU:N	4:E1:483:GLU:OE2	2.14	0.81
3:A1:114:LYS:NZ	4:E1:48:LEU:O	2.15	0.80
4:E1:177:ALA:O	4:E1:356:ARG:NH2	2.15	0.80
4:D1:415:LEU:O	4:D1:420:LYS:NZ	2.16	0.79
3:C1:39:ALA:HB3	3:C1:42:VAL:HG12	1.65	0.78
3:C1:487:LEU:HD21	3:C1:536:ILE:HG23	1.65	0.78
4:F1:415:LEU:O	4:F1:420:LYS:NZ	2.17	0.77
2:g1:286:THR:OG1	4:F1:297:ALA:O	2.02	0.77
4:D1:27:LYS:NZ	4:D1:29:ASN:OD1	2.15	0.76
4:D1:248:ARG:NH2	4:D1:286:GLU:OE1	2.20	0.74
3:B1:77:LYS:O	3:B1:121:ARG:NH1	2.21	0.74
3:B1:207:THR:N	9:B1:900:ATP:O2B	2.20	0.74
4:F1:355:ASN:HB3	4:F1:358:LEU:HD23	1.69	0.74
3:B1:82:GLU:OE2	3:B1:124:ALA:N	2.20	0.74
6:s:123:ASP:OD2	7:b:214:TYR:OH	2.05	0.73
1:G1:164:GLU:OE2	1:G1:180:TYR:OH	2.07	0.73
4:D1:48:LEU:HD21	4:D1:75:SER:HA	1.70	0.73
1:G1:168:LYS:O	1:G1:172:ALA:N	2.23	0.71
3:C1:517:SER:OG	3:C1:519:ASP:OD1	2.06	0.71
3:A1:171:GLN:OE1	3:A1:174:ARG:NH2	2.22	0.71
4:D1:385:GLU:O	4:D1:389:VAL:HG23	1.90	0.71
4:F1:150:GLU:N	4:F1:150:GLU:OE1	2.23	0.71
3:A1:210:ALA:HB1	3:A1:298:ILE:HD13	1.71	0.71
4:E1:335:ASP:OD1	4:E1:337:THR:OG1	2.09	0.70
3:C1:289:ARG:NH1	3:C1:339:ARG:O	2.24	0.70
6:s:141:LYS:NZ	8:d:106:GLU:OE2	2.23	0.70
3:B1:170:ARG:NH2	3:B1:338:GLU:O	2.24	0.70
4:F1:206:GLY:O	4:F1:279:ARG:NE	2.24	0.70
3:C1:156:GLN:N	3:C1:156:GLN:OE1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:241:ARG:NH1	4:D1:140:PRO:O	2.23	0.70
3:B1:165:PRO:O	3:B1:170:ARG:NH1	2.24	0.70
3:A1:522:GLU:O	3:A1:526:ASN:ND2	2.24	0.70
7:b:55:GLU:O	7:b:59:THR:HG23	1.91	0.70
4:E1:317:THR:HG23	4:E1:322:SER:HA	1.75	0.69
3:B1:407:SER:OG	3:B1:415:LYS:NZ	2.19	0.69
3:B1:289:ARG:NH1	3:B1:339:ARG:O	2.26	0.69
4:E1:231:GLU:O	4:E1:232:SER:OG	2.10	0.68
3:A1:35:SER:OG	7:b:329:GLU:OE1	2.12	0.68
7:b:374:LYS:O	7:b:378:THR:HG22	1.92	0.68
3:A1:454:ARG:NH2	3:A1:487:LEU:O	2.26	0.68
4:F1:275:ASP:OD2	4:F1:279:ARG:NH2	2.26	0.68
4:F1:256:LEU:HD21	4:F1:314:ARG:HB2	1.76	0.67
6:s:123:ASP:OD1	8:d:121:SER:OG	2.11	0.67
4:D1:68:VAL:HA	4:D1:79:THR:HG22	1.77	0.67
4:E1:54:ALA:O	4:E1:97:THR:OG1	2.10	0.67
3:B1:139:PHE:HE1	3:B1:152:LEU:HD13	1.60	0.67
3:A1:378:ASP:O	3:A1:404:ARG:NH1	2.28	0.67
7:b:282:GLU:N	7:b:282:GLU:OE1	2.28	0.67
6:s:143:ASP:O	8:d:99:ASN:ND2	2.28	0.67
3:C1:195:ARG:NH1	3:C1:376:ILE:O	2.29	0.66
4:D1:253:LEU:HD23	4:D1:311:LEU:HD13	1.75	0.66
3:B1:375:SER:O	4:E1:208:ARG:NH2	2.28	0.66
2:g1:46:MET:HE3	2:g1:259:MET:SD	2.36	0.66
4:F1:481:ASP:OD1	4:F1:482:LEU:N	2.28	0.66
4:F1:231:GLU:O	4:F1:232:SER:OG	2.12	0.66
3:A1:414:MET:HE3	3:A1:414:MET:HA	1.78	0.66
1:G1:152:ALA:HB2	1:G1:186:ILE:O	1.95	0.65
8:d:75:ILE:HD12	8:d:75:ILE:H	1.61	0.65
4:F1:98:GLY:C	4:F1:99:LEU:HD12	2.23	0.64
4:D1:416:SER:OG	4:D1:419:ASP:OD1	2.14	0.64
3:B1:208:ALA:N	9:B1:900:ATP:O2A	2.30	0.64
4:F1:452:ASN:OD1	4:F1:453:LEU:N	2.30	0.64
4:E1:382:ILE:HD12	4:E1:386:HIS:ND1	2.13	0.64
7:b:333:LEU:HG	7:b:334:ILE:HG23	1.80	0.64
1:G1:105:THR:HG22	1:G1:106:ASN:H	1.63	0.64
3:B1:378:ASP:OD2	4:E1:210:ARG:NE	2.30	0.64
8:d:82:GLU:O	8:d:86:VAL:HG12	1.97	0.64
4:E1:253:LEU:HD23	4:E1:311:LEU:HD13	1.77	0.64
2:g1:259:MET:HE2	2:g1:259:MET:HA	1.80	0.63
3:B1:57:THR:HG23	3:B1:58:GLU:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F1:389:VAL:O	4:F1:393:VAL:HG23	1.98	0.63
3:C1:67:ASP:OD1	4:D1:293:ARG:NH2	2.30	0.63
7:b:220:ASP:OD2	8:d:37:ILE:HD11	1.98	0.63
3:C1:68:GLY:O	3:C1:106:VAL:HG12	1.99	0.63
3:B1:446:GLN:O	3:B1:450:ASN:ND2	2.30	0.63
4:F1:210:ARG:NH2	4:F1:211:GLU:OE2	2.31	0.63
4:E1:235:ALA:C	4:E1:236:LEU:HD12	2.24	0.63
4:F1:363:ILE:HG23	4:F1:434:SER:HB3	1.80	0.63
4:F1:68:VAL:HA	4:F1:79:THR:HG22	1.81	0.63
3:C1:139:PHE:HE1	3:C1:152:LEU:HD22	1.63	0.63
8:d:86:VAL:HG13	8:d:87:ILE:H	1.62	0.63
1:G1:164:GLU:OE1	1:G1:178:VAL:HG21	1.98	0.63
2:g1:46:MET:SD	4:D1:410:LEU:HD21	2.40	0.62
4:F1:376:MET:HG3	4:F1:381:THR:HG21	1.80	0.62
4:E1:334:ASP:OD2	4:E1:356:ARG:NH1	2.32	0.62
4:D1:205:VAL:CG1	4:D1:251:VAL:HG13	2.29	0.62
3:A1:538:GLU:OE1	8:d:58:THR:HG22	2.00	0.62
4:D1:231:GLU:O	4:D1:232:SER:OG	2.11	0.62
3:B1:279:TYR:OH	3:B1:332:LEU:HD12	2.00	0.62
6:s:120:TYR:OH	7:b:211:HIS:ND1	2.25	0.62
3:B1:162:ILE:HD11	3:B1:286:GLU:OE1	2.01	0.61
3:A1:206:LYS:NZ	9:A1:900:ATP:O2B	2.27	0.61
4:D1:339:PRO:O	4:D1:343:THR:HG23	2.00	0.61
4:E1:112:ARG:NH2	4:E1:125:GLY:O	2.28	0.60
4:D1:152:LEU:HD13	4:D1:167:ARG:HG2	1.83	0.60
4:E1:377:LEU:HD12	4:E1:382:ILE:HD11	1.83	0.60
8:d:122:SER:O	8:d:125:LEU:N	2.34	0.60
3:C1:186:SER:O	3:C1:410:GLN:NE2	2.35	0.59
3:B1:127:ASP:OD1	3:B1:157:ARG:NH1	2.35	0.59
4:F1:303:THR:OG1	4:F1:307:ASP:OD2	2.18	0.59
3:C1:241:ARG:HG2	3:C1:266:THR:HG21	1.85	0.59
4:E1:141:SER:OG	4:E1:144:ASP:OD1	2.19	0.59
7:b:369:ILE:O	7:b:372:VAL:HG12	2.02	0.59
4:D1:112:ARG:NH2	4:D1:125:GLY:O	2.34	0.59
3:B1:107:LEU:HD13	3:B1:142:LEU:HD21	1.85	0.59
4:E1:68:VAL:HA	4:E1:79:THR:HG22	1.83	0.59
4:D1:235:ALA:C	4:D1:236:LEU:HD12	2.28	0.59
4:E1:225:ILE:HA	4:E1:232:SER:HA	1.83	0.59
8:d:54:ARG:O	8:d:58:THR:HG23	2.01	0.59
4:F1:235:ALA:C	4:F1:236:LEU:HD12	2.28	0.59
3:A1:201:ASP:O	3:A1:206:LYS:NZ	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:279:TYR:OH	3:C1:332:LEU:HD12	2.03	0.58
2:g1:26:LEU:HD12	2:g1:26:LEU:H	1.68	0.58
6:s:125:CYS:O	6:s:128:ILE:HG22	2.04	0.58
3:C1:139:PHE:CE1	3:C1:152:LEU:HD22	2.38	0.58
4:E1:300:TYR:OH	4:E1:338:ASP:OD2	2.16	0.58
3:B1:279:TYR:OH	3:B1:332:LEU:O	2.21	0.58
3:B1:186:SER:O	3:B1:410:GLN:NE2	2.37	0.58
3:A1:487:LEU:H	3:A1:487:LEU:HD23	1.69	0.57
4:D1:454:LYS:H	4:D1:454:LYS:HD2	1.70	0.57
3:A1:211:ILE:HD11	3:A1:247:LEU:HD11	1.87	0.57
4:F1:441:GLU:O	4:F1:445:GLY:N	2.36	0.57
3:C1:257:MET:O	3:C1:258:LYS:HG2	2.05	0.56
3:C1:501:GLU:O	3:C1:505:THR:HG23	2.04	0.56
3:B1:140:ASP:OD1	3:B1:144:ASN:N	2.36	0.56
3:B1:63:ILE:HD11	3:B1:73:PHE:HB2	1.86	0.56
3:A1:67:ASP:OD2	4:E1:293:ARG:NH2	2.38	0.56
4:E1:172:GLY:HA3	4:E1:348:LEU:HD13	1.87	0.56
1:G1:151:SER:O	1:G1:182:VAL:HG12	2.05	0.56
3:B1:209:ILE:O	3:B1:213:THR:HG23	2.05	0.56
3:B1:470:GLU:OE2	3:B1:515:ARG:NH2	2.38	0.56
4:F1:82:MET:HE2	4:F1:82:MET:HA	1.88	0.56
4:F1:301:GLN:OE1	4:F1:301:GLN:N	2.30	0.56
3:B1:461:GLN:NE2	3:B1:465:THR:O	2.37	0.56
4:F1:421:LEU:HD21	4:F1:425:ARG:NH1	2.21	0.56
3:A1:138:VAL:N	3:A1:147:ASP:OD2	2.36	0.56
7:b:315:ILE:O	7:b:319:VAL:HG23	2.06	0.55
4:D1:256:LEU:HD13	4:D1:315:ILE:HG12	1.86	0.55
3:A1:513:ARG:NH1	3:A1:524:ASP:OD1	2.36	0.55
4:E1:34:GLN:NE2	4:E1:41:ASP:OD2	2.37	0.55
5:i1:57:LEU:HD12	5:i1:58:LEU:N	2.21	0.55
3:B1:179:THR:HB	3:B1:213:THR:HG22	1.88	0.55
3:C1:83:MET:HE2	3:C1:126:VAL:HB	1.88	0.55
4:D1:239:GLY:HA3	4:D1:251:VAL:HG11	1.89	0.55
2:g1:261:ASN:OD1	2:g1:265:ASN:ND2	2.39	0.55
3:C1:86:PHE:HB3	3:C1:113:ILE:HG21	1.87	0.55
4:F1:103:VAL:HG11	4:F1:254:THR:HG23	1.86	0.55
3:A1:58:GLU:OE2	3:A1:76:THR:N	2.40	0.55
8:d:131:GLU:N	8:d:131:GLU:OE1	2.40	0.55
4:D1:376:MET:HG3	4:D1:381:THR:HG21	1.89	0.55
6:s:139:LEU:HD12	7:b:356:LEU:HD21	1.89	0.55
4:D1:82:MET:HE1	4:D1:250:ARG:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F1:135:ILE:HD12	4:F1:254:THR:HA	1.86	0.55
4:F1:385:GLU:O	4:F1:389:VAL:HG23	2.06	0.55
4:D1:205:VAL:HG12	4:D1:251:VAL:CG1	2.32	0.55
4:E1:67:GLU:OE2	4:E1:250:ARG:NH1	2.40	0.55
4:D1:406:ILE:HD11	4:D1:410:LEU:HD12	1.87	0.54
3:B1:441:LEU:HD13	3:B1:445:THR:HG21	1.88	0.54
3:B1:486:ALA:O	3:B1:544:LYS:N	2.33	0.54
3:A1:246:ASN:OD1	4:E1:147:THR:HG22	2.06	0.54
6:s:127:TYR:CE1	8:d:117:ILE:HG22	2.42	0.54
4:D1:441:GLU:O	4:D1:445:GLY:N	2.38	0.54
3:B1:485:ASP:OD1	3:B1:486:ALA:N	2.41	0.54
3:B1:52:GLN:HG2	3:B1:53:GLN:H	1.73	0.54
3:B1:139:PHE:CE1	3:B1:152:LEU:HD13	2.42	0.54
3:A1:206:LYS:HG2	3:A1:383:LEU:HD12	1.89	0.54
3:C1:375:SER:O	4:F1:241:MET:HE1	2.08	0.54
4:F1:275:ASP:O	4:F1:276:ASN:C	2.51	0.54
3:C1:163:LYS:NZ	4:F1:83:ASP:OD2	2.26	0.54
4:D1:266:GLU:N	4:D1:266:GLU:OE1	2.41	0.54
3:A1:239:GLN:NE2	3:A1:300:ASP:OD2	2.41	0.54
4:E1:236:LEU:O	4:E1:237:ILE:HD13	2.08	0.53
3:C1:532:ILE:HB	3:C1:533:PRO:HD3	1.90	0.53
4:D1:256:LEU:HD21	4:D1:314:ARG:HB2	1.90	0.53
4:F1:219:MET:O	4:F1:220:MET:HB2	2.08	0.53
4:F1:400:TYR:HE1	4:F1:423:VAL:HG13	1.74	0.53
3:A1:241:ARG:HG2	3:A1:266:THR:HG21	1.91	0.53
1:G1:56:SER:HB2	1:G1:61:LEU:HD11	1.89	0.53
1:G1:206:ARG:NE	7:b:305:ASP:OD2	2.42	0.53
3:A1:431:LEU:HD11	5:i:143:LYS:HD3	1.91	0.53
3:B1:83:MET:HE3	3:B1:126:VAL:HA	1.91	0.53
6:s:134:GLU:OE1	6:s:137:ARG:NH2	2.41	0.53
3:B1:34:LEU:HD12	3:B1:34:LEU:O	2.09	0.53
3:B1:527:GLU:O	3:B1:531:ILE:HG22	2.09	0.53
1:G1:141:LEU:O	1:G1:141:LEU:HD13	2.08	0.53
4:E1:80:ILE:N	4:E1:80:ILE:HD12	2.24	0.53
4:E1:110:LEU:HB3	4:E1:232:SER:O	2.09	0.53
1:G1:182:VAL:HG23	1:G1:182:VAL:O	2.09	0.52
4:F1:421:LEU:C	4:F1:421:LEU:HD23	2.34	0.52
8:d:87:ILE:O	8:d:88:SER:OG	2.16	0.52
3:B1:392:ILE:HG22	3:B1:392:ILE:O	2.09	0.52
4:D1:236:LEU:O	4:D1:237:ILE:HD13	2.09	0.52
3:C1:302:LEU:HD13	3:C1:302:LEU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D1:493:ALA:HB2	5:i1:57:LEU:HD11	1.92	0.52
3:B1:159:ARG:NH1	3:B1:162:ILE:HG22	2.24	0.52
4:E1:156:ILE:HA	4:E1:435:GLN:OE1	2.09	0.52
4:D1:208:ARG:NH2	3:A1:377:THR:O	2.42	0.52
4:D1:317:THR:HG23	4:D1:322:SER:HA	1.92	0.52
4:D1:172:GLY:HA3	4:D1:348:LEU:HD13	1.91	0.52
4:F1:449:ARG:NH2	4:F1:484:GLU:OE2	2.43	0.52
3:C1:543:LEU:N	3:C1:543:LEU:HD23	2.25	0.52
3:C1:69:ILE:HD12	3:C1:315:LEU:CB	2.40	0.52
8:d:30:ALA:HB3	8:d:31:PRO:HD3	1.92	0.52
3:A1:430:GLU:O	5:i1:40:SER:HB3	2.10	0.51
4:E1:304:LEU:HD23	4:E1:304:LEU:C	2.35	0.51
4:D1:189:ILE:O	4:D1:193:ALA:HB3	2.11	0.51
4:F1:376:MET:CG	4:F1:381:THR:HG21	2.39	0.51
3:C1:206:LYS:HG2	3:C1:383:LEU:HD12	1.91	0.51
3:A1:532:ILE:HB	3:A1:533:PRO:HD3	1.91	0.51
7:b:343:SER:O	7:b:347:ASN:ND2	2.37	0.51
3:C1:481:LYS:HE2	3:C1:481:LYS:HA	1.93	0.51
3:A1:241:ARG:CG	3:A1:266:THR:HG21	2.40	0.51
7:b:288:LEU:O	7:b:292:ILE:HD13	2.10	0.51
3:C1:113:ILE:HD12	3:C1:113:ILE:O	2.10	0.51
3:A1:266:THR:N	3:A1:269:ASP:OD2	2.43	0.51
4:D1:298:VAL:HG12	4:D1:298:VAL:O	2.11	0.51
3:B1:50:ILE:HD12	3:B1:50:ILE:O	2.11	0.51
4:D1:89:VAL:CG2	3:A1:77:LYS:HA	2.41	0.51
3:B1:383:LEU:HA	3:B1:395:ALA:O	2.11	0.50
3:B1:211:ILE:HD11	3:B1:247:LEU:HD11	1.93	0.50
3:A1:220:ALA:O	3:A1:223:THR:O	2.29	0.50
4:E1:113:ILE:HD11	4:E1:216:TYR:CD1	2.47	0.50
4:E1:271:LEU:HD23	4:E1:324:THR:HB	1.93	0.50
1:G1:183:ASP:N	1:G1:184:PRO:HD3	2.27	0.50
7:b:44:VAL:O	7:b:47:PHE:CD2	2.64	0.50
3:C1:65:ILE:HD13	3:C1:113:ILE:CD1	2.42	0.50
4:F1:34:GLN:HG2	4:F1:41:ASP:HB2	1.93	0.50
3:A1:37:GLY:O	3:A1:41:VAL:HG23	2.12	0.50
3:C1:98:GLU:HA	4:F1:34:GLN:HB2	1.92	0.50
3:C1:50:ILE:HG23	3:C1:50:ILE:O	2.11	0.50
3:A1:300:ASP:O	3:A1:301:ASP:C	2.54	0.50
1:G1:217:ILE:O	1:G1:218:SER:OG	2.22	0.49
4:E1:27:LYS:HD3	4:E1:27:LYS:O	2.12	0.49
4:E1:301:GLN:OE1	4:E1:301:GLN:N	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E1:329:ILE:HD12	4:E1:329:ILE:N	2.27	0.49
7:b:363:ASP:N	7:b:363:ASP:OD1	2.43	0.49
3:B1:114:LYS:NZ	4:F1:47:GLU:OE2	2.40	0.49
3:A1:83:MET:SD	3:A1:126:VAL:HG12	2.52	0.49
4:E1:328:ALA:C	4:E1:329:ILE:HD12	2.37	0.49
3:C1:165:PRO:O	3:C1:170:ARG:NH1	2.45	0.49
3:C1:211:ILE:HD11	3:C1:247:LEU:HD21	1.94	0.49
4:E1:131:LYS:C	4:E1:132:LEU:HD12	2.38	0.49
3:B1:416:LYS:H	3:B1:416:LYS:HD2	1.77	0.49
3:B1:433:ALA:O	3:B1:436:GLN:NE2	2.44	0.49
4:F1:225:ILE:HA	4:F1:232:SER:HA	1.94	0.49
7:b:360:PRO:HB2	7:b:362:LEU:HD11	1.94	0.49
4:F1:256:LEU:HD22	4:F1:311:LEU:CD1	2.34	0.49
4:F1:259:ALA:HB1	4:F1:270:VAL:HG11	1.94	0.49
4:F1:400:TYR:CE1	4:F1:423:VAL:HG13	2.48	0.49
3:C1:93:MET:HE1	3:C1:276:LEU:HD11	1.95	0.48
4:F1:494:LEU:C	4:F1:494:LEU:HD23	2.38	0.48
1:G1:184:PRO:HB2	1:G1:186:ILE:HG12	1.94	0.48
3:B1:111:ARG:O	4:F1:50:GLN:NE2	2.38	0.48
7:b:334:ILE:O	7:b:334:ILE:HG13	2.12	0.48
1:G1:51:LEU:HD22	1:G1:114:LEU:HD22	1.95	0.48
4:D1:166:ALA:HB2	4:D1:376:MET:HE3	1.96	0.48
3:B1:197:LEU:HD11	3:B1:358:ILE:CG1	2.43	0.48
4:F1:256:LEU:HD21	4:F1:314:ARG:CB	2.43	0.48
3:A1:134:MET:SD	3:A1:152:LEU:HD21	2.53	0.48
1:G1:113:ASN:N	1:G1:113:ASN:HD22	2.12	0.48
1:G1:149:ILE:CG2	1:G1:190:LEU:HD12	2.44	0.48
3:B1:50:ILE:HD12	3:B1:52:GLN:H	1.79	0.48
4:F1:114:MET:HE2	4:F1:237:ILE:HD12	1.96	0.48
4:E1:231:GLU:C	4:E1:232:SER:HG	2.16	0.48
4:E1:256:LEU:HD21	4:E1:314:ARG:HB2	1.94	0.48
4:E1:494:LEU:C	4:E1:494:LEU:HD23	2.39	0.48
1:G1:149:ILE:HD12	1:G1:149:ILE:N	2.29	0.48
4:D1:116:VAL:HG23	4:D1:251:VAL:HA	1.95	0.48
3:A1:314:LEU:HD21	3:A1:320:PRO:HB3	1.95	0.48
4:E1:276:ASN:HA	4:E1:328:ALA:O	2.13	0.48
4:D1:356:ARG:O	4:D1:359:THR:OG1	2.25	0.48
4:D1:361:LEU:HD21	5:i:1:39:LYS:HE2	1.95	0.48
3:B1:76:THR:HG22	3:B1:77:LYS:N	2.28	0.48
3:B1:392:ILE:HA	3:B1:460:LYS:HD3	1.96	0.48
3:C1:490:SER:O	3:C1:494:LYS:NZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D1:146:ALA:HB2	4:D1:319:GLN:CD	2.38	0.48
3:B1:173:VAL:O	3:B1:173:VAL:HG23	2.14	0.48
3:B1:412:LYS:HA	3:B1:415:LYS:HD3	1.96	0.48
1:G1:119:ILE:CD1	1:G1:124:LEU:HD22	2.44	0.47
3:C1:534:LEU:HD23	3:C1:534:LEU:C	2.39	0.47
4:F1:198:GLY:HA3	4:F1:269:ASP:O	2.14	0.47
1:G1:127:LEU:N	1:G1:128:PRO:HD2	2.30	0.47
3:C1:197:LEU:HD11	3:C1:358:ILE:CG1	2.44	0.47
4:D1:226:SER:H	4:D1:232:SER:HB3	1.79	0.47
4:F1:103:VAL:CG1	4:F1:135:ILE:HD11	2.44	0.47
1:G1:189:GLY:HA3	1:G1:202:SER:HA	1.96	0.47
3:C1:69:ILE:HD12	3:C1:315:LEU:HB3	1.96	0.47
3:C1:329:VAL:O	3:C1:332:LEU:HB3	2.14	0.47
3:B1:153:LYS:HG3	3:B1:153:LYS:O	2.15	0.47
3:A1:241:ARG:NH1	4:E1:140:PRO:O	2.46	0.47
3:B1:83:MET:HE2	3:B1:126:VAL:HG23	1.96	0.47
4:F1:418:GLU:O	4:F1:422:VAL:HG23	2.14	0.47
3:A1:365:VAL:HG11	3:A1:382:PHE:HE2	1.79	0.47
4:F1:243:GLU:O	4:F1:248:ARG:NH1	2.48	0.47
4:F1:356:ARG:O	4:F1:359:THR:OG1	2.26	0.47
4:E1:492:ASP:O	4:E1:495:LYS:HG2	2.15	0.47
7:b:40:TYR:O	7:b:44:VAL:HG23	2.13	0.47
1:G1:189:GLY:C	1:G1:190:LEU:HD22	2.39	0.47
4:D1:263:ARG:NH1	4:D1:316:THR:O	2.48	0.47
3:B1:407:SER:HG	3:B1:415:LYS:HZ2	1.54	0.47
4:F1:131:LYS:C	4:F1:132:LEU:HD12	2.40	0.47
3:A1:197:LEU:HD11	3:A1:358:ILE:CG1	2.44	0.47
4:E1:149:ALA:C	4:E1:376:MET:HE1	2.40	0.47
4:E1:240:GLN:OE1	4:E1:240:GLN:HA	2.15	0.47
3:A1:63:ILE:N	3:A1:71:ARG:O	2.46	0.47
8:d:92:LEU:C	8:d:92:LEU:HD23	2.40	0.47
3:B1:55:ASP:CG	3:B1:57:THR:HG22	2.39	0.47
4:F1:377:LEU:HD23	4:F1:377:LEU:O	2.15	0.47
7:b:242:LEU:HD13	8:d:78:ILE:CD1	2.45	0.47
1:G1:151:SER:HB2	1:G1:190:LEU:HD13	1.97	0.46
3:C1:491:GLU:OE2	3:C1:542:LYS:N	2.47	0.46
4:D1:470:GLU:O	5:i1:53:ALA:HB1	2.14	0.46
3:B1:83:MET:O	3:B1:122:THR:OG1	2.31	0.46
3:A1:279:TYR:OH	3:A1:332:LEU:HD12	2.15	0.46
4:E1:421:LEU:HD23	4:E1:421:LEU:C	2.40	0.46
1:G1:217:ILE:HG23	3:A1:46:LYS:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A1:277:ALA:HB3	3:A1:278:PRO:HD3	1.96	0.46
1:G1:127:LEU:HD13	1:G1:127:LEU:C	2.41	0.46
3:C1:58:GLU:HG2	3:C1:58:GLU:O	2.15	0.46
4:F1:391:ARG:NH1	4:F1:394:GLN:OE1	2.49	0.46
3:A1:130:ILE:HD12	3:A1:287:PHE:HB2	1.98	0.46
7:b:336:LEU:HD12	7:b:336:LEU:H	1.80	0.46
3:C1:182:LYS:NZ	3:C1:458:MET:O	2.37	0.46
