



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:26 PM UTC

PDB ID : 6LY8 / pdb_00006ly8
EMDB ID : EMD-30014
Title : V/A-ATPase from *Thermus thermophilus*, the soluble domain, including V1, d, two EG stalks, and N-terminal domain of α -subunit.
Authors : Kishikawa, J.; Nakanishi, A.; Furuta, A.; Kato, T.; Namba, K.; Tamakoshi, M.; Mitsuoka, K.; Yokoyama, K.
Deposited on : 2020-02-13
Resolution : 3.50 Å (reported)
Based on initial model : 5Y5Y

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:

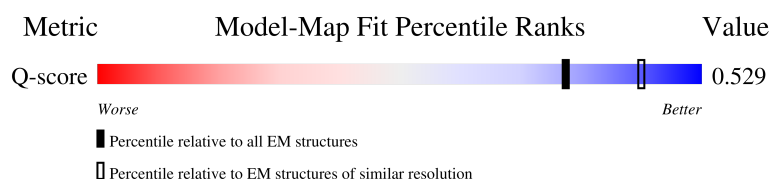
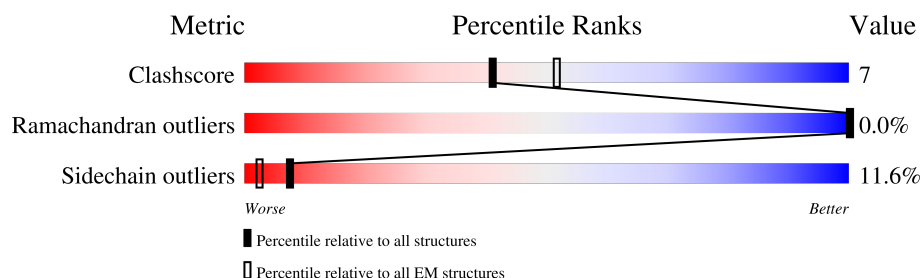
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.50 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	13950 (3.00 - 4.00)

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	578	
1	B	578	
1	C	578	

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Mol	Chain	Length	Quality of chain
2	D	478	75%20%
2	E	478	73%21%
2	F	478	75%19%
3	G	223	20%75%19%6%
4	H	104	37%67%23%6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26631 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	577	Total	C	N	O	S	0	0
			4472	2854	762	834	22		
1	B	577	Total	C	N	O	S	0	0
			4472	2854	762	834	22		
1	C	577	Total	C	N	O	S	0	0
			4472	2854	762	834	22		

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	459	Total	C	N	O	S	0	0
			3596	2278	622	686	10		
2	E	459	Total	C	N	O	S	0	0
			3596	2278	622	686	10		
2	F	459	Total	C	N	O	S	0	0
			3596	2278	622	686	10		

- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	210	Total	C	N	O	S	0	0
			1642	1033	307	300	2		

- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	100	Total	C	N	O	S	0	0
			758	479	131	145	3		

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

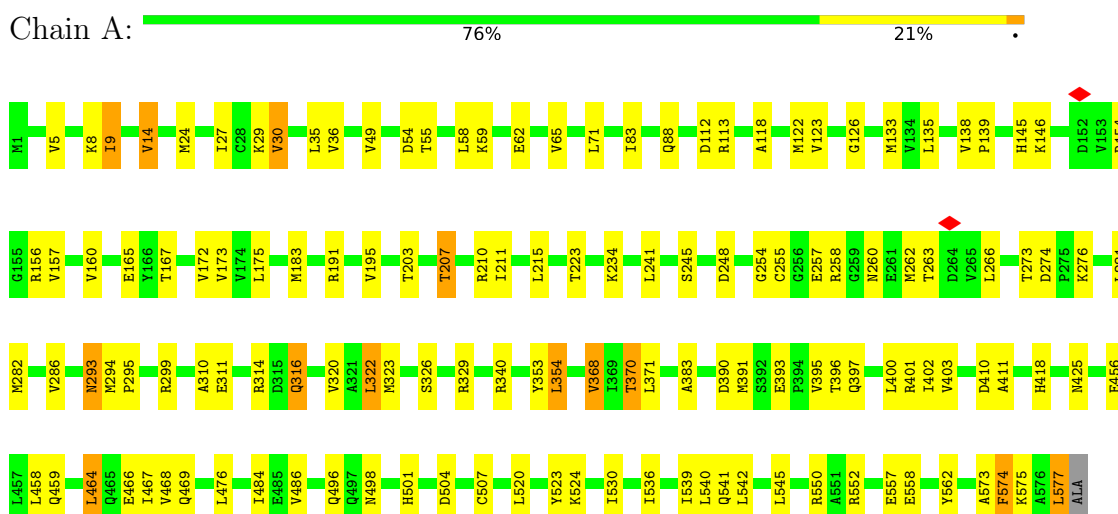


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

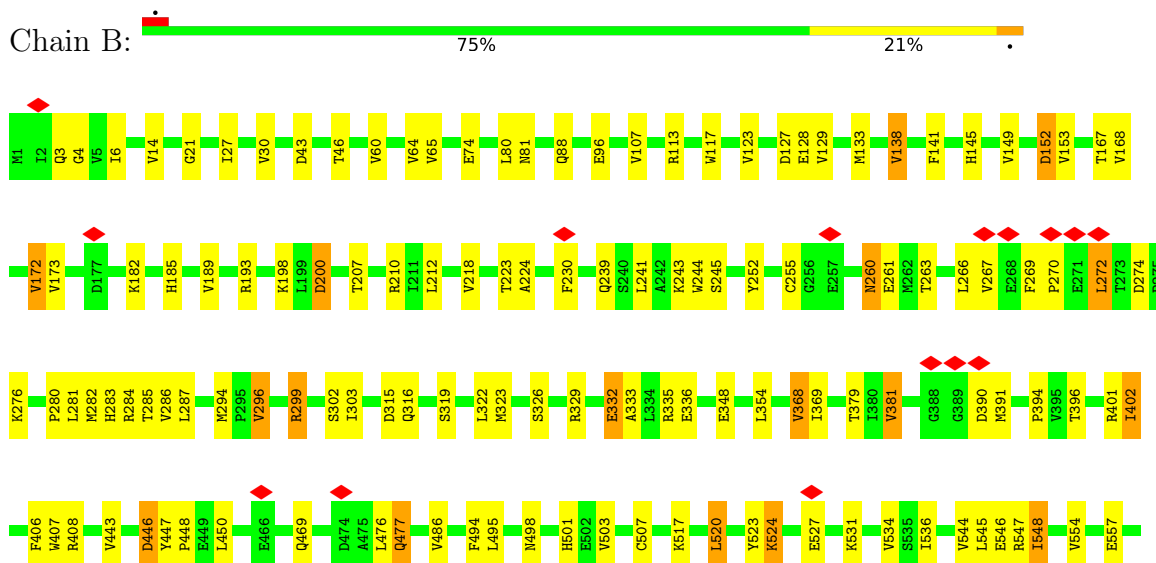
3 Residue-property plots

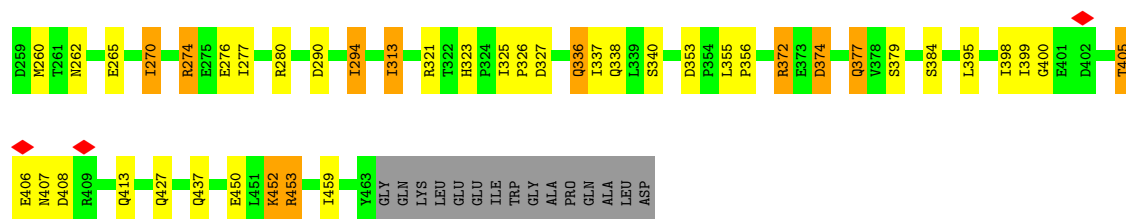
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: V-type ATP synthase alpha chain



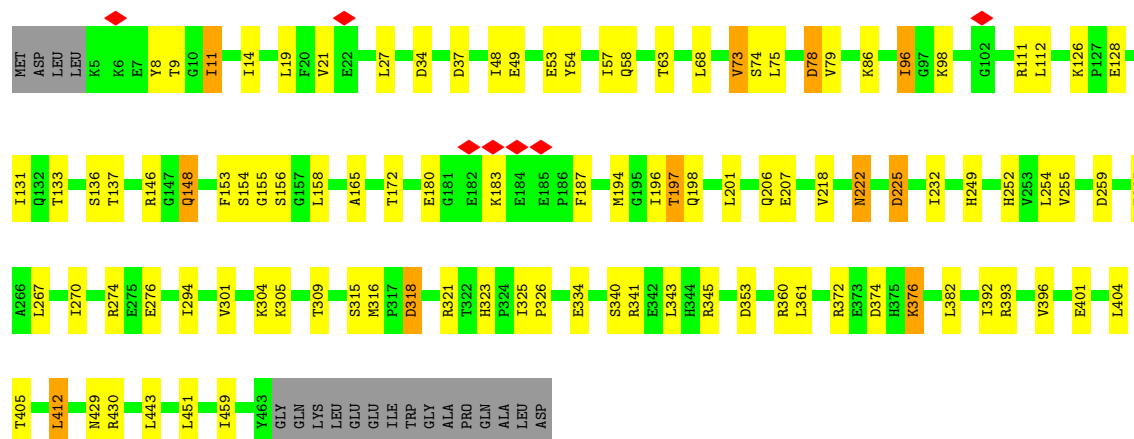
• Molecule 1: V-type ATP synthase alpha chain





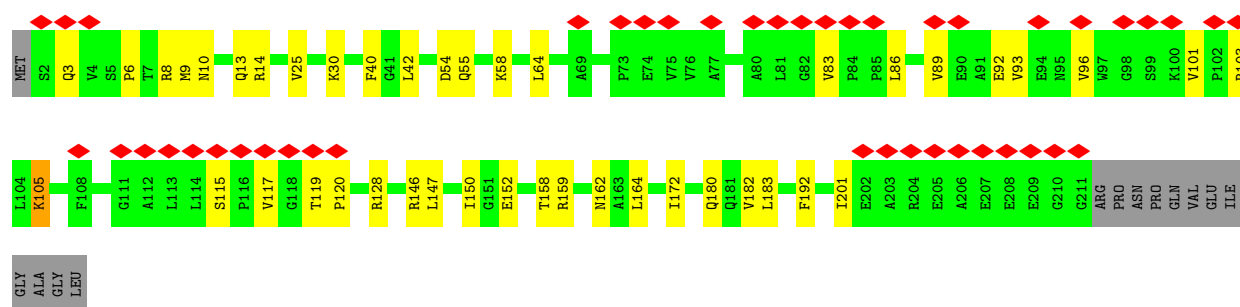
• Molecule 2: V-type ATP synthase beta chain

Chain F: 75% 19%



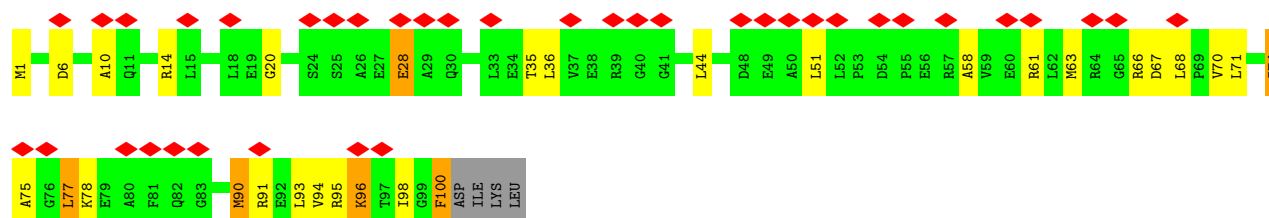
• Molecule 3: V-type ATP synthase subunit D

