



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:26 AM UTC

PDB ID : 6M5V / pdb_00006m5v
EMDB ID : EMD-30094
Title : The coordinate of the hexameric terminase complex in the presence of the ADP-BeF3
Authors : Yang, Y.X.; Yang, P.; Wang, N.; Chen, Z.H.; Zhou, Z.H.; Rao, Z.H.; Wang, X.X.
Deposited on : 2020-03-11
Resolution : 4.50 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:

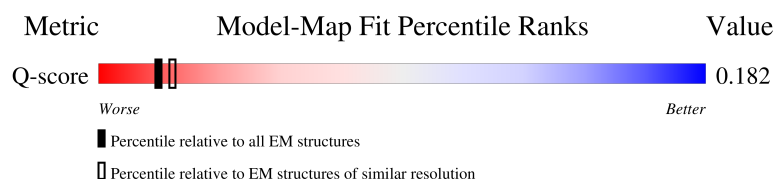
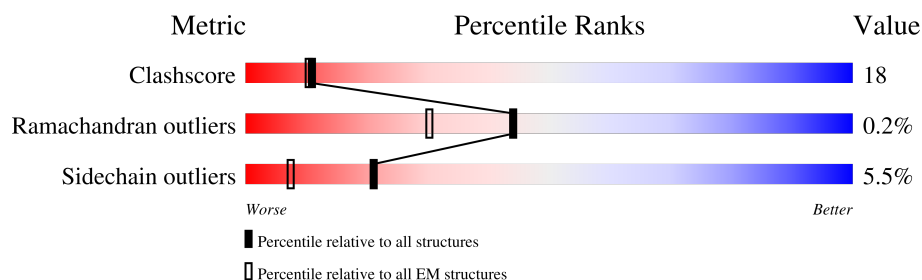
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.50 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	2937 (4.00 - 5.00)

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	690	
2	B	771	
3	C	117	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ADP	A	801	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10549 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 Tripartite terminase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	585	Total	C	N	O	S	0	0
			4482	2889	782	792	19		

- Molecule 2 is a protein called Tripartite terminase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	670	Total	C	N	O	S	0	0
			5208	3285	958	940	25		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	216	SER	ARG	engineered mutation	UNP P10212
B	312	GLN	ARG	engineered mutation	UNP P10212

- Molecule 3 is a protein called Tripartite terminase subunit 2.

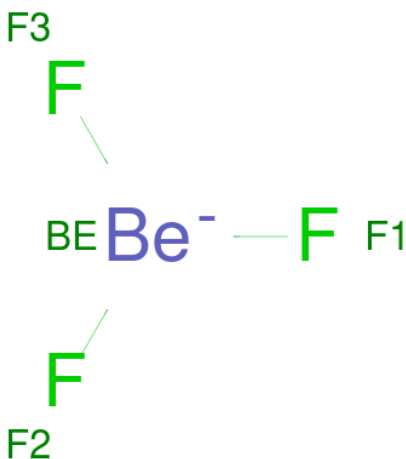
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	104	Total	C	N	O	S	0	0
			825	519	148	155	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

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



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

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

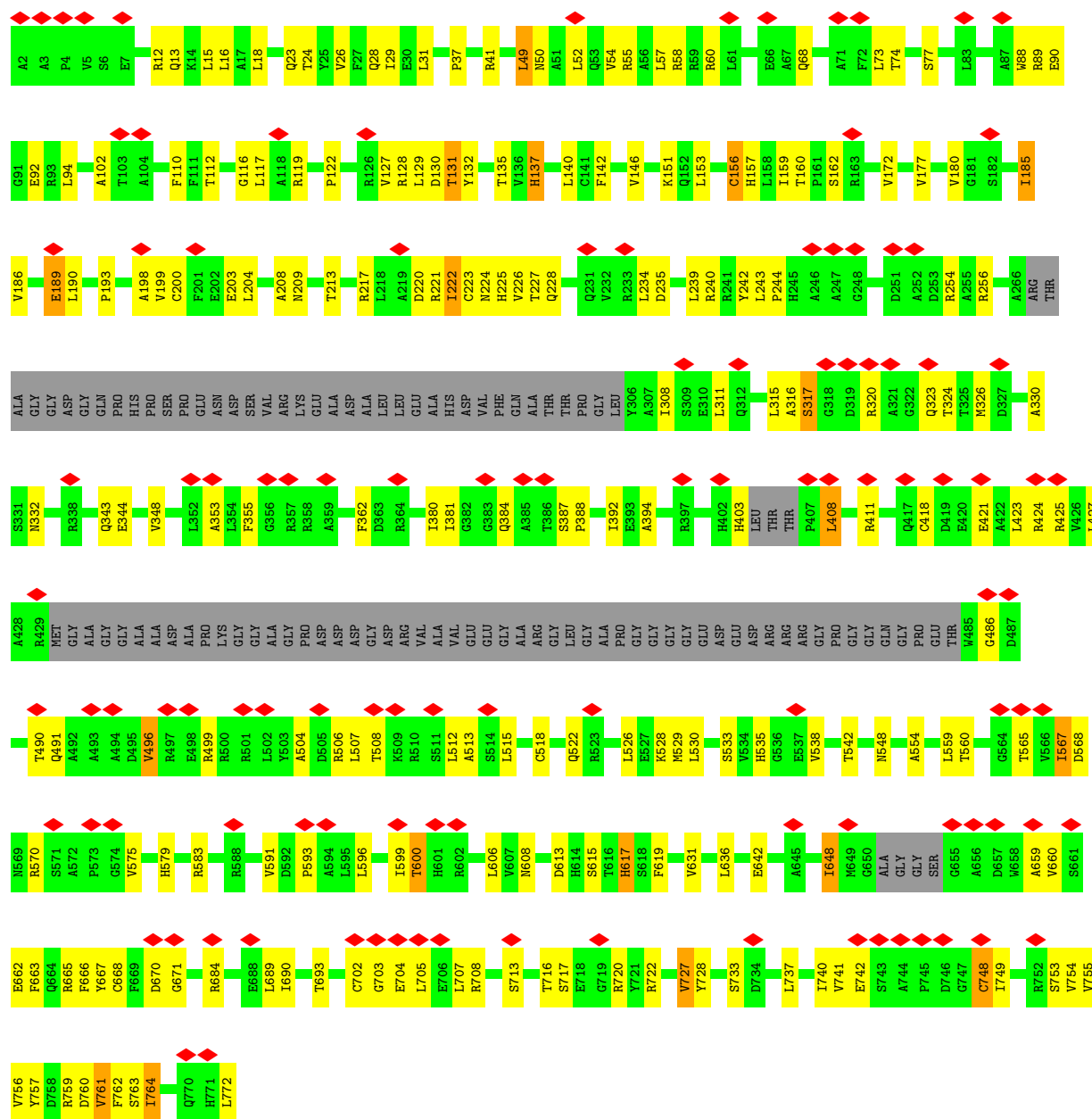
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total 1	Mg 1	0

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	B	2	Total 2	Zn 2	0

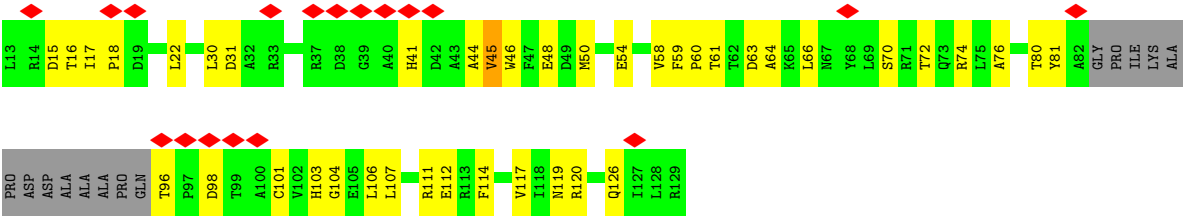


• Molecule 2: Tripartite terminase subunit 1



• Molecule 3: Tripartite terminase subunit 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7841	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 ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.258	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.0694	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.08, 2.08, 2.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	1/4589 (0.0%)	0.67	3/6240 (0.0%)
2	B	0.19	0/5316	0.44	0/7215
3	C	0.20	0/839	0.49	0/1140
All	All	0.33	1/10744 (0.0%)	0.55	3/14595 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	482	ALA	C-O	-5.49	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	CYS	CA-C-N	6.77	130.37	122.52
1	A	125	CYS	C-N-CA	6.77	130.37	122.52
1	A	477	VAL	N-CA-C	5.14	115.76	110.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4482	0	4414	195	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5208	0	5167	200	0
3	C	825	0	813	56	0
4	A	27	0	12	10	0
5	A	4	0	0	0	0
6	A	1	0	0	0	0
7	B	2	0	0	0	0
All	All	10549	0	10406	386	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 18.

