



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:39 AM UTC

PDB ID : 8JIF / pdb_00008jif
EMDB ID : EMD-36311
Title : Cryo-EM Structure of 3-axis block of AAV9P31-Car4 complex
Authors : Zhang, R.; Liu, Y.; Lou, Z.
Deposited on : 2023-05-26
Resolution : 2.28 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

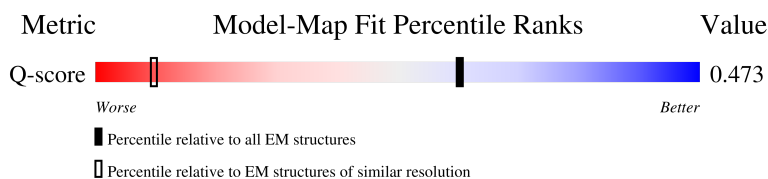
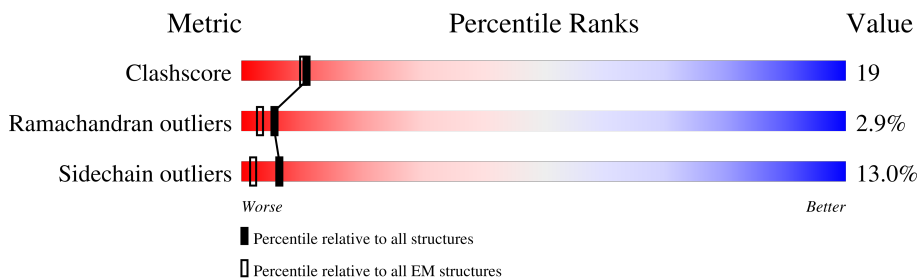
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.28 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	3643 (1.78 - 2.78)

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	R	256	
2	A	525	
2	B	525	
2	C	525	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14630 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 Carbonic anhydrase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	256	Total	C	N	O	S	0	0
			2056	1302	359	383	12		

- Molecule 2 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	525	Total	C	N	O	S	0	0
			4191	2647	726	804	14		
2	B	525	Total	C	N	O	S	0	0
			4191	2647	726	804	14		
2	C	525	Total	C	N	O	S	0	0
			4191	2647	726	804	14		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	588A	TRP	-	insertion	UNP Q6JC40
A	588B	PRO	-	insertion	UNP Q6JC40
A	588C	THR	-	insertion	UNP Q6JC40
A	588D	SER	-	insertion	UNP Q6JC40
A	588E	TYR	-	insertion	UNP Q6JC40
A	588F	ASP	-	insertion	UNP Q6JC40
A	588G	ALA	-	insertion	UNP Q6JC40
B	588A	TRP	-	insertion	UNP Q6JC40
B	588B	PRO	-	insertion	UNP Q6JC40
B	588C	THR	-	insertion	UNP Q6JC40
B	588D	SER	-	insertion	UNP Q6JC40
B	588E	TYR	-	insertion	UNP Q6JC40
B	588F	ASP	-	insertion	UNP Q6JC40
B	588G	ALA	-	insertion	UNP Q6JC40
C	588A	TRP	-	insertion	UNP Q6JC40
C	588B	PRO	-	insertion	UNP Q6JC40
C	588C	THR	-	insertion	UNP Q6JC40

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Chain	Residue	Modelled	Actual	Comment	Reference
C	588D	SER	-	insertion	UNP Q6JC40
C	588E	TYR	-	insertion	UNP Q6JC40
C	588F	ASP	-	insertion	UNP Q6JC40
C	588G	ALA	-	insertion	UNP Q6JC40

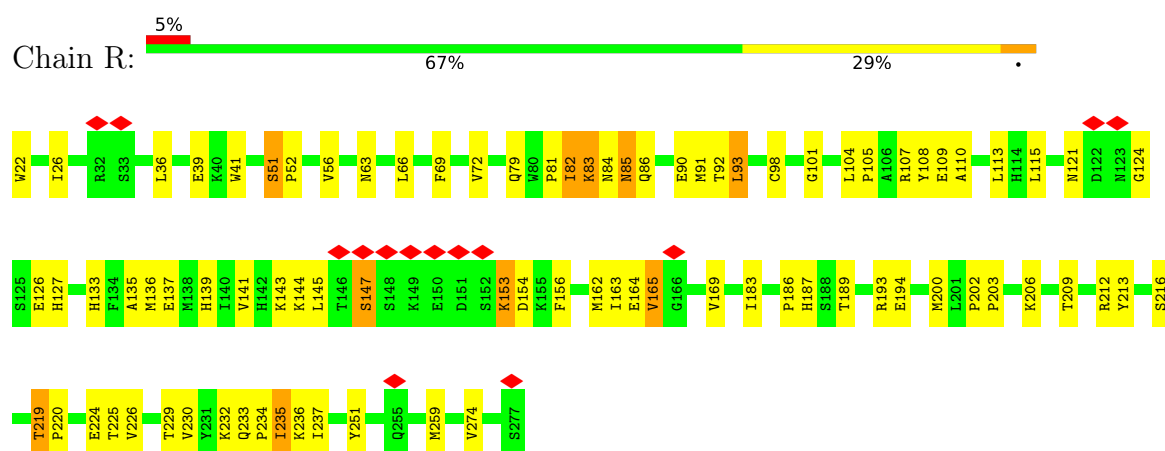
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	R	1	Total	Zn	0
			1	1	

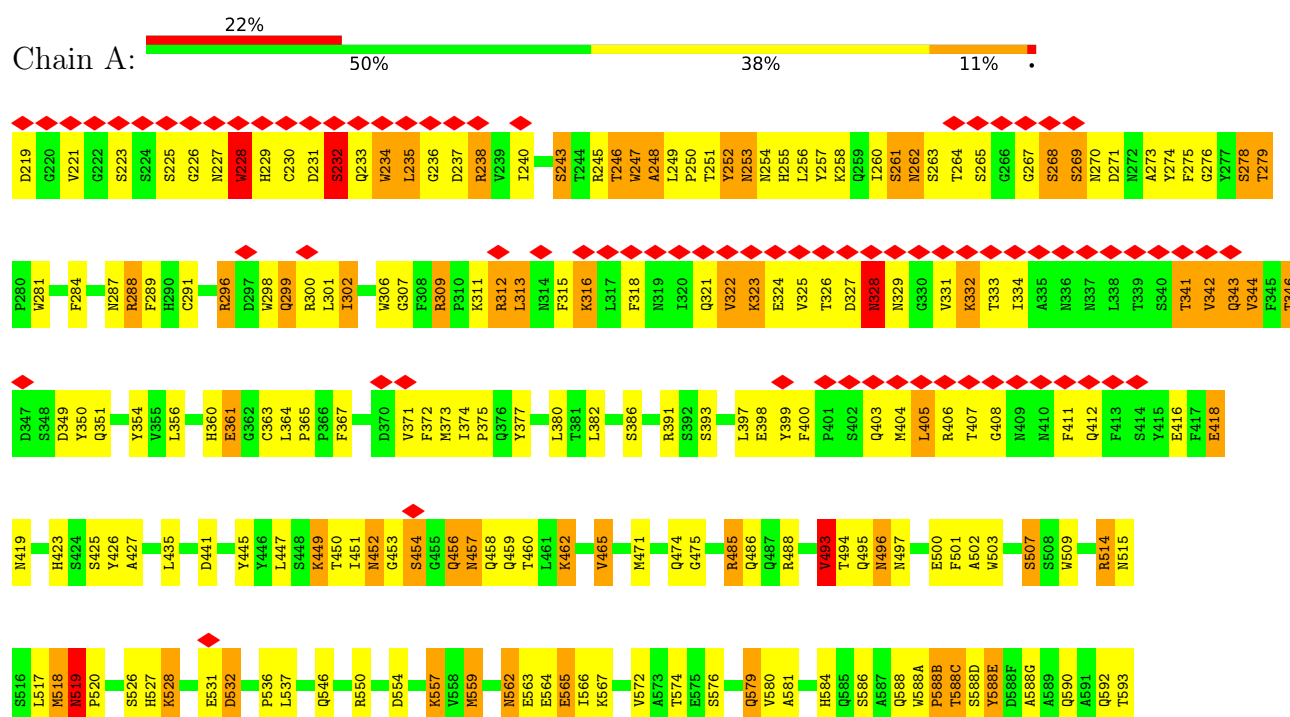
3 Residue-property plots

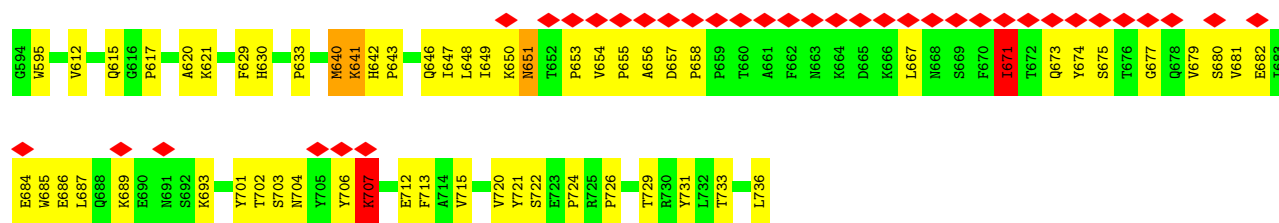
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Carbonic anhydrase 4

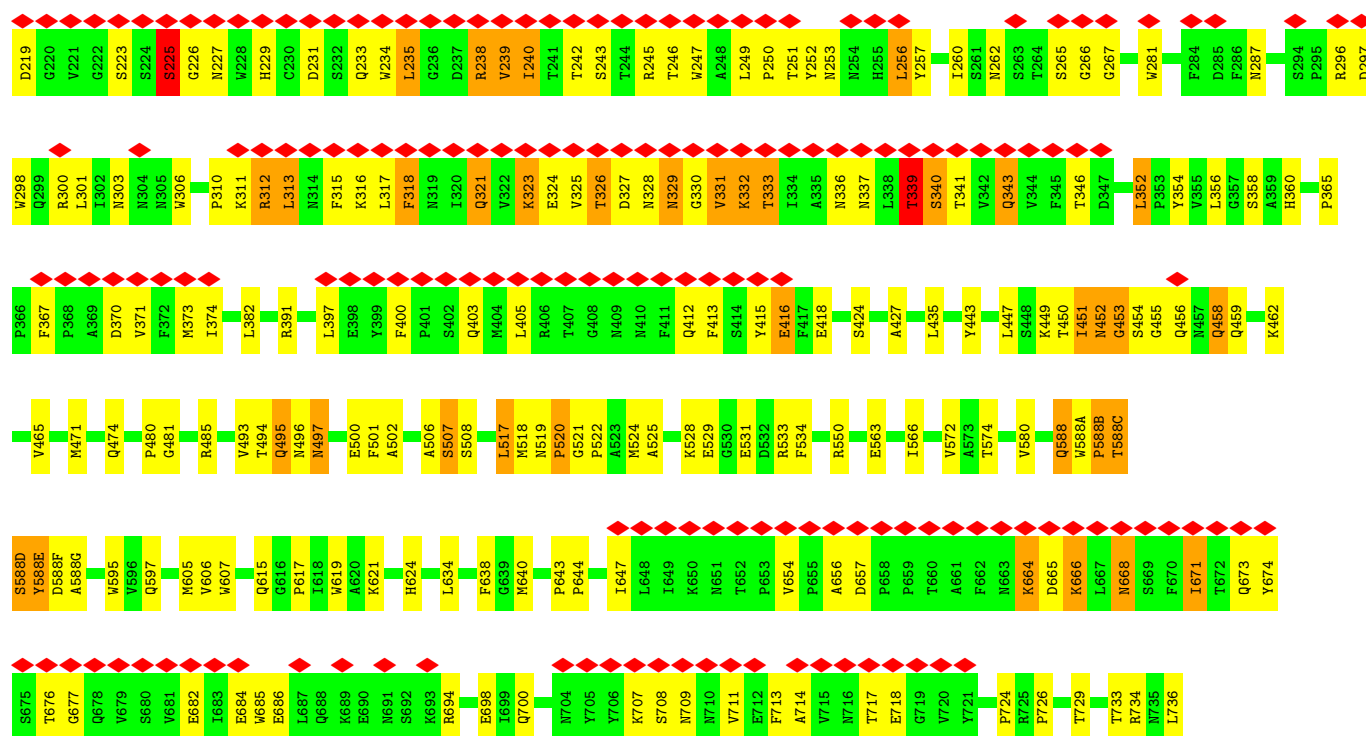


• Molecule 2: Capsid protein VP1

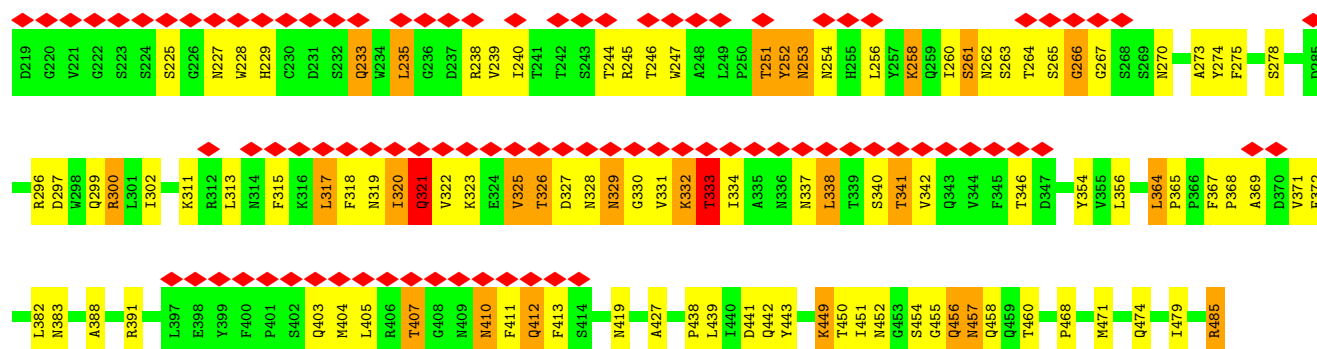


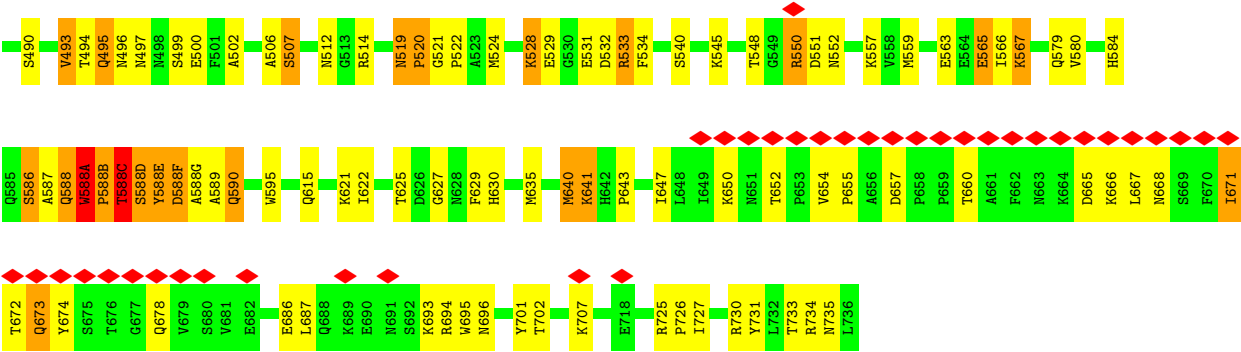


• Molecule 2: Capsid protein VP1



• Molecule 2: Capsid protein VP1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13604676	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.038	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	134.928, 134.928, 134.928	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8433, 0.8433, 0.8433	Depositor

