



Full wwPDB EM Validation Report ⓘ

May 18, 2026 – 02:01 PM EDT

PDB ID : 10BU / pdb_000010bu
EMDB ID : EMD-75053
Title : Adenovirus hexon displaying BAP insertion in the HVR5 region
Authors : Reddy, V.S.; Ma, O.X.
Deposited on : 2026-01-10
Resolution : 3.20 Å (reported)
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
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

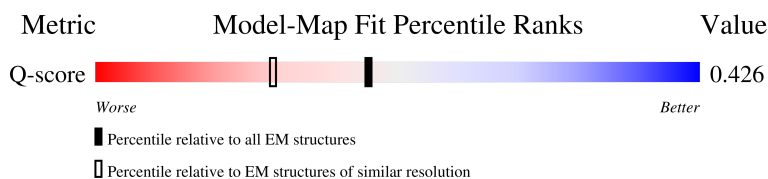
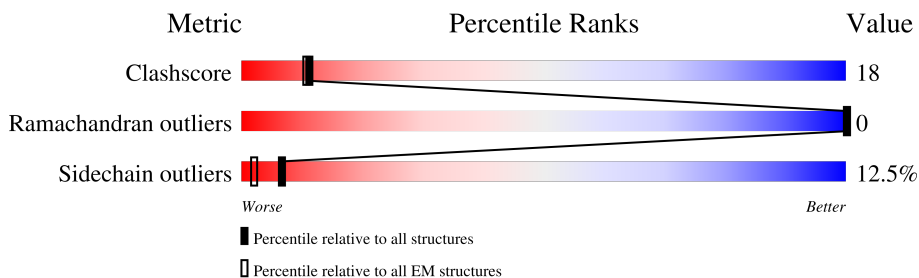
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	991	
1	B	991	
1	C	991	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23438 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.

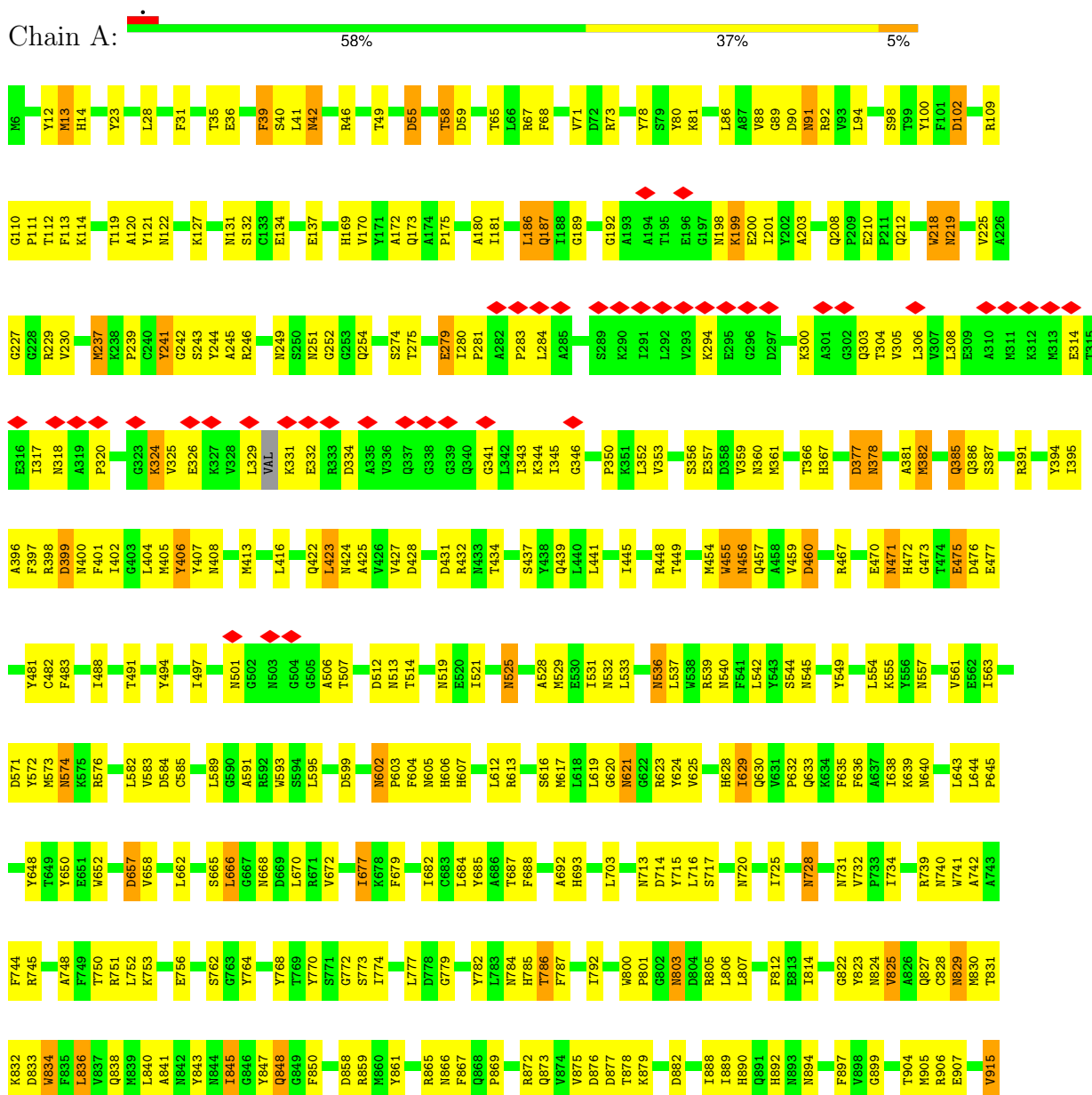
- Molecule 1 is a protein called BAP inserted Hexon protein.

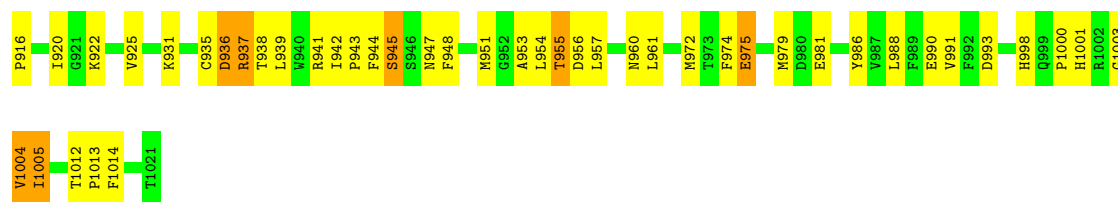
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	990	Total	C	N	O	S	0	0
			7820	4949	1327	1505	39		
1	B	990	Total	C	N	O	S	0	0
			7819	4950	1327	1503	39		
1	C	987	Total	C	N	O	S	0	0
			7799	4939	1323	1498	39		

3 Residue-property plots

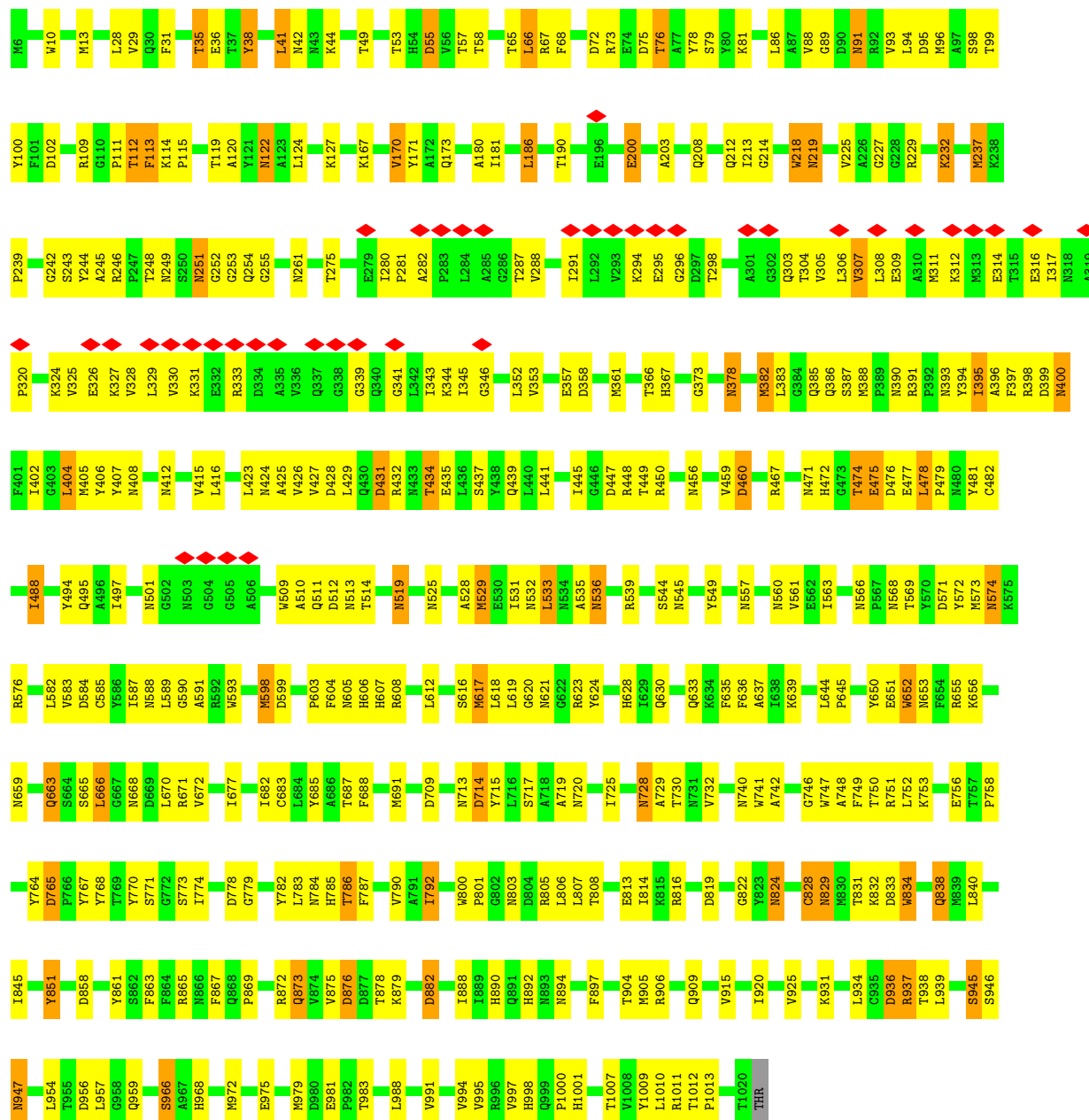
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



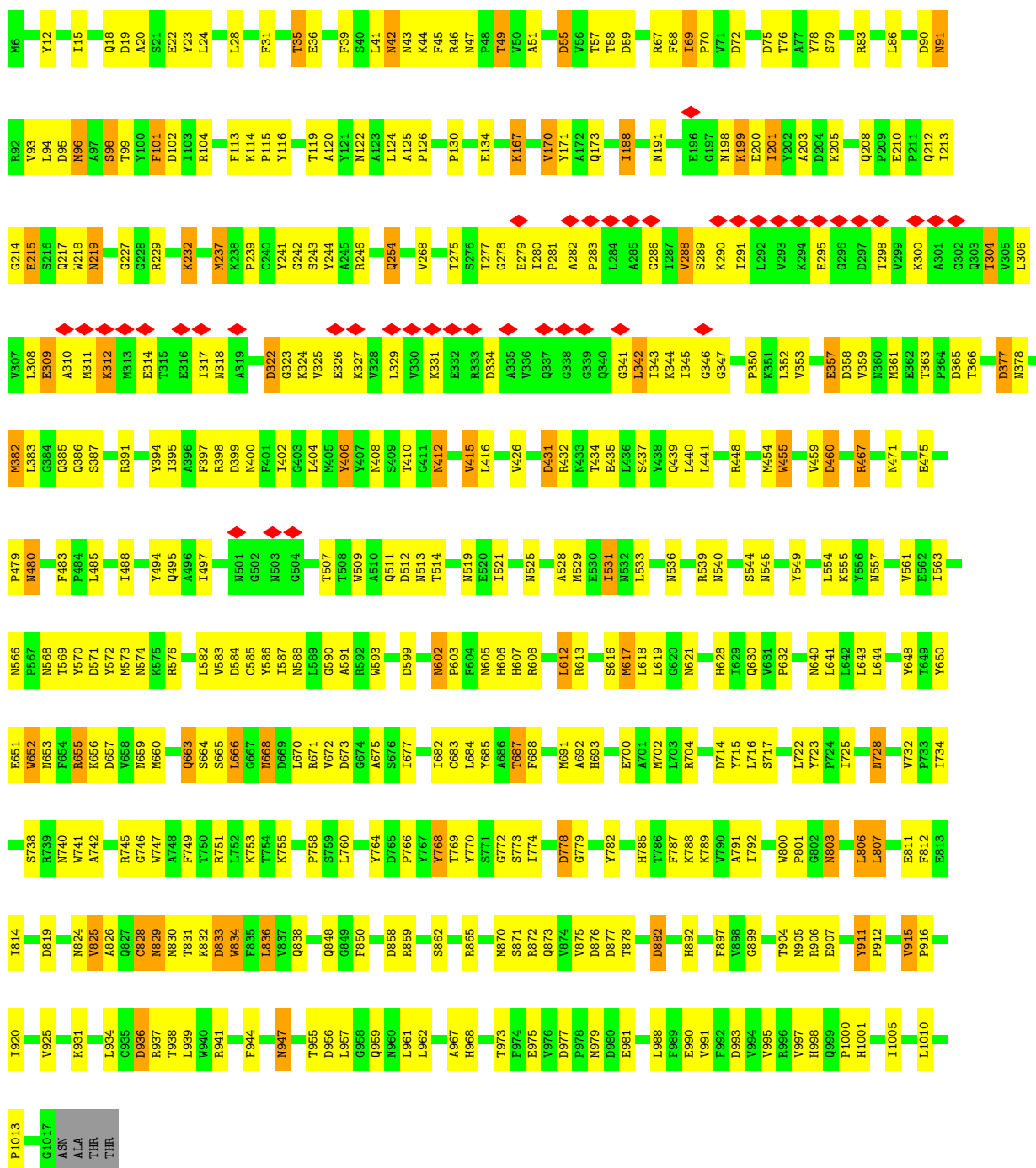


• Molecule 1: BAP inserted Hexon protein



• Molecule 1: BAP inserted Hexon protein

Chain C: 58% 35% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4440390	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.003	Depositor
Map size (Å)	225.28, 225.28, 225.28	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.408, 1.408, 1.408	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.26	0/8015	0.42	0/10892
1	B	0.25	0/8015	0.41	1/10895 (0.0%)
1	C	0.26	0/7995	0.42	0/10867
All	All	0.26	0/24025	0.42	1/32654 (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	C	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	746	GLY	N-CA-C	5.08	119.49	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	199	LYS	Peptide
1	C	915	VAL	Peptide

