



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 06:50 PM UTC

PDB ID : 6UZD / pdb_00006uzd
EMDB ID : EMD-20957
Title : Anthrax toxin protective antigen channels bound to edema factor
Authors : Hardenbrook, N.J.; Liu, S.; Zhou, K.; Zhou, Z.H.; Krantz, B.A.
Deposited on : 2019-11-14
Resolution : 3.40 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:

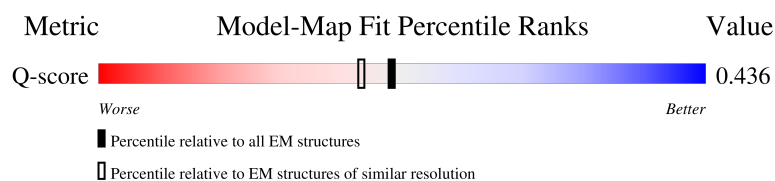
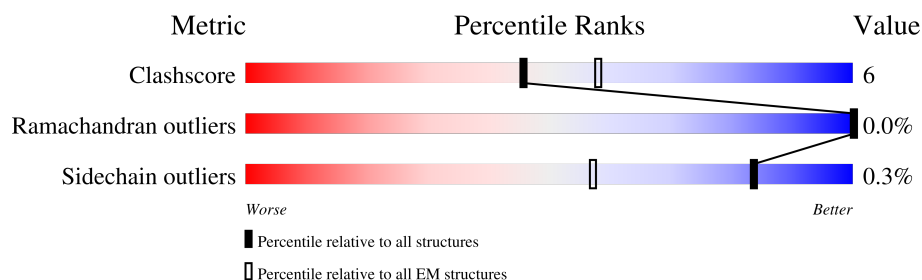
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.40 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	14717 (2.90 - 3.90)

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	735	24% 66% 11% 24%
1	B	735	24% 65% 11% 24%
1	C	735	24% 66% 10% 24%
1	D	735	24% 67% 9% 24%

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Mol	Chain	Length	Quality of chain
1	E	735	
1	F	735	
1	G	735	
2	H	767	
2	I	767	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 42822 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 Protective antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	562	Total	C	N	O	S	0	0
			4438	2772	765	895	6		
1	B	562	Total	C	N	O	S	0	0
			4438	2772	765	895	6		
1	C	562	Total	C	N	O	S	0	0
			4438	2772	765	895	6		
1	D	562	Total	C	N	O	S	0	0
			4438	2772	765	895	6		
1	E	562	Total	C	N	O	S	0	0
			4438	2772	765	895	6		
1	F	562	Total	C	N	O	S	0	0
			4438	2772	765	895	6		
1	G	562	Total	C	N	O	S	0	0
			4438	2772	765	895	6		

- Molecule 2 is a protein called Calmodulin-sensitive adenylate cyclase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	720	Total	C	N	O	S	0	0
			5871	3749	975	1141	6		
2	I	720	Total	C	N	O	S	0	0
			5871	3749	975	1141	6		

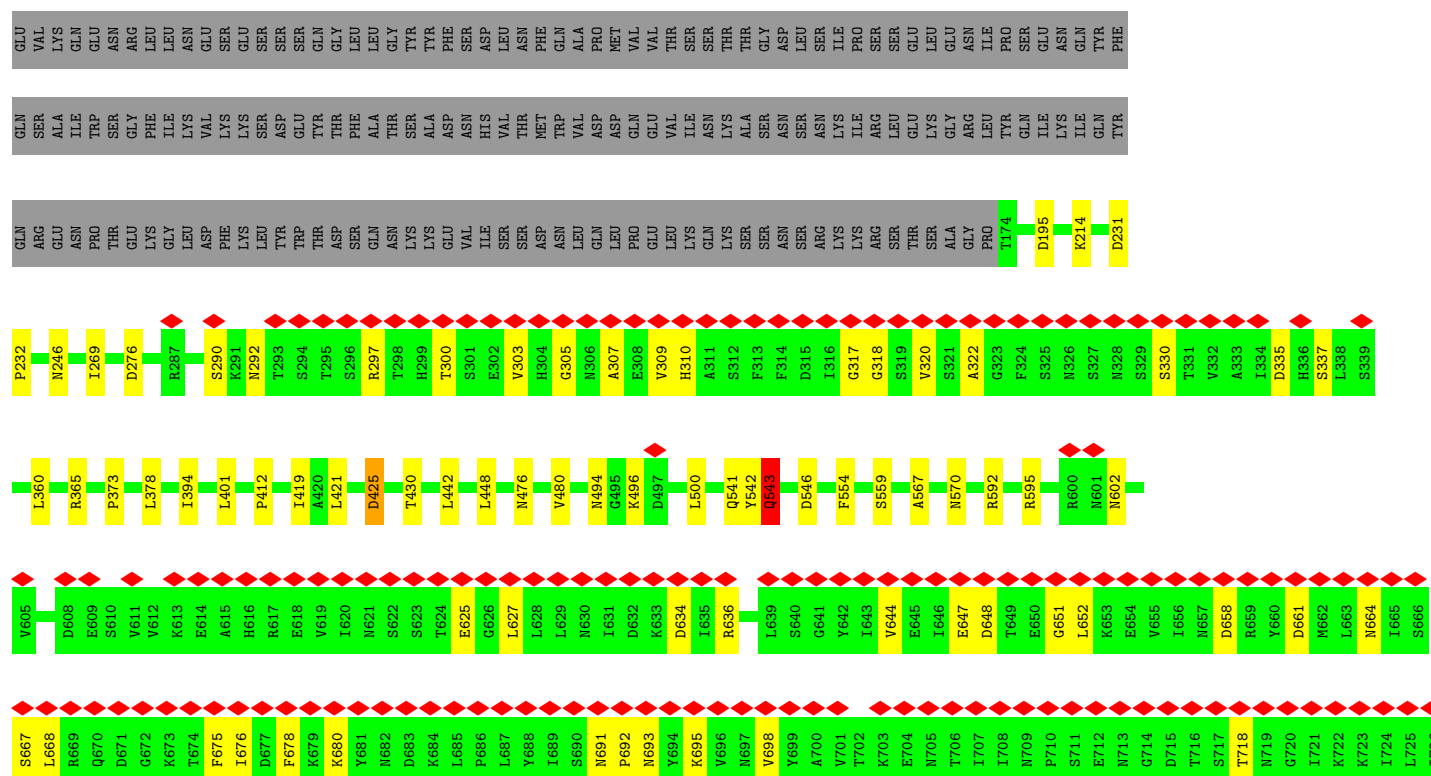
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Ca	0
			2	2	
3	B	2	Total	Ca	0
			2	2	
3	C	2	Total	Ca	0
			2	2	
3	D	2	Total	Ca	0
			2	2	

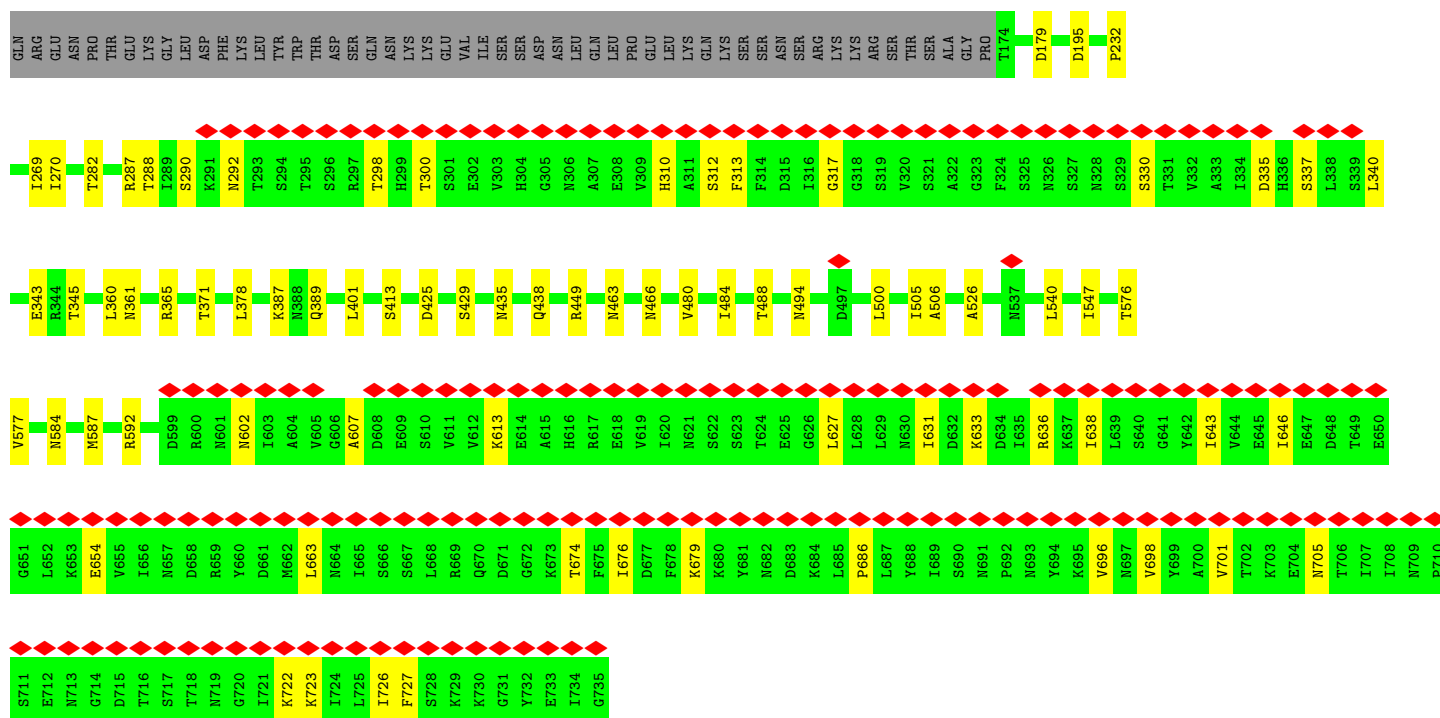
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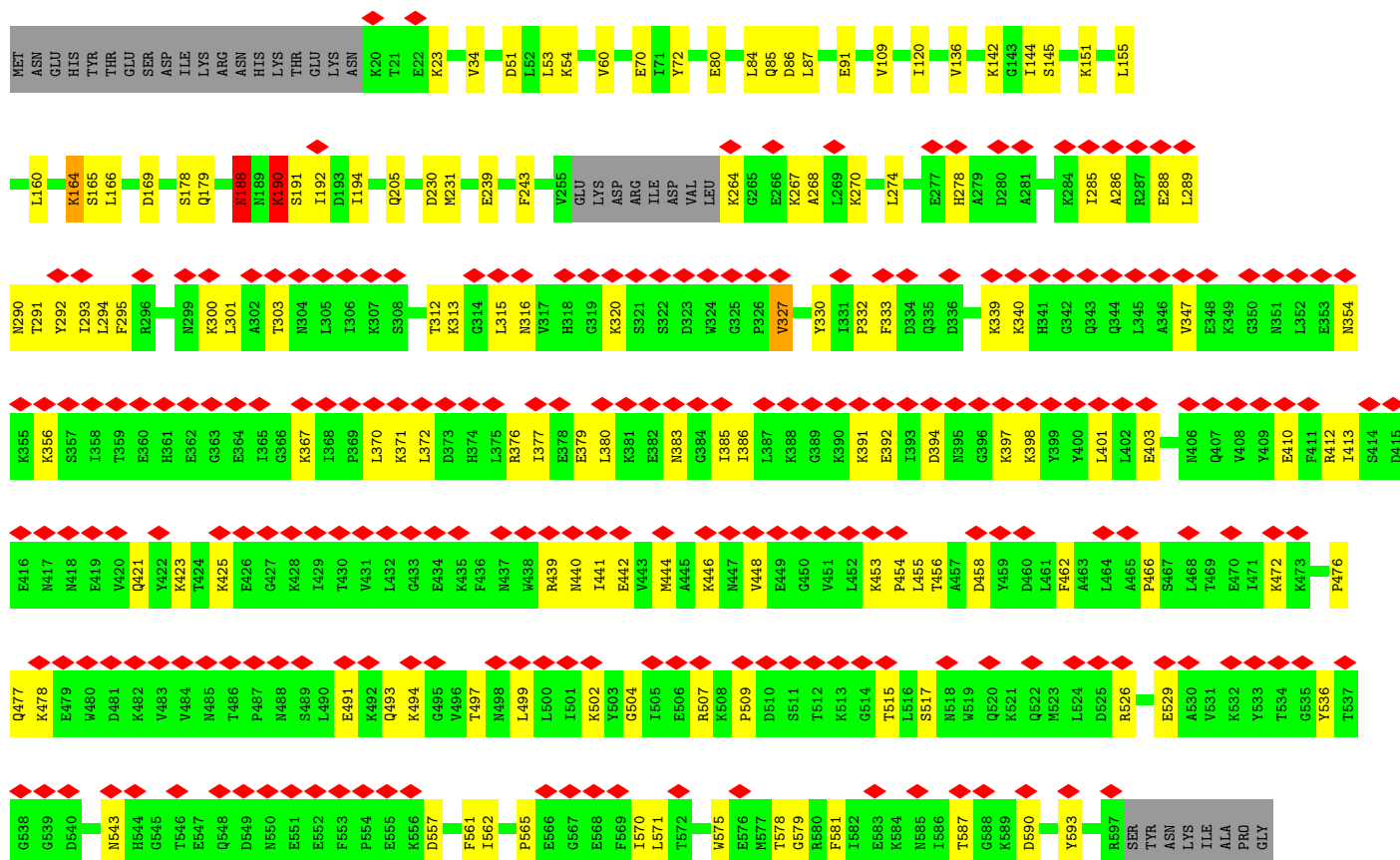
Mol	Chain	Residues	Atoms		AltConf
3	E	2	Total 2	Ca 2	0
3	F	2	Total 2	Ca 2	0
3	G	2	Total 2	Ca 2	0