5 Model quality

5.1 Standard geometry

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

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	R	0.16	0/2109	0.39	1/2855 (0.0%)
2	A	0.42	0/4320	0.85	9/5889 (0.2%)
2	B	0.36	0/4320	0.76	8/5889 (0.1%)
2	C	0.38	0/4320	0.80	5/5889 (0.1%)
All	All	0.36	0/15069	0.76	23/20522 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	247	TRP	N-CA-C	10.53	125.83	111.71
2	A	494	THR	N-CA-C	-8.28	104.32	114.75
2	C	494	THR	N-CA-C	-8.07	104.31	114.56
2	B	226	GLY	N-CA-C	7.25	121.14	110.63
2	A	341	THR	N-CA-C	6.97	119.67	109.07
2	B	405	LEU	N-CA-C	6.27	118.62	108.34
2	B	256	LEU	N-CA-C	6.17	119.61	109.85
2	C	725	ARG	N-CA-C	5.92	113.55	108.22
2	B	225	SER	N-CA-C	-5.85	105.72	112.92
2	B	318	PHE	N-CA-C	5.79	116.04	107.88
2	A	279	THR	CA-C-N	-5.76	114.96	120.83
2	A	279	THR	C-N-CA	-5.76	114.96	120.83
2	B	485	ARG	N-CA-C	5.62	118.63	110.42
2	C	485	ARG	N-CA-C	5.56	118.53	110.42
1	R	147	SER	CB-CA-C	-5.49	110.23	116.54
2	A	485	ARG	N-CA-C	5.42	117.94	110.35
2	C	627	GLY	N-CA-C	5.33	119.05	110.90
2	A	588(C)	THR	N-CA-C	-5.27	103.44	110.55
2	B	443	TYR	N-CA-C	-5.24	107.06	112.93
2	A	519	ASN	CA-C-N	-5.18	113.36	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	519	ASN	C-N-CA	-5.18	113.36	119.84
2	B	416	GLU	O-C-N	-5.12	117.49	123.27
2	C	479	ILE	N-CA-C	5.00	113.40	107.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	2056	0	2027	60	0
2	A	4191	0	3932	204	0
2	B	4191	0	3932	157	0
2	C	4191	0	3932	155	0
3	R	1	0	0	0	0
All	All	14630	0	13823	528	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 19.