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7820	0	7522	307	0
1	B	7819	0	7525	307	0
1	C	7799	0	7507	319	0
All	All	23438	0	22554	832	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (832) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:O	1:A:314:GLU:HA	1.67	0.92
1:C:98:SER:HG	1:C:687:THR:HG1	1.14	0.91
1:C:382:MET:SD	1:C:385:GLN:NE2	2.46	0.89
1:B:308:LEU:O	1:B:314:GLU:HA	1.73	0.88
1:C:308:LEU:O	1:C:314:GLU:HA	1.77	0.85
1:A:382:MET:SD	1:A:385:GLN:NE2	2.48	0.84
1:A:828:CYS:SG	1:A:829:ASN:N	2.51	0.84
1:C:828:CYS:SG	1:C:829:ASN:N	2.50	0.84
1:A:589:LEU:O	1:C:621:ASN:ND2	2.11	0.83
1:C:460:ASP:N	1:C:460:ASP:OD1	2.11	0.83
1:C:237:MET:SD	1:C:378:ASN:ND2	2.51	0.83
1:B:237:MET:SD	1:B:378:ASN:ND2	2.53	0.81
1:B:828:CYS:SG	1:B:829:ASN:N	2.53	0.81
1:B:460:ASP:OD1	1:B:460:ASP:N	2.13	0.81
1:B:88:VAL:HG21	1:B:94:LEU:HD22	1.64	0.80
1:C:605:ASN:ND2	1:C:770:TYR:OH	2.15	0.80
1:A:237:MET:SD	1:A:237:MET:N	2.57	0.78
1:A:906:ARG:O	1:A:906:ARG:NH1	2.17	0.77
1:C:906:ARG:O	1:C:906:ARG:NH1	2.17	0.77
1:A:399:ASP:OD1	1:A:400:ASN:ND2	2.18	0.76
1:A:621:ASN:ND2	1:B:589:LEU:O	2.18	0.76
1:B:88:VAL:O	1:B:645:PRO:HA	1.85	0.76
1:A:399:ASP:OD2	1:A:439:GLN:NE2	2.18	0.76
1:A:460:ASP:N	1:A:460:ASP:OD1	2.16	0.75
1:B:127:LYS:HD2	1:C:479:PRO:HB3	1.69	0.75
1:C:431:ASP:N	1:C:431:ASP:OD1	2.18	0.75
1:B:399:ASP:OD2	1:B:439:GLN:NE2	2.18	0.75
1:A:58:THR:HB	1:A:692:ALA:HA	1.68	0.75
1:A:848:GLN:NE2	1:C:95:ASP:OD2	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:MET:SD	1:B:385:GLN:NE2	2.60	0.74
1:B:431:ASP:OD1	1:B:431:ASP:N	2.18	0.74
1:C:725:ILE:HG12	1:C:732:VAL:HG21	1.69	0.74
1:A:814:ILE:HA	1:A:834:TRP:HD1	1.51	0.74
1:B:237:MET:SD	1:B:237:MET:N	2.61	0.74
1:B:100:TYR:OH	1:C:832:LYS:NZ	2.20	0.73
1:A:134:GLU:HB3	1:A:170:VAL:HG13	1.68	0.73
1:C:237:MET:SD	1:C:237:MET:N	2.61	0.73
1:B:400:ASN:OD1	1:B:439:GLN:NE2	2.22	0.72
1:B:906:ARG:O	1:B:906:ARG:NH1	2.22	0.72
1:B:67:ARG:HG3	1:B:685:TYR:HE1	1.54	0.72
1:A:394:TYR:OH	1:A:613:ARG:NH1	2.23	0.72
1:B:814:ILE:HA	1:B:834:TRP:HD1	1.54	0.72
1:A:127:LYS:HD2	1:B:479:PRO:HB3	1.72	0.71
1:C:96:MET:O	1:C:99:THR:OG1	2.08	0.71
1:A:751:ARG:NH1	1:A:979:MET:SD	2.64	0.71
1:B:304:THR:HG21	1:B:316:GLU:HB3	1.72	0.71
1:B:467:ARG:NH2	1:B:936:ASP:OD2	2.24	0.71
1:C:833:ASP:N	1:C:833:ASP:OD1	2.22	0.70
1:A:605:ASN:ND2	1:A:770:TYR:OH	2.23	0.70
1:B:111:PRO:HD3	1:B:623:ARG:HH21	1.55	0.70
1:A:102:ASP:OD1	1:A:630:GLN:NE2	2.24	0.70
1:A:218:TRP:NE1	1:A:219:ASN:OD1	2.24	0.70
1:B:67:ARG:NH2	1:B:683:CYS:SG	2.64	0.70
1:C:67:ARG:NH2	1:C:683:CYS:SG	2.64	0.70
1:A:229:ARG:NE	1:A:357:GLU:OE2	2.25	0.70
1:A:605:ASN:OD1	1:A:773:SER:OG	2.09	0.70
1:C:114:LYS:NZ	1:C:116:TYR:O	2.25	0.69
1:A:621:ASN:OD1	1:A:621:ASN:N	2.26	0.69
1:C:72:ASP:HB3	1:C:83:ARG:HB3	1.73	0.69
1:A:725:ILE:HG12	1:A:732:VAL:HG21	1.74	0.69
1:A:824:ASN:O	1:C:628:HIS:NE2	2.25	0.69
1:B:218:TRP:NE1	1:B:219:ASN:OD1	2.26	0.69
1:C:239:PRO:HG2	1:C:387:SER:HB2	1.73	0.68
1:C:602:ASN:OD1	1:C:602:ASN:N	2.18	0.68
1:B:96:MET:O	1:B:99:THR:OG1	2.10	0.68
1:B:109:ARG:NH2	1:B:620:GLY:O	2.26	0.68
1:C:659:ASN:HD21	1:C:671:ARG:HB2	1.57	0.68
1:C:668:ASN:HD21	1:C:670:LEU:HD23	1.59	0.68
1:A:829:ASN:ND2	1:A:931:LYS:O	2.27	0.68
1:B:605:ASN:ND2	1:B:770:TYR:OH	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:751:ARG:NH1	1:B:979:MET:SD	2.67	0.68
1:B:88:VAL:HG11	1:B:94:LEU:HB2	1.75	0.68
1:B:668:ASN:HD21	1:B:670:LEU:HD23	1.59	0.67
1:A:838:GLN:NE2	1:A:941:ARG:O	2.26	0.67
1:B:431:ASP:O	1:B:720:ASN:ND2	2.26	0.67
1:B:805:ARG:NH2	1:B:946:SER:O	2.27	0.67
1:A:431:ASP:O	1:A:720:ASN:ND2	2.26	0.67
1:A:31:PHE:O	1:A:35:THR:OG1	2.13	0.67
1:C:467:ARG:NH1	1:C:599:ASP:OD1	2.28	0.67
1:B:229:ARG:NE	1:B:357:GLU:OE2	2.25	0.67
1:B:557:ASN:OD1	1:B:576:ARG:NH1	2.28	0.67
1:C:242:GLY:HA3	1:C:366:THR:HG21	1.77	0.67
1:C:322:ASP:N	1:C:322:ASP:OD1	2.27	0.67
1:C:814:ILE:HA	1:C:834:TRP:HD1	1.60	0.67
1:A:557:ASN:OD1	1:A:576:ARG:NH1	2.29	0.66
1:A:192:GLY:O	1:A:198:ASN:ND2	2.29	0.66
1:B:57:THR:OG1	1:C:947:ASN:ND2	2.28	0.66
1:C:814:ILE:HG12	1:C:834:TRP:HE1	1.59	0.66
1:C:467:ARG:NH2	1:C:936:ASP:OD2	2.29	0.66
1:A:73:ARG:NH2	1:A:80:TYR:OH	2.28	0.66
1:B:512:ASP:OD1	1:B:513:ASN:N	2.28	0.66
1:B:621:ASN:ND2	1:C:590:GLY:O	2.29	0.66
1:A:189:GLY:O	1:A:201:ILE:N	2.28	0.65
1:C:512:ASP:OD1	1:C:513:ASN:N	2.29	0.65
1:A:512:ASP:OD1	1:A:513:ASN:N	2.28	0.65
1:B:246:ARG:NH1	1:C:882:ASP:OD2	2.29	0.65
1:A:882:ASP:OD2	1:C:246:ARG:NH1	2.30	0.65
1:A:936:ASP:N	1:A:936:ASP:OD1	2.29	0.65
1:B:876:ASP:OD2	1:B:879:LYS:N	2.30	0.65
1:C:280:ILE:HB	1:C:343:ILE:HB	1.79	0.65
1:B:991:VAL:HB	1:B:1013:PRO:HD2	1.77	0.65
1:C:663:GLN:NE2	1:C:664:SER:O	2.30	0.65
1:C:42:ASN:N	1:C:42:ASN:OD1	2.28	0.64
1:A:593:TRP:CE2	1:A:872:ARG:HD3	2.32	0.64
1:B:608:ARG:NH2	1:C:475:GLU:OE2	2.30	0.64
1:B:947:ASN:OD1	1:B:947:ASN:N	2.29	0.64
1:C:134:GLU:HB3	1:C:170:VAL:HG13	1.79	0.64
1:B:450:ARG:HH12	1:C:865:ARG:HH21	1.44	0.64
1:A:401:PHE:HB3	1:A:404:LEU:HD12	1.80	0.64
1:A:623:ARG:NH1	1:A:624:TYR:OH	2.30	0.64
1:A:748:ALA:HB3	1:A:988:LEU:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:ARG:NH1	1:B:599:ASP:OD1	2.31	0.63
1:A:519:ASN:OD1	1:B:170:VAL:N	2.29	0.63
1:A:602:ASN:OD1	1:A:602:ASN:N	2.22	0.63
1:B:725:ILE:HG12	1:B:732:VAL:HG21	1.79	0.63
1:C:557:ASN:OD1	1:C:576:ARG:NH1	2.32	0.63
1:B:95:ASP:OD2	1:C:848:GLN:NE2	2.30	0.63
1:C:309:GLU:HA	1:C:314:GLU:HG2	1.80	0.63
1:C:382:MET:O	1:C:385:GLN:NE2	2.22	0.63
1:B:382:MET:O	1:B:385:GLN:NE2	2.24	0.63
1:A:227:GLY:HA2	1:A:353:VAL:O	1.99	0.63
1:A:280:ILE:HD11	1:A:320:PRO:HD3	1.80	0.63
1:B:748:ALA:HB3	1:B:988:LEU:HB3	1.81	0.63
1:B:936:ASP:OD1	1:B:936:ASP:N	2.30	0.63
1:C:399:ASP:OD2	1:C:439:GLN:NE2	2.31	0.63
1:A:531:ILE:HB	1:B:482:CYS:HA	1.81	0.63
1:B:327:LYS:HE2	1:B:329:LEU:HD21	1.80	0.63
1:C:385:GLN:O	1:C:386:GLN:NE2	2.31	0.63
1:B:214:GLY:HA3	1:C:907:GLU:HB2	1.81	0.62
1:B:249:ASN:OD1	1:B:252:GLY:N	2.29	0.62
1:A:306:LEU:HB3	1:A:317:ILE:HB	1.82	0.62
1:A:476:ASP:OD2	1:A:532:ASN:ND2	2.31	0.62
1:B:391:ARG:NH1	1:B:573:MET:O	2.29	0.62
1:A:42:ASN:N	1:A:42:ASN:OD1	2.33	0.62
1:B:298:THR:HA	1:B:324:LYS:HA	1.82	0.62
1:C:203:ALA:HB1	1:C:208:GLN:HB2	1.80	0.62
1:A:325:VAL:HA	1:A:345:ILE:HA	1.81	0.62
1:C:412:ASN:OD1	1:C:412:ASN:N	2.33	0.62
1:B:476:ASP:OD2	1:B:532:ASN:ND2	2.32	0.62
1:A:58:THR:OG1	1:A:59:ASP:N	2.29	0.61
1:B:232:LYS:NZ	1:B:358:ASP:OD1	2.27	0.61
1:B:906:ARG:HH12	1:C:525:ASN:HD22	1.46	0.61
1:C:398:ARG:NH2	1:C:772:GLY:O	2.33	0.61
1:B:813:GLU:OE2	1:B:816:ARG:NE	2.30	0.61
1:A:279:GLU:HA	1:A:344:LYS:HA	1.82	0.61
1:A:324:LYS:N	1:A:346:GLY:O	2.32	0.61
1:A:382:MET:O	1:A:385:GLN:NE2	2.33	0.61
1:B:714:ASP:OD2	1:B:717:SER:N	2.30	0.61
1:C:398:ARG:HH12	1:C:774:ILE:H	1.47	0.61
1:C:593:TRP:CE2	1:C:872:ARG:HD3	2.35	0.61
1:C:652:TRP:HD1	1:C:653:ASN:H	1.49	0.61
1:A:841:ALA:HB1	1:A:943:PRO:HG3	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:PHE:HE1	1:B:619:LEU:HD11	1.65	0.61
1:C:229:ARG:NE	1:C:357:GLU:OE2	2.32	0.61
1:A:960:ASN:OD1	1:A:961:LEU:N	2.32	0.61
1:B:719:ALA:HB2	1:B:1011:ARG:HH12	1.66	0.61
1:B:829:ASN:N	1:B:829:ASN:OD1	2.32	0.61
1:C:191:ASN:H	1:C:200:GLU:HB2	1.66	0.61
1:C:936:ASP:N	1:C:936:ASP:OD1	2.31	0.61
1:A:542:LEU:HD11	1:A:583:VAL:HG12	1.82	0.61
1:B:652:TRP:HD1	1:B:653:ASN:H	1.49	0.61
1:A:237:MET:SD	1:A:378:ASN:ND2	2.74	0.60
1:A:501:ASN:ND2	1:A:506:ALA:O	2.35	0.60
1:B:395:ILE:O	1:B:616:SER:OG	2.19	0.60
1:A:829:ASN:N	1:A:829:ASN:OD1	2.34	0.60
1:C:892:HIS:O	1:C:892:HIS:ND1	2.33	0.60
1:A:109:ARG:NH2	1:A:620:GLY:O	2.34	0.60
1:A:36:GLU:OE2	1:A:42:ASN:ND2	2.35	0.59
1:A:536:ASN:HD21	1:C:124:LEU:HD11	1.67	0.59
1:C:306:LEU:HB3	1:C:317:ILE:HB	1.83	0.59
1:B:424:ASN:OD1	1:B:425:ALA:N	2.35	0.59
1:A:714:ASP:OD1	1:A:715:TYR:N	2.35	0.59
1:B:295:GLU:HB3	1:B:327:LYS:HA	1.84	0.59
1:A:199:LYS:H	1:A:199:LYS:HD2	1.66	0.59
1:A:331:LYS:NZ	1:A:332:GLU:O	2.35	0.59
1:C:938:THR:OG1	1:C:939:LEU:N	2.36	0.59
1:A:628:HIS:NE2	1:B:824:ASN:O	2.35	0.59
1:B:394:TYR:N	1:B:665:SER:OG	2.36	0.59
1:A:241:TYR:OH	1:B:476:ASP:OD2	2.22	0.58
1:B:792:ILE:HG22	1:B:972:MET:HG2	1.84	0.58
1:C:114:LYS:HE2	1:C:365:ASP:HB2	1.84	0.58
1:A:239:PRO:HG3	1:A:385:GLN:HB2	1.86	0.58
1:A:467:ARG:NH2	1:A:599:ASP:OD1	2.35	0.58
1:B:386:GLN:OE1	1:B:905:MET:N	2.36	0.58
1:B:904:THR:OG1	1:B:905:MET:N	2.36	0.58
1:C:227:GLY:HA2	1:C:353:VAL:O	2.03	0.58
1:C:829:ASN:N	1:C:829:ASN:OD1	2.36	0.58
1:A:391:ARG:NH1	1:A:573:MET:O	2.33	0.58
1:B:512:ASP:OD1	1:B:514:THR:N	2.35	0.58
1:C:90:ASP:N	1:C:90:ASP:OD1	2.35	0.58
1:A:731:ASN:ND2	1:A:975:GLU:OE2	2.37	0.58
1:A:786:THR:O	1:A:786:THR:OG1	2.22	0.58
1:B:876:ASP:CG	1:B:878:THR:H	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:938:THR:OG1	1:B:939:LEU:N	2.37	0.58
1:B:945:SER:OG	1:B:946:SER:N	2.36	0.58
1:C:18:GLN:HB3	1:C:22:GLU:HB2	1.84	0.58
1:A:300:LYS:HG2	1:A:303:GLN:HE21	1.69	0.58
1:B:652:TRP:CD1	1:B:653:ASN:H	2.22	0.58
1:A:395:ILE:O	1:A:616:SER:OG	2.22	0.57
1:B:227:GLY:HA2	1:B:353:VAL:O	2.04	0.57
1:C:286:GLY:HA3	1:C:310:ALA:HA	1.86	0.57
1:C:584:ASP:OD1	1:C:585:CYS:N	2.34	0.57
1:B:394:TYR:HB2	1:B:665:SER:HB3	1.86	0.57
1:C:652:TRP:CD1	1:C:653:ASN:H	2.22	0.57
1:A:455:TRP:CZ3	1:A:632:PRO:HB3	2.38	0.57
1:C:829:ASN:ND2	1:C:931:LYS:O	2.31	0.57
