



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:15 PM UTC

PDB ID : 9CLS / pdb_00009cls
EMDB ID : EMD-45729
Title : Cryo-EM model derived from localized reconstruction of human adenovirus 6 (Ad6)-hexon-FII complex
Authors : Reddy, V.S.; Ma, O.X.
Deposited on : 2024-07-12
Resolution : 3.70 Å(reported)
Based on initial model : 6BIT

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:

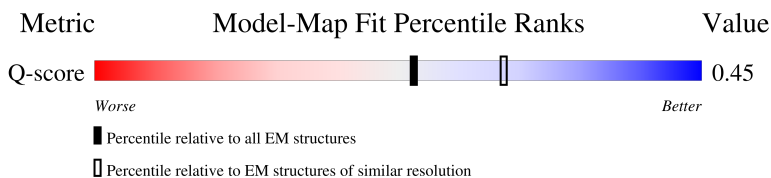
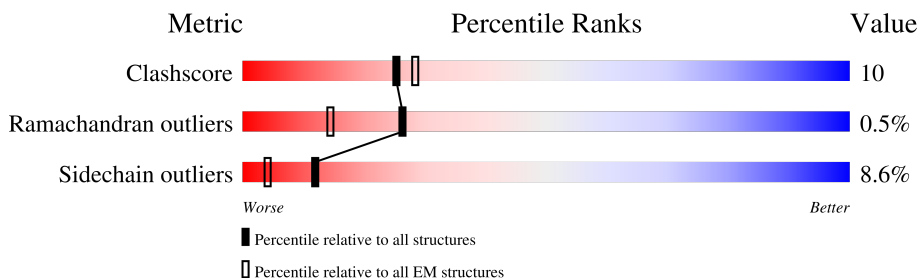
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.70 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	11569 (3.20 - 4.20)

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	J	963	
1	K	963	
1	L	963	
2	Z	622	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26845 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 Hexon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	931	Total	C	N	O	S	0	0
			7400	4691	1258	1413	38		
1	K	935	Total	C	N	O	S	0	0
			7426	4707	1262	1419	38		
1	L	930	Total	C	N	O	S	0	0
			7397	4691	1256	1412	38		

- Molecule 2 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	579	Total	C	N	O	S	0	0
			4615	2868	805	910	32		

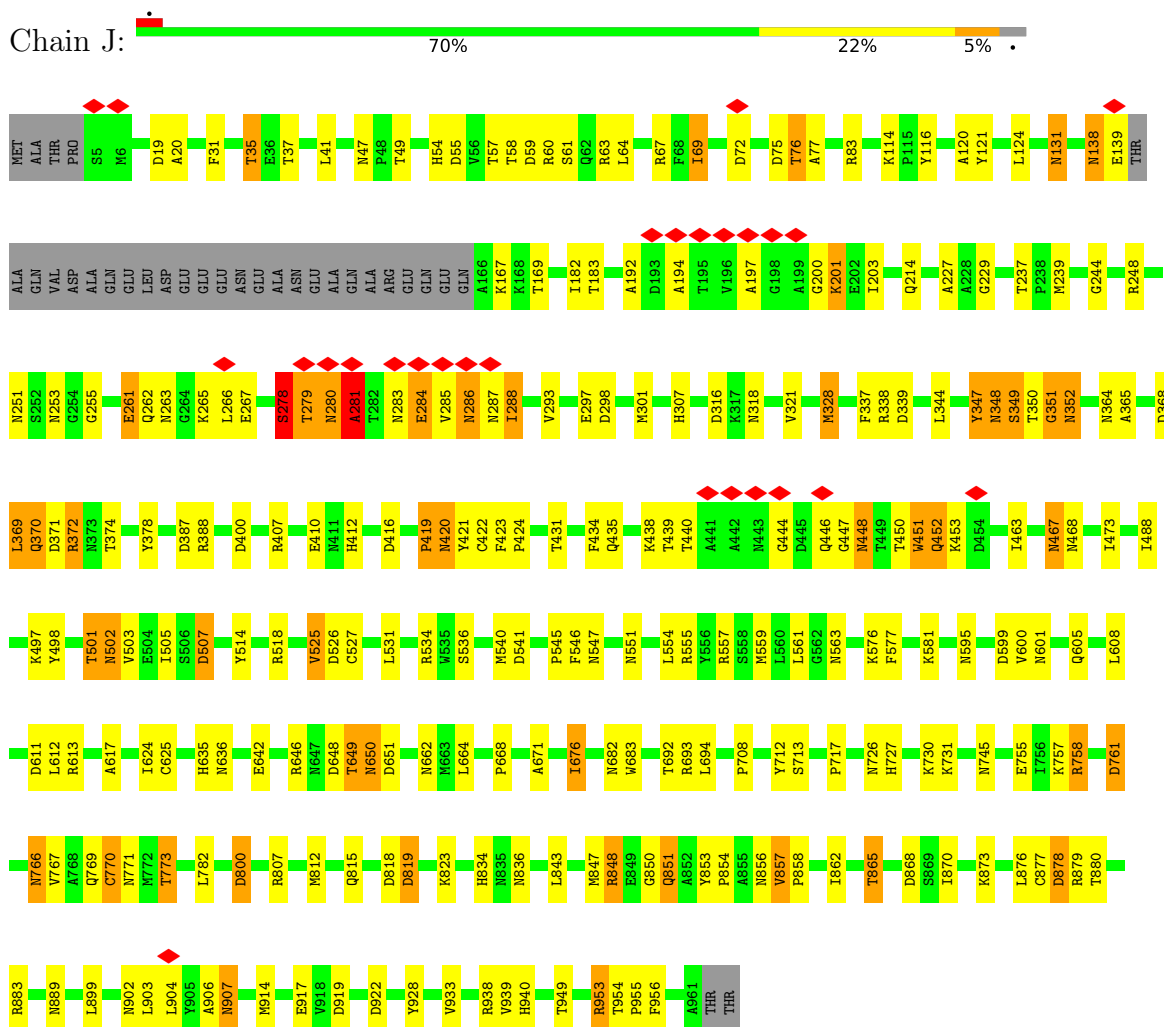
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	Z	7	Total	Ca	0
			7	7	

3 Residue-property plots

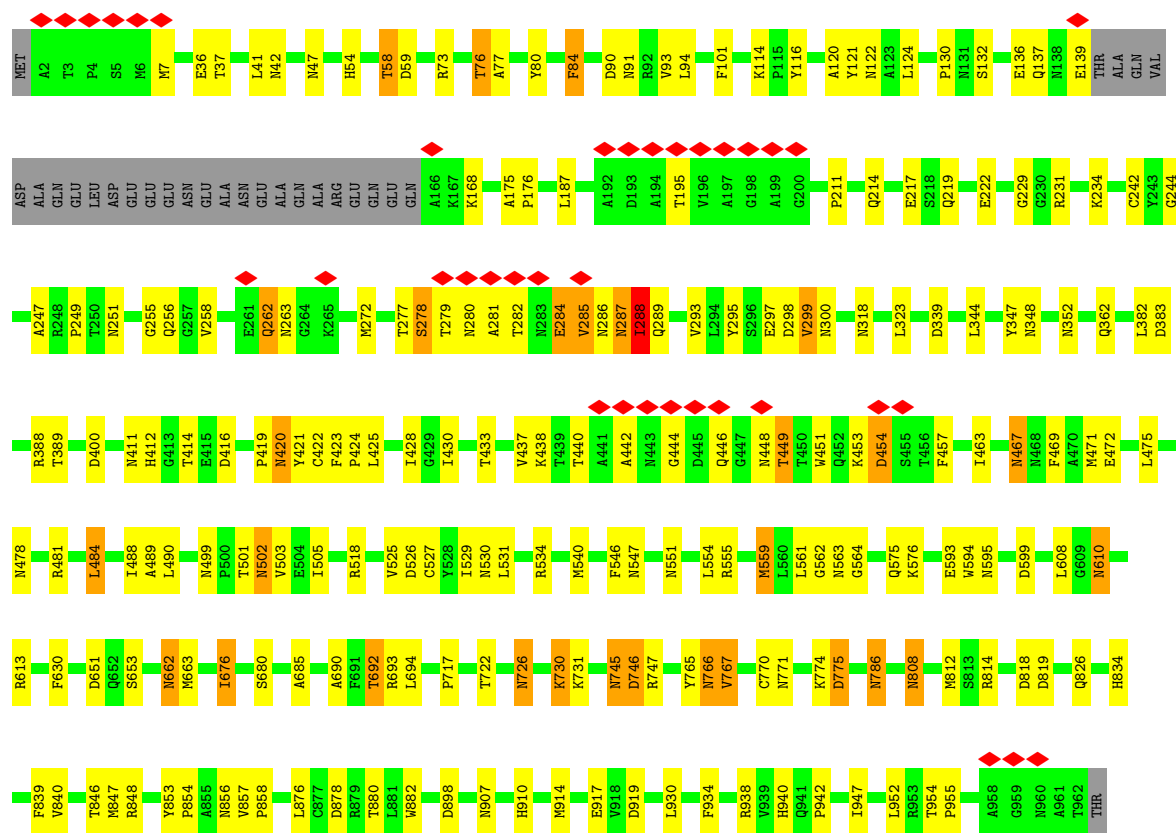
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Hexon protein