Chain G: 20% 75% 19% 6%



• Molecule 4: V-type ATP synthase subunit F

Chain H: 37% 67% 23% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	71196	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.512	Depositor
Minimum map value	-0.365	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.068	Depositor
Map size ($\text{\AA}$)	374.0, 374.0, 374.0	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/4568	0.40	0/6198
1	B	0.25	0/4568	0.41	0/6198
1	C	0.26	0/4568	0.40	0/6198
2	D	0.28	0/3663	0.40	0/4960
2	E	0.25	0/3663	0.40	0/4960
2	F	0.28	0/3663	0.42	0/4960
3	G	0.21	0/1662	0.40	0/2235
4	H	0.16	0/769	0.41	0/1039
All	All	0.26	0/27124	0.40	0/36748

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	419	PHE	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	A	4472	0	4490	63	0
1	B	4472	0	4491	66	0
1	C	4472	0	4491	62	0
2	D	3596	0	3624	44	0
2	E	3596	0	3624	58	0
2	F	3596	0	3624	47	0
3	G	1642	0	1718	24	0
4	H	758	0	764	19	0
5	A	27	0	12	0	0
All	All	26631	0	26838	368	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (368) 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:C:576:ALA:O	1:C:577:LEU:CD2	1.80	1.29
1:C:576:ALA:O	1:C:577:LEU:HD22	1.38	1.20
1:C:576:ALA:O	1:C:577:LEU:HD23	1.62	0.98
4:H:94:VAL:HG12	4:H:100:PHE:C	1.92	0.94
1:C:576:ALA:C	1:C:577:LEU:HD23	2.01	0.85
1:A:577:LEU:HD23	1:A:577:LEU:H	1.42	0.85
1:C:576:ALA:C	1:C:577:LEU:CD2	2.50	0.84
1:C:210:ARG:NH1	1:C:507:CYS:SG	2.51	0.82
2:E:91:ARG:NH2	2:E:104:PRO:O	2.15	0.80
1:C:401:ARG:NH2	2:F:265:GLU:OE2	2.15	0.79
2:F:225:ASP:OD1	2:F:225:ASP:N	2.18	0.75
1:B:294:MET:O	1:B:299:ARG:NH1	2.20	0.74
1:A:210:ARG:NH1	1:A:507:CYS:SG	2.60	0.74
1:C:547:ARG:O	1:C:562:TYR:OH	2.04	0.74
1:C:74:GLU:OE2	1:C:113:ARG:NH2	2.22	0.73
2:E:85:SER:H	2:E:88:MET:HE2	1.53	0.73
1:B:74:GLU:OE1	1:B:113:ARG:NH2	2.23	0.72
1:B:210:ARG:NH1	1:B:494:PHE:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ALA:HB3	1:B:381:VAL:HG12	1.75	0.69
1:C:113:ARG:NH1	1:C:169:GLU:OE2	2.25	0.68
2:E:274:ARG:NH1	2:E:276:GLU:OE2	2.25	0.68
2:F:318:ASP:N	2:F:318:ASP:OD1	2.25	0.68
1:A:550:ARG:NH1	1:A:562:TYR:OH	2.26	0.68
2:D:406:GLU:OE1	2:D:409:ARG:NH1	2.26	0.68
1:C:234:LYS:HD2	1:C:383:ALA:HB1	1.77	0.67
4:H:63:MET:HG2	4:H:68:LEU:HD12	1.76	0.67
1:C:1:MET:HG2	1:C:2:ILE:HG13	1.75	0.66
1:C:470:LEU:HG	1:C:471:VAL:HG13	1.76	0.66
1:B:391:MET:HE3	1:B:396:THR:HG21	1.79	0.65
2:E:374:ASP:OD1	2:E:374:ASP:N	2.30	0.65
1:A:29:LYS:HG2	1:A:36:VAL:HG12	1.78	0.65
1:A:340:ARG:NH2	2:F:276:GLU:OE2	2.30	0.65
2:D:318:ASP:OD1	2:D:318:ASP:N	2.29	0.65
2:F:197:THR:OG1	2:F:198:GLN:N	2.31	0.64
2:E:323:HIS:HB3	2:E:326:PRO:HD2	1.79	0.64
2:D:197:THR:OG1	2:D:198:GLN:N	2.30	0.64
2:F:11:ILE:HG22	2:F:21:VAL:HG12	1.79	0.64
2:E:407:ASN:ND2	2:E:408:ASP:OD1	2.31	0.64
1:B:326:SER:HB3	1:B:329:ARG:HB2	1.79	0.63
3:G:103:ARG:HH21	3:G:146:ARG:HD3	1.62	0.63
1:A:391:MET:O	1:A:397:GLN:NE2	2.30	0.62
3:G:25:VAL:HG23	3:G:164:LEU:HD23	1.81	0.61
1:B:332:GLU:OE1	1:B:335:ARG:NH1	2.32	0.61
1:A:577:LEU:HD23	1:A:577:LEU:N	2.14	0.61
1:B:200:ASP:OD1	1:B:200:ASP:N	2.31	0.61
1:A:467:ILE:HD11	2:D:394:LYS:HG2	1.83	0.61
1:C:576:ALA:C	1:C:577:LEU:HD22	2.21	0.60
1:A:370:THR:OG1	1:A:371:LEU:N	2.32	0.60
1:B:207:THR:HG23	1:B:241:LEU:HD13	1.83	0.60
1:B:401:ARG:NH2	2:E:265:GLU:OE2	2.34	0.60
2:F:325:ILE:HB	2:F:326:PRO:HD3	1.82	0.60
1:B:185:HIS:HE1	1:B:193:ARG:HH12	1.50	0.59
1:C:167:THR:OG1	1:C:168:VAL:N	2.32	0.59
1:B:4:GLY:O	1:B:64:VAL:N	2.32	0.59
2:D:325:ILE:HB	2:D:326:PRO:HD3	1.84	0.59
2:F:78:ASP:OD1	2:F:78:ASP:N	2.34	0.59
1:A:210:ARG:NH2	1:A:496:GLN:O	2.36	0.59
1:B:517:LYS:HD3	1:B:563:PHE:HZ	1.68	0.59
1:A:293:ASN:OD1	1:A:293:ASN:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:ASP:N	2:D:37:ASP:OD1	2.35	0.59
1:C:393:GLU:HB3	1:C:396:THR:HG22	1.85	0.59
1:A:577:LEU:H	1:A:577:LEU:CD2	2.13	0.58
1:B:270:PRO:HA	1:B:280:PRO:HA	1.85	0.58
4:H:66:ARG:HB3	4:H:68:LEU:HG	1.83	0.58
1:A:504:ASP:OD2	1:A:552:ARG:NH1	2.36	0.58
1:C:127:ASP:OD1	1:C:128:GLU:N	2.32	0.58
2:E:325:ILE:HB	2:E:326:PRO:HD3	1.84	0.58
2:E:405:THR:OG1	2:E:406:GLU:N	2.36	0.58
2:E:150:LEU:HD21	2:E:337:ILE:HD12	1.85	0.58
1:B:260:ASN:ND2	1:B:261:GLU:OE2	2.36	0.58
1:B:252:TYR:HB3	1:B:287:LEU:HD12	1.86	0.58
2:E:340:SER:HB2	2:E:353:ASP:HB2	1.85	0.57
1:C:311:GLU:OE2	1:C:364:ARG:NE	2.35	0.57
1:B:336:GLU:OE2	2:D:289:THR:OG1	2.17	0.57
2:F:154:SER:OG	2:F:155:GLY:N	2.36	0.57
1:A:393:GLU:HG2	1:A:395:VAL:H	1.70	0.57
2:D:455:SER:OG	2:D:457:ASP:OD1	2.16	0.56
2:F:27:LEU:HD23	2:F:75:LEU:HD13	1.86	0.56
2:F:49:GLU:OE1	2:F:274:ARG:NH2	2.38	0.56
4:H:100:PHE:CD2	4:H:100:PHE:N	2.73	0.56
1:A:459:GLN:HG3	2:D:345:ARG:HD2	1.87	0.56
4:H:14:ARG:NH1	4:H:20:GLY:O	2.37	0.56
1:C:315:ASP:HA	1:C:370:THR:HG21	1.86	0.56
2:E:169:ARG:NH1	2:E:207:GLU:OE2	2.38	0.56
2:F:11:ILE:HD13	2:F:11:ILE:H	1.71	0.56
2:F:136:SER:OG	2:F:430:ARG:NH1	2.39	0.56
2:E:154:SER:OG	2:E:155:GLY:N	2.39	0.56
3:G:158:THR:HG22	3:G:162:ASN:HD21	1.70	0.56
2:D:154:SER:OG	2:D:155:GLY:N	2.40	0.55
2:E:51:SER:OG	2:E:52:GLU:N	2.40	0.55
2:F:148:GLN:NE2	2:F:361:LEU:HB2	2.22	0.55
3:G:8:ARG:HD3	3:G:9:MET:H	1.72	0.55
1:A:558:GLU:OE1	1:A:558:GLU:N	2.39	0.54
2:F:318:ASP:O	3:G:3:GLN:NE2	2.35	0.54
1:B:446:ASP:OD1	1:B:446:ASP:N	2.41	0.54
1:C:473:PRO:HA	1:C:476:LEU:HD23	1.88	0.54
2:D:317:PRO:HG3	2:D:323:HIS:CD2	2.42	0.54
1:A:126:GLY:HA2	1:A:156:ARG:HH21	1.73	0.54
2:D:418:PHE:HA	2:D:442:LEU:HD21	1.90	0.53
1:C:400:LEU:O	1:C:401:ARG:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:194:MET:HE3	2:D:263:TYR:HB2	1.89	0.53
2:D:13:TYR:HB3	2:D:20:PHE:HB2	1.90	0.53
2:E:210:ARG:HD2	2:E:211:THR:HG23	1.90	0.53
1:B:270:PRO:HG3	1:B:280:PRO:HB3	1.91	0.53
2:E:9:THR:OG1	2:E:10:GLY:N	2.42	0.53
1:A:112:ASP:OD1	1:A:113:ARG:N	2.41	0.53
1:A:118:ALA:HB3	1:A:139:PRO:HD2	1.90	0.53
4:H:67:ASP:OD1	4:H:67:ASP:N	2.36	0.53
1:A:468:VAL:HG22	1:A:476:LEU:HD11	1.91	0.52
1:B:547:ARG:O	1:B:562:TYR:OH	2.26	0.52
2:D:457:ASP:OD1	2:D:457:ASP:N	2.35	0.52
2:F:153:PHE:HB3	2:F:316:MET:HE3	1.91	0.52
2:E:76:VAL:HG12	2:E:77:GLU:HG2	1.91	0.52