1:A:740:ASN:OD1	1:A:741:TRP:N	2.38	0.57
1:B:242:GLY:HA3	1:B:366:THR:HG21	1.87	0.57
1:C:232:LYS:NZ	1:C:358:ASP:OD1	2.28	0.57
1:C:876:ASP:CG	1:C:878:THR:H	2.13	0.57
1:C:947:ASN:N	1:C:947:ASN:OD1	2.38	0.57
1:C:814:ILE:HG12	1:C:834:TRP:NE1	2.20	0.57
1:A:938:THR:OG1	1:A:939:LEU:N	2.38	0.57
1:B:584:ASP:OD1	1:B:585:CYS:N	2.37	0.57
1:B:668:ASN:O	1:B:771:SER:OG	2.23	0.57
1:B:725:ILE:HG23	1:B:729:ALA:HB3	1.85	0.57
1:C:331:LYS:H	1:C:334:ASP:HB2	1.69	0.57
1:C:714:ASP:OD1	1:C:715:TYR:N	2.38	0.57
1:A:572:TYR:OH	1:A:576:ARG:NH2	2.33	0.56
1:B:621:ASN:N	1:C:873:GLN:OE1	2.37	0.56
1:A:494:TYR:HD1	1:B:275:THR:HA	1.71	0.56
1:A:739:ARG:HD3	1:A:1014:PHE:HE1	1.70	0.56
1:A:770:TYR:OH	1:A:772:GLY:O	2.15	0.56
1:C:714:ASP:OD1	1:C:716:LEU:N	2.36	0.56
1:A:378:ASN:OD1	1:A:378:ASN:N	2.37	0.56
1:A:394:TYR:N	1:A:665:SER:OG	2.36	0.56
1:B:471:ASN:HD21	1:B:589:LEU:HD12	1.69	0.56
1:C:605:ASN:OD1	1:C:773:SER:OG	2.13	0.56
1:C:828:CYS:SG	1:C:830:MET:N	2.74	0.56
1:C:876:ASP:OD1	1:C:877:ASP:N	2.38	0.56
1:A:528:ALA:HB2	1:C:906:ARG:HE	1.69	0.56
1:C:394:TYR:N	1:C:665:SER:OG	2.38	0.56
1:C:102:ASP:OD1	1:C:630:GLN:NE2	2.35	0.56
1:A:540:ASN:ND2	1:B:475:GLU:O	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:SER:O	1:B:545:ASN:ND2	2.39	0.56
1:C:191:ASN:ND2	1:C:200:GLU:OE2	2.37	0.56
1:A:800:TRP:CG	1:A:801:PRO:HA	2.41	0.56
1:C:859:ARG:O	1:C:865:ARG:NH1	2.39	0.56
1:A:476:ASP:OD2	1:C:241:TYR:OH	2.24	0.56
1:A:648:TYR:HE1	1:A:1003:GLY:HA2	1.70	0.56
1:C:753:LYS:NZ	1:C:981:GLU:OE2	2.29	0.56
1:A:890:HIS:ND1	1:C:210:GLU:OE2	2.29	0.55
1:B:814:ILE:HA	1:B:834:TRP:CD1	2.37	0.55
1:C:800:TRP:CD1	1:C:801:PRO:HA	2.41	0.55
1:A:199:LYS:HG2	1:A:200:GLU:H	1.71	0.55
1:A:325:VAL:HG13	1:A:345:ILE:HG13	1.89	0.55
1:C:991:VAL:HB	1:C:1013:PRO:HD2	1.87	0.55
1:A:906:ARG:HB3	1:B:481:TYR:CD2	2.40	0.55
1:B:714:ASP:OD1	1:B:715:TYR:N	2.40	0.55
1:A:512:ASP:OD1	1:A:514:THR:N	2.31	0.55
1:A:170:VAL:N	1:C:519:ASN:OD1	2.37	0.55
1:A:131:ASN:ND2	1:A:132:SER:O	2.39	0.55
1:A:947:ASN:OD1	1:C:57:THR:OG1	2.21	0.55
1:B:67:ARG:HG3	1:B:685:TYR:CE1	2.39	0.55
1:B:112:THR:O	1:B:112:THR:OG1	2.21	0.55
1:C:655:ARG:HH22	1:C:760:LEU:HD23	1.70	0.55
1:A:329:LEU:O	1:A:331:LYS:N	2.39	0.55
1:A:876:ASP:OD1	1:A:877:ASP:N	2.40	0.55
1:A:482:CYS:HA	1:C:531:ILE:HB	1.89	0.55
1:B:471:ASN:HD22	1:B:590:GLY:H	1.55	0.55
1:C:415:VAL:HG23	1:C:651:GLU:HB3	1.89	0.55
1:A:750:THR:OG1	1:A:784:ASN:OD1	2.23	0.55
1:B:72:ASP:OD1	1:B:73:ARG:N	2.40	0.55
1:C:740:ASN:OD1	1:C:742:ALA:N	2.40	0.55
1:A:892:HIS:O	1:A:892:HIS:ND1	2.40	0.54
1:A:246:ARG:NH1	1:B:882:ASP:OD2	2.40	0.54
1:A:398:ARG:NH2	1:A:774:ILE:HG13	2.23	0.54
1:A:801:PRO:HB2	1:A:805:ARG:HG3	1.90	0.54
1:B:709:ASP:OD1	1:B:998:HIS:ND1	2.37	0.54
1:A:636:PHE:CE1	1:A:714:ASP:HB2	2.43	0.54
1:C:83:ARG:NE	1:C:651:GLU:OE2	2.39	0.54
1:C:800:TRP:CG	1:C:801:PRO:HA	2.43	0.54
1:C:751:ARG:NH1	1:C:979:MET:SD	2.81	0.54
1:A:621:ASN:N	1:B:873:GLN:OE1	2.41	0.54
1:C:323:GLY:HA3	1:C:347:GLY:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:TYR:OH	1:A:607:HIS:HB2	2.07	0.53
1:B:324:LYS:N	1:B:346:GLY:O	2.41	0.53
1:C:283:PRO:HG3	1:C:317:ILE:HG13	1.89	0.53
1:C:570:TYR:OH	1:C:574:ASN:ND2	2.41	0.53
1:C:572:TYR:OH	1:C:576:ARG:NH2	2.32	0.53
1:A:111:PRO:HD3	1:A:623:ARG:HH21	1.73	0.53
1:A:867:PHE:HD1	1:A:869:PRO:HD3	1.74	0.53
1:C:803:ASN:OD1	1:C:803:ASN:N	2.41	0.53
1:C:218:TRP:NE1	1:C:219:ASN:HD22	2.05	0.53
1:B:181:ILE:HG22	1:B:186:LEU:HA	1.90	0.53
1:B:582:LEU:HD12	1:B:888:ILE:HG12	1.90	0.53
1:C:31:PHE:O	1:C:35:THR:OG1	2.21	0.53
1:C:915:VAL:HG13	1:C:916:PRO:HD3	1.89	0.53
1:A:280:ILE:HB	1:A:343:ILE:HG13	1.91	0.53
1:C:836:LEU:HD12	1:C:850:PHE:HZ	1.73	0.53
1:A:100:TYR:OH	1:B:832:LYS:NZ	2.23	0.53
1:A:806:LEU:HD13	1:A:833:ASP:HB3	1.91	0.53
1:C:432:ARG:NH1	1:C:993:ASP:OD2	2.42	0.53
1:A:180:ALA:HA	1:A:225:VAL:HG11	1.91	0.53
1:A:397:PHE:HE1	1:A:619:LEU:HD11	1.74	0.53
1:A:408:ASN:N	1:A:428:ASP:OD2	2.32	0.53
1:A:840:LEU:HA	1:A:845:ILE:O	2.08	0.53
1:B:495:GLN:NE2	1:C:326:GLU:OE2	2.35	0.53
1:C:36:GLU:OE2	1:C:42:ASN:ND2	2.40	0.53
1:C:113:PHE:CE2	1:C:115:PRO:HD3	2.44	0.53
1:B:511:GLN:H	1:C:324:LYS:NZ	2.06	0.53
1:C:325:VAL:HG13	1:C:345:ILE:HG12	1.90	0.53
1:A:907:GLU:N	1:A:907:GLU:OE1	2.42	0.53
1:A:915:VAL:HG22	1:A:916:PRO:HA	1.89	0.53
1:B:549:TYR:OH	1:B:607:HIS:HB2	2.09	0.53
1:C:377:ASP:N	1:C:377:ASP:OD1	2.42	0.53
1:C:545:ASN:HD21	1:C:608:ARG:HH21	1.57	0.53
1:A:744:PHE:HB3	1:A:944:PHE:HD2	1.74	0.52
1:A:785:HIS:O	1:A:785:HIS:ND1	2.42	0.52
1:A:847:TYR:O	1:A:848:GLN:NE2	2.41	0.52
1:C:76:THR:OG1	1:C:79:SER:O	2.24	0.52
1:C:606:HIS:CD2	1:C:607:HIS:H	2.27	0.52
1:A:800:TRP:CD1	1:A:801:PRO:HA	2.44	0.52
1:C:612:LEU:HD21	1:C:663:GLN:HE22	1.75	0.52
1:B:758:PRO:HA	1:B:768:TYR:HE2	1.73	0.52
1:B:813:GLU:CD	1:B:816:ARG:HE	2.15	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:966:SER:OG	1:B:968:HIS:NE2	2.43	0.52
1:C:300:LYS:C	1:C:322:ASP:HB3	2.35	0.52
1:A:843:TYR:HB2	1:A:845:ILE:HG22	1.91	0.52
1:A:110:GLY:O	1:A:112:THR:N	2.41	0.52
1:A:589:LEU:HD21	1:C:116:TYR:CE2	2.45	0.52
1:A:657:ASP:HB2	1:A:764:TYR:HE2	1.74	0.52
1:C:395:ILE:O	1:C:616:SER:OG	2.15	0.52
1:A:814:ILE:HG12	1:A:834:TRP:HE1	1.75	0.52
1:A:876:ASP:CG	1:A:878:THR:H	2.17	0.52
1:A:907:GLU:HB2	1:C:214:GLY:HA3	1.92	0.52
1:B:325:VAL:HA	1:B:345:ILE:HA	1.91	0.52
1:B:399:ASP:OD1	1:B:400:ASN:ND2	2.42	0.52
1:A:122:ASN:OD1	1:B:894:ASN:N	2.43	0.52
1:A:181:ILE:HG22	1:A:186:LEU:HA	1.92	0.51
1:A:470:GLU:HG2	1:A:472:HIS:HE1	1.75	0.51
1:A:643:LEU:HG	1:A:648:TYR:HE2	1.75	0.51
1:B:326:GLU:N	1:B:344:LYS:O	2.43	0.51
1:B:617:MET:HE2	1:C:591:ALA:N	2.25	0.51
1:C:91:ASN:OD1	1:C:91:ASN:N	2.43	0.51
1:A:584:ASP:OD1	1:A:585:CYS:N	2.39	0.51
1:A:779:GLY:O	1:A:861:TYR:OH	2.23	0.51
1:B:434:THR:O	1:B:437:SER:HB2	2.09	0.51
1:B:786:THR:O	1:B:786:THR:OG1	2.27	0.51
1:C:239:PRO:HG3	1:C:385:GLN:HB2	1.91	0.51
1:A:714:ASP:OD1	1:A:716:LEU:N	2.41	0.51
1:B:75:ASP:OD1	1:B:76:THR:N	2.40	0.51
1:C:399:ASP:OD2	1:C:400:ASN:ND2	2.44	0.51
1:A:434:THR:O	1:A:437:SER:HB2	2.09	0.51
1:B:398:ARG:HH12	1:B:774:ILE:H	1.57	0.51
1:B:519:ASN:OD1	1:C:170:VAL:N	2.37	0.51
1:B:713:ASN:HB3	1:B:994:VAL:HG12	1.93	0.51
1:C:398:ARG:NH1	1:C:774:ILE:H	2.08	0.51
1:A:12:TYR:CD2	1:A:13:MET:HE3	2.46	0.51
1:A:242:GLY:HA3	1:A:366:THR:HG21	1.93	0.51
1:A:416:LEU:HD13	1:A:650:TYR:HD1	1.74	0.51
1:B:906:ARG:HE	1:C:528:ALA:HB2	1.76	0.51
1:C:391:ARG:NH1	1:C:573:MET:O	2.40	0.51
1:C:398:ARG:NH2	1:C:774:ILE:HG13	2.25	0.51
1:A:905:MET:HE1	1:C:218:TRP:HA	1.92	0.51
1:A:956:ASP:OD1	1:A:956:ASP:N	2.40	0.51
1:B:671:ARG:NH1	1:B:764:TYR:OH	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:829:ASN:HD21	1:B:931:LYS:C	2.19	0.51
1:C:188:ILE:HD11	1:C:203:ALA:N	2.25	0.51
1:C:700:GLU:OE2	1:C:704:ARG:NE	2.43	0.51
1:A:121:TYR:HB2	1:A:242:GLY:HA2	1.93	0.51
1:A:807:LEU:HD13	1:A:823:TYR:CZ	2.46	0.51
1:B:98:SER:O	1:B:98:SER:OG	2.26	0.51
1:B:593:TRP:CE2	1:B:872:ARG:HD3	2.45	0.51
1:C:130:PRO:HG3	1:C:383:LEU:HB3	1.91	0.51
1:C:555:LYS:HD3	1:C:576:ARG:HB3	1.93	0.51
1:A:88:VAL:HG12	1:A:645:PRO:HA	1.92	0.50
1:A:391:ARG:HD3	1:A:574:ASN:HA	1.92	0.50
1:B:239:PRO:HG2	1:B:387:SER:HB2	1.91	0.50
1:C:603:PRO:O	1:C:606:HIS:HB2	2.11	0.50
1:B:765:ASP:CG	1:B:767:TYR:H	2.19	0.50
1:C:69:ILE:HG22	1:C:70:PRO:HD2	1.92	0.50
1:C:512:ASP:OD1	1:C:514:THR:N	2.43	0.50
1:B:325:VAL:HG13	1:B:345:ILE:HG12	1.92	0.50
1:B:800:TRP:CG	1:B:801:PRO:HA	2.46	0.50
1:A:119:THR:OG1	1:A:120:ALA:N	2.43	0.50
1:A:824:ASN:HB2	1:C:628:HIS:CD2	2.46	0.50
1:A:955:THR:OG1	1:A:956:ASP:N	2.44	0.50
1:B:398:ARG:NH2	1:B:774:ILE:HG13	2.27	0.50
1:B:425:ALA:HB1	1:B:1007:THR:HG21	1.93	0.50
1:C:20:ALA:HB2	1:C:47:ASN:HD21	1.76	0.50
1:A:753:LYS:NZ	1:A:981:GLU:OE2	2.37	0.50
1:B:525:ASN:N	1:B:525:ASN:OD1	2.45	0.50
1:B:814:ILE:HG12	1:B:834:TRP:HE1	1.77	0.50
1:B:740:ASN:OD1	1:B:741:TRP:N	2.45	0.50
1:B:408:ASN:O	1:B:408:ASN:ND2	2.46	0.49
1:C:588:ASN:HD21	1:C:872:ARG:HH11	1.60	0.49
1:C:791:ALA:HB3	1:C:973:THR:HB	1.94	0.49
1:A:728:ASN:OD1	1:A:728:ASN:N	2.45	0.49
1:A:803:ASN:OD1	1:A:803:ASN:N	2.45	0.49
1:A:906:ARG:HE	1:B:528:ALA:HB2	1.77	0.49
1:C:324:LYS:O	1:C:346:GLY:N	2.31	0.49
1:C:758:PRO:HB3	1:C:768:TYR:CZ	2.47	0.49
1:B:31:PHE:O	1:B:35:THR:OG1	2.25	0.49
1:B:119:THR:OG1	1:B:120:ALA:N	2.44	0.49
1:B:306:LEU:HG	1:B:317:ILE:HB	1.94	0.49
1:C:455:TRP:NE1	1:C:632:PRO:HG3	2.27	0.49
1:B:603:PRO:O	1:B:606:HIS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:THR:HB	1:C:509:TRP:HE1	1.77	0.49
1:A:814:ILE:HG12	1:A:834:TRP:NE1	2.27	0.49
1:B:36:GLU:OE2	1:B:42:ASN:ND2	2.31	0.49
1:B:618:LEU:O	1:C:871:SER:OG	2.24	0.49
1:B:728:ASN:N	1:B:728:ASN:OD1	2.44	0.49
1:C:119:THR:OG1	1:C:120:ALA:N	2.44	0.49
1:B:482:CYS:HB2	1:B:529:MET:HB2	1.94	0.49
1:B:872:ARG:HA	1:B:873:GLN:HE21	1.76	0.49
1:C:740:ASN:OD1	1:C:741:TRP:N	2.45	0.49
1:B:605:ASN:OD1	1:B:773:SER:N	2.45	0.49
1:C:397:PHE:CE1	1:C:619:LEU:HD11	2.47	0.49
1:C:402:ILE:HD11	1:C:435:GLU:HB3	1.94	0.49
1:C:480:ASN:N	1:C:480:ASN:HD22	2.10	0.49
1:A:640:ASN:HB3	1:C:44:LYS:NZ	2.28	0.49
1:B:122:ASN:OD1	1:B:122:ASN:N	2.45	0.49
1:A:55:ASP:OD1	1:A:55:ASP:N	2.46	0.49
1:A:441:LEU:O	1:A:445:ILE:HG12	2.13	0.49
1:B:628:HIS:NE2	1:C:824:ASN:O	2.44	0.49
1:B:892:HIS:O	1:B:892:HIS:ND1	2.37	0.49
1:A:836:LEU:HD12	1:A:850:PHE:HZ	1.78	0.48