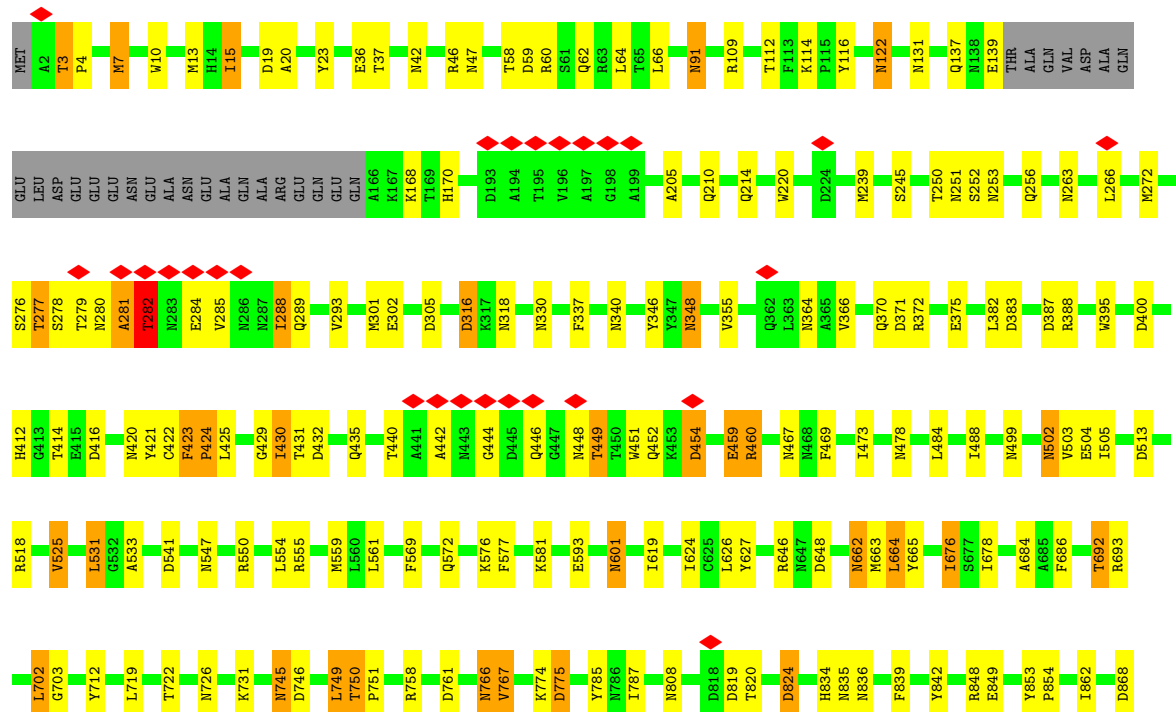
- Molecule 1: Hexon protein





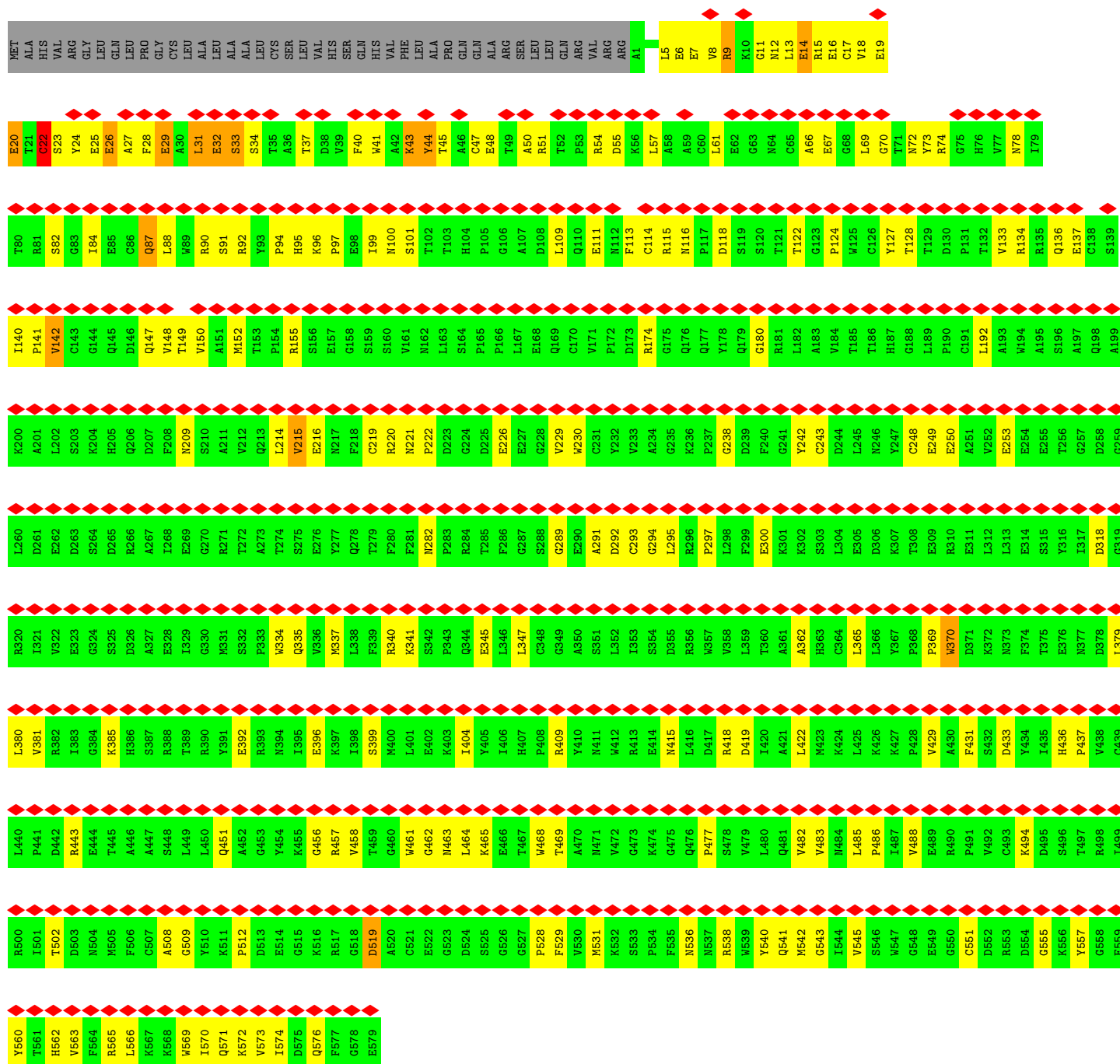
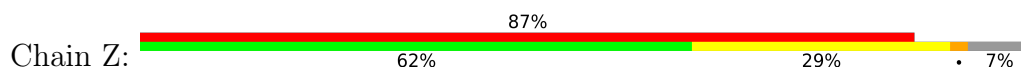
• Molecule 1: Hexon protein

Chain L: 75% 18%





• Molecule 2: Prothrombin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13045	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	81	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	130.944, 212.608, 115.456	wwPDB
Map dimensions	151, 82, 93	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.408, 1.408, 1.408	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CGU, 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	J	0.37	1/7592 (0.0%)	0.49	5/10326 (0.0%)
1	K	0.32	0/7619	0.46	3/10365 (0.0%)
1	L	0.32	2/7590 (0.0%)	0.47	3/10325 (0.0%)
2	Z	0.18	0/4597	0.46	1/6220 (0.0%)
All	All	0.32	3/27398 (0.0%)	0.47	12/37236 (0.0%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	278	SER	CA-C	-5.31	1.46	1.52
1	L	424	PRO	CA-C	-5.27	1.46	1.52
1	L	432	ASP	CA-C	-5.14	1.50	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	280	ASN	N-CA-C	-10.72	98.25	111.11
1	K	489	ALA	CA-C-N	-7.74	108.37	122.38
1	K	489	ALA	C-N-CA	-7.74	108.37	122.38
1	J	850	GLY	N-CA-C	7.11	121.63	112.68
2	Z	22	CYS	N-CA-C	6.87	120.80	110.14
1	J	281	ALA	N-CA-C	-6.49	96.97	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	425	LEU	N-CA-C	6.33	118.74	111.02
1	J	278	SER	N-CA-C	-5.63	104.83	110.97
1	L	432	ASP	N-CA-C	5.54	114.07	108.75
1	L	423	PHE	N-CA-C	5.42	116.82	110.31
1	L	432	ASP	CB-CA-C	-5.33	108.69	116.53
1	J	421	TYR	N-CA-C	5.14	118.13	109.95