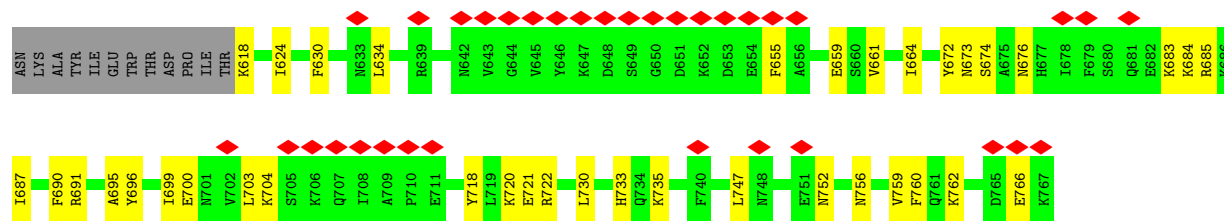




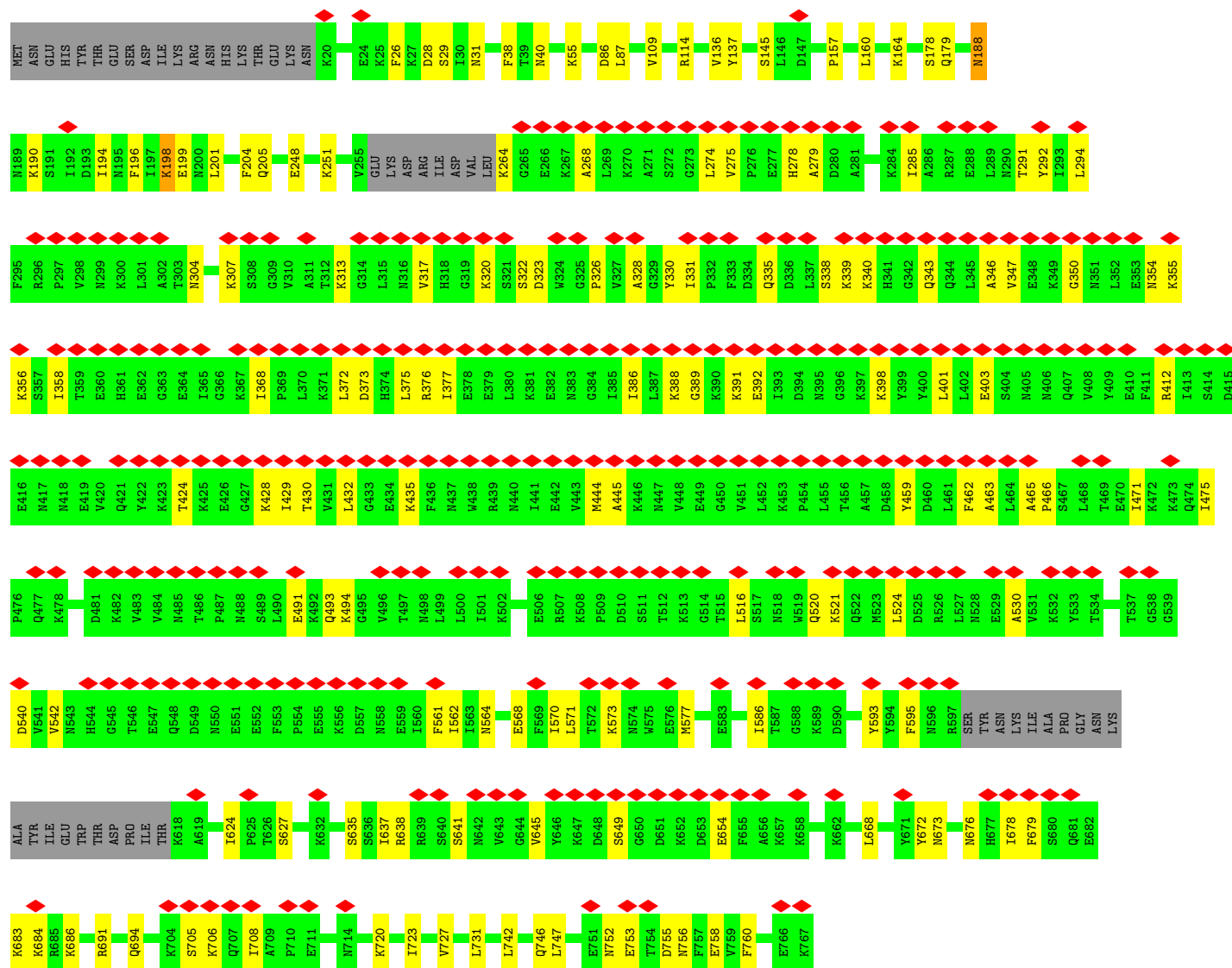
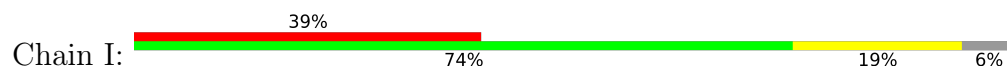


● Molecule 2: Calmodulin-sensitive adenylate cyclase





• Molecule 2: Calmodulin-sensitive adenylate cyclase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	72864	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 ($e^-/\text{\AA}^2$)	62.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.201	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: CA