1:A:894:ASN:N	1:C:122:ASN:OD1	2.41	0.48
1:B:427:VAL:H	1:B:1009:TYR:HE2	1.61	0.48
1:C:94:LEU:HD13	1:C:688:PHE:CE1	2.47	0.48
1:B:124:LEU:HD21	1:C:536:ASN:CG	2.38	0.48
1:C:78:TYR:HA	1:C:656:LYS:HD3	1.95	0.48
1:C:298:THR:HG23	1:C:324:LYS:HA	1.94	0.48
1:B:81:LYS:NZ	1:B:651:GLU:OE2	2.25	0.48
1:C:198:ASN:OD1	1:C:199:LYS:N	2.39	0.48
1:C:212:GLN:NE2	1:C:213:ILE:HG13	2.29	0.48
1:B:612:LEU:HD21	1:B:663:GLN:HG2	1.95	0.48
1:A:525:ASN:OD1	1:A:525:ASN:N	2.46	0.48
1:B:287:THR:O	1:B:309:GLU:N	2.44	0.48
1:B:447:ASP:OD1	1:B:448:ARG:N	2.46	0.48
1:B:756:GLU:OE1	1:B:782:TYR:OH	2.27	0.48
1:C:96:MET:SD	1:C:99:THR:OG1	2.72	0.48
1:A:481:TYR:CD2	1:C:906:ARG:HB3	2.47	0.48
1:A:481:TYR:OH	1:C:905:MET:HA	2.13	0.48
1:B:450:ARG:HH22	1:C:865:ARG:NE	2.11	0.48
1:A:303:GLN:HB3	1:A:305:VAL:HG13	1.96	0.48
1:A:998:HIS:CD2	1:A:1000:PRO:HD3	2.49	0.48
1:B:747:TRP:NE1	1:B:972:MET:SD	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:764:TYR:HD2	1:C:766:PRO:HG3	1.78	0.48
1:A:432:ARG:NH2	1:A:993:ASP:OD1	2.46	0.48
1:B:997:VAL:HG22	1:B:1007:THR:HG22	1.95	0.48
1:C:279:GLU:OE1	1:C:344:LYS:NZ	2.46	0.48
1:A:471:ASN:ND2	1:A:473:GLY:H	2.12	0.48
1:A:604:PHE:HZ	1:A:937:ARG:HD3	1.78	0.48
1:A:800:TRP:HA	1:A:801:PRO:C	2.38	0.48
1:C:58:THR:HB	1:C:692:ALA:HA	1.94	0.48
1:C:673:ASP:O	1:C:675:ALA:N	2.39	0.48
1:B:68:PHE:HE2	1:B:86:LEU:HD12	1.78	0.48
1:B:806:LEU:HD13	1:B:833:ASP:HB3	1.95	0.48
1:B:858:ASP:CG	1:B:865:ARG:HH22	2.22	0.48
1:C:454:MET:C	1:C:455:TRP:HE3	2.21	0.48
1:A:89:GLY:HA3	1:A:92:ARG:NH2	2.29	0.47
1:A:574:ASN:O	1:A:574:ASN:ND2	2.45	0.47
1:A:245:ALA:HB3	1:A:254:GLN:CD	2.39	0.47
1:A:876:ASP:OD2	1:A:879:LYS:N	2.42	0.47
1:B:36:GLU:CD	1:B:42:ASN:HD21	2.21	0.47
1:B:328:VAL:HG22	1:B:343:ILE:HD12	1.96	0.47
1:C:391:ARG:NH2	1:C:666:LEU:HD21	2.30	0.47
1:A:91:ASN:OD1	1:A:91:ASN:N	2.47	0.47
1:B:391:ARG:HD3	1:B:574:ASN:HA	1.95	0.47
1:C:789:LYS:HG2	1:C:975:GLU:HB3	1.97	0.47
1:B:441:LEU:O	1:B:445:ILE:HG12	2.14	0.47
1:B:740:ASN:OD1	1:B:742:ALA:N	2.47	0.47
1:B:785:HIS:O	1:B:785:HIS:ND1	2.47	0.47
1:C:967:ALA:O	1:C:968:HIS:CG	2.68	0.47
1:A:92:ARG:HD2	1:A:688:PHE:HE2	1.80	0.47
1:A:834:TRP:CZ3	1:A:838:GLN:HG2	2.49	0.47
1:B:41:LEU:HA	1:B:41:LEU:HD22	1.74	0.47
1:B:525:ASN:ND2	1:C:215:GLU:OE1	2.47	0.47
1:B:779:GLY:O	1:B:861:TYR:OH	2.22	0.47
1:C:408:ASN:ND2	1:C:408:ASN:O	2.48	0.47
1:A:91:ASN:HD22	1:A:693:HIS:CG	2.32	0.47
1:A:456:ASN:OD1	1:A:456:ASN:N	2.47	0.47
1:A:685:TYR:CD2	1:B:832:LYS:HE3	2.49	0.47
1:A:953:ALA:N	1:C:49:THR:OG1	2.29	0.47
1:B:398:ARG:HH22	1:B:774:ILE:HG13	1.79	0.47
1:B:405:MET:HB2	1:B:407:TYR:OH	2.14	0.47
1:B:448:ARG:NH2	1:B:459:VAL:HB	2.30	0.47
1:B:807:LEU:N	1:B:833:ASP:OD2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:SER:OG	1:C:687:THR:OG1	2.02	0.47
1:C:655:ARG:CZ	1:C:660:MET:HG3	2.45	0.47
1:B:867:PHE:HD1	1:B:869:PRO:HD3	1.80	0.47
1:A:539:ARG:NE	1:A:584:ASP:OD2	2.48	0.47
1:A:762:SER:OG	1:A:764:TYR:O	2.25	0.47
1:B:623:ARG:NH1	1:B:624:TYR:OH	2.48	0.47
1:C:511:GLN:NE2	1:C:512:ASP:O	2.48	0.47
1:A:381:ALA:HB1	1:C:217:GLN:HE22	1.80	0.47
1:A:582:LEU:HD12	1:A:888:ILE:HG12	1.96	0.47
1:A:905:MET:HA	1:B:481:TYR:OH	2.15	0.47
1:A:986:TYR:OH	1:A:988:LEU:HD21	2.15	0.47
1:C:101:PHE:HD1	1:C:101:PHE:HA	1.63	0.47
1:C:277:THR:OG1	1:C:278:GLY:N	2.47	0.47
1:A:281:PRO:HA	1:A:341:GLY:HA2	1.97	0.46
1:A:326:GLU:OE2	1:C:495:GLN:NE2	2.40	0.46
1:A:454:MET:HE1	1:A:630:GLN:HB2	1.97	0.46
1:C:569:THR:OG1	1:C:570:TYR:N	2.48	0.46
1:C:955:THR:OG1	1:C:956:ASP:N	2.46	0.46
1:A:555:LYS:HD3	1:A:576:ARG:HG3	1.98	0.46
1:A:899:GLY:HA2	1:A:907:GLU:OE1	2.15	0.46
1:B:758:PRO:HA	1:B:768:TYR:CE2	2.50	0.46
1:A:39:PHE:HD1	1:A:40:SER:H	1.62	0.46
1:A:713:ASN:CG	1:C:46:ARG:HE	2.23	0.46
1:A:858:ASP:OD2	1:A:865:ARG:NH1	2.47	0.46
1:B:327:LYS:HD3	1:B:344:LYS:HD2	1.97	0.46
1:B:635:PHE:HE1	1:B:637:ALA:HB3	1.81	0.46
1:B:814:ILE:HG12	1:B:834:TRP:NE1	2.31	0.46
1:B:829:ASN:ND2	1:B:931:LYS:O	2.43	0.46
1:C:907:GLU:N	1:C:907:GLU:OE1	2.48	0.46
1:A:897:PHE:CE2	1:C:125:ALA:HA	2.50	0.46
1:B:296:GLY:HA2	1:B:324:LYS:HD3	1.96	0.46
1:B:114:LYS:NZ	1:B:390:ASN:HB2	2.30	0.46
1:C:641:LEU:HD21	1:C:997:VAL:HG11	1.97	0.46
1:A:239:PRO:HG2	1:A:387:SER:HB2	1.97	0.46
1:A:639:LYS:O	1:A:640:ASN:ND2	2.49	0.46
1:B:68:PHE:HE2	1:B:86:LEU:HA	1.80	0.46
1:B:281:PRO:HA	1:B:341:GLY:HA2	1.98	0.46
1:B:471:ASN:OD1	1:B:472:HIS:N	2.49	0.46
1:B:245:ALA:HB3	1:B:254:GLN:CD	2.40	0.46
1:B:612:LEU:HD12	1:B:612:LEU:HA	1.75	0.46
1:B:633:GLN:OE1	1:B:650:TYR:OH	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:915:VAL:HG13	1:C:916:PRO:CD	2.46	0.46
1:A:90:ASP:OD1	1:A:90:ASP:N	2.48	0.46
1:A:111:PRO:HD3	1:A:623:ARG:NH2	2.31	0.46
1:A:991:VAL:HB	1:A:1013:PRO:HD2	1.98	0.46
1:B:488:ILE:HG13	1:C:171:TYR:OH	2.16	0.46
1:C:593:TRP:CD2	1:C:872:ARG:HB3	2.51	0.46
1:A:173:GLN:OE1	1:C:488:ILE:HA	2.16	0.45
1:A:218:TRP:HA	1:B:905:MET:HE1	1.99	0.45
1:A:401:PHE:CE1	1:A:629:ILE:HD12	2.51	0.45
1:C:644:LEU:HD22	1:C:700:GLU:HG2	1.96	0.45
1:C:644:LEU:HD23	1:C:644:LEU:HA	1.75	0.45
1:C:904:THR:OG1	1:C:905:MET:N	2.49	0.45
1:C:967:ALA:O	1:C:968:HIS:ND1	2.49	0.45
1:A:396:ALA:HB2	1:A:616:SER:HA	1.99	0.45
1:B:396:ALA:HB2	1:B:616:SER:HA	1.98	0.45
1:B:426:VAL:HA	1:B:1009:TYR:OH	2.16	0.45
1:B:840:LEU:HA	1:B:845:ILE:O	2.17	0.45
1:C:323:GLY:HA3	1:C:346:GLY:HA2	1.98	0.45
1:C:663:GLN:HE21	1:C:663:GLN:C	2.24	0.45
1:C:723:TYR:CE2	1:C:734:ILE:HG21	2.52	0.45
1:A:398:ARG:HH12	1:A:774:ILE:H	1.65	0.45
1:A:602:ASN:CG	1:A:782:TYR:CZ	2.94	0.45
1:B:55:ASP:OD1	1:B:55:ASP:N	2.49	0.45
1:B:494:TYR:HD1	1:C:275:THR:HA	1.82	0.45
1:A:408:ASN:ND2	1:A:408:ASN:O	2.49	0.45
1:A:491:THR:HB	1:A:521:ILE:O	2.16	0.45
1:B:402:ILE:HD11	1:B:435:GLU:HB3	1.98	0.45
1:B:621:ASN:HD21	1:C:591:ALA:HB2	1.82	0.45
1:B:946:SER:HB3	1:B:957:LEU:HD11	1.99	0.45
1:C:602:ASN:CG	1:C:782:TYR:CZ	2.94	0.45
1:A:172:ALA:O	1:C:521:ILE:HG13	2.15	0.45
1:A:249:ASN:OD1	1:A:252:GLY:N	2.50	0.45
1:B:91:ASN:N	1:B:91:ASN:OD1	2.49	0.45
1:B:456:ASN:N	1:B:456:ASN:HD22	2.15	0.45
1:C:205:LYS:HB2	1:C:268:VAL:HG11	1.98	0.45
1:C:728:ASN:OD1	1:C:728:ASN:N	2.49	0.45
1:A:94:LEU:HD23	1:A:643:LEU:HD23	1.99	0.45
1:A:752:LEU:HA	1:A:752:LEU:HD23	1.69	0.45
1:A:897:PHE:CE2	1:C:126:PRO:HD3	2.52	0.45
1:B:644:LEU:HA	1:B:644:LEU:HD23	1.69	0.45
1:C:75:ASP:OD1	1:C:76:THR:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:SER:OG	1:A:687:THR:HB	2.17	0.45
1:A:212:GLN:N	1:A:212:GLN:OE1	2.50	0.45
1:A:406:TYR:HD1	1:A:406:TYR:HA	1.71	0.45
1:A:539:ARG:CZ	1:B:478:LEU:HD11	2.47	0.45
1:B:383:LEU:HD23	1:B:383:LEU:HA	1.77	0.45
1:C:612:LEU:HD21	1:C:663:GLN:NE2	2.32	0.45
1:C:819:ASP:OD2	1:C:824:ASN:N	2.49	0.45
1:A:331:LYS:HZ2	1:A:334:ASP:HB2	1.81	0.45
1:A:397:PHE:CE1	1:A:619:LEU:HD11	2.51	0.45
1:B:367:HIS:NE2	1:B:388:MET:SD	2.90	0.45
1:B:428:ASP:OD1	1:B:429:LEU:N	2.50	0.45
1:B:539:ARG:NE	1:B:584:ASP:OD2	2.48	0.45
1:A:377:ASP:N	1:A:377:ASP:OD1	2.49	0.44
1:B:218:TRP:HA	1:C:905:MET:HE1	1.99	0.44
1:B:636:PHE:HA	1:B:639:LYS:HD3	1.99	0.44
1:C:58:THR:OG1	1:C:59:ASP:N	2.50	0.44
1:C:397:PHE:HE1	1:C:619:LEU:HD11	1.82	0.44
1:C:507:THR:HB	1:C:509:TRP:NE1	2.31	0.44
1:C:870:MET:HE3	1:C:934:LEU:HB2	1.99	0.44
1:A:454:MET:HE2	1:A:455:TRP:CE3	2.52	0.44
1:B:593:TRP:CD2	1:B:872:ARG:HD3	2.52	0.44
1:C:304:THR:HB	1:C:318:ASN:HB3	1.98	0.44
1:C:899:GLY:HA2	1:C:907:GLU:OE1	2.17	0.44
1:A:137:GLU:OE1	1:A:169:HIS:NE2	2.50	0.44
1:B:806:LEU:HA	1:B:806:LEU:HD23	1.64	0.44
1:A:275:THR:HA	1:C:494:TYR:HD1	1.82	0.44
1:B:13:MET:HG3	1:C:1010:LEU:HD23	2.00	0.44
1:B:307:VAL:HG12	1:B:314:GLU:HB2	1.99	0.44
1:B:432:ARG:HH11	1:B:636:PHE:HE1	1.65	0.44
1:B:510:ALA:HA	1:C:324:LYS:HD2	1.99	0.44
1:B:824:ASN:N	1:B:824:ASN:OD1	2.50	0.44
1:C:281:PRO:HA	1:C:341:GLY:HA2	1.99	0.44
1:C:621:ASN:OD1	1:C:621:ASN:N	2.46	0.44
1:A:41:LEU:HA	1:A:41:LEU:HD23	1.72	0.44
1:A:866:ASN:O	1:A:935:CYS:HA	2.17	0.44
1:B:10:TRP:CZ3	1:C:962:LEU:HD22	2.53	0.44
1:C:448:ARG:NH2	1:C:459:VAL:HB	2.32	0.44
1:C:459:VAL:HG22	1:C:460:ASP:H	1.83	0.44
1:C:825:VAL:HG11	1:C:832:LYS:HA	2.00	0.44
1:B:53:THR:HG22	1:C:959:GLN:HG3	2.00	0.44
1:A:413:MET:SD	1:A:428:ASP:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:SER:OG	1:A:948:PHE:N	2.51	0.44
1:B:120:ALA:HB1	1:C:586:TYR:HB3	2.00	0.44
1:B:239:PRO:HG3	1:B:385:GLN:HB2	2.00	0.44
1:B:303:GLN:HE21	1:B:305:VAL:CG1	2.31	0.44
1:B:533:LEU:HA	1:B:533:LEU:HD22	1.83	0.44
1:B:691:MET:HE3	1:B:691:MET:HB2	1.86	0.44
1:C:961:LEU:HD23	1:C:961:LEU:HA	1.82	0.44
1:A:13:MET:HG3	1:B:1010:LEU:HD23	1.99	0.44
1:A:593:TRP:CE3	1:A:872:ARG:HB3	2.53	0.44
1:A:740:ASN:OD1	1:A:742:ALA:N	2.51	0.44
1:B:536:ASN:ND2	1:C:480:ASN:OD1	2.51	0.44
1:C:406:TYR:HD1	1:C:406:TYR:HA	1.70	0.44
1:A:668:ASN:HD21	1:A:670:LEU:HD23	1.83	0.43
1:A:812:PHE:HE2	1:A:942:ILE:HD13	1.83	0.43
1:B:327:LYS:HG2	1:B:344:LYS:HB2	2.00	0.43
1:C:643:LEU:HG	1:C:648:TYR:HE2	1.83	0.43
1:A:658:VAL:HB	1:A:662:LEU:HD12	2.00	0.43
1:B:212:GLN:NE2	1:B:213:ILE:HG13	2.33	0.43
1:B:509:TRP:CZ2	1:C:350:PRO:HG3	2.53	0.43
1:B:574:ASN:O	1:B:574:ASN:ND2	2.50	0.43
1:B:591:ALA:O	1:B:593:TRP:N	2.51	0.43
1:B:725:ILE:HB	1:B:983:THR:OG1	2.18	0.43
1:C:243:SER:HB3	1:C:361:MET:SD	2.58	0.43
1:C:295:GLU:HA	1:C:327:LYS:HA	2.00	0.43
1:C:406:TYR:CZ	1:C:655:ARG:HG3	2.54	0.43