All (386) 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:A:395:PHE:CZ	2:B:427:LEU:HD23	1.63	1.32
2:B:381:ILE:CG2	3:C:74:ARG:HB3	1.61	1.28
2:B:180:VAL:HG13	2:B:535:HIS:CE1	1.71	1.25
2:B:381:ILE:HG22	3:C:74:ARG:CB	1.74	1.15
1:A:525:VAL:CG1	1:A:537:ALA:HB3	1.78	1.13
1:A:616:GLU:CG	1:A:618:LEU:HD11	1.78	1.13
3:C:17:ILE:HG13	3:C:18:PRO:HD3	1.27	1.13
2:B:667:TYR:HD2	2:B:733:SER:HA	1.14	1.08
1:A:395:PHE:HZ	2:B:427:LEU:CD2	1.68	1.06
3:C:17:ILE:HD13	3:C:46:TRP:HZ3	1.15	1.06
1:A:298:PHE:HD1	1:A:336:PHE:CE2	1.74	1.04
2:B:49:LEU:HG	3:C:17:ILE:HG22	1.35	1.03
2:B:180:VAL:HG13	2:B:535:HIS:HE1	1.24	1.02
1:A:616:GLU:HG3	1:A:618:LEU:HD11	1.41	1.01
2:B:667:TYR:CD2	2:B:733:SER:HA	1.94	1.01
1:A:525:VAL:HG12	1:A:537:ALA:HB3	1.42	1.01
2:B:392:ILE:CD1	2:B:530:LEU:HD12	1.91	1.01
1:A:395:PHE:HZ	2:B:427:LEU:HD23	0.87	1.00
1:A:430:CYS:SG	4:A:801:ADP:C8	2.56	0.98
1:A:298:PHE:CD1	1:A:322:ILE:HD11	1.97	0.98
1:A:298:PHE:CE1	1:A:322:ILE:CG1	2.47	0.97
1:A:487:LEU:HD21	2:B:506:ARG:NH1	1.82	0.94
1:A:616:GLU:HG3	1:A:618:LEU:CD1	1.98	0.93
3:C:17:ILE:CD1	3:C:46:TRP:HZ3	1.81	0.93
1:A:525:VAL:HG11	1:A:537:ALA:HB3	1.50	0.91
2:B:392:ILE:HD11	2:B:530:LEU:HD12	1.52	0.90
1:A:298:PHE:CD1	1:A:336:PHE:CE2	2.59	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:LEU:HD21	2:B:506:ARG:CZ	2.00	0.90
1:A:681:LEU:HD23	1:A:709:MET:HG3	1.53	0.90
2:B:381:ILE:HG22	3:C:74:ARG:HB3	0.92	0.89
3:C:17:ILE:HG13	3:C:18:PRO:CD	2.02	0.89
1:A:49:ALA:HB3	1:A:123:LYS:HB3	1.52	0.88
1:A:298:PHE:HE1	1:A:322:ILE:CG1	1.86	0.86
3:C:17:ILE:HD13	3:C:46:TRP:CZ3	2.07	0.86
1:A:492:SER:HB3	2:B:317:SER:HB2	1.56	0.85
1:A:358:ALA:O	1:A:395:PHE:HD2	1.60	0.83
2:B:667:TYR:CE2	2:B:733:SER:N	2.47	0.83
2:B:667:TYR:HE2	2:B:733:SER:N	1.77	0.83
1:A:298:PHE:CE1	1:A:322:ILE:HG12	2.13	0.83
2:B:411:ARG:NH1	2:B:418:CYS:SG	2.53	0.82
1:A:358:ALA:O	1:A:395:PHE:CD2	2.33	0.82
1:A:488:LEU:HD21	2:B:515:LEU:HA	1.62	0.82
3:C:17:ILE:CG1	3:C:18:PRO:HD3	2.10	0.82
1:A:525:VAL:CG1	1:A:537:ALA:CB	2.57	0.81
1:A:395:PHE:CZ	2:B:427:LEU:CD2	2.51	0.81
2:B:392:ILE:HD13	2:B:530:LEU:HD12	1.61	0.81
1:A:298:PHE:HE1	1:A:322:ILE:HG13	1.45	0.79
2:B:667:TYR:CD2	2:B:733:SER:CA	2.64	0.79
1:A:298:PHE:CE1	1:A:322:ILE:HD11	2.18	0.79
1:A:113:LEU:O	1:A:117:VAL:HG23	1.82	0.78
1:A:636:LEU:HD21	1:A:640:LYS:HB2	1.66	0.77
1:A:616:GLU:CG	1:A:618:LEU:CD1	2.59	0.74
2:B:223:CYS:O	2:B:225:HIS:ND1	2.21	0.74
1:A:353:LEU:HD23	1:A:380:ILE:HG12	1.70	0.73
2:B:180:VAL:HA	2:B:535:HIS:NE2	2.04	0.72
1:A:486:PHE:HE2	1:A:674:VAL:HG13	1.54	0.72
2:B:49:LEU:CG	3:C:17:ILE:HG22	2.16	0.72
2:B:180:VAL:CG1	2:B:535:HIS:HE1	2.01	0.71
1:A:298:PHE:CE1	1:A:322:ILE:CD1	2.74	0.71
1:A:530:ARG:HG3	1:A:531:ASP:H	1.55	0.71
2:B:132:TYR:HE2	2:B:667:TYR:CZ	2.09	0.71
2:B:180:VAL:CG1	2:B:535:HIS:CE1	2.63	0.70
2:B:132:TYR:HE2	2:B:667:TYR:OH	1.73	0.70
3:C:101:CYS:O	3:C:104:GLY:N	2.22	0.70
2:B:737:LEU:HB3	2:B:764:ILE:HG13	1.72	0.70
1:A:263:GLY:HA2	4:A:801:ADP:O2A	1.91	0.69
1:A:525:VAL:HG12	1:A:537:ALA:CB	2.21	0.69
1:A:487:LEU:O	1:A:487:LEU:HD23	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:THR:HG22	3:C:63:ASP:H	1.57	0.69
1:A:525:VAL:HG11	1:A:537:ALA:CB	2.22	0.69
1:A:298:PHE:HD1	1:A:336:PHE:HE2	1.40	0.69
2:B:239:LEU:CD2	2:B:343:GLN:NE2	2.55	0.69
1:A:289:HIS:HE1	1:A:361:ILE:HG12	1.58	0.68
1:A:620:TYR:CD2	1:A:725:PRO:HB3	2.29	0.68
1:A:616:GLU:CD	1:A:618:LEU:HD11	2.19	0.68
1:A:46:LEU:HD22	2:B:13:GLN:HG2	1.75	0.67
1:A:63:VAL:HG12	1:A:64:GLY:N	2.08	0.67
1:A:489:TYR:CE1	3:C:120:ARG:HG2	2.28	0.67
2:B:117:LEU:HA	3:C:80:THR:HG22	1.74	0.67
2:B:157:HIS:NE2	2:B:608:ASN:O	2.27	0.67
1:A:489:TYR:HE1	1:A:657:MET:SD	2.18	0.67
1:A:636:LEU:C	1:A:636:LEU:HD23	2.20	0.67
2:B:381:ILE:HG21	3:C:74:ARG:HB3	1.74	0.67
1:A:654:GLY:O	3:C:120:ARG:NH1	2.28	0.67
2:B:50:ASN:ND2	3:C:50:MET:SD	2.68	0.67
3:C:17:ILE:CD1	3:C:46:TRP:CZ3	2.70	0.67
1:A:495:THR:O	2:B:320:ARG:NH2	2.28	0.66
3:C:17:ILE:HG21	3:C:48:GLU:OE2	1.95	0.66
2:B:239:LEU:HD23	2:B:343:GLN:NE2	2.11	0.66
2:B:244:PRO:O	2:B:254:ARG:HD2	1.95	0.66
1:A:487:LEU:HD23	1:A:487:LEU:C	2.20	0.65
2:B:565:THR:HB	2:B:754:VAL:HG23	1.79	0.65
2:B:156:CYS:HB3	2:B:159:ILE:HD11	1.78	0.65
1:A:289:HIS:CG	1:A:360:PHE:HD2	2.14	0.65
1:A:480:LYS:NZ	1:A:480:LYS:HB3	2.12	0.65
1:A:487:LEU:HD11	2:B:506:ARG:HH12	1.62	0.65
2:B:693:THR:HG23	2:B:705:LEU:HD12	1.79	0.65
1:A:430:CYS:SG	4:A:801:ADP:H8	2.16	0.65
1:A:206:LYS:HG2	1:A:210:MET:HE2	1.78	0.64
1:A:538:LEU:HD22	1:A:708:LEU:HD11	1.79	0.64
1:A:86:ASN:HD21	1:A:103:THR:HB	1.62	0.64
1:A:620:TYR:CZ	1:A:725:PRO:HG3	2.33	0.64
2:B:132:TYR:CE2	2:B:667:TYR:OH	2.51	0.64
1:A:516:THR:HG22	1:A:518:ALA:H	1.62	0.63
2:B:52:LEU:HD11	3:C:30:LEU:HB3	1.80	0.63
1:A:490:ARG:NH2	2:B:506:ARG:HH22	1.96	0.63
2:B:239:LEU:CD2	2:B:343:GLN:HE22	2.11	0.63
1:A:252:ARG:HA	1:A:379:LYS:HG3	1.81	0.63
1:A:388:THR:HA	1:A:391:ALA:HB2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:GLU:CB	2:B:496:VAL:CG2	2.77	0.62
1:A:67:HIS:CD2	1:A:69:CYS:H	2.18	0.62
2:B:223:CYS:O	2:B:225:HIS:N	2.33	0.62
1:A:408:ASN:HB3	2:B:208:ALA:HA	1.82	0.62
2:B:119:ARG:HG3	2:B:122:PRO:HD3	1.82	0.62
2:B:324:THR:OG1	3:C:126:GLN:NE2	2.33	0.62
2:B:667:TYR:CE2	2:B:733:SER:CA	2.83	0.62
2:B:132:TYR:HE2	2:B:667:TYR:HH	1.48	0.62
2:B:737:LEU:HD22	2:B:761:VAL:HA	1.82	0.62
1:A:370:MET:HA	1:A:373:LEU:HD12	1.81	0.62
2:B:185:ILE:HD11	3:C:70:SER:HB2	1.81	0.61
1:A:651:PHE:HA	1:A:656:VAL:HG13	1.82	0.61
2:B:151:LYS:HD3	2:B:198:ALA:HB2	1.82	0.61
1:A:113:LEU:HD21	2:B:15:LEU:HD11	1.83	0.61
1:A:269:VAL:HG22	1:A:270:PRO:HD3	1.82	0.61
1:A:620:TYR:CE2	1:A:725:PRO:HG3	2.36	0.61
1:A:616:GLU:HG2	1:A:618:LEU:HD11	1.79	0.60
2:B:243:LEU:N	2:B:244:PRO:CD	2.65	0.60
1:A:86:ASN:ND2	1:A:107:GLU:OE2	2.34	0.60
1:A:63:VAL:HG21	2:B:16:LEU:HB3	1.83	0.60
1:A:302:ASP:OD2	1:A:316:HIS:NE2	2.35	0.60
1:A:351:ASN:HA	1:A:378:CYS:HA	1.83	0.60
2:B:226:VAL:HG13	2:B:227:THR:HG23	1.85	0.59
1:A:63:VAL:HG12	1:A:64:GLY:H	1.66	0.59
1:A:413:ILE:HG12	1:A:420:ARG:HD2	1.85	0.59
1:A:490:ARG:NH2	2:B:506:ARG:NH2	2.51	0.58
3:C:17:ILE:CG1	3:C:18:PRO:CD	2.75	0.58
2:B:24:THR:O	2:B:28:GLN:HG2	2.03	0.58
2:B:193:PRO:HB2	2:B:222:ILE:HG22	1.84	0.58
1:A:559:VAL:HG13	1:A:600:MET:CE	2.34	0.58
1:A:618:LEU:HB3	1:A:726:HIS:O	2.03	0.58
1:A:489:TYR:CE1	1:A:657:MET:SD	2.97	0.58
2:B:529:MET:O	3:C:74:ARG:NH2	2.37	0.58
2:B:570:ARG:HG2	2:B:759:ARG:HG2	1.84	0.57
1:A:480:LYS:HB3	1:A:480:LYS:HZ3	1.69	0.57
1:A:395:PHE:CE1	2:B:427:LEU:HA	2.39	0.57
2:B:600:THR:HA	2:B:648:ILE:HD12	1.85	0.57
1:A:616:GLU:HG3	1:A:618:LEU:HD12	1.86	0.57
2:B:666:PHE:HB3	2:B:759:ARG:O	2.04	0.57
1:A:284:ILE:HG12	1:A:352:LEU:HD12	1.87	0.57
1:A:298:PHE:CE1	1:A:322:ILE:HG13	2.29	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LEU:HD13	1:A:354:PHE:HE2	1.70	0.56
3:C:17:ILE:HD13	3:C:48:GLU:OE2	2.06	0.56
2:B:55:ARG:NH2	3:C:31:ASP:OD1	2.36	0.56
2:B:381:ILE:HG21	3:C:74:ARG:C	2.31	0.56
1:A:111:PRO:O	1:A:115:ARG:NH1	2.38	0.55
1:A:360:PHE:CG	1:A:360:PHE:O	2.59	0.55
2:B:741:VAL:HG23	2:B:742:GLU:HG2	1.87	0.55
1:A:525:VAL:HG13	1:A:537:ALA:N	2.21	0.55
2:B:760:ASP:HB2	2:B:763:SER:HB3	1.89	0.55
2:B:208:ALA:O	2:B:217:ARG:NH1	2.40	0.55
2:B:18:LEU:HD11	2:B:57:LEU:HD11	1.88	0.55
2:B:381:ILE:CG2	3:C:74:ARG:CB	2.53	0.55
1:A:530:ARG:HG3	1:A:531:ASP:N	2.19	0.55
2:B:129:LEU:HD11	2:B:153:LEU:HD13	1.89	0.55
1:A:67:HIS:HD2	1:A:69:CYS:H	1.53	0.54
2:B:311:LEU:HD12	2:B:330:ALA:HB2	1.88	0.54
1:A:525:VAL:CG1	1:A:537:ALA:N	2.71	0.54
2:B:662:GLU:OE1	2:B:663:PHE:N	2.41	0.54
1:A:360:PHE:O	1:A:360:PHE:CD2	2.62	0.53
1:A:63:VAL:CG1	1:A:64:GLY:N	2.71	0.53
2:B:37:PRO:HG3	2:B:110:PHE:CD2	2.42	0.53
1:A:374:ASN:ND2	2:B:424:ARG:HH22	2.06	0.53
2:B:239:LEU:HD12	2:B:240:ARG:N	2.23	0.53
2:B:392:ILE:HD13	2:B:530:LEU:CD1	2.35	0.53
2:B:41:ARG:HD2	2:B:102:ALA:HB2	1.91	0.53
1:A:559:VAL:HG13	1:A:600:MET:HE2	1.91	0.53
1:A:361:ILE:HD12	1:A:395:PHE:HE2	1.74	0.53
2:B:234:LEU:HD13	3:C:64:ALA:HB2	1.91	0.53
2:B:381:ILE:HG21	3:C:74:ARG:O	2.08	0.53
2:B:204:LEU:O	2:B:217:ARG:NH2	2.42	0.52
1:A:321:THR:HG22	1:A:335:VAL:HB	1.91	0.52
2:B:23:GLN:HA	2:B:26:VAL:HG12	1.91	0.52
1:A:63:VAL:CG1	1:A:64:GLY:H	2.22	0.52
2:B:418:CYS:O	2:B:421:GLU:HG3	2.10	0.52
1:A:93:LEU:HD22	1:A:235:VAL:HG22	1.92	0.51
1:A:96:ARG:NH2	2:B:615:SER:O	2.36	0.51
3:C:76:ALA:O	3:C:80:THR:HG23	2.10	0.51
1:A:576:VAL:HG22	1:A:617:LEU:HD12	1.93	0.51
1:A:52:THR:HG21	1:A:67:HIS:HB2	1.91	0.51
1:A:167:LEU:HD11	1:A:201:LEU:HG	1.93	0.51
2:B:323:GLN:NE2	2:B:324:THR:O	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASP:OD1	2:B:717:SER:OG	2.29	0.51
3:C:15:ASP:HA	3:C:44:ALA:CB	2.41	0.51
1:A:211:HIS:HB3	1:A:379:LYS:NZ	2.26	0.51
1:A:233:ARG:NH2	1:A:243:ASP:OD1	2.44	0.51
1:A:267:PHE:C	1:A:270:PRO:HD2	2.35	0.51
