



Full wwPDB EM Validation Report ⓘ

Apr 9, 2026 – 11:23 PM UTC

PDB ID : 9L6I / pdb_00009l6i
EMDB ID : EMD-62853
Title : Glycogen phosphorylase from Segatella copri
Authors : Shobu, K.; Fukuda, Y.; Inoue, T.
Deposited on : 2024-12-25
Resolution : 2.98 Å(reported)
Based on initial model : .

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:

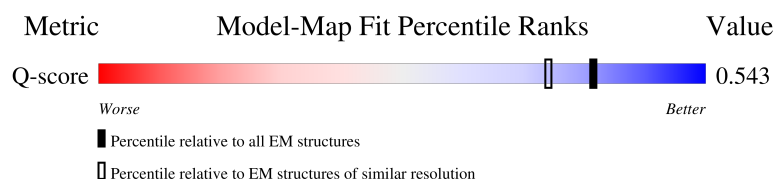
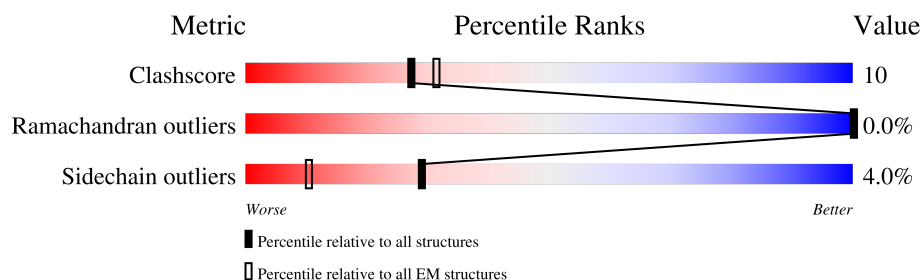
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 2.98 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	13236 (2.48 - 3.48)

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	852	
1	B	852	
1	C	852	
1	D	852	

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Mol	Chain	Length	Quality of chain
1	E	852	

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
1	LLP	B	609	-	-	X	-

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 34770 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 Alpha-glucan family phosphorylase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	852	Total	C	N	O	P	S	0	0
			6957	4453	1169	1295	1	39		
1	B	852	Total	C	N	O	P	S	0	0
			6957	4453	1169	1295	1	39		
1	C	852	Total	C	N	O	S		0	0
			6942	4445	1168	1290	39			
1	D	852	Total	C	N	O	P	S	0	0
			6957	4453	1169	1295	1	39		
1	E	852	Total	C	N	O	P	S	0	0
			6957	4453	1169	1295	1	39		

There are 5 discrepancies between the modelled and reference sequences:

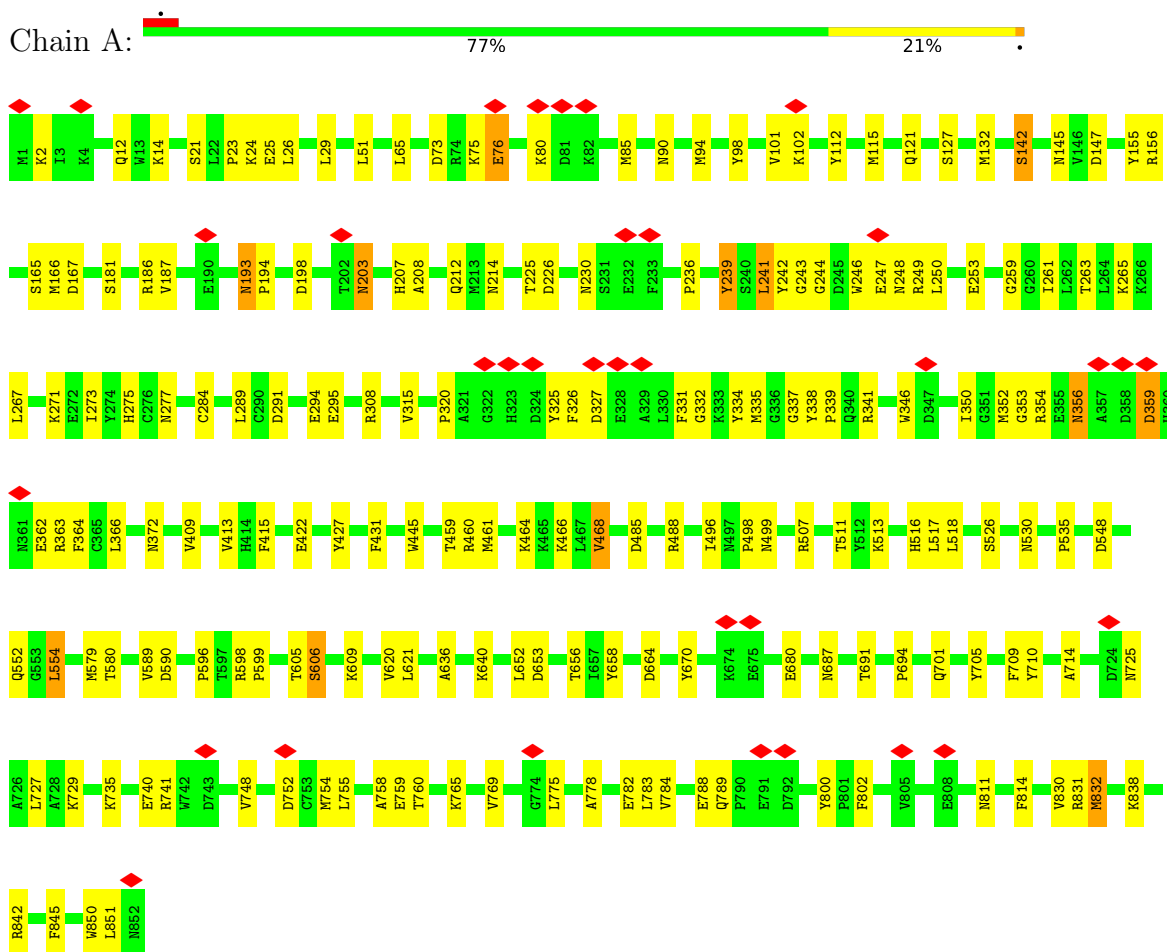
Chain	Residue	Modelled	Actual	Comment	Reference
A	239	TYR	HIS	conflict	UNP A0AA93BMC9
B	239	TYR	HIS	conflict	UNP A0AA93BMC9
C	239	TYR	HIS	conflict	UNP A0AA93BMC9
D	239	TYR	HIS	conflict	UNP A0AA93BMC9
E	239	TYR	HIS	conflict	UNP A0AA93BMC9

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.

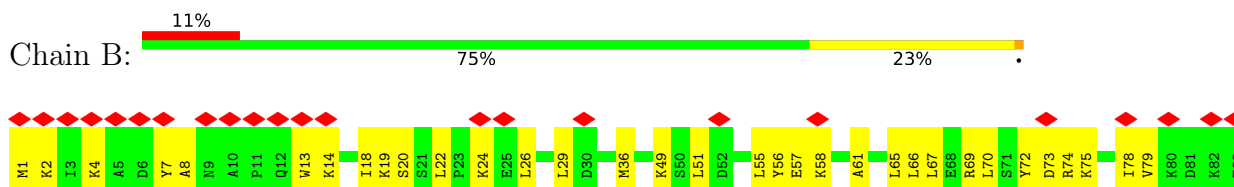
• Molecule 1: Alpha-glucan family phosphorylase

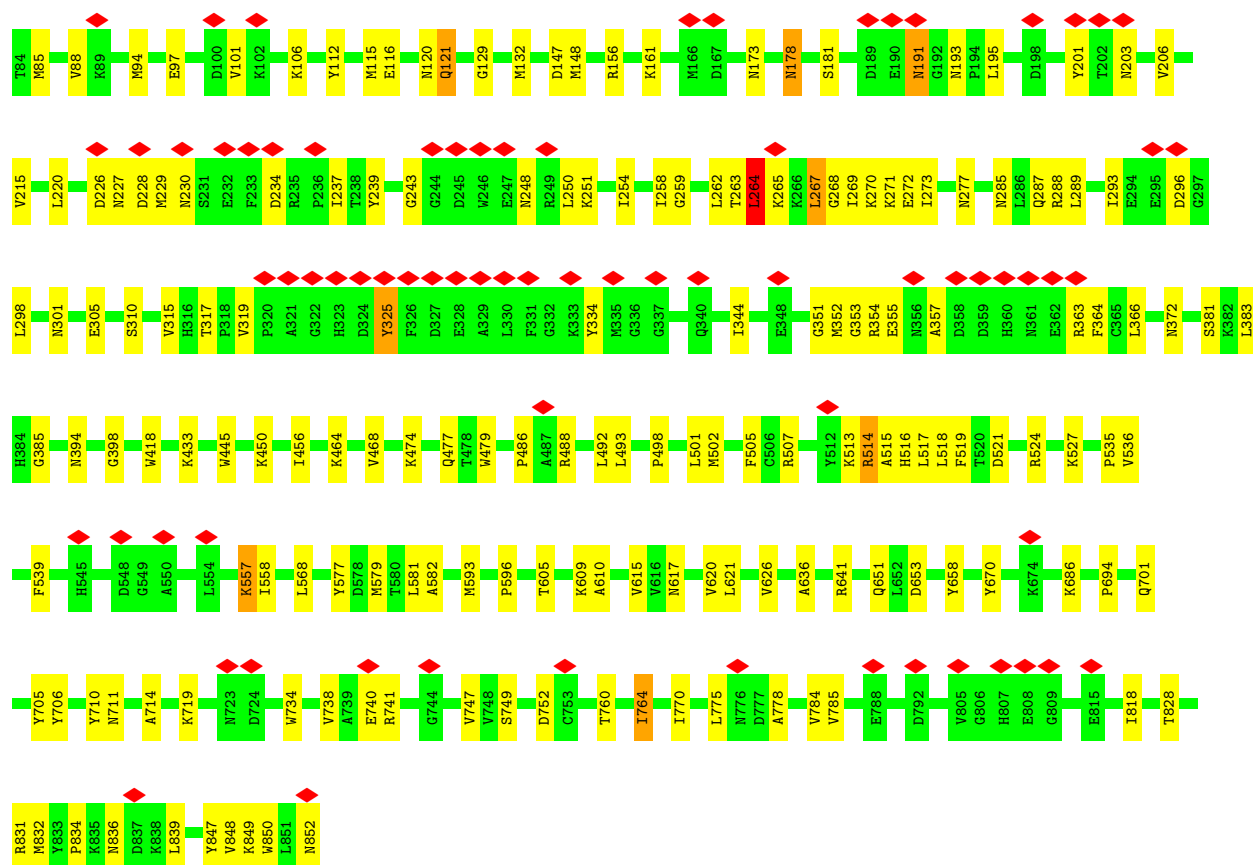
Chain A:



• Molecule 1: Alpha-glucan family phosphorylase

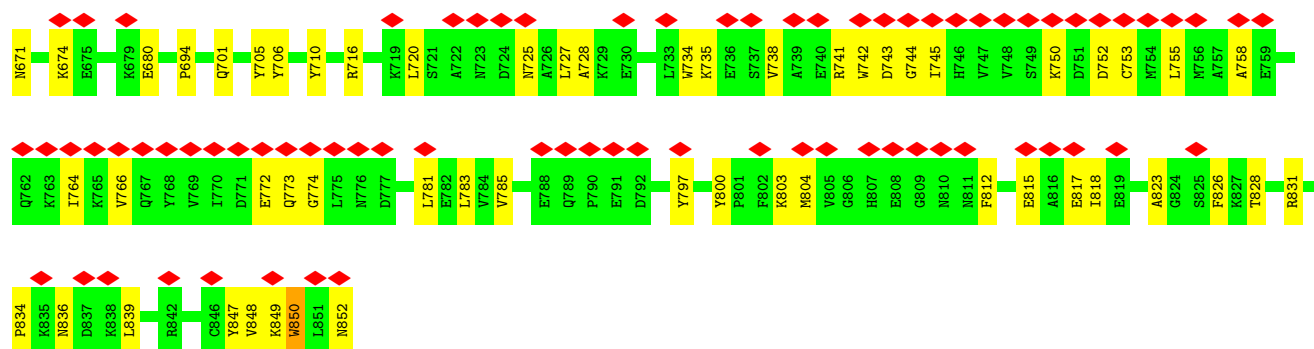
Chain B:



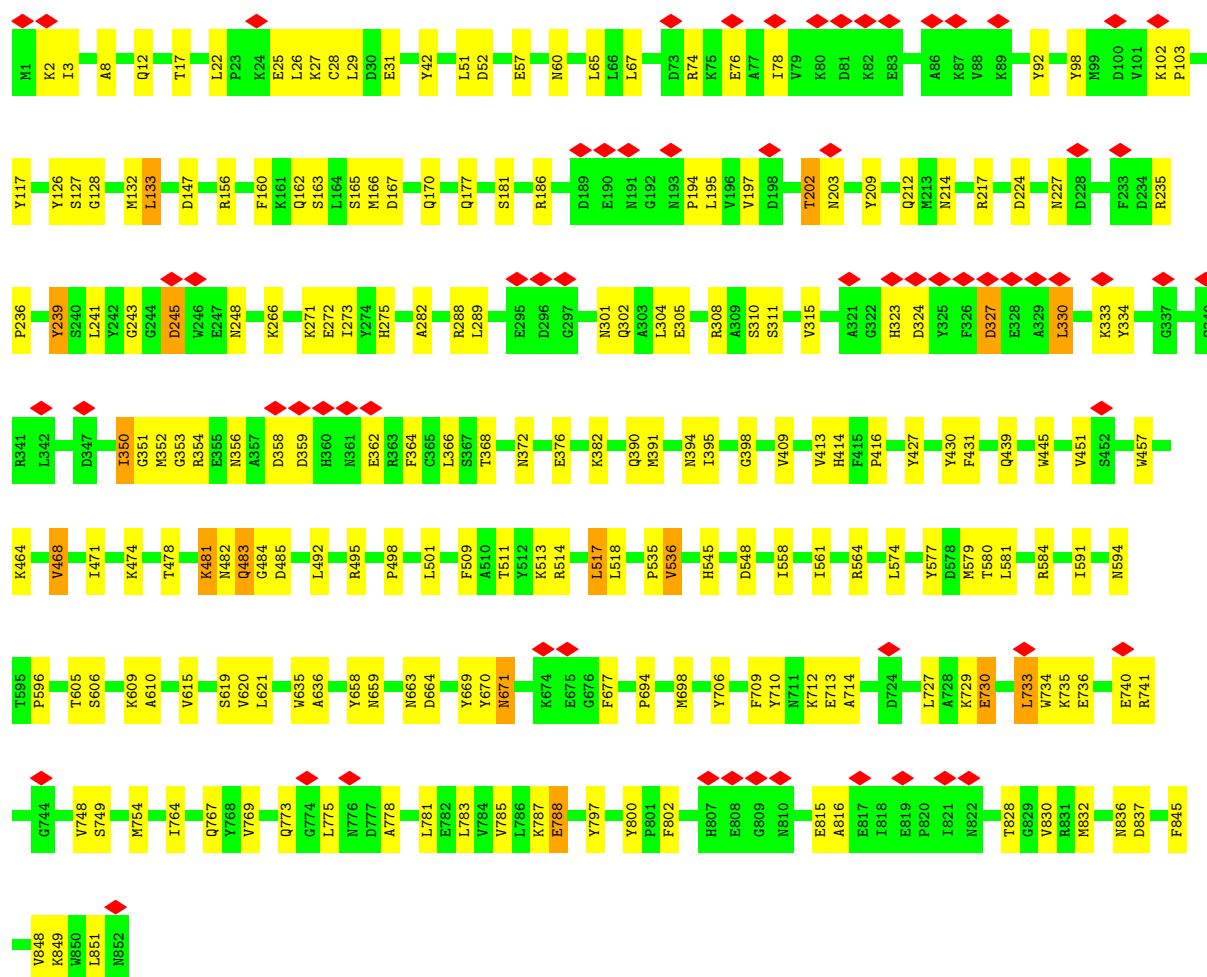
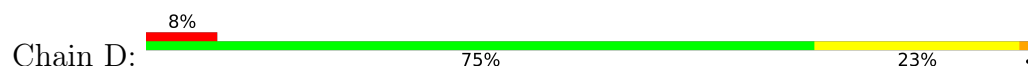