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	905	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	7400	0	7100	175	0
1	K	7426	0	7126	155	0
1	L	7397	0	7100	142	0
2	Z	4615	0	4345	143	0
3	Z	7	0	0	0	0
All	All	26845	0	25671	548	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 (548) 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:L:277:THR:OG1	1:L:279:THR:HG22	1.43	1.17
1:K:279:THR:HG21	2:Z:25:CGU:HA	1.33	1.07
1:L:277:THR:HG1	1:L:279:THR:HG22	1.22	0.96
2:Z:31:LEU:HD13	2:Z:37:THR:HA	1.48	0.94
1:K:279:THR:HG23	2:Z:28:PHE:CB	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:277:THR:HG21	1:K:280:ASN:HB2	1.53	0.89
1:K:287:ASN:HB2	1:K:289:GLN:HE21	1.37	0.88
1:K:277:THR:CG2	1:K:280:ASN:HB2	2.04	0.86
1:K:279:THR:CG2	2:Z:28:PHE:HB2	2.12	0.79
1:J:836:ASN:HD21	1:K:124:LEU:H	1.31	0.78
1:K:279:THR:HG23	2:Z:28:PHE:CG	2.19	0.77
1:J:239:MET:HG3	1:J:318:ASN:HD22	1.50	0.75
2:Z:66:ALA:HB1	2:Z:70:GLY:HA2	1.69	0.74
1:L:348:ASN:ND2	1:L:372:ARG:O	2.21	0.73
1:J:407:ARG:HH21	1:J:545:PRO:HG3	1.53	0.73
2:Z:43:LYS:HG2	2:Z:61:LEU:HD23	1.71	0.72
1:J:251:ASN:ND2	1:J:253:ASN:OD1	2.21	0.72
1:K:279:THR:CG2	2:Z:28:PHE:CB	2.68	0.71
1:J:439:THR:HG22	1:J:447:GLY:HA2	1.72	0.71
1:L:601:ASN:ND2	1:L:712:TYR:O	2.23	0.71
1:K:114:LYS:NZ	1:K:116:TYR:O	2.24	0.70
1:K:287:ASN:HB2	1:K:289:GLN:NE2	2.05	0.70
1:J:72:ASP:HB3	1:J:83:ARG:HB3	1.72	0.70
1:K:651:ASP:OD2	1:K:938:ARG:NH1	2.25	0.69
1:K:217:GLU:HB3	1:L:467:ASN:HD21	1.57	0.69
1:J:348:ASN:HD21	1:J:374:THR:H	1.40	0.69
1:K:211:PRO:HG3	1:K:295:TYR:CD2	2.28	0.69
1:K:747:ARG:HB3	1:L:64:LEU:HD12	1.75	0.69
1:J:507:ASP:OD1	1:J:507:ASP:N	2.26	0.69
1:J:114:LYS:NZ	1:J:116:TYR:O	2.26	0.68
1:L:646:ARG:NH1	1:L:943:HIS:O	2.26	0.68
1:J:281:ALA:C	1:J:283:ASN:H	2.01	0.68
1:K:279:THR:CG2	2:Z:25:CGU:HA	2.17	0.68
1:J:63:ARG:NE	1:L:746:ASP:OD2	2.27	0.68
2:Z:543:GLY:HA2	2:Z:563:VAL:HG22	1.76	0.68
1:J:251:ASN:OD1	1:J:255:GLY:N	2.21	0.67
1:K:726:ASN:ND2	1:K:880:THR:O	2.24	0.67
1:J:261:GLU:HB2	1:J:265:LYS:HG2	1.74	0.67
1:J:435:GLN:N	1:L:278:SER:HB2	2.09	0.67
2:Z:292:ASP:O	2:Z:436:HIS:NE2	2.27	0.67
1:J:651:ASP:OD2	1:J:938:ARG:NH1	2.27	0.67
1:K:279:THR:HG21	2:Z:28:PHE:HB2	1.75	0.66
1:L:499:ASN:OD1	1:L:518:ARG:NH1	2.28	0.66
1:J:726:ASN:ND2	1:J:880:THR:O	2.24	0.66
2:Z:48:GLU:OE1	2:Z:51:ARG:NH2	2.29	0.66
1:L:371:ASP:O	1:L:662:ASN:ND2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:277:THR:HG21	1:K:280:ASN:CB	2.26	0.65
1:J:601:ASN:ND2	1:J:712:TYR:O	2.29	0.65
1:J:834:HIS:O	1:J:834:HIS:ND1	2.30	0.65
1:L:758:ARG:NH1	1:L:761:ASP:OD2	2.30	0.65
1:K:534:ARG:HB2	1:L:559:MET:HE2	1.79	0.65
1:K:767:VAL:HG12	1:L:572:GLN:HE21	1.62	0.65
1:K:766:ASN:N	1:K:766:ASN:OD1	2.28	0.64
2:Z:69:LEU:O	2:Z:116:ASN:ND2	2.26	0.64
1:J:770:CYS:SG	1:J:771:ASN:N	2.70	0.64
1:L:907:ASN:OD1	1:L:907:ASN:N	2.29	0.64
1:L:452:GLN:NE2	1:L:454:ASP:OD2	2.30	0.64
2:Z:243:CYS:O	2:Z:409:ARG:NH2	2.28	0.63
1:J:131:ASN:HD22	1:L:854:PRO:HD3	1.63	0.63
1:L:541:ASP:OD2	1:L:874:LYS:NZ	2.27	0.63
1:K:287:ASN:HB3	1:L:448:ASN:O	1.98	0.63
1:L:775:ASP:N	1:L:775:ASP:OD1	2.31	0.63
2:Z:221:ASN:HB2	2:Z:229:VAL:HA	1.79	0.63
1:J:650:ASN:OD1	1:J:650:ASN:N	2.31	0.62
1:K:412:HIS:CE1	1:L:555:ARG:HD3	2.34	0.62
1:J:547:ASN:O	1:J:547:ASN:ND2	2.32	0.62
1:J:878:ASP:N	1:J:878:ASP:OD1	2.32	0.62
1:J:954:THR:HB	1:J:955:PRO:HD3	1.81	0.62
2:Z:291:ALA:O	2:Z:538:ARG:NH2	2.32	0.62
1:L:4:PRO:HA	1:L:7:MET:HB2	1.81	0.62
1:J:420:ASN:OD1	1:K:478:ASN:ND2	2.33	0.62
1:J:642:GLU:OE2	1:J:646:ARG:NE	2.31	0.62
1:K:272:MET:HG2	1:K:295:TYR:CD1	2.34	0.62
1:L:355:VAL:HB	1:L:593:GLU:HG2	1.81	0.61
2:Z:519:ASP:N	2:Z:519:ASP:OD1	2.33	0.61
1:L:878:ASP:N	1:L:878:ASP:OD1	2.33	0.61
2:Z:96:LYS:O	2:Z:134:ARG:NH2	2.33	0.61
1:L:114:LYS:NZ	1:L:116:TYR:O	2.34	0.60
1:K:420:ASN:ND2	1:K:475:LEU:HD12	2.15	0.60
1:L:442:ALA:HA	1:L:446:GLN:HB2	1.83	0.60
1:J:192:ALA:HB3	1:J:200:GLY:HA2	1.82	0.60
1:K:47:ASN:O	1:K:47:ASN:ND2	2.35	0.60
1:L:902:ASN:O	1:L:906:ALA:N	2.33	0.60
2:Z:78:ASN:HB3	2:Z:113:PHE:HD1	1.65	0.60
1:J:423:PHE:HB3	1:J:424:PRO:HD2	1.82	0.60
1:J:546:PHE:O	1:J:551:ASN:ND2	2.33	0.60
1:J:262:GLN:NE2	1:J:267:GLU:OE1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:262:GLN:O	1:J:263:ASN:ND2	2.35	0.60
1:K:58:THR:OG1	1:K:59:ASP:N	2.32	0.60
1:J:731:LYS:HG2	1:J:917:GLU:HB3	1.84	0.60
1:K:770:CYS:SG	1:K:771:ASN:N	2.74	0.60
1:J:348:ASN:HD21	1:J:374:THR:N	2.00	0.60
1:J:902:ASN:O	1:J:906:ALA:N	2.35	0.59
2:Z:90:ARG:NH2	2:Z:111:GLU:OE1	2.35	0.59
1:K:775:ASP:OD1	1:K:775:ASP:N	2.31	0.59
1:L:745:ASN:OD1	1:L:745:ASN:N	2.35	0.59
2:Z:97:PRO:HB2	2:Z:100:ASN:HB3	1.85	0.59
1:K:121:TYR:HB2	1:K:244:GLY:HA2	1.84	0.59
1:L:731:LYS:HG2	1:L:917:GLU:HB3	1.83	0.59
2:Z:174:ARG:NE	2:Z:226:GLU:O	2.35	0.59
1:J:557:ARG:NH2	1:J:605:GLN:OE1	2.36	0.59
1:K:411:ASN:ND2	1:K:529:ILE:O	2.34	0.59
1:L:281:ALA:O	1:L:282:THR:C	2.46	0.59
1:K:745:ASN:OD1	1:K:745:ASN:N	2.36	0.59
1:K:262:GLN:O	1:K:263:ASN:ND2	2.36	0.58
2:Z:54:ARG:NH1	2:Z:55:ASP:OD1	2.35	0.58
1:K:411:ASN:HB3	1:K:531:LEU:HD23	1.85	0.58
2:Z:219:CYS:O	2:Z:220:ARG:NH1	2.35	0.58
1:K:284:GLU:CD	1:K:284:GLU:H	2.12	0.58
1:K:442:ALA:HA	1:K:446:GLN:HB2	1.86	0.58
2:Z:17:CYS:HA	2:Z:22:CYS:HB3	1.85	0.58
1:J:287:ASN:HD22	1:K:449:THR:HA	1.68	0.58
2:Z:282:ASN:H	2:Z:571:GLN:HE22	1.51	0.58
1:L:933:VAL:HB	1:L:955:PRO:HD2	1.85	0.58
2:Z:31:LEU:O	2:Z:33:SER:N	2.36	0.58
1:K:662:ASN:OD1	1:K:662:ASN:N	2.37	0.58
1:J:348:ASN:ND2	1:J:374:THR:H	2.01	0.58
1:K:424:PRO:HD3	1:K:469:PHE:O	2.03	0.58
2:Z:73:TYR:O	2:Z:74:ARG:NH1	2.33	0.58
2:Z:293:CYS:O	2:Z:538:ARG:NH1	2.37	0.58
1:K:416:ASP:N	1:K:416:ASP:OD1	2.37	0.57
2:Z:32:CGU:O	2:Z:34:SER:N	2.37	0.57
1:J:75:ASP:OD1	1:J:76:THR:N	2.38	0.57
1:J:467:ASN:OD1	1:J:467:ASN:N	2.37	0.57
2:Z:464:LEU:HD12	2:Z:468:TRP:HD1	1.68	0.57
1:J:526:ASP:OD1	1:J:527:CYS:N	2.31	0.57
1:K:217:GLU:HG2	1:K:222:GLU:HB3	1.85	0.57
1:K:878:ASP:OD1	1:K:878:ASP:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:97:PRO:O	2:Z:100:ASN:ND2	2.37	0.57
1:K:501:THR:OG1	1:K:502:ASN:OD1	2.18	0.57
1:J:682:ASN:OD1	1:J:683:TRP:N	2.37	0.57
1:J:755:GLU:O	1:J:773:THR:OG1	2.23	0.57
2:Z:137:GLU:HG3	2:Z:150:VAL:HG21	1.87	0.57
1:K:499:ASN:OD1	1:K:518:ARG:NH1	2.37	0.57
1:K:847:MET:HE1	1:L:220:TRP:HB3	1.85	0.57
2:Z:70:GLY:HA3	2:Z:124:PRO:HG3	1.87	0.57
1:J:599:ASP:OD2	1:J:613:ARG:NH2	2.38	0.57
2:Z:214:LEU:HD21	2:Z:222:PRO:HG3	1.86	0.57
1:J:194:ALA:HB1	1:J:197:ALA:HA	1.86	0.57
1:J:692:THR:HG22	1:J:693:ARG:H	1.69	0.56
1:K:278:SER:C	1:K:282:THR:HG23	2.30	0.56
1:K:423:PHE:CZ	1:L:839:PHE:HB3	2.40	0.56
1:J:237:THR:OG1	1:J:298:ASP:OD1	2.23	0.56
1:J:387:ASP:OD1	1:J:388:ARG:N	2.39	0.56
1:K:287:ASN:O	1:K:288:ILE:C	2.48	0.56
1:L:954:THR:HB	1:L:955:PRO:HD3	1.88	0.56
1:L:137:GLN:OE1	1:L:170:HIS:NE2	2.38	0.56
1:J:279:THR:O	1:J:280:ASN:C	2.49	0.56
1:K:746:ASP:OD1	1:K:746:ASP:N	2.37	0.56
1:J:903:LEU:HD22	1:J:907:ASN:HB2	1.88	0.56
1:J:201:LYS:H	1:J:201:LYS:HD3	1.71	0.56
1:K:826:GLN:NE2	1:L:250:THR:O	2.37	0.56
2:Z:250:GLU:O	2:Z:565:ARG:NH2	2.39	0.55
1:J:281:ALA:C	1:J:283:ASN:N	2.62	0.55
1:L:440:THR:HG21	1:L:449:THR:HG22	1.87	0.55
2:Z:536:ASN:ND2	2:Z:540:TYR:OH	2.39	0.55
1:J:412:HIS:CE1	1:K:555:ARG:HH21	2.24	0.55
1:J:497:LYS:O	1:J:518:ARG:NH1	2.38	0.55
1:L:364:ASN:ND2	1:L:366:VAL:H	2.04	0.55
1:J:819:ASP:OD1	1:J:819:ASP:N	2.39	0.55
1:K:676:ILE:HG23	1:K:914:MET:HB2	1.87	0.55
2:Z:90:ARG:HH22	2:Z:111:GLU:HA	1.72	0.55
1:J:541:ASP:OD1	1:J:727:HIS:NE2	2.40	0.55
1:J:800:ASP:OD2	1:J:807:ARG:NH1	2.40	0.55
1:K:420:ASN:OD1	1:L:478:ASN:ND2	2.40	0.55
1:L:280:ASN:O	1:L:281:ALA:C	2.50	0.55
2:Z:87:GLN:N	2:Z:127:TYR:O	2.33	0.55
1:K:818:ASP:OD1	1:K:819:ASP:N	2.39	0.55
1:J:169:THR:HB	1:K:457:PHE:HD1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:94:PRO:HG2	2:Z:95:HIS:CD2	2.42	0.54
2:Z:114:CYS:O	2:Z:115:ARG:NH1	2.36	0.54
1:K:898:ASP:N	1:K:898:ASP:OD1	2.40	0.54
1:K:36:GLU:OE1	1:K:42:ASN:ND2	2.40	0.54
1:K:278:SER:O	1:K:279:THR:C	2.50	0.54
1:J:766:ASN:OD1	1:J:766:ASN:N	2.40	0.54
1:L:550:ARG:HA	1:L:555:ARG:HH11	1.71	0.54
2:Z:101:SER:HA	2:Z:109:LEU:HD12	1.90	0.54
1:J:439:THR:HA	1:J:450:THR:HG22	1.88	0.54
1:L:692:THR:HG22	1:L:693:ARG:H	1.73	0.54
1:J:851:GLN:HG2	1:K:176:PRO:HG3	1.89	0.54
1:J:922:ASP:OD1	1:J:922:ASP:N	2.37	0.54
1:J:288:ILE:HD13	1:J:288:ILE:H	1.72	0.54
1:J:440:THR:OG1	1:J:446:GLN:OE1	2.25	0.54
1:L:400:ASP:OD1	1:L:400:ASP:N	2.38	0.54
1:L:440:THR:HG22	1:L:451:TRP:CE2	2.43	0.54
1:L:767:VAL:HG13	1:L:774:LYS:HG2	1.90	0.54
1:K:272:MET:SD	1:K:295:TYR:HE1	2.31	0.53
2:Z:465:LYS:O	2:Z:469:THR:OG1	2.20	0.53
1:L:58:THR:OG1	1:L:59:ASP:N	2.41	0.53
1:L:750:THR:HG22	1:L:751:PRO:HD2	1.90	0.53
1:J:818:ASP:HB2	1:J:870:ILE:HG23	1.89	0.53
2:Z:335:GLN:HG2	2:Z:461:TRP:HZ3	1.73	0.53
2:Z:25:CGU:HG	2:Z:29:CGU:OE21	2.09	0.53
1:K:287:ASN:C	1:K:288:ILE:HG12	2.31	0.53
1:K:258:VAL:HG23	1:K:298:ASP:O	2.09	0.53
1:L:348:ASN:OD1	1:L:348:ASN:N	2.42	0.53
2:Z:229:VAL:HG23	2:Z:243:CYS:HB2	1.90	0.53
1:K:231:ARG:HE	1:K:297:GLU:CD	2.17	0.53
1:J:423:PHE:HB3	1:J:424:PRO:CD	2.38	0.53
1:J:649:THR:OG1	1:J:650:ASN:OD1	2.25	0.53
1:K:122:ASN:ND2	1:K:242:CYS:SG	2.73	0.53
2:Z:122:THR:HB	2:Z:137:GLU:HB3	1.91	0.53
1:J:138:ASN:OD1	1:J:138:ASN:N	2.41	0.52
1:J:348:ASN:ND2	1:J:372:ARG:O	2.42	0.52
1:K:272:MET:HG2	1:K:295:TYR:HD1	1.73	0.52
1:L:288:ILE:HD13	1:L:288:ILE:H	1.73	0.52
2:Z:47:CYS:HB3	2:Z:50:ALA:HB3	1.91	0.52
1:K:187:LEU:HB2	1:K:293:VAL:HG11	1.91	0.52
1:J:116:TYR:CG	1:L:531:LEU:HD13	2.44	0.52
1:K:400:ASP:OD1	1:K:400:ASP:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:730:LYS:NZ	1:K:919:ASP:OD1	2.42	0.52
2:Z:6:CGU:O	2:Z:9:ARG:HG3	2.10	0.52
2:Z:24:TYR:HA	2:Z:27:ALA:HB3	1.92	0.52
1:L:3:THR:O	1:L:7:MET:N	2.42	0.52
1:L:459:GLU:C	1:L:460:ARG:HG2	2.33	0.52
2:Z:226:GLU:HB2	2:Z:565:ARG:HB3	1.92	0.52
1:K:610:ASN:OD1	1:K:610:ASN:N	2.42	0.52
1:J:847:MET:HA	1:L:421:TYR:OH	2.10	0.52
2:Z:67:GLU:N	2:Z:72:ASN:OD1	2.35	0.52
1:J:58:THR:OG1	1:J:59:ASP:N	2.43	0.51
1:J:423:PHE:CE1	1:K:839:PHE:HD1	2.27	0.51
1:L:684:ALA:HB2	1:L:904:LEU:HG	1.92	0.51
1:J:473:ILE:HB	1:L:422:CYS:SG	2.50	0.51
1:J:514:TYR:OH	1:J:518:ARG:NH2	2.39	0.51
2:Z:34:SER:HA	2:Z:37:THR:HB	1.90	0.51
1:J:933:VAL:HB	1:J:955:PRO:HD2	1.92	0.51
2:Z:99:ILE:HD13	2:Z:118:ASP:HB3	1.91	0.51
1:L:424:PRO:HD3	1:L:469:PHE:O	2.11	0.51
2:Z:141:PRO:HA	2:Z:148:VAL:HA	1.93	0.51
2:Z:295:LEU:H	2:Z:436:HIS:HD2	1.58	0.51
1:J:531:LEU:HD11	1:K:120:ALA:HB2	1.93	0.51
1:J:676:ILE:HG23	1:J:914:MET:HB2	1.92	0.51
1:K:423:PHE:CE2	1:L:839:PHE:HB3	2.46	0.51
1:K:546:PHE:O	1:K:551:ASN:ND2	2.44	0.51
1:K:745:ASN:ND2	1:L:60:ARG:O	2.38	0.51
1:J:555:ARG:HH11	1:L:412:HIS:CE1	2.28	0.51
1:K:136:GLU:OE1	1:K:137:GLN:N	2.44	0.51
1:J:67:ARG:NH2	1:J:625:CYS:SG	2.85	0.50
1:J:131:ASN:OD1	1:J:131:ASN:N	2.43	0.50
1:K:808:ASN:OD1	1:K:808:ASN:N	2.44	0.50
1:J:121:TYR:HB2	1:J:244:GLY:HA2	1.93	0.50
1:K:692:THR:HG22	1:K:693:ARG:H	1.77	0.50
1:J:758:ARG:NH1	1:J:761:ASP:OD2	2.44	0.50
1:L:897:THR:OG1	1:L:898:ASP:N	2.44	0.50
2:Z:43:LYS:O	2:Z:44:TYR:C	2.55	0.50
2:Z:347:LEU:O	2:Z:463:ASN:ND2	2.43	0.50
1:J:611:ASP:OD1	1:J:612:LEU:N	2.45	0.50
2:Z:253:GLU:O	2:Z:451:GLN:NE2	2.41	0.50
1:K:526:ASP:OD1	1:K:527:CYS:N	2.39	0.50
1:J:407:ARG:HH12	1:J:876:LEU:HD11	1.77	0.50
1:L:504:GLU:OE1	1:L:505:ILE:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:757:LYS:HB2	1:J:771:ASN:HD22	1.76	0.49
1:J:297:GLU:OE2	1:L:853:TYR:OH	2.21	0.49
1:K:438:LYS:HE3	1:K:453:LYS:HG3	1.95	0.49
1:L:420:ASN:OD1	1:L:420:ASN:N	2.45	0.49
1:L:572:GLN:OE1	1:L:572:GLN:N	2.45	0.49
2:Z:41:TRP:O	2:Z:45:THR:HG23	2.12	0.49
2:Z:215:VAL:HG21	2:Z:220:ARG:HH21	1.77	0.49
1:J:939:VAL:HG22	1:J:949:THR:HG22	1.94	0.49
1:K:454:ASP:N	1:K:454:ASP:OD1	2.46	0.49
1:J:815:GLN:HE22	1:K:562:GLY:HA3	1.77	0.49
2:Z:88:LEU:HB2	2:Z:91:SER:HB3	1.94	0.49
2:Z:485:LEU:HB3	2:Z:509:GLY:HA2	1.94	0.49
2:Z:97:PRO:HB3	2:Z:127:TYR:CZ	2.46	0.49
1:L:686:PHE:HB3	1:L:886:PHE:HD2	1.78	0.49
1:K:211:PRO:HG3	1:K:295:TYR:CE2	2.47	0.49
2:Z:238:GLY:HA3	2:Z:576:GLN:HG2	1.95	0.49
1:K:594:TRP:CD1	1:K:595:ASN:H	2.31	0.49
1:J:501:THR:OG1	1:J:502:ASN:OD1	2.29	0.49
1:J:31:PHE:O	1:J:35:THR:OG1	2.31	0.48
1:K:421:TYR:HE1	1:K:472:GLU:OE2	1.95	0.48
2:Z:294:GLY:N	2:Z:437:PRO:O	2.39	0.48
1:J:368:ASP:OD1	1:J:369:LEU:N	2.46	0.48
1:J:139:GLU:N	1:J:139:GLU:OE1	2.44	0.48
