



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 11:57 PM UTC

PDB ID : 8CVZ / pdb_00008cvz
EMDB ID : EMD-27022
Title : Human glycogenin-1 and glycogen synthase-1 complex in the apo ordered state
Authors : Liu, Y.; Fastman, N.M.; Tzitzilonis, C.
Deposited on : 2022-05-18
Resolution : 3.52 Å(reported)
Based on initial models : 3Q4S, 4QLB

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

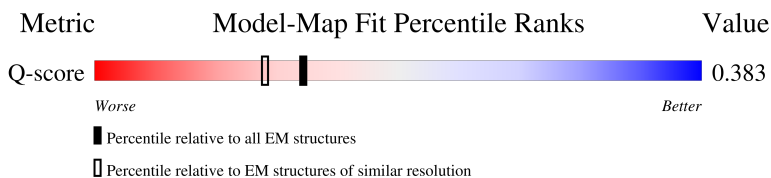
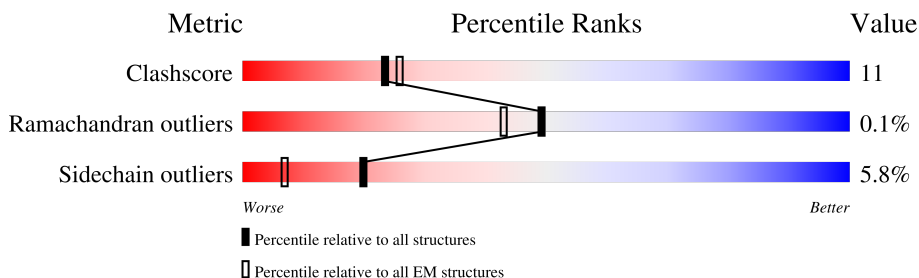
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.52 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	13017 (3.02 - 4.02)

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	E	352	8% . 90%
1	F	352	9% . 90%
1	G	352	5% . 90%
1	H	352	8% .. 90%

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Mol	Chain	Length	Quality of chain
1	I	352	59%15%24%
1	J	352	21%60%13%26%
2	A	634	67%25%5%
2	B	634	41%67%25%5%
2	C	634	65%27%5%
2	D	634	70%23%5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24517 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 Glycogenin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	261	Total	C	N	O	S	0	0
			2057	1334	333	381	9		
1	E	35	Total	C	N	O	S	0	0
			295	180	52	62	1		
1	I	267	Total	C	N	O	S	0	0
			2100	1360	342	389	9		
1	F	35	Total	C	N	O	S	0	0
			295	180	52	62	1		
1	G	34	Total	C	N	O	S	0	0
			285	175	50	59	1		
1	H	34	Total	C	N	O	S	0	0
			285	175	50	59	1		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-1	GLY	-	expression tag	UNP P46976
J	0	PRO	-	expression tag	UNP P46976
J	195	PHE	TYR	engineered mutation	UNP P46976
E	-1	GLY	-	expression tag	UNP P46976
E	0	PRO	-	expression tag	UNP P46976
E	195	PHE	TYR	engineered mutation	UNP P46976
I	-1	GLY	-	expression tag	UNP P46976
I	0	PRO	-	expression tag	UNP P46976
I	195	PHE	TYR	engineered mutation	UNP P46976
F	-1	GLY	-	expression tag	UNP P46976
F	0	PRO	-	expression tag	UNP P46976
F	195	PHE	TYR	engineered mutation	UNP P46976
G	-1	GLY	-	expression tag	UNP P46976
G	0	PRO	-	expression tag	UNP P46976
G	195	PHE	TYR	engineered mutation	UNP P46976
H	-1	GLY	-	expression tag	UNP P46976
H	0	PRO	-	expression tag	UNP P46976
H	195	PHE	TYR	engineered mutation	UNP P46976

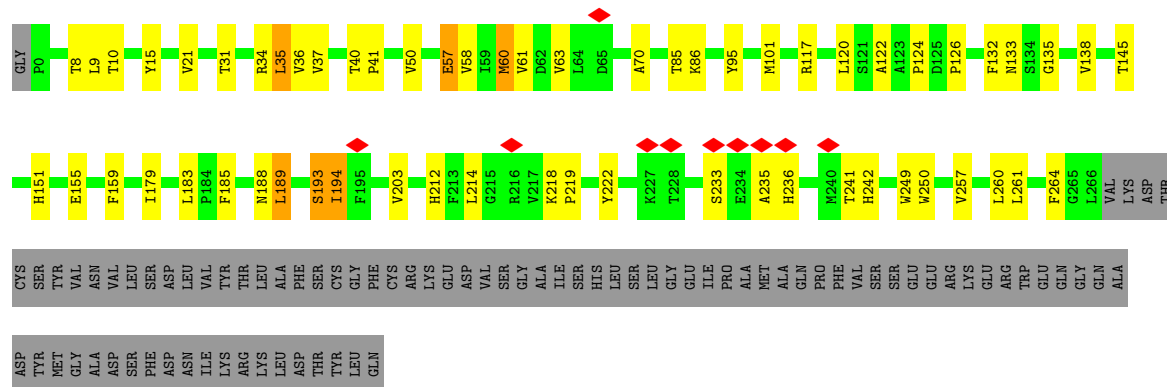
- Molecule 2 is a protein called Glycogen [starch] synthase, muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	602	Total	C	N	O	S	0	0
			4808	3095	822	867	24		
2	C	600	Total	C	N	O	S	0	0
			4781	3075	824	857	25		
2	D	601	Total	C	N	O	S	0	0
			4777	3078	814	860	25		
2	A	601	Total	C	N	O	S	0	0
			4834	3108	834	869	23		