• Molecule 1: Alpha-glucan family phosphorylase

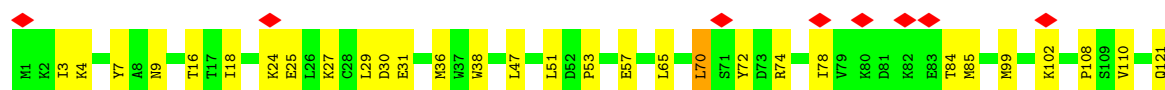
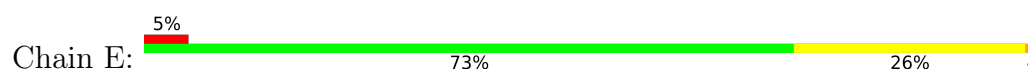


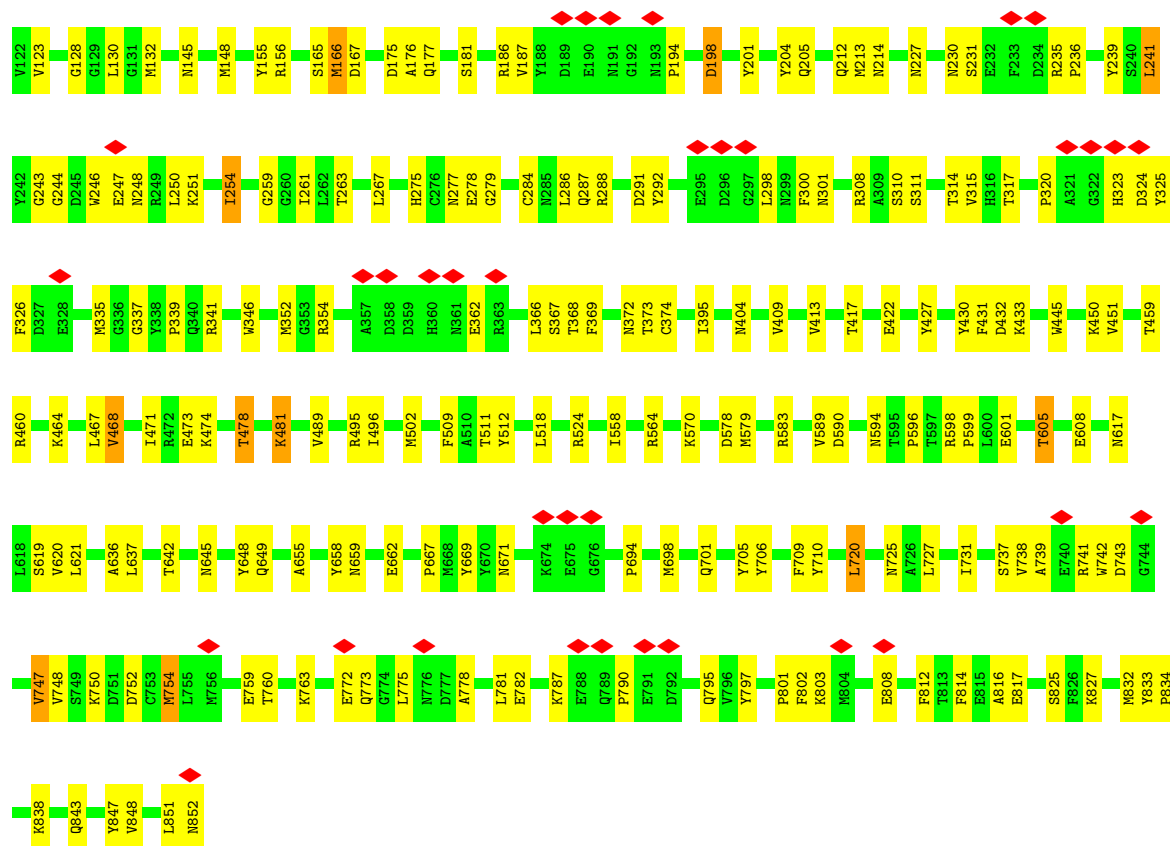


• Molecule 1: Alpha-glucan family phosphorylase



• Molecule 1: Alpha-glucan family phosphorylase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	531360	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	JEOL CRYO ARM 200	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.561	Depositor
Minimum map value	-0.326	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.0689	Depositor
Map size (\AA)	212.48, 212.48, 212.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	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: LLP

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	0.32	0/7110	0.41	0/9621
1	B	0.28	0/7110	0.45	2/9621 (0.0%)
1	C	0.21	0/7110	0.36	0/9621
1	D	0.26	0/7110	0.38	0/9621
1	E	0.28	0/7110	0.36	0/9621
All	All	0.27	0/35550	0.39	2/48105 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	LEU	N-CA-C	-5.50	107.21	114.31
1	B	264	LEU	N-CA-C	-5.06	105.85	111.36

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	6957	0	6747	115	0
1	B	6957	0	6747	142	0
1	C	6942	0	6740	161	0
1	D	6957	0	6747	131	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	6957	0	6747	148	0
All	All	34770	0	33728	669	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 10.