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	0.31	0/4515	0.51	3/6125 (0.0%)
1	B	0.32	0/4515	0.48	0/6125
1	C	0.34	0/4515	0.52	0/6125
1	D	0.31	0/4515	0.50	0/6125
1	E	0.30	0/4515	0.49	0/6125
1	F	0.30	0/4515	0.50	0/6125
1	G	0.30	0/4515	0.48	0/6125
2	H	0.23	0/5976	0.52	3/8024 (0.0%)
2	I	0.23	0/5976	0.51	3/8024 (0.0%)
All	All	0.29	0/43557	0.50	9/58923 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	708	ILE	CA-C-N	8.58	133.72	120.68
1	A	708	ILE	C-N-CA	8.58	133.72	120.68
1	A	708	ILE	N-CA-C	-6.12	106.94	111.90
2	H	188	ASN	CA-C-N	5.51	132.06	121.54
2	H	188	ASN	C-N-CA	5.51	132.06	121.54
2	H	327	VAL	N-CA-C	-5.47	107.65	112.90
2	I	188	ASN	N-CA-C	-5.08	105.84	112.23
2	I	38	PHE	CA-C-N	5.04	131.17	121.54
2	I	38	PHE	C-N-CA	5.04	131.17	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4438	0	4378	48	0
1	B	4438	0	4378	52	0
1	C	4438	0	4378	50	0
1	D	4438	0	4378	42	0
1	E	4438	0	4378	48	0
1	F	4438	0	4378	50	0
1	G	4438	0	4378	46	0
2	H	5871	0	5890	117	0
2	I	5871	0	5890	103	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
All	All	42822	0	42426	532	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (532) 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)
2:I:164:LYS:CE	2:I:190:LYS:HZ2	1.62	1.11
2:I:164:LYS:HE2	2:I:190:LYS:HZ2	1.17	1.06
2:I:164:LYS:CE	2:I:190:LYS:NZ	2.33	0.91
2:I:164:LYS:HD3	2:I:190:LYS:NZ	1.97	0.80
2:I:164:LYS:CD	2:I:190:LYS:NZ	2.52	0.71
1:C:543:GLN:HA	1:C:543:GLN:HE21	1.55	0.71
2:I:164:LYS:NZ	2:I:190:LYS:NZ	2.43	0.67
1:F:659:ARG:HB3	1:F:662:MET:HB2	1.78	0.66
1:A:627:LEU:HB3	1:A:676:ILE:HB	1.77	0.66
1:D:310:HIS:HB2	1:D:317:GLY:H	1.61	0.66
1:G:698:VAL:H	1:G:727:PHE:HB3	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:164:LYS:HD3	2:I:190:LYS:HZ1	1.60	0.66
2:I:164:LYS:HE2	2:I:190:LYS:NZ	2.03	0.65
1:E:648:ASP:HB2	1:E:651:GLY:H	1.61	0.64
1:F:232:PRO:HD3	1:F:480:VAL:HG11	1.81	0.62
1:E:232:PRO:HD3	1:E:480:VAL:HG11	1.81	0.62
2:I:194:ILE:O	2:I:198:LYS:HB2	2.00	0.62
1:G:269:ILE:HD11	1:G:360:LEU:HD22	1.81	0.61
2:I:294:LEU:HB3	2:I:462:PHE:HB3	1.81	0.61
1:D:627:LEU:HB3	1:D:676:ILE:HB	1.82	0.61
1:B:292:ASN:HB3	1:B:335:ASP:HB3	1.81	0.61
1:G:270:ILE:HB	1:G:361:ASN:HB3	1.83	0.61
1:A:312:SER:HB2	1:A:315:ASP:HB3	1.84	0.60
1:C:307:ALA:HA	1:C:320:VAL:HA	1.83	0.60
1:F:282:THR:HB	1:F:345:THR:HB	1.84	0.60
1:C:292:ASN:HB3	1:C:335:ASP:HB2	1.83	0.59
1:A:292:ASN:HB3	1:A:335:ASP:HB3	1.82	0.59
1:G:282:THR:HB	1:G:345:THR:HB	1.85	0.59
2:H:291:THR:HA	2:H:466:PRO:HA	1.84	0.59
1:B:232:PRO:HD3	1:B:480:VAL:HG11	1.84	0.59
2:H:685:ARG:HB3	2:H:730:LEU:HD21	1.85	0.59
2:H:367:LYS:HD2	2:H:442:GLU:HB2	1.86	0.58
1:D:278:SER:HB3	1:D:349:THR:HB	1.86	0.58
1:E:406:ALA:HB3	1:E:409:ASN:HD22	1.67	0.58
1:C:541:GLN:HG2	1:C:546:ASP:HA	1.85	0.58
2:H:84:LEU:HD11	2:H:120:ILE:HD13	1.85	0.58
2:H:472:LYS:NZ	2:H:477:GLN:OE1	2.36	0.58
2:H:109:VAL:HG21	2:H:136:VAL:HG22	1.86	0.57
2:H:294:LEU:HB3	2:H:462:PHE:HB3	1.85	0.57
2:I:55:LYS:NZ	2:I:137:TYR:OH	2.37	0.57
2:I:164:LYS:NZ	2:I:190:LYS:HZ2	1.98	0.57
1:B:326:ASN:HD22	1:C:303:VAL:HG23	1.69	0.57
2:H:51:ASP:HA	2:H:54:LYS:HG2	1.84	0.57
1:D:646:ILE:HB	1:D:654:GLU:HB3	1.86	0.57
2:I:145:SER:OG	2:I:205:GLN:NE2	2.37	0.57
1:B:643:ILE:HB	1:B:699:TYR:HB2	1.87	0.57
1:F:463:ASN:ND2	1:F:466:ASN:OD1	2.37	0.57
1:F:524:LYS:HD2	1:F:579:ASP:HB3	1.87	0.56
2:I:444:MET:SD	2:I:444:MET:N	2.78	0.56
1:C:269:ILE:HD11	1:C:360:LEU:HD22	1.86	0.56
2:H:294:LEU:HD13	2:H:562:ILE:HB	1.86	0.56
2:H:397:LYS:NZ	2:H:398:LYS:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:SER:OG	1:B:292:ASN:ND2	2.37	0.56
1:D:276:ASP:OD1	1:D:276:ASP:N	2.37	0.56
1:C:627:LEU:HB3	1:C:676:ILE:HB	1.88	0.56
1:D:645:GLU:HG2	1:D:697:ASN:HD22	1.69	0.56
1:A:731:GLY:HA2	1:A:734:ILE:HD12	1.88	0.56
1:B:395:LYS:O	1:B:397:LYS:NZ	2.38	0.56
1:E:665:ILE:HG13	1:E:680:LYS:HB2	1.88	0.56
1:A:299:HIS:ND1	1:G:330:SER:O	2.39	0.56
1:D:269:ILE:HD11	1:D:360:LEU:HD22	1.88	0.56
2:H:676:ASN:HB2	2:H:684:LYS:HD2	1.88	0.56
2:I:343:GLN:HB3	2:I:347:VAL:HG13	1.86	0.56
2:H:718:TYR:OH	2:H:722:ARG:NH2	2.38	0.56
1:B:515:GLU:HG3	1:B:518:LYS:HE2	1.87	0.55
1:G:646:ILE:HB	1:G:654:GLU:HB2	1.88	0.55
2:H:330:TYR:HA	2:H:456:THR:HA	1.88	0.55
1:F:592:ARG:NH1	1:F:602:ASN:OD1	2.40	0.55
2:H:292:TYR:HB3	2:H:562:ILE:HD11	1.87	0.55
1:A:463:ASN:ND2	1:A:466:ASN:OD1	2.38	0.55
1:G:592:ARG:NH1	1:G:602:ASN:OD1	2.39	0.55
2:H:274:LEU:O	2:H:300:LYS:NZ	2.40	0.55
2:H:380:LEU:HA	2:H:383:ASN:HB2	1.89	0.55
1:D:524:LYS:HG3	1:D:540:LEU:HD22	1.89	0.55
1:F:331:THR:HG22	1:G:298:THR:HG23	1.89	0.55
1:D:625:GLU:HB2	1:D:679:LYS:HE2	1.88	0.55
2:I:516:LEU:HB2	2:I:521:LYS:HG3	1.89	0.55
1:E:698:VAL:H	1:E:727:PHE:HB3	1.72	0.55
2:I:40:ASN:ND2	2:I:746:GLN:OE1	2.41	0.55
2:I:350:GLY:O	2:I:354:ASN:ND2	2.40	0.55
1:D:624:THR:HG21	1:D:689:ILE:HD11	1.88	0.54
1:E:523:LEU:HD13	1:E:583:LEU:HD21	1.89	0.54
2:H:562:ILE:HG23	2:H:570:ILE:HB	1.90	0.54
1:C:232:PRO:HD3	1:C:480:VAL:HG11	1.89	0.54
1:F:494:ASN:HB3	1:F:500:LEU:HD23	1.89	0.54
1:C:595:ARG:NH2	1:C:634:ASP:OD2	2.41	0.54
1:F:711:SER:HB3	1:F:715:ASP:HB2	1.89	0.54
2:H:87:LEU:HD12	2:H:91:GLU:HB3	1.89	0.54
1:B:497:ASP:O	1:B:637:LYS:NZ	2.38	0.54
1:C:664:ASN:O	1:C:680:LYS:NZ	2.41	0.54
2:H:379:GLU:O	2:H:383:ASN:ND2	2.41	0.54
2:H:499:LEU:HA	2:H:502:LYS:HE2	1.90	0.54
1:A:476:ASN:OD1	1:A:476:ASN:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:676:ASN:HB2	2:I:684:LYS:HE3	1.90	0.53
1:C:425:ASP:OD1	1:C:430:THR:OG1	2.26	0.53
1:E:224:GLU:OE1	1:F:242:ARG:NH2	2.40	0.53
2:H:439:ARG:NH1	2:H:440:ASN:O	2.41	0.53
1:E:323:GLY:HA2	1:F:306:ASN:HA	1.91	0.53
1:E:328:ASN:OD1	1:F:301:SER:OG	2.27	0.53
1:F:560:GLN:O	1:F:564:ASN:ND2	2.42	0.53
1:B:523:LEU:HD13	1:B:583:LEU:HD21	1.91	0.53
1:E:282:THR:HB	1:E:345:THR:HB	1.91	0.53
1:F:179:ASP:OD1	1:F:179:ASP:N	2.38	0.53
1:F:498:LEU:HD13	1:F:604:ALA:HB3	1.91	0.53
1:E:729:LYS:HD2	1:E:733:GLU:HB2	1.91	0.52
1:A:269:ILE:HD11	1:A:360:LEU:HD22	1.91	0.52
1:A:642:TYR:HB2	1:A:665:ILE:HG12	1.89	0.52
2:H:756:ASN:HA	2:H:759:VAL:HG22	1.91	0.52
1:D:282:THR:HB	1:D:345:THR:HB	1.91	0.52
1:F:620:ILE:HB	1:F:628:LEU:HD23	1.90	0.52
1:G:179:ASP:OD1	1:G:179:ASP:N	2.34	0.52
2:I:248:GLU:OE1	2:I:251:LYS:NZ	2.40	0.52
2:I:275:VAL:HB	2:I:278:HIS:HB2	1.91	0.52
1:E:463:ASN:ND2	1:E:466:ASN:OD1	2.42	0.52
1:F:623:SER:OG	1:F:624:THR:N	2.43	0.52
2:H:507:ARG:NH1	2:H:515:THR:O	2.42	0.52
2:H:587:THR:O	2:H:684:LYS:NZ	2.34	0.52
1:C:305:GLY:HA2	1:C:322:ALA:HA	1.92	0.52
1:G:584:ASN:HB2	1:G:587:MET:HE3	1.90	0.52
2:H:313:LYS:HB3	2:H:455:LEU:HB3	1.92	0.52
2:I:201:LEU:HA	2:I:204:PHE:HB2	1.92	0.52
1:B:329:SER:HA	1:C:300:THR:HA	1.92	0.52
1:C:592:ARG:NH1	1:C:602:ASN:OD1	2.40	0.52
1:F:329:SER:HA	1:G:300:THR:HA	1.92	0.52
1:F:640:SER:HB3	1:F:701:VAL:HG13	1.91	0.52
2:H:340:LYS:HB3	2:H:347:VAL:HG12	1.92	0.52
1:B:203:LEU:HD23	2:H:34:VAL:HG22	1.92	0.52
1:D:627:LEU:HD21	1:D:629:LEU:HD12	1.91	0.52
1:C:567:ALA:O	1:C:570:ASN:ND2	2.43	0.52
2:H:286:ALA:HB1	2:H:565:PRO:HA	1.91	0.52
1:G:312:SER:OG	1:G:313:PHE:N	2.43	0.51
2:H:683:LYS:HE2	2:H:687:ILE:HD11	1.92	0.51
1:A:695:LYS:NZ	1:A:697:ASN:OD1	2.43	0.51
2:H:268:ALA:HB2	2:H:571:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:SER:HA	1:E:302:GLU:HA	1.92	0.51
2:H:720:LYS:NZ	2:H:721:GLU:OE2	2.43	0.51
2:I:335:GLN:HB3	2:I:340:LYS:HB2	1.93	0.51
1:A:715:ASP:OD2	1:A:719:ASN:ND2	2.43	0.51
1:E:551:ASP:N	1:E:551:ASP:OD1	2.41	0.51
1:F:292:ASN:HB3	1:F:335:ASP:HB3	1.92	0.51
2:H:86:ASP:N	2:H:86:ASP:OD1	2.42	0.51
1:F:300:THR:HB	1:F:327:SER:HB2	1.91	0.51
1:G:505:ILE:HD13	1:G:526:ALA:HB1	1.92	0.51
2:H:762:LYS:NZ	2:H:766:GLU:OE1	2.38	0.51
2:I:194:ILE:O	2:I:194:ILE:HG22	2.10	0.51
1:D:613:LYS:O	1:D:617:ARG:NH1	2.44	0.51
2:H:188:ASN:CB	2:H:191:SER:OG	2.59	0.50
2:H:733:HIS:O	2:H:735:LYS:NZ	2.44	0.50
1:C:661:ASP:N	1:C:661:ASP:OD1	2.43	0.50
2:H:446:LYS:HG2	2:H:448:VAL:HG13	1.93	0.50
1:B:336:HIS:O	1:C:292:ASN:ND2	2.44	0.50
1:G:290:SER:HB3	1:G:337:SER:HB2	1.93	0.50
1:C:394:ILE:HG21	1:C:421:LEU:HD11	1.94	0.50
1:G:387:LYS:O	1:G:449:ARG:NH1	2.41	0.50
1:F:645:GLU:OE1	1:F:697:ASN:ND2	2.44	0.50
1:C:231:ASP:OD1	1:C:231:ASP:N	2.45	0.50
1:E:302:GLU:HG2	1:E:325:SER:HB2	1.94	0.50
2:I:328:ALA:O	2:I:376:ARG:NH2	2.45	0.50
1:A:298:THR:HB	1:A:329:SER:HB3	1.94	0.50
1:C:442:LEU:HD13	1:C:448:LEU:HD23	1.92	0.50
2:I:335:GLN:HA	2:I:338:SER:HB2	1.94	0.50
2:I:673:ASN:O	2:I:676:ASN:ND2	2.45	0.50
2:I:683:LYS:HA	2:I:686:LYS:HB2	1.93	0.50
1:G:705:ASN:HD21	1:G:722:LYS:HB3	1.77	0.50
1:E:183:ILE:HD12	1:E:203:LEU:HD11	1.94	0.49
1:F:265:ASP:N	1:F:265:ASP:OD1	2.44	0.49
1:B:280:GLN:HB3	1:B:347:ALA:HB3	1.93	0.49
1:D:365:ARG:NH1	1:D:412:PRO:O	2.45	0.49
1:F:365:ARG:NH1	1:F:412:PRO:O	2.43	0.49
1:G:613:LYS:HD3	1:G:726:ILE:HA	1.93	0.49
1:A:178:ARG:NH1	1:A:224:GLU:OE2	2.41	0.49
1:A:288:THR:HB	1:A:339:SER:HB2	1.93	0.49
1:C:290:SER:HB3	1:C:337:SER:HB3	1.93	0.49
1:A:494:ASN:HB3	1:A:500:LEU:HD23	1.93	0.49
1:B:488:THR:HG22	1:B:506:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:343:GLN:HG3	2:I:346:ALA:H	1.78	0.49
2:I:635:SER:HA	2:I:638:ARG:HG2	1.94	0.49
1:A:640:SER:HB3	1:A:701:VAL:HB	1.94	0.49
1:B:374:ILE:HG12	1:B:377:VAL:HG22	1.94	0.49
1:B:658:ASP:OD1	1:B:718:THR:OG1	2.31	0.49
1:E:365:ARG:NH1	1:E:412:PRO:O	2.44	0.49
2:H:166:LEU:HD11	2:H:231:MET:HB2	1.94	0.49
2:H:403:GLU:OE2	2:H:425:LYS:NZ	2.44	0.49
1:B:286:THR:HB	1:B:341:ALA:HB3	1.94	0.49
1:C:658:ASP:OD1	1:C:718:THR:OG1	2.30	0.49
1:E:494:ASN:HB3	1:E:500:LEU:HD23	1.93	0.49
2:I:340:LYS:HD2	2:I:343:GLN:HG2	1.94	0.49
1:G:633:LYS:HA	1:G:636:ARG:HG2	1.95	0.49
2:I:564:ASN:OD1	2:I:568:GLU:N	2.43	0.49
2:I:540:ASP:OD1	2:I:540:ASP:N	2.45	0.49
2:I:691:ARG:NH1	2:I:694:GLN:OE1	2.46	0.49
1:A:276:ASP:OD1	1:A:276:ASP:N	2.45	0.48
2:H:274:LEU:HA	2:H:303:THR:HG21	1.93	0.48
2:I:264:LYS:HD2	2:I:570:ILE:HA	1.95	0.48
2:I:320:LYS:HB2	2:I:339:LYS:HD2	1.95	0.48
2:I:389:GLY:H	2:I:403:GLU:H	1.61	0.48
1:F:630:ASN:HD22	1:F:673:LYS:HG2	1.78	0.48
1:A:286:THR:HG23	1:G:343:GLU:HG2	1.94	0.48
1:C:644:VAL:HG13	1:C:698:VAL:HG22	1.95	0.48
1:C:648:ASP:HB3	1:C:651:GLY:H	1.79	0.48
1:G:613:LYS:NZ	1:G:726:ILE:O	2.41	0.48
1:A:698:VAL:H	1:A:727:PHE:HB3	1.78	0.48
2:H:673:ASN:O	2:H:676:ASN:ND2	2.46	0.48
1:A:612:VAL:O	1:A:616:HIS:ND1	2.44	0.48
2:H:392:GLU:HB2	2:H:401:LEU:HD22	1.94	0.48
1:C:309:VAL:HA	1:C:318:GLY:HA2	1.96	0.48
1:G:701:VAL:HG22	1:G:723:LYS:HG2	1.96	0.48
2:I:368:ILE:HG12	2:I:445:ALA:HB2	1.95	0.48
2:I:373:ASP:HB3	2:I:375:LEU:HD23	1.96	0.48
2:I:752:ASN:OD1	2:I:756:ASN:ND2	2.46	0.48
1:D:316:ILE:H	1:E:313:PHE:HZ	1.62	0.48
1:D:623:SER:OG	1:D:626:GLY:O	2.32	0.48
1:E:332:VAL:O	1:F:296:SER:OG	2.27	0.48
1:E:659:ARG:NH1	1:E:716:THR:OG1	2.47	0.48
2:I:516:LEU:HD23	2:I:520:GLN:HB3	1.95	0.48
1:D:408:ASN:O	1:D:409:ASN:ND2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:80:GLU:HA	2:H:85:GLN:HE22	1.79	0.48
1:F:705:ASN:HB3	1:F:722:LYS:HD3	1.96	0.48
1:G:232:PRO:HD3	1:G:480:VAL:HG11	1.96	0.48
2:H:700:GLU:O	2:H:704:LYS:N	2.42	0.48
2:I:26:PHE:O	2:I:29:SER:OG	2.31	0.48
2:I:294:LEU:HB2	2:I:463:ALA:HB3	1.96	0.48
1:A:179:ASP:OD1	1:A:179:ASP:N	2.40	0.47
2:I:304:ASN:HA	2:I:307:LYS:HE3	1.96	0.47
2:H:312:THR:OG1	2:H:543:ASN:OD1	2.32	0.47
1:A:515:GLU:OE1	1:A:518:LYS:NZ	2.37	0.47
1:A:666:SER:HG	1:A:674:THR:HG1	1.58	0.47
1:B:621:ASN:HB3	1:B:628:LEU:HB2	1.95	0.47
2:H:696:TYR:HA	2:H:699:ILE:HB	1.96	0.47
2:I:196:PHE:HA	2:I:199:GLU:HG2	1.96	0.47
2:I:377:ILE:HB	2:I:388:LYS:HD2	1.95	0.47
2:I:428:LYS:NZ	2:I:429:ILE:O	2.48	0.47
1:B:290:SER:HB3	1:B:337:SER:HB2	1.95	0.47
1:C:300:THR:O	1:C:300:THR:OG1	2.30	0.47
2:I:268:ALA:HB2	2:I:571:LEU:HB2	1.95	0.47
2:I:705:SER:OG	2:I:706:LYS:N	2.44	0.47
1:B:179:ASP:OD1	1:B:179:ASP:N	2.35	0.47
1:E:554:PHE:HB2	1:E:559:SER:HB3	1.96	0.47
1:D:579:ASP:OD1	1:D:579:ASP:N	2.48	0.47
1:A:300:THR:HB	1:A:327:SER:HB2	1.97	0.47
1:A:378:LEU:HD21	1:A:401:LEU:HD12	1.97	0.47
1:B:276:ASP:OD1	1:B:276:ASP:N	2.47	0.47
1:C:494:ASN:HB3	1:C:500:LEU:HD23	1.97	0.47
1:E:482:PRO:HG2	1:F:404:ILE:HD13	1.96	0.47
2:H:188:ASN:HB3	2:H:191:SER:OG	2.15	0.47
2:H:372:LEU:HD11	2:H:376:ARG:HG2	1.97	0.47
2:H:491:GLU:HA	2:H:494:LYS:HG2	1.96	0.47
2:I:330:TYR:HE2	2:I:372:LEU:HB3	1.80	0.47
1:B:298:THR:HG22	1:B:329:SER:H	1.80	0.47
1:C:496:LYS:HB2	1:C:542:TYR:OH	2.15	0.47
1:G:679:LYS:HD3	1:G:686:PRO:HA	1.96	0.47
2:I:275:VAL:O	2:I:279:ALA:N	2.47	0.47
1:B:365:ARG:NH1	1:B:412:PRO:O	2.48	0.47
2:H:230:ASP:N	2:H:230:ASP:OD1	2.42	0.47
1:B:387:LYS:O	1:B:449:ARG:NH1	2.40	0.46
1:A:272:SER:OG	1:G:435:ASN:ND2	2.48	0.46
1:A:500:LEU:HD11	1:A:602:ASN:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:ASN:OD1	1:B:476:ASN:N	2.49	0.46