3:C1:211:ILE:CD1	3:C1:247:LEU:HD21	2.46	0.46
3:C1:340:ALA:HB1	3:C1:352:LEU:O	2.15	0.46
3:B1:45:GLU:HA	3:B1:48:LYS:HE2	1.97	0.46
4:F1:419:ASP:O	4:F1:423:VAL:HG23	2.15	0.46
3:A1:458:MET:SD	3:A1:475:ILE:HG22	2.55	0.46
4:E1:103:VAL:HG11	4:E1:254:THR:HG23	1.96	0.46
4:D1:172:GLY:C	4:D1:173:LEU:HD12	2.41	0.46
3:C1:215:LEU:HA	3:C1:256:CYS:SG	2.56	0.46
3:B1:478:ALA:HB2	3:B1:532:ILE:HD13	1.98	0.46
3:A1:479:GLY:HA2	3:A1:484:LEU:HD12	1.98	0.46
3:A1:481:LYS:HE2	3:A1:481:LYS:HA	1.98	0.46
1:G1:161:GLN:NE2	1:G1:165:GLN:OE1	2.48	0.46
2:g1:38:SER:O	2:g1:42:ILE:HD13	2.16	0.45
3:C1:421:LEU:O	3:C1:425:LEU:HD23	2.16	0.45
4:D1:276:ASN:HA	4:D1:328:ALA:O	2.16	0.45
4:F1:139:ALA:HB1	4:F1:140:PRO:HD2	1.96	0.45
4:E1:92:GLN:HG3	4:E1:93:PRO:HD2	1.98	0.45
3:B1:72:VAL:HG12	3:B1:73:PHE:N	2.32	0.45
3:B1:334:SER:HB2	4:E1:241:MET:HB3	1.97	0.45
3:B1:487:LEU:HD21	3:B1:536:ILE:HG23	1.99	0.45
4:F1:219:MET:HB3	4:F1:225:ILE:HG12	1.98	0.45
3:A1:197:LEU:HD11	3:A1:358:ILE:HG12	1.98	0.45
4:E1:339:PRO:O	4:E1:343:THR:HG23	2.16	0.45
3:C1:76:THR:HG22	3:C1:77:LYS:H	1.81	0.45
4:F1:114:MET:HE2	4:F1:237:ILE:CD1	2.47	0.45
4:F1:101:ILE:O	4:F1:135:ILE:HG12	2.16	0.45
4:F1:173:LEU:HD23	4:F1:173:LEU:C	2.41	0.45
6:s:144:LEU:HD21	7:b:241:ALA:HA	1.97	0.45
8:d:86:VAL:HG13	8:d:87:ILE:N	2.29	0.45
3:B1:203:GLN:HA	9:B1:900:ATP:O1B	2.17	0.45
3:C1:434:PHE:HB3	3:C1:441:LEU:HD11	1.98	0.45
4:F1:377:LEU:HD23	4:F1:377:LEU:C	2.42	0.45
7:b:353:LYS:O	7:b:357:GLU:HG2	2.17	0.45
8:d:117:ILE:HD12	8:d:118:SER:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C1:83:MET:HE1	3:C1:107:LEU:HD11	1.97	0.45
4:E1:62:HIS:O	4:E1:63:ARG:C	2.59	0.45
3:C1:461:GLN:NE2	3:C1:465:THR:O	2.49	0.45
4:D1:103:VAL:HG11	4:D1:254:THR:HG23	1.98	0.45
4:D1:187:GLU:HG2	4:D1:437:PHE:CD1	2.51	0.45
4:D1:241:MET:HE1	3:A1:376:ILE:HA	1.99	0.45
6:s:123:ASP:OD1	8:d:122:SER:OG	2.33	0.45
6:s:130:VAL:HG13	6:s:131:ALA:H	1.82	0.45
3:C1:167:ILE:HD11	4:F1:240:GLN:NE2	2.32	0.45
4:F1:156:ILE:HD12	4:F1:156:ILE:N	2.32	0.45
3:A1:96:ASN:OD1	3:A1:318:ARG:NH2	2.40	0.45
4:D1:262:PHE:O	4:D1:266:GLU:O	2.35	0.45
3:B1:443:ALA:O	3:B1:444:LYS:HB3	2.17	0.45
4:E1:256:LEU:HD13	4:E1:315:ILE:HG12	1.97	0.45
1:G1:165:GLN:HA	1:G1:165:GLN:NE2	2.32	0.44
1:G1:206:ARG:O	1:G1:210:LEU:HD13	2.17	0.44
3:C1:510:LEU:HD21	3:C1:524:ASP:HB3	1.98	0.44
3:A1:62:VAL:HG23	3:A1:62:VAL:O	2.15	0.44
3:C1:125:ILE:HG22	3:C1:126:VAL:N	2.33	0.44
3:C1:195:ARG:HD3	3:C1:337:LEU:O	2.17	0.44
4:E1:67:GLU:OE2	4:E1:250:ARG:NE	2.50	0.44
7:b:352:ARG:O	7:b:356:LEU:HD23	2.16	0.44
3:A1:62:VAL:HG23	3:A1:115:GLU:HA	1.99	0.44
3:A1:107:LEU:HD23	3:A1:272:PRO:HB2	1.99	0.44
3:A1:450:ASN:O	3:A1:454:ARG:HG2	2.17	0.44
3:A1:510:LEU:HD23	3:A1:510:LEU:C	2.42	0.44
4:E1:356:ARG:O	4:E1:359:THR:OG1	2.30	0.44
1:G1:200:ASP:OD1	1:G1:202:SER:OG	2.29	0.44
4:F1:423:VAL:O	4:F1:427:ARG:HG3	2.17	0.44
6:s:117:ALA:HB2	8:d:44:LEU:HD11	1.98	0.44
3:B1:76:THR:HG22	3:B1:77:LYS:H	1.83	0.44
4:F1:147:THR:O	4:F1:148:SER:OG	2.32	0.44
3:A1:472:GLN:O	3:A1:476:ILE:HG12	2.18	0.44
4:E1:253:LEU:CD2	4:E1:311:LEU:HD13	2.48	0.44
4:E1:410:LEU:HD12	4:E1:410:LEU:O	2.16	0.44
6:s:130:VAL:HG13	6:s:131:ALA:N	2.32	0.44
8:d:86:VAL:HG22	8:d:87:ILE:HG22	1.99	0.44
1:G1:190:LEU:HD21	7:b:288:LEU:HD23	1.99	0.44
4:D1:271:LEU:HD23	4:D1:324:THR:HB	2.00	0.44
4:D1:304:LEU:C	4:D1:304:LEU:HD23	2.43	0.44
3:B1:43:LEU:O	3:B1:47:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B1:507:HIS:NE2	3:B1:531:ILE:HD12	2.32	0.44
4:F1:418:GLU:OE1	4:F1:418:GLU:N	2.37	0.44
3:A1:397:ASN:CG	3:A1:400:LEU:HD23	2.42	0.44
4:E1:354:LEU:HA	4:E1:366:ALA:O	2.18	0.44
1:G1:148:THR:C	1:G1:149:ILE:HD12	2.43	0.44
1:G1:159:GLU:OE1	1:G1:159:GLU:HA	2.18	0.44
3:C1:431:LEU:HD11	3:C1:448:GLN:OE1	2.17	0.44
4:D1:225:ILE:HA	4:D1:232:SER:HA	2.00	0.44
3:B1:458:MET:SD	3:B1:475:ILE:HG22	2.57	0.44
4:F1:158:VAL:HG11	4:F1:367:VAL:HG21	1.99	0.44
3:A1:40:SER:OG	7:b:319:VAL:HG22	2.18	0.44
4:E1:219:MET:HG3	4:E1:224:VAL:HB	1.99	0.44
6:s:136:VAL:HG22	7:b:356:LEU:HD12	1.99	0.44
1:G1:115:LEU:O	1:G1:119:ILE:HG12	2.17	0.44
4:E1:153:VAL:HG23	4:E1:153:VAL:O	2.18	0.44
4:E1:376:MET:HE3	4:E1:381:THR:CG2	2.48	0.44
1:G1:145:GLU:N	1:G1:145:GLU:OE1	2.51	0.44
3:C1:302:LEU:HD13	3:C1:302:LEU:C	2.43	0.44
4:D1:301:GLN:OE1	4:D1:301:GLN:N	2.34	0.44
4:D1:329:ILE:N	4:D1:329:ILE:HD12	2.33	0.44
4:F1:240:GLN:HA	4:F1:240:GLN:OE1	2.18	0.44
4:F1:335:ASP:OD1	4:F1:337:THR:OG1	2.33	0.44
4:F1:471:TYR:HB3	4:F1:472:PRO:HD2	2.00	0.44
7:b:356:LEU:O	7:b:379:TRP:NE1	2.51	0.44
1:G1:164:GLU:OE1	1:G1:164:GLU:HA	2.18	0.43
3:B1:130:ILE:HD13	3:B1:158:ALA:HB2	2.00	0.43
4:F1:276:ASN:HD21	4:F1:279:ARG:CZ	2.31	0.43
3:A1:442:ASP:OD1	3:A1:443:ALA:N	2.50	0.43
6:s:138:ILE:HG23	8:d:106:GLU:CB	2.49	0.43
3:C1:203:GLN:CD	4:D1:373:THR:HG21	2.43	0.43
3:C1:392:ILE:C	3:C1:393:ARG:HD2	2.43	0.43
3:B1:376:ILE:HA	4:E1:241:MET:HE1	2.00	0.43
3:B1:472:GLN:O	3:B1:476:ILE:HG13	2.18	0.43
3:A1:140:ASP:OD1	3:A1:144:ASN:N	2.51	0.43
6:s:145:ILE:HD12	6:s:145:ILE:C	2.43	0.43
7:b:248:ALA:O	7:b:252:GLU:HG3	2.18	0.43
7:b:362:LEU:HD12	7:b:362:LEU:N	2.33	0.43
8:d:60:LEU:C	8:d:60:LEU:HD13	2.42	0.43
3:C1:155:THR:HB	3:C1:156:GLN:OE1	2.18	0.43
4:D1:194:LYS:HD3	4:D1:222:SER:OG	2.18	0.43
3:B1:417:ILE:CG2	3:B1:476:ILE:HG22	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E1:385:GLU:O	4:E1:389:VAL:HG23	2.18	0.43
4:E1:423:VAL:O	4:E1:427:ARG:HG2	2.18	0.43
8:d:44:LEU:HD13	8:d:44:LEU:C	2.44	0.43
4:D1:113:ILE:HD11	4:D1:216:TYR:CD1	2.54	0.43
4:D1:228:LYS:HD3	4:D1:229:GLU:O	2.19	0.43
3:B1:365:VAL:HG12	3:B1:365:VAL:O	2.18	0.43
3:A1:182:LYS:NZ	3:A1:458:MET:O	2.28	0.43
3:A1:427:THR:O	3:A1:431:LEU:HD13	2.18	0.43
6:s:131:ALA:HB1	7:b:229:GLU:HG2	2.01	0.43
3:C1:76:THR:HG22	3:C1:77:LYS:N	2.33	0.43
4:D1:380:ILE:N	4:D1:380:ILE:HD12	2.34	0.43
3:B1:277:ALA:HB3	3:B1:278:PRO:HD3	2.00	0.43
3:A1:125:ILE:HG22	3:A1:126:VAL:N	2.33	0.43
4:E1:425:ARG:O	4:E1:429:VAL:HG23	2.18	0.43
3:C1:475:ILE:HD13	3:C1:500:LEU:HD21	2.00	0.43
4:D1:354:LEU:HA	4:D1:366:ALA:O	2.18	0.43
3:B1:329:VAL:O	3:B1:332:LEU:HB3	2.19	0.43
4:F1:226:SER:H	4:F1:232:SER:HB3	1.83	0.43
3:A1:83:MET:HG2	3:A1:126:VAL:HG12	2.01	0.43
1:G1:203:LEU:C	1:G1:203:LEU:HD23	2.44	0.43
3:A1:55:ASP:O	3:A1:57:THR:HG23	2.18	0.43
7:b:353:LYS:HA	7:b:353:LYS:HE2	2.00	0.43
4:D1:242:ASN:OD1	4:D1:242:ASN:N	2.51	0.43
3:A1:344:ASN:OD1	3:A1:347:LEU:HD13	2.19	0.43
7:b:361:LYS:O	7:b:361:LYS:HG3	2.19	0.43
3:B1:75:LEU:HD21	3:B1:84:VAL:HG11	2.01	0.43
4:F1:110:LEU:HB3	4:F1:232:SER:O	2.18	0.43
7:b:42:ALA:HB3	8:d:114:SER:HB2	2.01	0.43
3:B1:436:GLN:HG2	3:B1:437:PHE:CD1	2.54	0.42
3:A1:43:LEU:HD21	7:b:264:ILE:HD11	2.00	0.42
3:A1:378:ASP:O	3:A1:404:ARG:HD3	2.19	0.42
3:C1:277:ALA:HB3	3:C1:278:PRO:HD3	2.01	0.42
4:D1:446:ILE:HG13	4:D1:447:PRO:HD2	2.00	0.42
4:F1:486:LEU:O	4:F1:490:ARG:HG3	2.19	0.42
3:A1:147:ASP:HB3	3:A1:149:LEU:HG	2.00	0.42
4:E1:277:ILE:O	4:E1:280:PHE:HB3	2.18	0.42
3:C1:168:ILE:HB	3:C1:169:PRO:HD3	2.01	0.42
3:C1:420:ASN:O	3:C1:424:THR:HG23	2.19	0.42
3:C1:457:GLU:O	3:C1:493:LEU:HD21	2.20	0.42
4:D1:355:ASN:O	4:D1:366:ALA:HB1	2.18	0.42
3:B1:46:LYS:O	3:B1:50:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B1:246:ASN:O	3:B1:250:ILE:HD13	2.20	0.42
4:F1:104:PRO:HB2	4:F1:129:ALA:HB2	2.00	0.42
4:F1:113:ILE:HD11	4:F1:216:TYR:CD1	2.54	0.42
3:A1:63:ILE:HD11	3:A1:73:PHE:HB2	2.02	0.42
4:E1:378:ASP:O	4:E1:382:ILE:HG12	2.19	0.42
2:g1:255:ARG:O	2:g1:259:MET:HG2	2.20	0.42
3:C1:268:SER:HB3	4:D1:313:GLU:HG3	2.01	0.42
4:D1:395:LYS:NZ	4:D1:395:LYS:HB3	2.34	0.42
4:F1:82:MET:HE1	4:F1:246:GLY:C	2.44	0.42
4:F1:459:SER:OG	4:F1:482:LEU:HB2	2.19	0.42
3:A1:58:GLU:OE2	3:A1:76:THR:HG22	2.19	0.42
4:E1:405:ASP:OD2	5:i1:28:THR:HA	2.19	0.42
8:d:72:VAL:HG13	8:d:72:VAL:O	2.20	0.42
3:C1:454:ARG:HH22	3:C1:488:VAL:HA	1.85	0.42
3:C1:534:LEU:HD23	3:C1:534:LEU:O	2.18	0.42
3:A1:83:MET:CG	3:A1:126:VAL:HG12	2.49	0.42
3:A1:454:ARG:HH22	3:A1:488:VAL:HA	1.84	0.42
4:E1:60:THR:HG23	4:E1:92:GLN:HE22	1.84	0.42
1:G1:187:LEU:N	1:G1:187:LEU:HD12	2.34	0.42
7:b:33:TYR:O	7:b:37:ARG:HG2	2.20	0.42
7:b:234:GLN:OE1	8:d:104:ILE:HD12	2.20	0.42
4:D1:340:ALA:HB3	4:D1:341:PRO:CD	2.50	0.42
3:B1:98:GLU:HA	4:E1:34:GLN:HB2	2.01	0.42
4:E1:340:ALA:HB3	4:E1:341:PRO:CD	2.50	0.42
3:C1:510:LEU:HD13	3:C1:510:LEU:C	2.45	0.42
3:B1:201:ASP:O	3:B1:206:LYS:NZ	2.51	0.42
4:F1:116:VAL:HG13	4:F1:117:ILE:HG23	2.02	0.42
4:F1:157:LYS:HG2	4:F1:451:VAL:HG11	2.01	0.42
4:F1:270:VAL:HG12	4:F1:271:LEU:N	2.35	0.42
4:F1:396:LEU:CD2	4:F1:426:ALA:HB2	2.49	0.42
3:A1:383:LEU:HA	3:A1:395:ALA:O	2.19	0.42
1:G1:199:LEU:HD13	1:G1:199:LEU:C	2.45	0.42
1:G1:208:ASN:O	1:G1:212:THR:HG23	2.20	0.42
3:C1:301:ASP:HB3	3:C1:304:LYS:HG3	2.02	0.42
3:C1:378:ASP:O	3:C1:404:ARG:HG2	2.19	0.42
4:D1:135:ILE:HA	4:D1:257:THR:OG1	2.20	0.42
4:F1:438:PHE:O	4:F1:441:GLU:HG2	2.20	0.42
3:C1:329:VAL:HG13	3:C1:330:PHE:N	2.35	0.42
3:C1:411:ILE:O	3:C1:415:LYS:HG3	2.20	0.42
3:B1:484:LEU:HD12	3:B1:484:LEU:N	2.34	0.42
4:E1:56:GLU:OE2	4:E1:63:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B1:179:THR:CB	3:B1:213:THR:HG22	2.49	0.41
4:F1:271:LEU:HD12	4:F1:324:THR:O	2.20	0.41
3:A1:65:ILE:HD12	3:A1:69:ILE:O	2.19	0.41
6:s:145:ILE:O	8:d:96:VAL:HG22	2.20	0.41
7:b:336:LEU:HD12	7:b:336:LEU:N	2.34	0.41
3:C1:65:ILE:HD13	3:C1:113:ILE:HD12	2.02	0.41
4:F1:132:LEU:HD12	4:F1:132:LEU:N	2.34	0.41
3:A1:397:ASN:ND2	3:A1:400:LEU:HD23	2.35	0.41
2:g1:259:MET:HE2	2:g1:259:MET:CA	2.50	0.41
3:C1:302:LEU:HD11	3:C1:333:HIS:NE2	2.34	0.41
4:D1:110:LEU:HB3	4:D1:232:SER:O	2.20	0.41
4:D1:318:THR:OG1	4:D1:319:GLN:N	2.53	0.41
4:D1:363:ILE:N	4:D1:363:ILE:HD12	2.35	0.41
3:B1:393:ARG:HD3	9:B1:900:ATP:C4	2.56	0.41
4:E1:421:LEU:HD23	4:E1:421:LEU:O	2.20	0.41
4:D1:236:LEU:HD12	4:D1:236:LEU:N	2.36	0.41
3:B1:34:LEU:HD12	3:B1:34:LEU:C	2.46	0.41
3:B1:168:ILE:N	3:B1:169:PRO:CD	2.84	0.41
3:B1:443:ALA:C	3:B1:445:THR:H	2.28	0.41
4:F1:284:CYS:O	4:F1:287:VAL:HG22	2.21	0.41
6:s:138:ILE:HG23	8:d:106:GLU:HB2	2.02	0.41
3:A1:168:ILE:HB	3:A1:169:PRO:HD3	2.02	0.41
7:b:290:SER:OG	7:b:300:MET:HE1	2.20	0.41
4:D1:34:GLN:HB3	4:D1:41:ASP:HB2	2.03	0.41
4:D1:261:TYR:CE1	4:D1:265:GLU:HG3	2.56	0.41
3:B1:315:LEU:CD2	4:F1:293:ARG:HD3	2.51	0.41
3:B1:320:PRO:HB2	3:B1:324:ALA:HA	2.02	0.41
4:F1:103:VAL:HG13	4:F1:135:ILE:HD11	2.02	0.41
4:F1:222:SER:HB2	4:F1:439:MET:HE3	2.01	0.41
6:s:132:ASN:O	6:s:136:VAL:HG23	2.21	0.41
1:G1:206:ARG:HD2	3:A1:52:GLN:OE1	2.20	0.41
3:C1:472:GLN:O	3:C1:476:ILE:HG12	2.21	0.41
3:C1:526:ASN:O	3:C1:530:THR:HG23	2.20	0.41
4:F1:407:ILE:CG2	4:F1:415:LEU:HD11	2.50	0.41
3:A1:534:LEU:O	3:A1:538:GLU:HG2	2.20	0.41
7:b:234:GLN:O	7:b:238:THR:HG22	2.21	0.41
7:b:279:LYS:O	7:b:279:LYS:HG2	2.21	0.41
7:b:337:THR:OG1	7:b:340:GLN:HB2	2.20	0.41
3:B1:160:VAL:HG11	3:B1:276:LEU:HD11	2.02	0.41
3:B1:241:ARG:HE	3:B1:266:THR:HG21	1.86	0.41
7:b:233:LEU:C	7:b:233:LEU:HD23	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G1:105:THR:HG22	1:G1:106:ASN:N	2.32	0.41
3:C1:246:ASN:OD1	4:D1:147:THR:HG21	2.20	0.41
3:C1:372:ASN:O	3:C1:376:ILE:HG13	2.21	0.41
4:D1:365:PRO:HD3	4:D1:437:PHE:CZ	2.55	0.41
4:D1:425:ARG:O	4:D1:429:VAL:HG23	2.21	0.41
3:B1:113:ILE:HG22	3:B1:114:LYS:N	2.36	0.41
3:B1:137:ARG:NH2	3:B1:150:GLY:O	2.37	0.41
3:B1:493:LEU:N	3:B1:493:LEU:HD12	2.36	0.41
4:F1:263:ARG:HD3	4:F1:323:ILE:HG13	2.02	0.41
4:F1:357:GLY:O	4:F1:361:LEU:HD13	2.21	0.41
3:A1:154:THR:HG22	3:A1:155:THR:N	2.36	0.41
4:E1:132:LEU:HD12	4:E1:132:LEU:N	2.35	0.41
4:E1:168:GLY:O	4:E1:317:THR:OG1	2.29	0.41
7:b:244:ILE:HG13	7:b:344:ILE:CG2	2.50	0.41
8:d:113:ILE:N	8:d:113:ILE:HD12	2.36	0.41
3:C1:78:VAL:HG23	3:C1:82:GLU:OE1	2.21	0.41
3:C1:398:VAL:HG23	3:C1:429:ARG:NH1	2.36	0.41
3:C1:450:ASN:O	3:C1:454:ARG:HG2	2.21	0.41
4:D1:286:GLU:HG2	3:A1:327:GLY:O	2.21	0.41
4:D1:438:PHE:O	4:D1:441:GLU:HG3	2.20	0.41
4:F1:248:ARG:NH2	4:F1:286:GLU:OE1	2.53	0.41
4:F1:276:ASN:HA	4:F1:328:ALA:HB3	2.03	0.41
3:A1:501:GLU:O	3:A1:505:THR:HG23	2.21	0.41
4:E1:386:HIS:CD2	4:E1:457:ILE:HD11	2.56	0.41
4:E1:433:LEU:HD23	4:E1:460:PHE:HZ	1.86	0.41
7:b:271:ILE:HD11	7:b:311:ILE:CD1	2.51	0.41
3:C1:414:MET:O	3:C1:415:LYS:C	2.64	0.40
4:D1:116:VAL:HG13	4:D1:117:ILE:HG23	2.02	0.40
3:B1:128:VAL:HG12	3:B1:142:LEU:O	2.21	0.40
4:F1:276:ASN:HD21	4:F1:279:ARG:NH1	2.19	0.40
3:A1:171:GLN:HG2	3:A1:172:SER:N	2.36	0.40
4:E1:471:TYR:HB3	4:E1:472:PRO:HD2	2.03	0.40
2:g1:57:GLU:O	2:g1:61:LEU:N	2.47	0.40
3:C1:134:MET:HE1	3:C1:284:ILE:HD13	2.02	0.40
4:D1:207:GLU:HA	4:D1:207:GLU:OE1	2.20	0.40
4:D1:277:ILE:O	4:D1:280:PHE:HB3	2.21	0.40
8:d:33:ASN:OD1	8:d:34:GLN:HG3	2.21	0.40
3:C1:57:THR:O	3:C1:58:GLU:HB3	2.22	0.40
4:D1:296:SER:OG	4:D1:297:ALA:N	2.52	0.40
3:B1:282:CYS:O	3:B1:286:GLU:HG3	2.22	0.40
4:F1:396:LEU:O	4:F1:396:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A1:268:SER:HB3	4:E1:313:GLU:HG3	2.04	0.40
6:s:144:LEU:C	6:s:145:ILE:HG13	2.46	0.40
3:B1:225:ASP:OD2	3:B1:228:LYS:HD3	2.22	0.40
4:F1:219:MET:C	4:F1:221:ASP:H	2.29	0.40
4:F1:259:ALA:CB	4:F1:270:VAL:HG11	2.52	0.40
4:F1:384:GLU:O	4:F1:388:THR:HG23	2.21	0.40
3:A1:138:VAL:HB	3:A1:147:ASP:OD1	2.21	0.40
7:b:362:LEU:CD2	8:d:63:LEU:HD23	2.51	0.40
8:d:44:LEU:HD13	8:d:44:LEU:O	2.21	0.40
8:d:125:LEU:HD23	8:d:125:LEU:C	2.46	0.40
4:D1:313:GLU:OE1	4:D1:313:GLU:HA	2.21	0.40
3:B1:70:ALA:HB3	3:B1:104:VAL:HG13	2.04	0.40
3:A1:329:VAL:O	3:A1:332:LEU:HB3	2.22	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	G1	186/219 (85%)	171 (92%)	15 (8%)	0	100	100
2	g1	86/299 (29%)	84 (98%)	2 (2%)	0	100	100
3	A1	510/546 (93%)	501 (98%)	9 (2%)	0	100	100
3	B1	509/546 (93%)	495 (97%)	14 (3%)	0	100	100
3	C1	511/546 (94%)	496 (97%)	15 (3%)	0	100	100
4	D1	468/497 (94%)	453 (97%)	15 (3%)	0	100	100
4	E1	468/497 (94%)	449 (96%)	19 (4%)	0	100	100
4	F1	467/497 (94%)	444 (95%)	23 (5%)	0	100	100
5	i1	34/108 (32%)	34 (100%)	0	0	100	100
6	s	29/145 (20%)	28 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	b	201/381 (53%)	192 (96%)	9 (4%)	0	100	100
8	d	101/234 (43%)	92 (91%)	9 (9%)	0	100	100
All	All	3570/4515 (79%)	3439 (96%)	131 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G1	166/195 (85%)	163 (98%)	3 (2%)	51	80
2	g1	73/254 (29%)	72 (99%)	1 (1%)	59	85
3	A1	422/453 (93%)	422 (100%)	0	100	100
3	B1	422/453 (93%)	420 (100%)	2 (0%)	81	93
3	C1	424/453 (94%)	423 (100%)	1 (0%)	87	96
4	D1	381/402 (95%)	381 (100%)	0	100	100
4	E1	381/402 (95%)	381 (100%)	0	100	100
4	F1	380/402 (94%)	379 (100%)	1 (0%)	86	96
5	i1	35/101 (35%)	35 (100%)	0	100	100
6	s	26/131 (20%)	26 (100%)	0	100	100
7	b	173/331 (52%)	173 (100%)	0	100	100
8	d	95/206 (46%)	95 (100%)	0	100	100
All	All	2978/3783 (79%)	2970 (100%)	8 (0%)	84	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G1	154	GLU
1	G1	163	VAL
1	G1	165	GLN
2	g1	298	ILE