All (528) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:327:ASP:HA	2:A:332:LYS:HA	1.29	1.12
1:R:51:SER:C	1:R:213:TYR:HH	1.58	1.12
1:R:51:SER:O	1:R:213:TYR:OH	1.68	1.10
2:B:327:ASP:HA	2:B:332:LYS:HA	1.32	1.08
2:C:519:ASN:HB3	2:C:520:PRO:HD2	1.35	1.08
2:C:327:ASP:HA	2:C:332:LYS:HA	1.41	0.98
2:C:403:GLN:HE22	2:C:411:PHE:HB2	1.33	0.93
1:R:51:SER:C	1:R:213:TYR:OH	2.12	0.90
2:C:588(A):TRP:HB2	2:C:588(B):PRO:HD2	1.53	0.90
1:R:51:SER:CA	1:R:213:TYR:OH	2.21	0.88
2:A:327:ASP:HA	2:A:332:LYS:CA	2.04	0.87
2:A:497:ASN:HD21	2:C:590:GLN:HE21	1.25	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:418:GLU:HG3	2:A:640:MET:HE2	1.60	0.84
1:R:51:SER:HA	1:R:213:TYR:OH	1.76	0.84
2:A:260:ILE:HA	2:A:264:THR:HG21	1.59	0.82
2:C:519:ASN:HB3	2:C:520:PRO:CD	2.09	0.81
2:A:238:ARG:HG3	2:A:686:GLU:HA	1.63	0.81
2:B:225:SER:HB2	2:B:318:PHE:HB2	1.64	0.80
2:B:312:ARG:HD3	2:B:416:GLU:HG3	1.63	0.80
2:B:262:ASN:O	2:B:267:GLY:N	2.13	0.77
2:A:327:ASP:CA	2:A:332:LYS:HA	2.14	0.76
2:B:238:ARG:HH12	2:B:686:GLU:HG3	1.49	0.76
1:R:51:SER:O	1:R:213:TYR:CZ	2.38	0.76
2:A:588(A):TRP:CD1	2:A:588(B):PRO:HD3	2.20	0.75
2:A:284:PHE:HD2	2:A:647:ILE:HB	1.52	0.75
2:A:255:HIS:CG	2:A:653:PRO:HB3	2.22	0.74
2:B:413:PHE:HE1	2:B:647:ILE:HD11	1.53	0.74
2:C:322:VAL:HG12	2:C:323:LYS:H	1.54	0.72
2:A:372:PHE:HZ	2:A:375:PRO:HD3	1.54	0.72
2:A:296:ARG:HD3	2:A:300:ARG:HE	1.54	0.71
2:B:296:ARG:HG3	2:B:300:ARG:HH21	1.56	0.71
2:B:711:VAL:HG13	2:B:714:ALA:HB3	1.72	0.71
1:R:145:LEU:HD11	2:B:595:TRP:HZ2	1.55	0.71
2:B:327:ASP:HB2	2:B:332:LYS:HD2	1.71	0.71
2:C:341:THR:HG21	2:C:404:MET:HE2	1.74	0.70
2:A:588:GLN:HB3	2:A:588(D):SER:HA	1.71	0.70
2:B:327:ASP:CA	2:B:332:LYS:HA	2.18	0.70
2:A:262:ASN:HB2	2:A:273:ALA:HA	1.71	0.70
2:B:250:PRO:HG3	2:B:373:MET:HE3	1.72	0.70
2:B:519:ASN:O	2:B:520:PRO:C	2.34	0.70
2:A:245:ARG:HH21	2:A:365:PRO:HB2	1.54	0.70
2:C:519:ASN:O	2:C:520:PRO:C	2.33	0.70
2:C:615:GLN:HE22	2:C:726:PRO:HA	1.57	0.70
2:B:718:GLU:N	2:B:718:GLU:OE1	2.24	0.69
2:A:255:HIS:CD2	2:A:653:PRO:HB3	2.28	0.69
2:A:527:HIS:HB2	2:A:531:GLU:HB3	1.76	0.68
2:A:588:GLN:HG2	2:A:588(G):ALA:HB2	1.75	0.68
2:C:262:ASN:HB3	2:C:273:ALA:HA	1.76	0.68
1:R:136:MET:HB3	1:R:163:ILE:HB	1.75	0.68
2:C:327:ASP:HB3	2:C:332:LYS:HE3	1.75	0.67
2:A:449:LYS:HB2	2:A:462:LYS:HB2	1.75	0.67
2:A:237:ASP:HA	2:A:689:LYS:HE3	1.76	0.66
2:A:554:ASP:HB2	2:A:557:LYS:HZ2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:235:LEU:HD12	2:A:238:ARG:HB3	1.77	0.66
2:A:471:MET:HA	2:A:474:GLN:HG3	1.78	0.66
2:C:654:VAL:O	2:C:671:ILE:HG12	1.95	0.66
2:B:452:ASN:HD21	2:B:458:GLN:HB2	1.61	0.65
2:B:471:MET:HA	2:B:474:GLN:HG3	1.78	0.65
2:A:226:GLY:HA3	2:A:318:PHE:CD2	2.32	0.65
2:A:397:LEU:HD13	2:A:648:LEU:HD13	1.77	0.65
2:C:640:MET:HG3	2:C:643:PRO:HB3	1.79	0.64
2:B:323:LYS:HG3	2:B:674:TYR:CZ	2.32	0.64
1:R:206:LYS:HB3	1:R:233:GLN:HG2	1.79	0.63
2:A:313:LEU:HA	2:A:682:GLU:O	1.98	0.63
2:C:382:LEU:HD12	2:C:391:ARG:HB3	1.80	0.63
1:R:156:PHE:HB2	1:R:226:VAL:HG22	1.81	0.63
2:C:263:SER:HA	2:C:267:GLY:H	1.64	0.63
1:R:162:MET:HB2	1:R:234:PRO:HB3	1.80	0.62
1:R:98:CYS:SG	1:R:107:ARG:NH2	2.72	0.62
1:R:153:LYS:HA	1:R:225:THR:HG22	1.80	0.62
2:A:306:TRP:HD1	2:A:426:TYR:HB3	1.65	0.62
2:A:296:ARG:O	2:A:300:ARG:HG3	2.00	0.62
2:A:342:VAL:HA	2:A:651:ASN:HA	1.80	0.62
2:B:312:ARG:HG3	2:B:416:GLU:HA	1.80	0.62
1:R:66:LEU:HD21	1:R:212:ARG:HG3	1.81	0.62
2:A:299:GLN:HG3	2:A:701:TYR:HD2	1.65	0.61
2:C:588(A):TRP:HB2	2:C:588(B):PRO:CD	2.29	0.61
2:B:227:ASN:HB2	2:B:229:HIS:CE1	2.36	0.61
2:B:235:LEU:HD23	2:B:238:ARG:HB2	1.83	0.61
2:B:382:LEU:HD12	2:B:391:ARG:HB3	1.83	0.61
2:B:328:ASN:O	2:B:329:ASN:C	2.43	0.61
2:B:588(B):PRO:HG3	2:C:495:GLN:HB2	1.81	0.60
1:R:86:GLN:HE21	1:R:186:PRO:HB2	1.67	0.60
2:A:453:GLY:O	2:A:454:SER:C	2.45	0.59
2:A:588(A):TRP:CG	2:A:588(B):PRO:HD3	2.37	0.59
2:A:528:LYS:HG2	2:A:572:VAL:HG21	1.83	0.59
1:R:187:HIS:CD2	2:A:456:GLN:N	2.71	0.59
1:R:187:HIS:CD2	2:A:456:GLN:H	2.20	0.59
2:A:249:LEU:HD12	2:A:250:PRO:HD2	1.85	0.59
2:B:588:GLN:HG2	2:B:588(G):ALA:HB2	1.85	0.59
2:C:337:ASN:OD1	2:C:340:SER:HB3	2.03	0.59
2:A:281:TRP:HA	2:A:650:LYS:HB2	1.85	0.59
2:A:588(A):TRP:CD2	2:B:495:GLN:HB3	2.37	0.59
2:A:562:ASN:HD21	2:A:564:GLU:HG3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:666:LYS:HZ1	2:B:668:ASN:HB2	1.68	0.58
2:B:297:ASP:HA	2:B:300:ARG:NH1	2.19	0.58
2:A:588(A):TRP:CE2	2:B:495:GLN:HB3	2.38	0.58
1:R:93:LEU:HD23	1:R:110:ALA:HB1	1.85	0.58
2:A:656:ALA:HB2	2:A:671:ILE:HG12	1.86	0.57
2:B:451:ILE:HG12	2:C:499:SER:C	2.29	0.57
2:B:315:PHE:CE2	2:B:647:ILE:HD13	2.38	0.57
1:R:83:LYS:HG2	1:R:84:ASN:N	2.19	0.57
2:A:227:ASN:O	2:A:228:TRP:C	2.46	0.57
2:B:297:ASP:HA	2:B:300:ARG:HH12	1.70	0.57
2:A:281:TRP:CG	2:A:397:LEU:HD12	2.40	0.57
2:C:239:VAL:HG12	2:C:687:LEU:HD21	1.85	0.57
2:A:315:PHE:CE2	2:A:679:VAL:HG23	2.40	0.57
1:R:66:LEU:HG	1:R:212:ARG:HE	1.69	0.56
1:R:82:ILE:HG12	1:R:183:ILE:HD13	1.87	0.56
2:B:711:VAL:HG13	2:B:714:ALA:CB	2.35	0.56
2:C:354:TYR:CE2	2:C:356:LEU:HB2	2.41	0.56
2:A:245:ARG:NH2	2:A:365:PRO:HB2	2.20	0.56
2:A:343:GLN:HE22	2:A:650:LYS:HE3	1.70	0.56
2:A:615:GLN:HE22	2:A:726:PRO:HA	1.70	0.56
2:C:403:GLN:NE2	2:C:411:PHE:HB2	2.13	0.56
2:A:493:VAL:HA	2:A:496:ASN:HD22	1.70	0.56
2:B:522:PRO:HG2	2:B:524:MET:HE2	1.87	0.56
2:C:328:ASN:O	2:C:329:ASN:C	2.49	0.56
2:C:588(C):THR:HA	2:C:588(E):TYR:CZ	2.40	0.56
2:B:249:LEU:HD12	2:B:250:PRO:HD2	1.87	0.56
2:A:313:LEU:HD13	2:A:681:VAL:HG23	1.87	0.56
2:B:413:PHE:CE1	2:B:647:ILE:HD11	2.37	0.56
2:C:311:LYS:HD3	2:C:686:GLU:HB2	1.88	0.56
2:A:372:PHE:CZ	2:A:375:PRO:HD3	2.38	0.55
2:A:503:TRP:CZ3	2:A:517:LEU:HB2	2.40	0.55
2:B:240:ILE:HD13	2:B:684:GLU:OE1	2.06	0.55
2:A:427:ALA:O	2:A:733:THR:HA	2.06	0.55
1:R:98:CYS:HA	1:R:109:GLU:HA	1.87	0.55
2:A:641:LYS:H	2:A:641:LYS:HZ3	1.55	0.55
1:R:219:THR:HG21	2:A:588(D):SER:CB	2.37	0.55
2:B:346:THR:HG22	2:B:647:ILE:HG12	1.88	0.55
2:A:230:CYS:SG	2:A:243:SER:HA	2.47	0.55
2:A:298:TRP:O	2:A:299:GLN:C	2.49	0.55
2:B:324:GLU:OE1	2:B:671:ILE:HG22	2.07	0.54
2:A:299:GLN:O	2:A:302:ILE:HG12	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:325:VAL:HA	2:C:334:ILE:HA	1.89	0.54
2:A:456:GLN:O	2:A:457:ASN:C	2.50	0.54
2:B:231:ASP:H	2:B:242:THR:HB	1.71	0.54
2:A:315:PHE:HA	2:A:680:SER:O	2.07	0.54
2:A:509:TRP:HD1	2:A:518:MET:HG2	1.73	0.54
2:C:471:MET:HA	2:C:474:GLN:HG3	1.88	0.54
2:B:219:ASP:HB2	2:B:223:SER:HB3	1.90	0.54
2:B:452:ASN:HD21	2:B:458:GLN:CB	2.20	0.54
2:B:327:ASP:H	2:B:333:THR:H	1.55	0.54
2:C:245:ARG:CZ	2:C:368:PRO:HA	2.38	0.54
2:A:250:PRO:HG2	2:A:252:TYR:CE1	2.43	0.54
2:B:459:GLN:HB2	2:C:493:VAL:O	2.07	0.54
1:R:165:VAL:HG11	1:R:236:LYS:HB3	1.90	0.54
2:B:451:ILE:O	2:B:452:ASN:C	2.51	0.54
2:A:360:HIS:HA	2:C:442:GLN:HA	1.90	0.54
2:B:452:ASN:ND2	2:B:458:GLN:HB2	2.22	0.54
2:A:289:PHE:HE2	2:A:612:VAL:HB	1.73	0.53
2:B:450:THR:OG1	2:C:500:GLU:HA	2.08	0.53
2:C:227:ASN:HB2	2:C:229:HIS:NE2	2.22	0.53
1:R:203:PRO:HD2	1:R:206:LYS:HD2	1.89	0.53
2:A:265:SER:HB3	2:A:274:TYR:OH	2.08	0.53
1:R:39:GLU:N	1:R:39:GLU:OE1	2.41	0.53
2:A:452:ASN:HB2	2:A:458:GLN:NE2	2.24	0.53
2:C:468:PRO:O	2:C:471:MET:HG3	2.08	0.53
2:A:232:SER:HA	2:A:240:ILE:O	2.08	0.53
2:A:306:TRP:CD1	2:A:426:TYR:HB3	2.44	0.53
2:A:322:VAL:HG13	2:A:675:SER:HB3	1.91	0.53
2:C:325:VAL:HG13	2:C:334:ILE:HG12	1.89	0.53
2:C:629:PHE:O	2:C:630:HIS:C	2.52	0.53
2:B:427:ALA:O	2:B:733:THR:HA	2.09	0.53
2:C:233:GLN:HG2	2:C:240:ILE:HB	1.91	0.53
2:A:250:PRO:HG3	2:A:373:MET:HE3	1.91	0.52
2:C:519:ASN:O	2:C:521:GLY:N	2.42	0.52
2:B:451:ILE:HG21	2:C:499:SER:N	2.24	0.52
2:B:315:PHE:CD2	2:B:647:ILE:HD13	2.45	0.52
1:R:216:SER:HA	1:R:224:GLU:HA	1.92	0.52
2:C:341:THR:HG22	2:C:652:THR:OG1	2.09	0.52
2:C:496:ASN:O	2:C:497:ASN:HB2	2.10	0.52
2:C:529:GLU:N	2:C:567:LYS:NZ	2.58	0.52
2:B:621:LYS:HB2	2:B:643:PRO:HG3	1.90	0.52
2:A:667:LEU:N	2:A:667:LEU:HD12	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:502:ALA:O	2:B:506:ALA:HB2	2.10	0.52
1:R:105:PRO:HD2	1:R:108:TYR:HE1	1.74	0.52
2:C:531:GLU:HB3	2:C:534:PHE:HD2	1.75	0.52
2:C:672:THR:O	2:C:673:GLN:HG2	2.10	0.52
2:B:240:ILE:HG23	2:B:684:GLU:HB2	1.91	0.52
2:B:506:ALA:HB3	2:B:517:LEU:HD11	1.92	0.52
2:A:235:LEU:N	2:A:238:ARG:O	2.41	0.51
2:B:563:GLU:O	2:B:566:ILE:HG12	2.10	0.51
2:C:326:THR:N	2:C:333:THR:O	2.38	0.51
2:A:311:LYS:N	2:A:684:GLU:O	2.40	0.51
2:B:265:SER:OG	2:B:266:GLY:N	2.43	0.51
2:B:310:PRO:C	2:B:311:LYS:HD2	2.35	0.51
2:C:315:PHE:HB3	2:C:413:PHE:CE1	2.45	0.51
2:C:302:ILE:HD12	2:C:731:TYR:CE1	2.45	0.51
2:A:296:ARG:CZ	2:A:300:ARG:HG2	2.40	0.51
2:B:496:ASN:O	2:B:497:ASN:HB2	2.10	0.51
1:R:127:HIS:HE1	1:R:213:TYR:CE1	2.29	0.51
2:B:313:LEU:HD22	2:B:415:TYR:HB3	1.93	0.51
2:C:233:GLN:CG	2:C:240:ILE:HB	2.41	0.51
2:B:325:VAL:HG13	2:B:332:LYS:HE2	1.93	0.51
2:B:326:THR:O	2:B:327:ASP:C	2.53	0.51
1:R:193:ARG:HG3	1:R:194:GLU:H	1.76	0.51
1:R:145:LEU:HD11	2:B:595:TRP:CZ2	2.43	0.51
2:A:312:ARG:HD2	2:A:684:GLU:OE1	2.10	0.51
2:A:693:LYS:HG3	2:B:400:PHE:CZ	2.46	0.51
2:B:328:ASN:O	2:B:330:GLY:N	2.43	0.51
2:A:328:ASN:O	2:A:329:ASN:C	2.54	0.51
2:C:323:LYS:HG3	2:C:674:TYR:CZ	2.45	0.51
1:R:91:MET:HE2	1:R:113:LEU:HD22	1.93	0.50
2:C:328:ASN:HB2	2:C:331:VAL:HG13	1.92	0.50
1:R:121:ASN:HB3	1:R:135:ALA:HB2	1.94	0.50
2:A:655:PRO:HB3	2:A:667:LEU:CD2	2.42	0.50
2:B:580:VAL:HG22	2:C:485:ARG:HB3	1.93	0.50
2:A:519:ASN:HB2	2:A:520:PRO:HD3	1.92	0.50
2:B:253:ASN:HB3	2:B:256:LEU:O	2.11	0.50
2:A:344:VAL:HG13	2:A:649:ILE:HB	1.94	0.50
2:B:316:LYS:HD3	2:B:412:GLN:HB2	1.94	0.50
2:C:693:LYS:HB3	2:C:693:LYS:HZ3	1.75	0.50
2:A:261:SER:O	2:A:262:ASN:C	2.55	0.50
2:A:271:ASP:HA	2:A:514:ARG:HG2	1.92	0.50
2:C:247:TRP:HB3	2:C:372:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:263:SER:H	2:A:386:SER:HB2	1.77	0.50
2:C:531:GLU:HB3	2:C:534:PHE:CD2	2.46	0.50
2:A:300:ARG:O	2:A:301:LEU:C	2.55	0.50
2:C:296:ARG:NH1	2:C:299:GLN:HB3	2.27	0.50
1:R:251:TYR:CE1	1:R:259:MET:HG3	2.46	0.50
2:A:261:SER:HA	2:A:275:PHE:HA	1.93	0.49
2:B:337:ASN:ND2	2:B:340:SER:HB3	2.27	0.49
2:C:615:GLN:NE2	2:C:726:PRO:HA	2.25	0.49
2:A:288:ARG:HB2	2:A:291:CYS:SG	2.52	0.49
2:A:546:GLN:HG2	2:A:721:TYR:O	2.12	0.49
2:B:588(B):PRO:HG3	2:C:495:GLN:CB	2.41	0.49
2:C:588(C):THR:HB	2:C:588(E):TYR:CE2	2.47	0.49
2:A:588(A):TRP:CG	2:B:495:GLN:HB3	2.47	0.49
2:A:267:GLY:O	2:A:268:SER:C	2.56	0.49
2:A:361:GLU:HG2	2:C:441:ASP:O	2.12	0.49
2:A:309:ARG:O	2:A:309:ARG:HG2	2.10	0.49
2:C:329:ASN:HD22	2:C:330:GLY:H	1.59	0.49
2:A:503:TRP:HZ3	2:A:517:LEU:HB2	1.78	0.49
2:A:565:GLU:CD	2:A:565:GLU:H	2.20	0.49
2:B:296:ARG:HD2	2:B:296:ARG:HA	1.56	0.49
2:B:315:PHE:HB3	2:B:413:PHE:CE1	2.47	0.49
2:B:323:LYS:HE3	2:B:336:ASN:HD22	1.78	0.49
2:B:597:GLN:OE1	2:B:597:GLN:HA	2.13	0.49
2:C:256:LEU:HB2	2:C:258:LYS:HE3	1.95	0.49
2:B:246:THR:HB	2:B:371:VAL:HG22	1.95	0.49
2:C:261:SER:H	2:C:264:THR:HB	1.77	0.49
2:C:621:LYS:HB2	2:C:643:PRO:HG3	1.94	0.49
1:R:163:ILE:HG12	1:R:235:ILE:HG22	1.95	0.48
2:A:251:THR:O	2:A:252:TYR:HB2	2.12	0.48
2:C:528:LYS:O	2:C:529:GLU:C	2.55	0.48
2:A:287:ASN:O	2:A:617:PRO:HA	2.13	0.48
2:A:288:ARG:HD3	2:C:443:TYR:CZ	2.48	0.48
2:A:296:ARG:HB3	2:A:300:ARG:HH21	1.77	0.48
2:B:324:GLU:HG2	2:B:673:GLN:HG2	1.95	0.48
2:C:529:GLU:CA	2:C:567:LYS:NZ	2.76	0.48
2:A:234:TRP:HE1	2:A:687:LEU:CD2	2.26	0.48
2:A:296:ARG:HH21	2:A:299:GLN:HB3	1.78	0.48
2:C:262:ASN:CB	2:C:273:ALA:HA	2.42	0.48
2:C:296:ARG:HG3	2:C:300:ARG:NH1	2.28	0.48
2:B:287:ASN:O	2:B:617:PRO:HA	2.13	0.48
2:A:621:LYS:NZ	2:A:643:PRO:HD2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:588:GLN:HA	2:C:588(D):SER:HA	1.96	0.48
2:C:641:LYS:HE2	2:C:641:LYS:HB3	1.52	0.48
1:R:81:PRO:HG2	1:R:92:THR:HB	1.96	0.48
2:B:354:TYR:CE2	2:B:356:LEU:HB2	2.49	0.48
2:A:629:PHE:O	2:A:630:HIS:C	2.57	0.48
2:C:297:ASP:HA	2:C:300:ARG:HH11	1.78	0.48
2:B:708:SER:O	2:B:709:ASN:C	2.55	0.48
2:C:548:THR:HG23	2:C:557:LYS:HB3	1.96	0.48