1:C:729:LYS:HE3	1:C:733:GLU:HB3	1.96	0.46
2:I:109:VAL:HG11	2:I:136:VAL:HG22	1.96	0.46
2:I:391:LYS:HE2	2:I:398:LYS:HG3	1.96	0.46
1:A:551:ASP:OD1	1:A:551:ASP:N	2.44	0.46
1:B:378:LEU:HD21	1:B:401:LEU:HD12	1.96	0.46
1:E:315:ASP:HA	1:F:313:PHE:HE2	1.81	0.46
1:G:607:ALA:HB2	1:G:638:ILE:HD11	1.96	0.46
2:H:695:ALA:O	2:H:699:ILE:N	2.42	0.46
2:I:28:ASP:HA	2:I:31:ASN:HB2	1.96	0.46
2:I:355:LYS:HA	2:I:358:ILE:HD12	1.96	0.46
1:G:292:ASN:HB3	1:G:335:ASP:HB2	1.97	0.46
2:H:410:GLU:OE2	2:H:423:LYS:NZ	2.46	0.46
2:H:458:ASP:OD1	2:H:458:ASP:N	2.49	0.46
2:I:691:ARG:NH1	2:I:753:GLU:OE1	2.42	0.46
1:B:667:SER:OG	1:B:677:ASP:OD1	2.34	0.46
1:C:667:SER:O	1:C:675:PHE:N	2.47	0.46
1:D:488:THR:HG22	1:D:506:ALA:HA	1.97	0.46
1:D:496:LYS:HD2	1:D:496:LYS:HA	1.76	0.46
1:G:484:ILE:O	1:G:488:THR:OG1	2.27	0.46
2:H:630:PHE:O	2:H:634:LEU:N	2.48	0.46
1:B:669:ARG:NH1	1:B:671:ASP:OD2	2.49	0.46
1:C:297:ARG:HA	1:C:330:SER:HA	1.98	0.46
1:A:290:SER:HB3	1:A:337:SER:HB2	1.98	0.46
1:G:643:ILE:HG21	1:G:723:LYS:HE2	1.97	0.46
2:H:145:SER:OG	2:H:205:GLN:NE2	2.41	0.46
2:H:624:ILE:O	2:H:672:TYR:OH	2.31	0.46
1:C:310:HIS:N	1:C:317:GLY:O	2.44	0.46
1:C:692:PRO:HB2	1:C:732:TYR:HD2	1.81	0.46
2:I:322:SER:HB3	2:I:338:SER:HA	1.98	0.46
1:D:674:THR:OG1	1:D:675:PHE:N	2.48	0.46
2:H:155:LEU:HD23	2:H:160:LEU:HD22	1.98	0.46
2:I:323:ASP:OD1	2:I:323:ASP:N	2.46	0.45
2:I:491:GLU:HA	2:I:494:LYS:HB2	1.98	0.45
1:B:528:LYS:HB2	1:B:528:LYS:HE3	1.76	0.45
1:D:179:ASP:OD1	1:D:179:ASP:N	2.43	0.45
2:H:391:LYS:HA	2:H:401:LEU:HB3	1.98	0.45
1:D:642:TYR:HA	1:D:700:ALA:HA	1.98	0.45
2:H:557:ASP:OD1	2:H:557:ASP:N	2.50	0.45
2:I:86:ASP:O	2:I:114:ARG:NH2	2.48	0.45
2:I:516:LEU:HD13	2:I:524:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:SER:HB3	1:E:337:SER:HB3	1.98	0.45
1:E:632:ASP:HB3	1:E:635:ILE:HG12	1.98	0.45
2:H:412:ARG:O	2:H:421:GLN:N	2.49	0.45
1:C:378:LEU:HD21	1:C:401:LEU:HD12	1.98	0.45
1:D:664:ASN:OD1	1:D:681:TYR:OH	2.34	0.45
1:E:329:SER:HA	1:F:300:THR:HA	1.97	0.45
1:E:717:SER:OG	1:E:718:THR:N	2.47	0.45
2:H:267:LYS:HA	2:H:270:LYS:HE3	1.98	0.45
2:H:661:VAL:HG23	2:H:664:ILE:HD12	1.99	0.45
2:I:747:LEU:HD21	2:I:760:PHE:HB2	1.98	0.45
2:I:755:ASP:HA	2:I:758:GLU:HB3	1.99	0.45
1:B:224:GLU:HG3	1:B:517:THR:HG21	1.98	0.45
1:D:636:ARG:HH22	1:D:668:LEU:HB2	1.80	0.45
1:D:700:ALA:H	1:D:726:ILE:HD13	1.81	0.45
1:E:312:SER:OG	1:E:313:PHE:N	2.49	0.45
1:F:488:THR:HG22	1:F:506:ALA:HA	1.99	0.45
2:I:274:LEU:HD22	2:I:561:PHE:HE2	1.82	0.45
1:G:378:LEU:HD21	1:G:401:LEU:HD12	1.99	0.45
2:H:192:ILE:HG12	2:H:192:ILE:O	2.15	0.45
2:H:444:MET:SD	2:H:444:MET:N	2.88	0.45
1:E:268:ASN:HB2	1:E:363:ASN:HB2	1.99	0.45
1:C:647:GLU:HB3	1:C:695:LYS:HB2	2.00	0.44
1:F:341:ALA:HB2	1:G:288:THR:HG23	1.98	0.44
2:H:476:PRO:HB2	2:H:478:LYS:HG2	1.98	0.44
2:I:87:LEU:HA	2:I:114:ARG:HH12	1.81	0.44
2:I:285:ILE:HD11	2:I:530:ALA:HB3	1.99	0.44
1:B:620:ILE:HG13	1:B:673:LYS:HD3	2.00	0.44
1:C:627:LEU:HD22	1:C:676:ILE:HD13	2.00	0.44
1:G:463:ASN:ND2	1:G:466:ASN:OD1	2.50	0.44
2:H:493:GLN:O	2:H:497:THR:OG1	2.30	0.44
2:H:504:GLY:O	2:H:517:SER:OG	2.30	0.44
2:I:178:SER:OG	2:I:179:GLN:N	2.49	0.44
1:D:425:ASP:OD2	1:D:429:SER:OG	2.35	0.44
2:H:655:PHE:O	2:H:659:GLU:N	2.50	0.44
1:F:496:LYS:HA	1:F:496:LYS:HD3	1.77	0.44
1:G:425:ASP:OD2	1:G:429:SER:OG	2.35	0.44
2:H:151:LYS:HA	2:H:151:LYS:HD3	1.73	0.44
2:H:590:ASP:N	2:H:590:ASP:OD1	2.48	0.44
2:I:335:GLN:HB2	2:I:347:VAL:HA	1.99	0.44
1:A:231:ASP:OD1	1:A:231:ASP:N	2.45	0.44
2:I:313:LYS:HE3	2:I:317:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:LEU:O	1:A:703:LYS:NZ	2.40	0.44
1:E:395:LYS:O	1:E:397:LYS:NZ	2.37	0.44
1:E:505:ILE:HD13	1:E:526:ALA:HB1	1.99	0.44
1:F:225:LYS:HE2	1:F:518:LYS:HD3	2.00	0.44
2:H:190:LYS:HD2	2:H:190:LYS:HA	1.63	0.44
2:H:333:PHE:H	2:H:441:ILE:HG23	1.82	0.44
2:H:687:ILE:HA	2:H:690:PHE:HB3	1.98	0.44
2:I:356:LYS:HA	2:I:356:LYS:HD3	1.85	0.44
1:G:540:LEU:HD23	1:G:547:ILE:HG12	2.00	0.44
2:H:60:VAL:HG13	2:H:144:ILE:HD13	1.99	0.44
2:H:332:PRO:O	2:H:354:ASN:ND2	2.50	0.44
2:I:392:GLU:H	2:I:401:LEU:HB3	1.83	0.44
2:I:649:SER:OG	2:I:654:GLU:OE1	2.32	0.44
2:I:720:LYS:HA	2:I:723:ILE:HG22	1.99	0.44
1:B:657:ASN:OD1	1:B:657:ASN:N	2.50	0.44
1:C:494:ASN:HD21	1:C:592:ARG:HG2	1.81	0.44
1:D:232:PRO:HG3	1:D:459:ILE:HD13	1.99	0.44
2:H:264:LYS:HA	2:H:570:ILE:HA	2.00	0.44
2:H:356:LYS:HD2	2:H:356:LYS:HA	1.72	0.44
2:H:394:ASP:OD1	2:H:394:ASP:N	2.50	0.44
2:H:53:LEU:HD12	2:H:53:LEU:HA	1.87	0.44
2:H:448:VAL:HG21	2:H:453:LYS:HD2	1.99	0.44
2:I:326:PRO:HG3	2:I:386:ILE:HD13	2.00	0.44
2:I:430:THR:HG22	2:I:432:LEU:H	1.82	0.44
2:I:637:ILE:O	2:I:641:SER:OG	2.30	0.44
1:E:692:PRO:HB2	1:E:732:TYR:HB3	1.99	0.43
1:F:629:LEU:N	1:F:674:THR:O	2.46	0.43
1:G:287:ARG:HG2	1:G:340:LEU:HD22	2.00	0.43
2:I:627:SER:HB3	2:I:668:LEU:HB3	2.00	0.43
1:B:624:THR:HB	1:B:687:LEU:H	1.84	0.43
1:D:609:GLU:O	1:D:613:LYS:NZ	2.39	0.43
2:H:23:LYS:HB2	2:H:23:LYS:HE3	1.87	0.43
2:H:70:GLU:OE1	2:H:72:TYR:OH	2.34	0.43
2:H:367:LYS:HD3	2:H:367:LYS:HA	1.70	0.43
1:A:508:VAL:HG13	1:A:516:THR:HA	2.01	0.43
1:C:636:ARG:HH22	1:C:668:LEU:HD13	1.82	0.43
1:D:476:ASN:OD1	1:D:476:ASN:N	2.51	0.43
1:D:665:ILE:HD12	1:D:681:TYR:HD2	1.84	0.43
1:E:422:ASN:OD1	1:E:422:ASN:N	2.51	0.43
1:F:360:LEU:HD23	1:F:360:LEU:HA	1.89	0.43
2:H:333:PHE:O	2:H:354:ASN:ND2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:371:LYS:H	2:H:454:PRO:HG2	1.84	0.43
1:E:276:ASP:OD1	1:E:276:ASP:N	2.35	0.43
1:E:423:ALA:HB1	1:E:428:SER:HA	2.00	0.43
1:G:631:ILE:HD13	1:G:674:THR:HB	1.99	0.43
1:G:643:ILE:HD11	1:G:663:LEU:HD13	1.99	0.43
2:I:493:GLN:HG3	2:I:678:ILE:HD11	2.00	0.43
1:B:282:THR:HB	1:B:345:THR:HB	2.00	0.43
1:C:276:ASP:OD1	1:C:276:ASP:N	2.48	0.43
1:F:276:ASP:OD1	1:F:276:ASP:N	2.52	0.43
1:F:502:GLU:O	1:F:503:ARG:NH1	2.52	0.43
2:H:164:LYS:HD2	2:H:164:LYS:HA	1.76	0.43
2:H:178:SER:OG	2:H:179:GLN:N	2.52	0.43
2:H:320:LYS:HA	2:H:320:LYS:HD3	1.85	0.43
2:H:575:TRP:O	2:H:579:GLY:N	2.39	0.43
1:D:595:ARG:HD2	1:D:611:VAL:HG21	2.00	0.43
2:I:291:THR:HA	2:I:466:PRO:HA	2.00	0.43
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.91	0.43
1:D:306:ASN:HB3	1:D:321:SER:HB2	2.01	0.43
2:H:142:LYS:O	2:H:145:SER:OG	2.33	0.43
2:H:295:PHE:N	2:H:561:PHE:O	2.52	0.43
2:H:509:PRO:HA	2:H:515:THR:HG22	2.01	0.43
2:I:157:PRO:HA	2:I:160:LEU:HB3	2.00	0.43
1:D:270:ILE:HB	1:D:361:ASN:HB3	2.01	0.43
1:D:425:ASP:HB2	1:D:430:THR:HB	2.00	0.43
1:E:265:ASP:OD1	1:E:265:ASP:N	2.46	0.43
1:E:300:THR:HB	1:E:327:SER:HB3	2.00	0.43
1:B:306:ASN:N	1:B:321:SER:OG	2.52	0.43
1:B:647:GLU:HB2	1:B:697:ASN:HD21	1.83	0.43
1:B:682:ASN:HD21	1:B:687:LEU:HA	1.84	0.43
1:D:508:VAL:HG23	1:D:516:THR:HA	2.01	0.43
1:E:179:ASP:OD1	1:E:179:ASP:N	2.52	0.43
1:F:476:ASN:OD1	1:F:476:ASN:N	2.49	0.43
2:H:618:LYS:NZ	2:H:718:TYR:O	2.52	0.43
2:I:593:TYR:CZ	2:I:595:PHE:HB3	2.54	0.43
1:A:454:GLN:NE2	1:B:401:LEU:O	2.44	0.42
1:A:545:LYS:HE2	1:A:545:LYS:HB3	1.92	0.42
1:A:612:VAL:HG21	1:A:724:ILE:HD12	2.00	0.42
1:B:494:ASN:HB3	1:B:500:LEU:HD23	2.00	0.42
1:B:645:GLU:HG3	1:B:697:ASN:HD22	1.84	0.42
1:C:195:ASP:OD2	1:C:214:LYS:NZ	2.38	0.42
1:G:488:THR:HG22	1:G:506:ALA:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:676:ASN:HB3	2:H:684:LYS:HA	2.00	0.42
2:I:424:THR:HG21	2:I:430:THR:HG23	2.01	0.42
1:A:188:GLU:OE1	1:A:221:SER:OG	2.32	0.42
2:I:391:LYS:HA	2:I:401:LEU:HB3	2.01	0.42
2:I:727:VAL:O	2:I:731:LEU:N	2.52	0.42
1:A:365:ARG:NH1	1:A:412:PRO:O	2.49	0.42
1:F:379:PRO:HB3	1:F:455:VAL:HG22	2.01	0.42
2:H:301:LEU:O	2:H:376:ARG:NH2	2.52	0.42
2:H:752:ASN:OD1	2:H:756:ASN:ND2	2.49	0.42
1:A:231:ASP:OD2	1:A:238:LYS:NZ	2.43	0.42
1:A:484:ILE:O	1:A:488:THR:OG1	2.34	0.42
1:B:606:GLY:HA3	1:B:704:GLU:HG3	2.01	0.42
1:E:278:SER:HB2	1:E:349:THR:HB	2.01	0.42
1:G:494:ASN:HB3	1:G:500:LEU:HD23	2.01	0.42
2:I:164:LYS:CD	2:I:190:LYS:HZ1	2.27	0.42
1:B:183:ILE:HD12	1:B:203:LEU:HD21	2.02	0.42
2:H:526:ARG:NE	2:H:529:GLU:OE2	2.52	0.42
1:E:662:MET:HE2	1:E:662:MET:HB3	1.99	0.42
1:B:285:GLN:O	1:B:287:ARG:NH1	2.51	0.42
1:E:250:GLU:OE2	1:E:503:ARG:NE	2.41	0.42
1:F:444:LYS:HE2	1:F:444:LYS:HB3	1.77	0.42
1:G:627:LEU:HB2	1:G:676:ILE:HB	2.02	0.42
1:G:696:VAL:HG23	1:G:727:PHE:HE2	1.85	0.42
2:I:188:ASN:ND2	2:I:190:LYS:O	2.52	0.42
1:F:605:VAL:HB	1:F:703:LYS:HB3	2.02	0.42
2:I:294:LEU:HA	2:I:562:ILE:HG22	2.01	0.42
2:I:586:ILE:HG22	2:I:593:TYR:HB2	2.01	0.42
1:A:560:GLN:O	1:A:564:ASN:ND2	2.53	0.42
1:C:648:ASP:H	1:C:652:LEU:H	1.67	0.42
2:H:194:ILE:O	2:H:194:ILE:HG22	2.20	0.42
2:I:471:ILE:HG22	2:I:475:ILE:HG12	2.01	0.42
1:C:691:ASN:OD1	1:C:693:ASN:ND2	2.52	0.41
1:C:732:TYR:HD1	1:C:733:GLU:HG3	1.85	0.41
1:E:326:ASN:O	1:F:303:VAL:N	2.53	0.41
1:F:523:LEU:HD13	1:F:583:LEU:HD21	2.02	0.41
1:G:576:THR:HG23	1:G:577:VAL:HG13	2.02	0.41
2:H:327:VAL:HG23	2:H:370:LEU:HD13	2.01	0.41
1:C:476:ASN:OD1	1:C:476:ASN:N	2.53	0.41
2:H:291:THR:HG23	2:H:293:ILE:HD11	2.01	0.41
2:H:313:LYS:HA	2:H:455:LEU:HD22	2.02	0.41
1:A:232:PRO:HD3	1:A:480:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ASN:HB2	1:B:405:LEU:HG	2.01	0.41
1:B:482:PRO:HB3	1:C:246:ASN:HD21	1.85	0.41
1:C:625:GLU:HA	1:C:678:PHE:HB2	2.02	0.41
1:G:310:HIS:N	1:G:317:GLY:O	2.52	0.41
2:H:747:LEU:HD11	2:H:760:PHE:HB2	2.02	0.41
2:I:292:TYR:N	2:I:465:ALA:O	2.52	0.41
2:I:398:LYS:HD2	2:I:398:LYS:HA	1.83	0.41
2:I:412:ARG:HE	2:I:412:ARG:HB3	1.76	0.41
1:A:286:THR:HB	1:A:341:ALA:HB3	2.02	0.41
1:A:296:SER:HB2	1:A:331:THR:HB	2.03	0.41
1:B:246:ASN:HB2	1:B:373:PRO:HG3	2.03	0.41
1:B:659:ARG:HE	1:B:659:ARG:HB3	1.67	0.41
1:D:218:LYS:HE2	1:D:220:LYS:HE2	2.02	0.41
1:E:631:ILE:HG12	1:E:674:THR:HG21	2.02	0.41
2:H:290:ASN:HA	2:H:565:PRO:HB3	2.02	0.41
2:I:706:LYS:HB3	2:I:706:LYS:HE3	1.89	0.41
1:A:534:ASN:OD1	1:A:534:ASN:N	2.54	0.41
1:D:261:ILE:HD12	1:D:370:GLY:HA2	2.03	0.41
2:H:385:ILE:HG22	2:H:386:ILE:HG23	2.02	0.41
2:H:288:GLU:HG2	2:H:289:LEU:HG	2.02	0.41
1:D:323:GLY:HA3	1:E:306:ASN:HA	2.02	0.41
1:E:183:ILE:HA	1:E:184:PRO:HD3	1.91	0.41
1:G:389:GLN:NE2	1:G:438:GLN:HE21	2.19	0.41
2:H:278:HIS:CE1	2:H:536:TYR:HB2	2.55	0.41
2:H:316:ASN:OD1	2:H:316:ASN:N	2.52	0.41
2:H:691:ARG:O	2:H:695:ALA:N	2.47	0.41
1:C:554:PHE:HB2	1:C:559:SER:HB2	2.02	0.41
1:D:197:LYS:HD3	1:D:197:LYS:HA	1.90	0.41
1:G:365:ARG:NH1	1:G:413:SER:O	2.53	0.41
2:H:700:GLU:HA	2:H:703:LEU:HD12	2.02	0.41
2:I:752:ASN:O	2:I:756:ASN:ND2	2.53	0.41
1:A:670:GLN:H	1:A:670:GLN:HG2	1.70	0.41
1:B:389:GLN:HE21	1:B:438:GLN:HE21	1.68	0.41
1:B:425:ASP:OD2	1:B:429:SER:OG	2.39	0.41
1:C:412:PRO:HD3	1:C:419:ILE:HG23	2.01	0.41
1:D:308:GLU:HB2	1:D:319:SER:HB3	2.03	0.41
1:E:646:ILE:HB	1:E:654:GLU:HG2	2.03	0.41
1:G:195:ASP:N	1:G:195:ASP:OD1	2.52	0.41
2:H:239:GLU:HA	2:H:243:PHE:HD2	1.86	0.41
2:H:377:ILE:HG22	2:H:413:ILE:HD13	2.03	0.41
2:H:593:TYR:H	2:H:674:SER:HB3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:313:LYS:HB3	2:I:331:ILE:HG13	2.01	0.41
2:I:624:ILE:O	2:I:672:TYR:OH	2.35	0.41
2:I:645:VAL:HG23	2:I:708:ILE:HG21	2.02	0.41
2:I:742:LEU:HD23	2:I:742:LEU:HA	1.89	0.41
1:B:647:GLU:HG2	1:B:651:GLY:HA2	2.03	0.41
1:C:246:ASN:HB2	1:C:373:PRO:HG3	2.02	0.41
2:I:435:LYS:HD2	2:I:435:LYS:HA	1.89	0.41
1:A:509:ASN:HA	1:A:510:PRO:HD3	1.95	0.40
2:H:188:ASN:C	2:H:190:LYS:H	2.28	0.40
2:H:315:LEU:HD23	2:H:315:LEU:HA	1.92	0.40
2:H:320:LYS:HB2	2:H:339:LYS:HB2	2.03	0.40
2:I:459:TYR:HD2	2:I:542:VAL:HG22	1.86	0.40
1:C:365:ARG:NH1	1:C:412:PRO:O	2.54	0.40
1:F:183:ILE:HA	1:F:184:PRO:HD3	1.92	0.40
2:I:373:ASP:HB2	2:I:376:ARG:HB2	2.01	0.40
2:I:573:LYS:HE2	2:I:577:MET:HG2	2.02	0.40
1:B:642:TYR:H	1:B:663:LEU:HB3	1.85	0.40
1:E:405:LEU:HA	1:E:405:LEU:HD12	1.80	0.40
1:F:269:ILE:HG12	1:F:448:LEU:HD23	2.03	0.40
1:F:595:ARG:HE	1:F:595:ARG:HB2	1.70	0.40
2:H:285:ILE:HA	2:H:288:GLU:HB3	2.02	0.40
1:B:667:SER:OG	1:B:675:PHE:O	2.33	0.40
1:F:271:LEU:HD13	1:F:439:PHE:HE1	1.86	0.40
2:H:762:LYS:HD3	2:H:762:LYS:HA	1.85	0.40
1:F:545:LYS:HE2	1:F:545:LYS:HB3	1.93	0.40
1:F:616:HIS:HD2	1:F:726:ILE:HD12	1.87	0.40
1:G:389:GLN:HE21	1:G:438:GLN:HE21	1.70	0.40
2:H:578:THR:HA	2:H:581:PHE:HB2	2.04	0.40
2:I:493:GLN:HE22	2:I:679:PHE:HB2	1.87	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	560/735 (76%)	523 (93%)	37 (7%)	0	100	100
1	B	560/735 (76%)	530 (95%)	30 (5%)	0	100	100
1	C	560/735 (76%)	532 (95%)	27 (5%)	1 (0%)	43	71
1	D	560/735 (76%)	528 (94%)	32 (6%)	0	100	100
1	E	560/735 (76%)	529 (94%)	31 (6%)	0	100	100
1	F	560/735 (76%)	524 (94%)	36 (6%)	0	100	100
1	G	560/735 (76%)	531 (95%)	29 (5%)	0	100	100
2	H	714/767 (93%)	677 (95%)	36 (5%)	1 (0%)	48	78
2	I	714/767 (93%)	667 (93%)	47 (7%)	0	100	100
All	All	5348/6679 (80%)	5041 (94%)	305 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	543	GLN
2	H	190	LYS