1:B:172:VAL:HG13	1:B:173:VAL:HG23	1.91	0.52
2:E:321:ARG:NH1	2:E:338:GLN:OE1	2.43	0.52
2:F:323:HIS:HD2	2:F:325:ILE:H	1.58	0.52
1:B:266:LEU:O	1:B:270:PRO:HG2	2.10	0.52
1:C:201:PRO:HB2	1:C:219:ALA:HB1	1.91	0.52
2:D:180:GLU:HG3	2:D:181:GLY:H	1.73	0.52
1:B:524:LYS:O	1:B:527:GLU:HG3	2.10	0.52
1:B:127:ASP:OD1	1:B:128:GLU:N	2.41	0.51
1:C:83:ILE:HD12	1:C:266:LEU:HD11	1.92	0.51
2:E:86:LYS:HG3	2:E:249:HIS:HD2	1.74	0.51
2:F:156:SER:OG	2:F:341:ARG:NH2	2.43	0.51
2:F:340:SER:HB2	2:F:353:ASP:HB2	1.91	0.51
2:D:115:THR:OG1	2:D:116:GLY:N	2.42	0.51
1:A:400:LEU:O	1:A:401:ARG:HG2	2.10	0.51
2:E:67:ASP:OD1	2:E:68:LEU:N	2.43	0.51
1:C:396:THR:HA	1:C:399:THR:HG22	1.92	0.51
2:F:196:ILE:HD12	2:F:201:LEU:HB2	1.93	0.51
1:A:326:SER:H	1:A:383:ALA:HB3	1.76	0.51
1:B:299:ARG:O	1:B:302:SER:OG	2.26	0.51
1:C:27:ILE:O	1:C:67:THR:OG1	2.29	0.51
1:A:390:ASP:OD1	1:A:390:ASP:N	2.44	0.51
1:A:9:ILE:HD12	1:A:58:LEU:HB2	1.93	0.51
2:F:148:GLN:HE21	2:F:361:LEU:HB2	1.76	0.51
4:H:14:ARG:HG2	4:H:20:GLY:H	1.75	0.51
1:A:310:ALA:HB2	1:A:322:LEU:HD23	1.93	0.50
1:B:527:GLU:O	1:B:531:LYS:HG2	2.11	0.50
2:E:194:MET:HA	2:E:222:ASN:HB3	1.93	0.50
1:A:172:VAL:HG23	1:A:173:VAL:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:ASP:OD1	1:C:475:ALA:N	2.43	0.50
1:B:43:ASP:N	1:B:43:ASP:OD1	2.42	0.50
2:E:377:GLN:H	2:E:377:GLN:NE2	2.09	0.50
2:F:194:MET:HA	2:F:222:ASN:HB3	1.93	0.50
1:C:7:GLN:HG3	1:C:17:LYS:HE2	1.94	0.50
1:B:145:HIS:CE1	1:B:316:GLN:HE22	2.29	0.50
2:E:321:ARG:NH2	2:E:336:GLN:OE1	2.45	0.50
1:B:252:TYR:HD2	1:B:323:MET:HE3	1.77	0.50
1:C:246:ASN:O	1:C:246:ASN:ND2	2.45	0.49
1:B:129:VAL:HA	1:B:133:MET:HE2	1.94	0.49
1:B:576:ALA:HB3	1:B:577:LEU:HD23	1.94	0.49
1:C:482:LEU:HD22	1:C:530:ILE:HD12	1.93	0.49
2:F:96:ILE:HD13	2:F:98:LYS:HG2	1.95	0.49
1:C:212:LEU:HD21	1:C:422:ILE:HD13	1.94	0.49
3:G:8:ARG:C	3:G:10:ASN:H	2.20	0.49
1:B:210:ARG:NE	1:B:507:CYS:SG	2.83	0.49
1:B:296:VAL:HG12	1:B:333:ALA:HB1	1.95	0.48
1:B:43:ASP:OD1	1:B:46:THR:OG1	2.28	0.48
1:B:576:ALA:C	1:B:577:LEU:HD23	2.39	0.48
1:C:303:ILE:O	1:C:307:VAL:HG23	2.14	0.48
2:D:395:LEU:HD22	3:G:30:LYS:HG2	1.95	0.48
3:G:8:ARG:HG2	3:G:183:LEU:HD21	1.94	0.48
1:A:557:GLU:N	1:A:557:GLU:OE1	2.46	0.48
1:C:12:PRO:HA	1:C:55:THR:HG21	1.96	0.48
2:D:110:LYS:HD3	2:D:112:LEU:HD21	1.94	0.48
1:B:544:VAL:O	1:B:548:ILE:HG23	2.14	0.48
1:C:447:TYR:HB3	1:C:448:PRO:HD3	1.95	0.48
3:G:119:THR:N	3:G:120:PRO:HD3	2.29	0.48
4:H:100:PHE:N	4:H:100:PHE:HD2	2.12	0.48
1:A:257:GLU:HG2	1:A:258:ARG:H	1.79	0.48
1:A:322:LEU:HD13	1:A:323:MET:H	1.79	0.48
1:C:41:ARG:HG2	1:C:42:LEU:H	1.79	0.47
4:H:10:ALA:O	4:H:14:ARG:HG3	2.14	0.47
1:C:532:ARG:HH12	1:C:577:LEU:HA	1.79	0.47
1:B:486:VAL:HG21	1:B:523:TYR:HD1	1.79	0.47
1:A:260:ASN:HA	1:A:263:THR:HG22	1.95	0.47
2:E:120:ASN:ND2	2:E:122:VAL:HG22	2.29	0.47
1:B:239:GLN:HB3	1:B:269:PHE:HZ	1.80	0.47
1:C:97:LYS:HG3	1:C:98:THR:OG1	2.14	0.47
2:D:207:GLU:OE1	2:D:210:ARG:NH2	2.47	0.47
2:F:165:ALA:HB1	2:F:207:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:85:SER:OG	2:E:86:LYS:N	2.47	0.47
2:E:195:GLY:HA3	2:E:262:ASN:HD22	1.78	0.47
4:H:74:ILE:HG23	4:H:75:ALA:H	1.78	0.47
1:B:498:ASN:HD22	1:B:501:HIS:HB2	1.80	0.47
1:C:39:ILE:HG23	1:C:47:ALA:HB1	1.97	0.47
2:F:34:ASP:OD1	2:F:34:ASP:N	2.48	0.47
1:C:326:SER:HB3	1:C:329:ARG:HD2	1.95	0.47
2:E:175:PRO:HG2	2:E:182:GLU:HG3	1.97	0.47
2:D:37:ASP:OD2	2:D:43:ARG:NH1	2.48	0.47
2:D:340:SER:HB2	2:D:353:ASP:HB2	1.98	0.46
2:E:11:ILE:HG22	2:E:21:VAL:HG22	1.97	0.46
2:F:155:GLY:HA3	2:F:158:LEU:HD12	1.96	0.46
2:D:373:GLU:OE1	2:D:373:GLU:N	2.47	0.46
1:B:117:TRP:HB3	1:B:138:VAL:HG21	1.97	0.46
1:B:391:MET:SD	1:B:391:MET:N	2.88	0.46
4:H:90:MET:O	4:H:94:VAL:HG22	2.16	0.46
3:G:42:LEU:HD22	3:G:150:ILE:HD12	1.96	0.46
1:B:269:PHE:CD2	1:B:281:LEU:HD23	2.50	0.46
1:C:41:ARG:HG2	1:C:42:LEU:N	2.31	0.46
2:D:229:ILE:H	2:D:229:ILE:HD12	1.80	0.46
2:D:60:PHE:HD1	2:D:229:ILE:HD13	1.80	0.46
4:H:1:MET:SD	4:H:1:MET:N	2.70	0.46
2:D:263:TYR:OH	2:D:290:ASP:OD1	2.30	0.46
1:B:390:ASP:OD1	1:B:390:ASP:N	2.49	0.45
2:E:207:GLU:CD	2:E:210:ARG:HH12	2.24	0.45
2:E:353:ASP:O	2:E:356:PRO:HD2	2.16	0.45
2:F:392:ILE:HG22	2:F:412:LEU:HD23	1.98	0.45
1:A:464:LEU:HB3	1:A:484:ILE:HD11	1.98	0.45
1:C:172:VAL:HG23	1:C:173:VAL:HG23	1.98	0.45
1:C:322:LEU:HD23	1:C:323:MET:N	2.31	0.45
2:D:8:TYR:OH	2:D:26:ASP:HB3	2.16	0.45
2:D:250:ASP:N	2:D:250:ASP:OD1	2.50	0.45
1:A:418:HIS:CD2	1:A:496:GLN:HE21	2.34	0.45
1:B:185:HIS:CE1	1:B:193:ARG:HH12	2.32	0.45
2:E:450:GLU:O	2:E:452:LYS:HD3	2.16	0.45
2:F:222:ASN:O	2:F:222:ASN:ND2	2.43	0.45
2:F:318:ASP:HB2	3:G:3:GLN:NE2	2.32	0.45
1:A:154:ARG:HE	1:A:154:ARG:HB3	1.59	0.45
1:B:274:ASP:O	1:B:276:LYS:N	2.50	0.45
2:E:399:ILE:HG13	2:E:400:GLY:H	1.80	0.45
4:H:77:LEU:HD13	4:H:78:LYS:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:334:GLU:HA	2:F:360:ARG:HH11	1.82	0.45
2:F:396:VAL:HG22	2:F:404:LEU:HD11	1.99	0.45
3:G:93:VAL:HG13	3:G:103:ARG:H	1.82	0.45
3:G:105:LYS:HE2	3:G:105:LYS:HB3	1.73	0.45
4:H:28:GLU:CD	4:H:28:GLU:H	2.25	0.45
2:E:60:PHE:CE1	2:E:229:ILE:HG12	2.53	0.44
2:E:372:ARG:NH1	2:E:374:ASP:OD2	2.50	0.44
4:H:58:ALA:HA	4:H:61:ARG:HD2	1.99	0.44
1:A:8:LYS:NZ	2:F:49:GLU:OE2	2.40	0.44
1:A:30:VAL:HG22	1:A:35:LEU:HB2	1.99	0.44
1:C:480:GLU:O	1:C:484:ILE:HG12	2.17	0.44
2:E:61:GLU:HG3	2:E:227:PRO:HG3	1.99	0.44
1:B:402:ILE:HD13	1:B:402:ILE:HA	1.80	0.44
1:B:520:LEU:HD12	1:B:520:LEU:HA	1.69	0.44
1:C:391:MET:HE2	1:C:408:ARG:HG3	1.99	0.44
3:G:158:THR:O	3:G:162:ASN:ND2	2.51	0.44
1:A:486:VAL:HG21	1:A:523:TYR:HD1	1.82	0.44
2:D:194:MET:HE2	2:D:194:MET:HB2	1.73	0.44
2:D:244:TYR:O	2:D:248:GLU:HB2	2.17	0.44
1:A:316:GLN:HE21	1:A:316:GLN:HB2	1.54	0.44
1:C:413:LEU:HD22	1:C:418:HIS:CD2	2.53	0.43
1:C:413:LEU:HD22	1:C:418:HIS:HD2	1.83	0.43
2:E:138:ILE:HG12	2:E:337:ILE:HD13	1.99	0.43
1:A:138:VAL:HG21	1:A:183:MET:HE3	1.99	0.43
1:A:248:ASP:OD1	1:A:276:LYS:NZ	2.51	0.43
1:B:81:ASN:HD22	1:B:282:MET:HB3	1.83	0.43
1:B:152:ASP:OD1	1:B:152:ASP:N	2.51	0.43
2:E:91:ARG:HG3	2:E:92:ARG:H	1.83	0.43
1:A:294:MET:HB3	1:A:295:PRO:HD2	2.00	0.43
1:B:198:LYS:HA	1:B:368:VAL:HG23	2.00	0.43