2:B:713:SER:O	2:B:713:SER:OG	2.28	0.51
1:A:480:LYS:NZ	1:A:480:LYS:CB	2.73	0.51
2:B:486:GLY:O	2:B:490:THR:HG23	2.11	0.51
2:B:332:ASN:HB3	2:B:394:ALA:HB1	1.92	0.51
2:B:54:VAL:O	2:B:58:ARG:HG2	2.11	0.50
2:B:708:ARG:HB2	2:B:728:TYR:CE1	2.47	0.50
2:B:203:GLU:OE1	2:B:221:ARG:NH2	2.45	0.50
2:B:315:LEU:H	3:C:119:ASN:HD21	1.60	0.50
2:B:408:LEU:HD23	2:B:512:LEU:HD21	1.93	0.50
1:A:211:HIS:HD2	1:A:254:THR:HG21	1.77	0.49
2:B:667:TYR:CD2	2:B:733:SER:N	2.80	0.49
1:A:211:HIS:CD2	1:A:254:THR:HG21	2.47	0.49
1:A:282:ILE:N	1:A:332:SER:OG	2.45	0.49
1:A:349:ASP:HA	1:A:375:GLN:HE22	1.76	0.49
1:A:361:ILE:HD12	1:A:395:PHE:CE2	2.47	0.49
1:A:636:LEU:C	1:A:636:LEU:CD2	2.85	0.49
1:A:263:GLY:HA2	4:A:801:ADP:H5'2	1.94	0.49
2:B:518:CYS:O	2:B:522:GLN:HG2	2.13	0.49
3:C:15:ASP:OD1	3:C:16:THR:N	2.45	0.49
1:A:387:ASN:O	1:A:388:THR:OG1	2.28	0.49
1:A:166:LEU:HD21	1:A:308:TRP:CD2	2.48	0.49
2:B:568:ASP:OD1	2:B:570:ARG:N	2.38	0.49
1:A:487:LEU:C	1:A:487:LEU:CD2	2.86	0.49
2:B:617:HIS:C	2:B:619:PHE:H	2.21	0.49
1:A:252:ARG:HB2	1:A:379:LYS:HA	1.93	0.48
2:B:308:ILE:H	2:B:308:ILE:HD12	1.78	0.48
2:B:116:GLY:HA3	2:B:119:ARG:HD2	1.94	0.48
1:A:490:ARG:NH2	1:A:674:VAL:HB	2.28	0.48
1:A:202:GLU:CD	1:A:428:THR:HG22	2.38	0.48
1:A:577:ARG:HA	1:A:618:LEU:O	2.13	0.48
2:B:140:LEU:HD11	2:B:172:VAL:HG22	1.96	0.48
2:B:256:ARG:NH2	2:B:353:ALA:O	2.45	0.48
2:B:529:MET:HE3	3:C:114:PHE:HB2	1.95	0.48
1:A:325:SER:OG	1:A:326:PHE:N	2.47	0.48
2:B:332:ASN:ND2	2:B:394:ALA:O	2.44	0.48
2:B:689:LEU:HD21	2:B:707:LEU:HD11	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:716:THR:OG1	2:B:720:ARG:HB3	2.14	0.48
1:A:39:ASP:H	1:A:87:SER:HB2	1.77	0.47
1:A:266:TRP:CZ2	4:A:801:ADP:H2	2.32	0.47
1:A:487:LEU:HD11	2:B:506:ARG:NH1	2.26	0.47
4:A:801:ADP:C2'	4:A:801:ADP:N3	2.78	0.47
2:B:606:LEU:HD12	2:B:690:ILE:HD11	1.96	0.47
3:C:22:LEU:HD12	3:C:22:LEU:HA	1.76	0.47
1:A:525:VAL:HG13	1:A:525:VAL:O	2.14	0.47
1:A:45:PHE:HD1	1:A:137:TYR:HD1	1.62	0.47
1:A:83:LEU:HD13	2:B:12:ARG:HD2	1.96	0.47
1:A:211:HIS:HB3	1:A:379:LYS:HZ1	1.79	0.47
1:A:399:LEU:HD21	1:A:406:LEU:HD23	1.97	0.47
1:A:505:TYR:CE2	1:A:577:ARG:HD2	2.50	0.47
2:B:128:ARG:HA	2:B:137:HIS:HB3	1.95	0.47
3:C:15:ASP:HB3	3:C:18:PRO:HD2	1.97	0.47
2:B:504:ALA:O	2:B:508:THR:HG23	2.15	0.47
1:A:489:TYR:CZ	3:C:120:ARG:HG2	2.50	0.46
1:A:661:GLU:CB	2:B:496:VAL:HG21	2.45	0.46
4:A:801:ADP:N3	4:A:801:ADP:H2'	2.30	0.46
1:A:414:CYS:HB2	1:A:419:PRO:HG2	1.97	0.46
2:B:344:GLU:O	2:B:348:VAL:HG23	2.15	0.46
2:B:355:PHE:CZ	3:C:54:GLU:HG3	2.51	0.46
1:A:156:LEU:O	1:A:160:VAL:HG22	2.15	0.46
2:B:529:MET:HE2	2:B:529:MET:HB2	1.76	0.46
1:A:255:VAL:HG22	1:A:382:PHE:HB2	1.98	0.46
2:B:599:ILE:HG22	2:B:648:ILE:HD13	1.98	0.46
1:A:163:PHE:CE2	1:A:171:PHE:HZ	2.34	0.46
1:A:266:TRP:HB2	4:A:801:ADP:H5'1	1.98	0.46
2:B:130:ASP:HA	2:B:135:THR:HB	1.97	0.46
2:B:388:PRO:O	2:B:392:ILE:HG12	2.15	0.46
1:A:202:GLU:HG2	4:A:801:ADP:N6	2.30	0.46
2:B:227:THR:OG1	2:B:528:LYS:NZ	2.42	0.46
1:A:155:GLN:HE21	1:A:280:ARG:HD2	1.81	0.46
1:A:207:MET:HA	1:A:210:MET:HE3	1.98	0.46
1:A:395:PHE:HE1	2:B:427:LEU:HA	1.77	0.45
1:A:534:ILE:HA	1:A:657:MET:O	2.15	0.45
2:B:74:THR:HG23	2:B:77:SER:H	1.81	0.45
2:B:667:TYR:CE2	2:B:733:SER:HB2	2.51	0.45
2:B:660:VAL:HG21	2:B:684:ARG:HB3	1.98	0.45
1:A:308:TRP:HD1	1:A:309:PHE:CD2	2.34	0.45
2:B:200:CYS:HB3	2:B:221:ARG:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:411:ARG:NH2	2:B:513:ALA:HA	2.31	0.45
2:B:667:TYR:HE2	2:B:733:SER:H	1.59	0.45
2:B:18:LEU:HD11	2:B:57:LEU:HD21	1.99	0.45
2:B:512:LEU:HD23	2:B:512:LEU:HA	1.75	0.45
2:B:579:HIS:CD2	2:B:762:PHE:HB2	2.51	0.45
1:A:269:VAL:HG12	1:A:297:VAL:HG13	1.99	0.45
1:A:491:PRO:HD2	1:A:658:ALA:O	2.16	0.45
1:A:516:THR:HB	1:A:519:SER:HB3	1.99	0.45
2:B:162:SER:OG	2:B:554:ALA:HB2	2.17	0.45
3:C:111:ARG:NH2	3:C:112:GLU:OE1	2.50	0.45
2:B:49:LEU:HD11	3:C:17:ILE:HG23	1.99	0.45
2:B:704:GLU:N	2:B:704:GLU:OE2	2.50	0.45
1:A:664:SER:HB3	2:B:499:ARG:HH12	1.82	0.45
2:B:186:VAL:HG13	2:B:186:VAL:O	2.17	0.45
3:C:101:CYS:O	3:C:103:HIS:N	2.50	0.45
1:A:210:MET:HG2	1:A:236:PHE:CE2	2.52	0.44
3:C:58:VAL:HG13	3:C:59:PHE:CD2	2.52	0.44
1:A:264:LYS:N	4:A:801:ADP:O2A	2.47	0.44
1:A:513:THR:O	1:A:519:SER:HB2	2.17	0.44
2:B:380:ILE:HG22	2:B:381:ILE:HG23	2.00	0.44
2:B:703:GLY:HA3	2:B:772:LEU:HD21	1.99	0.44
2:B:29:ILE:HG21	2:B:90:GLU:HB3	1.98	0.44
2:B:239:LEU:HD21	2:B:343:GLN:NE2	2.30	0.44
1:A:317:VAL:HG13	1:A:320:GLU:HB2	1.99	0.44
2:B:131:THR:HG22	2:B:160:THR:HG22	1.99	0.44
1:A:289:HIS:CD2	1:A:360:PHE:HB3	2.53	0.44
1:A:500:MET:HE2	1:A:500:MET:HB2	1.77	0.44
2:B:189:GLU:H	2:B:189:GLU:HG3	1.61	0.44
1:A:636:LEU:CD2	1:A:640:LYS:HB2	2.43	0.44
2:B:538:VAL:O	2:B:542:THR:HG23	2.18	0.44
2:B:702:CYS:SG	2:B:703:GLY:N	2.91	0.44
1:A:48:PHE:O	1:A:48:PHE:CG	2.71	0.43
1:A:233:ARG:HE	1:A:246:VAL:HG21	1.83	0.43
1:A:298:PHE:CD1	1:A:336:PHE:HE2	2.20	0.43
1:A:326:PHE:CD2	1:A:330:SER:HB2	2.54	0.43
1:A:621:HIS:HA	1:A:631:TYR:O	2.19	0.43
1:A:428:THR:HG1	1:A:431:SER:HG	1.59	0.43
2:B:49:LEU:CD1	3:C:17:ILE:CG2	2.96	0.43
2:B:722:ARG:HA	2:B:748:CYS:HA	2.00	0.43
1:A:240:LEU:HD12	2:B:199:VAL:HG21	2.01	0.43
2:B:189:GLU:HG2	3:C:81:TYR:HE2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:HIS:O	1:A:68:ASP:HB2	2.19	0.43
1:A:110:ALA:H	2:B:68:GLN:NE2	2.17	0.43
1:A:151:GLU:H	1:A:151:GLU:CD	2.27	0.43
2:B:665:ARG:HB3	2:B:668:CYS:HB3	2.00	0.43
1:A:352:LEU:HD13	1:A:354:PHE:CE2	2.51	0.43
2:B:209:ASN:HB3	2:B:217:ARG:NH2	2.34	0.43
2:B:362:PHE:HD2	3:C:72:THR:HB	1.83	0.43
2:B:596:LEU:O	2:B:600:THR:OG1	2.33	0.43
2:B:60:ARG:NH2	3:C:41:HIS:O	2.52	0.43
2:B:403:HIS:CE1	2:B:408:LEU:HD12	2.54	0.43
1:A:207:MET:HE2	1:A:256:PHE:HE1	1.84	0.43
1:A:560:HIS:CE1	2:B:491:GLN:NE2	2.87	0.43
2:B:560:THR:HG23	2:B:757:TYR:OH	2.19	0.43
1:A:119:ARG:HH21	2:B:60:ARG:CZ	2.31	0.42
1:A:382:PHE:HE1	2:B:423:LEU:HD21	1.84	0.42
2:B:740:ILE:HG12	2:B:755:VAL:HG12	2.01	0.42
2:B:764:ILE:HD13	2:B:764:ILE:HA	1.83	0.42
3:C:17:ILE:HD11	3:C:46:TRP:CZ3	2.51	0.42
1:A:404:ASP:OD2	1:A:404:ASP:N	2.52	0.42
2:B:228:GLN:O	2:B:533:SER:HA	2.19	0.42
2:B:239:LEU:HD12	2:B:239:LEU:C	2.44	0.42
2:B:583:ARG:NH2	2:B:659:ALA:HB1	2.34	0.42
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.77	0.42
2:B:88:TRP:O	2:B:92:GLU:HG2	2.19	0.42
2:B:135:THR:O	2:B:135:THR:OG1	2.38	0.42
1:A:51:ALA:HB2	3:C:46:TRP:CZ2	2.54	0.42
1:A:618:LEU:HD12	1:A:618:LEU:N	2.35	0.42
2:B:593:PRO:HA	2:B:596:LEU:HG	2.00	0.42
2:B:613:ASP:O	2:B:615:SER:N	2.52	0.42
1:A:55:ARG:HH12	2:B:242:TYR:HD1	1.67	0.42
2:B:234:LEU:HB3	2:B:387:SER:OG	2.19	0.42
2:B:670:ASP:OD1	2:B:671:GLY:N	2.53	0.42
1:A:361:ILE:CD1	1:A:395:PHE:HE2	2.33	0.42
2:B:156:CYS:O	2:B:160:THR:HG23	2.18	0.42
2:B:522:GLN:NE2	3:C:117:VAL:HG13	2.35	0.42
2:B:26:VAL:O	2:B:26:VAL:HG22	2.19	0.42
2:B:31:LEU:HA	2:B:31:LEU:HD23	1.76	0.42
2:B:89:ARG:HE	2:B:89:ARG:HB2	1.67	0.42
1:A:70:CYS:HB3	1:A:76:PHE:CE2	2.55	0.42
1:A:252:ARG:HH22	1:A:376:ALA:HA	1.85	0.42
1:A:298:PHE:CD1	1:A:322:ILE:CD1	2.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ALA:HB3	1:A:396:LEU:HD11	2.02	0.42
1:A:620:TYR:CZ	1:A:718:LEU:HG	2.55	0.42
2:B:49:LEU:CD1	3:C:17:ILE:HG22	2.50	0.41
2:B:239:LEU:HA	3:C:60:PRO:HG3	2.00	0.41
3:C:61:THR:HG22	3:C:63:ASP:N	2.30	0.41
2:B:636:LEU:HD12	2:B:636:LEU:HA	1.86	0.41
2:B:129:LEU:HG	2:B:131:THR:HG22	2.00	0.41
2:B:142:PHE:CE1	3:C:106:LEU:HD13	2.56	0.41
1:A:298:PHE:CZ	1:A:322:ILE:HG12	2.55	0.41
1:A:490:ARG:HA	1:A:491:PRO:HD3	1.95	0.41
2:B:112:THR:HA	2:B:117:LEU:HB2	2.02	0.41
2:B:180:VAL:HG22	2:B:535:HIS:CE1	2.55	0.41
1:A:412:TYR:O	1:A:423:THR:OG1	2.39	0.41
2:B:381:ILE:HG13	2:B:381:ILE:O	2.19	0.41
1:A:506:VAL:HA	1:A:524:ALA:O	2.21	0.41
2:B:73:LEU:N	2:B:548:ASN:OD1	2.54	0.41
2:B:316:ALA:HB2	2:B:326:MET:HE3	2.02	0.41
2:B:559:LEU:HD23	2:B:749:ILE:HD12	2.02	0.41
2:B:705:LEU:HB3	2:B:727:VAL:HG12	2.01	0.41
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.90	0.40
1:A:485:ARG:HB2	1:A:485:ARG:NH2	2.36	0.40
1:A:525:VAL:HG12	1:A:537:ALA:CA	2.51	0.40
1:A:83:LEU:HD12	2:B:16:LEU:HD21	2.03	0.40
2:B:421:GLU:OE1	2:B:425:ARG:NH2	2.50	0.40
2:B:613:ASP:C	2:B:615:SER:H	2.29	0.40
1:A:121:ARG:O	3:C:45:VAL:HG23	2.22	0.40
1:A:125:CYS:SG	1:A:126:ALA:N	2.94	0.40
2:B:200:CYS:SG	2:B:223:CYS:HB2	2.60	0.40
2:B:567:ILE:HG23	2:B:756:VAL:HG22	2.03	0.40
2:B:753:SER:O	2:B:753:SER:OG	2.29	0.40
2:B:507:LEU:HD12	2:B:507:LEU:HA	1.82	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	569/690 (82%)	532 (94%)	36 (6%)	1 (0%)	43	77
2	B	660/771 (86%)	591 (90%)	68 (10%)	1 (0%)	43	77
3	C	100/117 (86%)	85 (85%)	15 (15%)	0	100	100
All	All	1329/1578 (84%)	1208 (91%)	119 (9%)	2 (0%)	44	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	224	ASN
1	A	670	GLN