1:A:46:ARG:NE	1:B:713:ASN:OD1	2.52	0.43
1:B:44:LYS:NZ	1:C:640:ASN:HB3	2.33	0.43
1:B:111:PRO:N	1:B:623:ARG:HE	2.15	0.43
1:B:200:GLU:H	1:B:200:GLU:HG3	1.62	0.43
1:B:367:HIS:ND1	1:B:390:ASN:OD1	2.45	0.43
1:B:471:ASN:ND2	1:B:589:LEU:HD12	2.32	0.43
1:C:441:LEU:HD13	1:C:715:TYR:HB2	2.00	0.43
1:A:603:PRO:O	1:A:606:HIS:HB2	2.18	0.43
1:B:566:ASN:OD1	1:B:568:ASN:N	2.49	0.43
1:B:998:HIS:CD2	1:B:1000:PRO:HD3	2.53	0.43
1:C:68:PHE:HB2	1:C:684:LEU:HB3	1.99	0.43
1:C:309:GLU:OE1	1:C:312:LYS:N	2.47	0.43
1:C:656:LYS:HE2	1:C:656:LYS:HB3	1.85	0.43
1:A:475:GLU:O	1:C:540:ASN:ND2	2.46	0.43
1:B:38:TYR:HD1	1:B:38:TYR:H	1.66	0.43
1:B:415:VAL:HA	1:B:424:ASN:HD21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:845:ILE:HG12	1:B:851:TYR:HE1	1.84	0.43
1:C:55:ASP:N	1:C:55:ASP:OD1	2.47	0.43
1:C:437:SER:HB2	1:C:714:ASP:OD1	2.18	0.43
1:A:472:HIS:CD2	1:C:613:ARG:HD2	2.54	0.43
1:A:544:SER:OG	1:B:477:GLU:OE2	2.33	0.43
1:A:602:ASN:HD21	1:A:756:GLU:CD	2.25	0.43
1:A:858:ASP:CG	1:A:865:ARG:HH22	2.27	0.43
1:B:416:LEU:HD12	1:B:650:TYR:CD1	2.53	0.43
1:B:838:GLN:HB3	1:B:863:PHE:HE2	1.84	0.43
1:C:416:LEU:HD12	1:C:650:TYR:CD1	2.53	0.43
1:C:485:LEU:HD23	1:C:485:LEU:HA	1.89	0.43
1:C:755:LYS:HE2	1:C:755:LYS:HB3	1.75	0.43
1:A:243:SER:HB3	1:A:361:MET:SD	2.58	0.43
1:A:644:LEU:HA	1:A:644:LEU:HD23	1.77	0.43
1:B:397:PHE:CE1	1:B:619:LEU:HD11	2.49	0.43
1:B:671:ARG:HE	1:B:671:ARG:HB2	1.65	0.43
1:B:750:THR:OG1	1:B:751:ARG:N	2.51	0.43
1:A:684:LEU:HD12	1:A:685:TYR:H	1.84	0.43
1:C:584:ASP:HB3	1:C:586:TYR:CE1	2.54	0.43
1:C:746:GLY:C	1:C:747:TRP:HD1	2.27	0.43
1:A:318:ASN:OD1	1:A:318:ASN:N	2.52	0.43
1:A:423:LEU:H	1:A:423:LEU:HG	1.45	0.43
1:A:441:LEU:HD13	1:A:715:TYR:HB2	2.00	0.43
1:A:745:ARG:HB2	1:A:990:GLU:O	2.19	0.43
1:B:659:ASN:OD1	1:B:671:ARG:HB2	2.18	0.43
1:A:203:ALA:HB1	1:A:208:GLN:HB2	2.01	0.42
1:A:407:TYR:HD2	1:A:635:PHE:HB2	1.84	0.42
1:B:248:THR:OG1	1:B:255:GLY:O	2.30	0.42
1:B:352:LEU:HD23	1:B:352:LEU:HA	1.87	0.42
1:B:441:LEU:HD13	1:B:715:TYR:HB2	2.01	0.42
1:B:604:PHE:HZ	1:B:937:ARG:HD3	1.84	0.42
1:B:730:THR:O	1:B:975:GLU:HG3	2.19	0.42
1:C:91:ASN:HD22	1:C:693:HIS:CD2	2.37	0.42
1:C:605:ASN:ND2	1:C:772:GLY:HA3	2.34	0.42
1:C:714:ASP:O	1:C:717:SER:OG	2.36	0.42
1:B:68:PHE:CE2	1:B:86:LEU:HA	2.55	0.42
1:B:76:THR:OG1	1:B:79:SER:O	2.31	0.42
1:B:621:ASN:ND2	1:C:591:ALA:HB2	2.34	0.42
1:B:659:ASN:OD1	1:B:671:ARG:NE	2.43	0.42
1:B:832:LYS:HE2	1:B:832:LYS:HB2	1.83	0.42
1:B:934:LEU:HD23	1:B:934:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:ASN:OD1	1:C:525:ASN:N	2.49	0.42
1:C:659:ASN:ND2	1:C:671:ARG:HB2	2.31	0.42
1:A:13:MET:HB3	1:B:994:VAL:HG21	2.00	0.42
1:A:401:PHE:O	1:A:404:LEU:HB2	2.20	0.42
1:C:94:LEU:HD13	1:C:688:PHE:HE1	1.84	0.42
1:C:398:ARG:HG2	1:C:663:GLN:HB2	2.02	0.42
1:A:385:GLN:H	1:A:385:GLN:HG2	1.52	0.42
1:A:859:ARG:O	1:A:865:ARG:NH1	2.52	0.42
1:B:249:ASN:HD21	1:B:253:GLY:N	2.17	0.42
1:B:328:VAL:HG13	1:B:330:VAL:HG22	2.01	0.42
1:B:620:GLY:HA3	1:C:873:GLN:NE2	2.34	0.42
1:C:282:ALA:HB2	1:C:342:LEU:HD21	2.01	0.42
1:C:738:SER:HA	1:C:968:HIS:O	2.19	0.42
1:C:778:ASP:OD1	1:C:779:GLY:N	2.52	0.42
1:A:416:LEU:HD13	1:A:650:TYR:CD1	2.53	0.42
1:A:613:ARG:O	1:A:617:MET:HG3	2.19	0.42
1:B:180:ALA:HA	1:B:225:VAL:HG11	2.02	0.42
1:B:783:LEU:HD23	1:B:783:LEU:HA	1.86	0.42
1:B:819:ASP:CG	1:B:822:GLY:H	2.26	0.42
1:C:311:MET:HE3	1:C:311:MET:HB3	1.91	0.42
1:C:549:TYR:OH	1:C:607:HIS:HB2	2.19	0.42
1:A:677:ILE:HD11	1:A:679:PHE:CE1	2.55	0.42
1:A:806:LEU:HD23	1:A:806:LEU:HA	1.68	0.42
1:A:828:CYS:SG	1:A:830:MET:N	2.88	0.42
1:B:432:ARG:O	1:B:434:THR:N	2.52	0.42
1:B:659:ASN:ND2	1:B:670:LEU:HB2	2.35	0.42
1:C:455:TRP:CD1	1:C:632:PRO:HG3	2.54	0.42
1:C:785:HIS:O	1:C:785:HIS:ND1	2.53	0.42
1:A:612:LEU:HA	1:A:612:LEU:HD12	1.73	0.42
1:B:753:LYS:NZ	1:B:981:GLU:OE2	2.39	0.42
1:C:41:LEU:HD23	1:C:41:LEU:HA	1.78	0.42
1:A:274:SER:OG	1:A:275:THR:N	2.53	0.42
1:A:283:PRO:HG2	1:A:284:LEU:HD23	2.01	0.42
1:A:424:ASN:OD1	1:A:425:ALA:N	2.53	0.42
1:A:657:ASP:HB2	1:A:764:TYR:CE2	2.54	0.42
1:B:114:LYS:HZ2	1:B:390:ASN:HB2	1.84	0.42
1:B:588:ASN:OD1	1:B:872:ARG:NH1	2.49	0.42
1:C:24:LEU:HD11	1:C:45:PHE:CE2	2.55	0.42
1:C:96:MET:O	1:C:99:THR:N	2.53	0.42
1:C:593:TRP:CE3	1:C:872:ARG:HB3	2.55	0.42
1:C:944:PHE:CE2	1:C:957:LEU:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:HD11	1:A:777:LEU:HB3	2.01	0.42
1:A:591:ALA:N	1:C:617:MET:HE2	2.35	0.42
1:A:972:MET:HE2	1:A:974:PHE:HE1	1.84	0.42
1:B:467:ARG:HD3	1:B:603:PRO:HB3	2.01	0.42
1:C:304:THR:HA	1:C:318:ASN:HA	2.00	0.42
1:C:814:ILE:O	1:C:831:THR:HG23	2.20	0.42
1:C:826:ALA:C	1:C:828:CYS:H	2.28	0.42
1:A:402:ILE:CD1	1:A:777:LEU:HB3	2.50	0.42
1:A:822:GLY:HA3	1:C:104:ARG:NH1	2.35	0.42
1:B:474:THR:HG21	1:B:535:ALA:HA	2.01	0.42
1:B:566:ASN:CG	1:B:568:ASN:H	2.28	0.42
1:B:598:MET:HE3	1:B:598:MET:HB3	1.87	0.42
1:C:539:ARG:NE	1:C:584:ASP:OD2	2.51	0.42
1:C:566:ASN:CG	1:C:568:ASN:H	2.28	0.42
1:A:210:GLU:HB3	1:A:212:GLN:OE1	2.20	0.41
1:A:391:ARG:NH2	1:A:666:LEU:HD11	2.35	0.41
1:A:904:THR:OG1	1:A:905:MET:N	2.54	0.41
1:B:954:LEU:HD23	1:B:959:GLN:HE21	1.85	0.41
1:A:68:PHE:HE2	1:A:86:LEU:HD12	1.85	0.41
1:A:595:LEU:HD23	1:A:595:LEU:HA	1.88	0.41
1:C:432:ARG:O	1:C:434:THR:N	2.53	0.41
1:C:747:TRP:CZ3	1:C:792:ILE:HD12	2.55	0.41
1:A:892:HIS:NE2	1:C:254:GLN:OE1	2.45	0.41
1:C:19:ASP:OD1	1:C:19:ASP:N	2.52	0.41
1:A:407:TYR:CD2	1:A:635:PHE:HB2	2.55	0.41
1:A:825:VAL:HG11	1:A:832:LYS:HG3	2.01	0.41
1:C:998:HIS:CD2	1:C:1000:PRO:HD3	2.56	0.41
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.84	0.41
1:B:113:PHE:CZ	1:B:115:PRO:HD3	2.56	0.41
1:C:67:ARG:HG3	1:C:685:TYR:CE1	2.55	0.41
1:A:636:PHE:CZ	1:A:714:ASP:HB2	2.55	0.41
1:A:961:LEU:HD23	1:A:961:LEU:HA	1.91	0.41
1:B:249:ASN:OD1	1:B:251:ASN:N	2.54	0.41
1:B:280:ILE:HD11	1:B:320:PRO:HD3	2.02	0.41
1:B:450:ARG:HH22	1:C:865:ARG:HE	1.66	0.41
1:B:750:THR:OG1	1:B:784:ASN:OD1	2.23	0.41
1:B:752:LEU:HD23	1:B:752:LEU:HA	1.86	0.41
1:C:858:ASP:CG	1:C:865:ARG:HH22	2.29	0.41
1:A:367:HIS:O	1:A:387:SER:OG	2.24	0.41
1:A:483:PHE:CE1	1:C:897:PHE:HD2	2.39	0.41
1:A:827:GLN:OE1	1:C:618:LEU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:951:MET:HE3	1:C:51:ALA:HB1	2.03	0.41
1:B:89:GLY:HA2	1:B:645:PRO:HB3	2.02	0.41
1:B:402:ILE:C	1:B:404:LEU:H	2.28	0.41
1:B:834:TRP:CZ3	1:B:838:GLN:HG2	2.55	0.41
1:A:68:PHE:HE2	1:A:86:LEU:HA	1.86	0.41
1:A:477:GLU:OE2	1:C:544:SER:OG	2.33	0.41
1:A:734:ILE:CG1	1:A:972:MET:HB2	2.51	0.41
1:B:28:LEU:HD12	1:C:702:MET:HG2	2.02	0.41
1:B:203:ALA:HB1	1:B:208:GLN:HB2	2.03	0.41
1:B:393:ASN:OD1	1:B:666:LEU:HB2	2.21	0.41
1:B:656:LYS:HE2	1:B:656:LYS:HB3	1.93	0.41
1:C:68:PHE:HE2	1:C:86:LEU:HA	1.86	0.41
1:C:745:ARG:HB3	1:C:990:GLU:O	2.20	0.41
1:C:788:LYS:HD2	1:C:977:ASP:OD1	2.21	0.41
1:C:941:ARG:HH11	1:C:941:ARG:HB3	1.86	0.41
1:A:251:ASN:HA	1:B:890:HIS:HD2	1.85	0.41
1:A:405:MET:HE2	1:A:405:MET:HB3	1.82	0.41
1:A:643:LEU:HD12	1:A:643:LEU:HA	1.85	0.41
1:A:922:LYS:H	1:A:922:LYS:HG3	1.68	0.41
1:A:1004:VAL:HG12	1:A:1005:ILE:H	1.85	0.41
1:B:66:LEU:HD12	1:B:688:PHE:HE1	1.86	0.41
1:B:282:ALA:O	1:B:339:GLY:HA2	2.21	0.41
1:B:569:THR:HG23	1:B:572:TYR:H	1.85	0.41
1:B:572:TYR:CE1	1:B:576:ARG:HD3	2.56	0.41
1:B:956:ASP:O	1:B:959:GLN:N	2.38	0.41
1:C:200:GLU:HG3	1:C:201:ILE:HG12	2.03	0.41
1:C:288:VAL:HG12	1:C:289:SER:H	1.86	0.41
1:C:406:TYR:OH	1:C:655:ARG:HG3	2.20	0.41
1:C:915:VAL:HG22	1:C:916:PRO:HD3	2.03	0.41
1:A:814:ILE:HA	1:A:834:TRP:CD1	2.41	0.41
1:C:352:LEU:HD23	1:C:352:LEU:HA	1.88	0.41
1:C:806:LEU:HD22	1:C:807:LEU:H	1.86	0.41
1:C:814:ILE:HA	1:C:834:TRP:CD1	2.49	0.41
1:C:859:ARG:H	1:C:862:SER:HG	1.68	0.41
1:C:911:TYR:CD1	1:C:912:PRO:HD2	2.56	0.41
1:A:488:ILE:HG13	1:B:171:TYR:OH	2.21	0.40
1:A:640:ASN:HB3	1:C:44:LYS:HZ2	1.86	0.40
1:A:750:THR:OG1	1:A:751:ARG:N	2.54	0.40
1:A:957:LEU:HD23	1:A:957:LEU:HA	1.93	0.40
1:B:432:ARG:HE	1:B:432:ARG:HB2	1.69	0.40
1:C:440:LEU:HD23	1:C:440:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:806:LEU:HD23	1:C:806:LEU:HA	1.78	0.40
1:A:398:ARG:HH22	1:A:774:ILE:H	1.69	0.40
1:A:633:GLN:CD	1:A:638:ILE:HD11	2.46	0.40
1:B:311:MET:HE2	1:B:311:MET:HB3	1.98	0.40
1:B:373:GLY:C	1:B:560:ASN:HD22	2.29	0.40
1:A:14:HIS:CE1	1:A:23:TYR:CZ	3.09	0.40
1:A:81:LYS:HE3	1:A:81:LYS:HB2	1.75	0.40
1:A:175:PRO:HG3	1:B:909:GLN:HB3	2.03	0.40
1:A:230:VAL:O	1:A:356:SER:HA	2.21	0.40
1:A:448:ARG:NH2	1:A:459:VAL:HB	2.36	0.40
1:A:501:ASN:HB3	1:A:506:ALA:HB1	2.04	0.40
1:C:23:TYR:CE1	1:C:24:LEU:HG	2.56	0.40
1:C:167:LYS:H	1:C:167:LYS:HG2	1.46	0.40
1:C:295:GLU:CD	1:C:295:GLU:H	2.29	0.40
1:C:747:TRP:N	1:C:747:TRP:CD1	2.88	0.40
1:A:67:ARG:HG3	1:A:685:TYR:CE1	2.56	0.40
1:A:180:ALA:N	1:A:187:GLN:OE1	2.54	0.40
1:A:181:ILE:HD11	1:A:350:PRO:O	2.21	0.40
1:A:404:LEU:HD23	1:A:404:LEU:HA	1.83	0.40
1:B:863:PHE:C	1:B:863:PHE:CD1	2.99	0.40
1:C:691:MET:HE3	1:C:691:MET:HB2	1.87	0.40
1:B:243:SER:HB3	1:B:361:MET:SD	2.62	0.40
1:B:897:PHE:HD2	1:C:483:PHE:CZ	2.39	0.40
1:C:212:GLN:OE1	1:C:212:GLN:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	984/991 (99%)	845 (86%)	139 (14%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	986/991 (100%)	841 (85%)	145 (15%)	0	100	100
1	C	983/991 (99%)	822 (84%)	161 (16%)	0	100	100
All	All	2953/2973 (99%)	2508 (85%)	445 (15%)	0	100	100