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Mol	Chain	Res	Type
3	C1	302	LEU
3	B1	65	ILE
3	B1	300	ASP
4	F1	327	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	G1	106	ASN
1	G1	113	ASN
1	G1	196	ASN
3	C1	526	ASN
4	D1	196	HIS
3	B1	216	ASN
3	B1	502	HIS
3	B1	506	ASN
3	A1	333	HIS
4	E1	190	ASN
4	E1	217	HIS
4	E1	347	HIS
4	E1	452	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 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\# Z > 2$
11	ADP	D1	900	10	28,29,29	3.43	12 (42%)	43,45,45	3.19	14 (32%)
9	ATP	A1	900	10	32,33,33	3.47	12 (37%)	48,52,52	2.18	12 (25%)
9	ATP	C1	900	10	32,33,33	3.48	12 (37%)	48,52,52	2.07	12 (25%)
9	ATP	B1	900	10	32,33,33	3.49	12 (37%)	48,52,52	2.26	13 (27%)
11	ADP	E1	900	10	28,29,29	3.42	11 (39%)	43,45,45	3.19	16 (37%)

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
11	ADP	D1	900	10	-	4/16/32/32	0/3/3/3
9	ATP	A1	900	10	-	6/22/38/38	0/3/3/3
9	ATP	C1	900	10	-	6/22/38/38	0/3/3/3
9	ATP	B1	900	10	-	5/22/38/38	0/3/3/3
11	ADP	E1	900	10	-	2/16/32/32	0/3/3/3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D1	900	ADP	C2'-C3'	-10.96	1.23	1.53
11	E1	900	ADP	C2'-C3'	-10.77	1.24	1.53
9	C1	900	ATP	C3'-C4'	-9.62	1.28	1.53
9	B1	900	ATP	C3'-C4'	-9.62	1.28	1.53
9	A1	900	ATP	C3'-C4'	-9.51	1.28	1.53
9	A1	900	ATP	C2'-C1'	-8.42	1.27	1.53
9	B1	900	ATP	C2'-C1'	-8.33	1.27	1.53
9	C1	900	ATP	C2'-C1'	-8.19	1.27	1.53
11	E1	900	ADP	O4'-C4'	-6.61	1.30	1.45
11	D1	900	ADP	O4'-C4'	-6.28	1.31	1.45
9	C1	900	ATP	O4'-C1'	6.27	1.56	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A1	900	ATP	O4'-C1'	6.21	1.56	1.42
9	B1	900	ATP	O4'-C1'	6.15	1.56	1.42
11	D1	900	ADP	C3'-C4'	5.79	1.67	1.53
9	C1	900	ATP	PA-O3A	5.59	1.65	1.59
9	C1	900	ATP	PB-O3A	5.57	1.65	1.59
9	B1	900	ATP	PB-O3A	5.56	1.65	1.59
11	E1	900	ADP	C3'-C4'	5.46	1.66	1.53
9	B1	900	ATP	PA-O3A	5.30	1.65	1.59
9	A1	900	ATP	PA-O3A	5.25	1.65	1.59
9	B1	900	ATP	PB-O3B	5.18	1.65	1.59
9	A1	900	ATP	PB-O3A	5.16	1.65	1.59
11	D1	900	ADP	C1'-N9	-4.86	1.32	1.46
11	E1	900	ADP	C1'-N9	-4.83	1.33	1.46
9	C1	900	ATP	PB-O3B	4.81	1.64	1.59
9	A1	900	ATP	PB-O3B	4.75	1.64	1.59
9	B1	900	ATP	C2'-C3'	4.64	1.65	1.53
9	A1	900	ATP	C2'-C3'	4.60	1.65	1.53
9	A1	900	ATP	O4'-C4'	4.57	1.55	1.45
9	C1	900	ATP	C2'-C3'	4.46	1.65	1.53
9	B1	900	ATP	O4'-C4'	4.44	1.54	1.45
9	C1	900	ATP	O4'-C4'	4.39	1.54	1.45
9	B1	900	ATP	C6-N6	4.37	1.45	1.34
9	A1	900	ATP	C6-N6	4.36	1.45	1.34
11	D1	900	ADP	O4'-C1'	4.36	1.52	1.42
11	E1	900	ADP	C6-N6	4.35	1.45	1.34
11	E1	900	ADP	O4'-C1'	4.33	1.52	1.42
11	D1	900	ADP	C6-N6	4.32	1.45	1.34
9	C1	900	ATP	C6-N6	4.31	1.45	1.34
11	E1	900	ADP	PA-O3A	4.27	1.64	1.59
11	D1	900	ADP	PA-O3A	4.05	1.63	1.59
11	E1	900	ADP	C5-C4	-4.01	1.31	1.39
11	D1	900	ADP	C5-C4	-3.96	1.32	1.39
11	D1	900	ADP	O2'-C2'	3.57	1.51	1.43
11	E1	900	ADP	O2'-C2'	3.57	1.51	1.43
9	A1	900	ATP	C5-C4	-3.20	1.33	1.39
9	C1	900	ATP	C5-C4	-3.16	1.33	1.39
9	B1	900	ATP	C5-C4	-3.04	1.33	1.39
9	A1	900	ATP	C8-N9	-2.54	1.33	1.37
9	C1	900	ATP	C5-N7	-2.48	1.34	1.39
11	E1	900	ADP	C2'-C1'	2.46	1.61	1.53
9	B1	900	ATP	C5-N7	-2.44	1.34	1.39
9	B1	900	ATP	C8-N9	-2.43	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A1	900	ATP	C5-N7	-2.37	1.34	1.39
9	C1	900	ATP	C8-N9	-2.33	1.33	1.37
11	D1	900	ADP	C2'-C1'	2.33	1.60	1.53
11	D1	900	ADP	C5-N7	-2.03	1.35	1.39
11	E1	900	ADP	C5-N7	-2.02	1.35	1.39
11	D1	900	ADP	C8-N9	-2.00	1.34	1.37