All (669) 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:E:275:HIS:HD1	1:E:710:TYR:HH	1.13	0.90
1:B:582:ALA:HB2	1:B:609:LLP:C2'	2.08	0.84
1:B:582:ALA:HB2	1:B:609:LLP:H2'2	1.61	0.81
1:B:486:PRO:HB2	1:C:651:GLN:HG3	1.62	0.81
1:C:184:ILE:HG22	1:C:213:MET:HB2	1.61	0.80
1:B:741:ARG:HH21	1:B:775:LEU:HD12	1.46	0.79
1:E:236:PRO:HA	1:E:239:TYR:HD2	1.49	0.76
1:A:112:TYR:OH	1:A:277:ASN:ND2	2.19	0.75
1:E:763:LYS:HD3	1:E:817:GLU:HB2	1.70	0.74
1:E:417:THR:O	1:E:583:ARG:NH1	2.22	0.73
1:D:288:ARG:NH1	1:D:311:SER:OG	2.20	0.72
1:D:12:GLN:HB3	1:E:852:ASN:HD22	1.53	0.72
1:D:25:GLU:OE2	1:D:25:GLU:N	2.22	0.72
1:C:755:LEU:HD13	1:C:764:ILE:HG13	1.72	0.72
1:C:524:ARG:NH2	1:C:659:ASN:OD1	2.22	0.72
1:E:741:ARG:HD2	1:E:775:LEU:HG	1.70	0.72
1:D:781:LEU:HB3	1:D:802:PHE:HD2	1.56	0.71
1:E:27:LYS:NZ	1:E:27:LYS:O	2.23	0.71
1:B:262:LEU:HD23	1:B:265:LYS:HZ3	1.57	0.70
1:E:787:LYS:HB3	1:E:797:TYR:HB2	1.73	0.70
1:B:518:LEU:O	1:B:658:TYR:OH	2.09	0.70
1:E:720:LEU:HD12	1:E:727:LEU:HD12	1.75	0.69
1:C:741:ARG:HE	1:C:774:GLY:HA3	1.58	0.68
1:E:254:ILE:HD11	1:E:335:MET:HE1	1.75	0.68
1:D:282:ALA:HB3	1:D:366:LEU:HD22	1.74	0.68
1:E:596:PRO:HD2	1:E:620:VAL:HB	1.75	0.68
1:B:74:ARG:O	1:B:78:ILE:HG13	1.94	0.67
1:C:115:MET:HE3	1:C:280:HIS:HB3	1.75	0.67
1:D:212:GLN:NE2	1:D:214:ASN:OD1	2.27	0.67
1:D:518:LEU:O	1:D:658:TYR:OH	2.12	0.67
1:C:317:THR:HG21	1:C:322:GLY:HA3	1.74	0.67
1:D:754:MET:HG3	1:D:764:ILE:HG23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:790:PRO:HB3	1:E:795:GLN:HG2	1.75	0.67
1:A:850:TRP:H	1:E:9:ASN:HD21	1.42	0.67
1:B:121:GLN:HG2	1:B:579:MET:HB2	1.77	0.67
1:B:243:GLY:O	1:B:248:ASN:ND2	2.28	0.67
1:A:596:PRO:HD2	1:A:620:VAL:HB	1.77	0.67
1:D:596:PRO:HD2	1:D:620:VAL:HB	1.77	0.66
1:B:596:PRO:HD2	1:B:620:VAL:HB	1.76	0.66
1:D:202:THR:OG1	1:D:203:ASN:N	2.28	0.66
1:B:582:ALA:CB	1:B:609:LLP:H2'1	2.25	0.66
1:D:468:VAL:HG11	1:D:498:PRO:HB3	1.78	0.66
1:E:236:PRO:HA	1:E:239:TYR:CD2	2.31	0.65
1:C:836:ASN:HB3	1:C:839:LEU:HG	1.79	0.65
1:E:460:ARG:NH2	1:E:589:VAL:O	2.30	0.65
1:E:464:LYS:NZ	1:E:590:ASP:OD2	2.28	0.65
1:E:368:THR:HG23	1:E:395:ILE:HD12	1.79	0.65
1:A:12:GLN:OE1	1:B:852:ASN:ND2	2.29	0.65
1:B:582:ALA:CB	1:B:609:LLP:C2'	2.74	0.64
1:A:243:GLY:O	1:A:248:ASN:ND2	2.29	0.64
1:D:413:VAL:HG11	1:D:609:LLP:HG2	1.80	0.64
1:D:749:SER:HB3	1:D:769:VAL:HB	1.79	0.64
1:D:273:ILE:HD11	1:D:714:ALA:HB2	1.80	0.64
1:D:98:TYR:O	1:D:217:ARG:NH1	2.31	0.64
1:B:49:LYS:NZ	1:B:57:GLU:OE2	2.31	0.64
1:D:545:HIS:HB3	1:D:548:ASP:HB2	1.79	0.64
1:D:735:LYS:HE2	1:D:845:PHE:HB2	1.81	0.63
1:C:743:ASP:HA	1:C:849:LYS:HZ3	1.63	0.63
1:D:471:ILE:HD13	1:D:574:LEU:HD21	1.79	0.63
1:B:577:TYR:HA	1:B:581:LEU:HD23	1.81	0.63
1:A:275:HIS:ND1	1:A:710:TYR:OH	2.30	0.62
1:C:299:ASN:OD1	1:C:302:GLN:NE2	2.32	0.62
1:E:227:ASN:OD1	1:E:230:ASN:ND2	2.32	0.62
1:A:735:LYS:HB3	1:E:3:ILE:HD11	1.81	0.62
1:E:667:PRO:O	1:E:671:ASN:ND2	2.33	0.62
1:A:464:LYS:NZ	1:A:590:ASP:OD2	2.26	0.62
1:C:764:ILE:HG22	1:C:818:ILE:HB	1.81	0.62
1:B:8:ALA:HB1	1:C:848:VAL:HG12	1.82	0.62
1:C:156:ARG:NH1	1:C:177:GLN:O	2.32	0.62
1:C:288:ARG:NH2	1:C:310:SER:OG	2.32	0.62
1:C:508:ARG:O	1:C:508:ARG:NH1	2.33	0.61
1:D:102:LYS:HE2	1:D:103:PRO:HD2	1.82	0.61
1:E:298:LEU:HD11	1:E:725:ASN:HD22	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:635:TRP:HB3	1:C:660:LEU:HD21	1.82	0.61
1:C:750:LYS:HD3	1:C:753:CYS:HB3	1.83	0.61
1:A:782:GLU:OE1	1:A:842:ARG:NH2	2.32	0.61
1:A:193:ASN:OD1	1:A:193:ASN:N	2.33	0.61
1:D:236:PRO:HA	1:D:239:TYR:CD1	2.35	0.61
1:A:461:MET:HE1	1:A:499:ASN:HA	1.81	0.61
1:D:127:SER:HB3	1:D:241:LEU:HD22	1.81	0.61
1:C:745:ILE:HD12	1:C:772:GLU:HA	1.83	0.60
1:E:259:GLY:O	1:E:263:THR:OG1	2.20	0.60
1:B:764:ILE:HG12	1:B:818:ILE:HB	1.82	0.60
1:A:413:VAL:HG11	1:A:609:LLP:HG2	1.83	0.60
1:C:289:LEU:HG	1:C:307:VAL:HG21	1.83	0.60
1:C:598:ARG:HH21	1:C:621:LEU:HB2	1.67	0.60
1:E:74:ARG:HH22	1:E:78:ILE:HD11	1.67	0.60
1:E:156:ARG:NH1	1:E:177:GLN:O	2.34	0.59
1:E:701:GLN:HE21	1:E:705:TYR:HE2	1.50	0.59
1:A:468:VAL:HG11	1:A:498:PRO:HB3	1.83	0.59
1:E:308:ARG:NH1	1:E:372:ASN:O	2.35	0.59
1:E:655:ALA:O	1:E:659:ASN:ND2	2.35	0.59
1:A:166:MET:HE2	1:B:651:GLN:HG2	1.84	0.59
1:A:832:MET:HE2	1:A:851:LEU:HD21	1.84	0.59
1:C:381:SER:O	1:C:385:GLY:N	2.32	0.59
1:B:14:LYS:NZ	1:C:753:CYS:SG	2.76	0.59
1:D:351:GLY:HA2	1:D:354:ARG:HG3	1.85	0.59
1:B:325:TYR:HB2	1:B:363:ARG:HG2	1.85	0.58
1:C:506:CYS:O	1:C:507:ARG:HG2	2.03	0.58
1:D:787:LYS:HG3	1:D:797:TYR:HB2	1.85	0.58
1:B:582:ALA:HB2	1:B:609:LLP:H2'1	1.86	0.58
1:E:78:ILE:HD12	1:E:84:THR:HG21	1.84	0.58
1:A:187:VAL:HG11	1:A:267:LEU:HD21	1.86	0.58
1:A:242:TYR:O	1:A:249:ARG:NE	2.33	0.58
1:D:147:ASP:OD1	1:D:271:LYS:NZ	2.37	0.58
1:A:356:ASN:HB2	1:A:359:ASP:HB2	1.86	0.58
1:B:285:ASN:OD1	1:B:288:ARG:NH1	2.36	0.58
1:C:641:ARG:NH2	1:C:646:GLN:OE1	2.37	0.57
1:B:178:ASN:C	1:B:178:ASN:HD22	2.11	0.57
1:B:352:MET:O	1:B:372:ASN:ND2	2.37	0.57
1:E:642:THR:H	1:E:649:GLN:HE22	1.49	0.57
1:D:781:LEU:HB3	1:D:802:PHE:CD2	2.38	0.57
1:E:198:ASP:HB3	1:E:205:GLN:HB3	1.85	0.57
1:C:744:GLY:HA3	1:C:773:GLN:HE22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:592:TRP:CD1	1:C:610:ALA:HB2	2.39	0.57
1:B:65:LEU:HD13	1:B:181:SER:HB3	1.86	0.57
1:B:486:PRO:HB3	1:C:648:TYR:HD1	1.67	0.57
1:C:596:PRO:HD2	1:C:620:VAL:HB	1.85	0.57
1:D:156:ARG:NH1	1:D:177:GLN:O	2.36	0.57
1:E:130:LEU:HD11	1:E:277:ASN:HD22	1.70	0.57
1:B:227:ASN:OD1	1:B:230:ASN:ND2	2.38	0.57
1:C:596:PRO:HG2	1:C:622:ASP:HB3	1.87	0.57
1:C:621:LEU:HG	1:C:636:ALA:HB1	1.86	0.57
1:C:743:ASP:HA	1:C:849:LYS:NZ	2.20	0.57
1:D:783:LEU:HB3	1:D:800:TYR:HB2	1.87	0.57
1:E:27:LYS:HZ1	1:E:30:ASP:HB3	1.70	0.57
1:B:502:MET:HG2	1:B:539:PHE:CE2	2.39	0.56
1:D:671:ASN:ND2	1:D:671:ASN:O	2.37	0.56
1:E:432:ASP:OD1	1:E:433:LYS:N	2.38	0.56
1:B:831:ARG:HA	1:B:850:TRP:HA	1.87	0.56
1:D:635:TRP:NE1	1:D:664:ASP:OD2	2.38	0.56
1:A:156:ARG:NE	1:A:226:ASP:OD2	2.30	0.56
1:C:282:ALA:HB3	1:C:366:LEU:HG	1.86	0.56
1:D:354:ARG:HD3	1:D:362:GLU:HB3	1.87	0.56
1:C:725:ASN:HB2	1:C:728:ALA:HB3	1.87	0.56
1:E:311:SER:OG	1:E:374:CYS:SG	2.56	0.56
1:B:132:MET:HE3	1:B:609:LLP:C2	2.35	0.56
1:B:258:ILE:HG23	1:B:287:GLN:CG	2.35	0.56
1:C:706:TYR:HA	1:C:710:TYR:HB2	1.88	0.56
1:B:354:ARG:NH1	1:B:357:ALA:O	2.38	0.56
1:C:331:PHE:CD1	1:C:335:MET:HE3	2.41	0.56
1:C:516:HIS:CD2	1:C:554:LEU:HD13	2.40	0.56
1:A:12:GLN:OE1	1:A:12:GLN:N	2.38	0.56
1:A:350:ILE:HG23	1:A:354:ARG:NH2	2.21	0.56
1:A:165:SER:OG	1:A:167:ASP:OD1	2.22	0.56
1:B:55:LEU:HA	1:B:58:LYS:HD2	1.88	0.56
1:D:514:ARG:HB3	1:D:517:LEU:HD13	1.86	0.56
1:E:320:PRO:HA	1:E:323:HIS:CD2	2.41	0.56
1:E:244:GLY:HA3	1:E:248:ASN:HD22	1.71	0.55
1:A:273:ILE:HD11	1:A:714:ALA:HB2	1.87	0.55
1:A:327:ASP:HB3	1:A:363:ARG:HG2	1.88	0.55
1:D:767:GLN:NE2	1:D:815:GLU:OE1	2.40	0.55
1:E:243:GLY:O	1:E:248:ASN:ND2	2.39	0.55
1:A:308:ARG:NH1	1:A:372:ASN:O	2.33	0.55
1:E:288:ARG:NH2	1:E:310:SER:OG	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:ARG:HG2	1:C:649:GLN:HG2	1.87	0.55
1:C:738:VAL:O	1:C:742:TRP:HB2	2.06	0.55
1:B:785:VAL:HG13	1:B:828:THR:HG22	1.89	0.55
1:C:167:ASP:O	1:C:556:LYS:NZ	2.38	0.55
1:C:347:ASP:OD2	1:C:360:HIS:NE2	2.37	0.55
1:E:430:TYR:CD2	1:E:451:VAL:HG22	2.42	0.55
1:A:21:SER:O	1:A:75:LYS:NZ	2.31	0.55
1:E:65:LEU:HD13	1:E:181:SER:HB2	1.88	0.55
1:E:198:ASP:OD1	1:E:198:ASP:N	2.39	0.55
1:A:249:ARG:O	1:A:253:GLU:HG3	2.07	0.55
1:B:22:LEU:HB3	1:B:26:LEU:HB2	1.87	0.55
1:B:201:TYR:HE2	1:B:251:LYS:HG2	1.71	0.54
1:D:445:TRP:CD1	1:D:694:PRO:HB3	2.41	0.54
1:D:788:GLU:CD	1:D:788:GLU:H	2.16	0.54
1:C:577:TYR:HA	1:C:581:LEU:HD23	1.90	0.54
1:C:772:GLU:HB2	1:C:812:PHE:HD2	1.72	0.54
1:D:52:ASP:OD1	1:D:52:ASP:N	2.40	0.54
1:D:165:SER:OG	1:D:166:MET:N	2.39	0.54
1:A:208:ALA:HB2	1:A:225:THR:HG22	1.89	0.54
1:A:247:GLU:OE2	1:A:334:TYR:OH	2.24	0.54
1:D:308:ARG:NH1	1:D:372:ASN:O	2.41	0.54
1:E:212:GLN:OE1	1:E:214:ASN:ND2	2.31	0.54
1:A:102:LYS:O	1:A:145:ASN:ND2	2.40	0.54
1:B:258:ILE:HG23	1:B:287:GLN:HG2	1.88	0.54
1:C:464:LYS:NZ	1:C:590:ASP:OD2	2.40	0.54
1:D:478:THR:HA	1:D:481:LYS:HD3	1.88	0.54
1:D:501:LEU:HB3	1:D:536:VAL:HG22	1.90	0.54
1:D:621:LEU:HG	1:D:636:ALA:HB1	1.90	0.54
1:E:404:ASN:HA	1:E:843:GLN:NE2	2.23	0.54
1:E:464:LYS:HE3	1:E:502:MET:HE3	1.90	0.54
1:C:752:ASP:HB3	1:C:766:VAL:HA	1.90	0.54
1:A:741:ARG:HD2	1:A:775:LEU:HG	1.90	0.54
1:C:246:TRP:NE1	1:C:324:ASP:OD1	2.38	0.54
1:A:98:TYR:OH	1:A:142:SER:OG	2.26	0.54
1:A:350:ILE:HG23	1:A:354:ARG:HH22	1.73	0.54
1:B:288:ARG:HH22	1:B:310:SER:HB3	1.73	0.54
1:C:445:TRP:CD1	1:C:694:PRO:HB3	2.43	0.54
1:E:354:ARG:HD3	1:E:362:GLU:HB3	1.90	0.54
1:E:781:LEU:HD21	1:E:851:LEU:HD12	1.90	0.54
1:A:725:ASN:O	1:A:729:LYS:HG2	2.08	0.54
1:C:213:MET:HE2	1:C:220:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ARG:O	1:C:253:GLU:HG3	2.08	0.54
1:B:254:ILE:HD12	1:B:258:ILE:HG13	1.89	0.53
1:D:802:PHE:HD1	1:D:816:ALA:HB2	1.73	0.53
1:A:782:GLU:OE2	1:A:831:ARG:NE	2.40	0.53
1:D:356:ASN:OD1	1:D:356:ASN:N	2.42	0.53
1:D:561:ILE:HA	1:D:564:ARG:HD3	1.89	0.53
1:E:737:SER:HB2	1:E:741:ARG:HH21	1.73	0.53
1:A:485:ASP:HB3	1:A:488:ARG:HG3	1.91	0.53
1:C:336:GLY:HA2	1:C:346:TRP:CZ3	2.44	0.53
1:C:507:ARG:HG3	1:C:513:LYS:HE3	1.89	0.53
1:D:289:LEU:HD11	1:D:304:LEU:HD23	1.91	0.53
1:E:468:VAL:HG22	1:E:496:ILE:HG22	1.91	0.53
1:E:731:ILE:HD11	1:E:838:LYS:HB3	1.90	0.53
1:B:488:ARG:O	1:B:492:LEU:HG	2.08	0.53
1:B:706:TYR:HA	1:B:710:TYR:HB2	1.90	0.53
1:E:275:HIS:NE2	1:E:314:THR:OG1	2.37	0.53
1:B:325:TYR:HD1	1:B:325:TYR:H	1.57	0.53
1:C:593:MET:HG2	1:C:618:LEU:HB3	1.90	0.53
1:A:754:MET:HE3	1:A:765:LYS:H	1.74	0.53
1:D:202:THR:HG22	1:D:334:TYR:HA	1.91	0.53
1:B:740:GLU:OE1	1:B:740:GLU:N	2.31	0.53
1:E:110:VAL:HB	1:E:148:MET:HE2	1.91	0.53
1:B:502:MET:HG2	1:B:539:PHE:HE2	1.74	0.52
1:B:254:ILE:CD1	1:B:258:ILE:HG13	2.40	0.52
1:A:76:GLU:O	1:A:80:LYS:HG2	2.09	0.52
1:C:508:ARG:HE	1:C:540:PHE:HD2	1.57	0.52
1:D:492:LEU:O	1:D:495:ARG:HG2	2.09	0.52
1:A:244:GLY:HA3	1:A:248:ASN:HD22	1.75	0.52
1:B:516:HIS:HB3	1:B:557:LYS:NZ	2.24	0.52
1:E:802:PHE:HD1	1:E:816:ALA:HB2	1.74	0.52
1:A:687:ASN:O	1:A:691:THR:OG1	2.24	0.52
1:E:698:MET:O	1:E:698:MET:HG3	2.10	0.52
1:D:830:VAL:O	1:D:851:LEU:N	2.41	0.52
1:A:65:LEU:HD13	1:A:181:SER:HB3	1.92	0.52
1:B:237:ILE:HD11	1:B:251:LYS:HE2	1.92	0.52
1:C:743:ASP:OD1	1:C:849:LYS:NZ	2.37	0.52
1:D:275:HIS:ND1	1:D:710:TYR:OH	2.41	0.52
1:D:368:THR:HG23	1:D:395:ILE:HD11	1.91	0.52
1:D:698:MET:HG3	1:D:698:MET:O	2.09	0.52
1:B:19:LYS:NZ	1:C:758:ALA:O	2.39	0.52
1:C:161:LYS:HG2	1:C:173:ASN:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:GLY:O	1:D:248:ASN:ND2	2.31	0.52
1:E:369:PHE:O	1:E:373:THR:OG1	2.20	0.52
1:E:495:ARG:HD3	1:E:570:LYS:HE3	1.91	0.52
1:B:301:ASN:O	1:B:305:GLU:HG2	2.10	0.52
1:A:752:ASP:OD1	1:A:752:ASP:N	2.37	0.51
1:B:161:LYS:HB2	1:B:173:ASN:HB2	1.91	0.51
1:C:319:VAL:HG22	1:C:321:ALA:H	1.74	0.51
1:C:526:SER:O	1:C:530:ASN:HB2	2.10	0.51
1:D:398:GLY:HA3	1:D:848:VAL:HG11	1.90	0.51
1:A:518:LEU:O	1:A:658:TYR:OH	2.26	0.51
1:E:445:TRP:CD1	1:E:694:PRO:HB3	2.45	0.51
1:B:262:LEU:HA	1:B:265:LYS:HG2	1.91	0.51
1:B:398:GLY:HA3	1:B:848:VAL:HG11	1.93	0.51
1:E:165:SER:OG	1:E:167:ASP:OD1	2.26	0.51
1:A:354:ARG:HD2	1:A:362:GLU:HB3	1.92	0.51
1:B:51:LEU:O	1:B:74:ARG:NH2	2.43	0.51
1:A:516:HIS:HB3	1:A:554:LEU:HD21	1.92	0.51
1:C:617:ASN:HB3	1:C:619:SER:HB2	1.91	0.51
1:B:507:ARG:NH2	1:B:593:MET:O	2.43	0.51
1:C:831:ARG:HB2	1:C:848:VAL:CG2	2.40	0.51
1:D:414:HIS:CD2	1:D:416:PRO:HD2	2.46	0.51
1:A:783:LEU:HB3	1:A:800:TYR:HB2	1.92	0.51
1:C:296:ASP:HB3	1:C:298:LEU:HD13	1.93	0.51
1:D:3:ILE:HD12	1:E:300:PHE:CE2	2.46	0.50
1:E:278:GLU:HG3	1:E:279:GLY:H	1.76	0.50
1:A:445:TRP:CD1	1:A:694:PRO:HB3	2.45	0.50
1:A:460:ARG:NH2	1:A:589:VAL:O	2.44	0.50
1:B:7:TYR:HB3	1:C:847:TYR:CE1	2.47	0.50
1:C:25:GLU:CD	1:C:25:GLU:H	2.19	0.50
1:C:674:LYS:O	1:C:674:LYS:NZ	2.37	0.50
1:D:730:GLU:HA	1:D:733:LEU:HD23	1.93	0.50
1:A:526:SER:O	1:A:530:ASN:ND2	2.42	0.50
1:D:606:SER:HA	1:D:609:LLP:HD3	1.92	0.50
1:A:422:GLU:HB3	1:A:459:THR:HG23	1.93	0.50
1:B:477:GLN:HG2	1:C:643:TYR:HE2	1.77	0.50
1:C:212:GLN:OE1	1:C:214:ASN:ND2	2.28	0.50
1:D:272:GLU:O	1:D:310:SER:OG	2.30	0.50
1:A:606:SER:HA	1:A:609:LLP:HD3	1.93	0.50
1:C:147:ASP:OD1	1:C:271:LYS:NZ	2.44	0.50
1:E:246:TRP:NE1	1:E:325:TYR:O	2.42	0.50
1:C:507:ARG:HD2	1:C:604:GLY:HA2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:518:LEU:O	1:C:658:TYR:OH	2.24	0.50
1:A:23:PRO:HD2	1:A:26:LEU:HB2	1.94	0.50
1:A:147:ASP:OD1	1:A:271:LYS:NZ	2.45	0.50
1:C:250:LEU:HB2	1:C:326:PHE:CE1	2.47	0.50
1:D:482:ASN:O	1:D:483:GLN:C	2.55	0.49
1:D:741:ARG:HD2	1:D:775:LEU:HG	1.92	0.49
1:A:101:VAL:HG12	1:A:145:ASN:ND2	2.27	0.49
1:A:850:TRP:N	1:E:9:ASN:HD21	2.09	0.49
1:B:250:LEU:O	1:B:254:ILE:HG22	2.12	0.49
1:C:742:TRP:HA	1:C:745:ILE:HG12	1.94	0.49
1:E:782:GLU:HA	1:E:801:PRO:HA	1.93	0.49
1:D:368:THR:HG23	1:D:395:ILE:CD1	2.42	0.49
1:D:577:TYR:HA	1:D:581:LEU:HD23	1.94	0.49
1:B:832:MET:SD	1:B:849:LYS:NZ	2.85	0.49
1:D:327:ASP:OD1	1:D:327:ASP:N	2.31	0.49
1:B:501:LEU:HB3	1:B:536:VAL:HG22	1.94	0.49
1:D:65:LEU:HD13	1:D:181:SER:HB2	1.94	0.49
1:C:228:ASP:C	1:C:230:ASN:H	2.19	0.49
1:D:706:TYR:HA	1:D:710:TYR:HB2	1.93	0.49
1:E:24:LYS:HE2	1:E:24:LYS:HA	1.94	0.49
1:E:128:GLY:O	1:E:132:MET:HG2	2.12	0.49
1:A:85:MET:HE3	1:A:85:MET:O	2.13	0.49
1:B:26:LEU:HD21	1:B:85:MET:HE1	1.94	0.49
1:C:803:LYS:NZ	1:C:804:MET:O	2.45	0.49
1:D:376:GLU:OE2	1:D:712:LYS:NZ	2.46	0.49
1:E:25:GLU:HB3	1:E:85:MET:HE2	1.95	0.49
1:E:524:ARG:NH2	1:E:662:GLU:OE1	2.41	0.49
1:B:289:LEU:O	1:B:293:ILE:HG22	2.13	0.49
1:C:785:VAL:O	1:C:797:TYR:N	2.46	0.49
1:E:752:ASP:N	1:E:752:ASP:OD1	2.46	0.49
1:B:258:ILE:HD13	1:B:287:GLN:HB2	1.95	0.48
1:B:265:LYS:C	1:B:267:LEU:H	2.21	0.48
1:B:353:GLY:HA3	1:B:364:PHE:CE2	2.48	0.48
1:E:323:HIS:CG	1:E:367:SER:HG	2.28	0.48
1:C:160:PHE:O	1:C:543:LYS:NZ	2.39	0.48
1:A:339:PRO:HG3	1:A:346:TRP:HE3	1.78	0.48
1:C:189:ASP:OD2	1:C:191:ASN:ND2	2.47	0.48
1:D:734:TRP:CH2	1:D:836:ASN:HB2	2.48	0.48
1:E:51:LEU:O	1:E:74:ARG:NH2	2.43	0.48
1:A:24:LYS:HG2	1:A:25:GLU:HG3	1.95	0.48
1:A:90:ASN:O	1:A:94:MET:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:PHE:HD2	1:A:814:PHE:HB3	1.79	0.48
1:B:13:TRP:HA	1:B:13:TRP:CE3	2.48	0.48
1:B:621:LEU:HG	1:B:636:ALA:HB1	1.96	0.48
1:C:529:VAL:HG12	1:C:538:PHE:HE1	1.78	0.48
1:D:132:MET:HE1	1:D:579:MET:SD	2.53	0.48
1:D:167:ASP:OD1	1:D:167:ASP:N	2.36	0.48
1:B:521:ASP:OD1	1:B:524:ARG:HB2	2.13	0.48
1:C:396:TRP:CH2	1:C:405:HIS:HE1	2.31	0.48
1:C:620:VAL:HG12	1:C:622:ASP:HB2	1.95	0.48
1:A:259:GLY:O	1:A:263:THR:OG1	2.22	0.48
1:A:326:PHE:CE2	1:A:366:LEU:HD11	2.49	0.48
1:A:579:MET:HE2	1:A:579:MET:HB3	1.67	0.48
1:B:268:GLY:O	1:B:270:LYS:HD2	2.14	0.48
1:C:201:TYR:OH	1:C:251:LYS:O	2.31	0.48
1:C:518:LEU:HD21	1:C:538:PHE:CE2	2.49	0.48
1:D:748:VAL:HB	1:D:769:VAL:HG12	1.94	0.48
1:A:788:GLU:HG2	1:A:789:GLN:OE1	2.14	0.48
1:B:577:TYR:CZ	1:B:609:LLP:H2'2	2.48	0.48
1:C:607:GLY:O	1:C:611:GLU:HG2	2.13	0.48