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	501/661 (76%)	499 (100%)	2 (0%)	84	83
1	B	501/661 (76%)	501 (100%)	0	100	100
1	C	501/661 (76%)	499 (100%)	2 (0%)	84	83
1	D	501/661 (76%)	499 (100%)	2 (0%)	84	83
1	E	501/661 (76%)	500 (100%)	1 (0%)	87	85
1	F	501/661 (76%)	500 (100%)	1 (0%)	87	85
1	G	501/661 (76%)	500 (100%)	1 (0%)	87	85
2	H	651/698 (93%)	646 (99%)	5 (1%)	73	77
2	I	651/698 (93%)	650 (100%)	1 (0%)	87	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4809/6023 (80%)	4794 (100%)	15 (0%)	84 84

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	404	ILE
1	A	476	ASN
1	C	425	ASP
1	C	543	GLN
1	D	508	VAL
1	D	726	ILE
1	E	286	THR
1	F	276	ASP
1	G	371	THR
2	H	164	LYS
2	H	165	SER
2	H	169	ASP
2	H	188	ASN
2	H	190	LYS
2	I	198	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	ASN
1	A	304	HIS
1	A	363	ASN
1	A	437	ASN
1	A	564	ASN
1	A	602	ASN
1	A	691	ASN
1	B	280	GLN
1	B	292	ASN
1	B	326	ASN
1	B	363	ASN
1	B	376	ASN
1	B	389	GLN
1	B	437	ASN
1	B	458	ASN
1	B	463	ASN
1	B	601	ASN