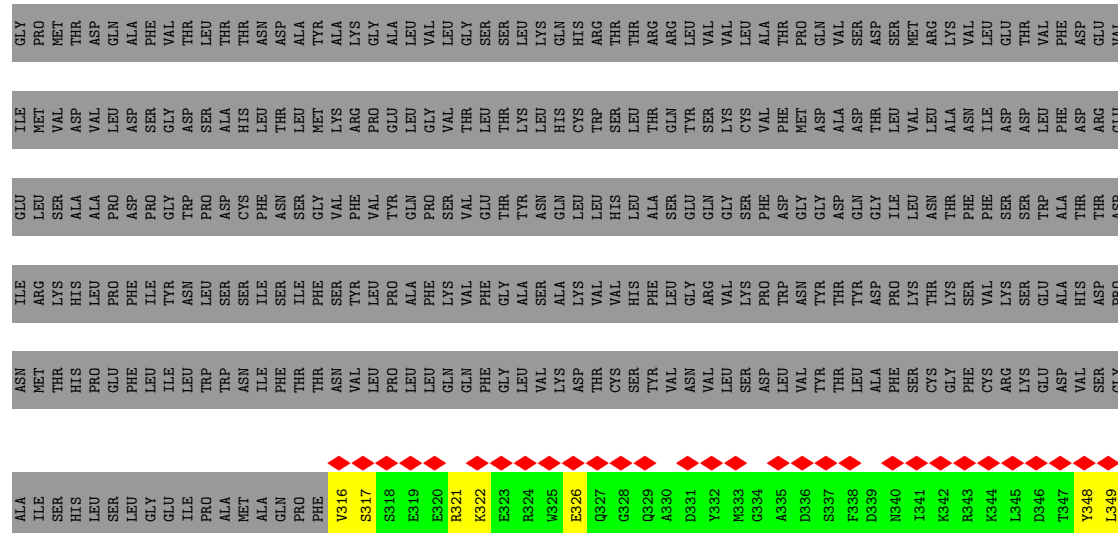
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLU	SER	engineered mutation	UNP P13807
B	11	GLU	SER	engineered mutation	UNP P13807
C	8	GLU	SER	engineered mutation	UNP P13807
C	11	GLU	SER	engineered mutation	UNP P13807
D	8	GLU	SER	engineered mutation	UNP P13807
D	11	GLU	SER	engineered mutation	UNP P13807
A	8	GLU	SER	engineered mutation	UNP P13807
A	11	GLU	SER	engineered mutation	UNP P13807