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	468/571 (82%)	445 (95%)	23 (5%)	22	44
2	B	536/606 (88%)	504 (94%)	32 (6%)	17	39
3	C	87/97 (90%)	82 (94%)	5 (6%)	18	41
All	All	1091/1274 (86%)	1031 (94%)	60 (6%)	21	42

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	GLU
1	A	130	VAL
1	A	131	VAL
1	A	235	VAL
1	A	241	PHE
1	A	250	ARG
1	A	268	LEU
1	A	269	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	276	LEU
1	A	290	ILE
1	A	317	VAL
1	A	335	VAL
1	A	366	VAL
1	A	383	VAL
1	A	408	ASN
1	A	480	LYS
1	A	504	LEU
1	A	558	VAL
1	A	561	SER
1	A	576	VAL
1	A	616	GLU
1	A	656	VAL
1	A	718	LEU
2	B	49	LEU
2	B	94	LEU
2	B	127	VAL
2	B	131	THR
2	B	137	HIS
2	B	146	VAL
2	B	156	CYS
2	B	177	VAL
2	B	185	ILE
2	B	189	GLU
2	B	190	LEU
2	B	213	THR
2	B	220	ASP
2	B	222	ILE
2	B	235	ASP
2	B	317	SER
2	B	384	GLN
2	B	408	LEU
2	B	496	VAL
2	B	526	LEU
2	B	567	ILE
2	B	575	VAL
2	B	591	VAL
2	B	600	THR
2	B	617	HIS
2	B	631	VAL
2	B	642	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	648	ILE
2	B	727	VAL
2	B	748	CYS
2	B	761	VAL
2	B	764	ILE
3	C	45	VAL
3	C	66	LEU
3	C	96	THR
3	C	98	ASP
3	C	107	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	67	HIS
1	A	135	ASN
1	A	165	GLN
1	A	211	HIS
1	A	224	HIS
1	A	248	HIS
1	A	374	ASN
1	A	375	GLN
1	A	377	ASN
1	A	670	GLN
2	B	68	GLN
2	B	124	HIS
2	B	137	HIS
2	B	144	HIS
2	B	195	HIS
2	B	312	GLN
2	B	323	GLN
2	B	343	GLN
2	B	384	GLN
2	B	491	GLN
2	B	522	GLN
2	B	621	GLN
2	B	664	GLN
2	B	679	GLN
3	C	25	GLN
3	C	119	ASN
3	C	126	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z > 2$
4	ADP	A	801	-	28,29,29	0.45	0	43,45,45	0.44	0
5	BEF	A	802	-	0,3,3	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	801	-	-	6/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