1:R:202:PRO:HG3	1:R:235:ILE:HG12	1.96	0.47
2:A:527:HIS:HB2	2:A:531:GLU:CB	2.43	0.47
2:A:531:GLU:O	2:A:532:ASP:C	2.57	0.47
2:C:330:GLY:C	2:C:332:LYS:HZ3	2.22	0.47
2:C:410:ASN:ND2	2:C:412:GLN:HE22	2.11	0.47
2:B:452:ASN:OD1	2:B:458:GLN:HB2	2.13	0.47
1:R:144:LYS:HD3	1:R:147:SER:HB2	1.97	0.47
2:A:559:MET:HE2	2:A:559:MET:HB2	1.78	0.47
2:B:517:LEU:HA	2:B:517:LEU:HD12	1.59	0.47
2:A:228:TRP:CZ3	2:A:230:CYS:HB2	2.49	0.47
2:B:219:ASP:HB2	2:B:223:SER:CB	2.43	0.47
2:B:588(E):TYR:O	2:B:588(E):TYR:CD1	2.67	0.47
2:B:249:LEU:HD13	2:B:374:ILE:HB	1.95	0.47
2:B:456:GLN:N	2:B:458:GLN:HE22	2.13	0.47
2:A:452:ASN:OD1	2:A:460:THR:HB	2.14	0.47
2:A:519:ASN:CB	2:A:520:PRO:HD3	2.44	0.47
2:B:358:SER:HB2	2:B:360:HIS:CD2	2.49	0.47
2:C:671:ILE:HG12	2:C:671:ILE:H	1.47	0.47
1:R:63:ASN:HB3	1:R:66:LEU:HD13	1.96	0.47
2:A:343:GLN:HE21	2:A:343:GLN:HB2	1.49	0.47
2:B:654:VAL:O	2:B:671:ILE:HG12	2.14	0.47
2:C:266:GLY:O	2:C:267:GLY:C	2.58	0.47
2:C:565:GLU:CD	2:C:565:GLU:H	2.23	0.47
1:R:165:VAL:HG12	1:R:237:ILE:O	2.15	0.47
2:A:701:TYR:HB2	2:A:731:TYR:CZ	2.50	0.47
2:B:245:ARG:HD2	2:B:365:PRO:HG2	1.96	0.47
2:C:225:SER:OG	2:C:319:ASN:N	2.35	0.47
1:R:232:LYS:HG2	1:R:233:GLN:H	1.80	0.47
2:A:275:PHE:C	2:A:275:PHE:CD1	2.93	0.47
2:A:315:PHE:HE1	2:A:411:PHE:CD2	2.33	0.47
2:A:586:SER:HA	2:B:496:ASN:O	2.15	0.47
2:C:502:ALA:O	2:C:506:ALA:HB2	2.15	0.47
2:A:485:ARG:HB3	2:C:580:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:520:PRO:HG2	2:C:635:MET:HG2	1.96	0.46
2:A:245:ARG:HD3	2:A:365:PRO:HD2	1.98	0.46
2:A:656:ALA:CB	2:A:671:ILE:HG12	2.44	0.46
2:A:667:LEU:N	2:A:667:LEU:CD1	2.79	0.46
2:B:281:TRP:CG	2:B:397:LEU:HD22	2.50	0.46
2:C:495:GLN:OE1	2:C:533:ARG:HD2	2.15	0.46
1:R:156:PHE:HE2	2:A:588(C):THR:HG21	1.79	0.46
2:C:322:VAL:C	2:C:323:LYS:HG2	2.40	0.46
2:A:495:GLN:HB2	2:C:588(A):TRP:CE3	2.50	0.46
2:A:245:ARG:NE	2:A:365:PRO:HD2	2.29	0.46
2:A:650:LYS:NZ	2:A:651:ASN:O	2.48	0.46
2:A:736:LEU:OXT	2:B:624:HIS:N	2.35	0.46
2:C:519:ASN:C	2:C:521:GLY:N	2.74	0.46
1:R:81:PRO:HD3	2:A:592:GLN:NE2	2.31	0.46
2:B:296:ARG:O	2:B:297:ASP:C	2.56	0.46
2:B:324:GLU:HG2	2:B:673:GLN:CG	2.46	0.46
2:B:321:GLN:OE1	2:B:677:GLY:HA2	2.16	0.46
2:B:519:ASN:O	2:B:521:GLY:N	2.47	0.46
2:C:251:THR:O	2:C:252:TYR:HB2	2.15	0.46
2:B:447:LEU:HD12	2:B:462:LYS:O	2.16	0.46
2:C:329:ASN:HD21	2:C:331:VAL:HG12	1.80	0.46
1:R:135:ALA:H	1:R:164:GLU:HB2	1.81	0.45
2:A:307:GLY:HA2	2:A:423:HIS:O	2.16	0.45
2:A:435:LEU:HD21	2:A:736:LEU:HD12	1.98	0.45
2:B:459:GLN:HG3	2:C:497:ASN:O	2.17	0.45
2:A:403:GLN:HG2	2:A:405:LEU:HD13	1.98	0.45
2:A:693:LYS:HG3	2:B:400:PHE:CE2	2.51	0.45
2:B:717:THR:OG1	2:B:718:GLU:OE1	2.15	0.45
2:C:318:PHE:CZ	2:C:678:GLN:HB3	2.50	0.45
2:A:309:ARG:O	2:A:685:TRP:HA	2.16	0.45
2:A:351:GLN:HB3	2:C:693:LYS:HG2	1.98	0.45
2:A:641:LYS:H	2:A:641:LYS:NZ	2.15	0.45
2:C:322:VAL:O	2:C:323:LYS:HG2	2.16	0.45
2:A:445:TYR:CZ	2:A:465:VAL:HG23	2.51	0.45
2:A:327:ASP:HA	2:A:332:LYS:N	2.32	0.45
2:A:363:CYS:O	2:A:365:PRO:HD3	2.16	0.45
2:C:338:LEU:HD11	2:C:407:THR:HG21	1.99	0.45
2:C:622:ILE:HD12	2:C:641:LYS:HD2	1.97	0.45
2:A:488:ARG:HB2	2:C:584:HIS:CD2	2.52	0.45
2:A:488:ARG:HG3	2:A:574:THR:HG21	1.97	0.45
2:B:247:TRP:HE1	2:B:317:LEU:HD11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:579:GLN:HG2	2:C:595:TRP:CE3	2.52	0.45
1:R:91:MET:HE1	1:R:200:MET:HE1	1.99	0.45
2:A:588(E):TYR:C	2:A:588(G):ALA:H	2.25	0.45
2:B:325:VAL:HG13	2:B:332:LYS:CE	2.46	0.45
2:C:454:SER:O	2:C:455:GLY:C	2.59	0.45
1:R:22:TRP:HE3	1:R:36:LEU:HD13	1.82	0.45
1:R:156:PHE:CE2	2:A:588(C):THR:HG21	2.51	0.45
2:A:247:TRP:O	2:A:248:ALA:C	2.59	0.45
2:A:323:LYS:HG3	2:A:674:TYR:CZ	2.51	0.45
1:R:124:GLY:HA2	1:R:133:HIS:HB3	1.98	0.45
2:A:246:THR:HA	2:A:677:GLY:O	2.17	0.45
2:A:475:GLY:HA2	2:B:519:ASN:HB3	1.98	0.45
2:A:528:LYS:O	2:A:531:GLU:HB2	2.16	0.45
2:A:562:ASN:HD21	2:A:564:GLU:CG	2.30	0.45
2:B:367:PHE:HB3	2:B:370:ASP:OD2	2.17	0.45
2:B:449:LYS:HB2	2:B:449:LYS:HE2	1.83	0.45
2:C:263:SER:O	2:C:264:THR:C	2.60	0.45
2:C:275:PHE:HB3	2:C:383:ASN:HB3	1.98	0.45
2:C:329:ASN:ND2	2:C:330:GLY:H	2.15	0.45
2:C:456:GLN:O	2:C:458:GLN:N	2.50	0.45
2:B:247:TRP:NE1	2:B:317:LEU:HD11	2.32	0.45
2:B:531:GLU:HB3	2:B:534:PHE:HD2	1.81	0.44
2:A:441:ASP:CG	2:B:550:ARG:HH21	2.24	0.44
2:B:480:PRO:O	2:B:605:MET:HG2	2.17	0.44
2:B:501:PHE:O	2:B:502:ALA:C	2.59	0.44
2:B:713:PHE:CE2	2:B:724:PRO:HD2	2.52	0.44
2:C:329:ASN:ND2	2:C:331:VAL:HG12	2.31	0.44
2:C:346:THR:HG22	2:C:647:ILE:HD12	1.98	0.44
2:A:258:LYS:HB2	2:A:278:SER:OG	2.16	0.44
2:B:619:TRP:CZ2	2:B:644:PRO:HG2	2.52	0.44
2:B:666:LYS:HZ2	2:B:666:LYS:HG3	1.70	0.44
2:A:588(A):TRP:CD1	2:B:495:GLN:HB3	2.52	0.44
2:A:279:THR:HG21	2:A:377:TYR:CD2	2.53	0.44
2:C:696:ASN:OD1	2:C:696:ASN:N	2.50	0.44
2:A:316:LYS:HE2	2:A:316:LYS:HB3	1.49	0.44
2:B:465:VAL:HG12	2:C:550:ARG:HH21	1.83	0.44
2:A:260:ILE:HG12	2:A:276:GLY:C	2.43	0.44
2:A:654:VAL:HG12	2:A:656:ALA:H	1.81	0.44
2:A:311:LYS:HB3	2:A:311:LYS:HE3	1.88	0.44
2:A:398:GLU:C	2:A:400:PHE:H	2.26	0.44
2:B:257:TYR:OH	2:B:397:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:352:LEU:HD12	2:B:352:LEU:HA	1.87	0.44
2:C:427:ALA:O	2:C:733:THR:HA	2.18	0.44
2:A:707:LYS:HE2	2:A:707:LYS:HB3	1.43	0.43
2:B:310:PRO:HD3	2:B:638:PHE:CE2	2.53	0.43
2:B:327:ASP:HA	2:B:332:LYS:CA	2.24	0.43
2:C:245:ARG:HD2	2:C:365:PRO:HG2	2.00	0.43
2:C:263:SER:HA	2:C:267:GLY:N	2.30	0.43
2:C:317:LEU:HD22	2:C:317:LEU:HA	1.74	0.43
2:C:522:PRO:HG2	2:C:524:MET:HE2	1.99	0.43
1:R:85:ASN:HB2	1:R:90:GLU:HG2	2.00	0.43
1:R:126:GLU:HG3	1:R:139:HIS:CE1	2.53	0.43
2:C:332:LYS:O	2:C:333:THR:C	2.61	0.43
2:A:219:ASP:HB2	2:A:408:GLY:O	2.18	0.43
2:C:327:ASP:HA	2:C:332:LYS:CA	2.30	0.43
1:R:127:HIS:CE1	1:R:213:TYR:CE1	3.06	0.43
2:A:245:ARG:CD	2:A:365:PRO:HD2	2.48	0.43
2:A:382:LEU:HD12	2:A:391:ARG:HB3	2.00	0.43
2:A:612:VAL:HG23	2:A:729:THR:HG21	1.99	0.43
2:C:545:LYS:HG3	2:C:557:LYS:O	2.18	0.43
2:A:271:ASP:OD1	2:A:515:ASN:N	2.50	0.43
2:B:508:SER:HB3	2:B:517:LEU:HD12	2.00	0.43
2:C:253:ASN:O	2:C:254:ASN:C	2.61	0.43
2:C:506:ALA:O	2:C:507:SER:HB2	2.18	0.43
1:R:108:TYR:OH	1:R:154:ASP:O	2.30	0.43
2:C:247:TRP:HA	2:C:372:PHE:O	2.18	0.43
2:C:253:ASN:HB3	2:C:258:LYS:NZ	2.34	0.43
1:R:51:SER:OG	1:R:52:PRO:HD3	2.17	0.43
1:R:187:HIS:HD2	2:A:456:GLN:N	2.16	0.43
2:A:327:ASP:O	2:A:328:ASN:C	2.61	0.43
2:B:306:TRP:CZ2	2:B:734:ARG:HB3	2.53	0.43
2:B:435:LEU:HD21	2:B:736:LEU:HD12	1.99	0.43
2:C:587:ALA:HB1	2:C:588:GLN:HE21	1.84	0.43
2:C:655:PRO:HB3	2:C:667:LEU:HD12	1.99	0.43
2:B:311:LYS:HD3	2:B:686:GLU:CB	2.49	0.43
2:B:453:GLY:O	2:B:454:SER:C	2.59	0.43
1:R:107:ARG:HD3	1:R:145:LEU:HD22	2.01	0.43
1:R:189:THR:HG23	2:A:590:GLN:HE22	1.83	0.43
2:A:500:GLU:HB2	2:C:451:ILE:HD11	2.01	0.43
2:A:641:LYS:HE2	2:A:641:LYS:HB2	1.78	0.43
2:C:405:LEU:N	2:C:405:LEU:HD12	2.34	0.43
2:A:245:ARG:NH2	2:A:367:PHE:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:572:VAL:HG12	2:A:574:THR:H	1.84	0.43
2:A:579:GLN:HG2	2:A:595:TRP:CE3	2.54	0.43
2:B:296:ARG:HH12	2:B:300:ARG:HG3	1.84	0.43
2:C:238:ARG:NH2	2:C:240:ILE:HD11	2.34	0.43
2:C:452:ASN:HD22	2:C:458:GLN:HB2	1.84	0.43
1:R:79:GLN:HG2	1:R:193:ARG:O	2.19	0.42
2:B:238:ARG:NH2	2:B:684:GLU:OE2	2.52	0.42
2:B:713:PHE:CZ	2:B:724:PRO:HD2	2.54	0.42
2:C:246:THR:HB	2:C:371:VAL:HG22	2.00	0.42
2:C:641:LYS:H	2:C:641:LYS:HG2	1.55	0.42
2:A:350:TYR:CE2	2:A:642:HIS:HB3	2.55	0.42
2:B:588(E):TYR:O	2:B:588(E):TYR:CG	2.72	0.42
2:A:252:TYR:O	2:A:253:ASN:C	2.61	0.42
2:A:712:GLU:HB2	2:A:724:PRO:HG2	2.02	0.42
2:B:239:VAL:HG13	2:B:685:TRP:HB2	2.00	0.42
2:C:320:ILE:HG22	2:C:321:GLN:N	2.34	0.42
2:C:410:ASN:C	2:C:410:ASN:HD22	2.27	0.42
2:C:490:SER:HB2	2:C:534:PHE:HE1	1.85	0.42
2:A:221:VAL:HG22	2:A:407:THR:HG21	2.01	0.42
2:C:228:TRP:O	2:C:244:THR:OG1	2.36	0.42
2:A:233:GLN:OE1	2:A:235:LEU:HD23	2.19	0.42
2:A:233:GLN:HB3	2:A:240:ILE:HG22	2.01	0.42
2:C:235:LEU:HD21	2:C:240:ILE:HD12	2.02	0.42
2:A:689:LYS:HA	2:A:689:LYS:HD3	1.63	0.42
2:B:234:TRP:HH2	2:B:301:LEU:HB2	1.85	0.42
2:C:338:LEU:HD13	2:C:338:LEU:HA	1.66	0.42
2:A:380:LEU:HD21	2:C:438:PRO:HB3	2.01	0.42
2:B:327:ASP:CG	2:B:332:LYS:HB2	2.45	0.42
2:C:275:PHE:CZ	2:C:388:ALA:HB2	2.55	0.42
1:R:69:PHE:HA	1:R:101:GLY:HA3	2.01	0.42
2:A:245:ARG:HH11	2:A:245:ARG:HB2	1.85	0.42
2:A:328:ASN:HB2	2:A:331:VAL:HB	2.01	0.42
2:A:654:VAL:HG12	2:A:656:ALA:N	2.34	0.42
2:B:312:ARG:CD	2:B:416:GLU:HG3	2.41	0.42
2:B:606:VAL:CG1	2:C:625:THR:HG21	2.50	0.42
2:A:312:ARG:NH2	2:A:416:GLU:CD	2.77	0.42
2:C:322:VAL:HG12	2:C:323:LYS:N	2.29	0.42
2:A:257:TYR:C	2:A:258:LYS:HD2	2.45	0.41
2:A:354:TYR:CE2	2:A:356:LEU:HB2	2.54	0.41
2:A:507:SER:O	2:A:517:LEU:HD12	2.19	0.41
2:B:481:GLY:HA3	2:B:607:TRP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:327:ASP:HB2	2:A:332:LYS:HE3	2.02	0.41
2:A:576:SER:HB2	2:A:595:TRP:CE3	2.55	0.41
2:B:615:GLN:HE22	2:B:726:PRO:HA	1.85	0.41
2:C:586:SER:N	2:C:589:ALA:HB3	2.34	0.41
2:A:346:THR:HA	2:A:646:GLN:O	2.20	0.41
2:A:458:GLN:O	2:A:459:GLN:C	2.63	0.41
2:A:536:PRO:O	2:A:537:LEU:C	2.63	0.41
2:B:296:ARG:HH22	2:B:300:ARG:CB	2.33	0.41
2:B:528:LYS:O	2:B:529:GLU:C	2.63	0.41
2:C:563:GLU:O	2:C:566:ILE:HG12	2.19	0.41
2:B:296:ARG:HG3	2:B:300:ARG:NH2	2.30	0.41
2:B:520:PRO:O	2:B:634:LEU:HB3	2.21	0.41
2:C:449:LYS:HB2	2:C:449:LYS:HE3	1.73	0.41
2:C:650:LYS:HE2	2:C:650:LYS:HB3	1.80	0.41
2:A:271:ASP:HA	2:A:514:ARG:CD	2.51	0.41
2:A:279:THR:HG21	2:A:377:TYR:HD2	1.85	0.41
2:A:447:LEU:HD12	2:A:462:LYS:O	2.19	0.41
2:A:563:GLU:O	2:A:566:ILE:HG12	2.20	0.41
2:B:619:TRP:CE2	2:B:644:PRO:HG2	2.55	0.41
2:B:640:MET:HB2	2:B:640:MET:HE3	1.75	0.41
2:A:399:TYR:HB2	2:C:695:TRP:HZ3	1.85	0.41
2:A:574:THR:O	2:C:584:HIS:NE2	2.53	0.41
2:C:262:ASN:HA	2:C:274:TYR:CE1	2.56	0.41
2:A:268:SER:HB2	2:A:269:SER:H	1.63	0.41
2:A:713:PHE:HA	2:A:722:SER:O	2.20	0.41
2:B:328:ASN:N	2:B:331:VAL:O	2.53	0.41
2:B:694:ARG:HD3	2:B:698:GLU:HG2	2.03	0.41
2:C:551:ASP:O	2:C:552:ASN:C	2.64	0.41
2:C:734:ARG:HG3	2:C:735:ASN:O	2.20	0.41
2:A:581:ALA:HA	2:A:593:THR:HG22	2.02	0.41
2:A:588(A):TRP:CE2	2:A:588(B):PRO:HG3	2.56	0.41
2:A:620:ALA:HB3	2:A:633:PRO:HG3	2.02	0.41
2:A:715:VAL:HA	2:A:720:VAL:O	2.20	0.41
2:B:310:PRO:O	2:B:311:LYS:HD2	2.21	0.41
2:B:317:LEU:HD12	2:B:317:LEU:HA	1.90	0.41
2:B:452:ASN:O	2:B:453:GLY:C	2.64	0.41
2:B:606:VAL:HG13	2:C:625:THR:OG1	2.21	0.41
2:A:495:GLN:HB2	2:C:588(A):TRP:CZ3	2.56	0.41
2:A:650:LYS:HZ2	2:A:650:LYS:HG2	1.72	0.41
2:C:364:LEU:HD22	2:C:372:PHE:CZ	2.56	0.41
2:A:501:PHE:O	2:A:502:ALA:C	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:ASN:HB3	2:B:700:GLN:NE2	2.36	0.40
2:B:339:THR:HB	2:B:340:SER:H	1.71	0.40
2:B:529:GLU:HB2	2:C:512:ASN:HD21	1.85	0.40
2:C:328:ASN:ND2	2:C:333:THR:OG1	2.54	0.40
1:R:22:TRP:HE3	1:R:36:LEU:CD1	2.35	0.40
1:R:41:TRP:CE2	1:R:220:PRO:HG3	2.57	0.40
2:A:246:THR:OG1	2:A:371:VAL:HG13	2.22	0.40
2:A:450:THR:HG23	2:B:500:GLU:OE1	2.21	0.40
2:A:584:HIS:NE2	2:B:574:THR:O	2.55	0.40
2:B:332:LYS:C	2:B:332:LYS:HZ3	2.29	0.40
2:C:258:LYS:HG3	2:C:278:SER:OG	2.22	0.40
2:C:450:THR:HA	2:C:460:THR:O	2.22	0.40
2:A:393:SER:HB2	2:C:694:ARG:HG3	2.03	0.40
2:A:485:ARG:HG3	2:A:486:GLN:N	2.37	0.40
2:B:240:ILE:H	2:B:240:ILE:HG12	1.61	0.40
2:B:343:GLN:HA	2:B:403:GLN:O	2.21	0.40
2:B:506:ALA:CB	2:B:517:LEU:HD11	2.51	0.40
2:B:525:ALA:HB3	2:B:572:VAL:HA	2.03	0.40
2:C:297:ASP:HA	2:C:300:ARG:HD2	2.02	0.40
2:C:490:SER:HB2	2:C:534:PHE:CE1	2.56	0.40
2:B:298:TRP:CZ2	2:B:729:THR:HG22	2.57	0.40
2:B:506:ALA:O	2:B:507:SER:HB2	2.21	0.40
2:C:367:PHE:C	2:C:369:ALA:H	2.30	0.40
2:C:701:TYR:HB2	2:C:731:TYR:CZ	2.56	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	R	254/256 (99%)	226 (89%)	27 (11%)	1 (0%)	30 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	523/525 (100%)	454 (87%)	49 (9%)	20 (4%)	2	1
2	B	523/525 (100%)	469 (90%)	40 (8%)	14 (3%)	4	2
2	C	523/525 (100%)	464 (89%)	42 (8%)	17 (3%)	3	1
All	All	1823/1831 (100%)	1613 (88%)	158 (9%)	52 (3%)	5	2