1:B:241:LEU:O	1:B:245:SER:HB3	2.18	0.43
1:C:161:LYS:HG2	1:C:172:VAL:HA	2.00	0.43
2:D:174:ARG:NH2	2:D:433:GLU:OE1	2.46	0.43
2:F:372:ARG:HH21	2:F:374:ASP:CG	2.26	0.43
3:G:58:LYS:HG2	4:H:78:LYS:HG3	2.00	0.43
1:B:212:LEU:HD22	1:B:407:TRP:CE2	2.53	0.43
2:E:151:PRO:HG2	2:E:336:GLN:HB2	2.00	0.43
2:F:301:VAL:HG23	2:F:304:LYS:HB2	2.01	0.43
1:A:59:LYS:N	1:A:62:GLU:OE2	2.51	0.43
1:A:464:LEU:HD13	1:A:464:LEU:HA	1.71	0.43
1:C:348:GLU:OE2	2:E:280:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:GLN:HA	1:C:468:VAL:HB	2.00	0.43
2:E:152:ILE:HB	2:E:313:ILE:HG13	2.01	0.43
2:E:232:ILE:HD12	2:E:270:ILE:HD12	2.00	0.43
2:D:292:ALA:HB2	2:D:332:ILE:HD13	2.01	0.43
2:E:26:ASP:N	2:E:26:ASP:OD1	2.52	0.43
2:F:341:ARG:O	2:F:345:ARG:HG2	2.19	0.43
4:H:96:LYS:HD3	4:H:96:LYS:HA	1.83	0.43
1:C:209:MET:HA	1:C:497:GLN:HE22	1.83	0.43
2:F:305:LYS:HE2	2:F:305:LYS:HB3	1.69	0.43
3:G:96:VAL:HG12	3:G:101:VAL:O	2.19	0.43
1:A:14:VAL:HG22	1:A:49:VAL:HB	2.01	0.43
2:E:218:VAL:HG12	2:E:219:LEU:H	1.83	0.43
2:F:14:ILE:HG12	2:F:19:LEU:HD13	2.01	0.43
1:A:393:GLU:OE1	1:A:396:THR:OG1	2.37	0.42
2:D:355:LEU:HD21	2:D:386:TYR:HD2	1.83	0.42
2:E:6:LYS:O	2:E:6:LYS:HG2	2.18	0.42
3:G:40:PHE:HD1	3:G:40:PHE:HA	1.72	0.42
1:A:498:ASN:ND2	1:A:501:HIS:HB2	2.34	0.42
1:B:406:PHE:CE2	1:B:408:ARG:HG2	2.54	0.42
2:E:181:GLY:HA3	2:E:184:GLU:CD	2.45	0.42
4:H:95:ARG:HD3	4:H:95:ARG:HA	1.62	0.42
1:C:314:ARG:HD2	1:C:368:VAL:HG12	2.02	0.42
2:D:8:TYR:HB2	2:D:73:VAL:O	2.19	0.42
1:B:3:GLN:HG2	1:B:65:VAL:HG22	2.01	0.42
2:D:396:VAL:CG2	2:D:404:LEU:HD11	2.50	0.42
2:E:120:ASN:HD22	2:E:122:VAL:H	1.66	0.42
2:D:194:MET:HA	2:D:222:ASN:HB3	2.00	0.42
1:A:311:GLU:HG2	1:A:314:ARG:NH1	2.35	0.42
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.78	0.42
1:A:573:ALA:O	1:A:577:LEU:CD2	2.67	0.42
2:E:175:PRO:HB2	2:E:182:GLU:HA	2.00	0.42
1:A:27:ILE:HD11	1:A:71:LEU:HB2	2.00	0.42
1:A:401:ARG:HD3	2:D:262:ASN:ND2	2.34	0.42
1:B:167:THR:OG1	1:B:168:VAL:N	2.52	0.42
1:B:272:LEU:HD23	1:B:272:LEU:HA	1.86	0.42
1:C:141:PHE:CG	1:C:283:HIS:HD2	2.38	0.42
2:E:399:ILE:HG13	2:E:400:GLY:N	2.35	0.42
1:B:477:GLN:HE21	1:B:477:GLN:HB2	1.59	0.42
2:D:22:GLU:HG2	2:D:23:ASN:H	1.84	0.42
1:A:254:GLY:HA3	1:A:262:MET:HE1	2.02	0.42
3:G:6:PRO:O	3:G:10:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:THR:O	1:A:207:THR:OG1	2.35	0.41
1:A:574:PHE:HA	1:A:577:LEU:HD21	2.01	0.41
1:C:299:ARG:O	1:C:302:SER:OG	2.33	0.41
1:C:406:PHE:CE2	1:C:408:ARG:HB2	2.56	0.41
3:G:42:LEU:HB3	3:G:147:LEU:HD13	2.01	0.41
1:A:241:LEU:O	1:A:245:SER:HB3	2.19	0.41
1:C:394:PRO:O	1:C:398:SER:OG	2.32	0.41
2:D:389:GLY:HA3	2:D:415:ALA:HB2	2.02	0.41
3:G:103:ARG:NH2	3:G:146:ARG:HB2	2.35	0.41
1:A:410:ASP:OD1	1:A:411:ALA:N	2.53	0.41
2:D:261:THR:O	2:D:265:GLU:HG2	2.20	0.41
2:F:86:LYS:HD2	2:F:249:HIS:CD2	2.55	0.41
1:C:256:GLY:HA3	1:C:329:ARG:HG2	2.03	0.41
2:E:377:GLN:H	2:E:377:GLN:HE21	1.68	0.41
2:F:96:ILE:H	2:F:96:ILE:HG13	1.43	0.41
2:F:267:LEU:HD12	2:F:267:LEU:HA	1.82	0.41
3:G:14:ARG:HD3	3:G:14:ARG:HA	1.80	0.41
2:D:374:ASP:OD1	2:D:374:ASP:N	2.33	0.41
3:G:180:GLN:HE21	3:G:180:GLN:HB2	1.69	0.41
1:B:447:TYR:HB3	1:B:448:PRO:HD3	2.03	0.41
1:B:545:LEU:HD23	1:B:545:LEU:HA	1.81	0.41
2:F:146:ARG:HD2	2:F:252:HIS:HD2	1.86	0.41
1:A:145:HIS:ND1	1:A:146:LYS:O	2.53	0.41
1:A:539:ILE:HG23	1:A:574:PHE:HZ	1.84	0.41
1:B:182:LYS:HE3	1:B:182:LYS:HB2	1.93	0.41
1:C:50:GLN:O	1:C:50:GLN:HG3	2.21	0.41
2:F:8:TYR:HB2	2:F:73:VAL:O	2.21	0.41
1:C:574:PHE:HD1	1:C:574:PHE:HA	1.72	0.41
2:E:23:ASN:ND2	2:E:23:ASN:O	2.54	0.41
2:E:453:ARG:HH11	2:E:453:ARG:HB2	1.86	0.41
1:A:323:MET:HB2	1:A:323:MET:HE3	1.67	0.41
1:A:402:ILE:HG23	1:A:403:VAL:HG13	2.03	0.41
1:B:6:ILE:HG23	1:B:14:VAL:HG13	2.03	0.41
2:E:201:LEU:HD11	2:E:221:LEU:HD13	2.02	0.41
2:E:260:MET:HE1	2:E:294:ILE:HD11	2.03	0.41
2:E:277:ILE:HG12	3:G:192:PHE:CZ	2.55	0.41
2:F:48:ILE:HD11	2:F:58:GLN:NE2	2.36	0.41
2:F:57:ILE:HG22	2:F:58:GLN:H	1.86	0.41
1:A:54:ASP:O	1:A:55:THR:OG1	2.30	0.41
1:A:195:VAL:HG11	1:A:368:VAL:HG21	2.03	0.41
1:B:21:GLY:HA2	2:E:67:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:509:MET:HE2	1:C:509:MET:HA	2.03	0.40
2:D:355:LEU:HB2	2:D:356:PRO:HD3	2.03	0.40
2:D:462:TYR:O	2:D:463:TYR:HB3	2.21	0.40
1:B:348:GLU:HG3	1:B:394:PRO:HD3	2.04	0.40
2:F:376:LYS:H	2:F:376:LYS:HG2	1.70	0.40
4:H:91:ARG:HA	4:H:91:ARG:HD3	1.74	0.40
2:D:67:ASP:OD1	2:D:67:ASP:N	2.54	0.40
2:E:395:LEU:O	2:E:399:ILE:HG12	2.21	0.40
2:F:443:LEU:HD23	2:F:443:LEU:HA	1.91	0.40
3:G:158:THR:HG22	3:G:162:ASN:ND2	2.36	0.40
1:A:255:CYS:SG	1:A:299:ARG:HB3	2.62	0.40
1:B:243:LYS:HD2	1:B:244:TRP:CZ3	2.57	0.40
1:B:572:GLY:O	1:B:575:LYS:HG2	2.21	0.40
1:C:344:MET:HG2	1:C:345:PRO:HD2	2.03	0.40
2:E:398:ILE:HD13	2:E:398:ILE:HA	1.90	0.40
1:A:9:ILE:CD1	1:A:58:LEU:HB2	2.51	0.40
1:B:141:PHE:HE2	1:B:283:HIS:CD2	2.39	0.40
1:C:237:THR:O	1:C:241:LEU:HG	2.21	0.40
1:C:365:ALA:HB2	1:C:380:ILE:HD12	2.03	0.40
1:C:458:LEU:HD21	1:C:490:ILE:HG21	2.02	0.40
2:E:153:PHE:CE2	2:E:336:GLN:HG3	2.56	0.40
2:F:321:ARG:HE	2:F:321:ARG:HB3	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	575/578 (100%)	515 (90%)	60 (10%)	0	100	100
1	B	575/578 (100%)	517 (90%)	58 (10%)	0	100	100
1	C	575/578 (100%)	516 (90%)	58 (10%)	1 (0%)	43	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	457/478 (96%)	407 (89%)	50 (11%)	0	100	100
2	E	457/478 (96%)	401 (88%)	56 (12%)	0	100	100
2	F	457/478 (96%)	400 (88%)	57 (12%)	0	100	100
3	G	208/223 (93%)	190 (91%)	18 (9%)	0	100	100
4	H	98/104 (94%)	78 (80%)	20 (20%)	0	100	100
All	All	3402/3495 (97%)	3024 (89%)	377 (11%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	420	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	468/468 (100%)	412 (88%)	56 (12%)	5	23
1	B	468/468 (100%)	410 (88%)	58 (12%)	4	22
1	C	468/468 (100%)	423 (90%)	45 (10%)	8	30
2	D	386/401 (96%)	343 (89%)	43 (11%)	6	25
2	E	386/401 (96%)	343 (89%)	43 (11%)	6	25
2	F	386/401 (96%)	338 (88%)	48 (12%)	4	22
3	G	166/176 (94%)	149 (90%)	17 (10%)	7	28
4	H	76/80 (95%)	61 (80%)	15 (20%)	1	8
All	All	2804/2863 (98%)	2479 (88%)	325 (12%)	7	24