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Mol	Chain	Res	Type
1	B	682	ASN
1	B	697	ASN
1	C	246	ASN
1	C	292	ASN
1	C	310	HIS
1	C	326	ASN
1	C	363	ASN
1	C	376	ASN
1	C	409	ASN
1	C	437	ASN
1	C	438	GLN
1	C	463	ASN
1	C	494	ASN
1	C	537	ASN
1	C	543	GLN
1	C	557	GLN
1	C	560	GLN
1	C	570	ASN
1	C	601	ASN
1	C	693	ASN
1	D	281	ASN
1	D	292	ASN
1	D	363	ASN
1	D	409	ASN
1	D	438	GLN
1	D	458	ASN
1	D	560	GLN
1	D	584	ASN
1	D	705	ASN
1	E	292	ASN
1	E	353	ASN
1	E	376	ASN
1	E	389	GLN
1	E	409	ASN
1	E	458	ASN
1	E	463	ASN
1	E	556	GLN
1	E	557	GLN
1	E	565	GLN
1	E	602	ASN
1	E	713	ASN
1	E	719	ASN

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Mol	Chain	Res	Type
1	F	292	ASN
1	F	336	HIS
1	F	363	ASN
1	F	389	GLN
1	F	499	ASN
1	F	539	ASN
1	F	557	GLN
1	F	561	ASN
1	F	588	ASN
1	F	630	ASN
1	F	705	ASN
1	F	709	ASN
1	G	198	ASN
1	G	253	HIS
1	G	310	HIS
1	G	376	ASN
1	G	438	GLN
1	G	458	ASN
1	G	463	ASN
1	G	537	ASN
1	G	560	GLN
1	G	705	ASN
2	H	85	GLN
2	H	93	ASN
2	H	200	ASN
2	H	206	HIS
2	H	220	HIS
2	H	341	HIS
2	H	351	ASN
2	H	447	ASN
2	H	633	ASN
2	H	676	ASN
2	H	701	ASN
2	H	725	ASN
2	H	726	GLN
2	I	32	ASN
2	I	40	ASN
2	I	81	HIS
2	I	189	ASN
2	I	205	GLN
2	I	206	HIS
2	I	278	HIS

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Mol	Chain	Res	Type
2	I	316	ASN
2	I	351	ASN
2	I	354	ASN
2	I	361	HIS
2	I	383	ASN
2	I	395	ASN
2	I	406	ASN
2	I	421	GLN
2	I	447	ASN
2	I	493	GLN
2	I	498	ASN
2	I	518	ASN
2	I	622	ASN
2	I	633	ASN
2	I	673	ASN
2	I	676	ASN
2	I	701	ASN
2	I	707	GLN
2	I	726	GLN
2	I	746	GLN
2	I	756	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

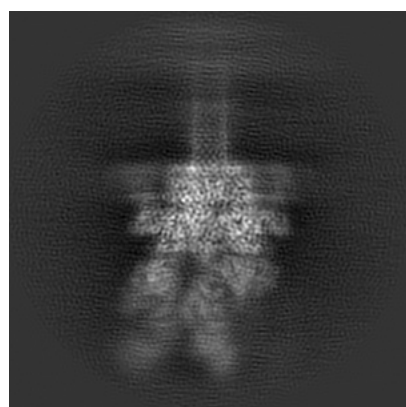
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20957. These allow visual inspection of the internal detail of the map and identification of artifacts.

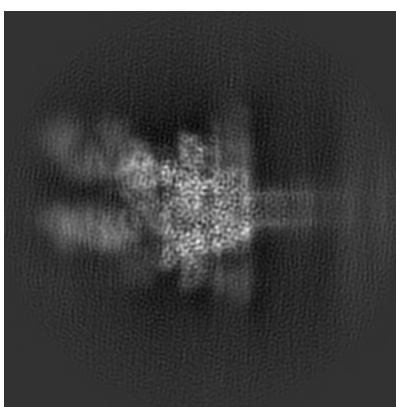
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

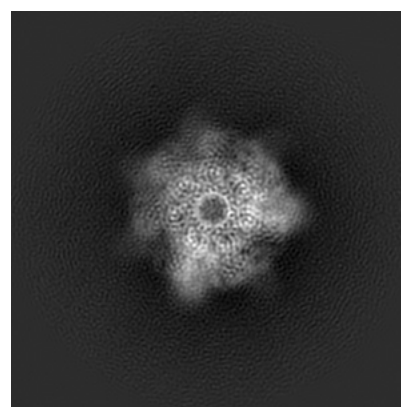
6.1.1 Primary map



X



Y

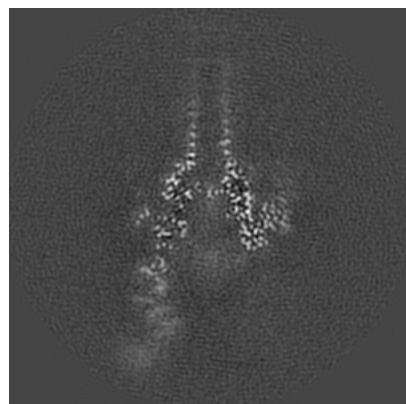


Z

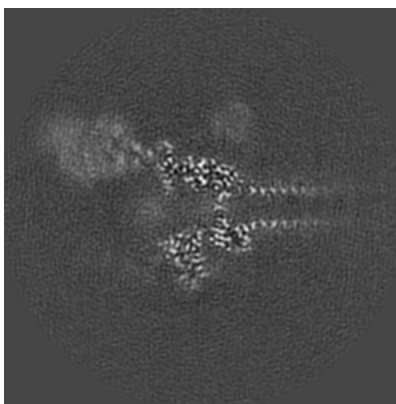
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

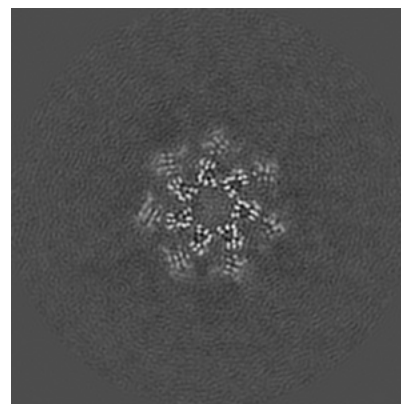
6.2.1 Primary map



X Index: 150



Y Index: 150

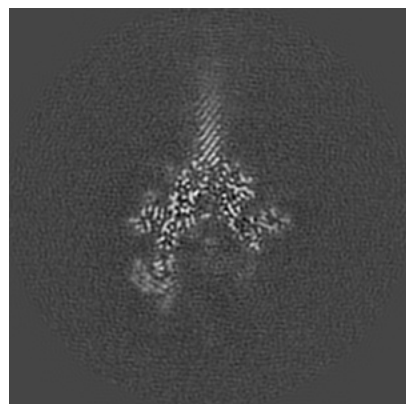


Z Index: 150

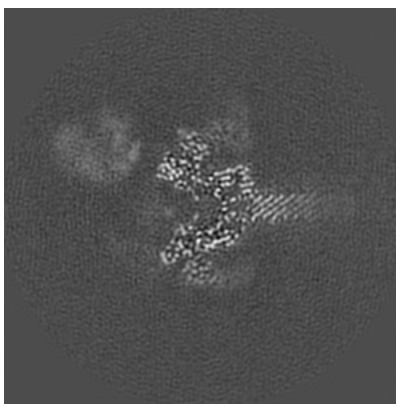
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