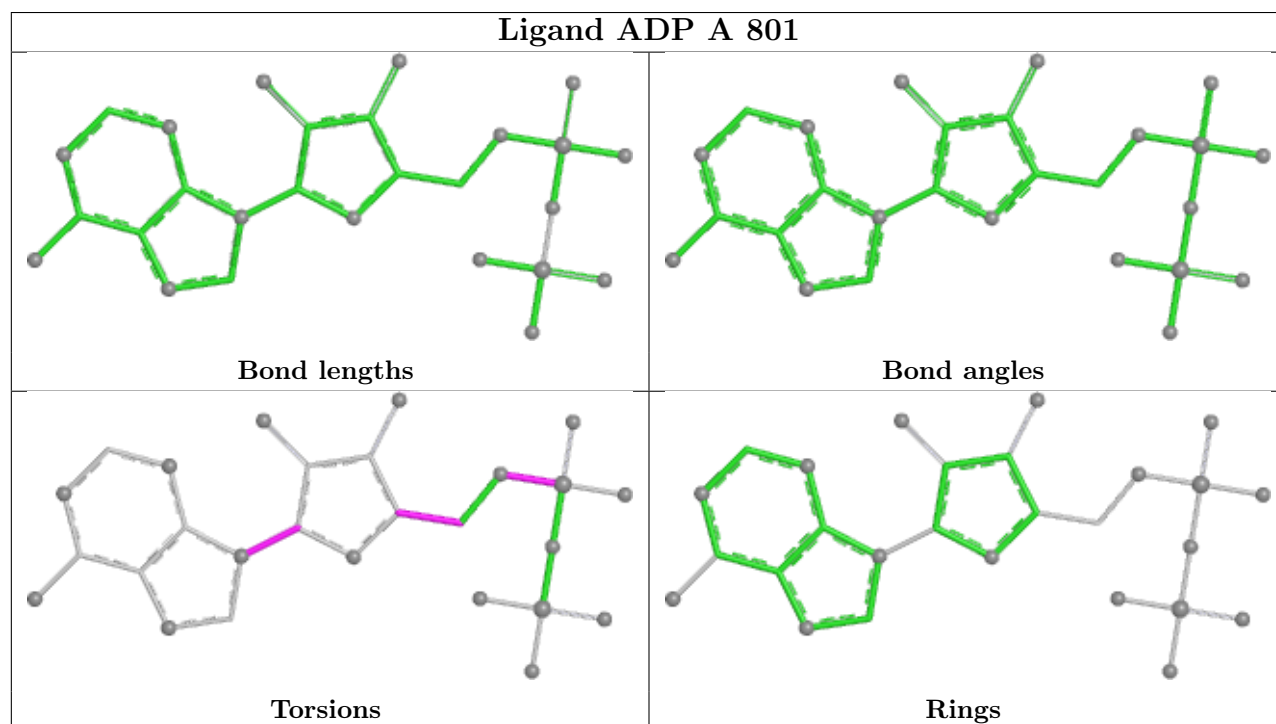
Mol	Chain	Res	Type	Atoms
4	A	801	ADP	C5'-O5'-PA-O3A
4	A	801	ADP	C3'-C4'-C5'-O5'
4	A	801	ADP	O4'-C4'-C5'-O5'
4	A	801	ADP	C2'-C1'-N9-C8
4	A	801	ADP	C2'-C1'-N9-C4
4	A	801	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	ADP	10	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.

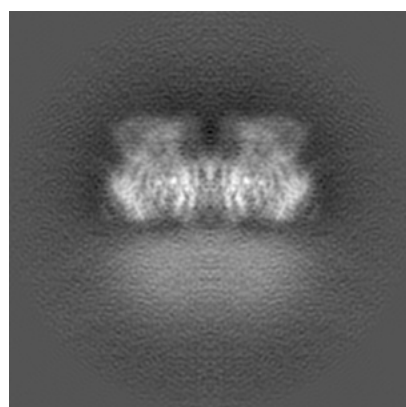
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30094. These allow visual inspection of the internal detail of the map and identification of artifacts.