All (325) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	9	ILE

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Mol	Chain	Res	Type
1	A	14	VAL
1	A	24	MET
1	A	30	VAL
1	A	65	VAL
1	A	83	ILE
1	A	88	GLN
1	A	122	MET
1	A	123	VAL
1	A	133	MET
1	A	135	LEU
1	A	157	VAL
1	A	160	VAL
1	A	165	GLU
1	A	167	THR
1	A	175	LEU
1	A	191	ARG
1	A	203	THR
1	A	207	THR
1	A	211	ILE
1	A	215	LEU
1	A	223	THR
1	A	234	LYS
1	A	266	LEU
1	A	273	THR
1	A	274	ASP
1	A	281	LEU
1	A	282	MET
1	A	286	VAL
1	A	293	ASN
1	A	316	GLN
1	A	320	VAL
1	A	322	LEU
1	A	329	ARG
1	A	353	TYR
1	A	354	LEU
1	A	368	VAL
1	A	370	THR
1	A	425	ASN
1	A	456	GLU
1	A	458	LEU
1	A	464	LEU
1	A	466	GLU

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Mol	Chain	Res	Type
1	A	469	GLN
1	A	520	LEU
1	A	524	LYS
1	A	530	ILE
1	A	536	ILE
1	A	540	LEU
1	A	541	GLN
1	A	542	LEU
1	A	545	LEU
1	A	574	PHE
1	A	575	LYS
1	A	577	LEU
1	B	27	ILE
1	B	30	VAL
1	B	60	VAL
1	B	80	LEU
1	B	88	GLN
1	B	96	GLU
1	B	107	VAL
1	B	123	VAL
1	B	138	VAL
1	B	149	VAL
1	B	152	ASP
1	B	153	VAL
1	B	172	VAL
1	B	189	VAL
1	B	200	ASP
1	B	218	VAL
1	B	223	THR
1	B	230	PHE
1	B	255	CYS
1	B	260	ASN
1	B	263	THR
1	B	267	VAL
1	B	272	LEU
1	B	284	ARG
1	B	285	THR
1	B	286	VAL
1	B	296	VAL
1	B	299	ARG
1	B	303	ILE
1	B	315	ASP

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Mol	Chain	Res	Type
1	B	319	SER
1	B	322	LEU
1	B	332	GLU
1	B	354	LEU
1	B	368	VAL
1	B	369	ILE
1	B	379	THR
1	B	381	VAL
1	B	402	ILE
1	B	443	VAL
1	B	446	ASP
1	B	450	LEU
1	B	469	GLN
1	B	476	LEU
1	B	477	GLN
1	B	495	LEU
1	B	503	VAL
1	B	520	LEU
1	B	524	LYS
1	B	534	VAL
1	B	536	ILE
1	B	546	GLU
1	B	548	ILE
1	B	554	VAL
1	B	557	GLU
1	B	565	GLU
1	B	574	PHE
1	B	577	LEU
1	C	20	LEU
1	C	50	GLN
1	C	83	ILE
1	C	96	GLU
1	C	103	THR
1	C	123	VAL
1	C	134	VAL
1	C	141	PHE
1	C	145	HIS
1	C	152	ASP
1	C	153	VAL
1	C	167	THR
1	C	168	VAL
1	C	186	THR

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Mol	Chain	Res	Type
1	C	200	ASP
1	C	207	THR
1	C	211	ILE
1	C	249	VAL
1	C	266	LEU
1	C	282	MET
1	C	284	ARG
1	C	287	LEU
1	C	293	ASN
1	C	315	ASP
1	C	320	VAL
1	C	329	ARG
1	C	337	ILE
1	C	340	ARG
1	C	354	LEU
1	C	363	GLU
1	C	368	VAL
1	C	369	ILE
1	C	379	THR
1	C	395	VAL
1	C	396	THR
1	C	461	GLU
1	C	517	LYS
1	C	520	LEU
1	C	531	LYS
1	C	538	GLU
1	C	568	LYS
1	C	570	ILE
1	C	571	GLN
1	C	574	PHE
1	C	577	LEU
2	D	7	GLU
2	D	25	LYS
2	D	37	ASP
2	D	50	VAL
2	D	59	VAL
2	D	94	ASN
2	D	103	LEU
2	D	119	LEU
2	D	126	LYS
2	D	130	PHE
2	D	131	ILE

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Mol	Chain	Res	Type
2	D	143	THR
2	D	183	LYS
2	D	189	VAL
2	D	194	MET
2	D	197	THR
2	D	214	LEU
2	D	216	ARG
2	D	250	ASP
2	D	258	THR
2	D	260	MET
2	D	268	ARG
2	D	270	ILE
2	D	294	ILE
2	D	309	THR
2	D	315	SER
2	D	318	ASP
2	D	322	THR
2	D	327	ASP
2	D	334	GLU
2	D	364	ASN
2	D	368	LYS
2	D	370	LYS
2	D	379	SER
2	D	381	GLN
2	D	390	VAL
2	D	398	ILE
2	D	399	ILE
2	D	401	GLU
2	D	424	ASN
2	D	429	ASN
2	D	442	LEU
2	D	457	ASP
2	E	7	GLU
2	E	26	ASP
2	E	43	ARG
2	E	73	VAL
2	E	82	LEU
2	E	89	LEU
2	E	94	ASN
2	E	100	ILE
2	E	111	ARG
2	E	119	LEU

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Mol	Chain	Res	Type
2	E	120	ASN
2	E	130	PHE
2	E	131	ILE
2	E	133	THR
2	E	137	THR
2	E	143	THR
2	E	173	VAL
2	E	180	GLU
2	E	183	LYS
2	E	194	MET
2	E	206	GLN
2	E	257	LEU
2	E	258	THR
2	E	270	ILE
2	E	274	ARG
2	E	290	ASP
2	E	294	ILE
2	E	313	ILE
2	E	327	ASP
2	E	336	GLN
2	E	355	LEU
2	E	372	ARG
2	E	374	ASP
2	E	377	GLN
2	E	379	SER
2	E	384	SER
2	E	405	THR
2	E	413	GLN
2	E	427	GLN
2	E	437	GLN
2	E	452	LYS
2	E	453	ARG
2	E	459	ILE
2	F	9	THR
2	F	11	ILE
2	F	37	ASP
2	F	53	GLU
2	F	54	TYR
2	F	63	THR
2	F	68	LEU
2	F	73	VAL
2	F	74	SER

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Mol	Chain	Res	Type
2	F	78	ASP
2	F	79	VAL
2	F	96	ILE
2	F	111	ARG
2	F	112	LEU
2	F	126	LYS
2	F	128	GLU
2	F	131	ILE
2	F	133	THR
2	F	137	THR
2	F	148	GLN
2	F	172	THR
2	F	180	GLU
2	F	183	LYS
2	F	187	PHE
2	F	197	THR
2	F	206	GLN
2	F	218	VAL
2	F	222	ASN
2	F	225	ASP
2	F	232	ILE
2	F	254	LEU
2	F	255	VAL
2	F	259	ASP
2	F	270	ILE
2	F	294	ILE
2	F	309	THR
2	F	315	SER
2	F	318	ASP
2	F	343	LEU
2	F	376	LYS
2	F	382	LEU
2	F	393	ARG
2	F	401	GLU
2	F	405	THR
2	F	412	LEU
2	F	429	ASN
2	F	451	LEU
2	F	459	ILE
3	G	13	GLN
3	G	54	ASP
3	G	55	GLN

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Mol	Chain	Res	Type
3	G	64	LEU
3	G	83	VAL
3	G	86	LEU
3	G	89	VAL
3	G	92	GLU
3	G	105	LYS
3	G	115	SER
3	G	117	VAL
3	G	128	ARG
3	G	152	GLU
3	G	159	ARG
3	G	172	ILE
3	G	182	VAL
3	G	201	ILE
4	H	6	ASP
4	H	28	GLU
4	H	35	THR
4	H	36	LEU
4	H	44	LEU
4	H	51	LEU
4	H	70	VAL
4	H	71	LEU
4	H	74	ILE
4	H	77	LEU
4	H	90	MET
4	H	93	LEU
4	H	96	LYS
4	H	98	ILE
4	H	100	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	81	ASN
1	A	88	GLN
1	A	196	GLN
1	A	442	ASN
1	A	469	GLN
1	A	477	GLN
1	A	496	GLN
1	A	571	GLN

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Mol	Chain	Res	Type
1	B	3	GLN
1	B	7	GLN
1	B	50	GLN
1	B	81	ASN
1	B	88	GLN
1	B	185	HIS
1	B	202	ASN
1	B	290	ASN
1	B	316	GLN
1	B	418	HIS
1	B	442	ASN
1	B	459	GLN
1	B	477	GLN
1	B	496	GLN
1	B	498	ASN
1	C	50	GLN
1	C	81	ASN
1	C	202	ASN
1	C	283	HIS
1	C	316	GLN
1	C	442	ASN
1	C	469	GLN
1	C	497	GLN
2	D	132	GLN
2	D	142	ASN
2	D	148	GLN
2	D	161	ASN
2	D	166	GLN
2	D	206	GLN
2	D	222	ASN
2	D	249	HIS
2	D	252	HIS
2	D	262	ASN
2	D	377	GLN
2	D	407	ASN
2	D	413	GLN
2	D	424	ASN
2	D	425	GLN
2	D	428	GLN
2	D	429	ASN
2	E	23	ASN
2	E	120	ASN

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Mol	Chain	Res	Type
2	E	142	ASN
2	E	148	GLN
2	E	222	ASN
2	E	252	HIS
2	E	323	HIS
2	E	363	ASN
2	E	377	GLN
2	E	427	GLN
2	E	429	ASN
2	E	437	GLN
2	E	448	GLN
2	E	458	HIS
2	F	46	GLN
2	F	58	GLN
2	F	129	GLN
2	F	142	ASN
2	F	148	GLN
2	F	170	GLN
2	F	252	HIS
2	F	310	GLN
2	F	323	HIS
2	F	363	ASN
2	F	413	GLN
2	F	429	ASN
2	F	448	GLN
3	G	13	GLN
3	G	17	GLN
3	G	55	GLN
3	G	95	ASN
3	G	162	ASN
3	G	166	GLN
3	G	175	GLN
3	G	180	GLN
3	G	185	GLN
4	H	11	GLN

5.3.3 RNA ⓘ

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	ADP	A	600	-	28,29,29	1.40	4 (14%)	43,45,45	1.81	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
5	ADP	A	600	-	-	5/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	600	ADP	C5-C4	4.60	1.47	1.39
5	A	600	ADP	C5-N7	-2.49	1.34	1.39
5	A	600	ADP	C5-C6	2.45	1.47	1.41
5	A	600	ADP	C8-N7	2.21	1.35	1.31

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	600	ADP	C5-C4-N3	-5.80	118.73	126.72
5	A	600	ADP	N3-C4-N9	4.72	135.19	127.17
5	A	600	ADP	C2-N3-C4	3.60	120.61	111.83
5	A	600	ADP	N3-C2-N1	-3.23	123.69	128.58
5	A	600	ADP	C4-C5-N7	-3.07	107.07	110.58
5	A	600	ADP	C4-N9-C8	2.47	108.33	105.74
5	A	600	ADP	C3'-C2'-C1'	2.42	106.05	101.46
5	A	600	ADP	C5-N7-C8	2.24	106.97	103.45
5	A	600	ADP	C2'-C3'-C4'	2.08	106.62	102.61
5	A	600	ADP	C2-N1-C6	2.01	122.03	118.73

There are no chirality outliers.