2:Z:569:TRP:O	2:Z:572:LYS:HB2	2.13	0.48
1:J:536:SER:HB3	1:J:812:MET:HE1	1.95	0.48
1:L:531:LEU:HD23	1:L:531:LEU:HA	1.71	0.48
1:L:785:TYR:HB2	1:L:787:ILE:HG12	1.95	0.48
1:J:337:PHE:HD2	1:J:561:LEU:HD11	1.79	0.48
1:L:444:GLY:H	1:L:446:GLN:HG2	1.78	0.48
2:Z:486:PRO:O	2:Z:509:GLY:N	2.32	0.48
1:J:412:HIS:CE1	1:K:555:ARG:HD3	2.49	0.48
1:L:678:ILE:HB	1:L:912:LEU:HB3	1.95	0.48
1:J:815:GLN:OE1	1:K:564:GLY:N	2.46	0.48
1:K:251:ASN:OD1	1:K:255:GLY:N	2.38	0.48
1:L:387:ASP:OD1	1:L:388:ARG:N	2.45	0.48
2:Z:529:PHE:HD2	2:Z:542:MET:HB2	1.79	0.48
1:L:20:ALA:HA	1:L:23:TYR:CE2	2.48	0.47
1:J:889:ASN:OD1	1:J:889:ASN:N	2.47	0.47
1:J:438:LYS:HB2	1:J:453:LYS:HD2	1.97	0.47
1:J:531:LEU:HD13	1:K:116:TYR:CG	2.49	0.47
1:L:853:TYR:CG	1:L:854:PRO:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:124:PRO:HD2	2:Z:149:THR:HG21	1.97	0.47
1:J:369:LEU:O	1:J:371:ASP:N	2.42	0.47
1:K:130:PRO:HG3	1:K:323:LEU:HG	1.95	0.47
1:L:577:PHE:O	1:L:581:LYS:HB2	2.14	0.47
2:Z:180:GLY:O	2:Z:220:ARG:NH2	2.36	0.47
2:Z:362:ALA:N	2:Z:419:ASP:OD1	2.45	0.47
2:Z:512:PRO:HG2	2:Z:555:GLY:HA2	1.97	0.47
1:J:435:GLN:HE22	1:L:281:ALA:HB2	1.79	0.47
2:Z:40:PHE:HA	2:Z:43:LYS:HZ2	1.79	0.47
2:Z:341:LYS:HG2	2:Z:380:LEU:HD23	1.96	0.47
1:K:694:LEU:HD21	1:K:717:PRO:HB2	1.95	0.47
1:L:47:ASN:ND2	1:L:47:ASN:O	2.47	0.47
1:L:547:ASN:ND2	1:L:547:ASN:O	2.47	0.47
1:L:922:ASP:OD1	1:L:922:ASP:N	2.42	0.47
2:Z:12:ASN:O	2:Z:13:LEU:C	2.56	0.47
1:J:169:THR:HB	1:K:457:PHE:CD1	2.49	0.47
2:Z:541:GLN:NE2	2:Z:543:GLY:O	2.30	0.47
1:J:865:THR:O	1:J:865:THR:OG1	2.33	0.47
1:K:547:ASN:O	1:K:547:ASN:ND2	2.47	0.47
1:J:412:HIS:NE2	1:K:559:MET:SD	2.84	0.47
1:L:205:ALA:HB1	1:L:210:GLN:HB3	1.95	0.47
1:J:419:PRO:O	1:J:420:ASN:CG	2.58	0.46
1:K:484:LEU:HD23	1:K:488:ILE:HD13	1.97	0.46
1:L:423:PHE:HB3	1:L:424:PRO:HD2	1.97	0.46
2:Z:128:THR:OG1	2:Z:133:VAL:O	2.34	0.46
1:J:120:ALA:HB2	1:L:531:LEU:HD12	1.97	0.46
1:L:337:PHE:HD2	1:L:561:LEU:HD11	1.80	0.46
1:L:429:GLY:O	1:L:430:ILE:C	2.58	0.46
1:J:284:GLU:HG3	1:J:286:ASN:OD1	2.15	0.46
1:J:352:ASN:HB3	1:J:595:ASN:ND2	2.30	0.46
1:J:400:ASP:OD1	1:J:400:ASP:N	2.38	0.46
2:Z:140:ILE:O	2:Z:149:THR:N	2.49	0.46
1:J:834:HIS:HB3	1:K:214:GLN:HG2	1.98	0.46
1:K:168:LYS:NZ	1:L:454:ASP:O	2.37	0.46
1:K:347:TYR:HE2	1:K:576:LYS:HD2	1.78	0.46
1:K:481:ARG:NH1	1:K:840:VAL:HG21	2.31	0.46
2:Z:78:ASN:HB3	2:Z:113:PHE:CD1	2.48	0.46
2:Z:334:TRP:HD1	2:Z:528:PRO:HG3	1.81	0.46
1:J:262:GLN:HE21	1:J:262:GLN:HB3	1.61	0.46
1:L:819:ASP:OD1	1:L:820:THR:N	2.49	0.46
1:J:364:ASN:OD1	1:J:365:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:726:ASN:OD1	1:K:726:ASN:N	2.49	0.46
1:K:834:HIS:O	1:K:834:HIS:ND1	2.48	0.46
1:K:846:THR:OG1	1:K:847:MET:N	2.49	0.46
1:K:857:VAL:HB	1:K:858:PRO:HD3	1.98	0.46
1:L:305:ASP:O	1:L:330:ASN:ND2	2.49	0.46
1:J:278:SER:C	1:J:280:ASN:H	2.24	0.46
1:J:555:ARG:HH11	1:L:412:HIS:CD2	2.34	0.46
1:L:664:LEU:HD11	1:L:702:LEU:HD21	1.98	0.46
2:Z:25:CGU:O	2:Z:29:CGU:N	2.49	0.46
1:J:338:ARG:HG2	1:J:339:ASP:H	1.80	0.45
1:J:713:SER:O	1:J:713:SER:OG	2.28	0.45
1:K:288:ILE:O	1:K:289:GLN:C	2.59	0.45
1:L:20:ALA:H	1:L:47:ASN:HB3	1.81	0.45
1:L:66:LEU:HD23	1:L:66:LEU:HA	1.84	0.45
2:Z:95:HIS:NE2	2:Z:134:ARG:HA	2.31	0.45
2:Z:96:LYS:HD2	2:Z:370:TRP:CH2	2.51	0.45
1:J:498:TYR:OH	1:J:843:LEU:O	2.33	0.45
2:Z:95:HIS:CD2	2:Z:134:ARG:HA	2.51	0.45
1:K:934:PHE:CE1	1:L:15:ILE:HD11	2.52	0.45
1:L:686:PHE:HB3	1:L:886:PHE:CD2	2.52	0.45
2:Z:293:CYS:SG	2:Z:538:ARG:NH1	2.90	0.45
1:J:857:VAL:HB	1:J:858:PRO:HD3	1.99	0.45
1:L:502:ASN:OD1	1:L:502:ASN:N	2.49	0.45
1:J:347:TYR:CZ	1:J:576:LYS:HB2	2.52	0.45
1:K:599:ASP:OD2	1:K:613:ARG:NH2	2.49	0.45
1:K:954:THR:HB	1:K:955:PRO:HD3	1.97	0.45
1:L:375:GLU:HG3	1:L:719:LEU:HD22	1.99	0.45
2:Z:230:TRP:HB3	2:Z:242:TYR:CD2	2.52	0.45
1:J:347:TYR:O	1:J:349:SER:N	2.50	0.45
1:J:757:LYS:HB2	1:J:771:ASN:ND2	2.31	0.45
1:J:662:ASN:OD1	1:J:928:TYR:OH	2.21	0.45
1:K:530:ASN:OD1	1:K:814:ARG:NH2	2.48	0.45
1:J:636:ASN:OD1	1:J:636:ASN:N	2.48	0.45
1:J:668:PRO:HG2	1:J:671:ALA:HB2	1.98	0.45
2:Z:13:LEU:HD12	2:Z:13:LEU:HA	1.71	0.45
1:J:69:ILE:HD13	1:J:69:ILE:H	1.81	0.45
1:L:122:ASN:OD1	1:L:122:ASN:N	2.49	0.45
1:L:550:ARG:HA	1:L:555:ARG:NH1	2.31	0.45
2:Z:297:PRO:HD2	2:Z:433:ASP:HA	1.97	0.45
1:J:692:THR:HG23	1:J:726:ASN:OD1	2.17	0.44
1:K:256:GLN:HB3	1:K:299:VAL:CG1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:36:GLU:OE2	1:L:42:ASN:ND2	2.40	0.44
1:L:277:THR:C	1:L:279:THR:H	2.25	0.44
1:L:836:ASN:ND2	1:L:836:ASN:O	2.50	0.44
1:K:279:THR:HG23	2:Z:28:PHE:HB3	1.95	0.44
1:J:61:SER:HA	1:L:745:ASN:HB3	1.99	0.44
1:J:488:ILE:HG21	1:J:525:VAL:HG11	1.98	0.44
1:J:577:PHE:O	1:J:581:LYS:HB2	2.18	0.44
1:L:423:PHE:HB3	1:L:424:PRO:CD	2.47	0.44
2:Z:18:VAL:C	2:Z:20:CGU:H	2.25	0.44
1:J:438:LYS:HD3	1:J:453:LYS:HE3	2.00	0.44
1:L:488:ILE:HG21	1:L:525:VAL:HG11	2.00	0.44
1:K:575:GLN:OE1	1:K:576:LYS:N	2.50	0.44
1:L:808:ASN:OD1	1:L:808:ASN:N	2.50	0.44
2:Z:47:CYS:O	2:Z:50:ALA:N	2.50	0.44
1:J:60:ARG:HD3	1:J:635:HIS:CE1	2.52	0.44
1:K:412:HIS:CE1	1:L:555:ARG:HH21	2.36	0.44
2:Z:381:VAL:HG23	2:Z:399:SER:HB2	2.00	0.44
1:J:131:ASN:ND2	1:L:854:PRO:HD3	2.32	0.44
1:J:307:HIS:CE1	1:J:328:MET:HE2	2.53	0.44
1:J:853:TYR:O	1:J:854:PRO:C	2.55	0.44
1:J:47:ASN:O	1:J:47:ASN:ND2	2.50	0.44
1:K:279:THR:HG23	2:Z:28:PHE:CD2	2.52	0.44
1:L:388:ARG:HD2	1:L:388:ARG:HA	1.78	0.44
2:Z:34:SER:HA	2:Z:37:THR:CB	2.47	0.44
2:Z:289:GLY:HA3	2:Z:431:PHE:CZ	2.53	0.44
2:Z:458:VAL:HG13	2:Z:545:VAL:HG21	1.99	0.44
1:K:467:ASN:N	1:K:467:ASN:OD1	2.49	0.44
2:Z:365:LEU:HD13	2:Z:404:ILE:HD13	1.99	0.44
1:J:239:MET:HG3	1:J:318:ASN:ND2	2.26	0.43
1:J:868:ASP:OD1	1:J:868:ASP:N	2.50	0.43
2:Z:12:ASN:C	2:Z:14:CGU:N	2.69	0.43
1:J:423:PHE:O	1:K:471:MET:HE2	2.18	0.43
1:J:502:ASN:OD1	1:J:502:ASN:N	2.51	0.43
1:L:364:ASN:HD22	1:L:366:VAL:H	1.64	0.43
2:Z:47:CYS:C	2:Z:50:ALA:H	2.25	0.43
1:J:182:ILE:HG13	1:J:227:ALA:HB1	2.01	0.43
1:J:192:ALA:HB2	1:J:203:ILE:HD11	2.00	0.43
1:J:352:ASN:OD1	1:J:352:ASN:N	2.50	0.43
1:J:440:THR:HG22	1:J:451:TRP:NE1	2.33	0.43
1:K:726:ASN:HB3	1:K:882:TRP:NE1	2.33	0.43
1:L:749:LEU:HD13	1:L:749:LEU:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:853:TYR:CG	1:K:854:PRO:HD2	2.53	0.43
1:L:316:ASP:OD1	1:L:316:ASP:N	2.51	0.43
2:Z:456:GLY:HA2	2:Z:531:MET:HG2	1.98	0.43
2:Z:458:VAL:HB	2:Z:483:VAL:HG13	1.99	0.43
1:K:277:THR:HG23	1:K:281:ALA:N	2.34	0.43
1:L:251:ASN:OD1	1:L:252:SER:N	2.51	0.43
1:L:665:TYR:CE2	1:L:676:ILE:HG13	2.54	0.43
1:J:20:ALA:H	1:J:47:ASN:HB3	1.83	0.43
1:J:416:ASP:OD1	1:J:416:ASP:N	2.50	0.43
2:Z:23:SER:OG	2:Z:26:CGU:N	2.51	0.43
2:Z:137:GLU:HG3	2:Z:150:VAL:HG11	2.01	0.43
2:Z:340:ARG:NH1	2:Z:345:GLU:OE1	2.51	0.43
2:Z:545:VAL:HG22	2:Z:560:TYR:HE2	1.84	0.43
1:J:563:ASN:HB3	1:L:533:ALA:HB2	2.00	0.43
1:K:217:GLU:HB3	1:L:467:ASN:ND2	2.27	0.43
1:K:448:ASN:OD1	1:K:449:THR:N	2.52	0.43
1:L:766:ASN:OD1	1:L:766:ASN:N	2.49	0.43
2:Z:422:LEU:HD23	2:Z:573:VAL:HG11	2.01	0.43
2:Z:40:PHE:HA	2:Z:43:LYS:NZ	2.34	0.43
1:J:694:LEU:HD22	1:J:717:PRO:HB2	2.00	0.43
1:K:247:ALA:O	1:K:256:GLN:NE2	2.32	0.43
1:L:301:MET:HE2	1:L:301:MET:HB2	1.93	0.43
2:Z:142:VAL:HG23	2:Z:147:GLN:O	2.18	0.43
2:Z:72:ASN:O	2:Z:74:ARG:HG2	2.18	0.42
1:K:175:ALA:HB1	1:K:229:GLY:O	2.19	0.42
1:K:786:ASN:OD1	1:K:786:ASN:N	2.50	0.42
1:L:440:THR:HA	1:L:451:TRP:CZ3	2.53	0.42
1:L:824:ASP:N	1:L:824:ASP:OD1	2.50	0.42
1:L:868:ASP:N	1:L:868:ASP:OD1	2.51	0.42
2:Z:545:VAL:HG22	2:Z:560:TYR:CE2	2.54	0.42
1:J:301:MET:HE2	1:J:301:MET:HB2	1.93	0.42
1:J:434:PHE:C	1:L:278:SER:HB2	2.45	0.42
1:K:76:THR:HG22	1:K:77:ALA:H	1.83	0.42
1:L:842:TYR:N	1:L:849:GLU:OE2	2.52	0.42
2:Z:335:GLN:HG2	2:Z:461:TRP:CZ3	2.54	0.42
1:K:690:ALA:HA	1:K:882:TRP:O	2.20	0.42
1:L:263:ASN:O	1:L:263:ASN:ND2	2.52	0.42
1:L:554:LEU:HA	1:L:554:LEU:HD23	1.81	0.42
1:J:76:THR:HG22	1:J:77:ALA:H	1.84	0.42
1:J:410:GLU:HG2	1:J:534:ARG:HG3	2.01	0.42
1:J:847:MET:SD	1:J:848:ARG:NH2	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:18:VAL:HG13	2:Z:57:LEU:HD23	2.02	0.42
2:Z:209:ASN:HB2	2:Z:222:PRO:O	2.19	0.42
2:Z:238:GLY:O	2:Z:576:GLN:NE2	2.53	0.42
2:Z:415:ASN:HD21	2:Z:502:THR:HG23	1.84	0.42
1:K:722:THR:O	1:K:722:THR:OG1	2.31	0.42
1:K:834:HIS:HB3	1:L:214:GLN:NE2	2.33	0.42
2:Z:11:GLY:HA2	2:Z:15:ARG:NH2	2.34	0.42
2:Z:92:ARG:HG2	2:Z:96:LYS:HG3	2.01	0.42
2:Z:219:CYS:HB3	2:Z:229:VAL:HB	2.02	0.42
1:J:613:ARG:HH12	1:J:708:PRO:HA	1.84	0.42
1:J:769:GLN:O	1:J:873:LYS:HD3	2.20	0.42
1:K:287:ASN:O	1:K:289:GLN:N	2.53	0.42
1:L:692:THR:HG23	1:L:726:ASN:OD1	2.19	0.42
1:J:138:ASN:HB3	1:J:167:LYS:HZ3	1.85	0.42
1:J:378:TYR:HD1	1:J:378:TYR:O	2.02	0.42
1:J:468:ASN:OD1	1:J:468:ASN:N	2.52	0.42
1:L:834:HIS:O	1:L:834:HIS:ND1	2.53	0.42
2:Z:12:ASN:HB3	2:Z:15:ARG:H	1.84	0.42
1:J:321:VAL:HG13	1:K:219:GLN:HE22	1.85	0.42
1:J:347:TYR:OH	1:J:576:LYS:HG3	2.20	0.42
1:L:239:MET:HG3	1:L:318:ASN:HD22	1.83	0.42
1:L:440:THR:HG22	1:L:451:TRP:CD2	2.54	0.42
1:L:835:ASN:OD1	1:L:836:ASN:N	2.53	0.42
2:Z:82:SER:O	2:Z:155:ARG:N	2.47	0.42
2:Z:87:GLN:OE1	2:Z:94:PRO:HD2	2.20	0.42
2:Z:95:HIS:CE1	2:Z:369:PRO:HB3	2.54	0.42
1:J:248:ARG:NH1	1:L:824:ASP:OD2	2.53	0.41
1:K:765:TYR:O	1:K:774:LYS:HG3	2.19	0.41
1:L:416:ASP:OD1	1:L:416:ASP:N	2.51	0.41
1:J:229:GLY:HA2	1:J:293:VAL:O	2.20	0.41
1:K:262:GLN:HE21	1:K:262:GLN:HB3	1.59	0.41
1:L:626:LEU:HD12	1:L:627:TYR:H	1.84	0.41
2:Z:215:VAL:HG12	2:Z:216:GLU:H	1.84	0.41
2:Z:295:LEU:H	2:Z:436:HIS:CD2	2.38	0.41
2:Z:571:GLN:CD	2:Z:574:ILE:HD11	2.44	0.41
1:K:285:VAL:O	1:K:286:ASN:C	2.63	0.41
1:K:388:ARG:HD2	1:K:388:ARG:HA	1.83	0.41
1:K:502:ASN:OD1	1:K:502:ASN:N	2.50	0.41
1:L:370:GLN:HE22	1:L:703:GLY:HA3	1.85	0.41
2:Z:41:TRP:HA	2:Z:41:TRP:CE3	2.55	0.41
2:Z:457:ARG:HG3	2:Z:482:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:448:ASN:OD1	1:J:448:ASN:N	2.54	0.41
1:K:653:SER:OG	1:L:46:ARG:HG2	2.19	0.41
2:Z:409:ARG:HB3	2:Z:418:ARG:HD3	2.02	0.41
2:Z:508:ALA:HB3	2:Z:560:TYR:CE1	2.54	0.41
1:J:444:GLY:O	1:J:446:GLN:NE2	2.31	0.41
1:J:600:VAL:HG11	1:J:617:ALA:HB3	2.03	0.41
1:K:73:ARG:HH21	1:K:80:TYR:HE1	1.67	0.41
1:K:731:LYS:HG2	1:K:917:GLU:HB3	2.02	0.41
1:J:423:PHE:CD1	1:K:839:PHE:HD1	2.38	0.41
1:K:278:SER:O	1:K:281:ALA:N	2.54	0.41
1:K:952:LEU:HD22	1:L:13:MET:HE3	2.02	0.41
1:J:287:ASN:OD1	1:J:287:ASN:N	2.54	0.41
1:J:349:SER:C	1:J:351:GLY:N	2.79	0.41
1:J:452:GLN:HE21	1:J:452:GLN:HB3	1.55	0.41
1:K:440:THR:HG22	1:K:451:TRP:CE2	2.56	0.41
2:Z:31:LEU:CD1	2:Z:37:THR:HA	2.35	0.41
2:Z:220:ARG:HA	2:Z:220:ARG:HD3	1.91	0.41
2:Z:469:THR:HG23	2:Z:551:CYS:HB3	2.03	0.41
1:K:94:LEU:HB2	1:K:630:PHE:CE1	2.56	0.41
1:K:422:CYS:SG	1:K:471:MET:HB2	2.61	0.41
2:Z:249:GLU:OE1	2:Z:494:LYS:NZ	2.46	0.41
1:J:540:MET:HE2	1:J:540:MET:HB3	1.98	0.41
1:J:782:LEU:HD23	1:J:782:LEU:HA	1.93	0.41
1:K:272:MET:SD	1:K:295:TYR:CE1	3.13	0.41
1:K:940:HIS:CE1	1:K:942:PRO:HD3	2.56	0.41
2:Z:250:GLU:OE2	2:Z:443:ARG:NH2	2.54	0.41
1:K:490:LEU:HD23	1:K:490:LEU:HA	1.81	0.41
1:K:685:ALA:HB2	1:L:10:TRP:CZ2	2.56	0.41
2:Z:116:ASN:HB2	2:Z:124:PRO:HA	2.03	0.41
1:J:57:THR:HG21	1:L:888:SER:HB3	2.02	0.40
1:K:84:PHE:HE2	1:K:101:PHE:HE1	1.69	0.40
1:L:91:ASN:OD1	1:L:91:ASN:N	2.53	0.40
2:Z:45:THR:O	2:Z:48:GLU:HB2	2.20	0.40
1:J:407:ARG:HH11	1:J:876:LEU:HD21	1.87	0.40
1:K:91:ASN:N	1:K:91:ASN:OD1	2.54	0.40
1:K:907:ASN:OD1	1:K:907:ASN:N	2.55	0.40
1:L:366:VAL:HG13	1:L:577:PHE:CE2	2.57	0.40
1:L:425:LEU:O	1:L:425:LEU:HD23	2.21	0.40
2:Z:566:LEU:O	2:Z:570:ILE:HG13	2.21	0.40
1:K:444:GLY:H	1:K:446:GLN:HG2	1.86	0.40
1:L:112:THR:O	1:L:112:THR:OG1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:834:HIS:O	1:L:834:HIS:CG	2.74	0.40
2:Z:84:ILE:HD12	2:Z:136:GLN:HE22	1.85	0.40
2:Z:392:GLU:O	2:Z:396:GLU:HG2	2.20	0.40
1:J:856:ASN:HB2	1:K:249:PRO:HG3	2.03	0.40
1:J:953:ARG:HB3	1:J:956:PHE:O	2.21	0.40
2:Z:385:LYS:HE3	2:Z:385:LYS:HB3	1.93	0.40
2:Z:462:GLY:HA3	2:Z:477:PRO:HD2	2.04	0.40
1:J:448:ASN:ND2	1:L:289:GLN:OE1	2.55	0.40
1:K:531:LEU:HD13	1:L:116:TYR:CG	2.56	0.40
1:K:680:SER:HA	1:K:910:HIS:O	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	J	927/963 (96%)	821 (89%)	97 (10%)	9 (1%)	12	43
1	K	931/963 (97%)	837 (90%)	89 (10%)	5 (0%)	24	56
1	L	926/963 (96%)	822 (89%)	102 (11%)	2 (0%)	43	72
2	Z	567/622 (91%)	532 (94%)	34 (6%)	1 (0%)	43	72
All	All	3351/3511 (95%)	3012 (90%)	322 (10%)	17 (0%)	26	56