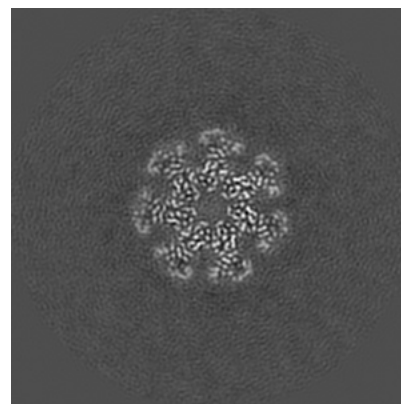
6.3.1 Primary map



X Index: 163



Y Index: 139

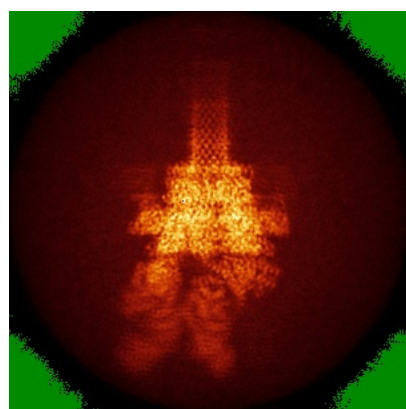


Z Index: 144

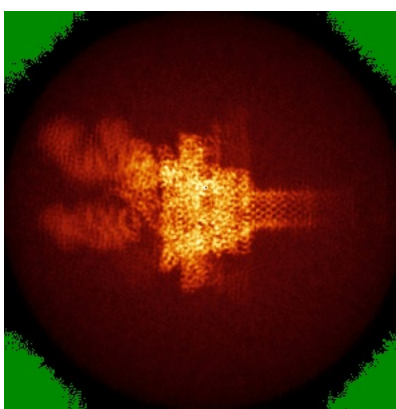
The images above show the largest variance slices of the map in three orthogonal directions.

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

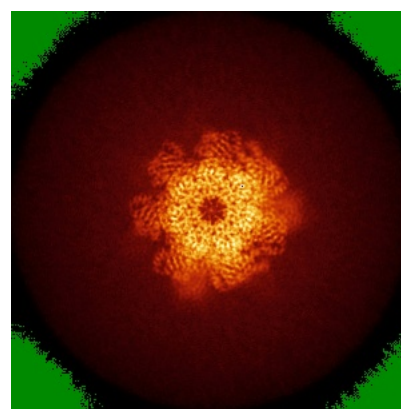
6.4.1 Primary map



X



Y

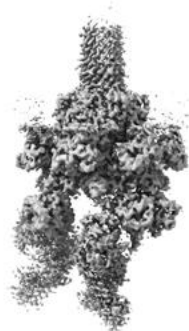


Z

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

6.5 Orthogonal surface views [i](#)

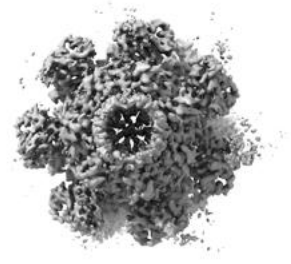
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

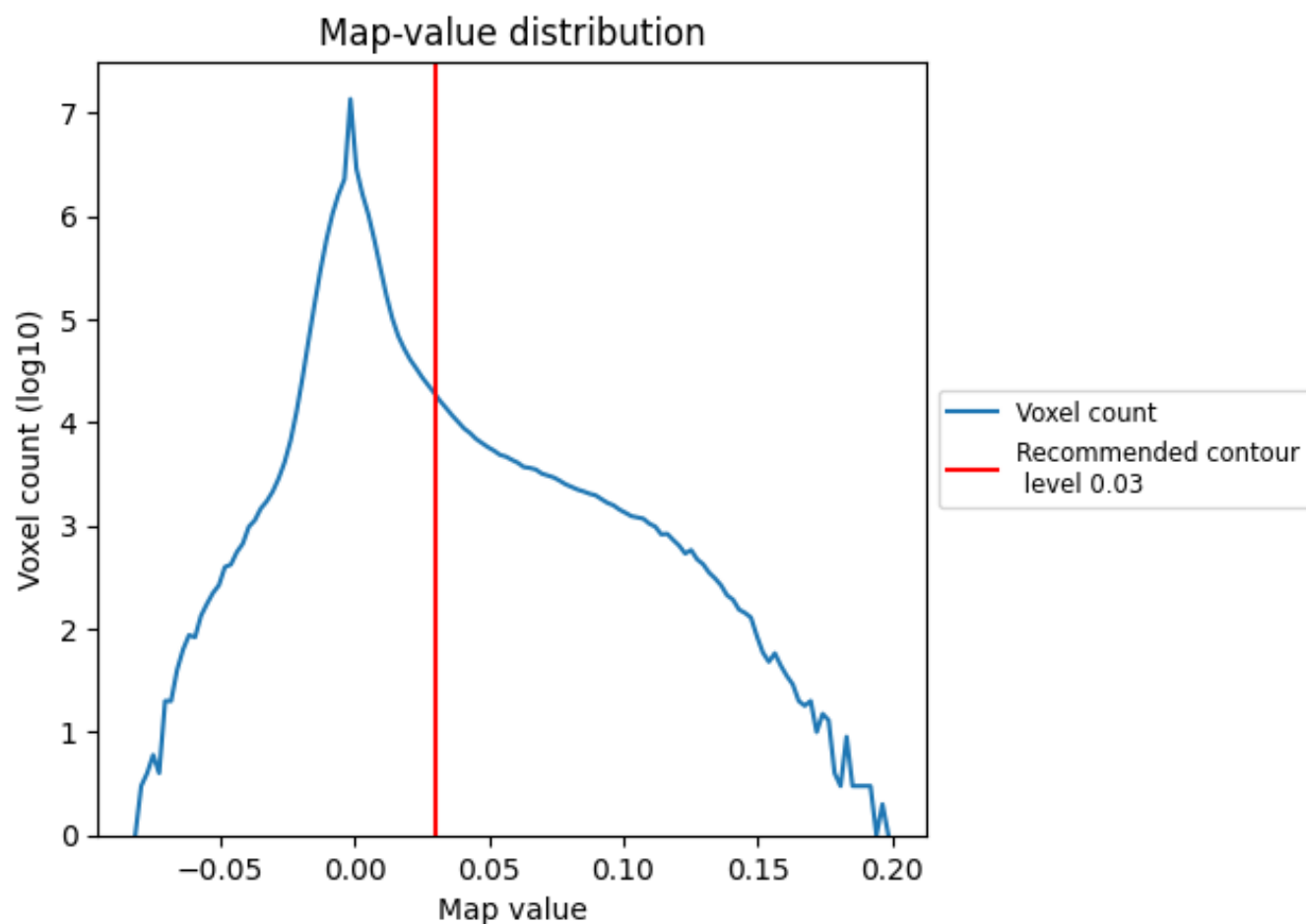
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

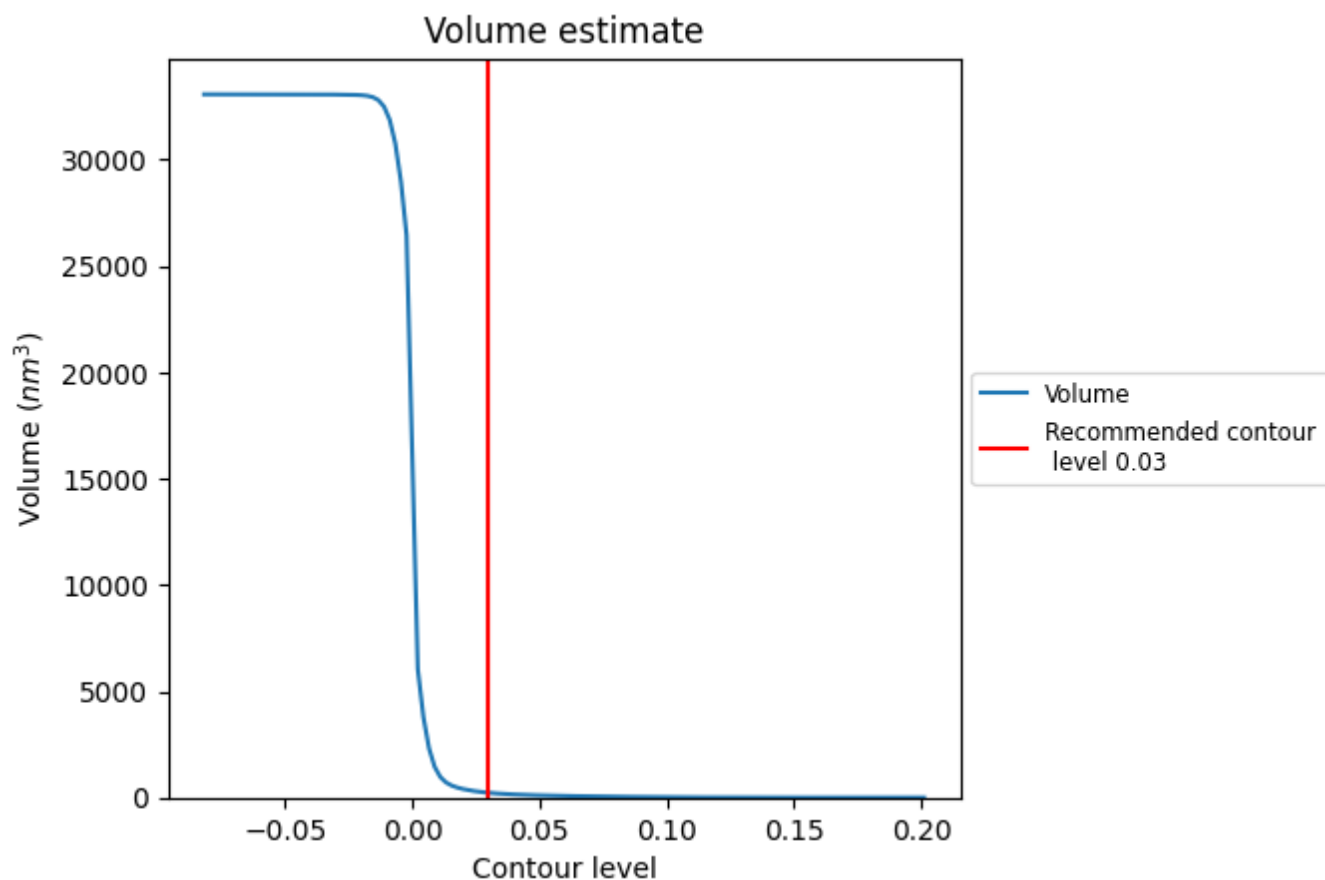
This section contains the results of statistical analysis of the map.

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.