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	51	SER
2	A	248	ALA
2	A	588(B)	PRO
2	B	329	ASN
2	B	497	ASN
2	B	520	PRO
2	B	664	LYS
2	C	320	ILE
2	C	333	THR
2	C	457	ASN
2	C	519	ASN
2	C	588(A)	TRP
2	A	328	ASN
2	A	454	SER
2	A	496	ASN
2	B	339	THR
2	B	588(D)	SER
2	B	656	ALA
2	C	252	TYR
2	A	228	TRP
2	A	671	ILE
2	B	340	SER
2	B	452	ASN
2	B	455	GLY
2	C	329	ASN
2	A	231	ASP
2	A	252	TYR
2	A	299	GLN
2	A	374	ILE
2	A	588(E)	TYR
2	A	658	PRO
2	A	706	TYR
2	A	707	LYS

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Mol	Chain	Res	Type
2	B	252	TYR
2	B	453	GLY
2	B	507	SER
2	C	588(F)	ASP
2	C	588(G)	ALA
2	A	456	GLN
2	C	253	ASN
2	C	321	GLN
2	C	507	SER
2	C	588(C)	THR
2	A	232	SER
2	B	588(C)	THR
2	C	493	VAL
2	C	266	GLY
2	C	325	VAL
2	A	236	GLY
2	A	519	ASN
2	C	520	PRO
2	A	493	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	R	232/232 (100%)	211 (91%)	21 (9%)	9	10
2	A	459/459 (100%)	377 (82%)	82 (18%)	2	1
2	B	459/459 (100%)	412 (90%)	47 (10%)	7	7
2	C	459/459 (100%)	400 (87%)	59 (13%)	4	4
All	All	1609/1609 (100%)	1400 (87%)	209 (13%)	6	4

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	26	ILE
1	R	56	VAL

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Mol	Chain	Res	Type
1	R	72	VAL
1	R	82	ILE
1	R	83	LYS
1	R	85	ASN
1	R	93	LEU
1	R	104	LEU
1	R	115	LEU
1	R	137	GLU
1	R	141	VAL
1	R	143	LYS
1	R	153	LYS
1	R	165	VAL
1	R	169	VAL
1	R	209	THR
1	R	219	THR
1	R	229	THR
1	R	230	VAL
1	R	235	ILE
1	R	274	VAL
2	A	223	SER
2	A	225	SER
2	A	228	TRP
2	A	229	HIS
2	A	232	SER
2	A	234	TRP
2	A	235	LEU
2	A	238	ARG
2	A	243	SER
2	A	246	THR
2	A	253	ASN
2	A	254	ASN
2	A	256	LEU
2	A	261	SER
2	A	262	ASN
2	A	268	SER
2	A	269	SER
2	A	270	ASN
2	A	278	SER
2	A	288	ARG
2	A	296	ARG
2	A	302	ILE
2	A	309	ARG

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Mol	Chain	Res	Type
2	A	312	ARG
2	A	313	LEU
2	A	316	LYS
2	A	321	GLN
2	A	322	VAL
2	A	323	LYS
2	A	324	GLU
2	A	325	VAL
2	A	326	THR
2	A	328	ASN
2	A	332	LYS
2	A	333	THR
2	A	334	ILE
2	A	341	THR
2	A	342	VAL
2	A	343	GLN
2	A	344	VAL
2	A	346	THR
2	A	349	ASP
2	A	361	GLU
2	A	364	LEU
2	A	404	MET
2	A	405	LEU
2	A	406	ARG
2	A	412	GLN
2	A	418	GLU
2	A	419	ASN
2	A	425	SER
2	A	449	LYS
2	A	451	ILE
2	A	452	ASN
2	A	457	ASN
2	A	462	LYS
2	A	465	VAL
2	A	493	VAL
2	A	507	SER
2	A	514	ARG
2	A	518	MET
2	A	526	SER
2	A	528	LYS
2	A	532	ASP
2	A	550	ARG

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Mol	Chain	Res	Type
2	A	557	LYS
2	A	559	MET
2	A	562	ASN
2	A	565	GLU
2	A	567	LYS
2	A	579	GLN
2	A	580	VAL
2	A	640	MET
2	A	641	LYS
2	A	651	ASN
2	A	657	ASP
2	A	671	ILE
2	A	673	GLN
2	A	702	THR
2	A	703	SER
2	A	704	ASN
2	A	707	LYS
2	B	225	SER
2	B	233	GLN
2	B	235	LEU
2	B	238	ARG
2	B	239	VAL
2	B	240	ILE
2	B	243	SER
2	B	251	THR
2	B	260	ILE
2	B	312	ARG
2	B	313	LEU
2	B	321	GLN
2	B	323	LYS
2	B	326	THR
2	B	331	VAL
2	B	332	LYS
2	B	333	THR
2	B	339	THR
2	B	341	THR
2	B	343	GLN
2	B	352	LEU
2	B	418	GLU
2	B	424	SER
2	B	451	ILE
2	B	458	GLN

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Mol	Chain	Res	Type
2	B	493	VAL
2	B	494	THR
2	B	495	GLN
2	B	517	LEU
2	B	518	MET
2	B	533	ARG
2	B	588	GLN
2	B	588(A)	TRP
2	B	588(B)	PRO
2	B	588(C)	THR
2	B	588(D)	SER
2	B	588(E)	TYR
2	B	588(F)	ASP
2	B	657	ASP
2	B	664	LYS
2	B	665	ASP
2	B	666	LYS
2	B	668	ASN
2	B	671	ILE
2	B	676	THR
2	B	682	GLU
2	B	707	LYS
2	C	233	GLN
2	C	235	LEU
2	C	251	THR
2	C	258	LYS
2	C	260	ILE
2	C	261	SER
2	C	265	SER
2	C	270	ASN
2	C	300	ARG
2	C	313	LEU
2	C	317	LEU
2	C	321	GLN
2	C	326	THR
2	C	332	LYS
2	C	333	THR
2	C	338	LEU
2	C	341	THR
2	C	342	VAL
2	C	364	LEU
2	C	407	THR