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	281	ALA
1	J	420	ASN
1	K	419	PRO
1	K	420	ASN
1	L	281	ALA

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Mol	Chain	Res	Type
2	Z	33	SER
1	J	279	THR
1	J	348	ASN
1	J	347	TYR
1	J	370	GLN
1	J	419	PRO
1	K	278	SER
1	L	282	THR
1	K	234	LYS
1	J	351	GLY
1	K	288	ILE
1	J	857	VAL

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	J	800/826 (97%)	721 (90%)	79 (10%)	7	30
1	K	803/826 (97%)	734 (91%)	69 (9%)	10	34
1	L	801/826 (97%)	723 (90%)	78 (10%)	8	31
2	Z	486/521 (93%)	463 (95%)	23 (5%)	23	48
All	All	2890/2999 (96%)	2641 (91%)	249 (9%)	12	34

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	19	ASP
1	J	35	THR
1	J	37	THR
1	J	41	LEU
1	J	49	THR
1	J	54	HIS
1	J	55	ASP
1	J	64	LEU
1	J	69	ILE

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Mol	Chain	Res	Type
1	J	76	THR
1	J	124	LEU
1	J	131	ASN
1	J	138	ASN
1	J	183	THR
1	J	201	LYS
1	J	214	GLN
1	J	261	GLU
1	J	266	LEU
1	J	278	SER
1	J	284	GLU
1	J	285	VAL
1	J	286	ASN
1	J	288	ILE
1	J	316	ASP
1	J	328	MET
1	J	344	LEU
1	J	349	SER
1	J	350	THR
1	J	352	ASN
1	J	369	LEU
1	J	370	GLN
1	J	372	ARG
1	J	422	CYS
1	J	431	THR
1	J	448	ASN
1	J	451	TRP
1	J	452	GLN
1	J	463	ILE
1	J	467	ASN
1	J	501	THR
1	J	502	ASN
1	J	503	VAL
1	J	505	ILE
1	J	507	ASP
1	J	525	VAL
1	J	554	LEU
1	J	559	MET
1	J	608	LEU
1	J	624	ILE
1	J	648	ASP
1	J	649	THR

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Mol	Chain	Res	Type
1	J	650	ASN
1	J	664	LEU
1	J	676	ILE
1	J	730	LYS
1	J	745	ASN
1	J	758	ARG
1	J	761	ASP
1	J	766	ASN
1	J	767	VAL
1	J	770	CYS
1	J	773	THR
1	J	800	ASP
1	J	819	ASP
1	J	823	LYS
1	J	848	ARG
1	J	851	GLN
1	J	862	ILE
1	J	865	THR
1	J	877	CYS
1	J	878	ASP
1	J	879	ARG
1	J	883	ARG
1	J	899	LEU
1	J	904	LEU
1	J	907	ASN
1	J	919	ASP
1	J	940	HIS
1	J	953	ARG
1	K	7	MET
1	K	37	THR
1	K	41	LEU
1	K	54	HIS
1	K	58	THR
1	K	76	THR
1	K	84	PHE
1	K	90	ASP
1	K	93	VAL
1	K	132	SER
1	K	139	GLU
1	K	195	THR
1	K	262	GLN
1	K	284	GLU

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Mol	Chain	Res	Type
1	K	285	VAL
1	K	287	ASN
1	K	288	ILE
1	K	299	VAL
1	K	300	ASN
1	K	318	ASN
1	K	339	ASP
1	K	344	LEU
1	K	348	ASN
1	K	352	ASN
1	K	362	GLN
1	K	382	LEU
1	K	383	ASP
1	K	389	THR
1	K	414	THR
1	K	428	ILE
1	K	430	ILE
1	K	433	THR
1	K	437	VAL
1	K	449	THR
1	K	454	ASP
1	K	463	ILE
1	K	467	ASN
1	K	484	LEU
1	K	502	ASN
1	K	503	VAL
1	K	505	ILE
1	K	525	VAL
1	K	540	MET
1	K	554	LEU
1	K	559	MET
1	K	561	LEU
1	K	563	ASN
1	K	593	GLU
1	K	608	LEU
1	K	610	ASN
1	K	662	ASN
1	K	663	MET
1	K	676	ILE
1	K	692	THR
1	K	726	ASN
1	K	730	LYS