There are no Ramachandran outliers to report.

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	844/845 (100%)	745 (88%)	99 (12%)	5	23
1	B	844/845 (100%)	734 (87%)	110 (13%)	4	20
1	C	842/845 (100%)	735 (87%)	107 (13%)	4	20
All	All	2530/2535 (100%)	2214 (88%)	316 (12%)	7	21

All (316) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MET
1	A	28	LEU
1	A	39	PHE
1	A	42	ASN
1	A	49	THR
1	A	55	ASP
1	A	58	THR
1	A	65	THR
1	A	71	VAL
1	A	78	TYR
1	A	91	ASN
1	A	102	ASP
1	A	113	PHE
1	A	114	LYS
1	A	186	LEU
1	A	187	GLN

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Mol	Chain	Res	Type
1	A	199	LYS
1	A	218	TRP
1	A	219	ASN
1	A	237	MET
1	A	241	TYR
1	A	244	TYR
1	A	279	GLU
1	A	294	LYS
1	A	304	THR
1	A	324	LYS
1	A	359	VAL
1	A	360	ASN
1	A	377	ASP
1	A	378	ASN
1	A	382	MET
1	A	385	GLN
1	A	386	GLN
1	A	399	ASP
1	A	406	TYR
1	A	422	GLN
1	A	423	LEU
1	A	427	VAL
1	A	449	THR
1	A	455	TRP
1	A	456	ASN
1	A	457	GLN
1	A	460	ASP
1	A	471	ASN
1	A	475	GLU
1	A	497	ILE
1	A	507	THR
1	A	525	ASN
1	A	529	MET
1	A	533	LEU
1	A	536	ASN
1	A	537	LEU
1	A	545	ASN
1	A	554	LEU
1	A	561	VAL
1	A	563	ILE
1	A	571	ASP
1	A	574	ASN

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Mol	Chain	Res	Type
1	A	602	ASN
1	A	621	ASN
1	A	625	VAL
1	A	629	ILE
1	A	652	TRP
1	A	657	ASP
1	A	666	LEU
1	A	672	VAL
1	A	677	ILE
1	A	682	ILE
1	A	703	LEU
1	A	717	SER
1	A	728	ASN
1	A	768	TYR
1	A	786	THR
1	A	787	PHE
1	A	792	ILE
1	A	803	ASN
1	A	825	VAL
1	A	829	ASN
1	A	831	THR
1	A	834	TRP
1	A	836	LEU
1	A	845	ILE
1	A	848	GLN
1	A	873	GLN
1	A	875	VAL
1	A	889	ILE
1	A	915	VAL
1	A	920	ILE
1	A	925	VAL
1	A	936	ASP
1	A	937	ARG
1	A	945	SER
1	A	954	LEU
1	A	955	THR
1	A	975	GLU
1	A	1001	HIS
1	A	1004	VAL
1	A	1005	ILE
1	A	1012	THR
1	B	29	VAL

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Mol	Chain	Res	Type
1	B	35	THR
1	B	38	TYR
1	B	41	LEU
1	B	49	THR
1	B	55	ASP
1	B	58	THR
1	B	65	THR
1	B	66	LEU
1	B	76	THR
1	B	78	TYR
1	B	91	ASN
1	B	93	VAL
1	B	102	ASP
1	B	112	THR
1	B	113	PHE
1	B	122	ASN
1	B	167	LYS
1	B	170	VAL
1	B	173	GLN
1	B	186	LEU
1	B	190	THR
1	B	200	GLU
1	B	218	TRP
1	B	219	ASN
1	B	232	LYS
1	B	237	MET
1	B	244	TYR
1	B	251	ASN
1	B	261	ASN
1	B	288	VAL
1	B	291	ILE
1	B	294	LYS
1	B	307	VAL
1	B	312	LYS
1	B	331	LYS
1	B	333	ARG
1	B	378	ASN
1	B	382	MET
1	B	395	ILE
1	B	400	ASN
1	B	404	LEU
1	B	406	TYR

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Mol	Chain	Res	Type
1	B	412	ASN
1	B	423	LEU
1	B	431	ASP
1	B	434	THR
1	B	449	THR
1	B	460	ASP
1	B	474	THR
1	B	475	GLU
1	B	478	LEU
1	B	488	ILE
1	B	497	ILE
1	B	501	ASN
1	B	519	ASN
1	B	529	MET
1	B	531	ILE
1	B	533	LEU
1	B	536	ASN
1	B	561	VAL
1	B	563	ILE
1	B	571	ASP
1	B	574	ASN
1	B	583	VAL
1	B	587	ILE
1	B	598	MET
1	B	617	MET
1	B	630	GLN
1	B	652	TRP
1	B	655	ARG
1	B	663	GLN
1	B	666	LEU
1	B	672	VAL
1	B	677	ILE
1	B	682	ILE
1	B	687	THR
1	B	714	ASP
1	B	728	ASN
1	B	749	PHE
1	B	765	ASP
1	B	778	ASP
1	B	786	THR
1	B	787	PHE
1	B	790	VAL

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Mol	Chain	Res	Type
1	B	792	ILE
1	B	803	ASN
1	B	808	THR
1	B	824	ASN
1	B	828	CYS
1	B	829	ASN
1	B	831	THR
1	B	834	TRP
1	B	838	GLN
1	B	851	TYR
1	B	873	GLN
1	B	875	VAL
1	B	876	ASP
1	B	882	ASP
1	B	915	VAL
1	B	920	ILE
1	B	925	VAL
1	B	936	ASP
1	B	937	ARG
1	B	945	SER
1	B	947	ASN
1	B	966	SER
1	B	995	VAL
1	B	1001	HIS
1	B	1012	THR
1	C	12	TYR
1	C	15	ILE
1	C	28	LEU
1	C	35	THR
1	C	39	PHE
1	C	42	ASN
1	C	43	ASN
1	C	49	THR
1	C	55	ASP
1	C	69	ILE
1	C	91	ASN
1	C	93	VAL
1	C	96	MET
1	C	98	SER
1	C	101	PHE
1	C	167	LYS
1	C	170	VAL

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Mol	Chain	Res	Type
1	C	173	GLN
1	C	188	ILE
1	C	201	ILE
1	C	215	GLU
1	C	219	ASN
1	C	232	LYS
1	C	237	MET
1	C	244	TYR
1	C	254	GLN
1	C	288	VAL
1	C	290	LYS
1	C	291	ILE
1	C	304	THR
1	C	309	GLU
1	C	312	LYS
1	C	322	ASP
1	C	329	LEU
1	C	342	LEU
1	C	357	GLU
1	C	359	VAL
1	C	363	THR
1	C	377	ASP
1	C	382	MET
1	C	404	LEU
1	C	406	TYR
1	C	410	THR
1	C	412	ASN
1	C	415	VAL
1	C	426	VAL
1	C	431	ASP
1	C	455	TRP
1	C	460	ASP
1	C	467	ARG
1	C	471	ASN
1	C	480	ASN
1	C	497	ILE
1	C	529	MET
1	C	531	ILE
1	C	533	LEU
1	C	554	LEU
1	C	561	VAL
1	C	563	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	571	ASP
1	C	582	LEU
1	C	583	VAL
1	C	587	ILE
1	C	602	ASN
1	C	612	LEU
1	C	617	MET
1	C	652	TRP
1	C	655	ARG
1	C	657	ASP
1	C	663	GLN
1	C	666	LEU
1	C	668	ASN
1	C	672	VAL
1	C	677	ILE
1	C	682	ILE
1	C	687	THR
1	C	722	LEU
1	C	728	ASN
1	C	749	PHE
1	C	768	TYR
1	C	769	THR
1	C	778	ASP
1	C	787	PHE
1	C	803	ASN
1	C	806	LEU
1	C	807	LEU
1	C	811	GLU
1	C	812	PHE
1	C	825	VAL
1	C	828	CYS
1	C	829	ASN
1	C	833	ASP
1	C	834	TRP
1	C	836	LEU
1	C	838	GLN
1	C	875	VAL
1	C	882	ASP
1	C	911	TYR
1	C	920	ILE
1	C	925	VAL
1	C	936	ASP

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Mol	Chain	Res	Type
1	C	937	ARG
1	C	947	ASN
1	C	988	LEU
1	C	995	VAL
1	C	1001	HIS
1	C	1005	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	173	GLN
1	A	303	GLN
1	A	439	GLN
1	A	472	HIS
1	A	536	ASN
1	A	653	ASN
1	A	720	ASN
1	A	999	GLN
1	B	187	GLN
1	B	303	GLN
1	B	456	ASN
1	B	536	ASN
1	B	602	ASN
1	B	621	ASN
1	B	668	ASN
1	C	217	GLN
1	C	219	ASN
1	C	360	ASN
1	C	386	GLN
1	C	400	ASN
1	C	456	ASN
1	C	574	ASN
1	C	693	HIS
1	C	710	GLN
1	C	844	ASN
1	C	965	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	139:ASP	C	165:GLY	N	9.42
1	B	139:ASP	C	165:GLY	N	8.85
1	C	139:ASP	C	165:GLY	N	6.22

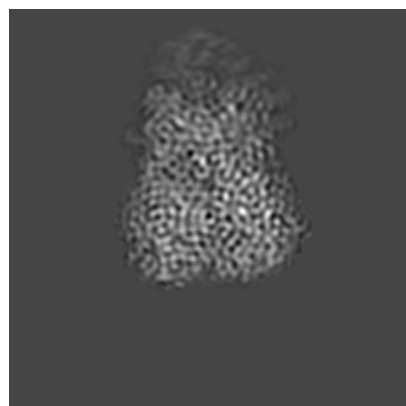
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75053. These allow visual inspection of the internal detail of the map and identification of artifacts.

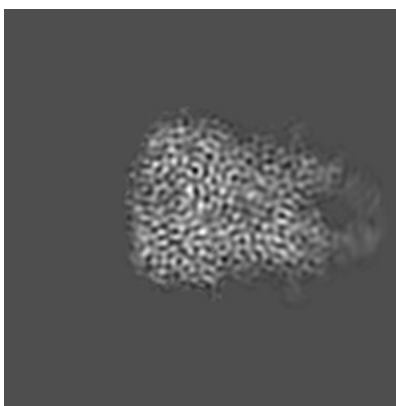
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

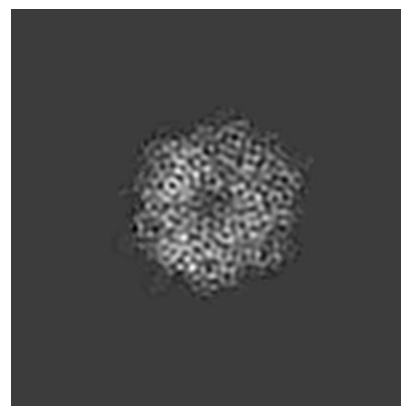
6.1.1 Primary map



X

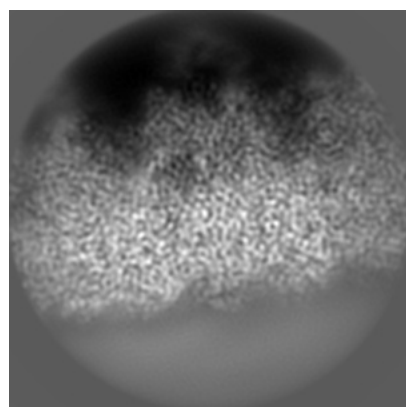


Y

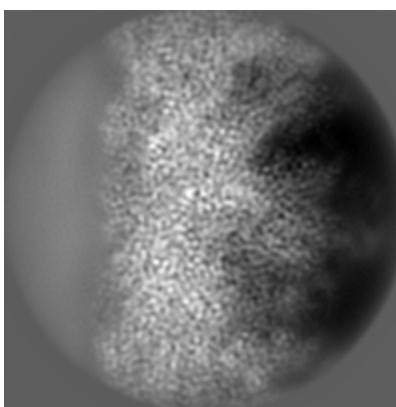


Z

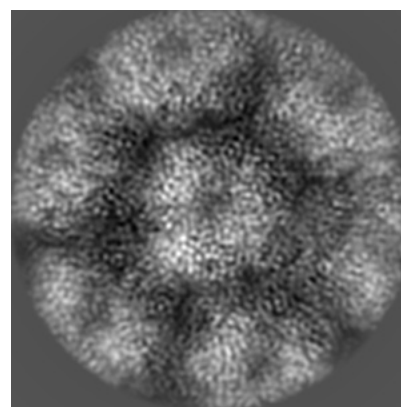
6.1.2 Raw map



X



Y

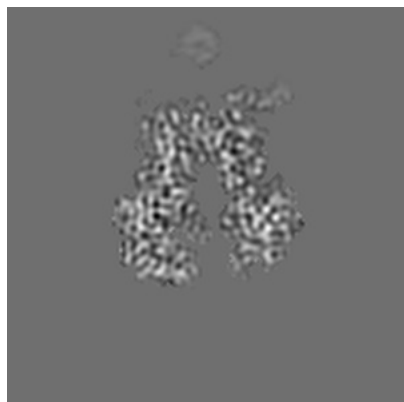


Z

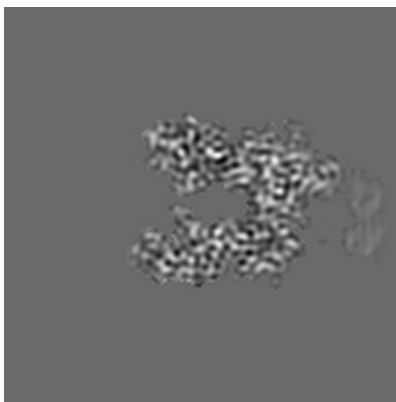
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

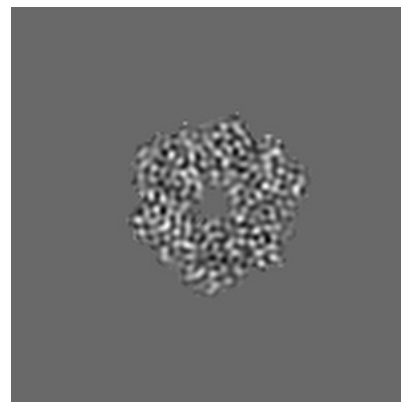
6.2.1 Primary map



X Index: 80

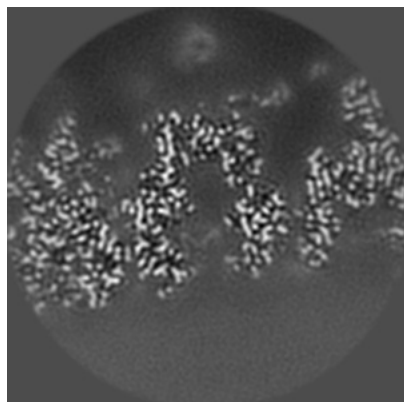


Y Index: 80

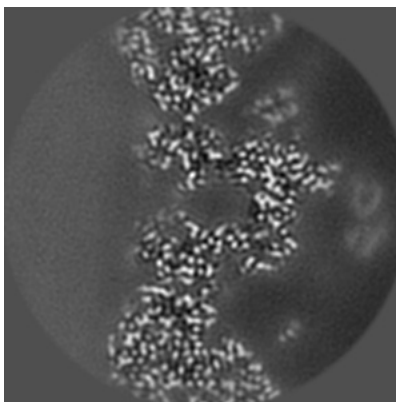


Z Index: 80

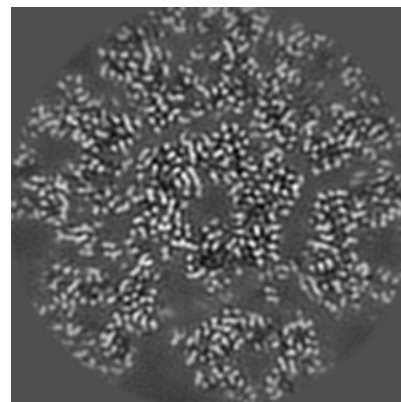
6.2.2 Raw map



X Index: 80



Y Index: 80

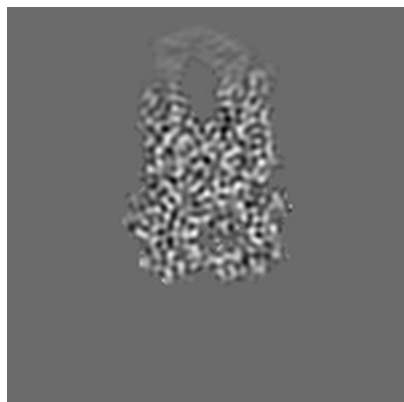


Z Index: 80

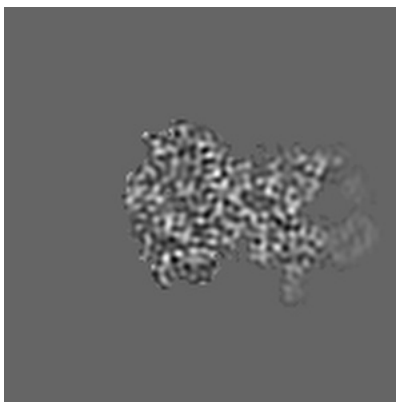
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