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D1	900	ADP	C1'-N9-C8	-11.53	101.51	127.09
11	E1	900	ADP	C1'-N9-C8	-11.18	102.29	127.09
11	D1	900	ADP	C4-N9-C1'	10.66	151.57	126.63
11	E1	900	ADP	C4-N9-C1'	10.32	150.76	126.63
9	B1	900	ATP	C1'-N9-C8	-5.67	114.51	127.09
9	A1	900	ATP	C1'-N9-C8	-5.65	114.56	127.09
11	D1	900	ADP	N3-C2-N1	-5.64	120.04	128.58
11	E1	900	ADP	N3-C2-N1	-5.63	120.06	128.58
9	C1	900	ATP	N3-C2-N1	-5.53	120.21	128.58
9	A1	900	ATP	N3-C2-N1	-5.53	120.21	128.58
9	B1	900	ATP	N3-C2-N1	-5.51	120.25	128.58
9	C1	900	ATP	C1'-N9-C8	-5.05	115.88	127.09
11	D1	900	ADP	C5-C4-N3	-5.03	119.79	126.72
11	E1	900	ADP	C5-C4-N3	-5.02	119.80	126.72
9	A1	900	ATP	N9-C8-N7	-4.68	107.30	113.94
11	D1	900	ADP	N6-C6-N1	-4.65	108.01	118.38
9	B1	900	ATP	C5-C4-N3	-4.64	120.33	126.72
11	E1	900	ADP	O4'-C1'-N9	4.57	116.86	108.09
9	C1	900	ATP	C5-C4-N3	-4.56	120.43	126.72
9	B1	900	ATP	N6-C6-N1	-4.54	108.26	118.38
9	A1	900	ATP	N6-C6-N1	-4.49	108.37	118.38
9	A1	900	ATP	C5-C4-N3	-4.46	120.57	126.72
9	B1	900	ATP	N9-C8-N7	-4.46	107.61	113.94
11	E1	900	ADP	N6-C6-N1	-4.43	108.50	118.38
9	C1	900	ATP	N6-C6-N1	-4.41	108.55	118.38
9	C1	900	ATP	N9-C8-N7	-4.27	107.88	113.94
9	B1	900	ATP	C4-N9-C1'	4.23	136.53	126.63
9	A1	900	ATP	C4-N9-C1'	4.06	136.12	126.63
11	E1	900	ADP	N9-C8-N7	-3.95	108.33	113.94
11	D1	900	ADP	N9-C8-N7	-3.88	108.44	113.94
11	D1	900	ADP	O4'-C1'-N9	3.82	115.43	108.09
9	C1	900	ATP	C4-N9-C1'	3.76	135.42	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D1	900	ADP	C5-C6-N6	3.49	131.94	123.29
9	A1	900	ATP	C4-N9-C8	3.41	109.32	105.74
11	D1	900	ADP	C2-N3-C4	3.40	120.14	111.83
11	E1	900	ADP	C2-N3-C4	3.37	120.07	111.83
9	B1	900	ATP	C5-C6-N6	3.30	131.46	123.29
11	E1	900	ADP	C5-C6-N6	3.30	131.45	123.29
9	A1	900	ATP	C5-C6-N6	3.25	131.34	123.29
9	B1	900	ATP	C2-N3-C4	3.25	119.77	111.83
9	B1	900	ATP	C3'-C2'-C1'	3.23	107.58	101.46
9	C1	900	ATP	C2-N3-C4	3.20	119.64	111.83
9	A1	900	ATP	C2-N3-C4	3.18	119.60	111.83
9	C1	900	ATP	C5-C6-N6	3.15	131.09	123.29
9	B1	900	ATP	N3-C4-N9	3.08	132.41	127.17
9	B1	900	ATP	C4-N9-C8	3.06	108.95	105.74
9	B1	900	ATP	C2'-C3'-C4'	3.02	108.45	102.61
9	C1	900	ATP	N3-C4-N9	3.02	132.31	127.17
9	A1	900	ATP	N3-C4-N9	3.00	132.27	127.17
11	E1	900	ADP	C5-N7-C8	2.94	108.08	103.45
11	D1	900	ADP	C5-N7-C8	2.91	108.03	103.45
11	E1	900	ADP	C4'-O4'-C1'	-2.88	103.11	109.47
9	C1	900	ATP	C4-N9-C8	2.80	108.67	105.74
9	A1	900	ATP	C5-N7-C8	2.76	107.78	103.45
9	B1	900	ATP	C5-N7-C8	2.73	107.74	103.45
11	D1	900	ADP	C5-C4-N9	2.70	108.75	105.81
11	E1	900	ADP	C3'-C2'-C1'	2.68	106.54	101.46
11	E1	900	ADP	C5-C4-N9	2.68	108.73	105.81
9	C1	900	ATP	C5-N7-C8	2.57	107.49	103.45
11	E1	900	ADP	N3-C4-N9	2.53	131.47	127.17
11	D1	900	ADP	N3-C4-N9	2.52	131.46	127.17
9	A1	900	ATP	C4'-O4'-C1'	-2.39	104.19	109.47
11	D1	900	ADP	C4-C5-N7	-2.37	107.87	110.58
11	E1	900	ADP	C4-C5-N7	-2.34	107.91	110.58
11	E1	900	ADP	C6-C5-C4	2.14	120.09	117.18
11	D1	900	ADP	C6-C5-C4	2.07	120.01	117.18
9	C1	900	ATP	C4'-O4'-C1'	-2.04	104.97	109.47