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Mol	Chain	Res	Type
1	K	745	ASN
1	K	746	ASP
1	K	766	ASN
1	K	767	VAL
1	K	775	ASP
1	K	786	ASN
1	K	808	ASN
1	K	812	MET
1	K	848	ARG
1	K	856	ASN
1	K	876	LEU
1	K	930	LEU
1	K	947	ILE
1	L	3	THR
1	L	7	MET
1	L	15	ILE
1	L	19	ASP
1	L	37	THR
1	L	62	GLN
1	L	91	ASN
1	L	109	ARG
1	L	122	ASN
1	L	131	ASN
1	L	139	GLU
1	L	168	LYS
1	L	245	SER
1	L	253	ASN
1	L	256	GLN
1	L	266	LEU
1	L	272	MET
1	L	276	SER
1	L	277	THR
1	L	282	THR
1	L	284	GLU
1	L	285	VAL
1	L	288	ILE
1	L	293	VAL
1	L	302	GLU
1	L	316	ASP
1	L	340	ASN
1	L	346	TYR
1	L	348	ASN

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Mol	Chain	Res	Type
1	L	382	LEU
1	L	383	ASP
1	L	395	TRP
1	L	414	THR
1	L	430	ILE
1	L	431	THR
1	L	435	GLN
1	L	449	THR
1	L	454	ASP
1	L	459	GLU
1	L	460	ARG
1	L	473	ILE
1	L	484	LEU
1	L	502	ASN
1	L	503	VAL
1	L	513	ASP
1	L	525	VAL
1	L	531	LEU
1	L	569	PHE
1	L	576	LYS
1	L	601	ASN
1	L	619	ILE
1	L	624	ILE
1	L	648	ASP
1	L	662	ASN
1	L	663	MET
1	L	664	LEU
1	L	676	ILE
1	L	692	THR
1	L	702	LEU
1	L	722	THR
1	L	745	ASN
1	L	749	LEU
1	L	750	THR
1	L	766	ASN
1	L	767	VAL
1	L	775	ASP
1	L	824	ASP
1	L	848	ARG
1	L	862	ILE
1	L	887	SER
1	L	897	THR

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Mol	Chain	Res	Type
1	L	899	LEU
1	L	903	LEU
1	L	904	LEU
1	L	907	ASN
1	L	918	VAL
1	L	930	LEU
1	L	936	VAL
2	Z	5	LEU
2	Z	8	VAL
2	Z	9	ARG
2	Z	22	CYS
2	Z	31	LEU
2	Z	43	LYS
2	Z	44	TYR
2	Z	87	GLN
2	Z	142	VAL
2	Z	152	MET
2	Z	192	LEU
2	Z	215	VAL
2	Z	248	CYS
2	Z	300	GLU
2	Z	318	ASP
2	Z	337	MET
2	Z	370	TRP
2	Z	379	LEU
2	Z	429	VAL
2	Z	488	VAL
2	Z	519	ASP
2	Z	557	TYR
2	Z	562	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	47	ASN
1	J	91	ASN
1	J	137	GLN
1	J	262	GLN
1	J	263	ASN
1	J	280	ASN
1	J	318	ASN
1	J	348	ASN

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Mol	Chain	Res	Type
1	J	601	ASN
1	J	635	HIS
1	J	745	ASN
1	J	771	ASN
1	J	960	ASN
1	K	214	GLN
1	K	262	GLN
1	K	263	ASN
1	K	289	GLN
1	K	326	GLN
1	K	348	ASN
1	K	476	ASN
1	K	635	HIS
1	K	670	ASN
1	L	47	ASN
1	L	219	GLN
1	L	435	GLN
1	L	452	GLN
1	L	467	ASN
1	L	478	ASN
1	L	551	ASN
1	L	670	ASN
1	L	673	ASN
1	L	901	GLN
2	Z	95	HIS
2	Z	147	GLN
2	Z	562	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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	$\# Z > 2$
2	CGU	Z	6	2,3	9,11,12	1.30	0	10,14,16	0.81	0
2	CGU	Z	26	2,3	9,11,12	1.41	0	10,14,16	1.03	1 (10%)
2	CGU	Z	19	2,3	9,11,12	1.49	1 (11%)	10,14,16	0.87	0
2	CGU	Z	20	2,3	9,11,12	1.50	1 (11%)	10,14,16	0.93	0
2	CGU	Z	25	2,3	9,11,12	1.44	0	10,14,16	0.78	0
2	CGU	Z	14	2,3	9,11,12	1.50	1 (11%)	10,14,16	0.84	0
2	CGU	Z	7	2,3	9,11,12	1.52	1 (11%)	10,14,16	0.80	0
2	CGU	Z	29	2,3	9,11,12	1.50	1 (11%)	10,14,16	0.85	0
2	CGU	Z	32	2	9,11,12	1.68	1 (11%)	10,14,16	0.81	0
2	CGU	Z	16	2,3	9,11,12	1.51	2 (22%)	10,14,16	0.84	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
2	CGU	Z	6	2,3	-	5/13/14/16	-
2	CGU	Z	26	2,3	-	2/13/14/16	-
2	CGU	Z	19	2,3	-	5/13/14/16	-
2	CGU	Z	20	2,3	-	6/13/14/16	-
2	CGU	Z	25	2,3	-	3/13/14/16	-
2	CGU	Z	14	2,3	-	6/13/14/16	-
2	CGU	Z	7	2,3	-	6/13/14/16	-
2	CGU	Z	29	2,3	-	7/13/14/16	-
2	CGU	Z	32	2	-	6/13/14/16	-
2	CGU	Z	16	2,3	-	2/13/14/16	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	32	CGU	CG-CD2	3.09	1.56	1.52
2	Z	7	CGU	CG-CD1	2.44	1.55	1.52
2	Z	19	CGU	CG-CD2	2.41	1.55	1.52
2	Z	20	CGU	CG-CD2	2.37	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	29	CGU	CG-CD1	2.18	1.54	1.52
2	Z	16	CGU	CG-CD2	2.11	1.54	1.52
2	Z	14	CGU	CG-CD1	2.09	1.54	1.52
2	Z	16	CGU	CG-CD1	2.00	1.54	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	26	CGU	CB-CG-CD2	-2.50	108.03	113.11

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Z	6	CGU	O-C-CA-CB
2	Z	6	CGU	CA-CB-CG-CD1
2	Z	6	CGU	CA-CB-CG-CD2
2	Z	7	CGU	N-CA-CB-CG
2	Z	7	CGU	C-CA-CB-CG
2	Z	7	CGU	CA-CB-CG-CD1
2	Z	7	CGU	CA-CB-CG-CD2
2	Z	14	CGU	C-CA-CB-CG
2	Z	14	CGU	CA-CB-CG-CD1
2	Z	14	CGU	CA-CB-CG-CD2
2	Z	16	CGU	N-CA-CB-CG
2	Z	16	CGU	C-CA-CB-CG
2	Z	19	CGU	O-C-CA-CB
2	Z	20	CGU	O-C-CA-CB
2	Z	20	CGU	C-CA-CB-CG
2	Z	20	CGU	OE22-CD2-CG-CB
2	Z	25	CGU	C-CA-CB-CG
2	Z	25	CGU	CA-CB-CG-CD1
2	Z	25	CGU	CA-CB-CG-CD2
2	Z	26	CGU	OE21-CD2-CG-CD1
2	Z	26	CGU	OE22-CD2-CG-CD1
2	Z	29	CGU	N-CA-CB-CG
2	Z	29	CGU	C-CA-CB-CG
2	Z	29	CGU	CA-CB-CG-CD1
2	Z	29	CGU	CA-CB-CG-CD2
2	Z	32	CGU	N-CA-CB-CG
2	Z	32	CGU	C-CA-CB-CG
2	Z	20	CGU	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	Z	6	CGU	OE21-CD2-CG-CB
2	Z	6	CGU	OE22-CD2-CG-CB
2	Z	7	CGU	OE11-CD1-CG-CB
2	Z	7	CGU	OE12-CD1-CG-CB
2	Z	19	CGU	OE21-CD2-CG-CB
2	Z	19	CGU	OE22-CD2-CG-CB
2	Z	20	CGU	OE21-CD2-CG-CB
2	Z	29	CGU	OE11-CD1-CG-CB
2	Z	14	CGU	OE11-CD1-CG-CD2
2	Z	19	CGU	OE21-CD2-CG-CD1
2	Z	19	CGU	OE22-CD2-CG-CD1
2	Z	20	CGU	OE11-CD1-CG-CD2
2	Z	29	CGU	OE11-CD1-CG-CD2
2	Z	14	CGU	N-CA-CB-CG
2	Z	14	CGU	OE11-CD1-CG-CB
2	Z	29	CGU	OE12-CD1-CG-CB
2	Z	32	CGU	OE21-CD2-CG-CB
2	Z	32	CGU	OE22-CD2-CG-CB
2	Z	32	CGU	OE21-CD2-CG-CD1
2	Z	32	CGU	OE22-CD2-CG-CD1

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Z	6	CGU	1	0
2	Z	26	CGU	1	0
2	Z	20	CGU	1	0
2	Z	25	CGU	4	0
2	Z	14	CGU	1	0
2	Z	29	CGU	2	0
2	Z	32	CGU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

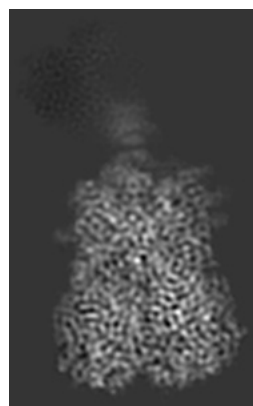
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45729. These allow visual inspection of the internal detail of the map and identification of artifacts.

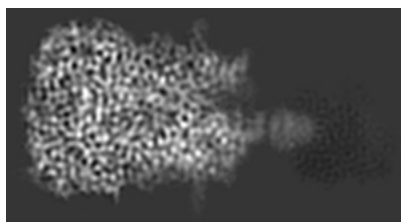
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

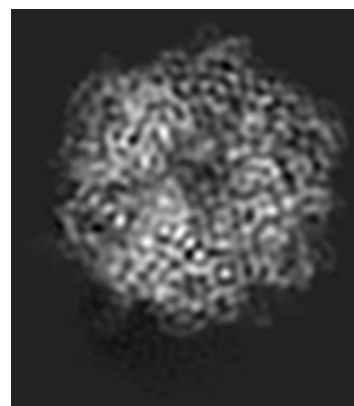
6.1.1 Primary map



X

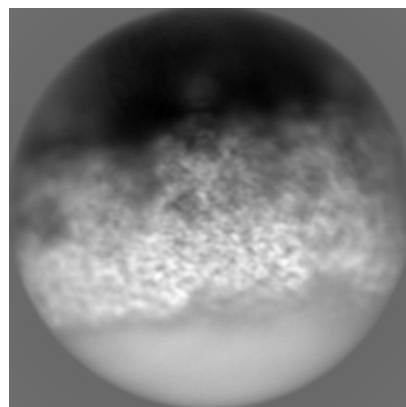


Y

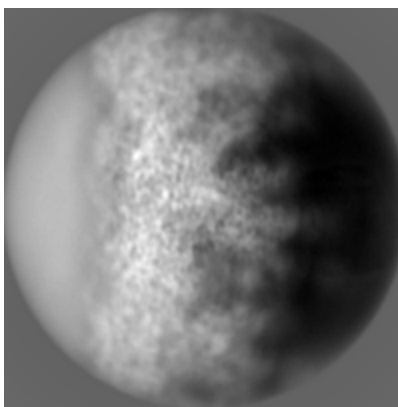


Z

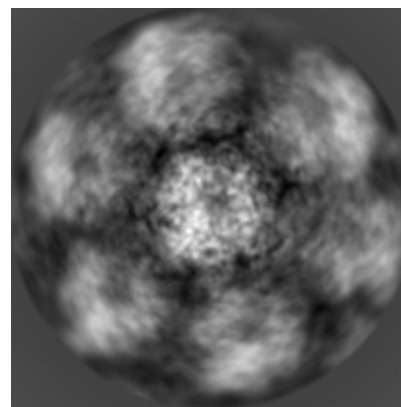
6.1.2 Raw map



X



Y

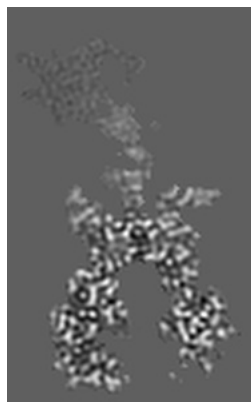


Z

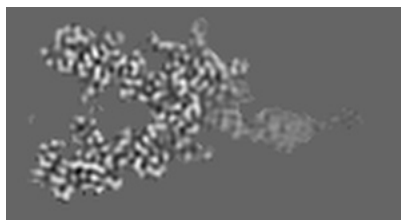
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