1:C:625:TRP:O	1:C:629:TYR:N	2.45	0.48
1:A:326:PHE:HE2	1:A:366:LEU:HD11	1.78	0.48
1:B:296:ASP:HB3	1:B:298:LEU:HD12	1.95	0.48
1:A:263:THR:HG22	1:A:267:LEU:HD12	1.95	0.47
1:A:727:LEU:HD11	1:A:838:LYS:HD2	1.95	0.47
1:B:298:LEU:HD12	1:B:298:LEU:H	1.79	0.47
1:E:775:LEU:HD13	1:E:778:ALA:HB3	1.96	0.47
1:A:352:MET:O	1:A:372:ASN:ND2	2.43	0.47
1:B:66:LEU:HD23	1:B:67:LEU:HD23	1.96	0.47
1:C:606:SER:HA	1:C:609:LLP:HD3	1.97	0.47
1:D:60:ASN:O	1:D:60:ASN:ND2	2.47	0.47
1:D:301:ASN:ND2	1:D:736:GLU:OE2	2.48	0.47
1:E:36:MET:SD	1:E:213:MET:HE3	2.55	0.47
1:E:422:GLU:HB3	1:E:459:THR:HG23	1.97	0.47
1:A:236:PRO:HA	1:A:239:TYR:CD1	2.49	0.47
1:C:476:THR:HG23	1:C:489:VAL:HG21	1.96	0.47
1:D:209:TYR:N	1:D:224:ASP:O	2.47	0.47
1:A:132:MET:HE3	1:A:132:MET:HB3	1.72	0.47
1:B:351:GLY:HA2	1:B:354:ARG:HG3	1.96	0.47
1:B:433:LYS:HD2	1:B:433:LYS:N	2.29	0.47
1:D:186:ARG:HH11	1:D:194:PRO:HB3	1.80	0.47
1:D:245:ASP:OD1	1:D:245:ASP:N	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:GLU:HA	1:D:305:GLU:OE1	2.15	0.47
1:E:645:ASN:HB3	1:E:648:TYR:CD2	2.49	0.47
1:A:155:TYR:CZ	1:A:241:LEU:HD13	2.49	0.47
1:C:619:SER:HB3	1:C:625:TRP:CD1	2.50	0.47
1:D:160:PHE:HE2	1:D:162:GLN:HB2	1.79	0.47
1:D:610:ALA:HB1	1:D:615:VAL:HB	1.97	0.47
1:A:466:LYS:HB3	1:A:466:LYS:HE3	1.62	0.46
1:E:747:VAL:HG21	1:E:750:LYS:HB3	1.97	0.46
1:A:121:GLN:OE1	1:A:580:THR:OG1	2.20	0.46
1:B:75:LYS:O	1:B:79:VAL:HG23	2.15	0.46
1:A:198:ASP:OD1	1:A:207:HIS:ND1	2.48	0.46
1:A:332:GLY:HA2	1:A:346:TRP:CH2	2.50	0.46
1:C:413:VAL:HG11	1:C:609:LLP:HG2	1.96	0.46
1:C:734:TRP:HH2	1:C:834:PRO:HB3	1.79	0.46
1:D:785:VAL:HG22	1:D:828:THR:HG23	1.96	0.46
1:E:427:TYR:O	1:E:431:PHE:HB2	2.15	0.46
1:E:368:THR:HG23	1:E:395:ILE:CD1	2.45	0.46
1:B:112:TYR:CZ	1:B:277:ASN:ND2	2.83	0.46
1:B:468:VAL:HG21	1:B:498:PRO:HB3	1.98	0.46
1:B:505:PHE:N	1:B:505:PHE:CD1	2.84	0.46
1:C:109:SER:HB2	1:C:271:LYS:HD3	1.98	0.46
1:B:120:ASN:OD1	1:B:121:GLN:N	2.41	0.46
1:B:129:GLY:HA2	1:B:609:LLP:HG2	1.98	0.46
1:B:519:PHE:CE2	1:B:558:ILE:HG12	2.51	0.46
1:B:535:PRO:O	1:B:670:TYR:OH	2.30	0.46
1:B:747:VAL:HA	1:B:770:ILE:HD12	1.98	0.46
1:C:481:LYS:HB3	1:C:481:LYS:HE3	1.71	0.46
1:D:430:TYR:CD2	1:D:451:VAL:HG22	2.50	0.46
1:E:186:ARG:HH11	1:E:194:PRO:HB3	1.79	0.46
1:C:47:LEU:HA	1:C:87:LYS:HD2	1.97	0.46
1:C:512:TYR:CE2	1:C:601:GLU:HA	2.50	0.46
1:C:750:LYS:HE2	1:C:750:LYS:HB3	1.86	0.46
1:D:22:LEU:HG	1:D:26:LEU:HB3	1.97	0.46
1:E:29:LEU:HD11	1:E:47:LEU:HD21	1.97	0.46
1:C:247:GLU:OE2	1:C:334:TYR:OH	2.27	0.46
1:C:395:ILE:HG22	1:C:396:TRP:CD1	2.51	0.46
1:A:748:VAL:HG21	1:A:811:ASN:OD1	2.15	0.46
1:B:383:LEU:HD22	1:B:626:VAL:HG21	1.98	0.46
1:C:508:ARG:HH21	1:C:540:PHE:HB3	1.81	0.46
1:D:659:ASN:OD1	1:D:663:ASN:ND2	2.49	0.46
1:A:203:ASN:N	1:A:203:ASN:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:THR:HG22	1:E:72:TYR:OH	2.16	0.46
1:B:18:ILE:HD13	1:C:826:PHE:HD2	1.81	0.46
1:D:535:PRO:O	1:D:670:TYR:OH	2.34	0.46
1:E:53:PRO:O	1:E:57:GLU:HG3	2.16	0.46
1:A:250:LEU:HD13	1:A:326:PHE:CE2	2.51	0.45
1:B:514:ARG:HB3	1:B:517:LEU:HD13	1.98	0.45
1:A:741:ARG:HE	1:A:741:ARG:HB3	1.59	0.45
1:B:1:MET:O	1:B:2:LYS:HD2	2.16	0.45
1:D:117:TYR:O	1:D:126:TYR:HB3	2.16	0.45
1:B:317:THR:OG1	1:B:319:VAL:O	2.34	0.45
1:D:353:GLY:HA3	1:D:364:PHE:CE1	2.51	0.45
1:E:467:LEU:O	1:E:471:ILE:HG12	2.15	0.45
1:A:207:HIS:O	1:A:230:ASN:ND2	2.44	0.45
1:C:3:ILE:HD13	1:D:735:LYS:HB3	1.97	0.45
1:C:535:PRO:O	1:C:670:TYR:OH	2.30	0.45
1:C:512:TYR:HE2	1:C:601:GLU:HA	1.80	0.45
1:E:261:ILE:HD11	1:E:284:CYS:HB2	1.98	0.45
1:E:698:MET:HE2	1:E:698:MET:HB2	1.83	0.45
1:A:621:LEU:HG	1:A:636:ALA:HB1	1.99	0.45
1:B:36:MET:HE2	1:B:36:MET:HB3	1.79	0.45
1:D:186:ARG:NH1	1:D:194:PRO:HB3	2.31	0.45
1:E:99:MET:HE3	1:E:99:MET:HB3	1.77	0.45
1:B:641:ARG:HE	1:B:641:ARG:HB3	1.51	0.45
1:C:224:ASP:N	1:C:224:ASP:OD1	2.50	0.45
1:C:250:LEU:HD11	1:C:335:MET:HE1	1.98	0.45
1:C:701:GLN:HE21	1:C:705:TYR:HE2	1.65	0.45
1:E:605:THR:HA	1:E:608:GLU:HG3	1.98	0.45
1:E:155:TYR:CZ	1:E:241:LEU:HD13	2.51	0.45
1:E:739:ALA:HA	1:E:847:TYR:HE2	1.81	0.45
1:B:13:TRP:H	1:C:850:TRP:HE1	1.65	0.44
1:B:366:LEU:HD12	1:B:366:LEU:HA	1.77	0.44
1:C:613:ASN:O	1:C:613:ASN:ND2	2.41	0.44
1:C:850:TRP:CD1	1:C:850:TRP:C	2.94	0.44
1:D:2:LYS:O	1:E:301:ASN:ND2	2.48	0.44
1:A:755:LEU:HD22	1:E:16:THR:HG21	1.98	0.44
1:E:827:LYS:HB2	1:E:827:LYS:NZ	2.31	0.44
1:A:337:GLY:O	1:A:341:ARG:HG3	2.17	0.44
1:A:427:TYR:O	1:A:431:PHE:HB2	2.18	0.44
1:C:783:LEU:HD23	1:C:800:TYR:HD2	1.82	0.44
1:D:166:MET:HE1	1:D:482:ASN:HA	1.98	0.44
1:A:758:ALA:HB3	1:E:18:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:CYS:HB2	1:D:92:TYR:CD1	2.52	0.44
1:E:352:MET:HE2	1:E:352:MET:HB2	1.87	0.44
1:E:802:PHE:CD1	1:E:816:ALA:HB2	2.51	0.44
1:B:836:ASN:HB3	1:B:839:LEU:HD23	1.97	0.44
1:D:457:TRP:CD1	1:D:677:PHE:HB3	2.53	0.44
1:E:413:VAL:HG13	1:E:608:GLU:HB2	2.00	0.44
1:E:474:LYS:HD2	1:E:474:LYS:HA	1.68	0.44
1:E:834:PRO:HD3	1:E:847:TYR:O	2.18	0.44
1:B:517:LEU:HD21	1:B:653:ASP:HB3	2.00	0.44
1:B:706:TYR:O	1:B:711:ASN:ND2	2.50	0.44
1:E:254:ILE:HD13	1:E:254:ILE:HA	1.85	0.44
1:E:478:THR:HA	1:E:481:LYS:HD3	1.99	0.44
1:E:518:LEU:O	1:E:658:TYR:OH	2.31	0.44
1:A:775:LEU:HD13	1:A:778:ALA:HB3	2.00	0.44
1:A:830:VAL:O	1:A:851:LEU:N	2.44	0.44
1:B:29:LEU:HD21	1:B:88:VAL:HG13	2.00	0.44
1:B:228:ASP:OD1	1:B:228:ASP:N	2.50	0.44
1:B:264:LEU:HD22	1:B:264:LEU:HA	1.74	0.44
1:B:269:ILE:HD12	1:B:269:ILE:O	2.18	0.44
1:C:136:ASP:HB3	1:C:414:HIS:HB2	1.98	0.44
1:C:766:VAL:O	1:C:815:GLU:HG2	2.18	0.44
1:B:51:LEU:HD23	1:B:66:LEU:HD21	2.00	0.44
1:C:165:SER:OG	1:C:167:ASP:OD1	2.24	0.44
1:D:330:LEU:HA	1:D:333:LYS:HD3	1.99	0.44
1:E:782:GLU:HG2	1:E:833:TYR:CE2	2.52	0.44
1:E:803:LYS:HE2	1:E:803:LYS:HB2	1.82	0.44
1:B:191:ASN:HB2	1:B:193:ASN:OD1	2.18	0.43
1:B:456:ILE:HD12	1:B:686:LYS:HE3	2.00	0.43
1:D:323:HIS:NE2	1:D:391:MET:SD	2.91	0.43
1:D:509:PHE:HE2	1:D:558:ILE:HD12	1.83	0.43
1:D:671:ASN:ND2	1:D:671:ASN:C	2.75	0.43
1:D:741:ARG:HD2	1:D:775:LEU:CG	2.48	0.43
1:E:645:ASN:HB3	1:E:648:TYR:HD2	1.83	0.43
1:D:74:ARG:HA	1:D:74:ARG:HD2	1.77	0.43
1:D:324:ASP:HB2	1:D:366:LEU:HB2	2.00	0.43
1:E:187:VAL:HG11	1:E:267:LEU:HD21	1.99	0.43
1:A:186:ARG:HD2	1:A:194:PRO:HB3	2.00	0.43
1:B:272:GLU:O	1:B:310:SER:OG	2.35	0.43
1:B:479:TRP:CZ3	1:B:568:LEU:HD21	2.53	0.43
1:C:430:TYR:CD2	1:C:451:VAL:HG22	2.54	0.43
1:D:160:PHE:CE2	1:D:162:GLN:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:VAL:HG23	1:D:709:PHE:HE2	1.83	0.43
1:D:775:LEU:HD13	1:D:778:ALA:HB3	2.00	0.43
1:E:102:LYS:O	1:E:145:ASN:ND2	2.48	0.43
1:E:227:ASN:O	1:E:235:ARG:NE	2.50	0.43
1:B:770:ILE:HG12	1:B:832:MET:HE1	2.01	0.43
1:C:448:ILE:HD11	1:C:456:ILE:HD11	2.00	0.43
1:D:197:VAL:HG12	1:D:266:LYS:HD2	2.00	0.43
1:D:350:ILE:HG12	1:D:354:ARG:NH2	2.33	0.43
1:B:273:ILE:HD11	1:B:714:ALA:HB2	2.01	0.43
1:B:775:LEU:HD23	1:B:778:ALA:HB3	2.00	0.43
1:C:108:PRO:HD2	1:C:706:TYR:CE1	2.54	0.43
1:C:508:ARG:HA	1:C:513:LYS:CG	2.49	0.43
1:C:513:LYS:HD2	1:C:596:PRO:HB3	1.99	0.43
1:D:162:GLN:NE2	1:D:170:GLN:OE1	2.39	0.43
1:D:484:GLY:O	1:D:485:ASP:C	2.61	0.43
1:A:212:GLN:OE1	1:A:214:ASN:ND2	2.40	0.43
1:A:517:LEU:HD21	1:A:653:ASP:HB3	1.99	0.43
1:B:258:ILE:O	1:B:262:LEU:HG	2.19	0.43
1:E:450:LYS:HB2	1:E:450:LYS:HE3	1.75	0.43
1:C:55:LEU:HD21	1:C:69:ARG:HB3	1.99	0.43
1:C:80:LYS:HB2	1:C:80:LYS:HE2	1.81	0.43
1:E:166:MET:HE3	1:E:166:MET:HB3	1.67	0.43
1:E:598:ARG:HA	1:E:599:PRO:HA	1.91	0.43
1:C:345:SER:N	1:C:348:GLU:OE2	2.35	0.43
1:D:302:GLN:HG2	1:D:729:LYS:HA	1.99	0.43
1:A:356:ASN:OD1	1:A:356:ASN:N	2.51	0.43
1:B:355:GLU:OE1	1:B:394:ASN:HB3	2.18	0.43
1:C:275:HIS:NE2	1:C:314:THR:OG1	2.34	0.43
1:C:431:PHE:CE2	1:C:445:TRP:HA	2.54	0.43
1:E:38:TRP:CD1	1:E:38:TRP:H	2.37	0.43
1:E:78:ILE:HD13	1:E:78:ILE:HA	1.85	0.43
1:A:338:TYR:N	1:A:339:PRO:HD2	2.33	0.42
1:B:258:ILE:HG23	1:B:287:GLN:HG3	2.00	0.42
1:B:513:LYS:O	1:B:515:ALA:N	2.51	0.42
1:C:207:HIS:O	1:C:230:ASN:ND2	2.52	0.42
1:E:323:HIS:CE1	1:E:367:SER:HG	2.33	0.42
1:E:337:GLY:O	1:E:341:ARG:HG3	2.18	0.42
1:E:433:LYS:HA	1:E:433:LYS:HD3	1.83	0.42
1:E:706:TYR:HA	1:E:710:TYR:HB2	2.01	0.42
1:B:527:LYS:HB3	1:B:527:LYS:HE3	1.75	0.42
1:C:380:VAL:HG23	1:C:603:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:LEU:HD23	1:C:502:MET:HE1	2.02	0.42
1:E:70:LEU:HD23	1:E:70:LEU:HA	1.78	0.42
1:E:250:LEU:HD11	1:E:335:MET:HE3	2.01	0.42
1:E:287:GLN:NE2	1:E:291:ASP:OD1	2.51	0.42
1:A:29:LEU:HD13	1:A:51:LEU:HD11	2.01	0.42
1:C:65:LEU:HD13	1:C:181:SER:HB2	2.01	0.42
1:C:102:LYS:HA	1:C:102:LYS:HD2	1.87	0.42
1:C:227:ASN:O	1:C:235:ARG:NE	2.52	0.42
1:C:412:GLY:N	1:C:701:GLN:OE1	2.47	0.42
1:D:445:TRP:CG	1:D:694:PRO:HB3	2.54	0.42
1:B:156:ARG:NE	1:B:226:ASP:OD2	2.40	0.42
1:B:621:LEU:HD22	1:B:626:VAL:HA	2.00	0.42
1:B:741:ARG:HH21	1:B:775:LEU:CD1	2.26	0.42
1:C:366:LEU:HD12	1:C:366:LEU:HA	1.77	0.42
1:C:513:LYS:CD	1:C:596:PRO:HB3	2.49	0.42
1:D:8:ALA:HA	1:E:848:VAL:O	2.19	0.42
1:D:509:PHE:CE2	1:D:558:ILE:HD12	2.55	0.42
1:E:24:LYS:NZ	1:E:27:LYS:HD3	2.34	0.42
1:A:320:PRO:O	1:A:325:TYR:OH	2.35	0.42
1:A:354:ARG:CD	1:A:362:GLU:HB3	2.49	0.42
1:A:701:GLN:HE21	1:A:705:TYR:HE2	1.68	0.42
1:A:735:LYS:HE2	1:A:845:PHE:HB2	2.02	0.42
1:C:620:VAL:HG22	1:C:637:LEU:HD22	2.00	0.42
1:C:154:LEU:HD12	1:C:154:LEU:HA	1.85	0.42
1:C:202:THR:OG1	1:C:334:TYR:O	2.38	0.42
1:C:514:ARG:HB3	1:C:595:THR:O	2.19	0.42
1:D:474:LYS:O	1:D:478:THR:HG22	2.19	0.42
1:E:741:ARG:HB3	1:E:741:ARG:NH1	2.34	0.42
1:A:548:ASP:O	1:A:552:GLN:HG3	2.18	0.42
1:C:755:LEU:HD22	1:C:764:ILE:HD12	2.01	0.42
1:D:51:LEU:HD22	1:D:78:ILE:HD13	2.01	0.42
1:D:288:ARG:HH12	1:D:311:SER:HG	1.56	0.42
1:D:741:ARG:HD3	1:D:773:GLN:OE1	2.19	0.42
1:E:464:LYS:NZ	1:E:669:TYR:OH	2.52	0.42
1:E:620:VAL:HA	1:E:637:LEU:HB2	2.02	0.42
1:C:29:LEU:HD21	1:C:88:VAL:HG21	2.00	0.42
1:C:353:GLY:HA3	1:C:364:PHE:CE1	2.55	0.42
1:C:388:SER:HA	1:C:391:MET:HG2	2.00	0.42
1:E:57:GLU:HG3	1:E:57:GLU:H	1.72	0.42
1:B:57:GLU:OE1	1:B:57:GLU:N	2.53	0.42
1:B:251:LYS:HE3	1:B:334:TYR:OH	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:TRP:CD2	1:B:609:LLP:HG3	2.54	0.42
1:B:719:LYS:HE3	1:B:719:LYS:HB2	1.88	0.42
1:E:286:LEU:HB2	1:E:369:PHE:CZ	2.55	0.42
1:B:147:ASP:OD1	1:B:271:LYS:NZ	2.53	0.42
1:B:203:ASN:OD1	1:B:203:ASN:N	2.51	0.42
1:B:734:TRP:O	1:B:738:VAL:HG23	2.20	0.42
1:C:356:ASN:N	1:C:362:GLU:OE1	2.48	0.42
1:C:781:LEU:HA	1:C:831:ARG:O	2.19	0.42
1:D:464:LYS:NZ	1:D:669:TYR:OH	2.53	0.42
1:E:409:VAL:HG23	1:E:709:PHE:HE2	1.85	0.42
1:A:2:LYS:HD2	1:B:344:ILE:HG12	2.01	0.41
1:B:610:ALA:HB1	1:B:615:VAL:HB	2.01	0.41
1:D:358:ASP:OD1	1:D:359:ASP:N	2.51	0.41
1:E:4:LYS:HD3	1:E:7:TYR:HD1	1.85	0.41
1:E:579:MET:HE2	1:E:579:MET:HB3	1.76	0.41
1:A:598:ARG:HA	1:A:599:PRO:HA	1.92	0.41
1:E:352:MET:O	1:E:372:ASN:ND2	2.49	0.41
1:E:832:MET:HE2	1:E:851:LEU:HD21	2.01	0.41
1:A:132:MET:HE1	1:A:579:MET:HE3	2.02	0.41
1:A:740:GLU:OE2	1:A:741:ARG:NH2	2.49	0.41
1:C:250:LEU:O	1:C:250:LEU:HD12	2.20	0.41
1:C:507:ARG:HE	1:C:606:SER:H	1.68	0.41
1:E:148:MET:HE3	1:E:148:MET:HB2	1.81	0.41
1:E:738:VAL:O	1:E:742:TRP:HB2	2.20	0.41
1:A:832:MET:HE3	1:A:832:MET:HB3	1.85	0.41
1:B:4:LYS:H	1:C:735:LYS:NZ	2.17	0.41
1:C:671:ASN:ND2	1:C:680:GLU:OE2	2.36	0.41
1:D:31:GLU:OE1	1:D:92:TYR:OH	2.32	0.41
1:E:175:ASP:OD1	1:E:176:ALA:N	2.53	0.41
1:E:772:GLU:HB2	1:E:812:PHE:CE1	2.56	0.41
1:A:468:VAL:HG22	1:A:496:ILE:HG22	2.01	0.41
1:A:640:LYS:HD3	1:A:640:LYS:HA	1.72	0.41
1:B:259:GLY:HA2	1:B:262:LEU:HD12	2.01	0.41
1:C:239:TYR:HD1	1:C:239:TYR:HA	1.71	0.41
1:C:318:PRO:HA	1:C:384:HIS:HE2	1.84	0.41
1:D:128:GLY:O	1:D:132:MET:HG2	2.20	0.41
1:E:201:TYR:HE2	1:E:251:LYS:HG2	1.85	0.41
1:E:339:PRO:HG2	1:E:346:TRP:HE3	1.85	0.41
1:A:653:ASP:HA	1:A:656:THR:HG22	2.02	0.41
1:B:106:LYS:HE2	1:B:106:LYS:HB3	1.84	0.41
1:C:288:ARG:NH1	1:C:311:SER:OG	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:PHE:HD1	1:C:335:MET:HE3	1.83	0.41
1:D:27:LYS:HD2	1:D:27:LYS:HA	1.74	0.41
1:E:324:ASP:HB2	1:E:366:LEU:HD12	2.03	0.41
1:B:56:TYR:CE1	1:B:61:ALA:HA	2.56	0.41
1:B:834:PRO:HD3	1:B:847:TYR:O	2.20	0.41
1:E:24:LYS:HZ1	1:E:27:LYS:HD3	1.85	0.41
1:A:409:VAL:HG23	1:A:709:PHE:HE2	1.86	0.41
1:B:20:SER:HB2	1:C:823:ALA:HB3	2.03	0.41
1:B:344:ILE:HD12	1:B:344:ILE:HA	1.88	0.41
1:C:509:PHE:HA	1:C:554:LEU:HD23	2.03	0.41
1:C:716:ARG:O	1:C:720:LEU:HB2	2.21	0.41
1:D:227:ASN:O	1:D:235:ARG:NH2	2.52	0.41
1:B:206:VAL:HG13	1:B:234:ASP:OD2	2.20	0.41
1:C:33:ALA:HB2	1:C:48:PHE:CZ	2.56	0.41
1:C:247:GLU:HG2	1:C:334:TYR:HE2	1.86	0.41
1:C:254:ILE:HG23	1:C:258:ILE:HD12	2.02	0.41
1:C:292:TYR:HD1	1:C:292:TYR:HA	1.77	0.41
1:C:506:CYS:HB2	1:C:592:TRP:CZ3	2.56	0.41
1:D:42:TYR:H	1:D:42:TYR:HD1	1.69	0.41
1:D:359:ASP:OD2	1:D:362:GLU:N	2.54	0.41
1:D:427:TYR:O	1:D:431:PHE:HB2	2.21	0.41
1:A:415:PHE:HZ	1:A:427:TYR:HD2	1.69	0.41
1:B:70:LEU:O	1:B:75:LYS:NZ	2.33	0.41
1:C:116:GLU:OE2	1:C:242:TYR:OH	2.37	0.41
1:C:348:GLU:H	1:C:348:GLU:HG3	1.65	0.41
1:D:17:THR:HA	1:E:825:SER:HA	2.01	0.41
1:E:246:TRP:CD1	1:E:326:PHE:HD1	2.39	0.41
1:E:754:MET:SD	1:E:754:MET:N	2.90	0.41
1:E:782:GLU:HG2	1:E:833:TYR:HE2	1.85	0.41
1:E:802:PHE:HB3	1:E:814:PHE:HB3	2.03	0.41
1:B:4:LYS:H	1:C:735:LYS:HZ3	1.69	0.40
1:B:94:MET:HA	1:B:97:GLU:HG2	2.03	0.40
1:B:263:THR:O	1:B:267:LEU:HD13	2.21	0.40
1:B:445:TRP:CD1	1:B:694:PRO:HB3	2.56	0.40
1:B:505:PHE:CZ	1:B:518:LEU:HD22	2.56	0.40
1:C:93:LYS:O	1:C:97:GLU:HG2	2.21	0.40
1:D:709:PHE:O	1:D:713:GLU:HB2	2.20	0.40
1:D:832:MET:HE2	1:D:849:LYS:HD2	2.02	0.40
1:E:108:PRO:HD2	1:E:706:TYR:CE1	2.56	0.40
1:E:594:ASN:O	1:E:619:SER:HA	2.21	0.40
1:A:353:GLY:HA3	1:A:364:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:PRO:O	1:A:670:TYR:OH	2.33	0.40
1:A:652:LEU:O	1:A:656:THR:HG22	2.22	0.40
1:B:72:TYR:CD1	1:B:72:TYR:C	2.99	0.40
1:D:29:LEU:HB3	1:D:67:LEU:HD11	2.03	0.40
1:D:102:LYS:HE2	1:D:103:PRO:CD	2.51	0.40
1:E:132:MET:HE1	1:E:579:MET:SD	2.61	0.40
1:E:621:LEU:HG	1:E:636:ALA:HB1	2.02	0.40
1:B:464:LYS:O	1:B:468:VAL:HG23	2.22	0.40
1:D:22:LEU:HD12	1:D:22:LEU:HA	1.88	0.40
1:A:14:LYS:HA	1:A:14:LYS:HD3	1.77	0.40
1:C:3:ILE:CD1	1:D:735:LYS:HB3	2.51	0.40
1:C:228:ASP:C	1:C:230:ASN:N	2.79	0.40
1:E:121:GLN:NE2	1:E:578:ASP:OD2	2.54	0.40
1:E:509:PHE:HE2	1:E:558:ILE:HD12	1.85	0.40
1:A:261:ILE:HD11	1:A:284:CYS:HB2	2.03	0.40
1:A:331:PHE:CE1	1:A:335:MET:HG3	2.56	0.40
1:B:381:SER:O	1:B:385:GLY:N	2.47	0.40
1:B:701:GLN:HE21	1:B:705:TYR:HE2	1.69	0.40
1:C:593:MET:SD	1:C:618:LEU:HD13	2.62	0.40
1:D:133:LEU:HD22	1:D:698:MET:HE1	2.02	0.40
1:D:439:GLN:O	1:D:445:TRP:NE1	2.54	0.40
1:D:594:ASN:O	1:D:619:SER:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	849/852 (100%)	803 (95%)	46 (5%)	0	100	100
1	B	849/852 (100%)	802 (94%)	46 (5%)	1 (0%)	48	78
1	C	849/852 (100%)	797 (94%)	52 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	849/852 (100%)	798 (94%)	50 (6%)	1 (0%)	48	78
1	E	849/852 (100%)	806 (95%)	43 (5%)	0	100	100
All	All	4245/4260 (100%)	4006 (94%)	237 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	514	ARG
1	D	202	THR