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C1	900	ATP	C5'-O5'-PA-O2A
9	C1	900	ATP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

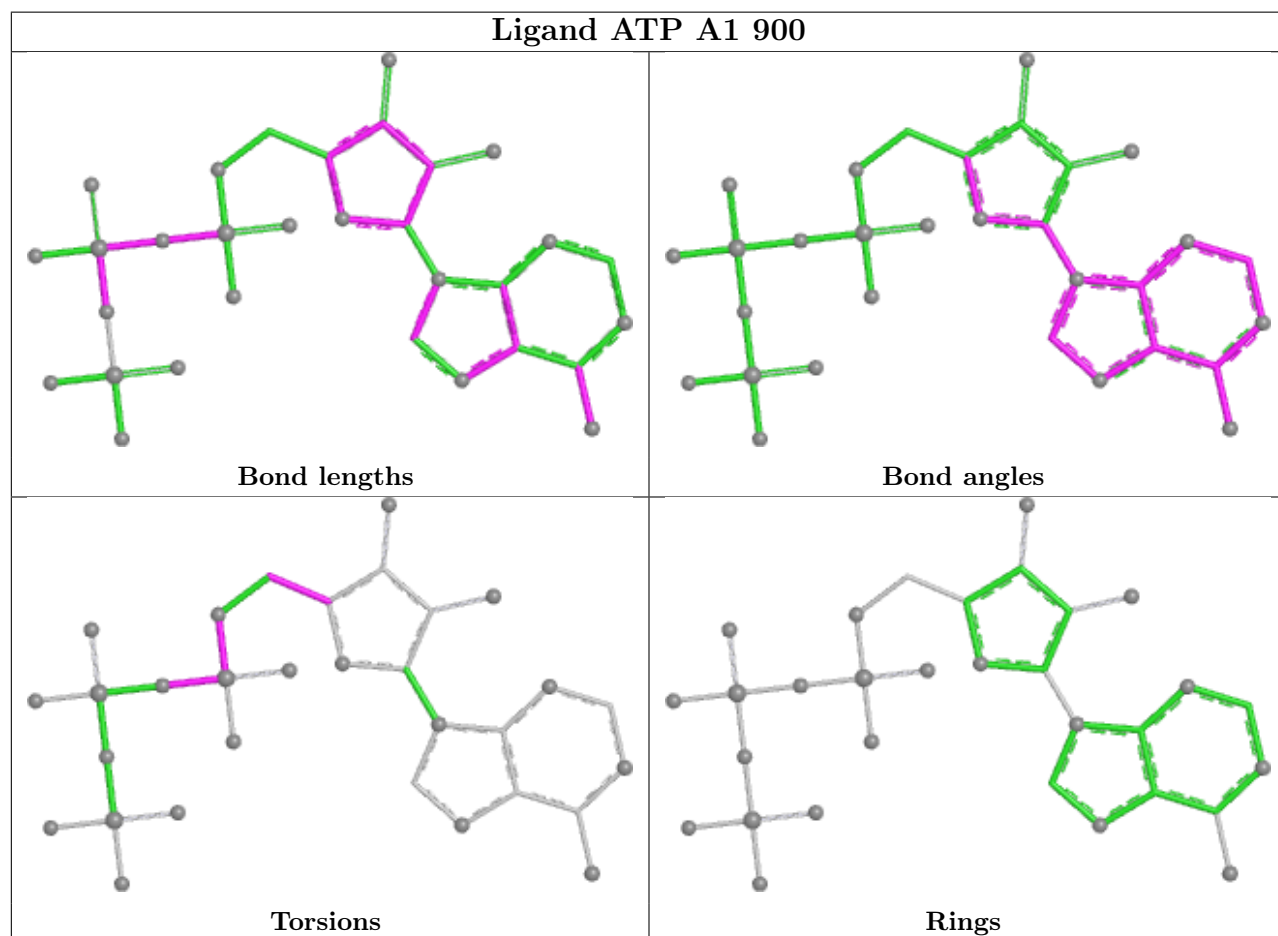
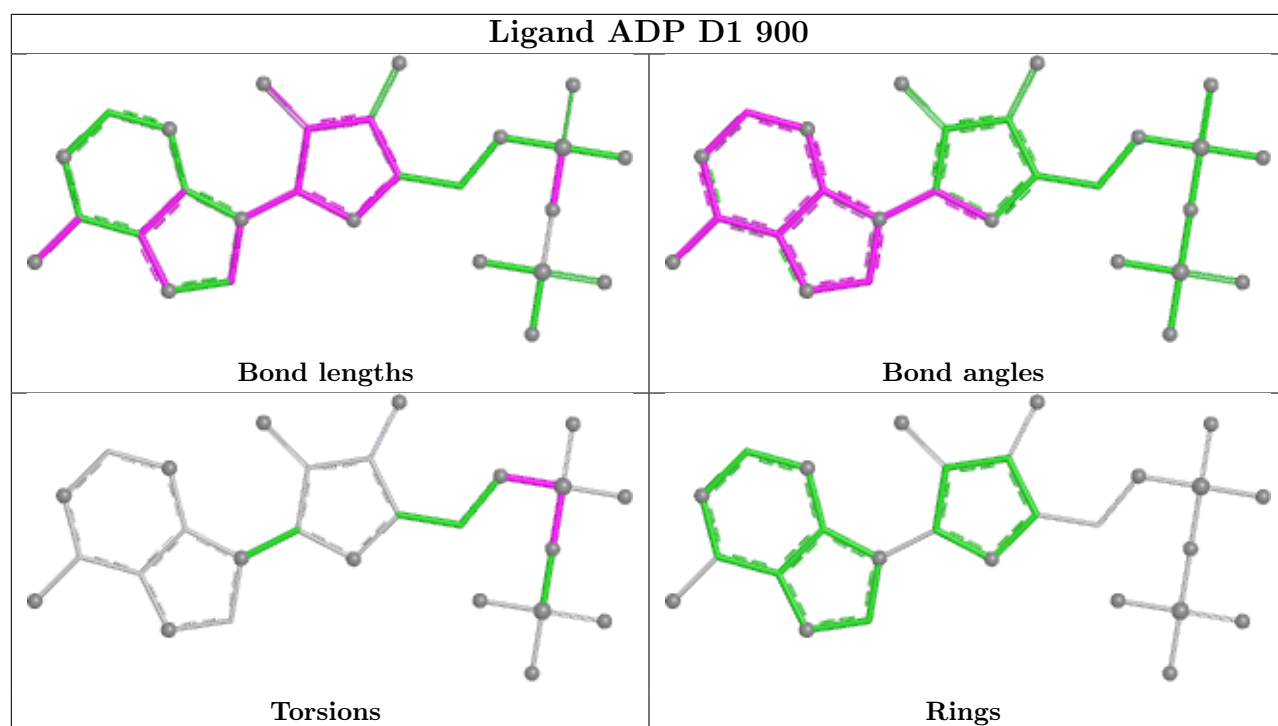
Mol	Chain	Res	Type	Atoms
9	A1	900	ATP	C5'-O5'-PA-O2A
9	A1	900	ATP	C5'-O5'-PA-O3A
11	D1	900	ADP	C5'-O5'-PA-O1A
11	D1	900	ADP	C5'-O5'-PA-O3A
9	A1	900	ATP	O4'-C4'-C5'-O5'
9	A1	900	ATP	C3'-C4'-C5'-O5'
11	E1	900	ADP	PA-O3A-PB-O2B
9	C1	900	ATP	C3'-C4'-C5'-O5'
9	C1	900	ATP	O4'-C4'-C5'-O5'
9	B1	900	ATP	C5'-O5'-PA-O1A
9	B1	900	ATP	C5'-O5'-PA-O2A
9	B1	900	ATP	C5'-O5'-PA-O3A
9	C1	900	ATP	PB-O3A-PA-O2A
9	B1	900	ATP	PB-O3A-PA-O1A
9	A1	900	ATP	PB-O3A-PA-O1A
11	D1	900	ADP	PB-O3A-PA-O2A
11	E1	900	ADP	PA-O3A-PB-O3B
9	C1	900	ATP	PB-O3A-PA-O1A
9	B1	900	ATP	PB-O3A-PA-O2A
11	D1	900	ADP	PB-O3A-PA-O1A
9	A1	900	ATP	PB-O3A-PA-O2A

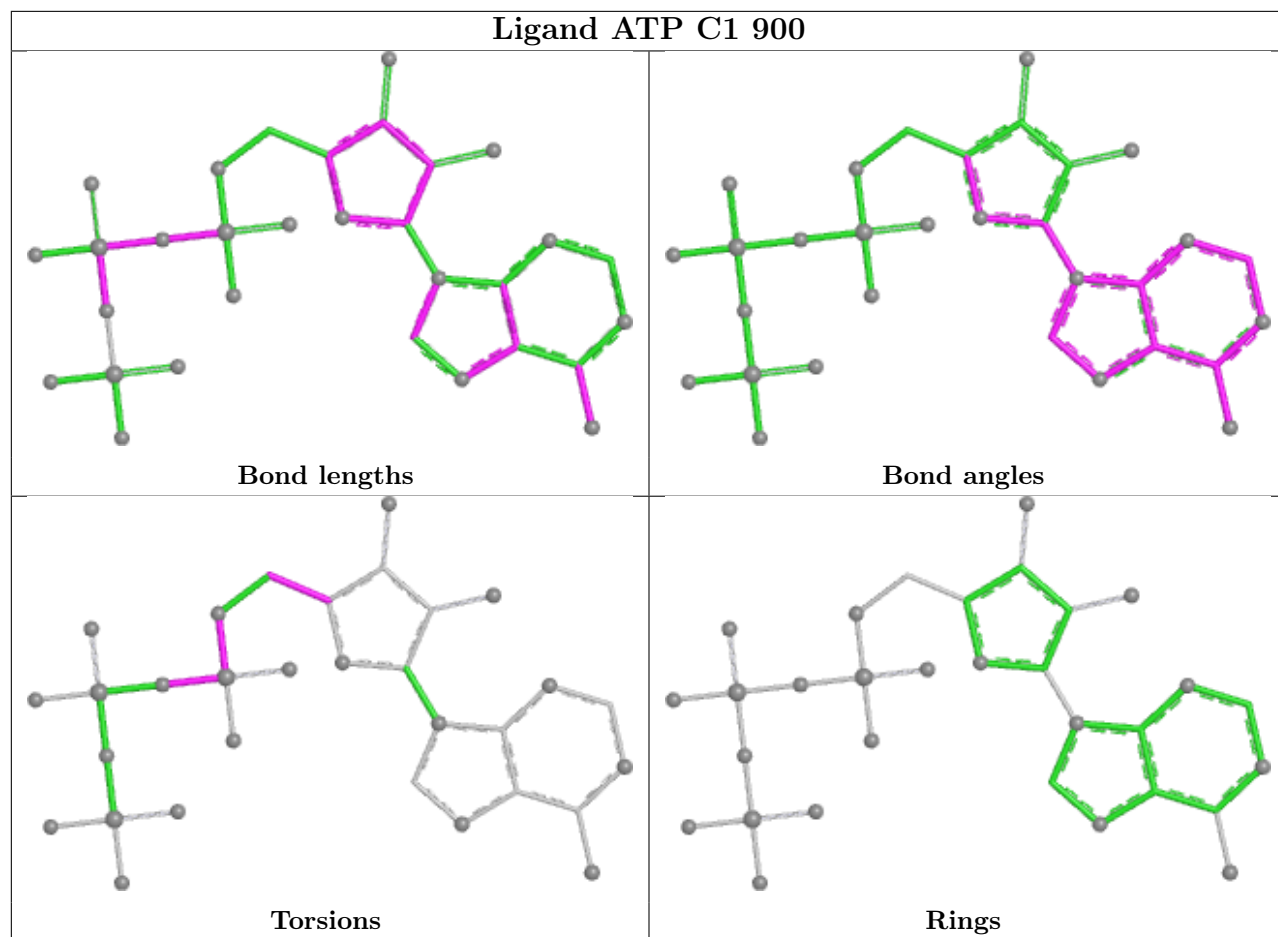
There are no ring outliers.