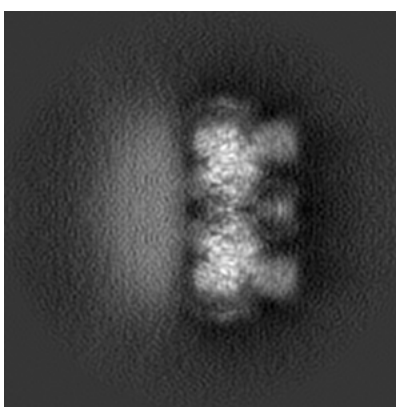
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

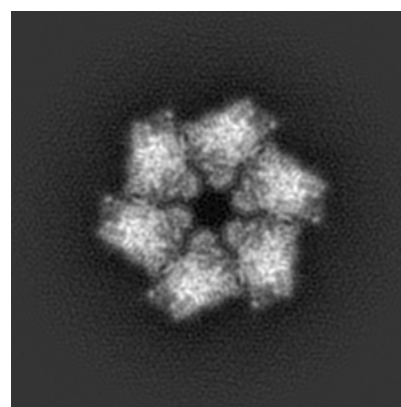
6.1.1 Primary map



X



Y

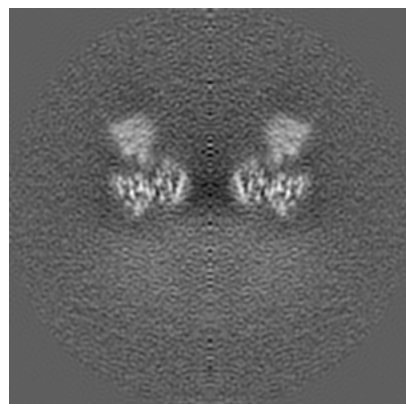


Z

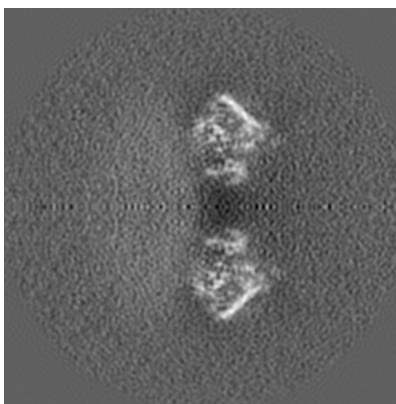
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

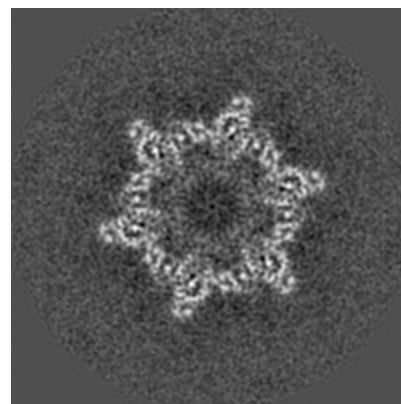
6.2.1 Primary map



X Index: 90



Y Index: 90

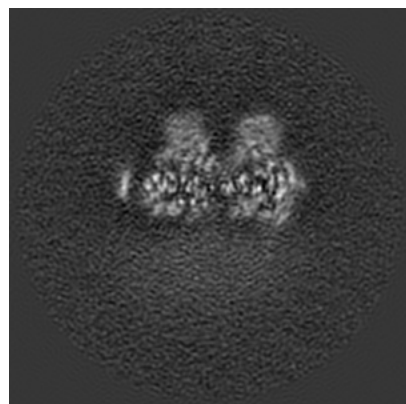


Z Index: 90

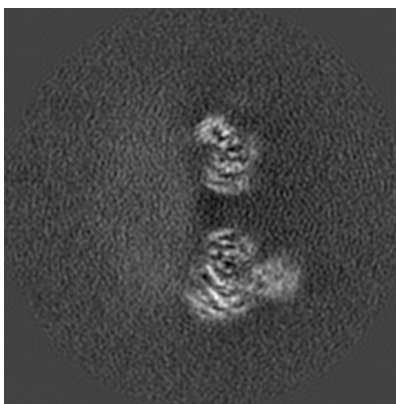
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

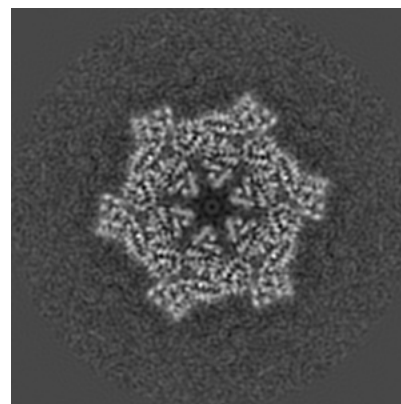
6.3.1 Primary map



X Index: 62



Y Index: 82

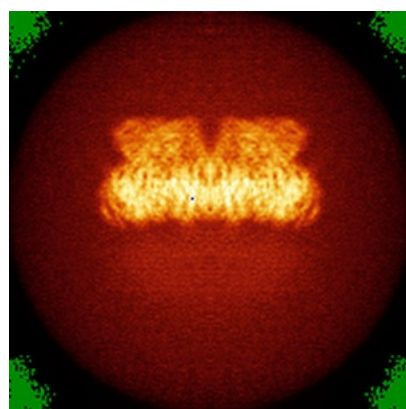


Z Index: 98

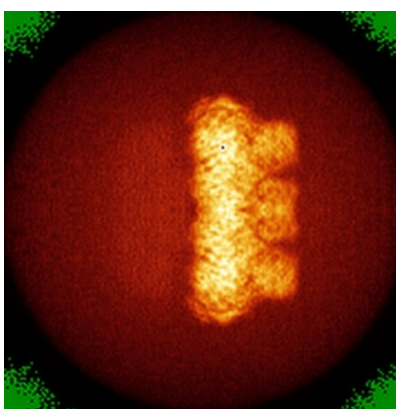
The images above show the largest variance slices of the map in three orthogonal directions.

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

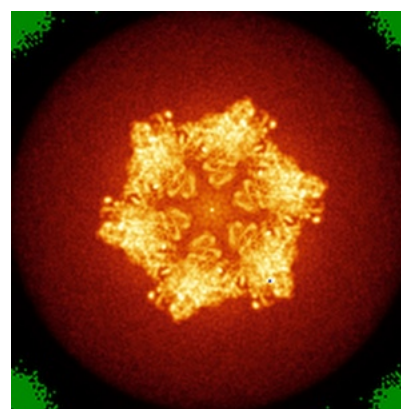
6.4.1 Primary map



X



Y

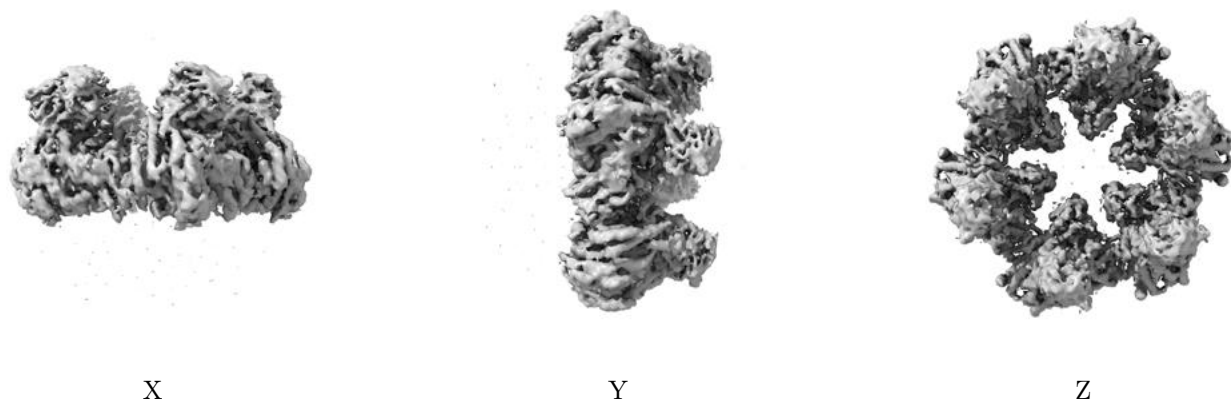


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0694. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