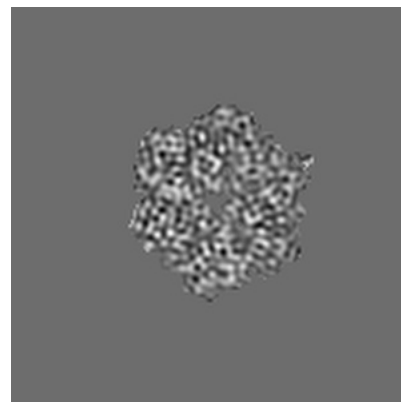
6.3.1 Primary map



X Index: 69

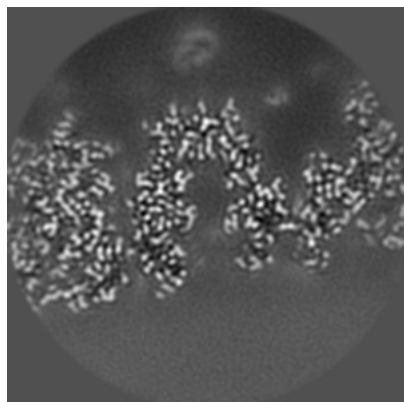


Y Index: 67

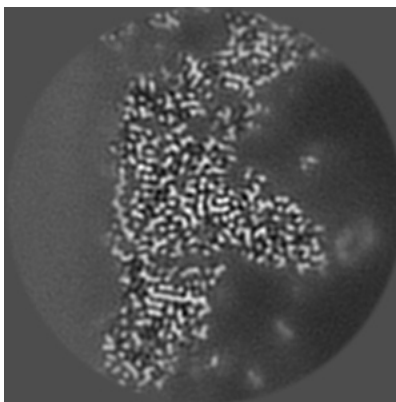


Z Index: 73

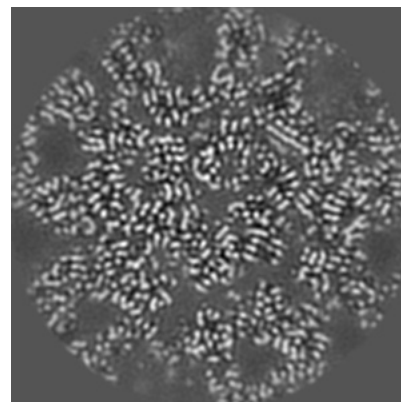
6.3.2 Raw map



X Index: 82



Y Index: 61

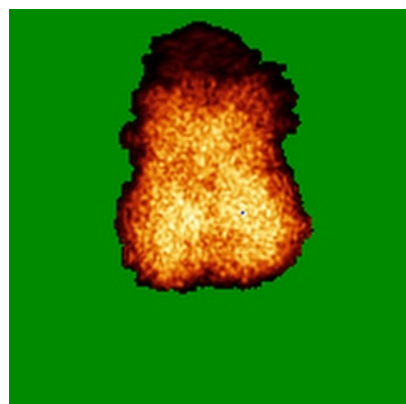


Z Index: 74

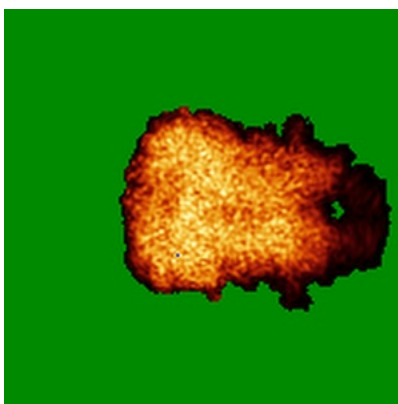
The images above show the largest variance slices of the map in three orthogonal directions.

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

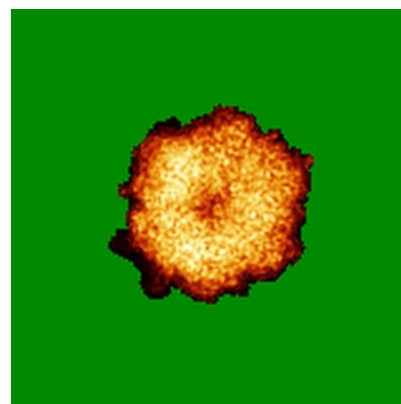
6.4.1 Primary map



X

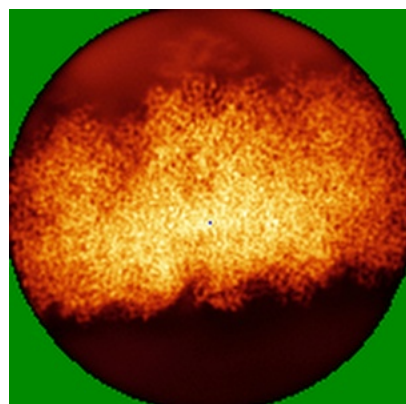


Y

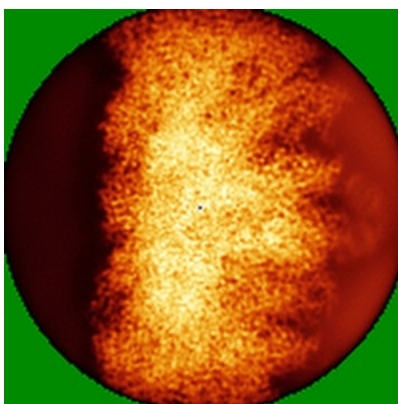


Z

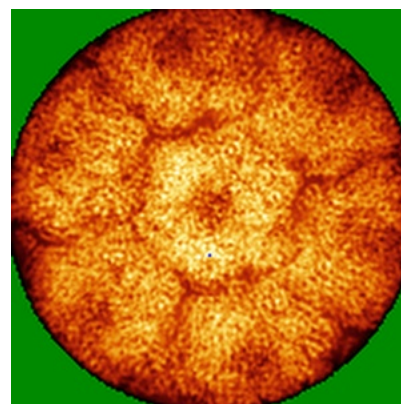
6.4.2 Raw map



X



Y

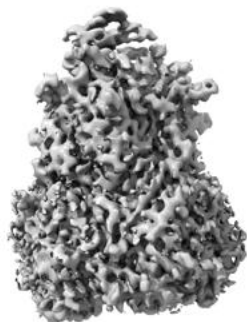


Z

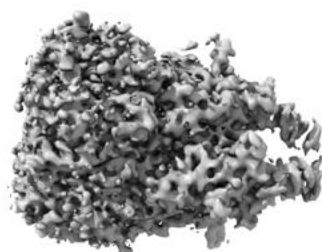
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

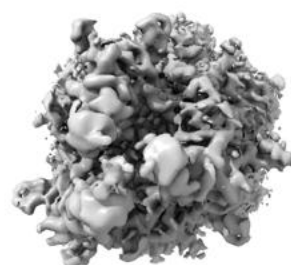
6.5.1 Primary map



X



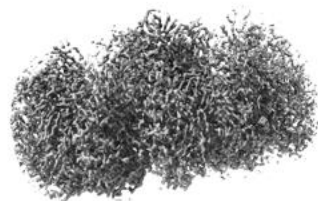
Y



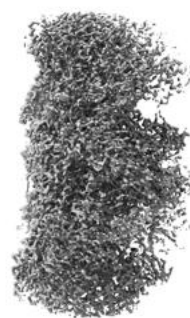
Z

The images above show the 3D surface view of the map at the recommended contour level 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

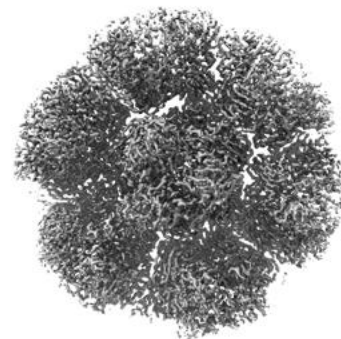
6.5.2 Raw map



X



Y



Z

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.

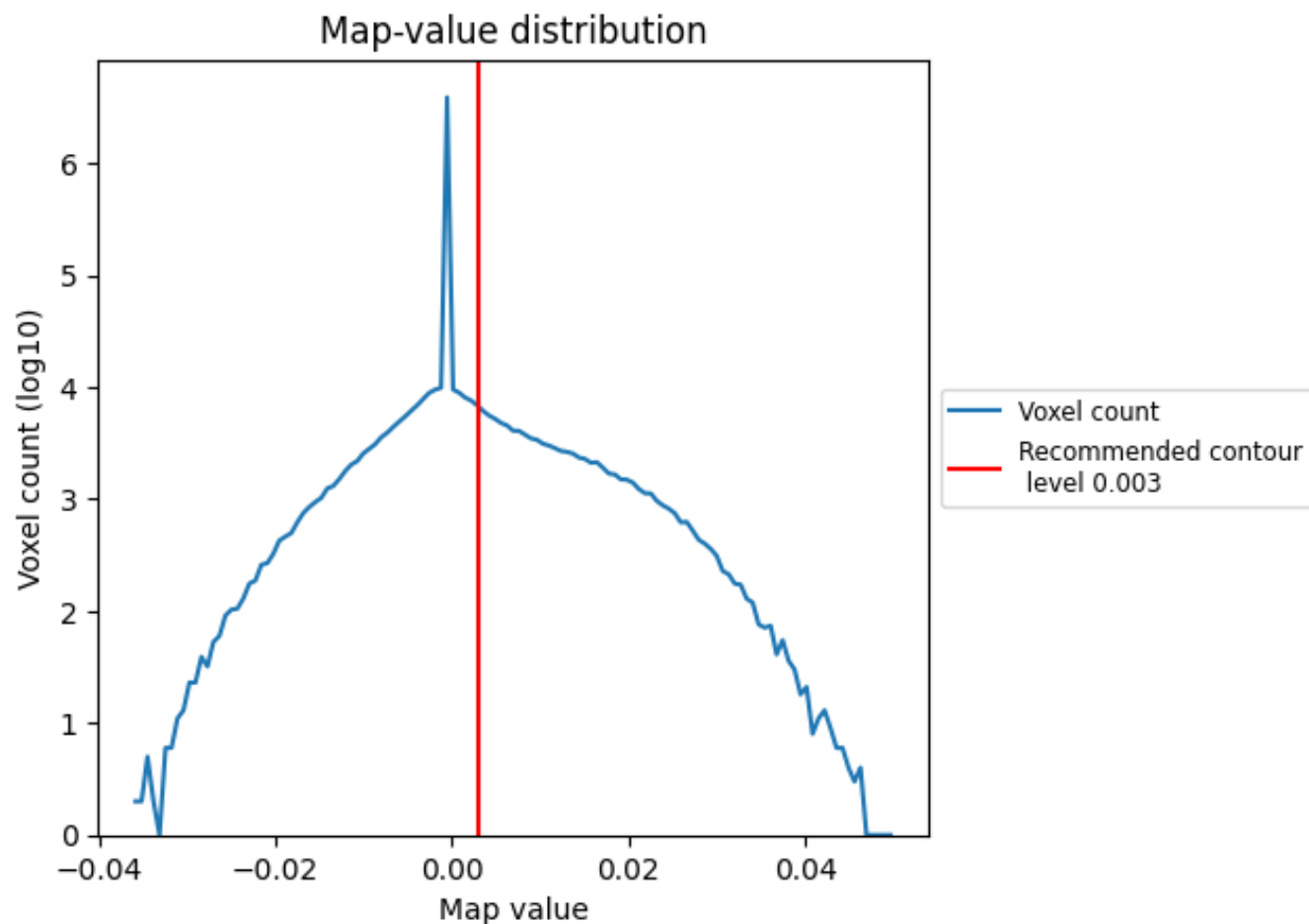
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

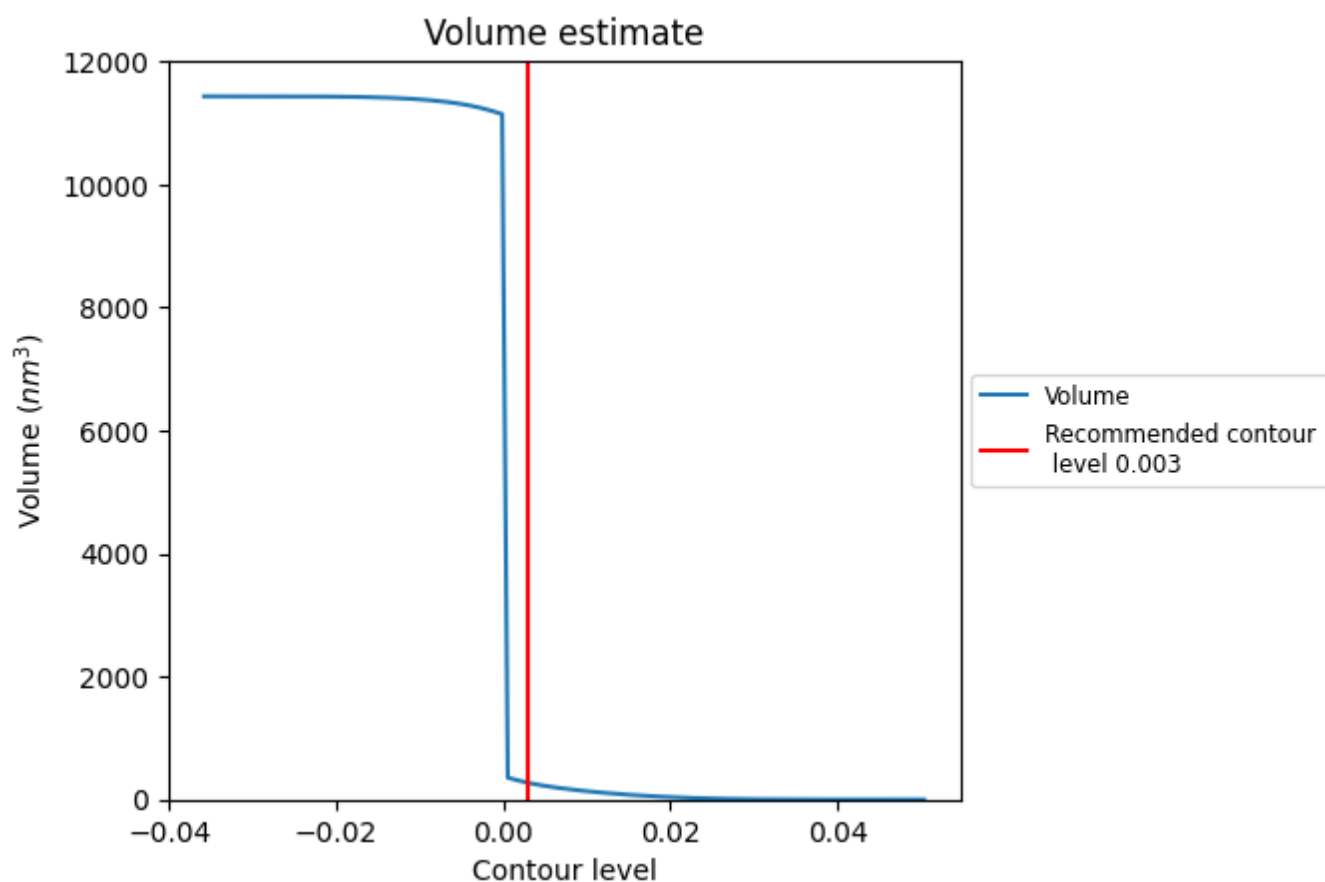
This section contains the results of statistical analysis of the map.

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.