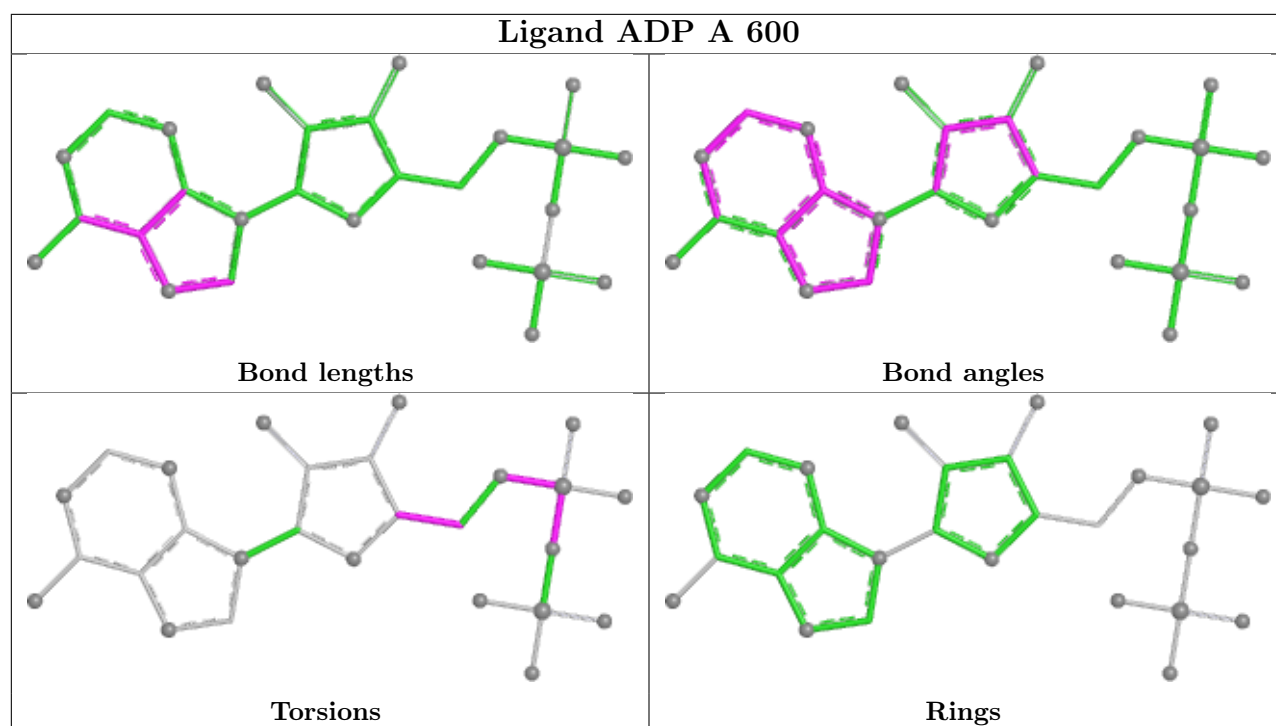
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	600	ADP	O4'-C4'-C5'-O5'
5	A	600	ADP	C3'-C4'-C5'-O5'
5	A	600	ADP	PB-O3A-PA-O1A
5	A	600	ADP	C5'-O5'-PA-O1A
5	A	600	ADP	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

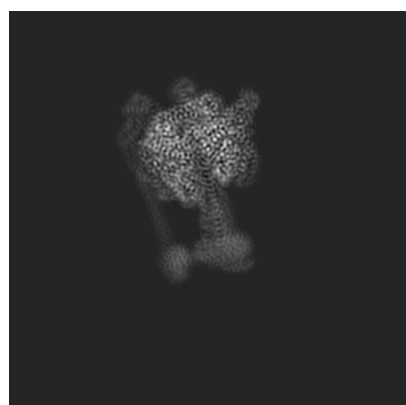
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30014. These allow visual inspection of the internal detail of the map and identification of artifacts.

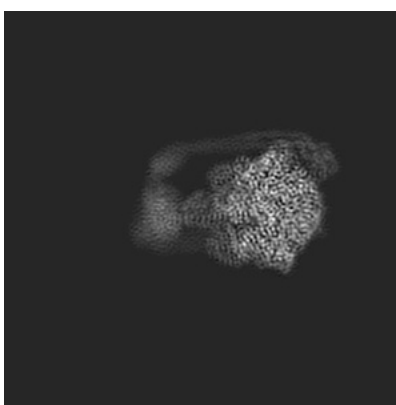
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

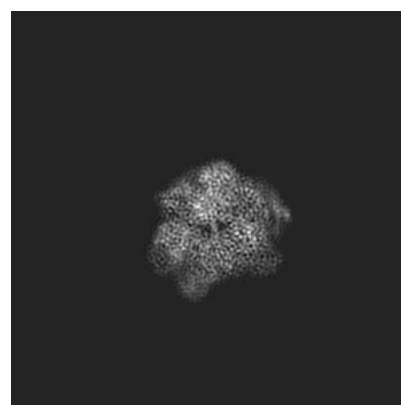
6.1.1 Primary map



X



Y

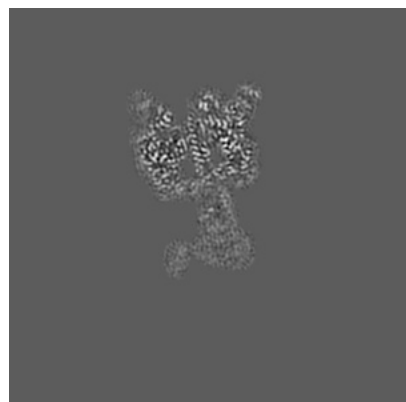


Z

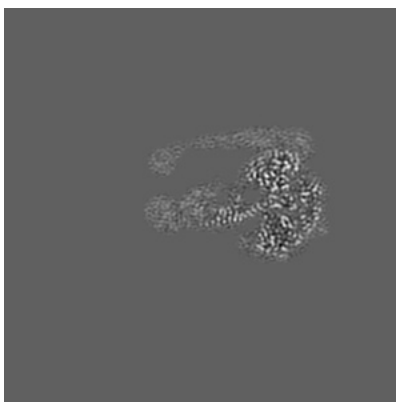
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 170



Y Index: 170

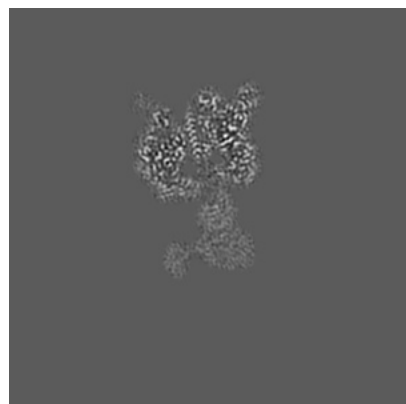


Z Index: 170

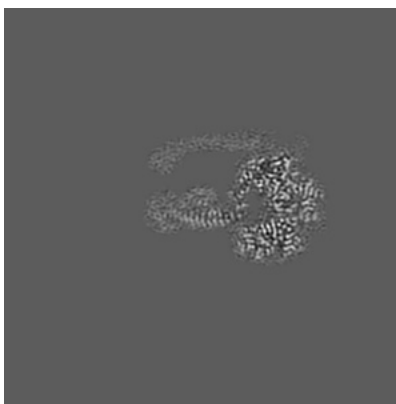
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

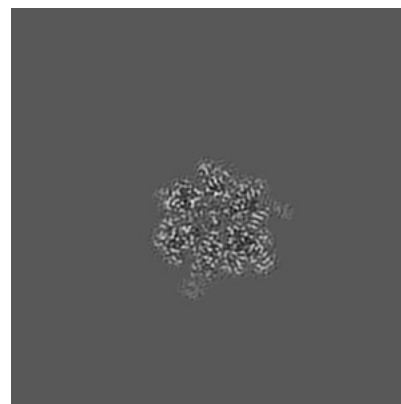
6.3.1 Primary map



X Index: 173



Y Index: 175

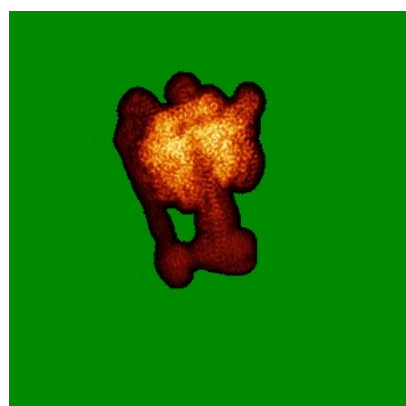


Z Index: 224

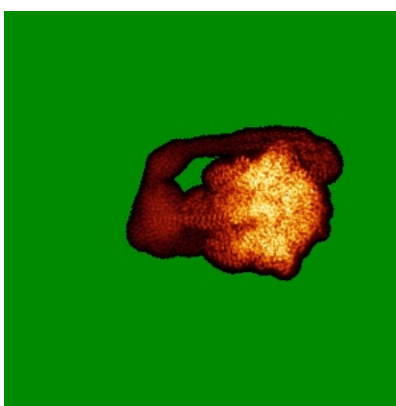
The images above show the largest variance slices of the map in three orthogonal directions.

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

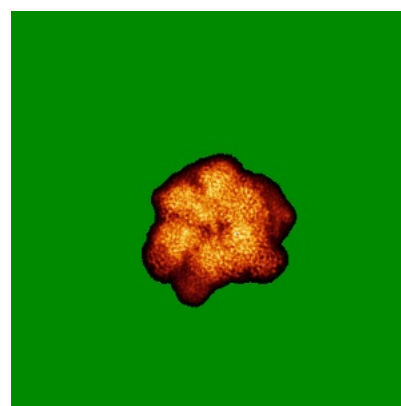
6.4.1 Primary map



X



Y

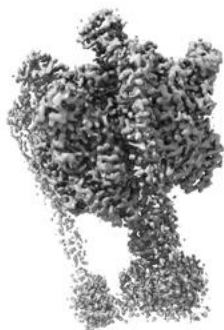


Z

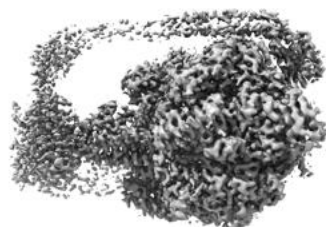
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

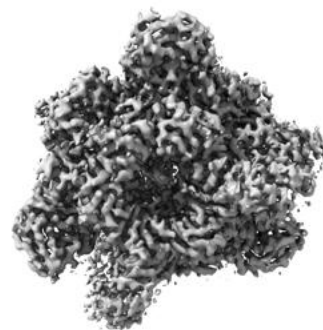
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.068. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