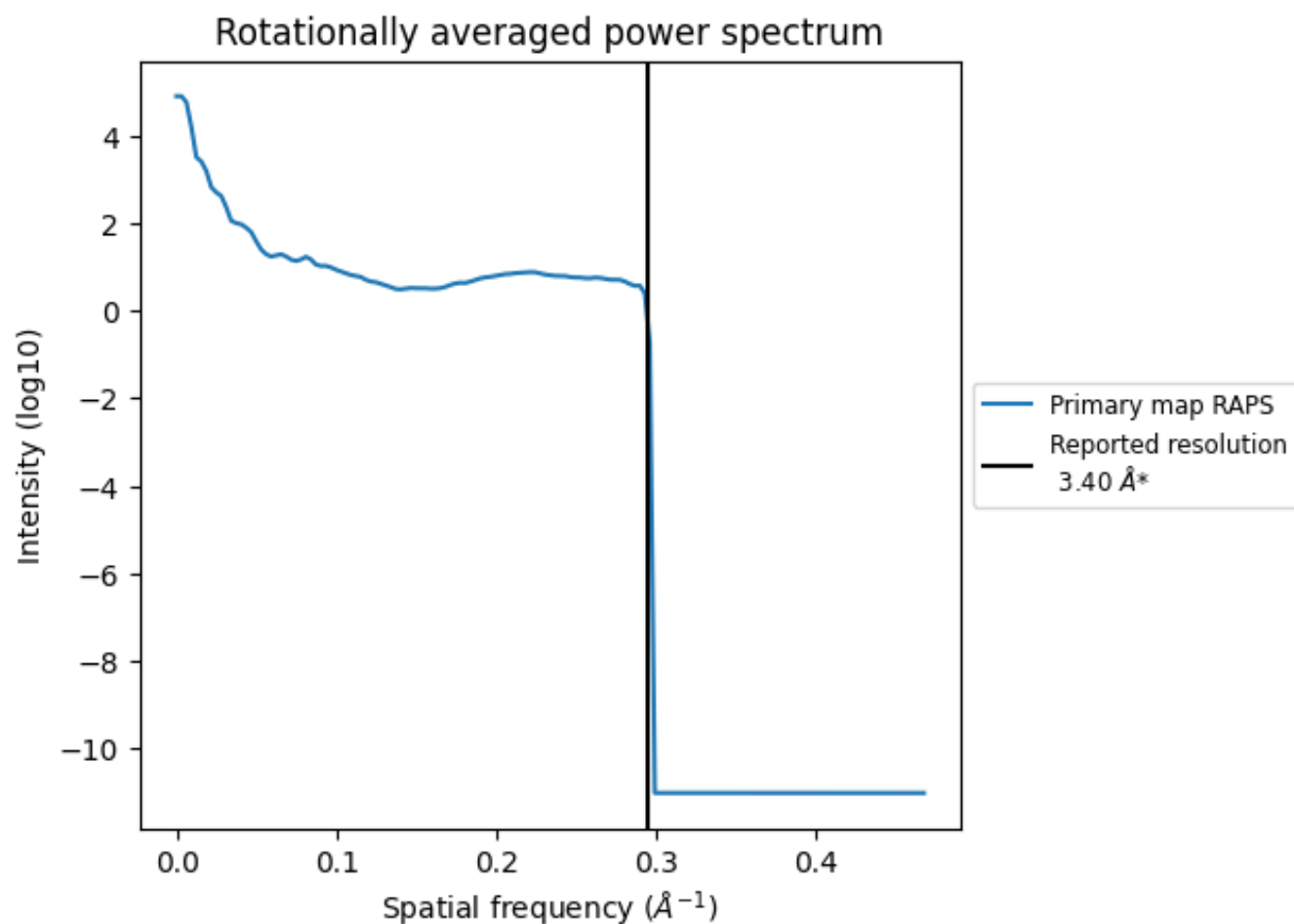
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 226 nm³; this corresponds to an approximate mass of 204 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 0.294 Å⁻¹

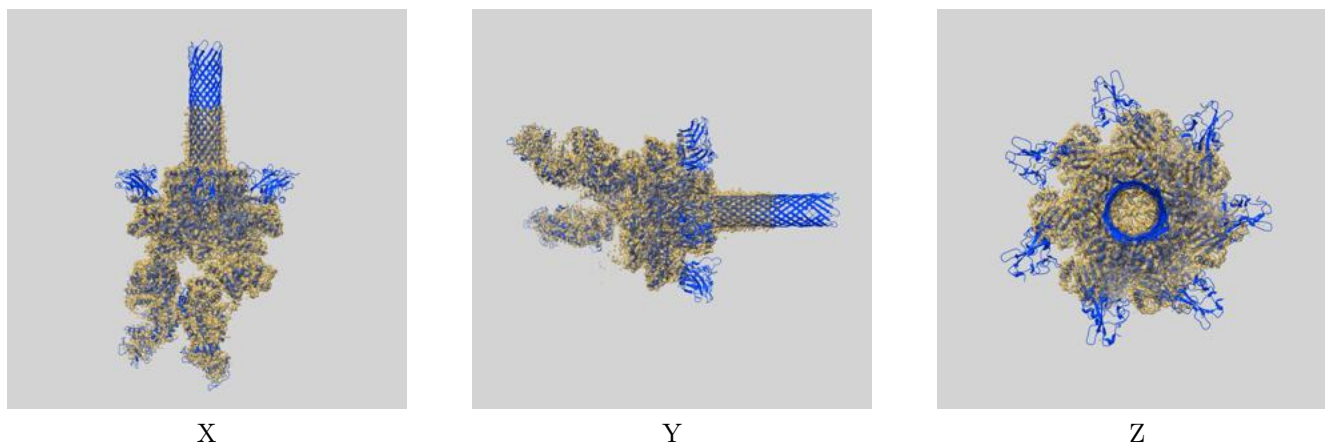
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

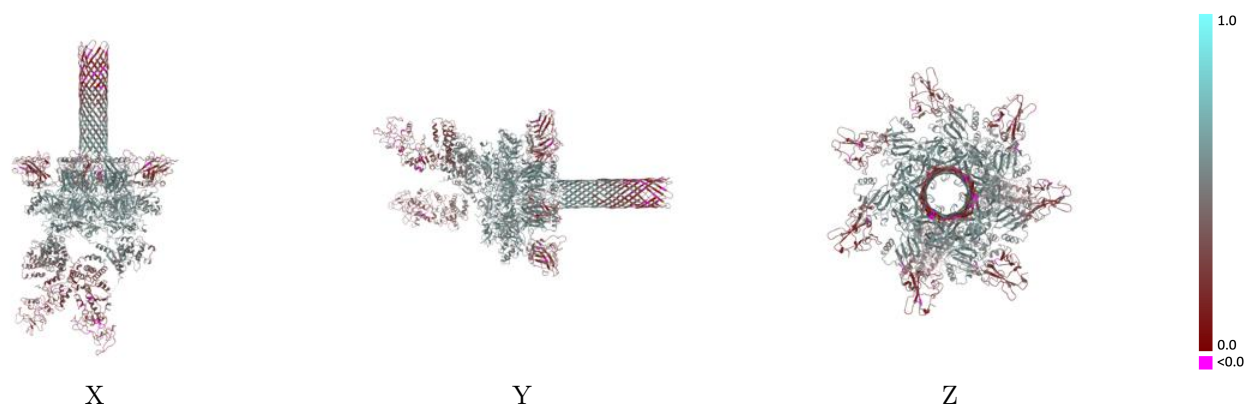
This section contains information regarding the fit between EMDB map EMD-20957 and PDB model 6UZD. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



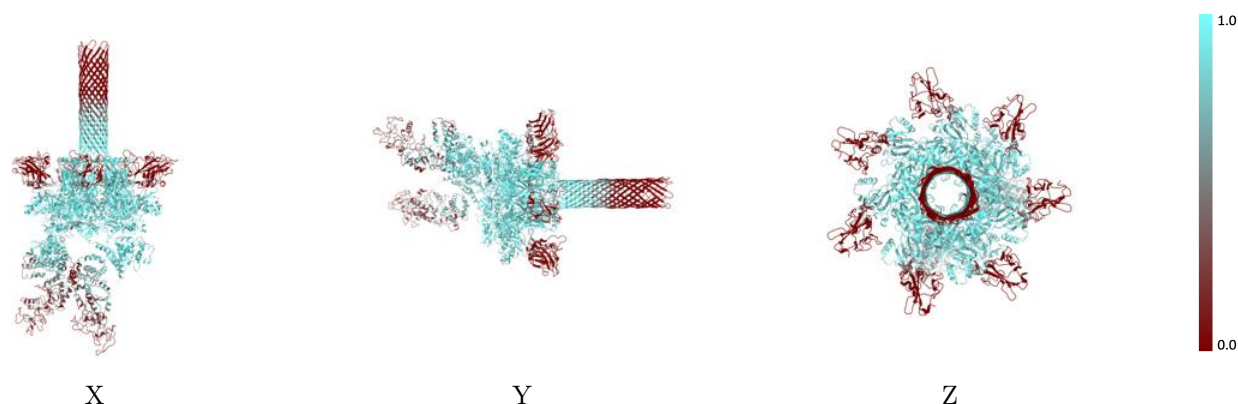
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



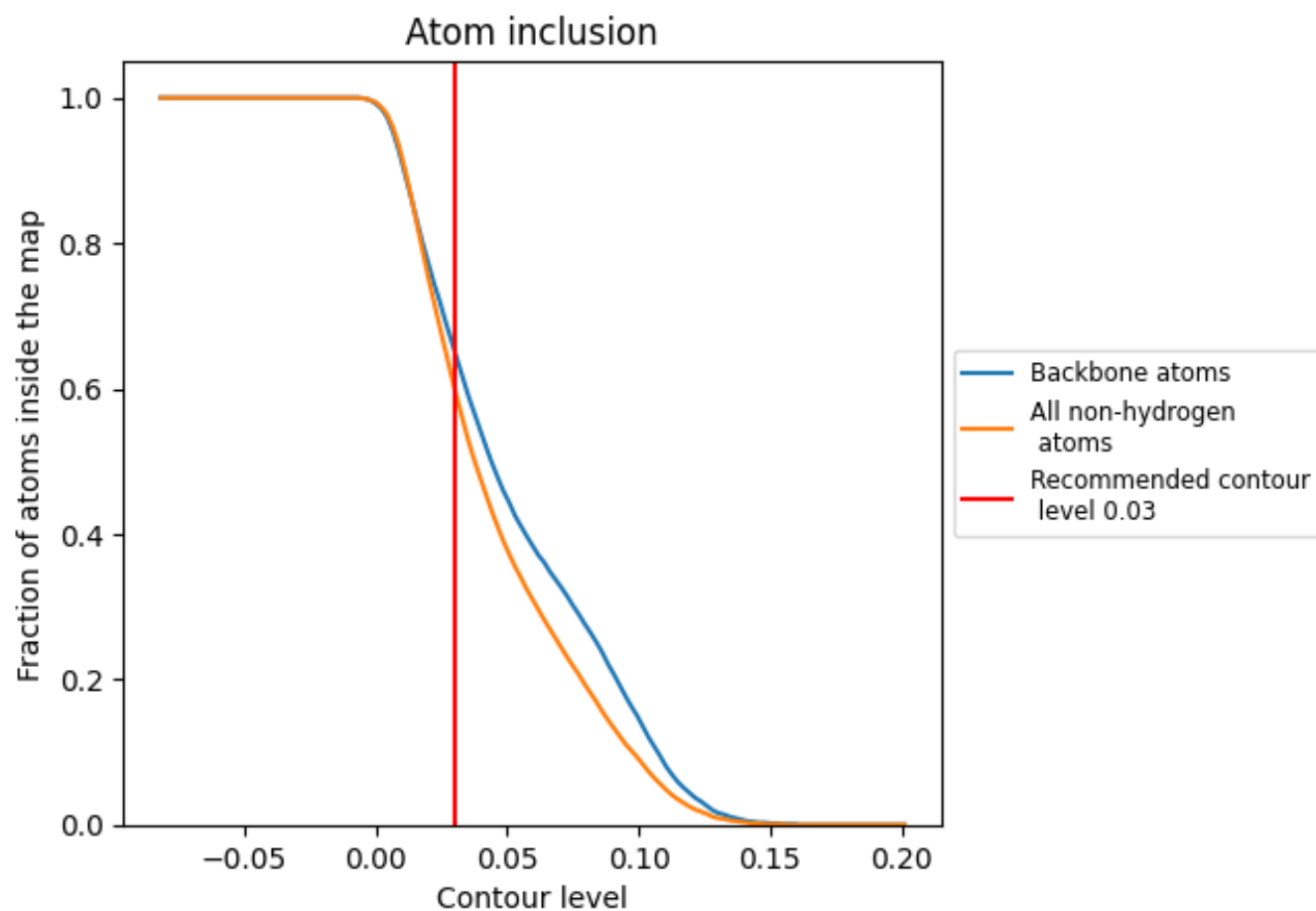
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 60% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6000	0.4360
A	0.6410	0.4730
B	0.6460	0.4800
C	0.6440	0.4710
D	0.6300	0.4730
E	0.6110	0.4670
F	0.6140	0.4650
G	0.6190	0.4690
H	0.5440	0.3390
I	0.5030	0.3440

1.0

0.0

<0.0