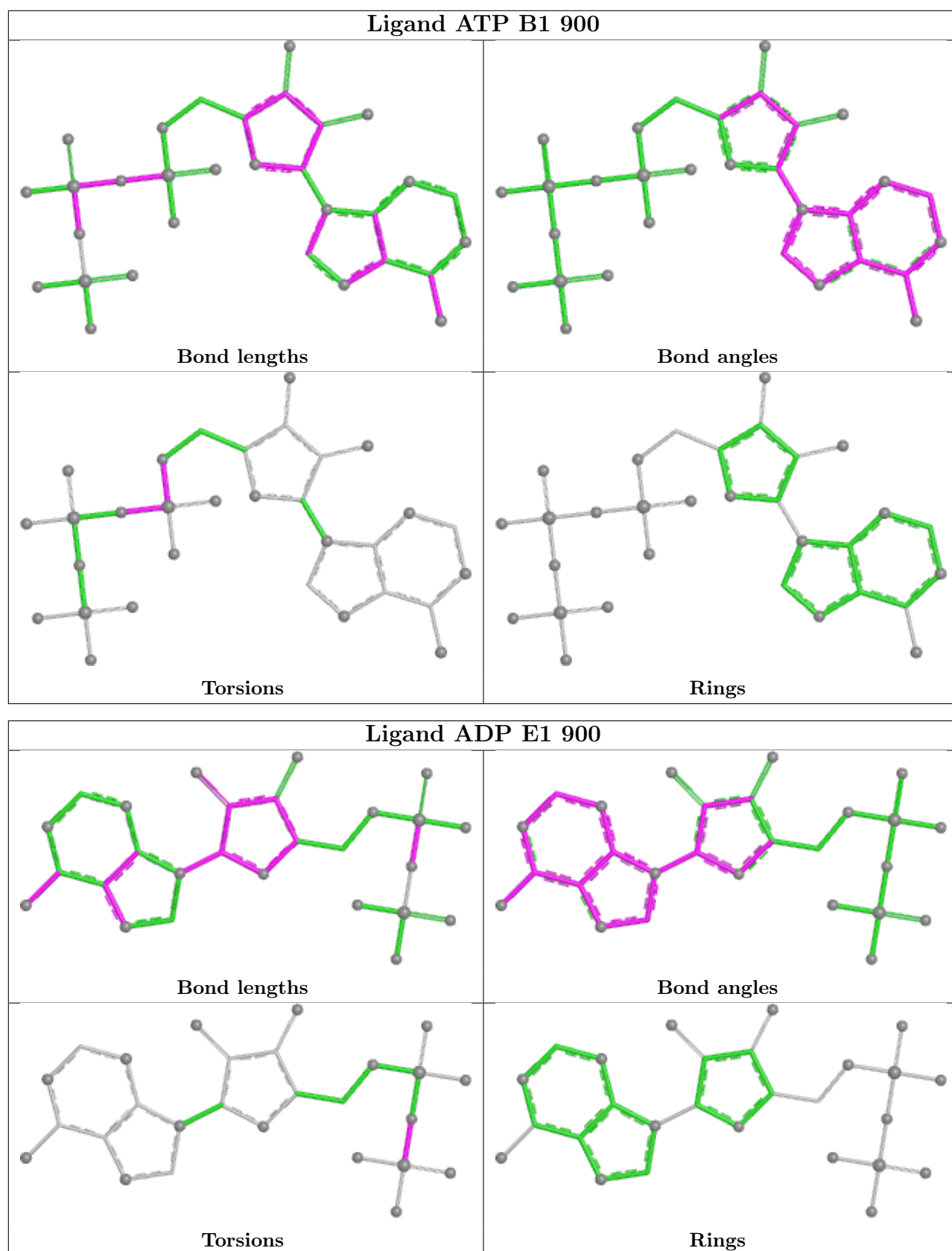
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D1	900	ADP	1	0
9	A1	900	ATP	1	0
9	B1	900	ATP	4	0

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







5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

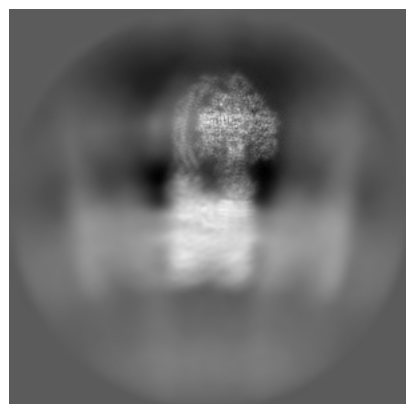
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10862. These allow visual inspection of the internal detail of the map and identification of artifacts.

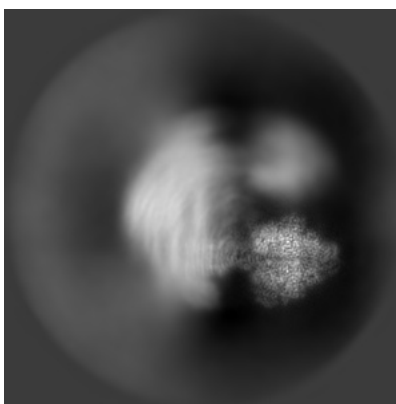
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

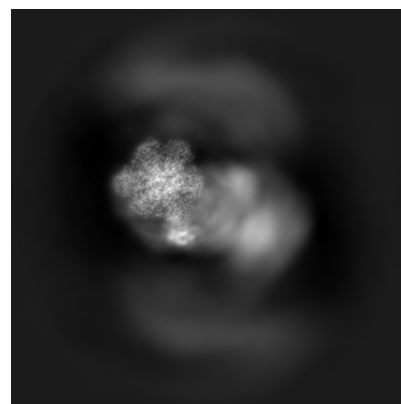
6.1.1 Primary map



X

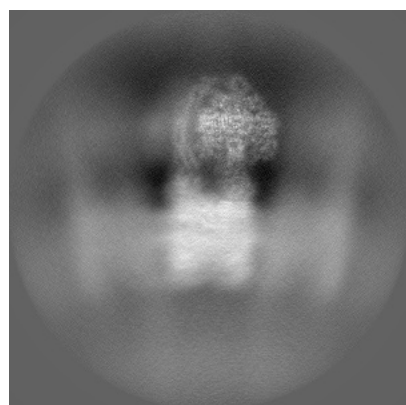


Y

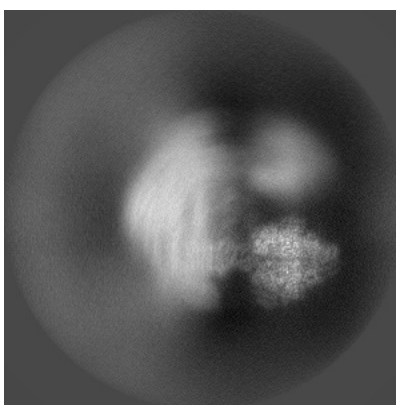


Z

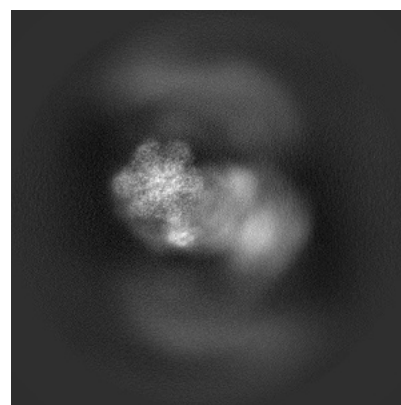
6.1.2 Raw map



X



Y

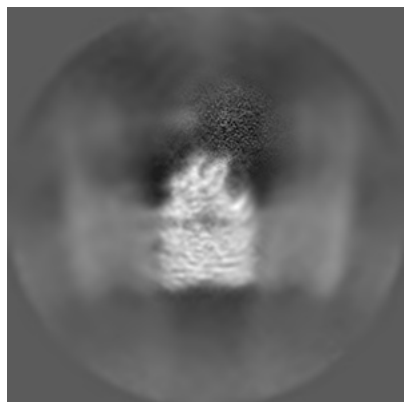


Z

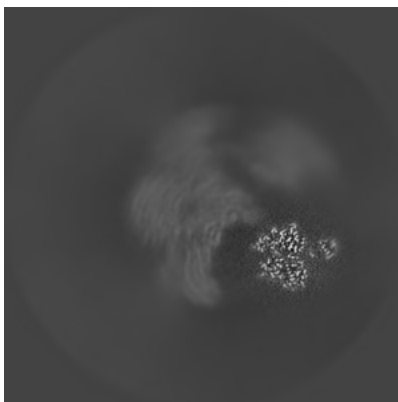
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

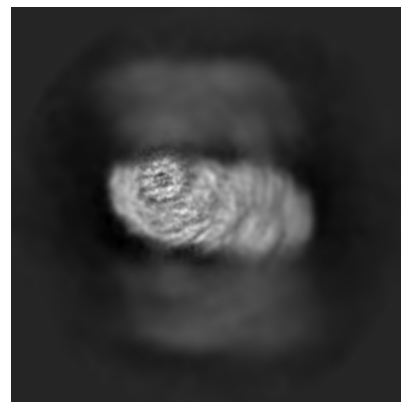
6.2.1 Primary map



X Index: 300

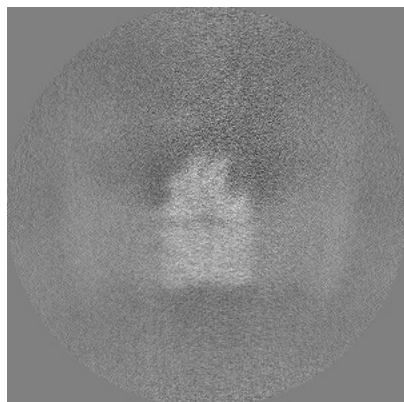


Y Index: 300

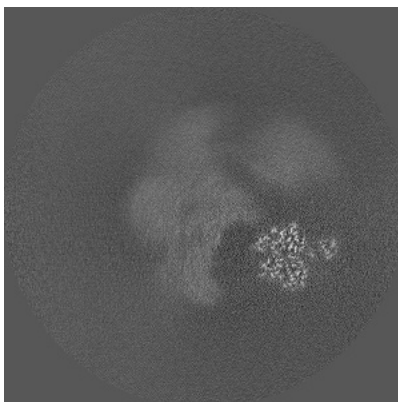


Z Index: 300

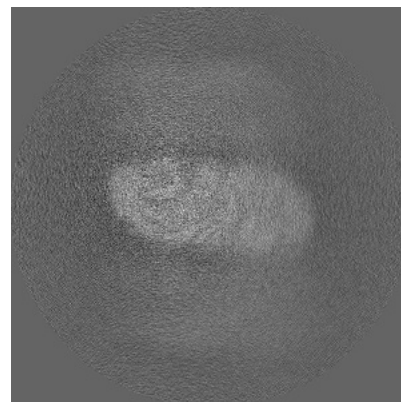
6.2.2 Raw map



X Index: 300



Y Index: 300



Z Index: 300

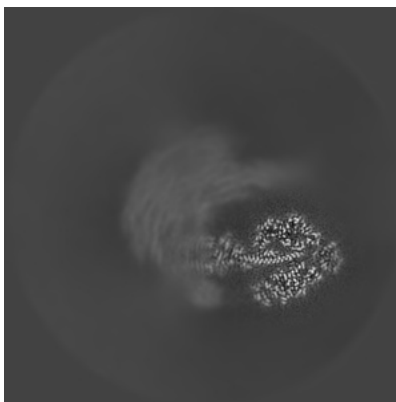
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

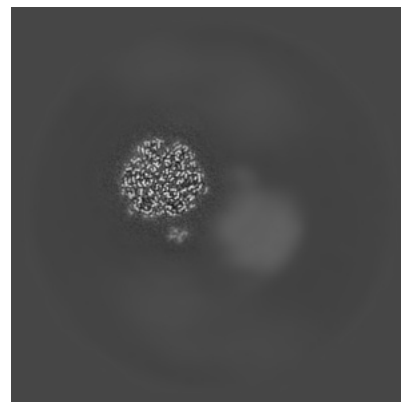
6.3.1 Primary map



X Index: 245



Y Index: 344

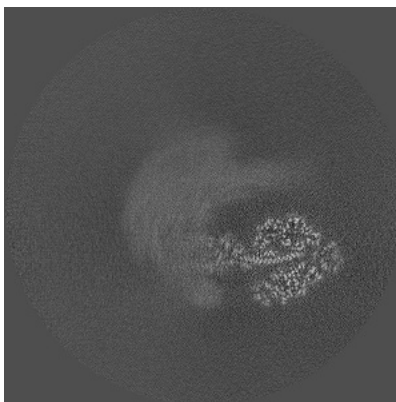


Z Index: 436

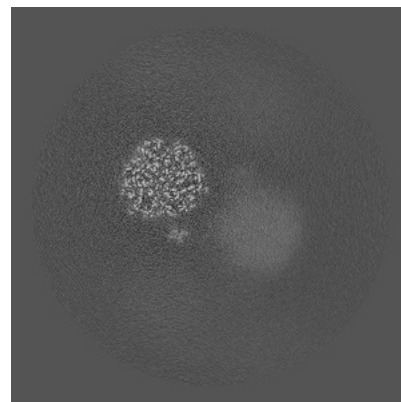
6.3.2 Raw map



X Index: 245



Y Index: 344

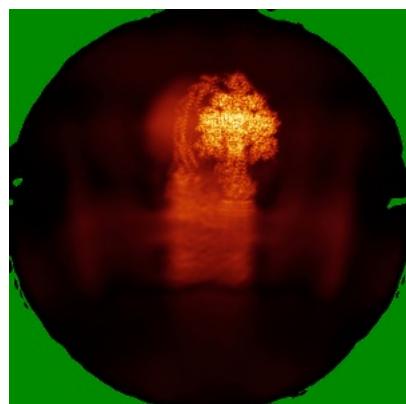


Z Index: 436

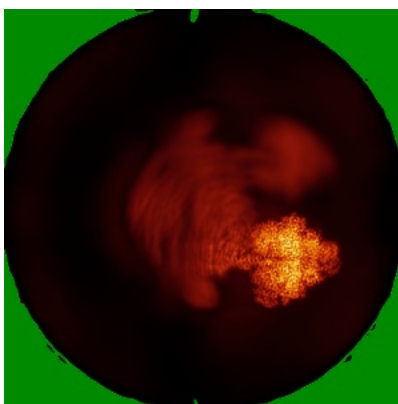
The images above show the largest variance slices of the map in three orthogonal directions.