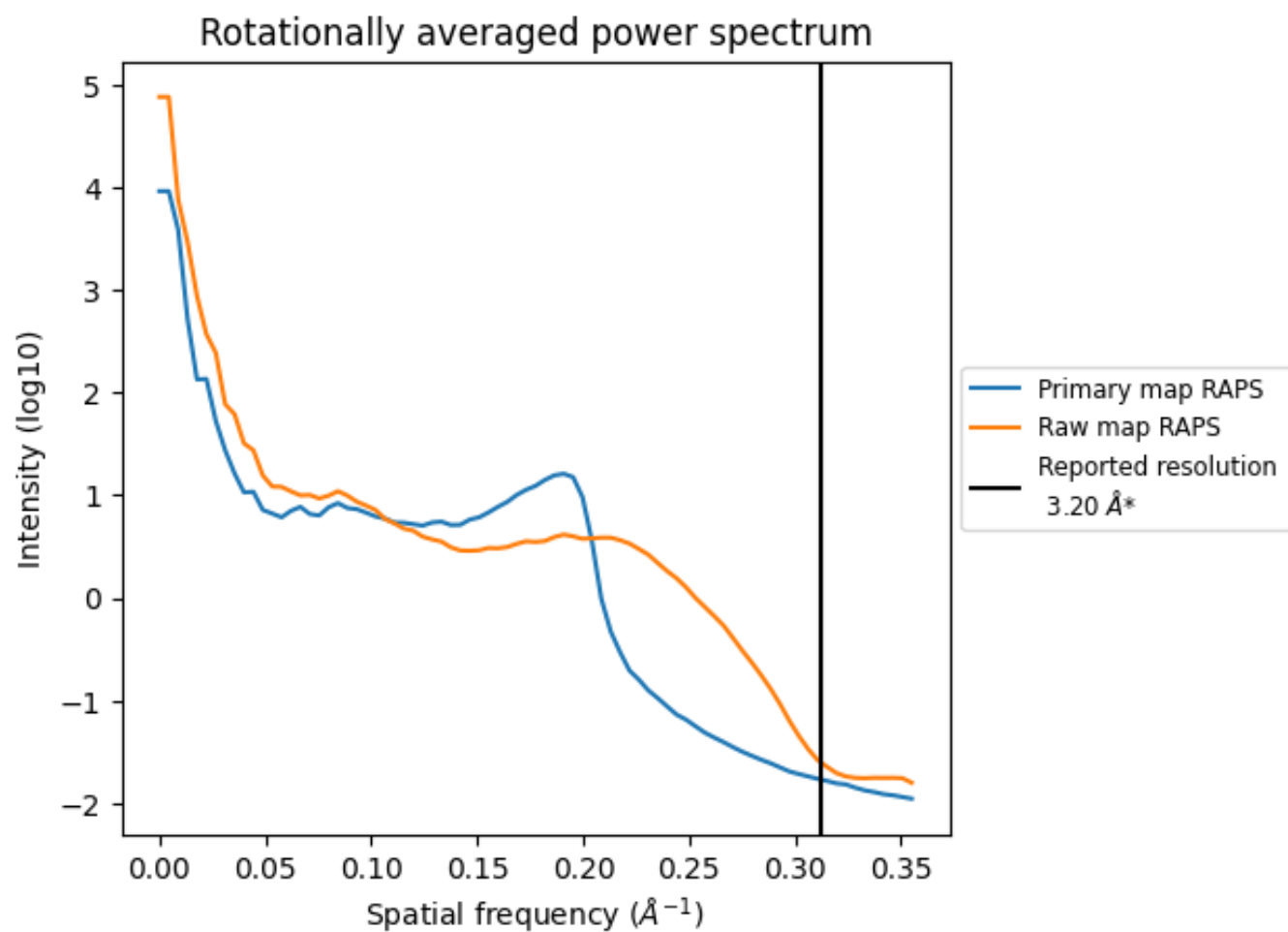
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 272 nm³; this corresponds to an approximate mass of 246 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 ⓘ

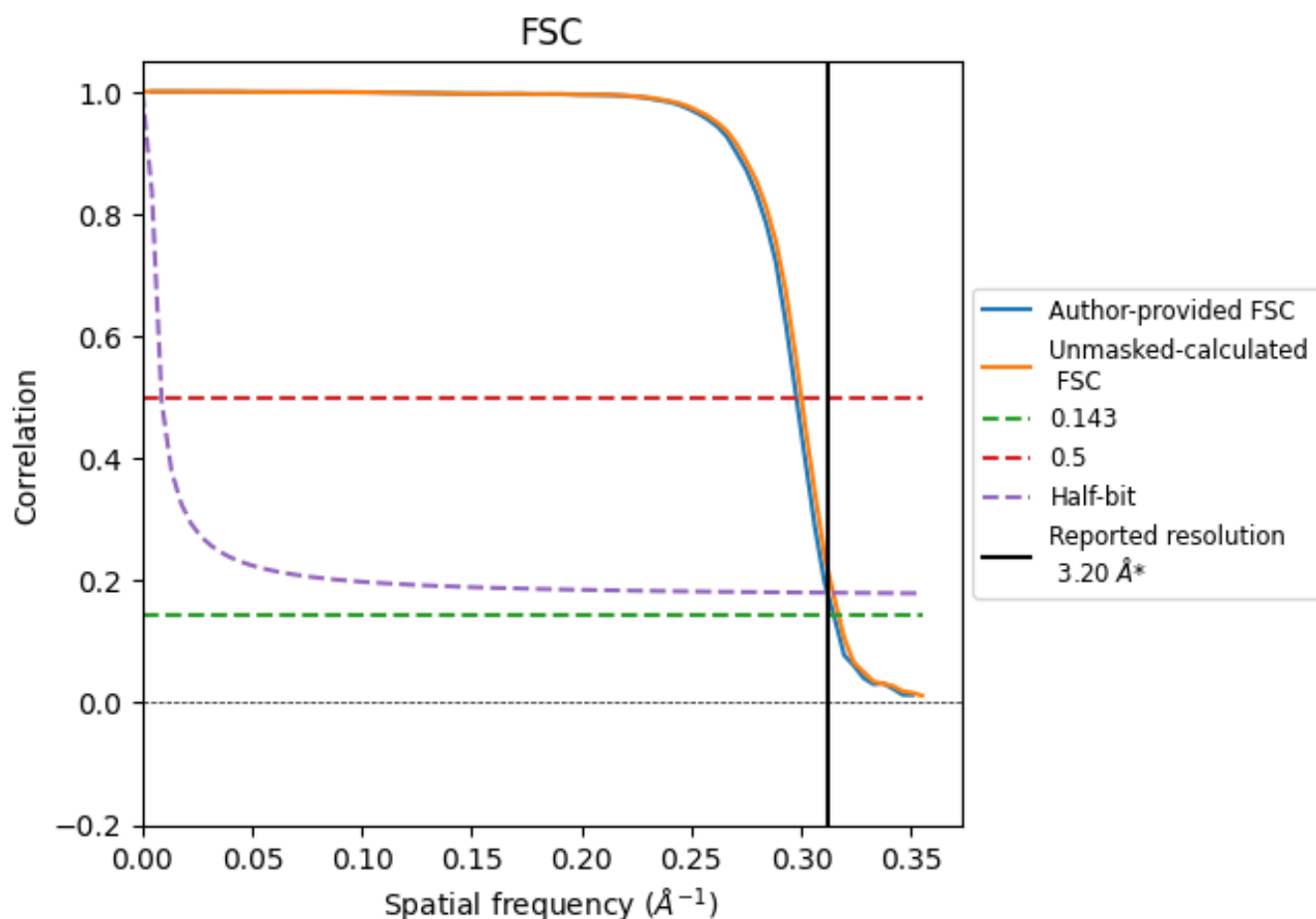


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

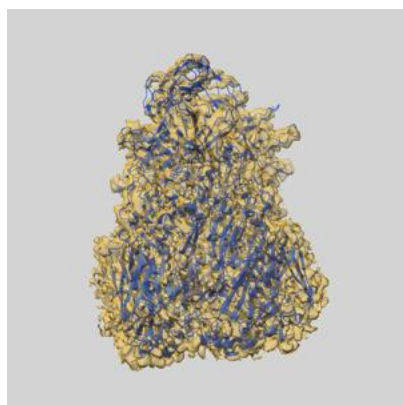
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.36	3.21
Unmasked-calculated*	3.15	3.33	3.18

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

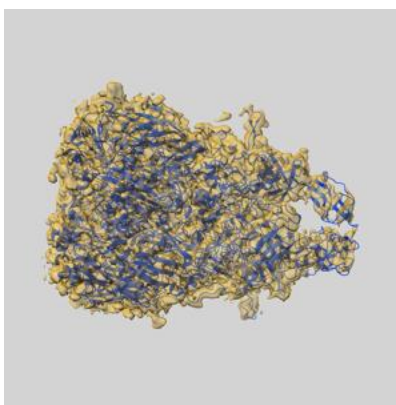
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-75053 and PDB model 10BU. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

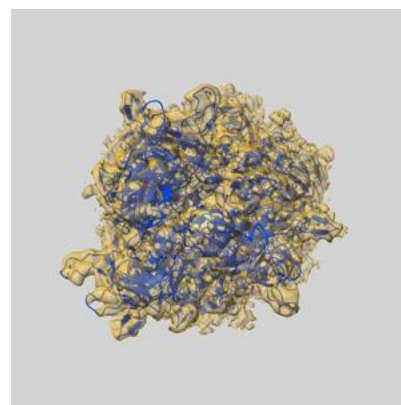
9.1 Map-model overlay [i](#)



X



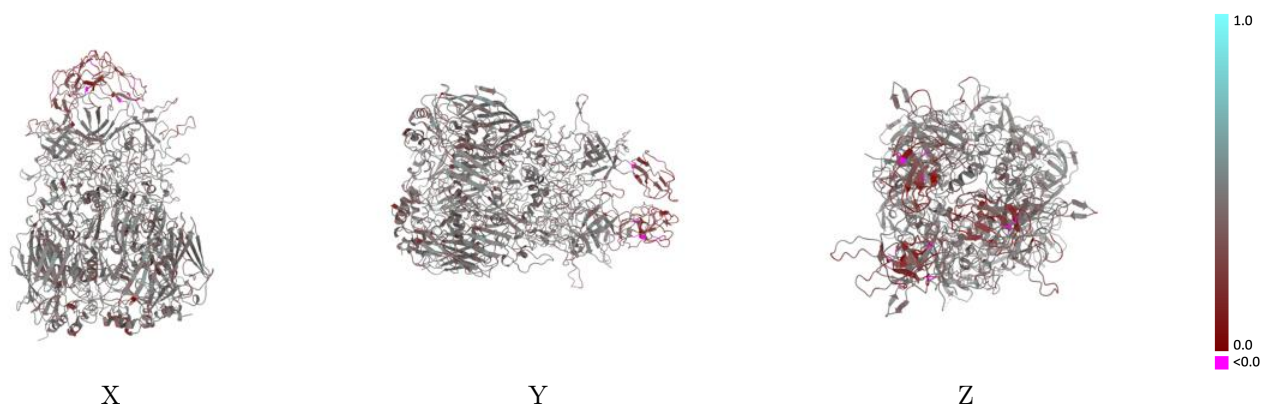
Y



Z

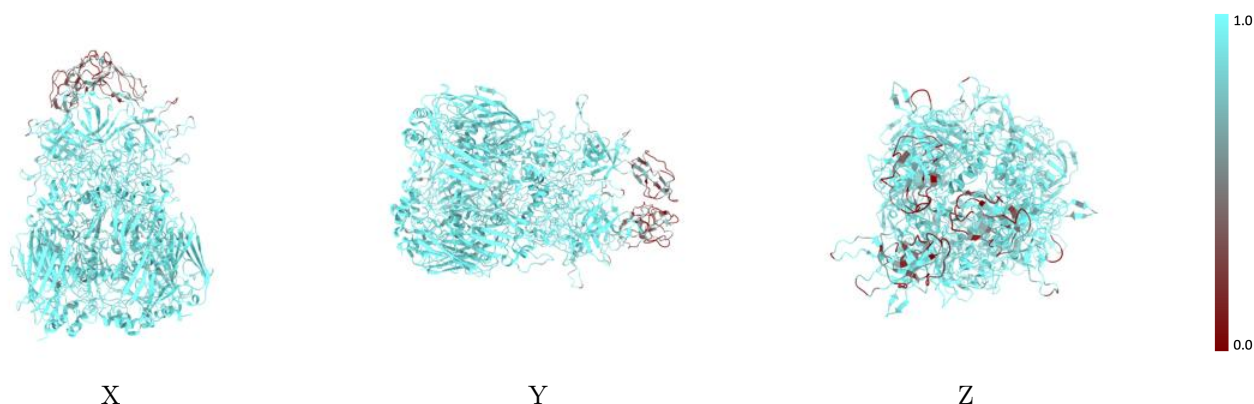
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



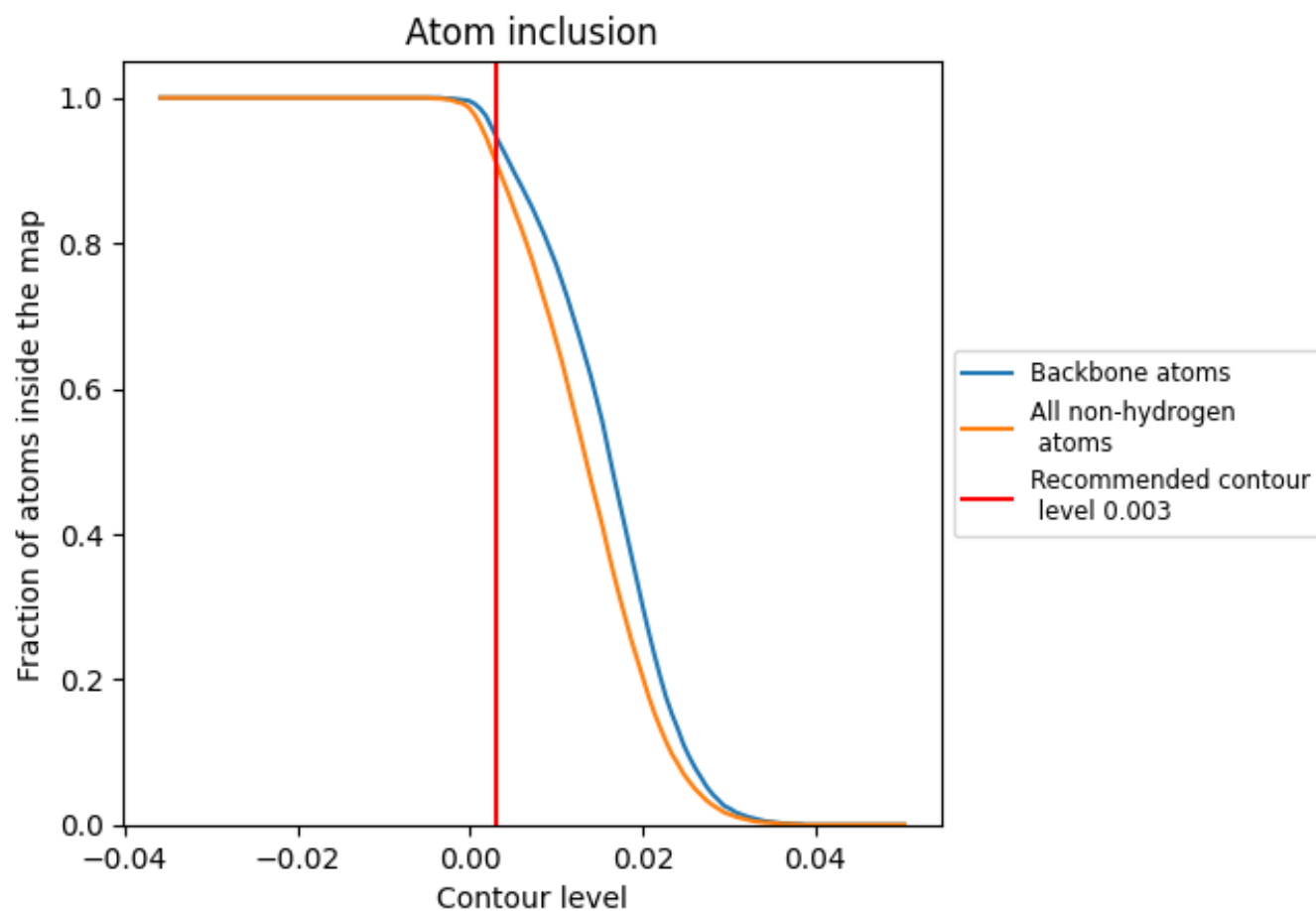
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9120	<div></div> 0.4260
A	<div></div> 0.9110	<div></div> 0.4270
B	<div></div> 0.9130	<div></div> 0.4250
C	<div></div> 0.9130	<div></div> 0.4260