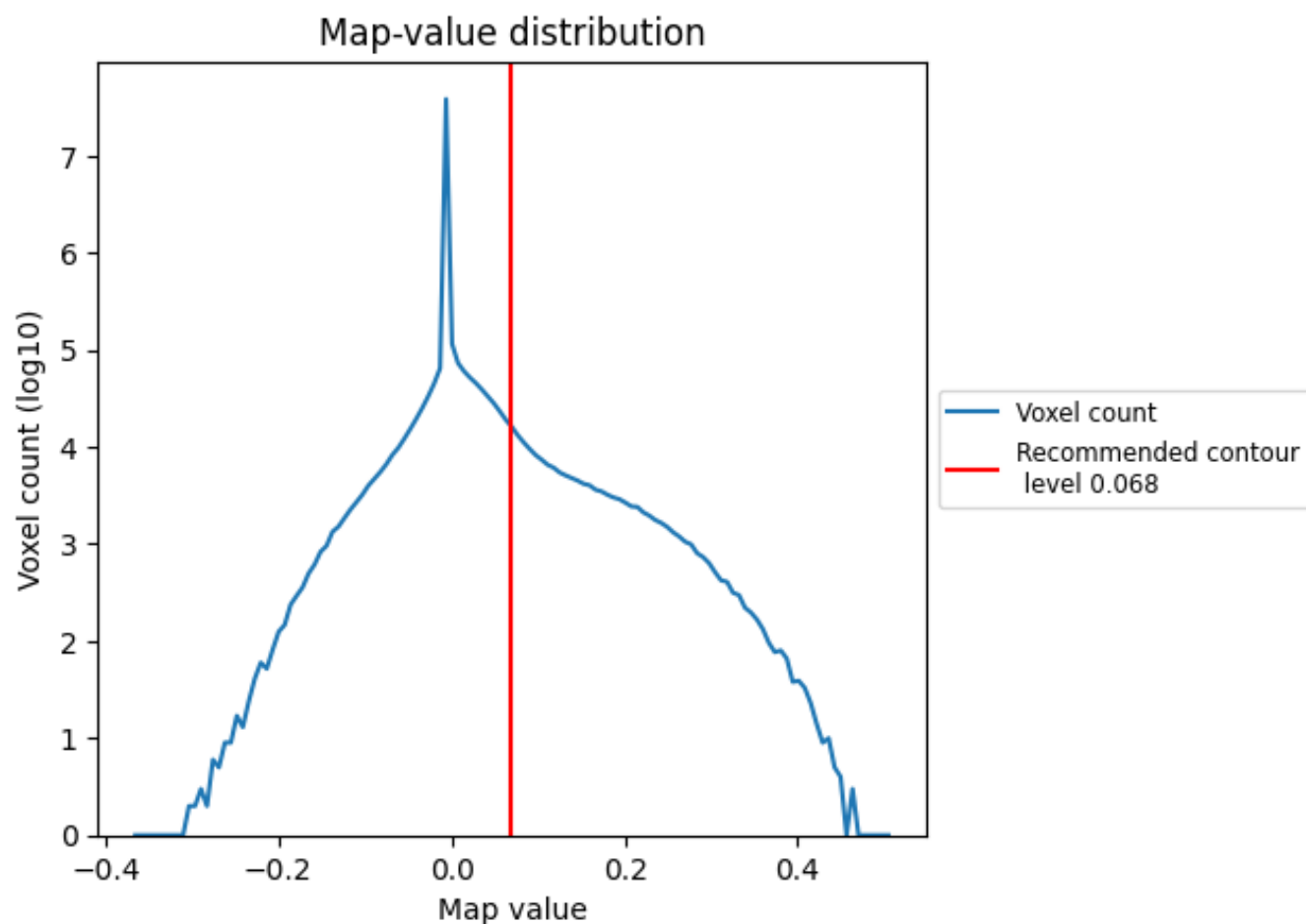
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

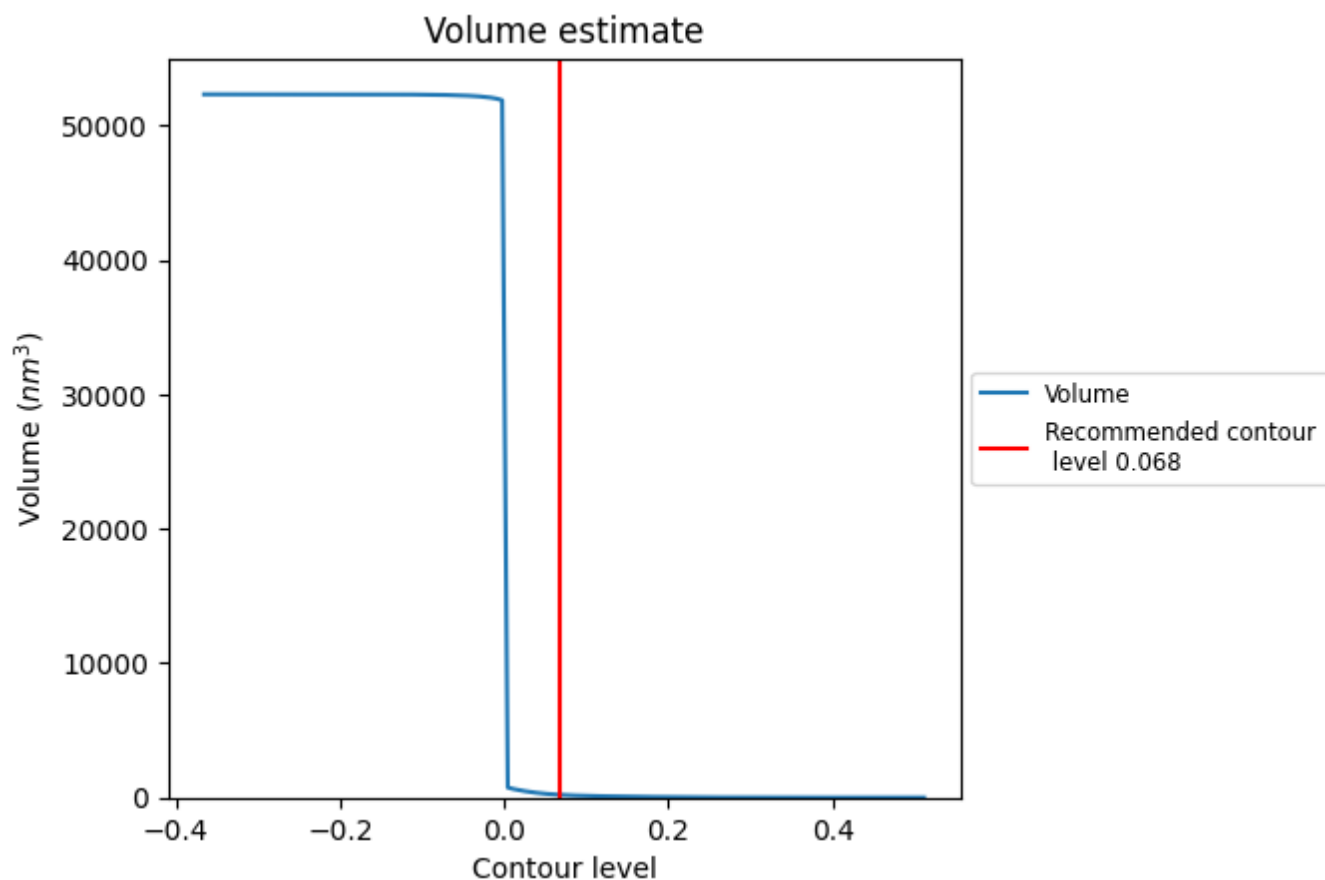
This section contains the results of statistical analysis of the map.

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.

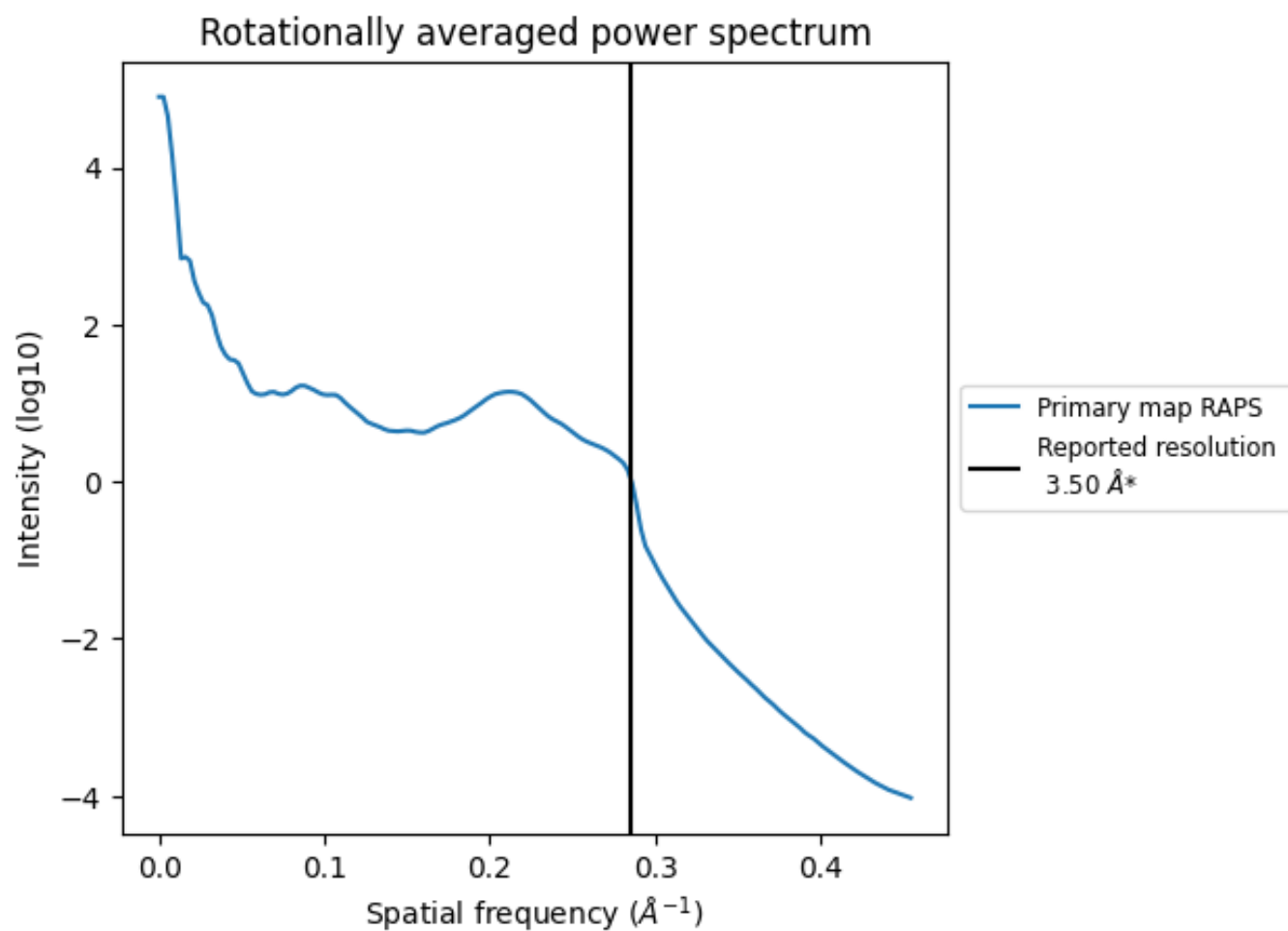
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 204 nm³; this corresponds to an approximate mass of 184 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 ⓘ