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Mol	Chain	Res	Type
2	C	410	ASN
2	C	412	GLN
2	C	419	ASN
2	C	439	LEU
2	C	449	LYS
2	C	456	GLN
2	C	457	ASN
2	C	495	GLN
2	C	514	ARG
2	C	528	LYS
2	C	532	ASP
2	C	533	ARG
2	C	540	SER
2	C	550	ARG
2	C	559	MET
2	C	565	GLU
2	C	567	LYS
2	C	586	SER
2	C	588	GLN
2	C	588(A)	TRP
2	C	588(B)	PRO
2	C	588(C)	THR
2	C	588(D)	SER
2	C	588(E)	TYR
2	C	588(F)	ASP
2	C	590	GLN
2	C	640	MET
2	C	641	LYS
2	C	657	ASP
2	C	660	THR
2	C	665	ASP
2	C	666	LYS
2	C	668	ASN
2	C	671	ILE
2	C	673	GLN
2	C	702	THR
2	C	707	LYS
2	C	727	ILE
2	C	730	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	85	ASN
1	R	127	HIS
2	A	254	ASN
2	A	255	HIS
2	A	314	ASN
2	A	321	GLN
2	A	351	GLN
2	A	412	GLN
2	A	419	ASN
2	A	458	GLN
2	A	470	ASN
2	A	497	ASN
2	A	498	ASN
2	A	590	GLN
2	A	628	ASN
2	A	646	GLN
2	A	678	GLN
2	A	688	GLN
2	A	691	ASN
2	A	710	ASN
2	A	735	ASN
2	B	229	HIS
2	B	233	GLN
2	B	255	HIS
2	B	290	HIS
2	B	351	GLN
2	B	419	ASN
2	B	452	ASN
2	B	459	GLN
2	B	470	ASN
2	B	496	ASN
2	B	519	ASN
2	B	663	ASN
2	B	668	ASN
2	B	678	GLN
2	B	688	GLN
2	B	700	GLN
2	C	227	ASN
2	C	329	ASN
2	C	403	GLN
2	C	410	ASN
2	C	452	ASN
2	C	456	GLN

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Mol	Chain	Res	Type
2	C	519	ASN
2	C	588	GLN
2	C	592	GLN
2	C	678	GLN
2	C	700	GLN
2	C	735	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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.

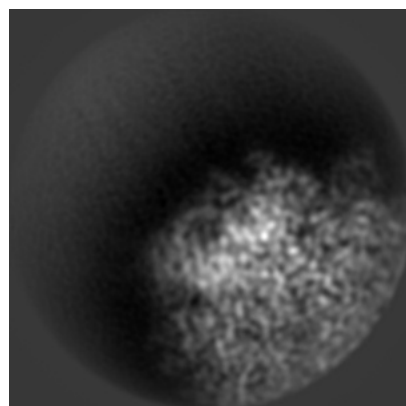
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36311. These allow visual inspection of the internal detail of the map and identification of artifacts.

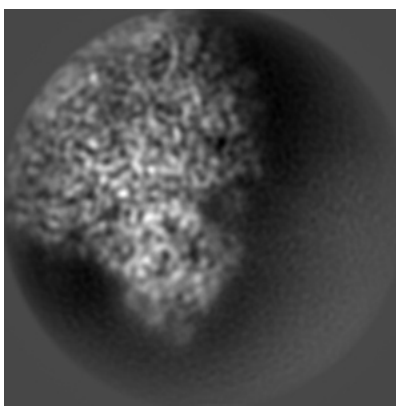
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

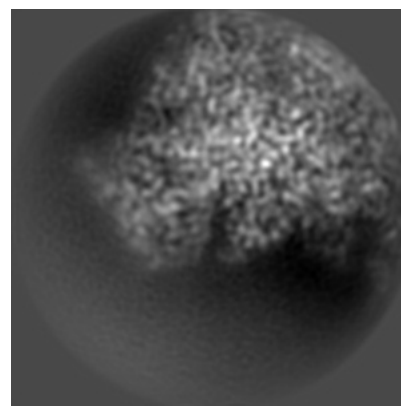
6.1.1 Primary map



X

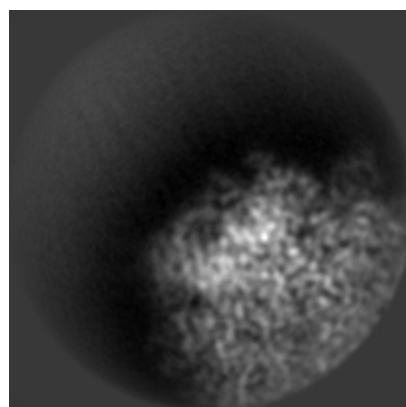


Y

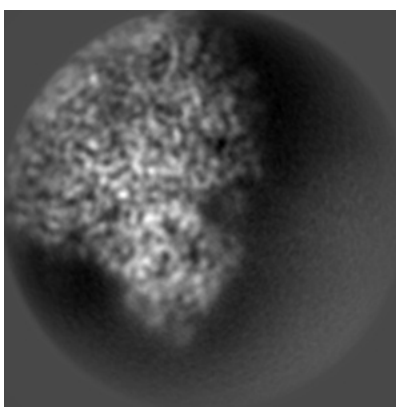


Z

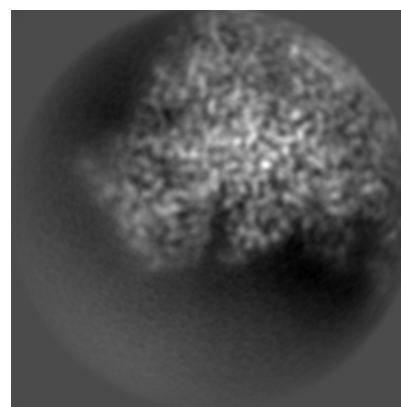
6.1.2 Raw map



X



Y

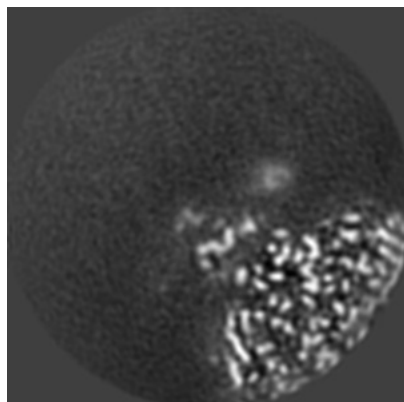


Z

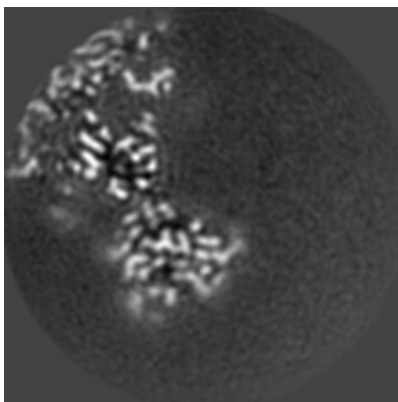
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

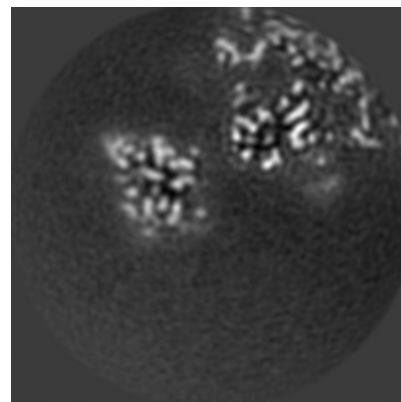
6.2.1 Primary map



X Index: 80

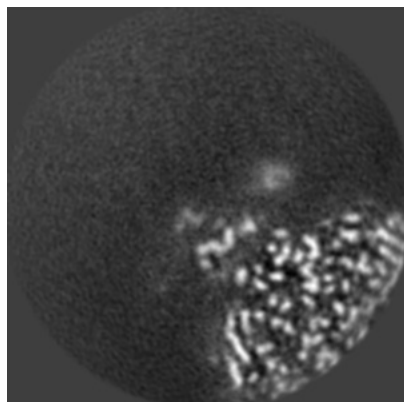


Y Index: 80

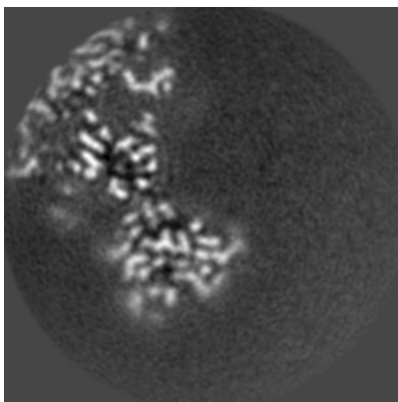


Z Index: 80

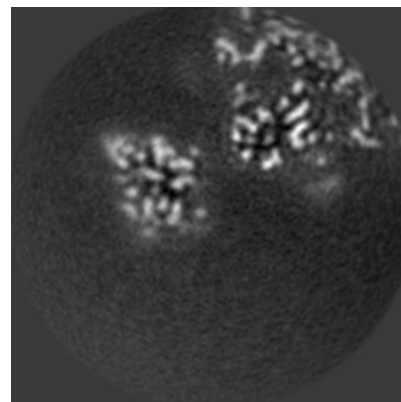
6.2.2 Raw map



X Index: 80



Y Index: 80

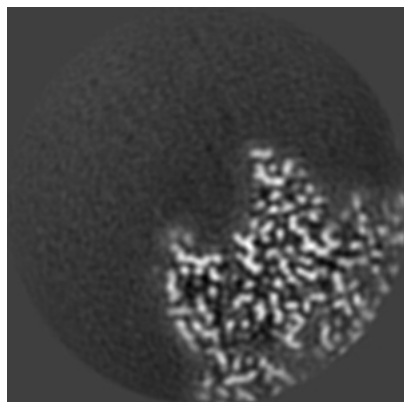


Z Index: 80

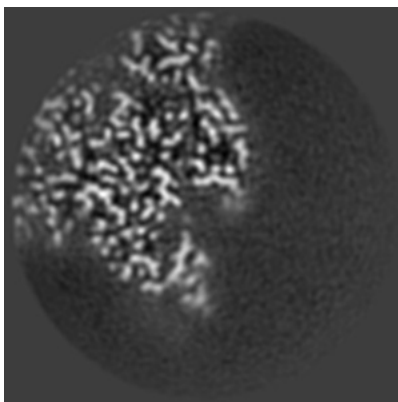
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

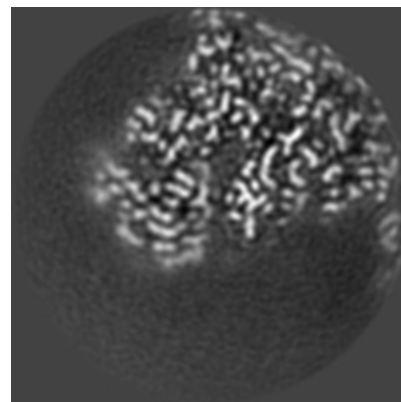
6.3.1 Primary map



X Index: 95

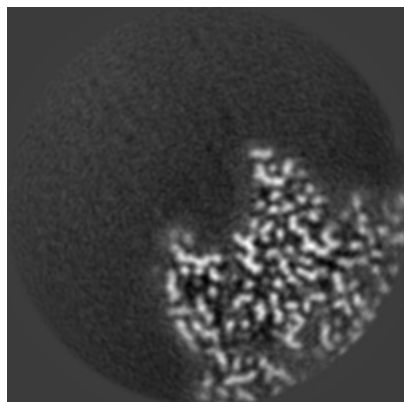


Y Index: 107

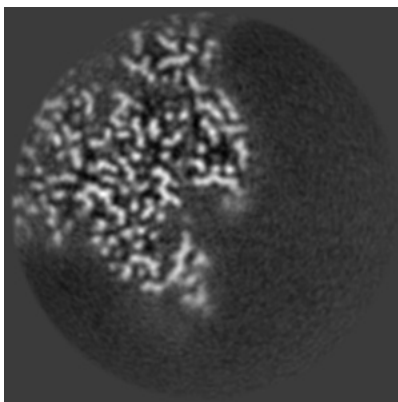


Z Index: 59

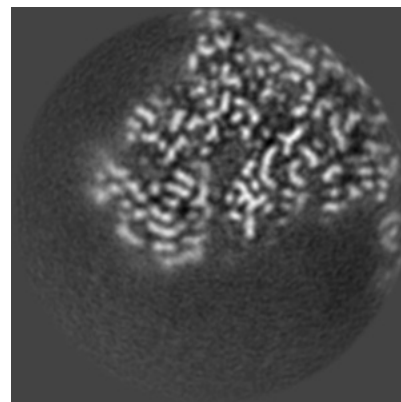
6.3.2 Raw map



X Index: 95



Y Index: 107

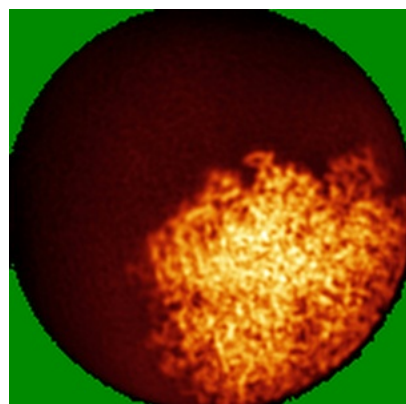


Z Index: 59

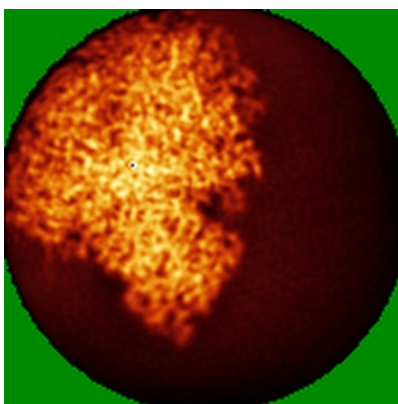
The images above show the largest variance slices of the map in three orthogonal directions.