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	737/737 (100%)	706 (96%)	31 (4%)	26	59
1	B	737/737 (100%)	708 (96%)	29 (4%)	28	60
1	C	737/737 (100%)	717 (97%)	20 (3%)	39	70
1	D	737/737 (100%)	704 (96%)	33 (4%)	24	57
1	E	737/737 (100%)	704 (96%)	33 (4%)	24	57
All	All	3685/3685 (100%)	3539 (96%)	146 (4%)	29	60

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ASP
1	A	76	GLU
1	A	115	MET
1	A	127	SER
1	A	142	SER
1	A	193	ASN
1	A	203	ASN
1	A	239	TYR
1	A	241	LEU

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Mol	Chain	Res	Type
1	A	246	TRP
1	A	265	LYS
1	A	289	LEU
1	A	291	ASP
1	A	294	GLU
1	A	295	GLU
1	A	315	VAL
1	A	356	ASN
1	A	359	ASP
1	A	468	VAL
1	A	507	ARG
1	A	511	THR
1	A	513	LYS
1	A	554	LEU
1	A	605	THR
1	A	606	SER
1	A	664	ASP
1	A	680	GLU
1	A	759	GLU
1	A	769	VAL
1	A	784	VAL
1	A	832	MET
1	B	24	LYS
1	B	69	ARG
1	B	73	ASP
1	B	101	VAL
1	B	115	MET
1	B	116	GLU
1	B	121	GLN
1	B	148	MET
1	B	178	ASN
1	B	191	ASN
1	B	195	LEU
1	B	215	VAL
1	B	220	LEU
1	B	229	MET
1	B	239	TYR
1	B	264	LEU
1	B	315	VAL
1	B	325	TYR
1	B	450	LYS
1	B	474	LYS