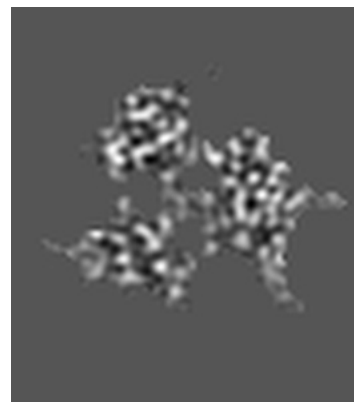
6.2.1 Primary map



X Index: 41

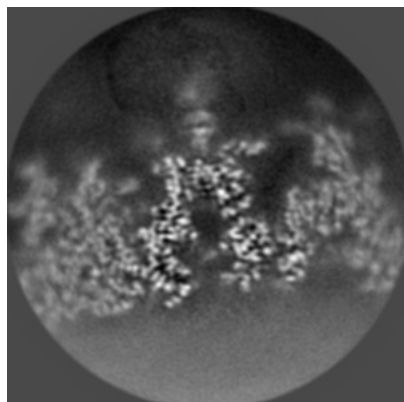


Y Index: 46

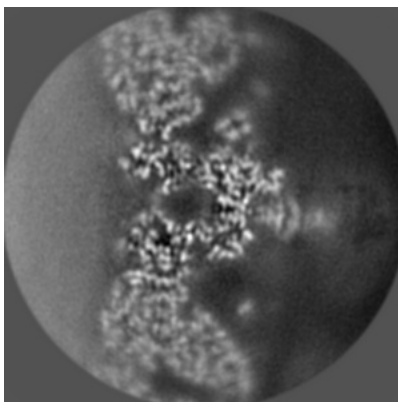


Z Index: 75

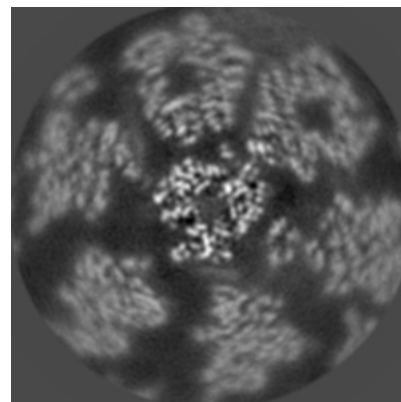
6.2.2 Raw map



X Index: 100



Y Index: 100

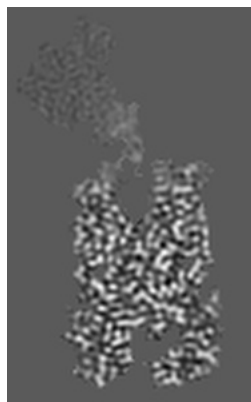


Z Index: 100

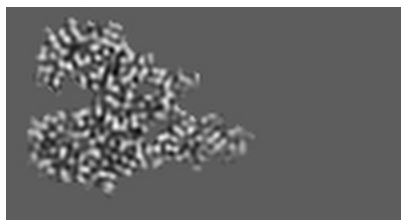
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

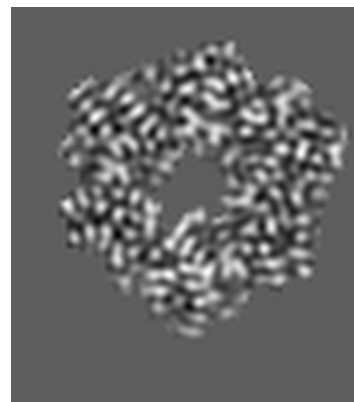
6.3.1 Primary map



X Index: 31

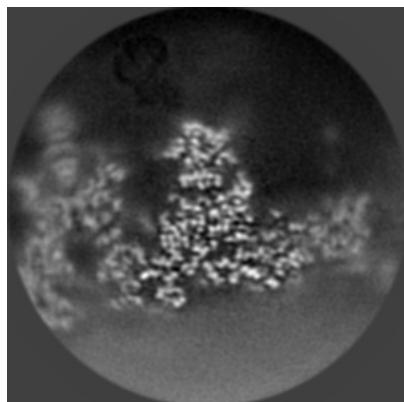


Y Index: 66

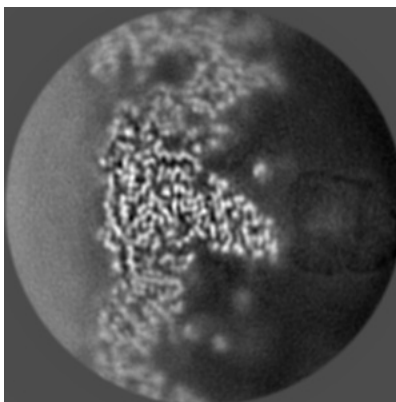


Z Index: 35

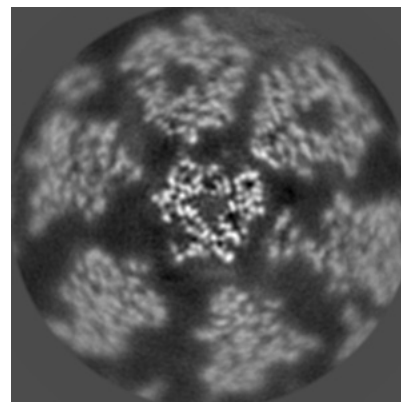
6.3.2 Raw map



X Index: 116



Y Index: 81

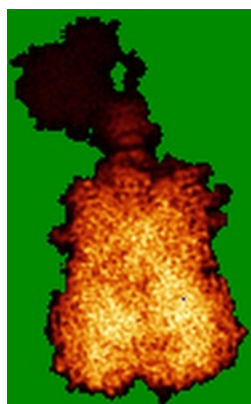


Z Index: 102

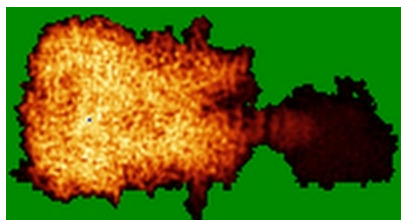
The images above show the largest variance slices of the map in three orthogonal directions.

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

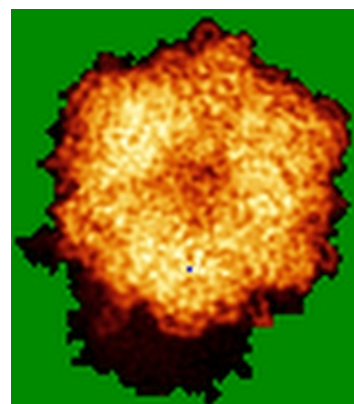
6.4.1 Primary map



X

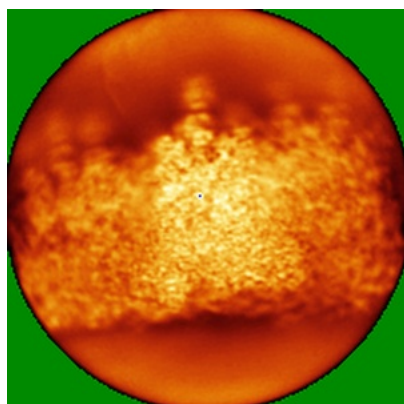


Y

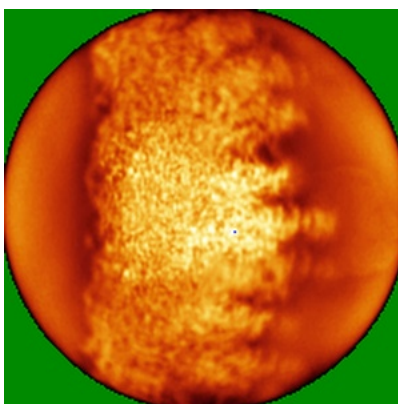


Z

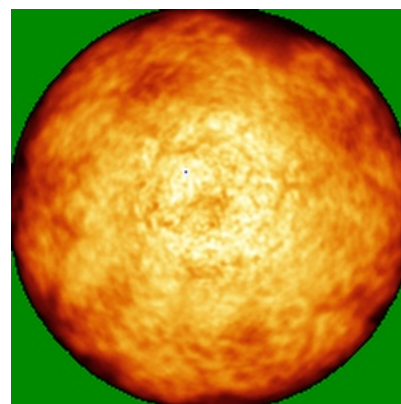
6.4.2 Raw map



X



Y

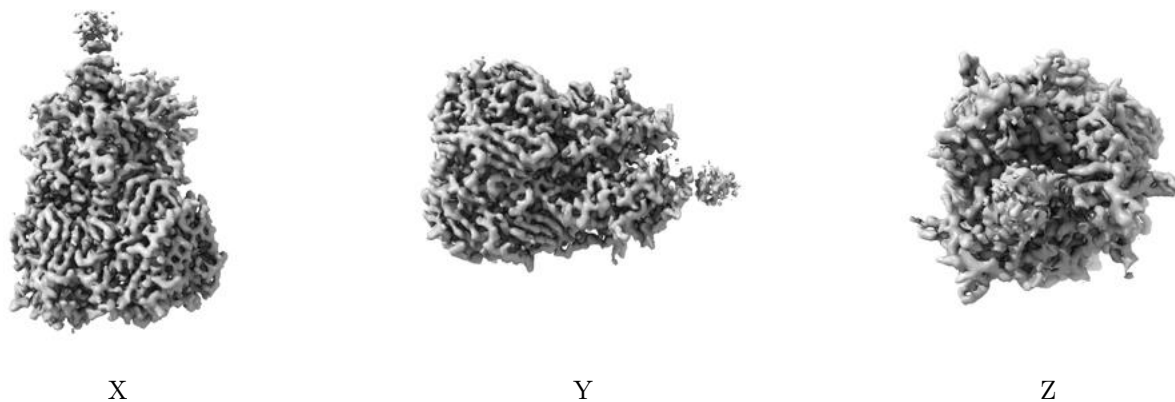


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

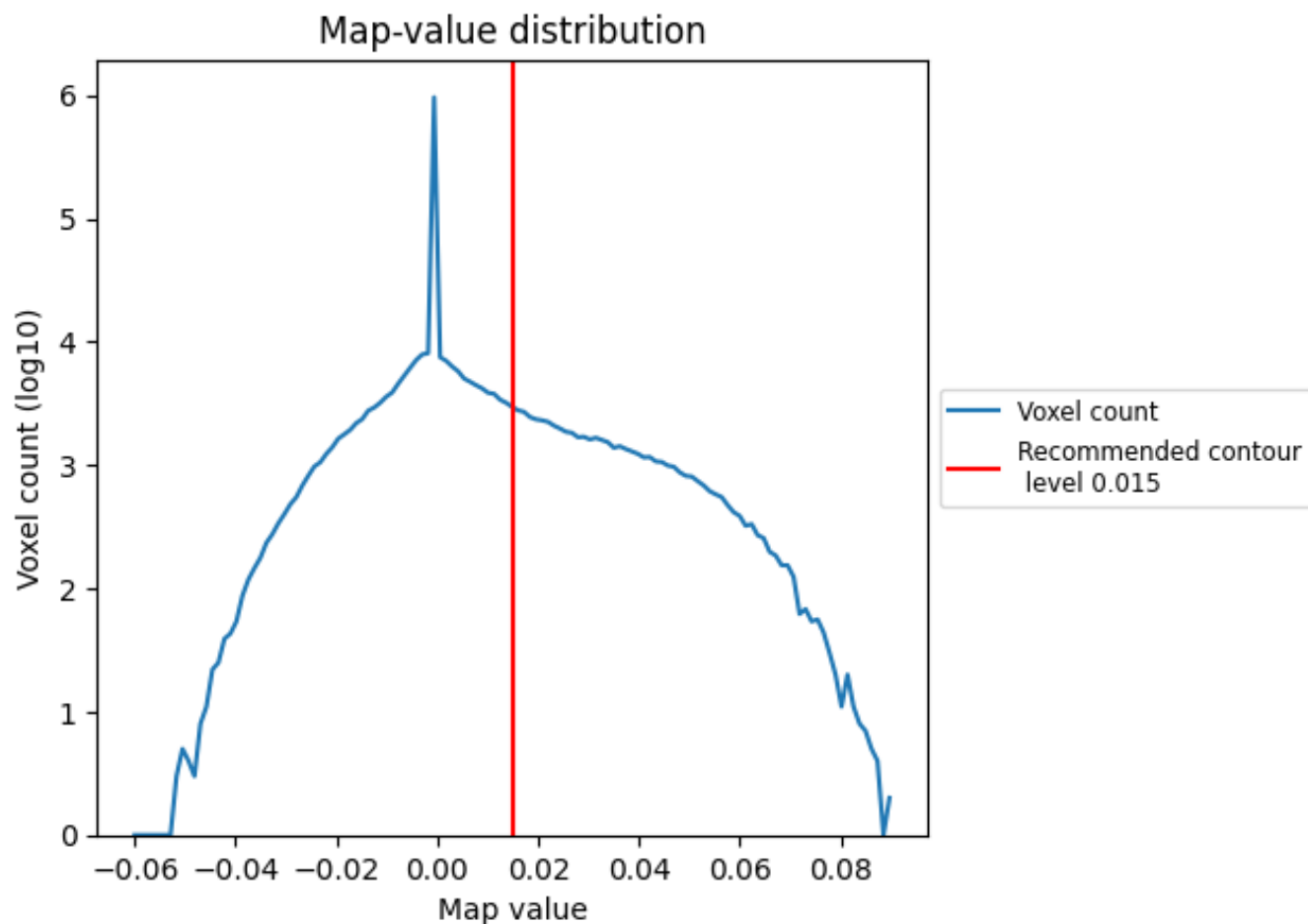
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