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

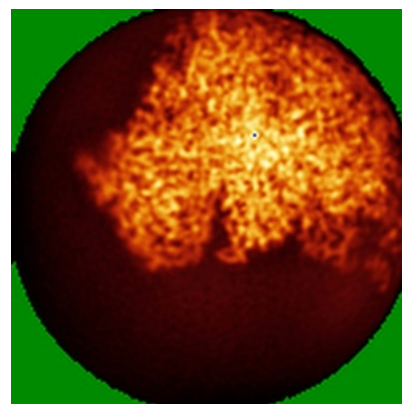
6.4.1 Primary map



X

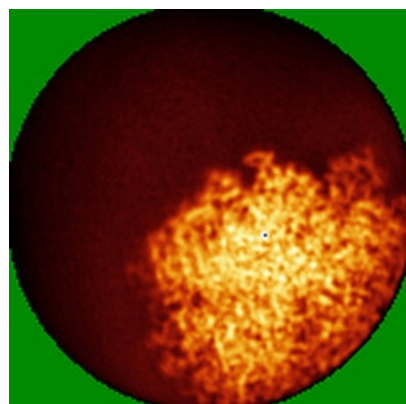


Y

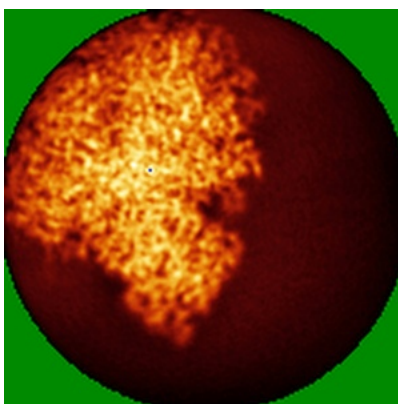


Z

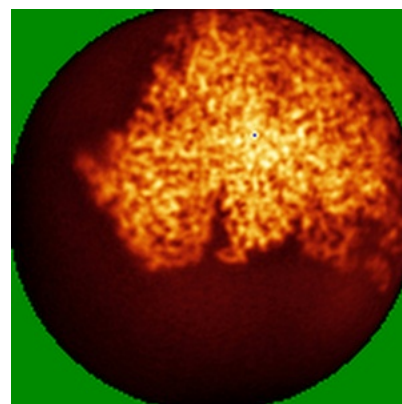
6.4.2 Raw map



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 0.01. 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.

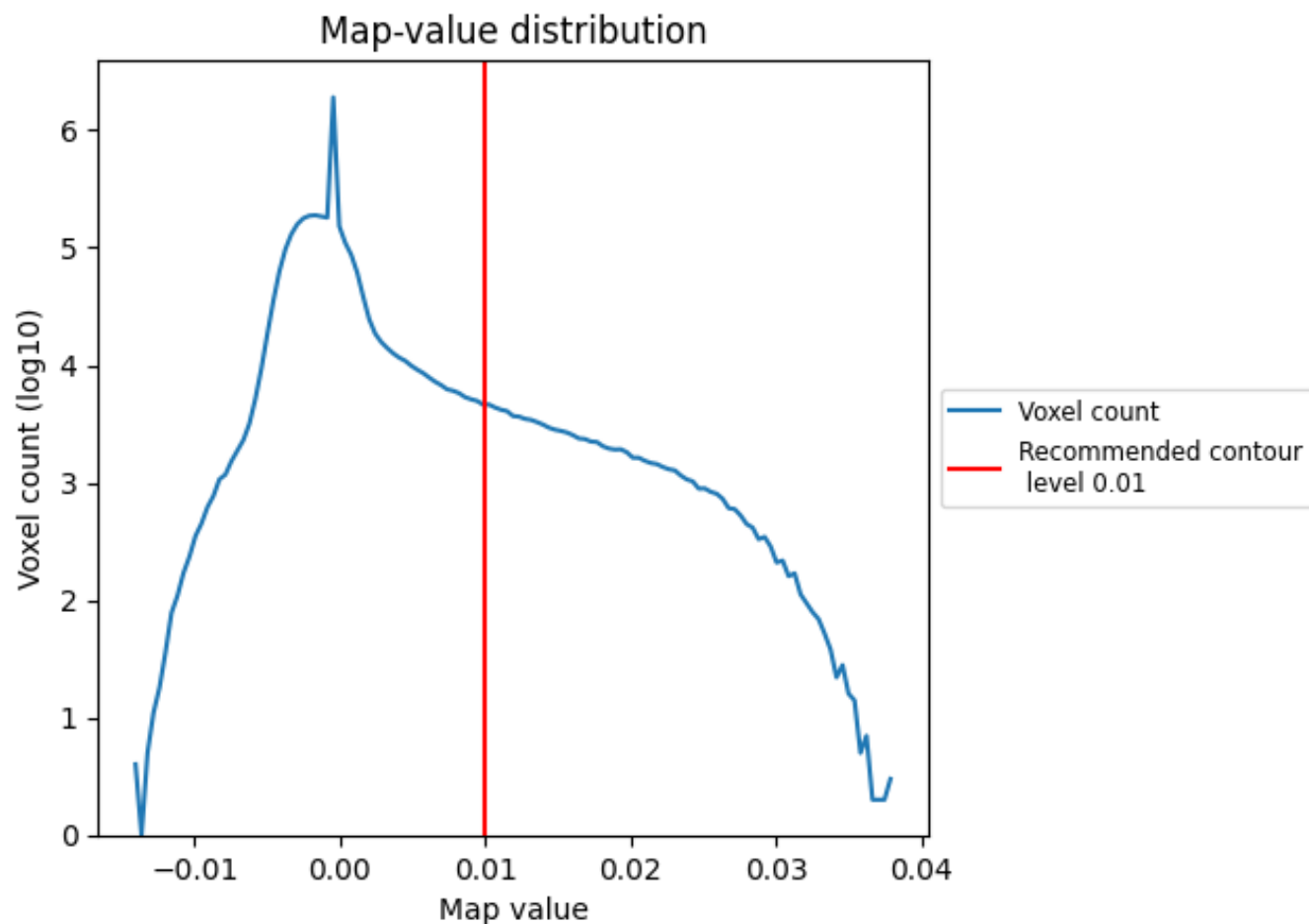
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

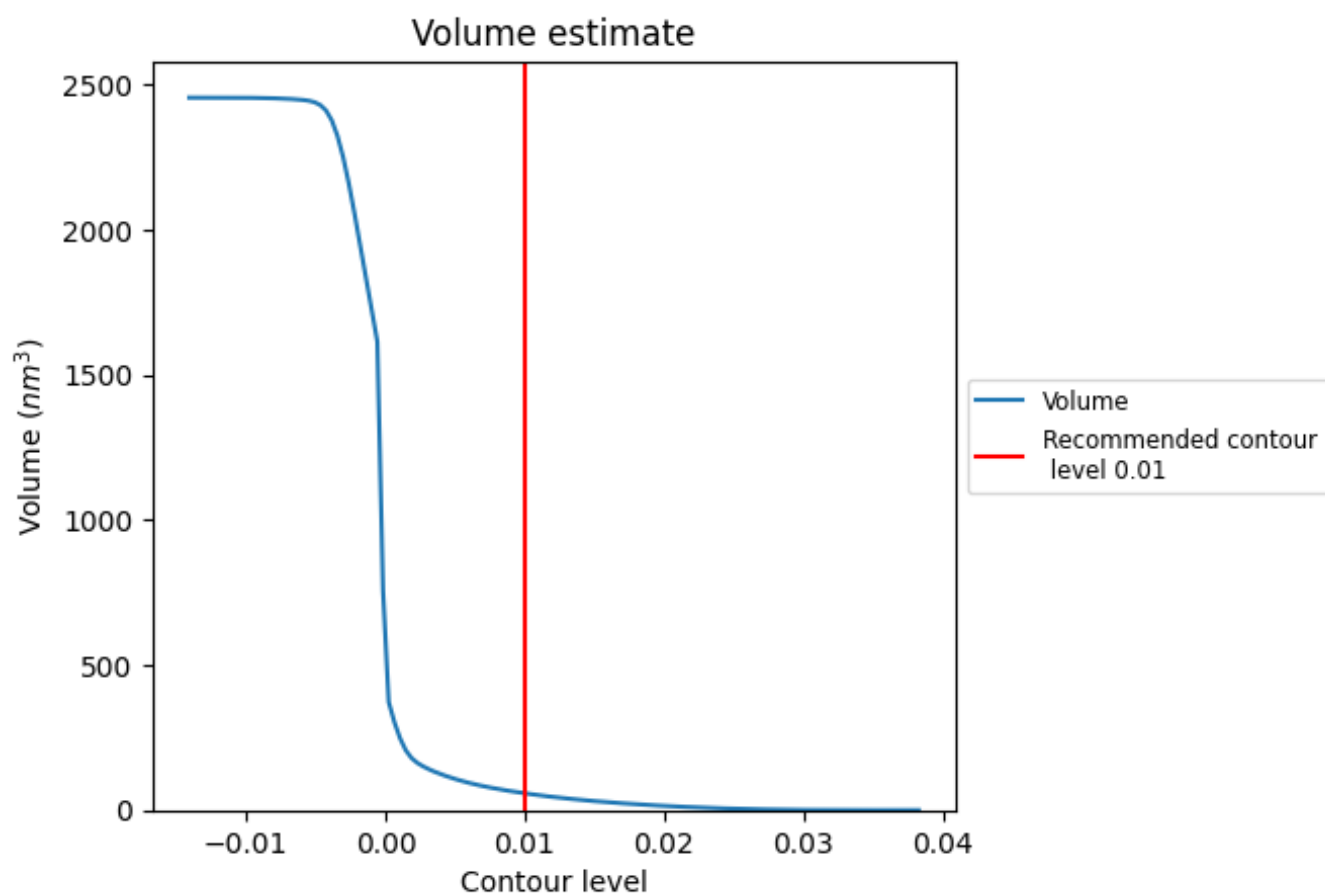
This section contains the results of statistical analysis of the map.

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.

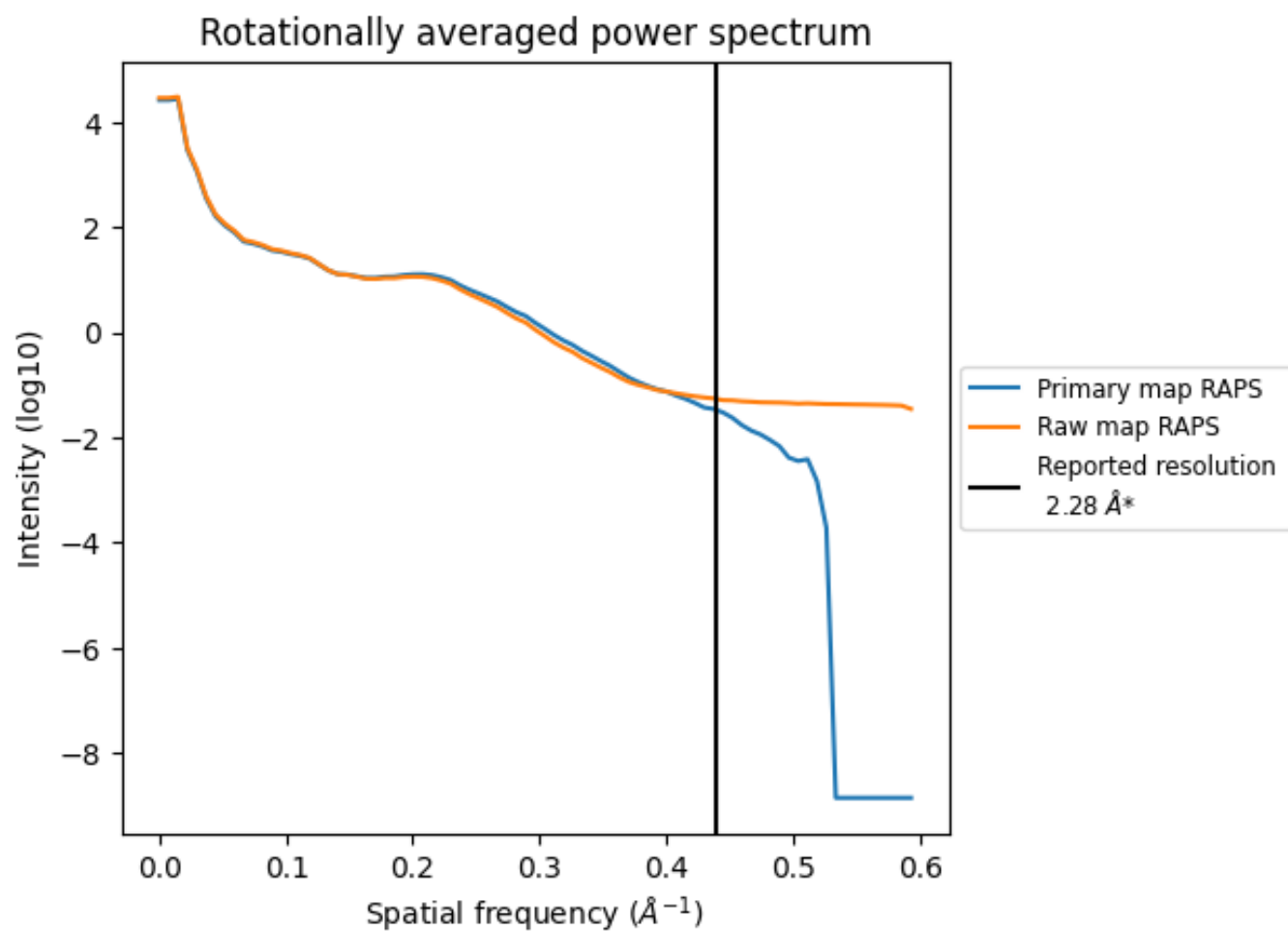
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 58 nm^3 ; this corresponds to an approximate mass of 53 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 ⓘ