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Mol	Chain	Res	Type
1	B	493	LEU
1	B	557	LYS
1	B	605	THR
1	B	617	ASN
1	B	749	SER
1	B	752	ASP
1	B	760	THR
1	B	764	ILE
1	B	784	VAL
1	C	110	VAL
1	C	116	GLU
1	C	119	ILE
1	C	121	GLN
1	C	166	MET
1	C	215	VAL
1	C	239	TYR
1	C	246	TRP
1	C	292	TYR
1	C	294	GLU
1	C	391	MET
1	C	456	ILE
1	C	518	LEU
1	C	613	ASN
1	C	618	LEU
1	C	727	LEU
1	C	817	GLU
1	C	828	THR
1	C	850	TRP
1	C	852	ASN
1	D	57	GLU
1	D	76	GLU
1	D	133	LEU
1	D	163	SER
1	D	195	LEU
1	D	239	TYR
1	D	245	ASP
1	D	315	VAL
1	D	327	ASP
1	D	330	LEU
1	D	350	ILE
1	D	352	MET
1	D	382	LYS

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Mol	Chain	Res	Type
1	D	390	GLN
1	D	394	ASN
1	D	468	VAL
1	D	481	LYS
1	D	483	GLN
1	D	511	THR
1	D	513	LYS
1	D	517	LEU
1	D	536	VAL
1	D	580	THR
1	D	584	ARG
1	D	591	ILE
1	D	605	THR
1	D	671	ASN
1	D	727	LEU
1	D	730	GLU
1	D	733	LEU
1	D	740	GLU
1	D	788	GLU
1	D	837	ASP
1	E	31	GLU
1	E	70	LEU
1	E	123	VAL
1	E	166	MET
1	E	198	ASP
1	E	204	TYR
1	E	231	SER
1	E	241	LEU
1	E	247	GLU
1	E	254	ILE
1	E	292	TYR
1	E	315	VAL
1	E	317	THR
1	E	468	VAL
1	E	473	GLU
1	E	478	THR
1	E	481	LYS
1	E	489	VAL
1	E	511	THR
1	E	512	TYR
1	E	564	ARG
1	E	601	GLU

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Mol	Chain	Res	Type
1	E	605	THR
1	E	617	ASN
1	E	720	LEU
1	E	743	ASP
1	E	747	VAL
1	E	748	VAL
1	E	754	MET
1	E	759	GLU
1	E	760	THR
1	E	773	GLN
1	E	808	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	GLN
1	A	277	ASN
1	A	299	ASN
1	A	301	ASN
1	A	394	ASN
1	A	434	ASN
1	A	437	ASN
1	A	659	ASN
1	A	663	ASN
1	A	671	ASN
1	A	795	GLN
1	B	35	ASN
1	B	121	GLN
1	B	205	GLN
1	B	230	ASN
1	B	248	ASN
1	B	378	ASN
1	B	394	ASN
1	B	434	ASN
1	B	439	GLN
1	B	497	ASN
1	B	499	ASN
1	B	644	GLN
1	B	663	ASN
1	C	177	GLN
1	C	180	ASN
1	C	302	GLN

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Mol	Chain	Res	Type
1	C	497	ASN
1	C	594	ASN
1	C	773	GLN
1	D	35	ASN
1	D	90	ASN
1	D	207	HIS
1	D	280	HIS
1	D	378	ASN
1	D	458	ASN
1	D	477	GLN
1	D	530	ASN
1	D	617	ASN
1	D	663	ASN
1	D	695	HIS
1	E	9	ASN
1	E	62	ASN
1	E	104	ASN
1	E	177	GLN
1	E	301	ASN
1	E	405	HIS
1	E	545	HIS
1	E	644	GLN
1	E	645	ASN
1	E	649	GLN
1	E	663	ASN
1	E	671	ASN
1	E	725	ASN
1	E	767	GLN
1	E	841	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	LLP	C	609	1	7,8,25	0.51	0	3,8,34	0.28	0
1	LLP	D	609	1	23,24,25	0.50	0	25,32,34	0.52	0
1	LLP	E	609	1	23,24,25	0.53	0	25,32,34	0.62	0
1	LLP	B	609	1	23,24,25	0.53	0	25,32,34	0.64	0
1	LLP	A	609	1	23,24,25	0.50	0	25,32,34	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	C	609	1	-	0/6/7/19	-
1	LLP	D	609	1	-	7/16/17/19	0/1/1/1
1	LLP	E	609	1	-	8/16/17/19	0/1/1/1
1	LLP	B	609	1	-	9/16/17/19	0/1/1/1
1	LLP	A	609	1	-	6/16/17/19	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	609	LLP	C5'-OP4-P-OP2
1	A	609	LLP	C5'-OP4-P-OP3
1	B	609	LLP	C4-C4'-NZ-CE
1	B	609	LLP	C5'-OP4-P-OP1
1	B	609	LLP	C5'-OP4-P-OP2
1	B	609	LLP	C5'-OP4-P-OP3
1	D	609	LLP	C4-C5-C5'-OP4
1	D	609	LLP	C5'-OP4-P-OP1
1	D	609	LLP	C5'-OP4-P-OP2
1	D	609	LLP	C5'-OP4-P-OP3
1	E	609	LLP	C5'-OP4-P-OP2
1	E	609	LLP	C5'-OP4-P-OP3

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Mol	Chain	Res	Type	Atoms
1	E	609	LLP	C4-C4'-NZ-CE
1	D	609	LLP	CD-CE-NZ-C4'
1	E	609	LLP	CG-CD-CE-NZ
1	D	609	LLP	C3-C4-C4'-NZ
1	A	609	LLP	CD-CE-NZ-C4'
1	A	609	LLP	C5-C4-C4'-NZ
1	A	609	LLP	C3-C4-C4'-NZ
1	B	609	LLP	CA-CB-CG-CD
1	A	609	LLP	C5'-OP4-P-OP1
1	E	609	LLP	C5'-OP4-P-OP1
1	E	609	LLP	C3-C4-C4'-NZ
1	D	609	LLP	C6-C5-C5'-OP4
1	B	609	LLP	CG-CD-CE-NZ
1	E	609	LLP	CD-CE-NZ-C4'
1	B	609	LLP	C3-C4-C4'-NZ
1	E	609	LLP	C5-C4-C4'-NZ
1	B	609	LLP	C4-C5-C5'-OP4
1	B	609	LLP	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	609	LLP	2	0
1	D	609	LLP	2	0
1	B	609	LLP	9	0
1	A	609	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

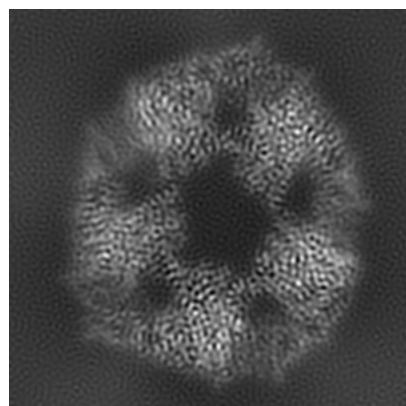
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62853. These allow visual inspection of the internal detail of the map and identification of artifacts.

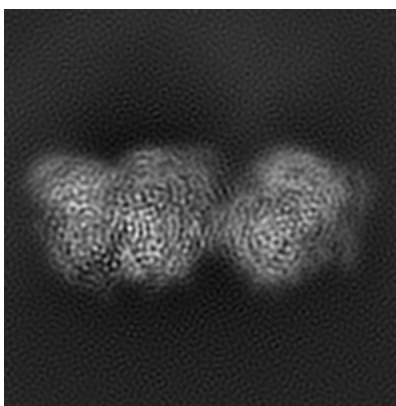
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

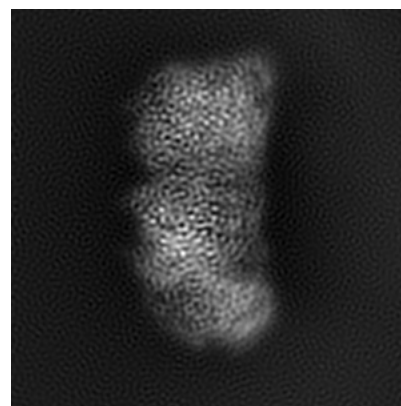
6.1.1 Primary map



X

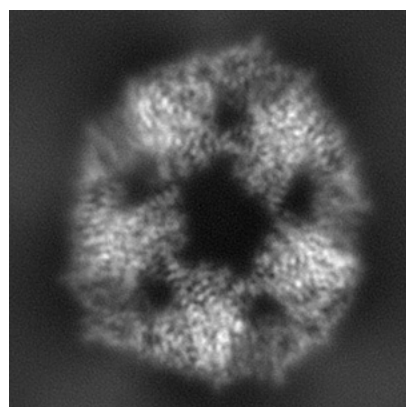


Y

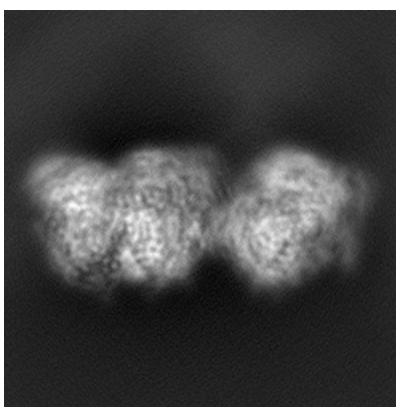


Z

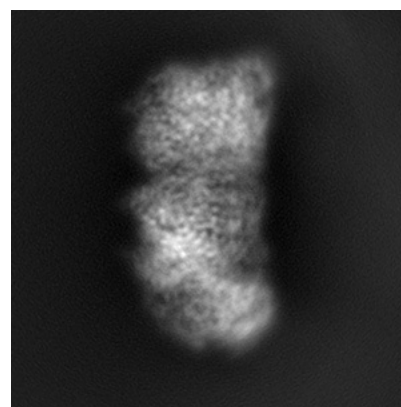
6.1.2 Raw map



X



Y

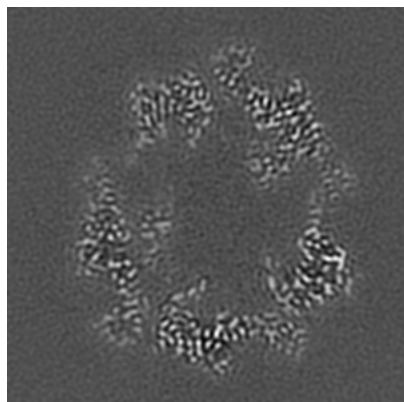


Z

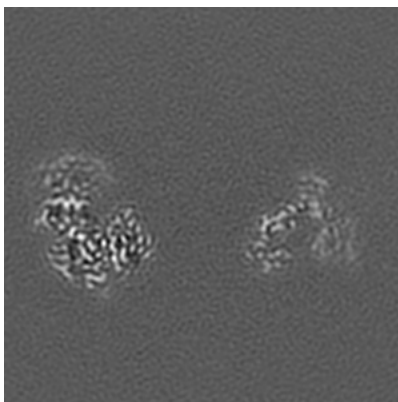
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

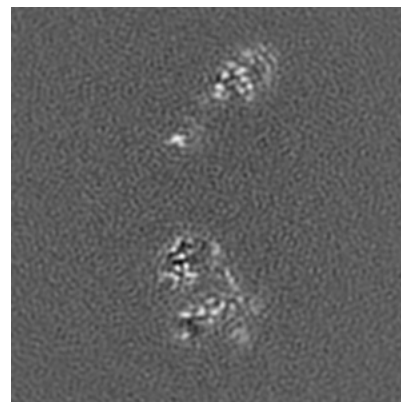
6.2.1 Primary map



X Index: 128

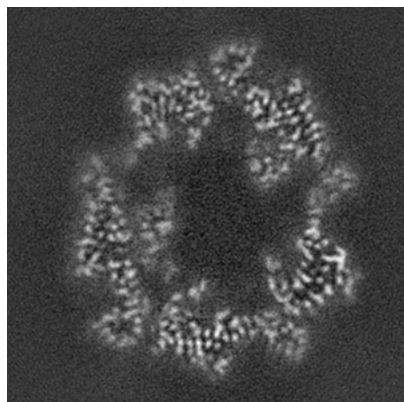


Y Index: 128

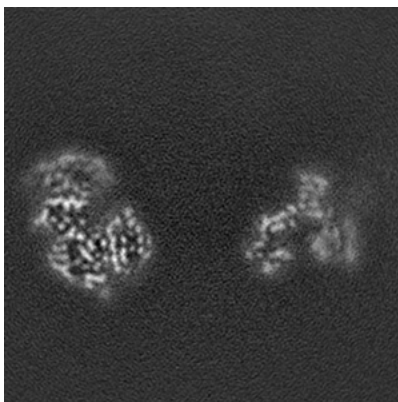


Z Index: 128

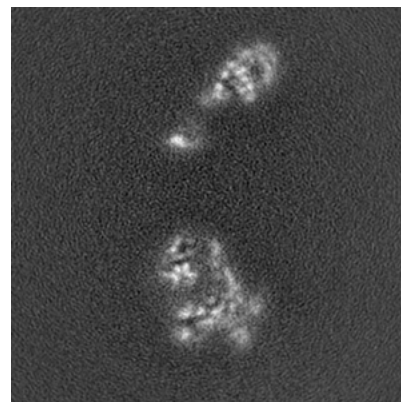
6.2.2 Raw map



X Index: 128



Y Index: 128

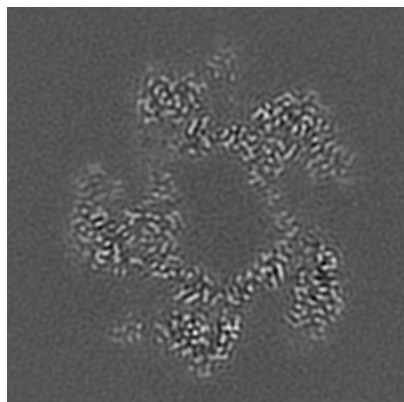


Z Index: 128

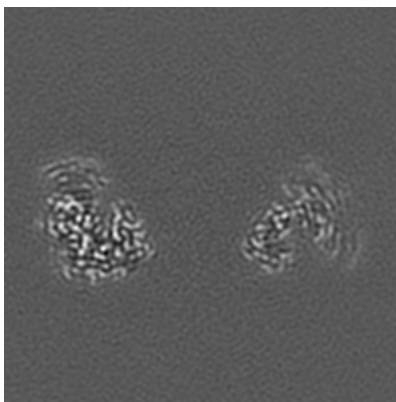
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

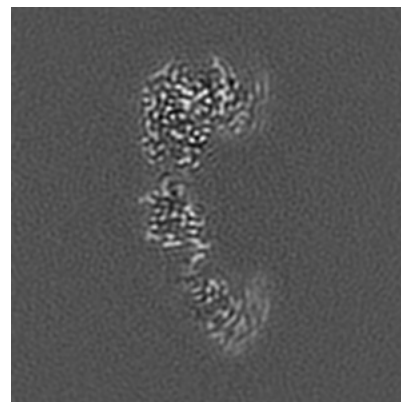
6.3.1 Primary map



X Index: 118

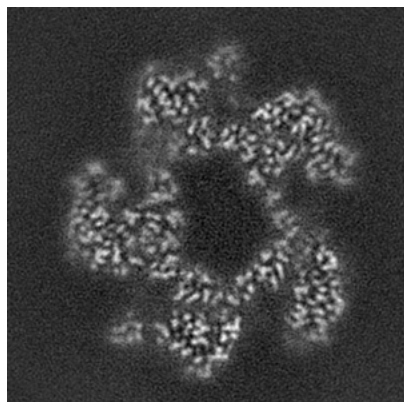


Y Index: 122

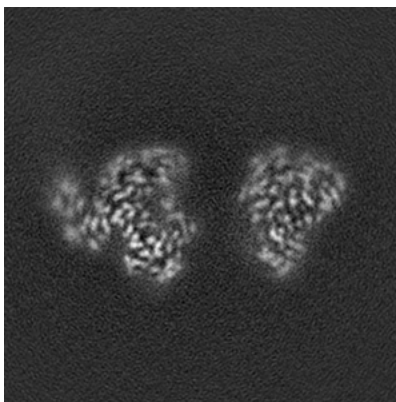


Z Index: 85

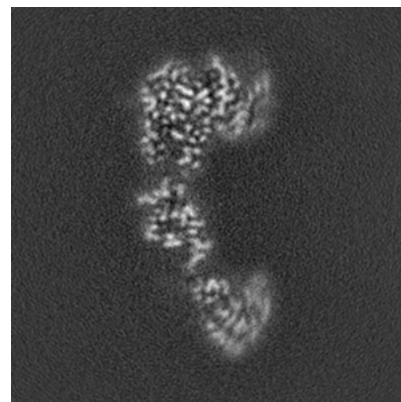
6.3.2 Raw map



X Index: 118



Y Index: 186

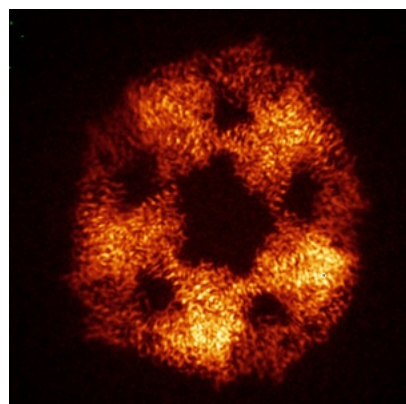


Z Index: 85

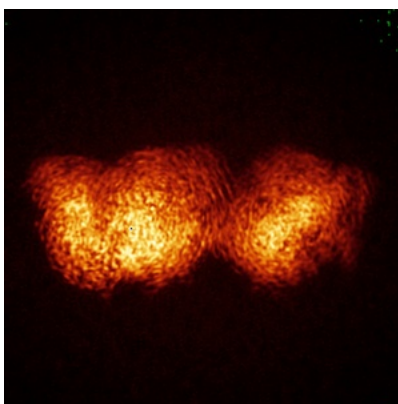
The images above show the largest variance slices of the map in three orthogonal directions.