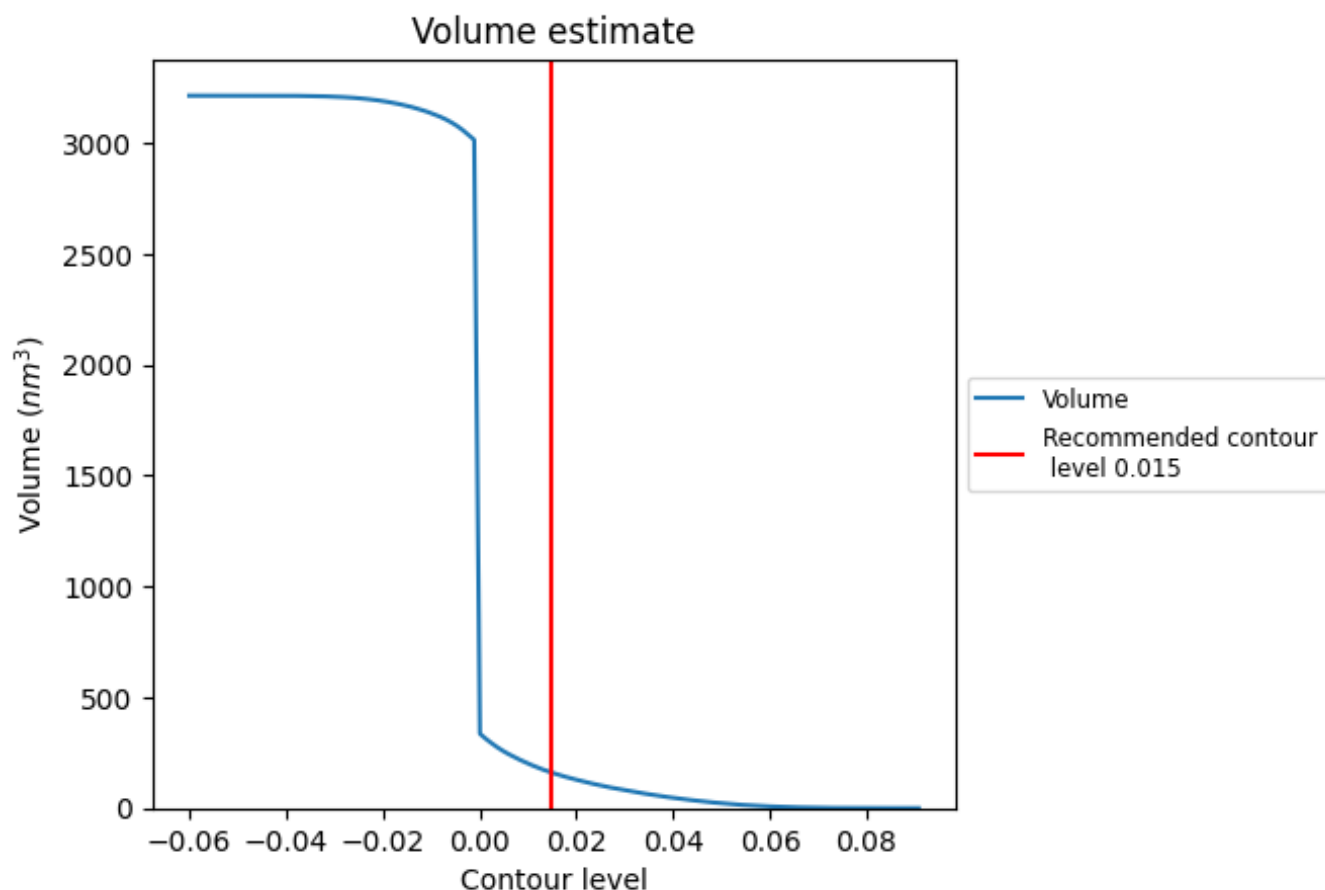
This section contains the results of statistical analysis of the map.

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 160 nm³; this corresponds to an approximate mass of 144 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.

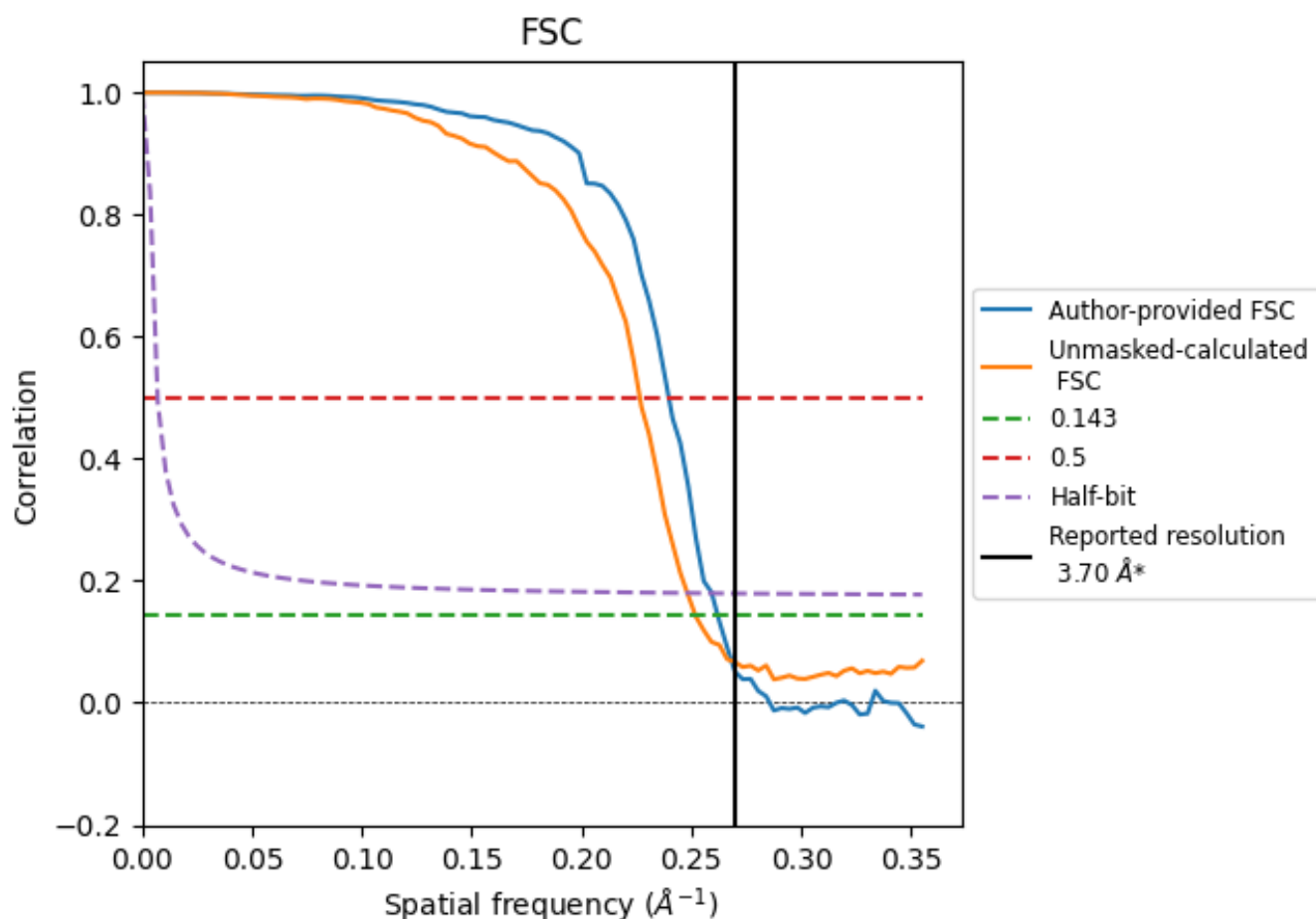
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

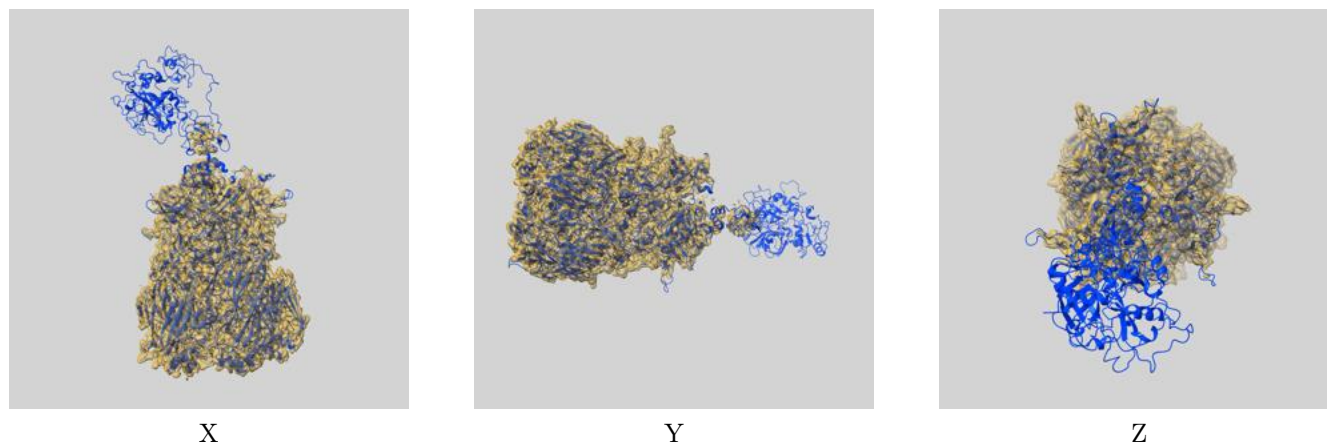
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.82	4.17	3.86
Unmasked-calculated*	3.97	4.41	4.03

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

9 Map-model fit [i](#)

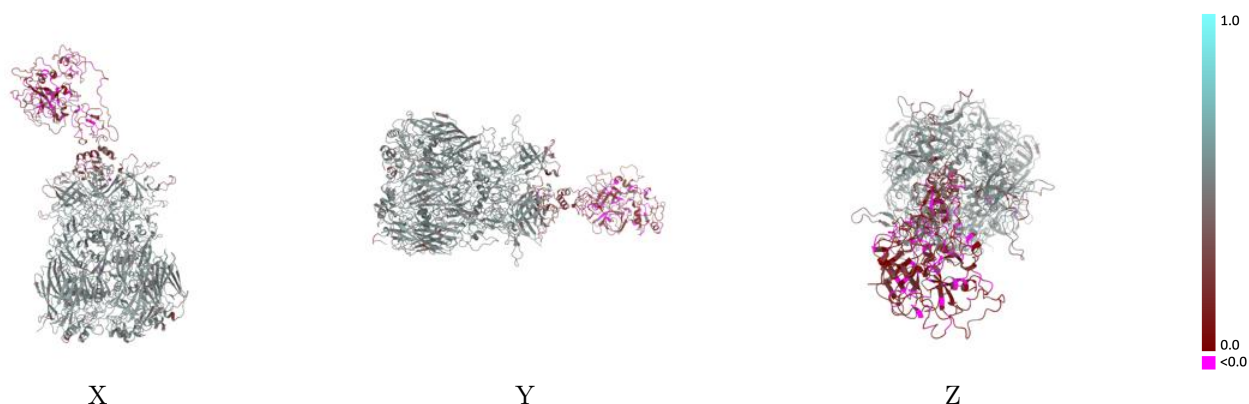
This section contains information regarding the fit between EMDB map EMD-45729 and PDB model 9CLS. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



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

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

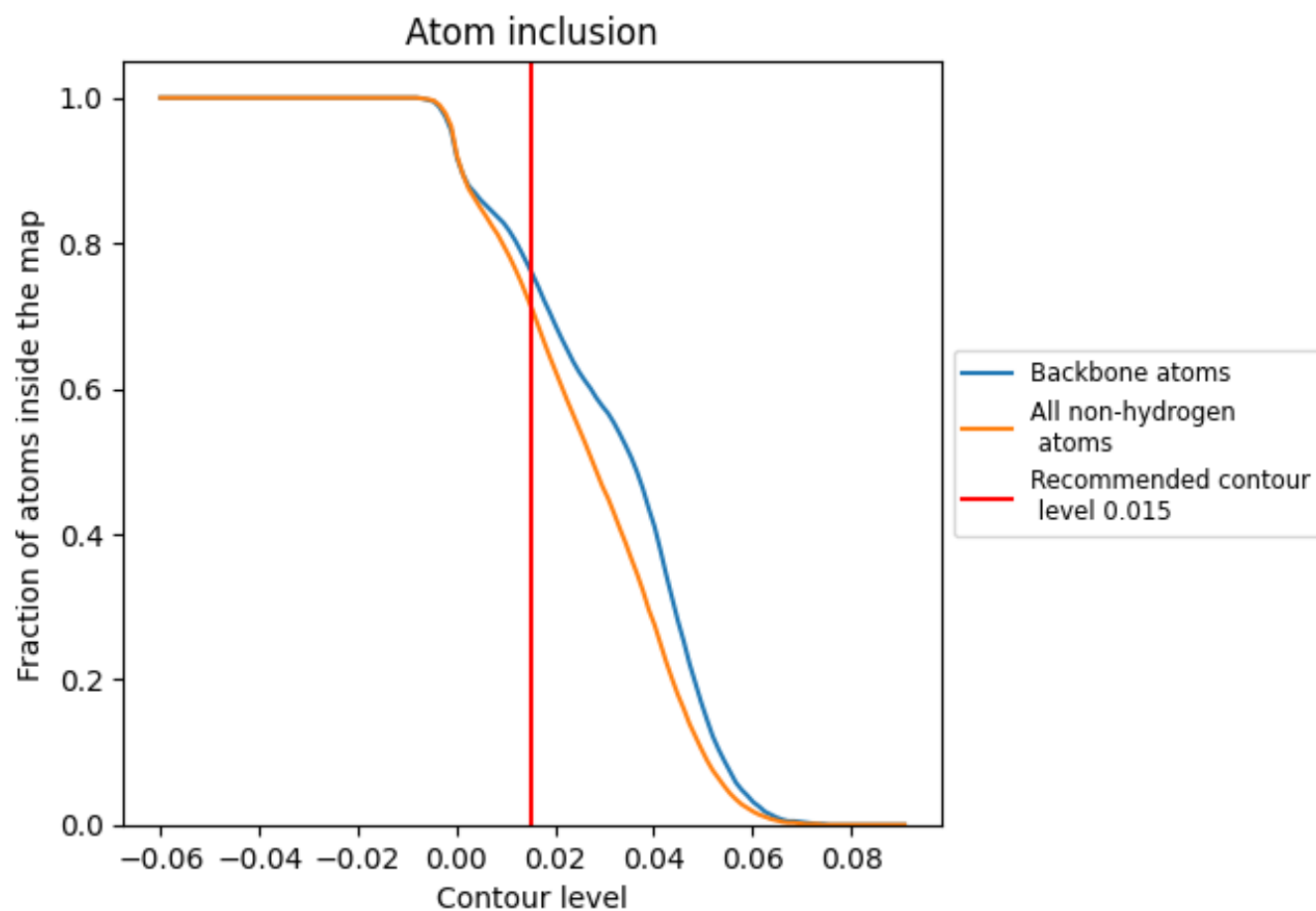


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7140	0.4500
J	0.8560	0.5100
K	0.8440	0.5140
L	0.8480	0.5110
Z	0.0630	0.1560