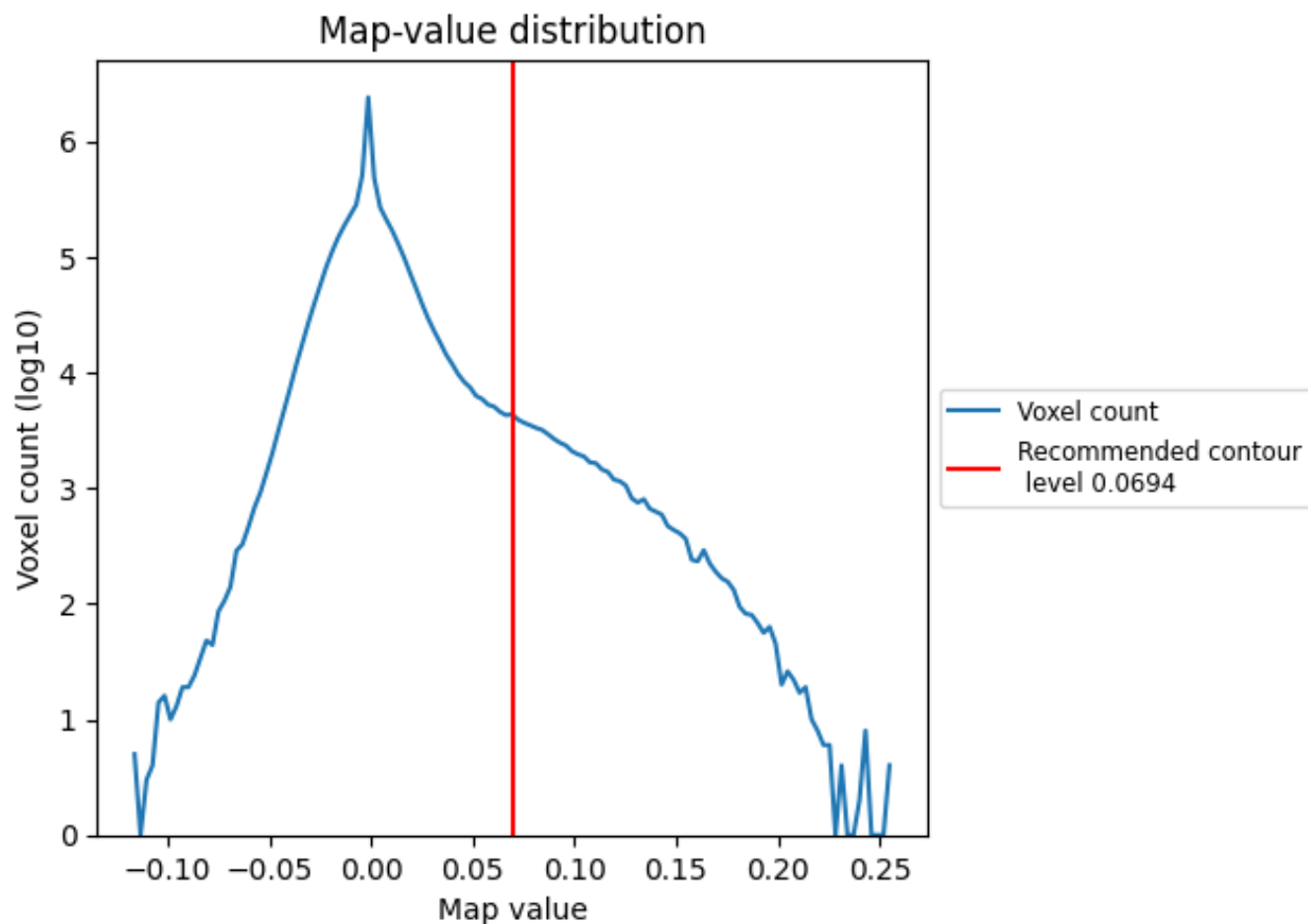
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

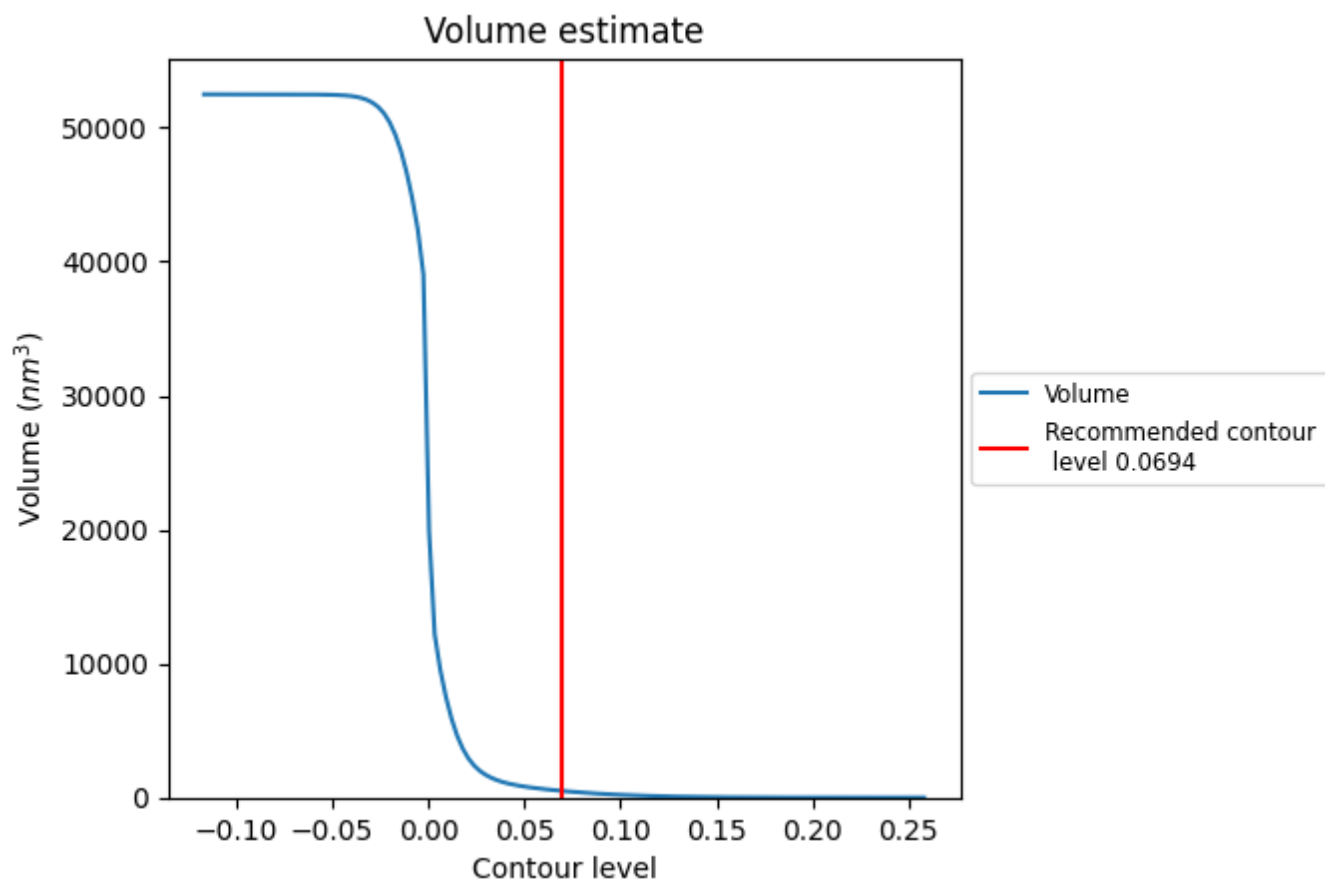
This section contains the results of statistical analysis of the map.

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.

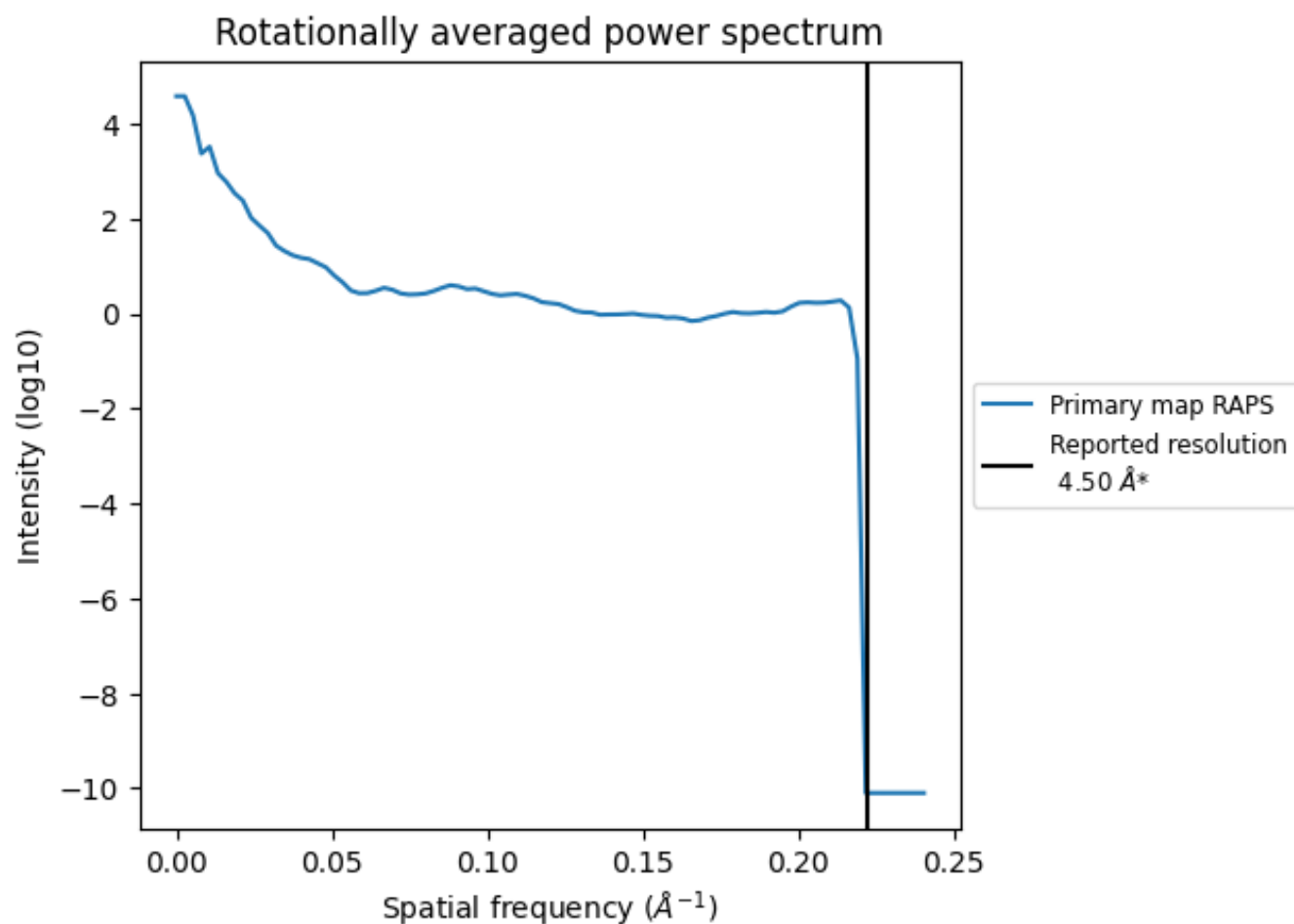
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 501 nm³; this corresponds to an approximate mass of 452 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 0.222 Å⁻¹