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

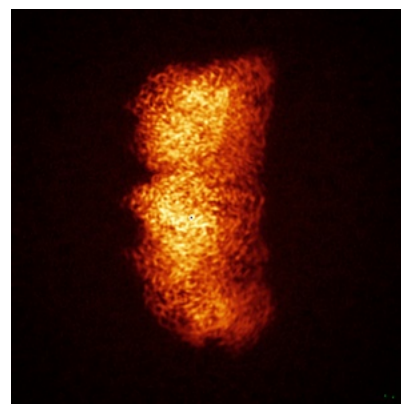
6.4.1 Primary map



X

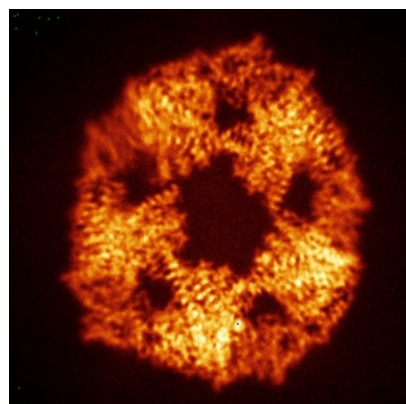


Y

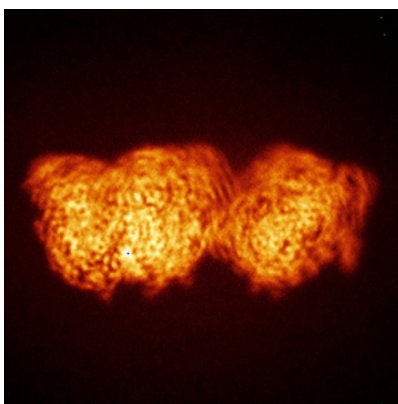


Z

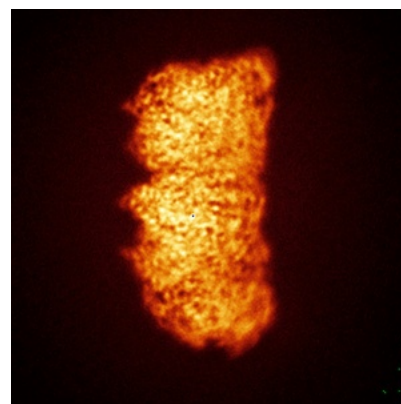
6.4.2 Raw map



X



Y

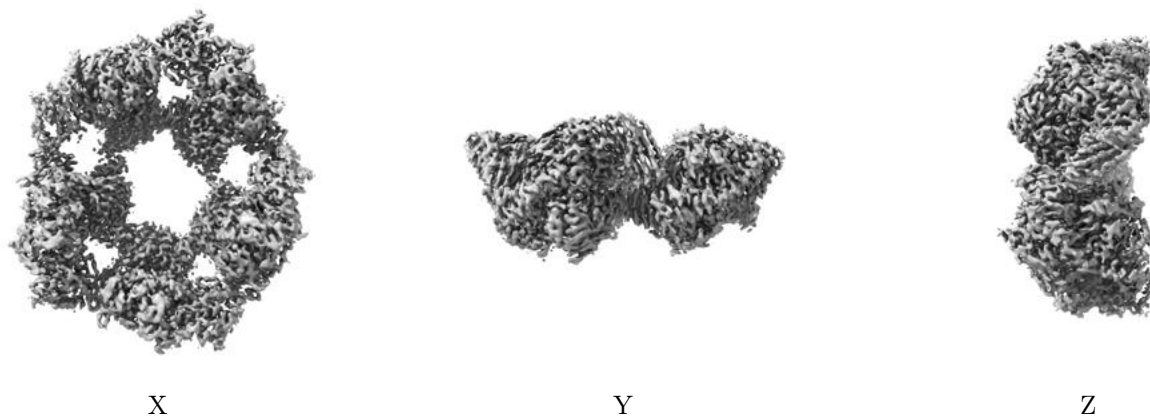


Z

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.

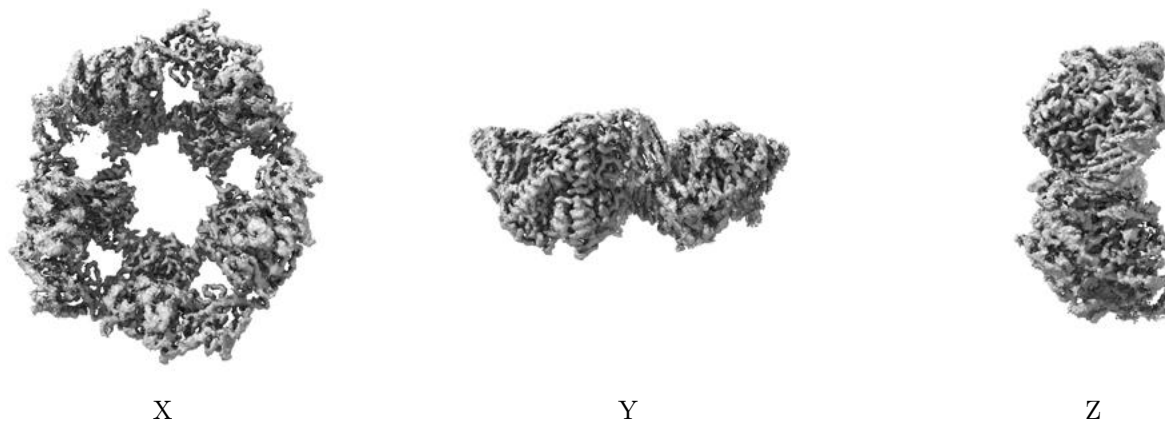
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0689. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

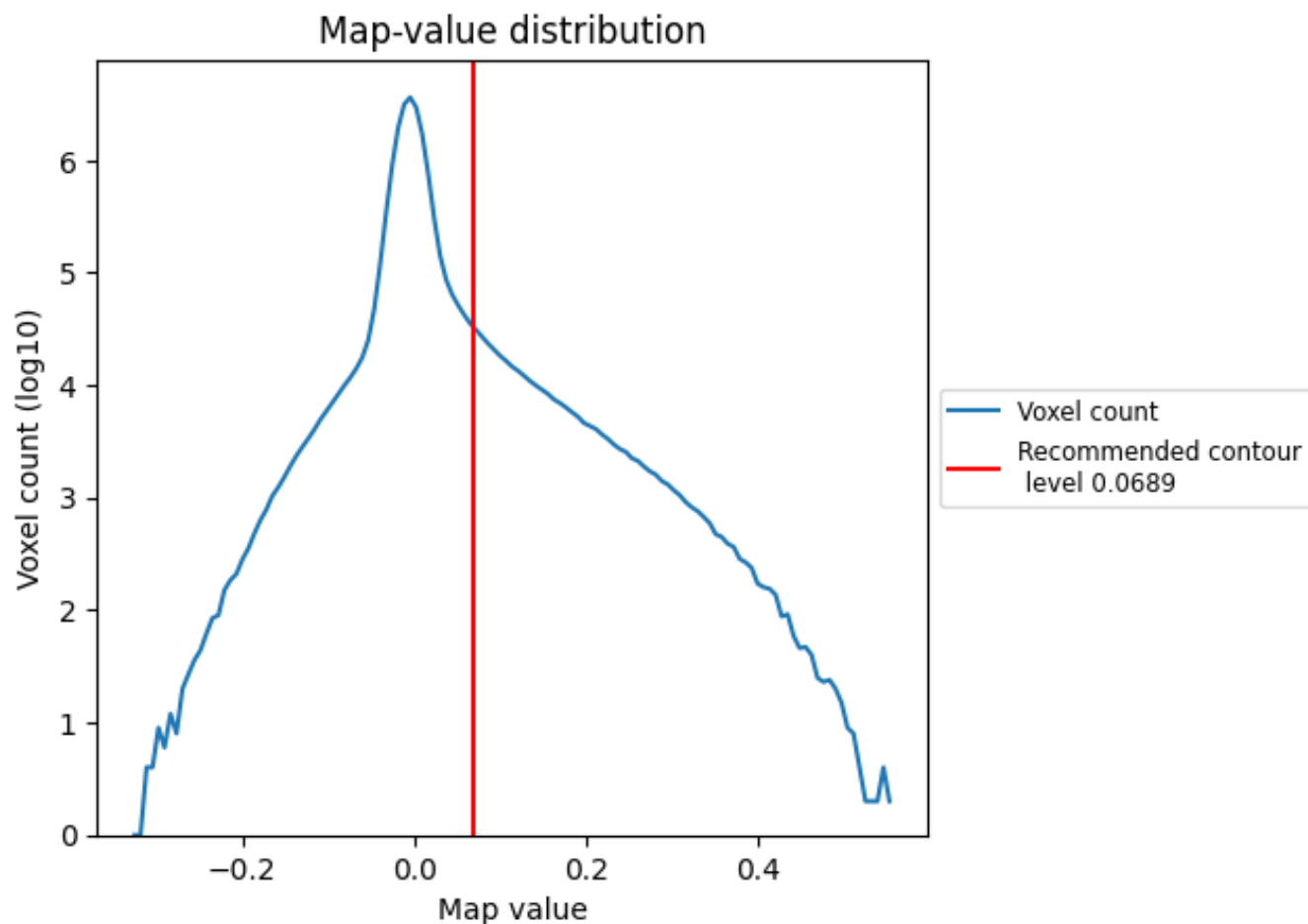
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

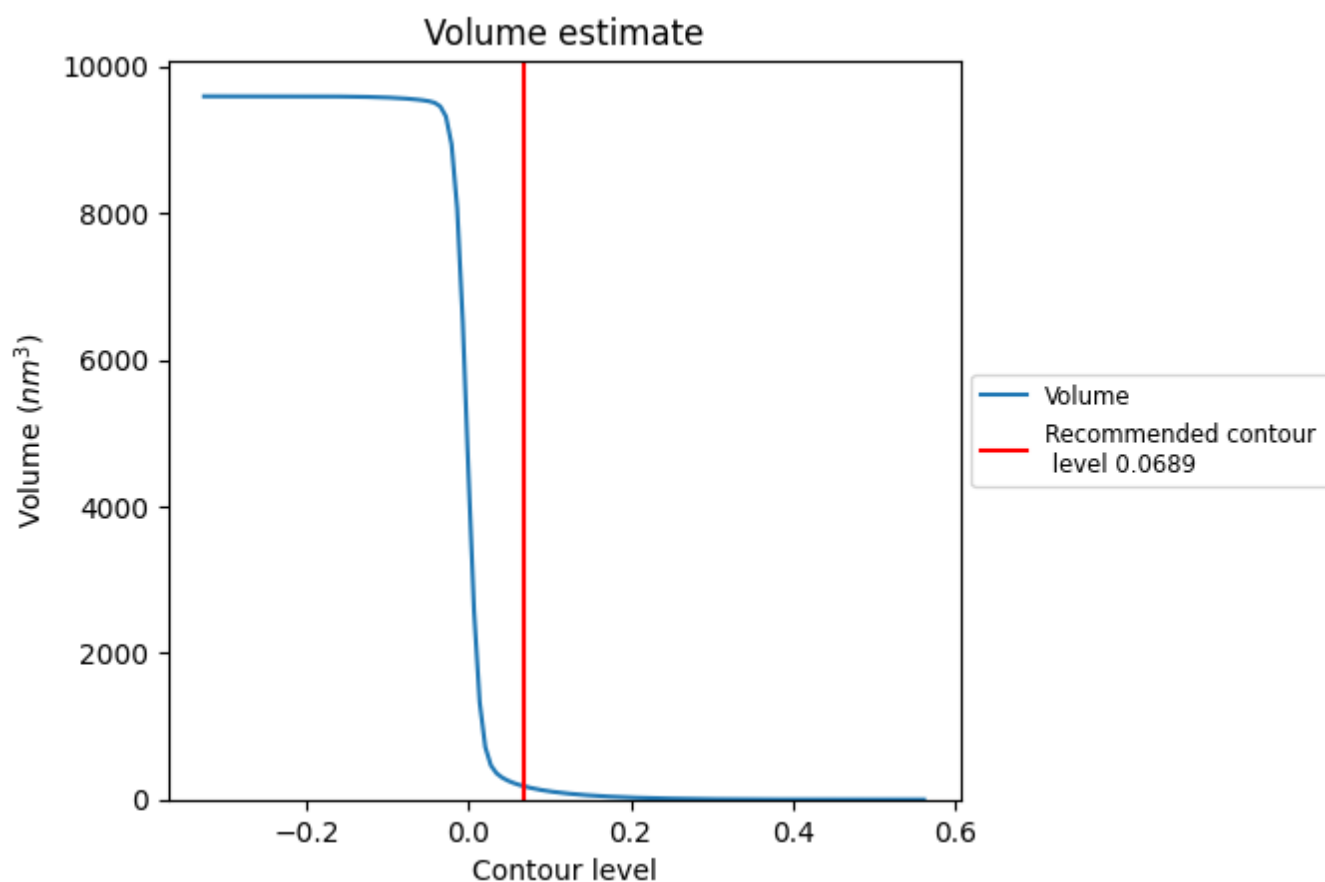
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