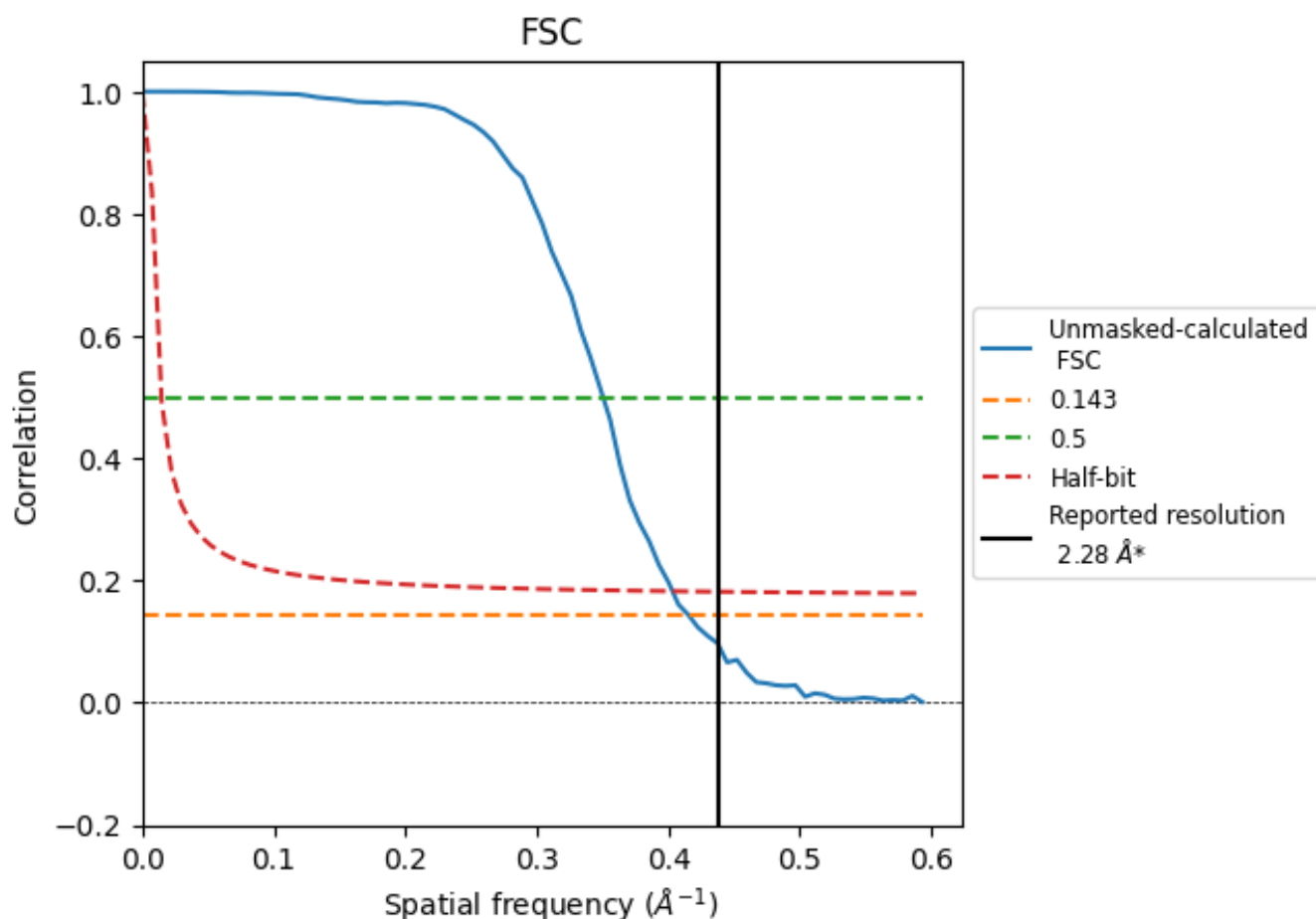


*Reported resolution corresponds to spatial frequency of 0.439 Å⁻¹

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 0.439 Å⁻¹

8.2 Resolution estimates [i](#)

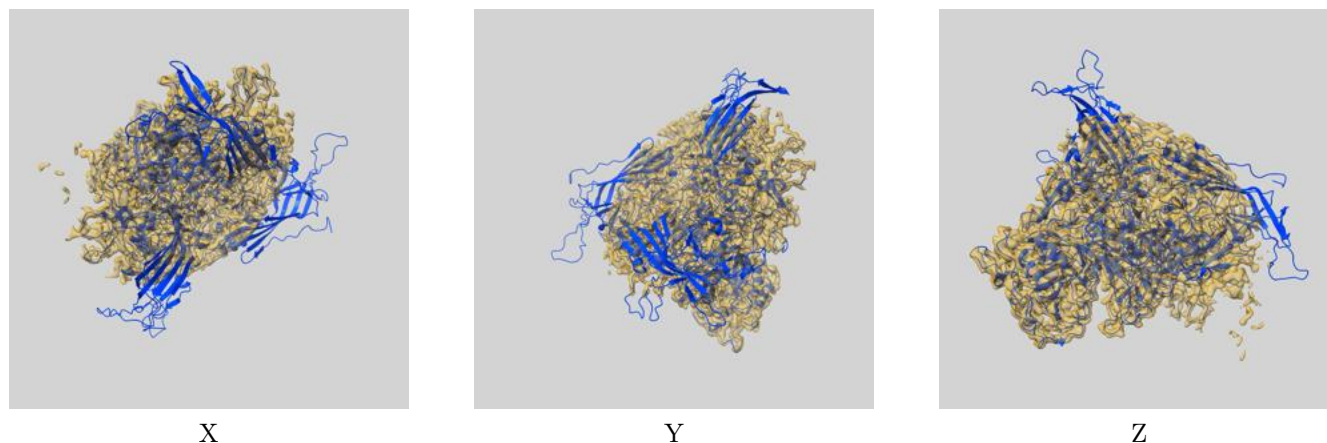
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.28	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.41	2.85	2.48

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

9 Map-model fit [i](#)

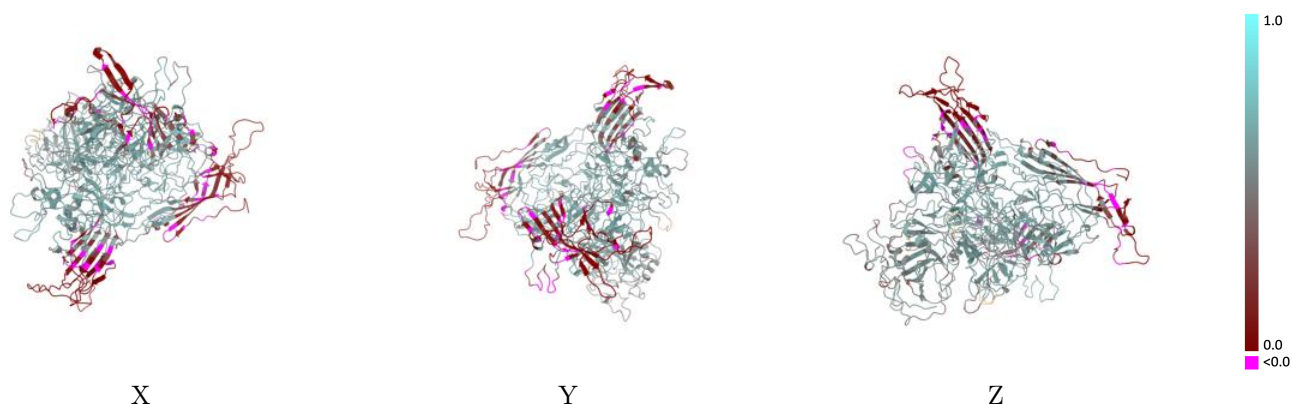
This section contains information regarding the fit between EMDB map EMD-36311 and PDB model 8JIF. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



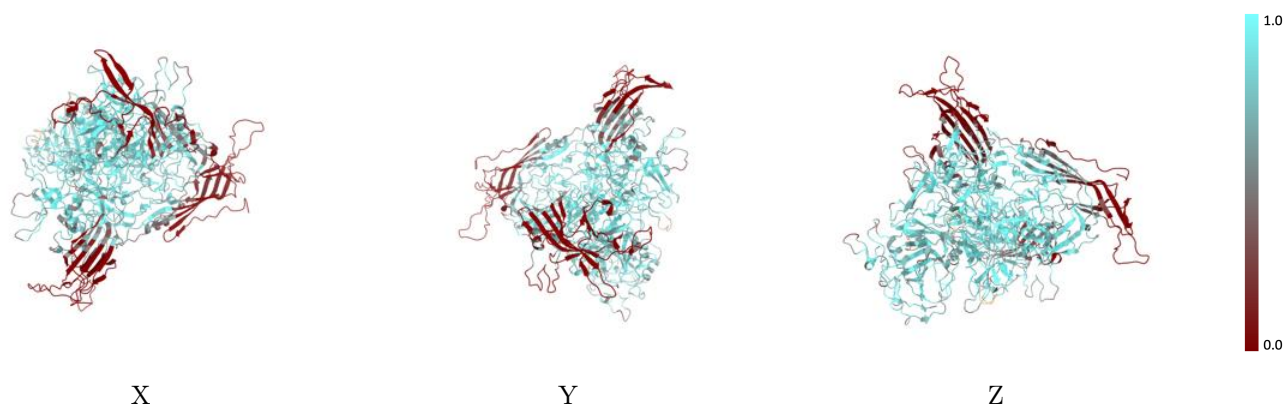
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



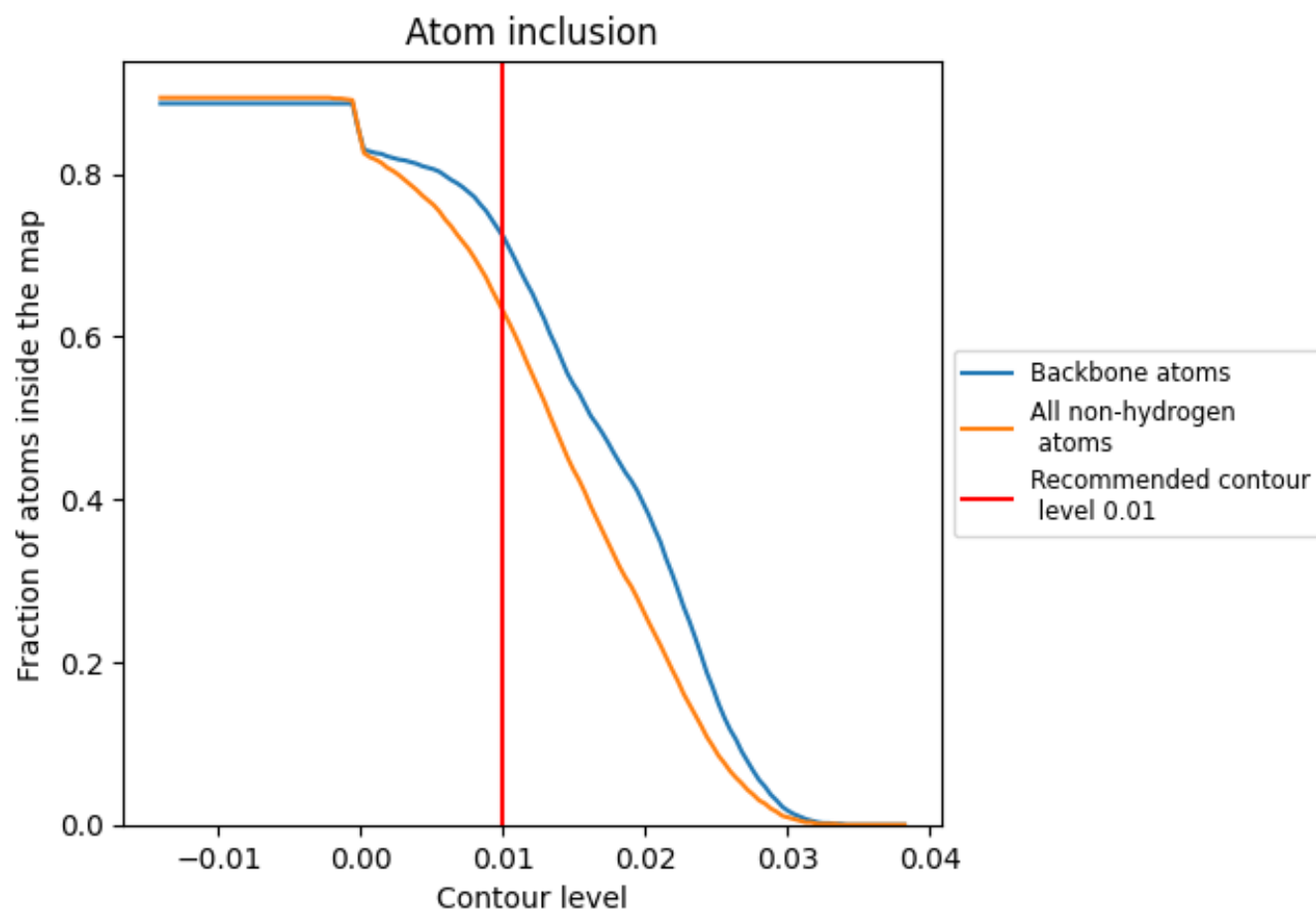
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 63% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6330	0.4730
A	0.6570	0.4910
B	0.5600	0.4320
C	0.6300	0.4770
R	0.7360	0.5090