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

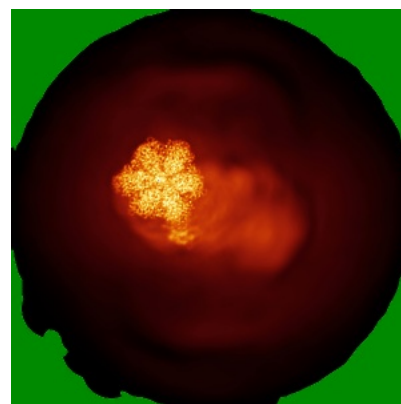
6.4.1 Primary map



X

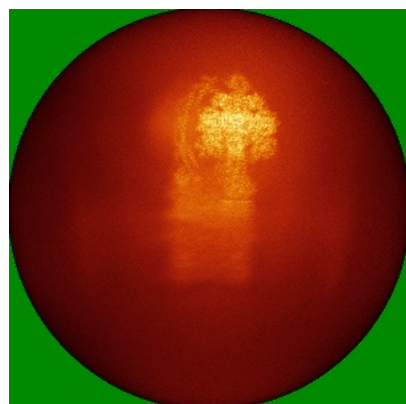


Y

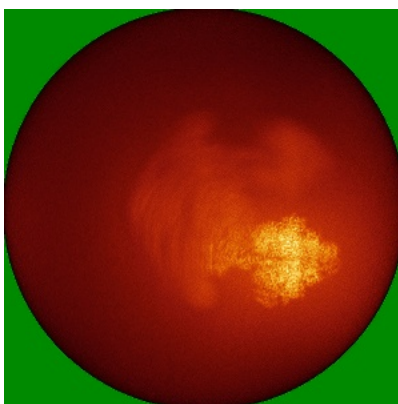


Z

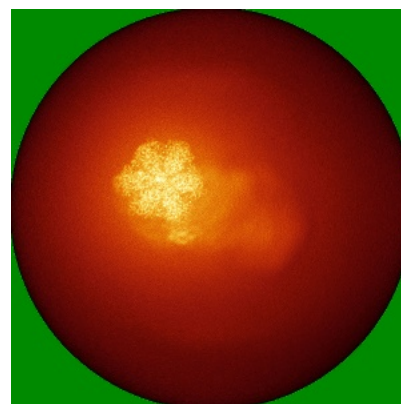
6.4.2 Raw map



X



Y

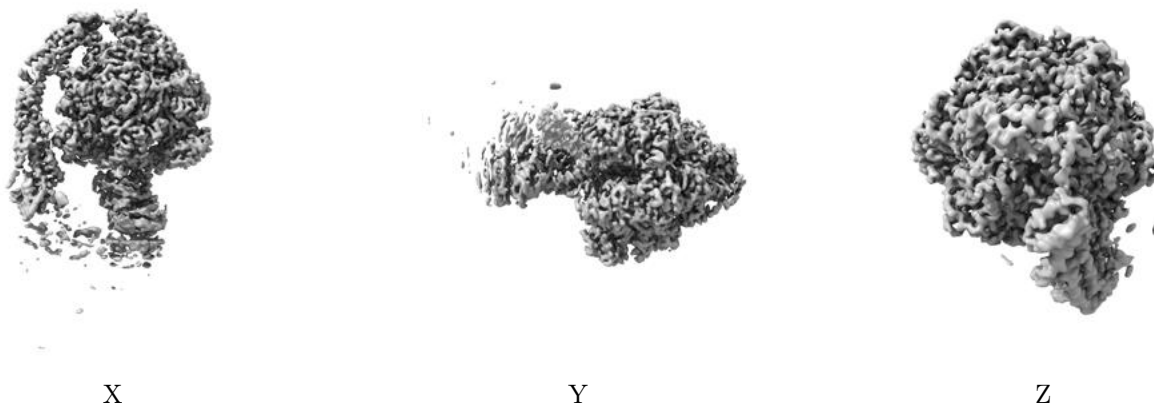


Z

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.

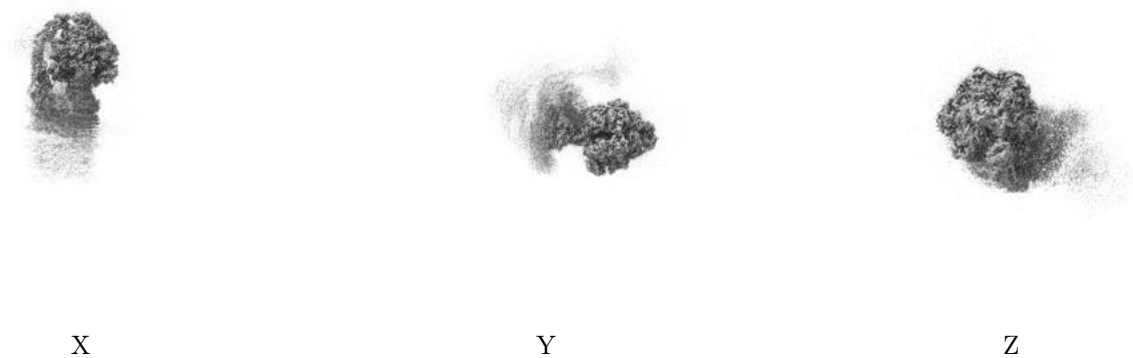
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

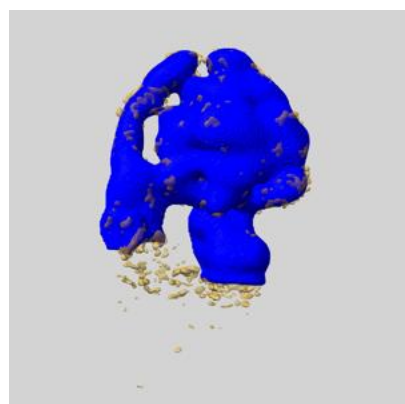
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

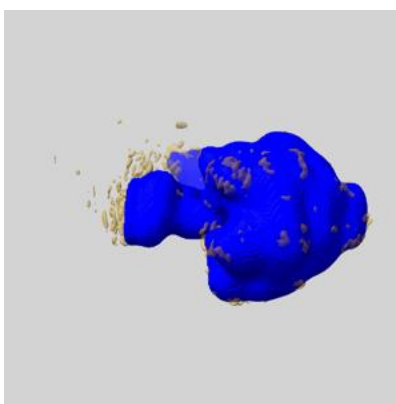
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

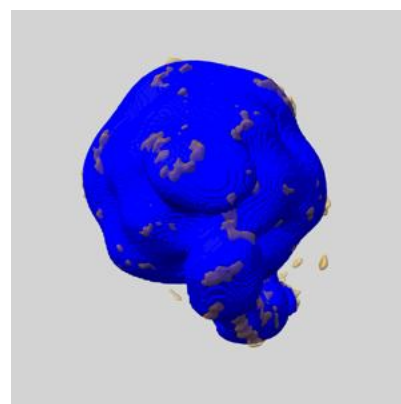
6.6.1 emd_10862_msk_1.map [i](#)



X



Y

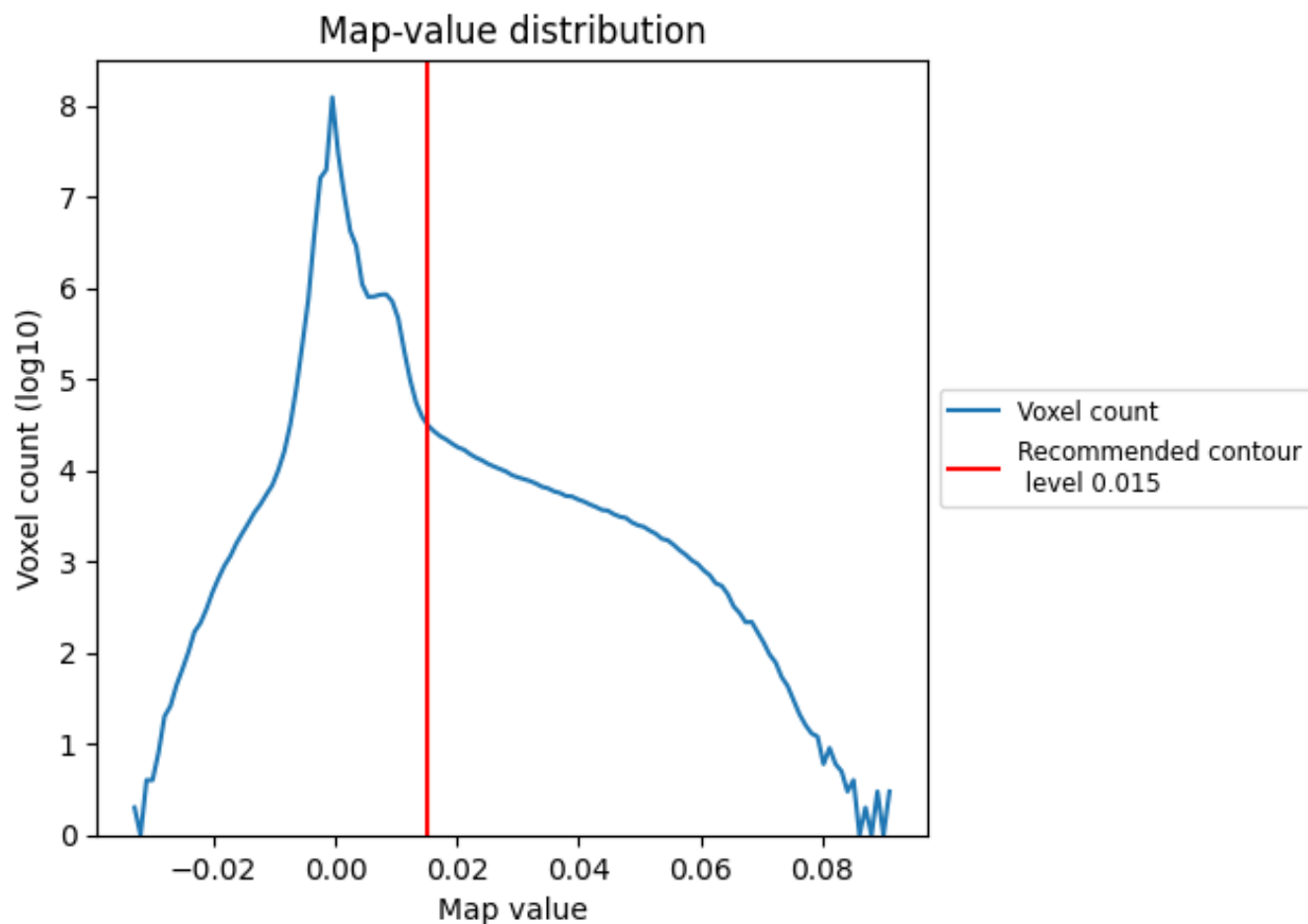


Z

7 Map analysis [i](#)

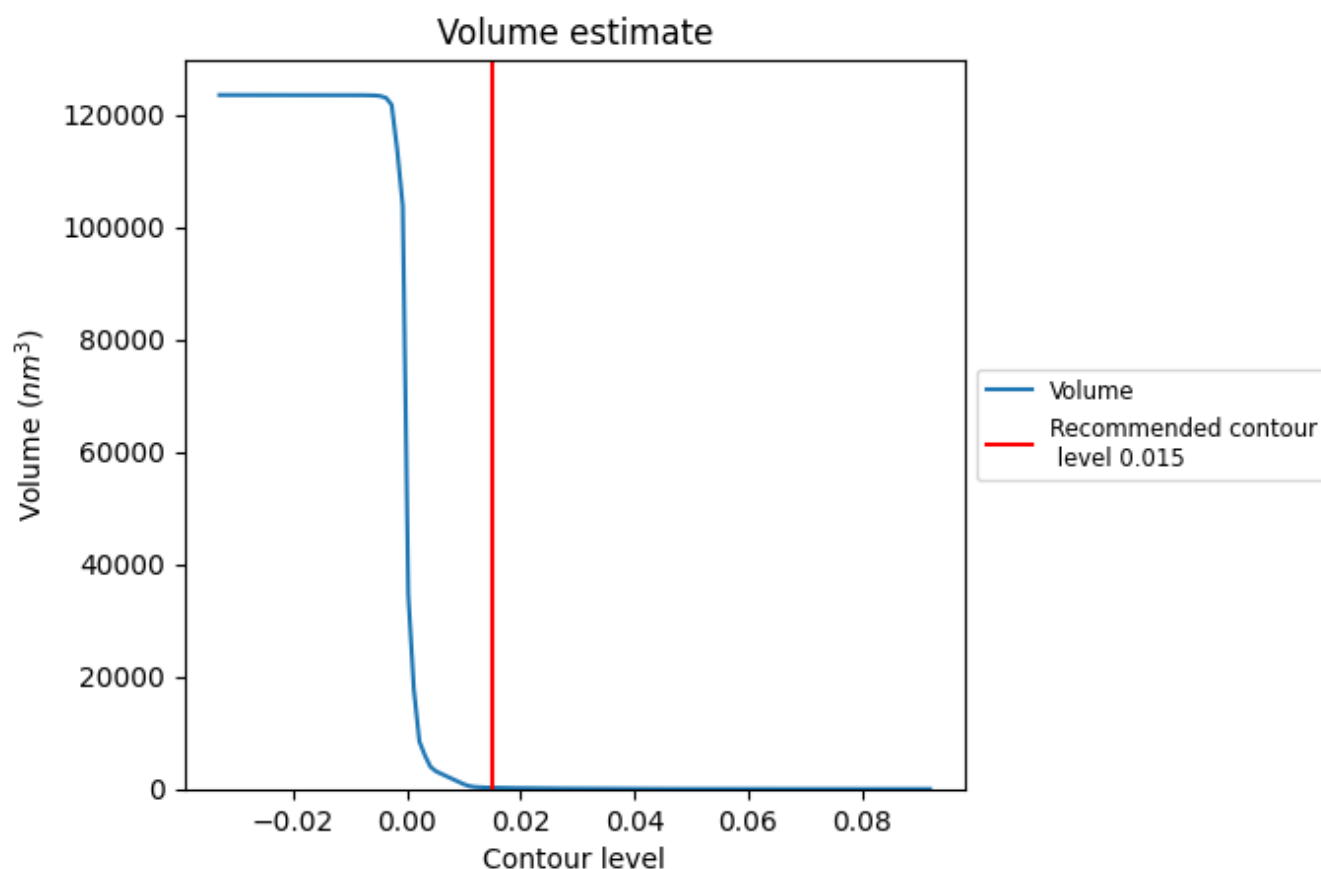
This section contains the results of statistical analysis of the map.

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.