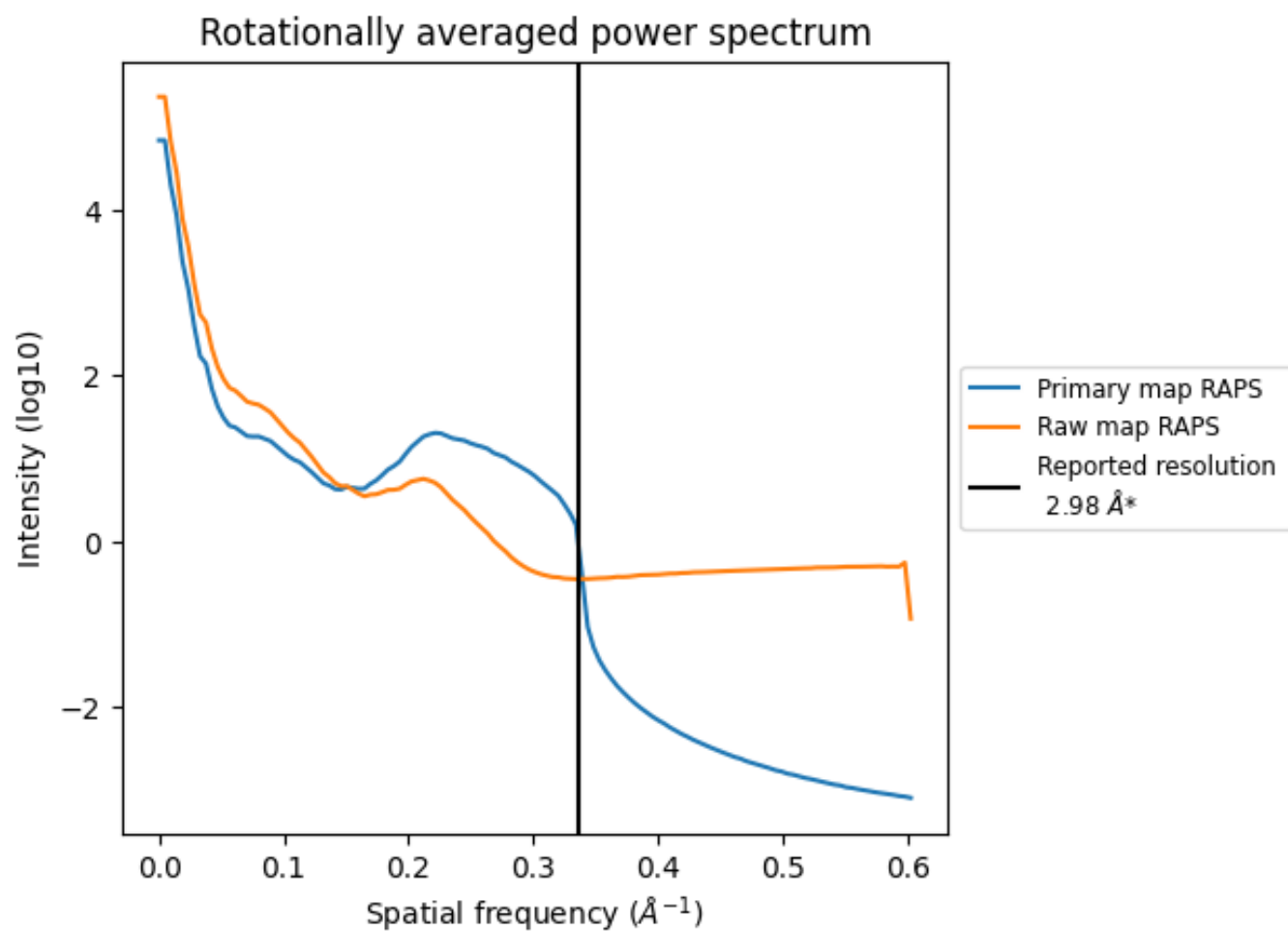
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm³; this corresponds to an approximate mass of 163 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 ⓘ

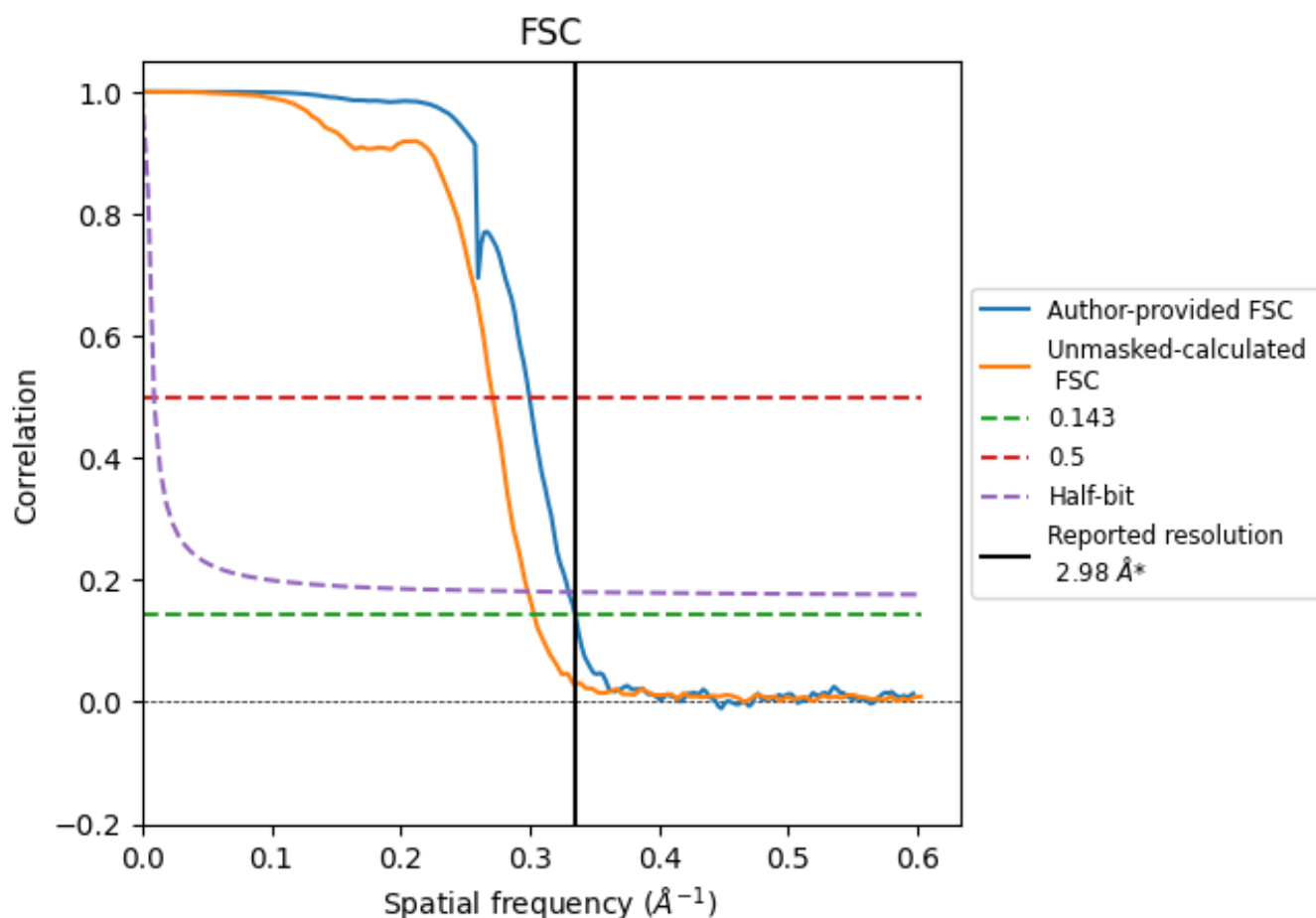


*Reported resolution corresponds to spatial frequency of 0.336 \AA^{-1}

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 0.336 \AA^{-1}

8.2 Resolution estimates [i](#)

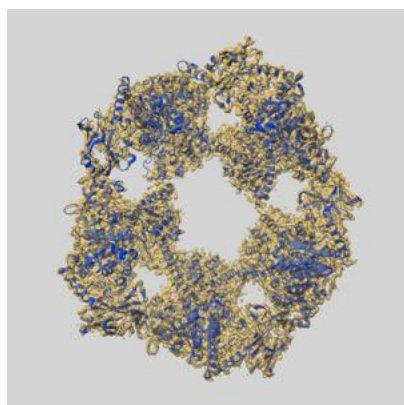
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.98	3.34	3.02
Unmasked-calculated*	3.30	3.69	3.35

*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 3.30 differs from the reported value 2.98 by more than 10 %

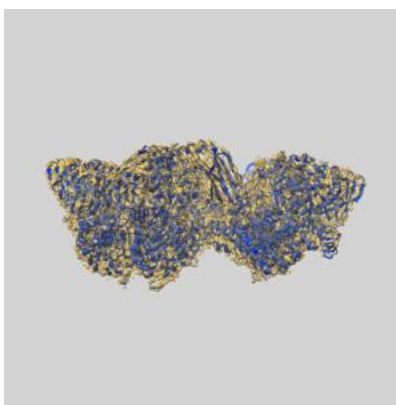
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62853 and PDB model 9L6I. Per-residue inclusion information can be found in section [3](#) on page [5](#).

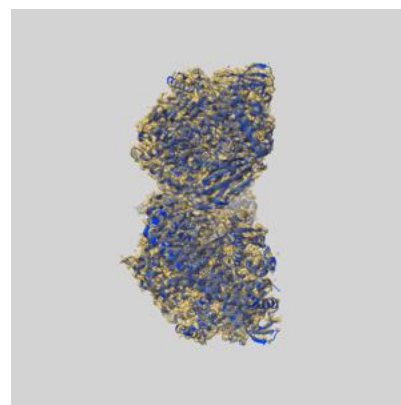
9.1 Map-model overlay [i](#)



X



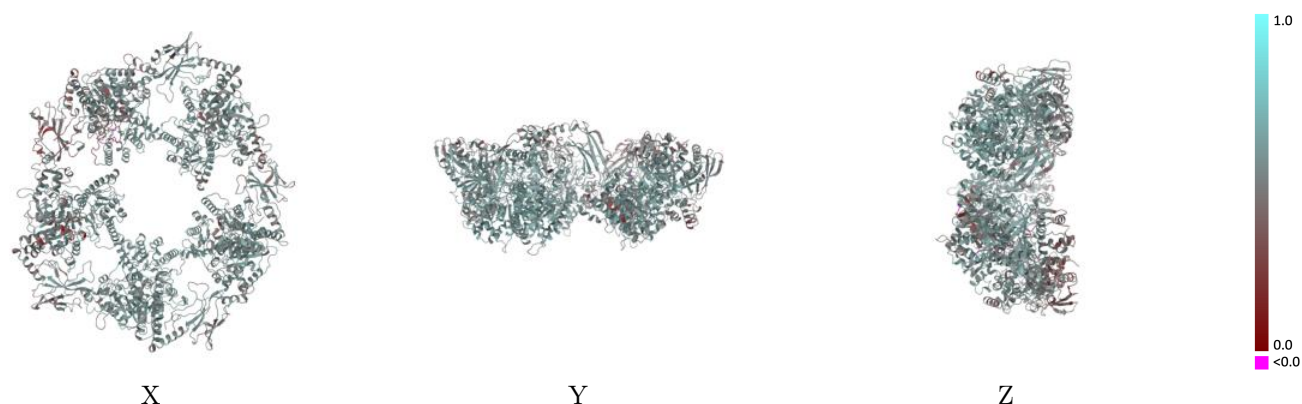
Y



Z

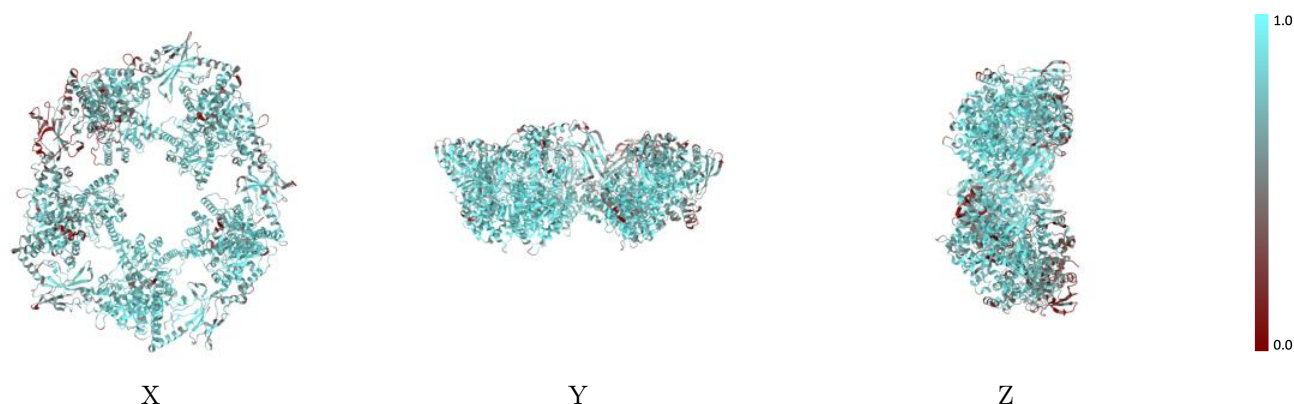
The images above show the 3D surface view of the map at the recommended contour level 0.0689 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



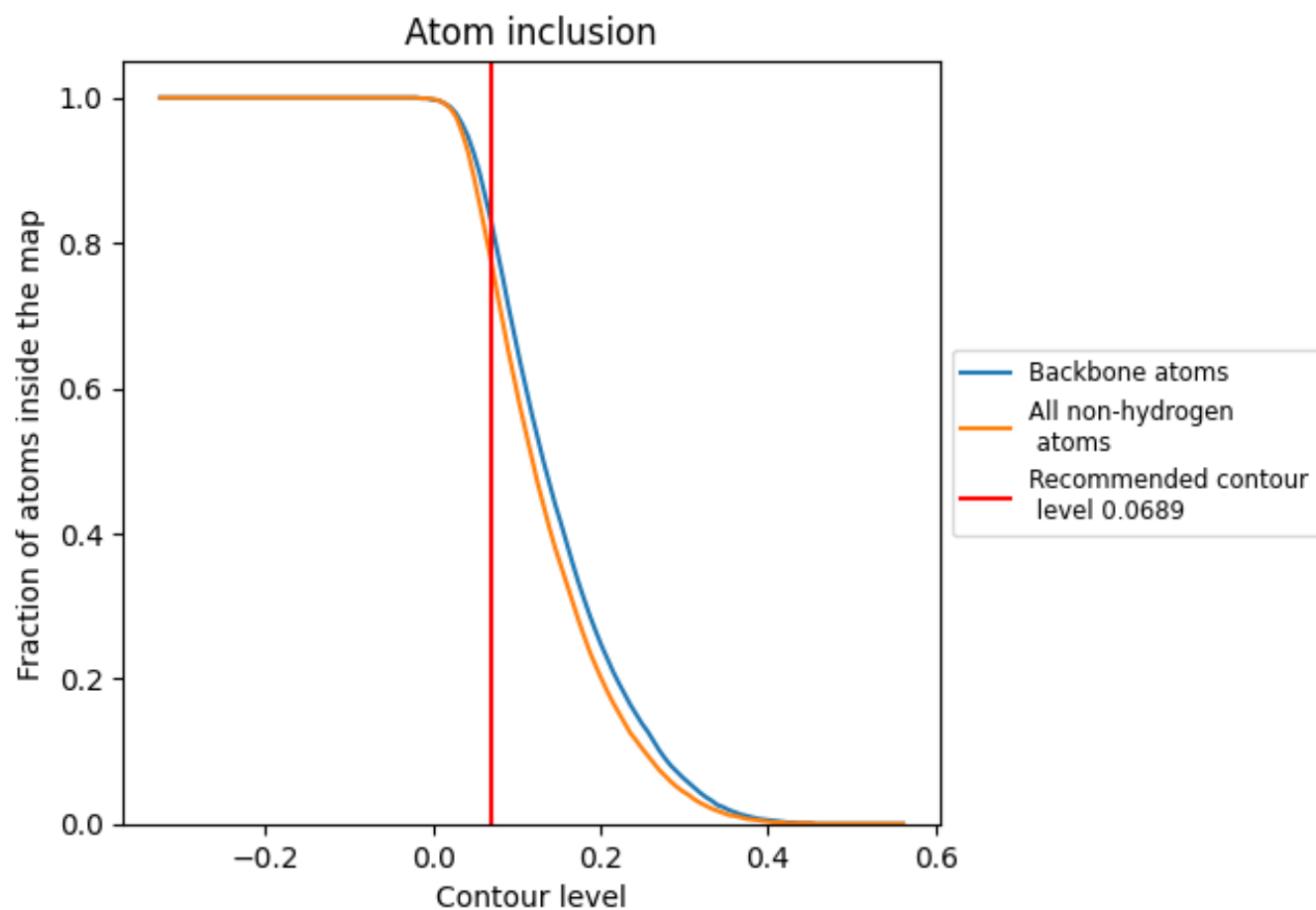
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0689).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (0.0689) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7780	<div></div> 0.5430
A	<div></div> 0.8540	<div></div> 0.5720
B	<div></div> 0.7510	<div></div> 0.5330
C	<div></div> 0.6630	<div></div> 0.5010
D	<div></div> 0.7910	<div></div> 0.5480
E	<div></div> 0.8280	<div></div> 0.5610