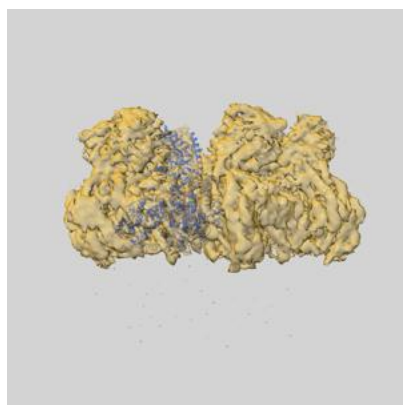
8 Fourier-Shell correlation ⓘ

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

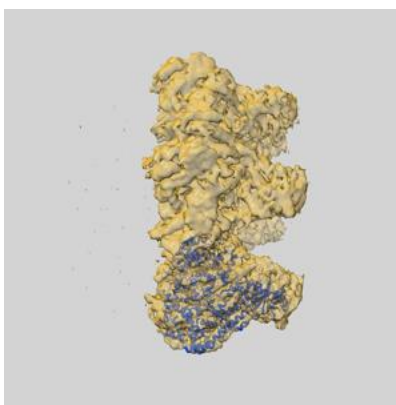
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30094 and PDB model 6M5V. Per-residue inclusion information can be found in section 3 on page 7.

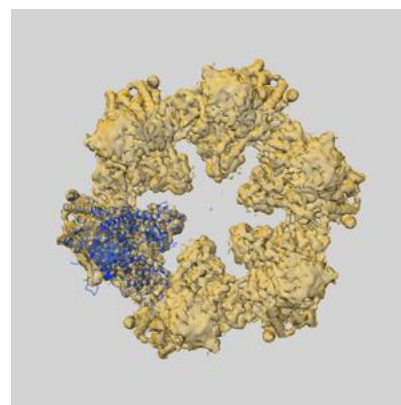
9.1 Map-model overlay [i](#)



X



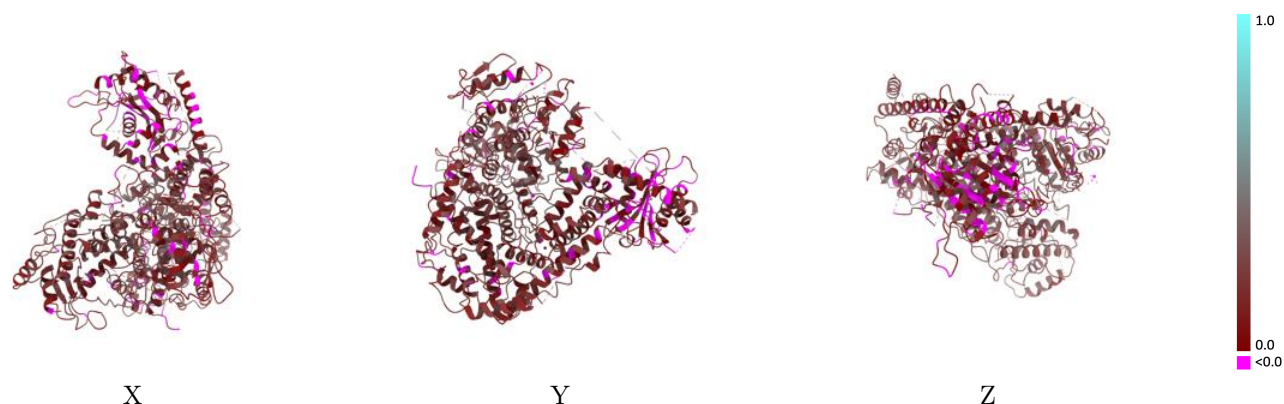
Y



Z

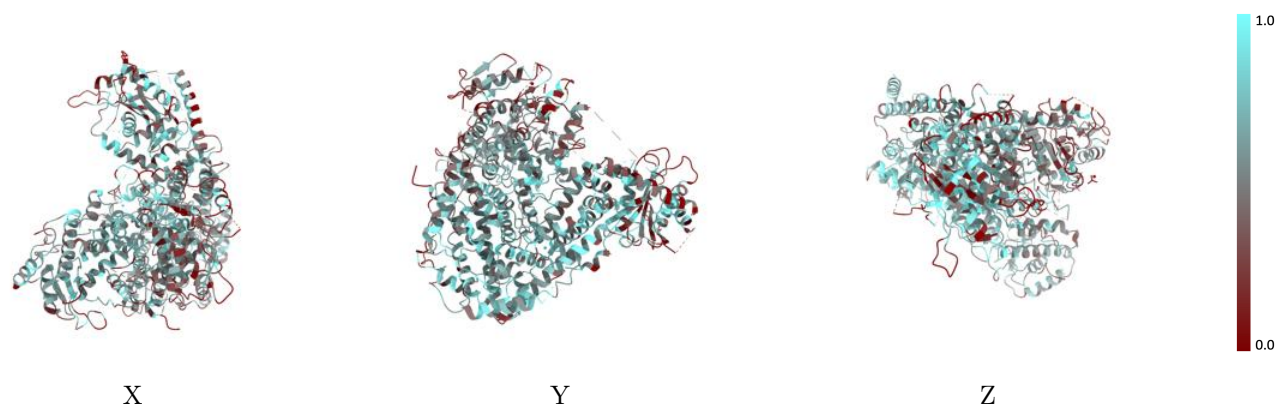
The images above show the 3D surface view of the map at the recommended contour level 0.0694 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



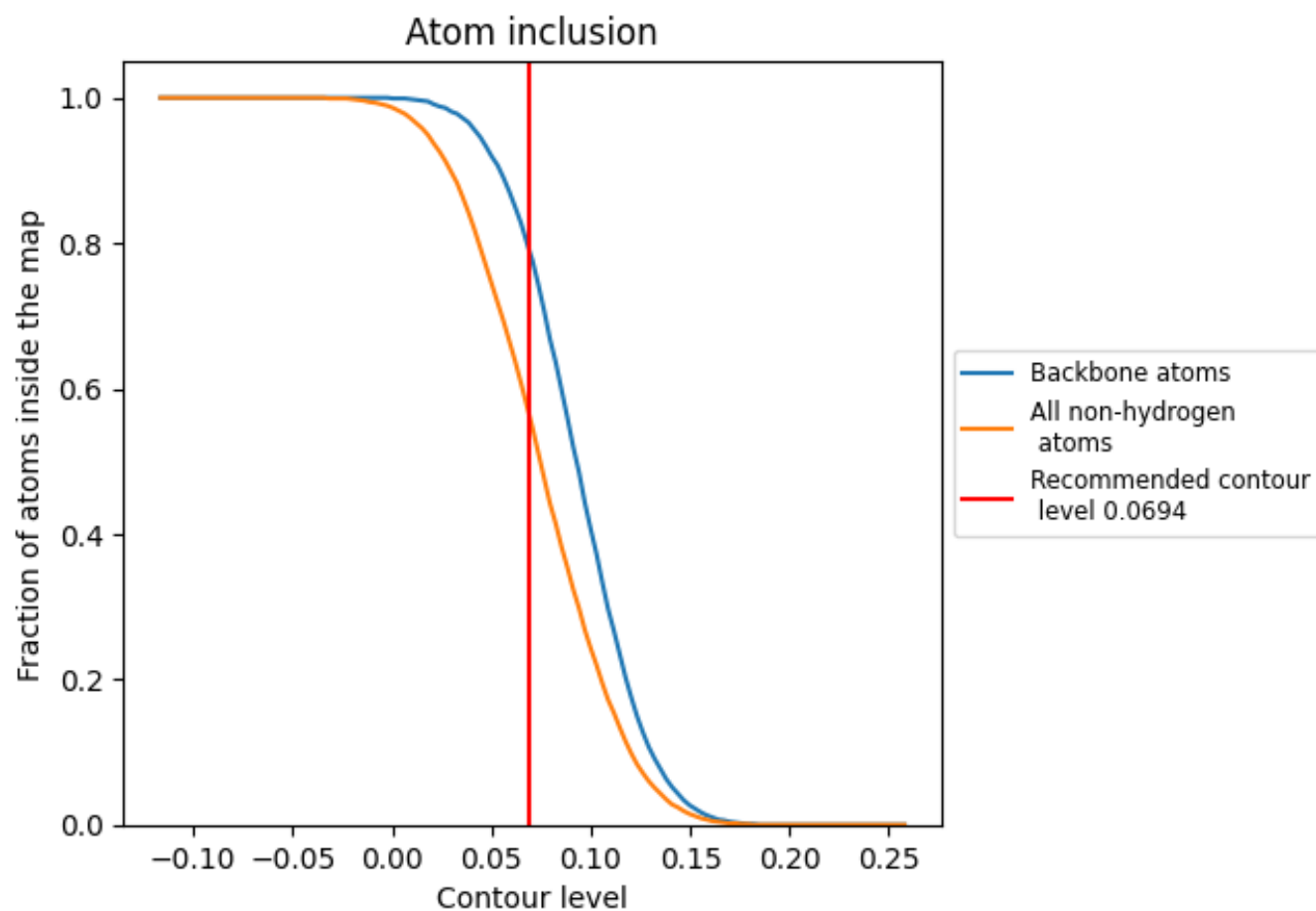
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0694).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 56% 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 (0.0694) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5600	0.1820
A	0.4900	0.1580
B	0.6100	0.2040
C	0.6250	0.1810