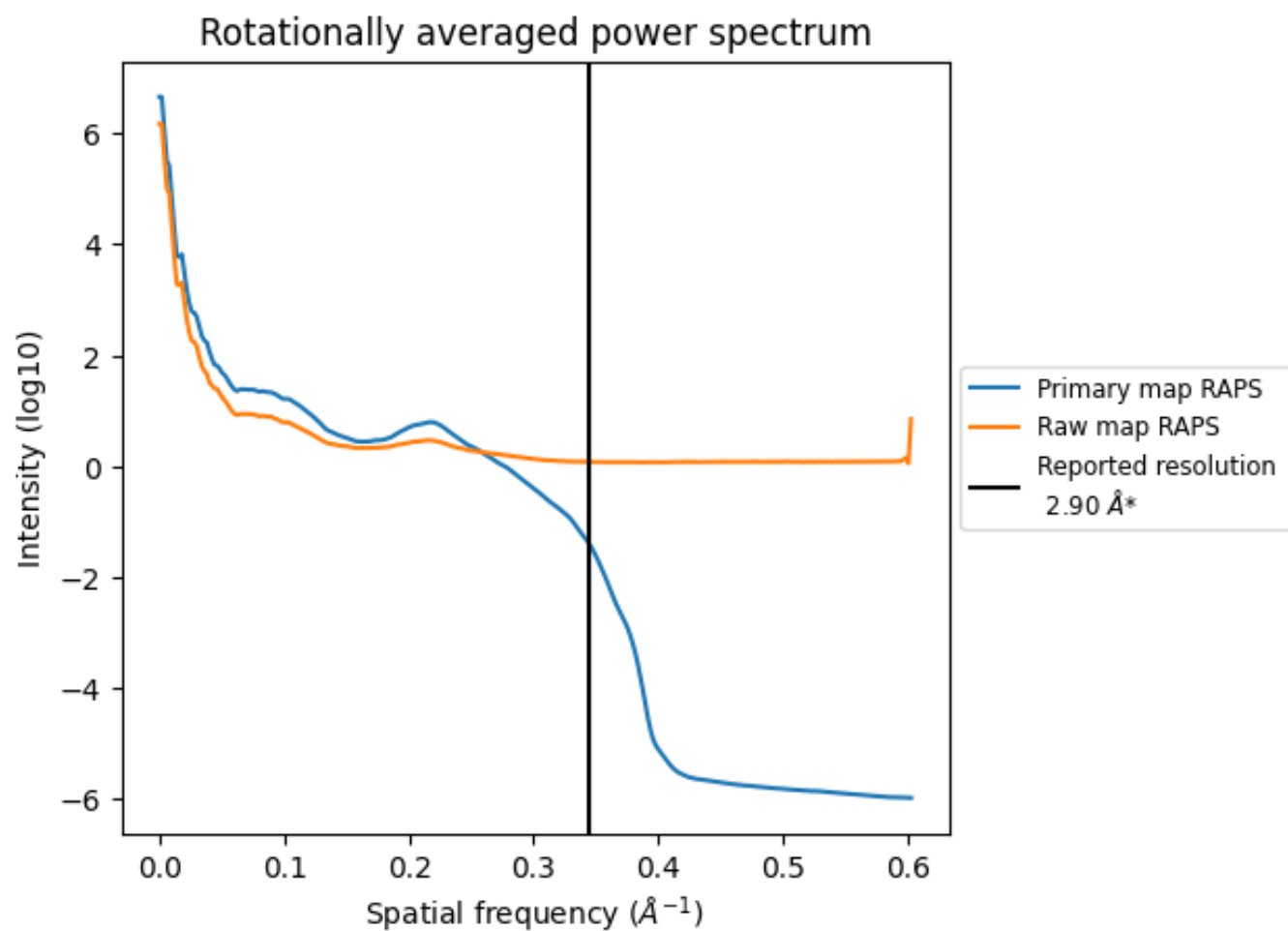
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 220 nm^3 ; this corresponds to an approximate mass of 199 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 ⓘ

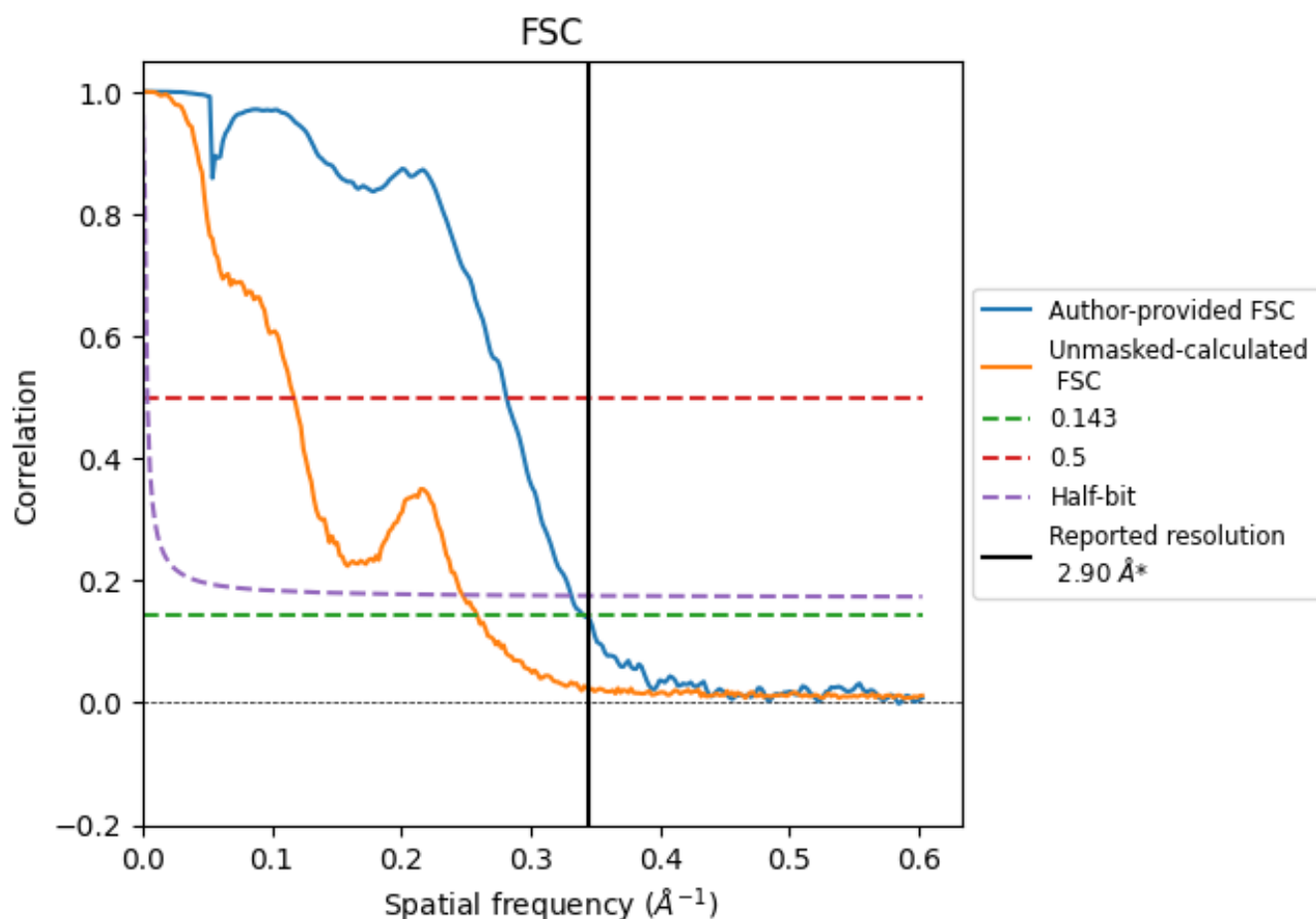


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

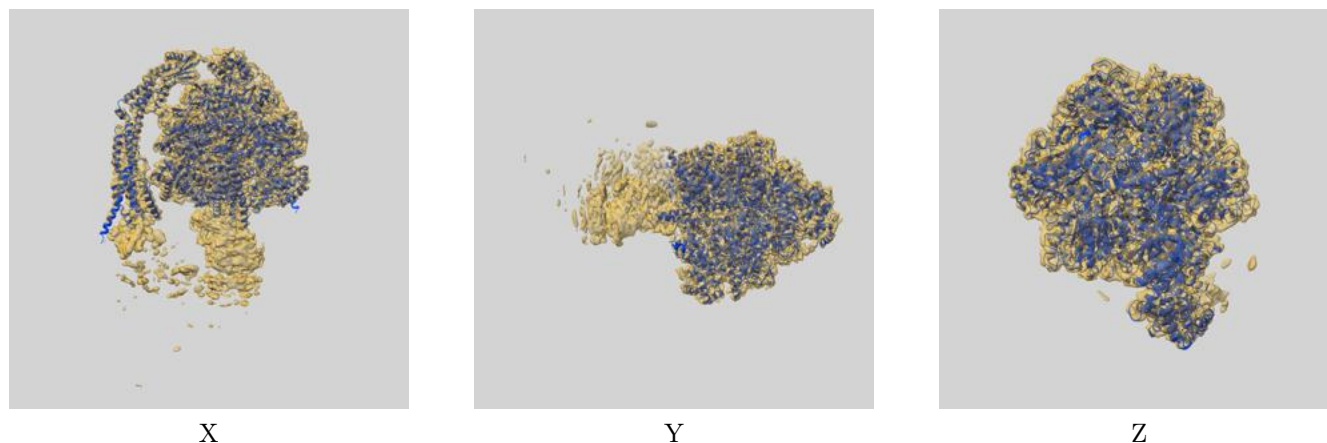
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.93	3.55	3.02
Unmasked-calculated*	3.87	8.54	4.04

*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 3.87 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

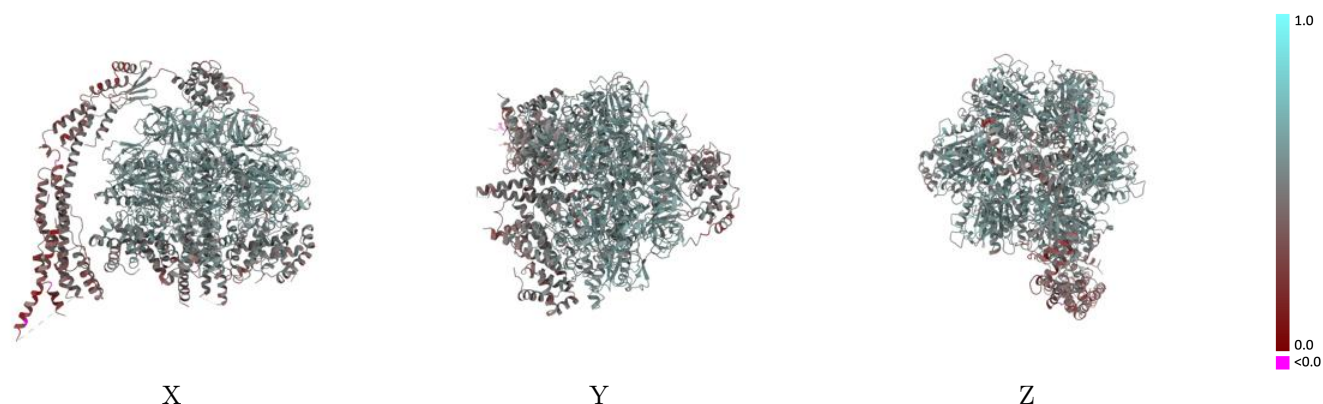
This section contains information regarding the fit between EMDB map EMD-10862 and PDB model 6YO0. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



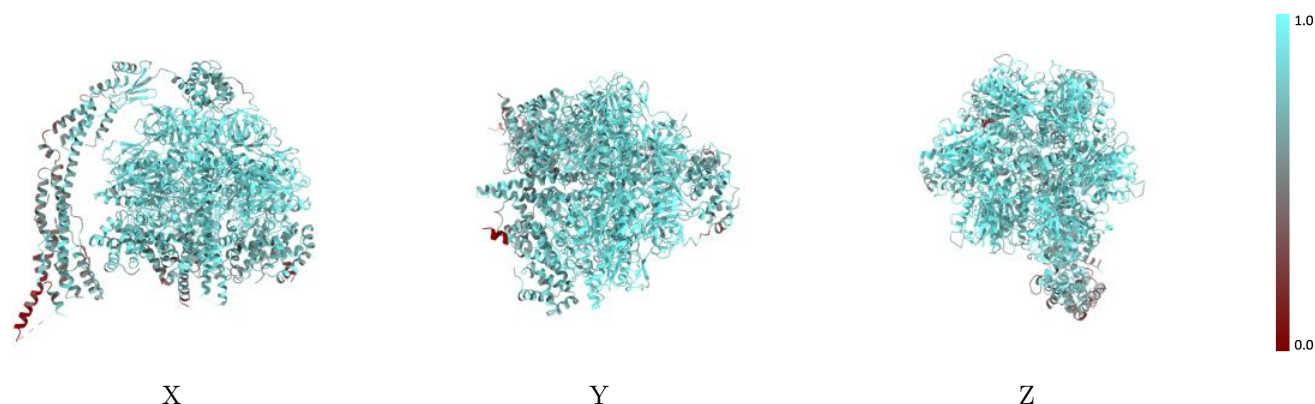
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



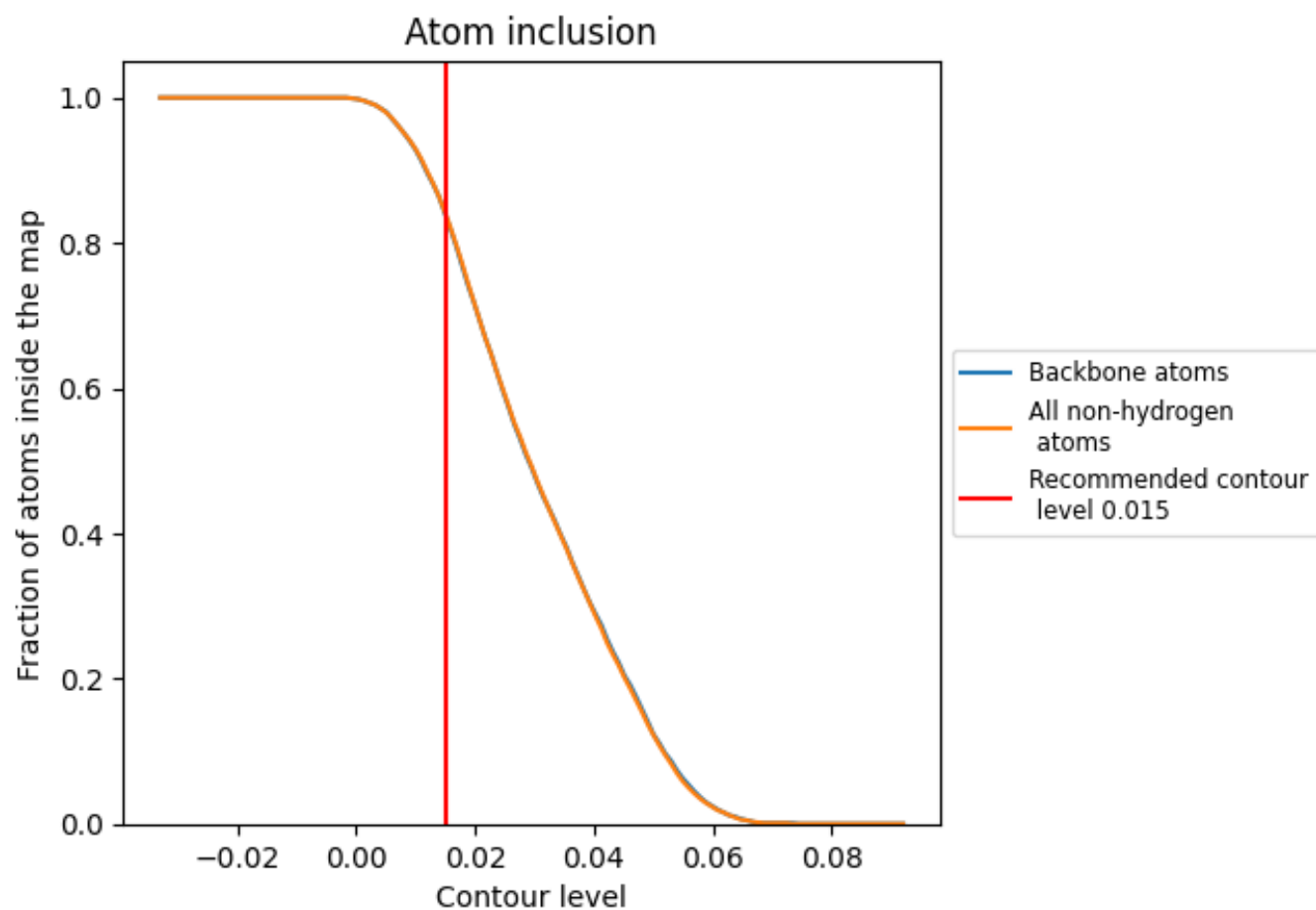
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 84% of all backbone atoms, 84% 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	0.8410	0.5120
A1	0.8750	0.5410
B1	0.8720	0.5200
C1	0.8560	0.5320
D1	0.8950	0.5530
E1	0.9020	0.5460
F1	0.8620	0.5270
G1	0.7730	0.4440
b	0.6260	0.3500
d	0.6050	0.3590
g1	0.8530	0.5120
i1	0.6750	0.4600
s	0.6710	0.3680

1.0

0.0

<0.0