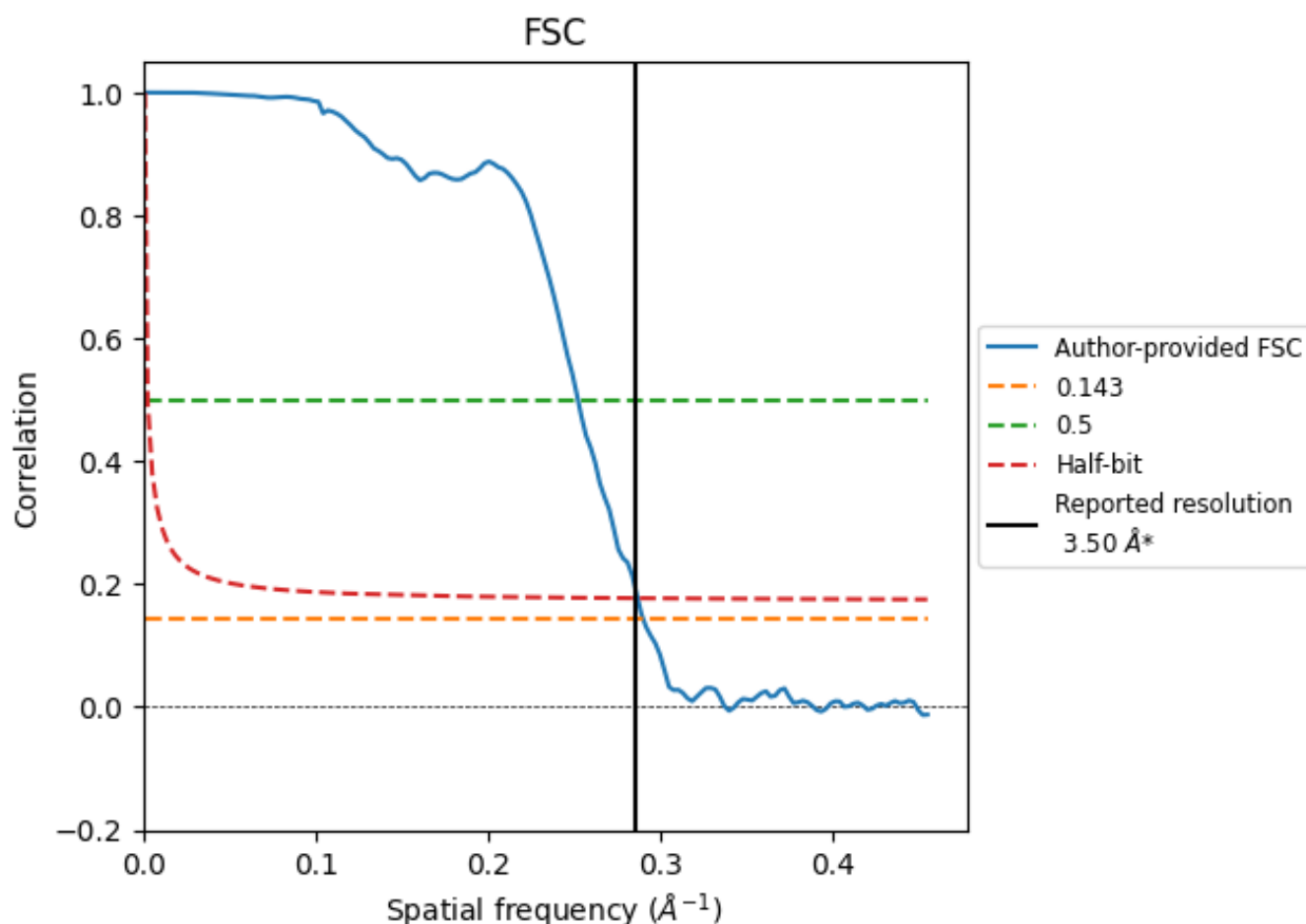


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.45	3.97	3.49
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

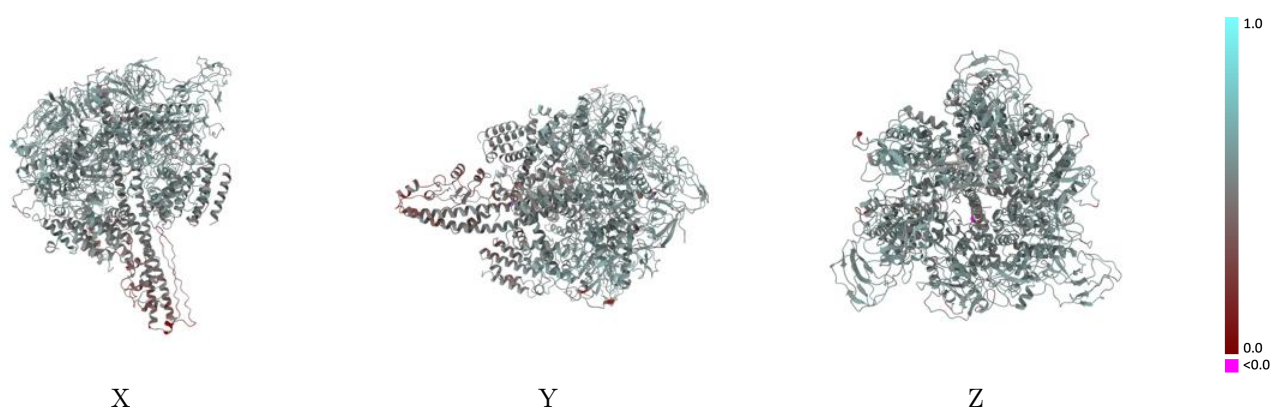
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-30014 and PDB model 6LY8. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

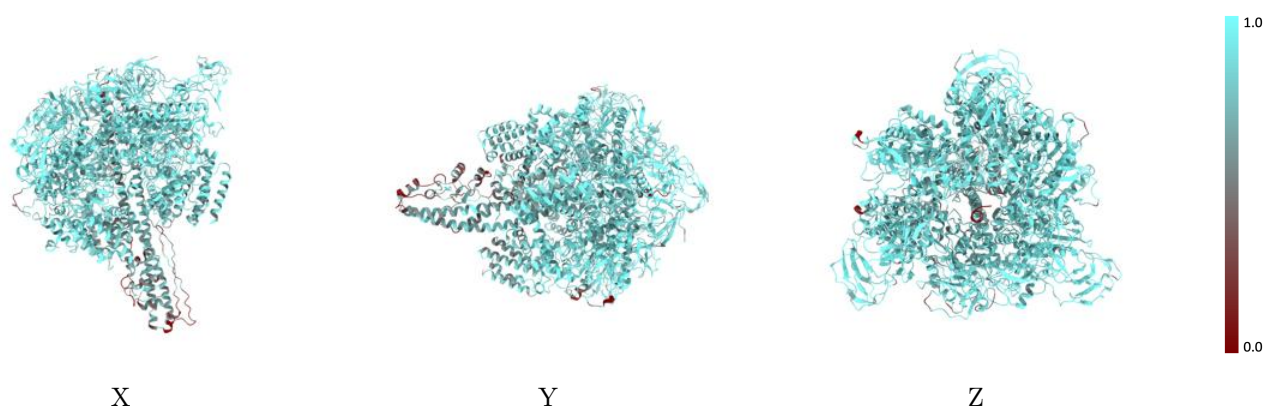
This section was not generated.

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



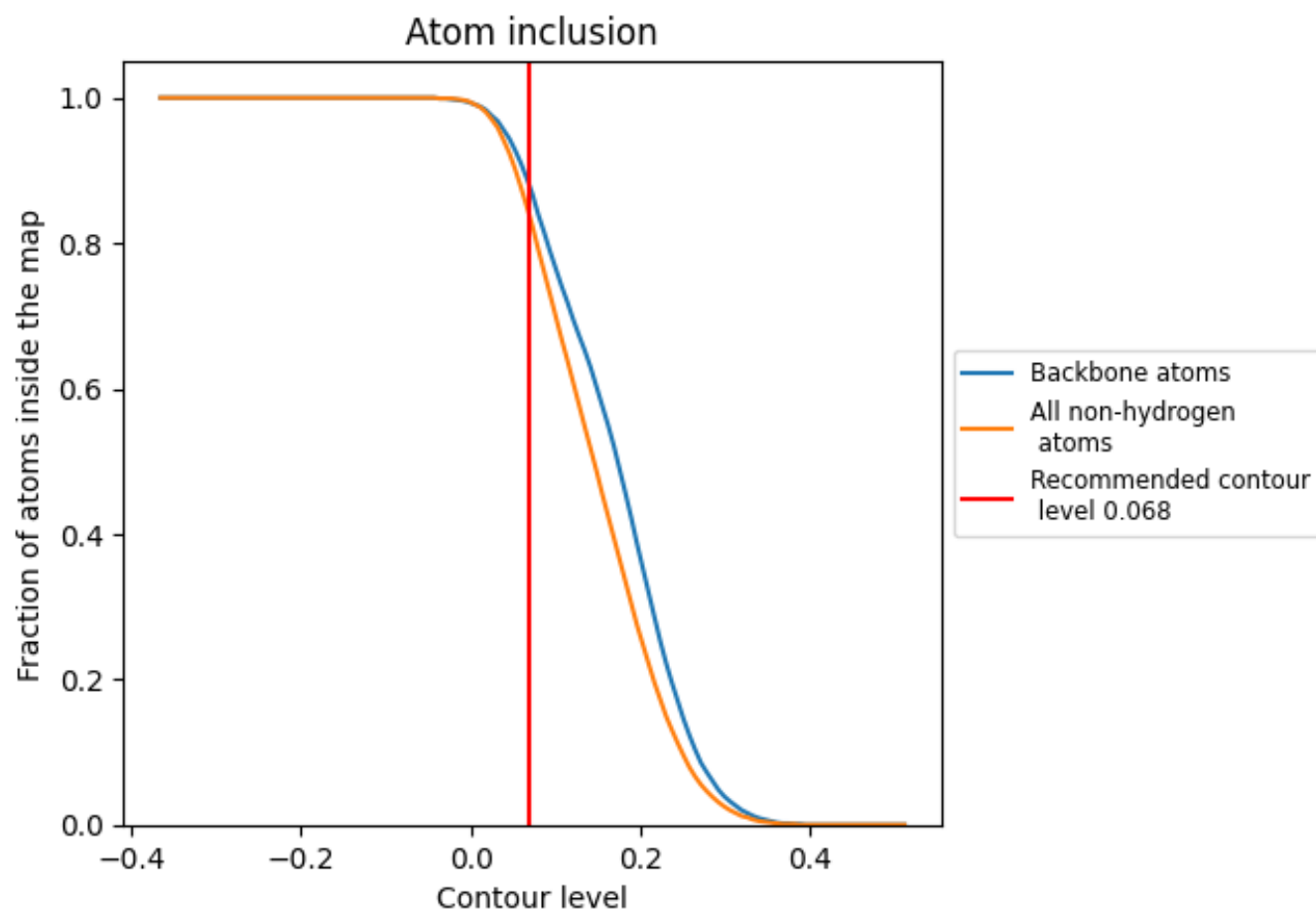
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.068).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% 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 (0.068) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8440	0.5290
A	0.8750	0.5390
B	0.8530	0.5280
C	0.8790	0.5430
D	0.8870	0.5470
E	0.8430	0.5300
F	0.8800	0.5460
G	0.6390	0.4500
H	0.4950	0.3820

1.0

0.0

<0.0