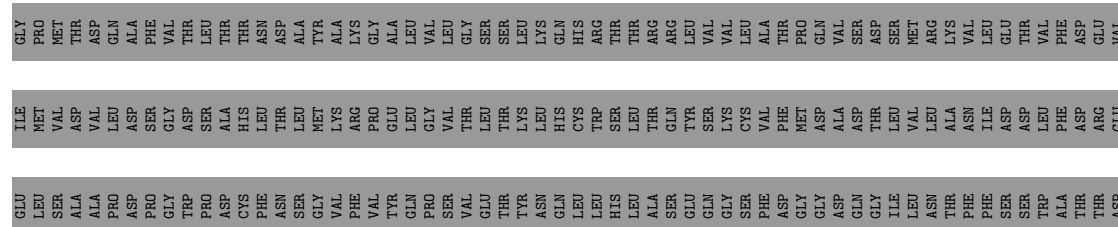
- Molecule 1: Glycogenin-1

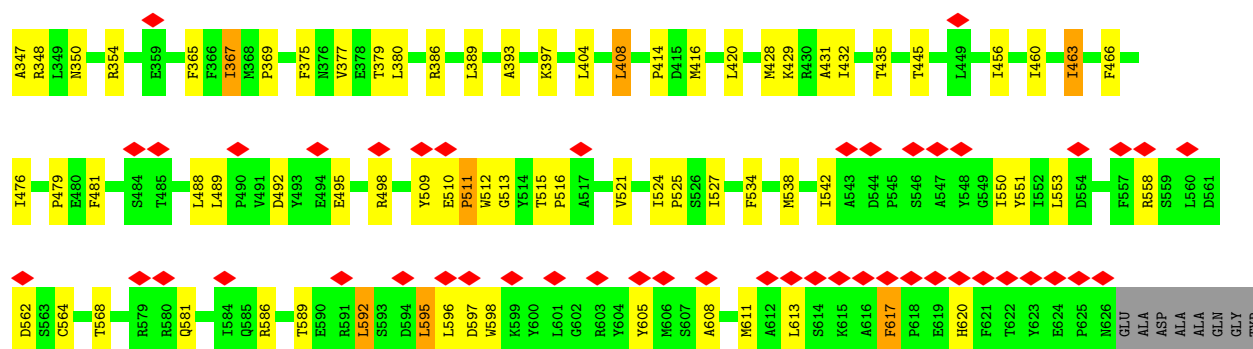


- Molecule 1: Glycogenin-1



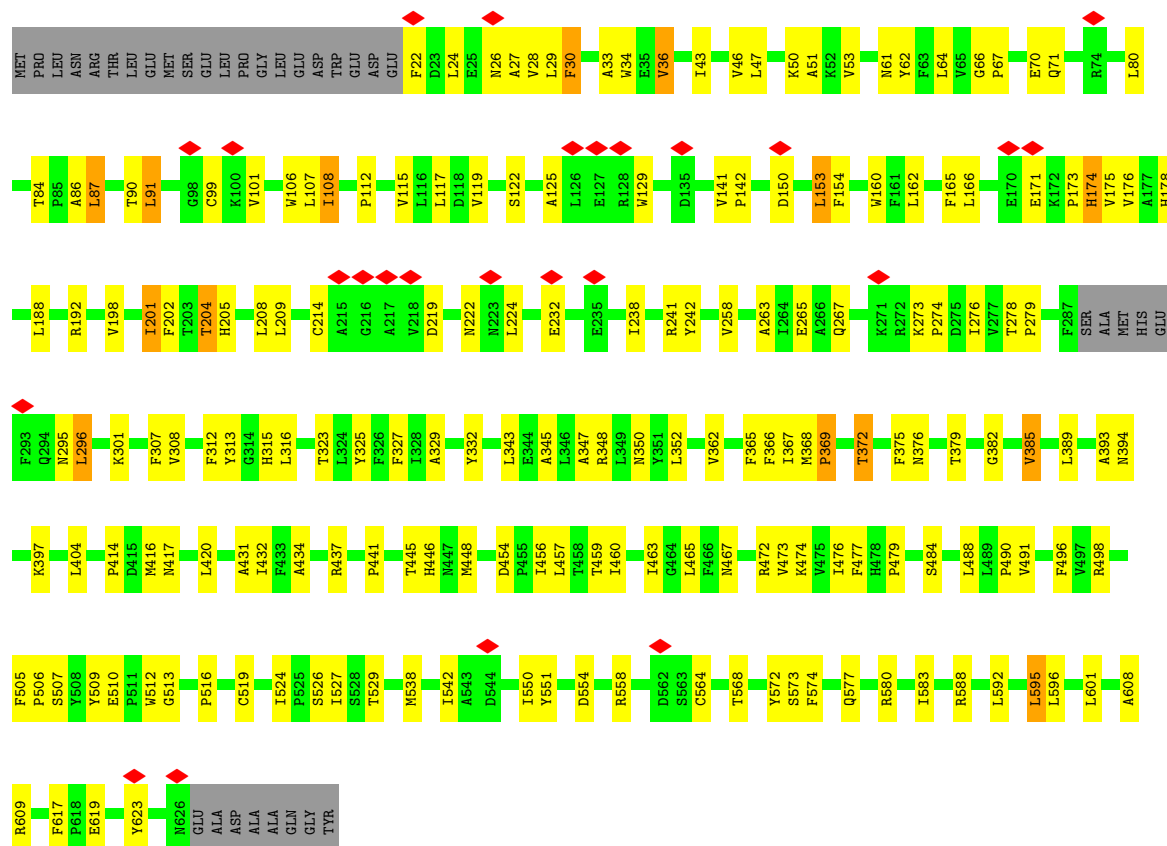
- Molecule 1: Glycogenin-1





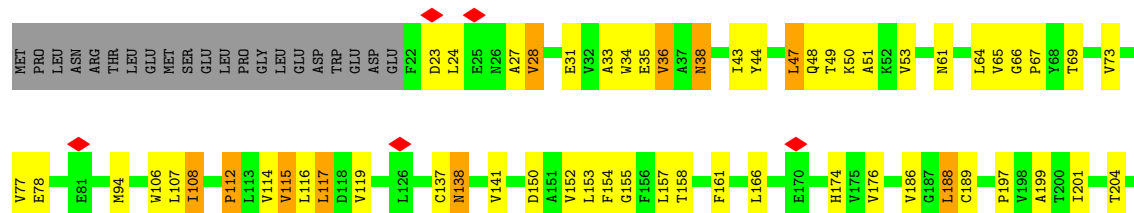
• Molecule 2: Glycogen [starch] synthase, muscle

Chain C: 65% 27% 5%



• Molecule 2: Glycogen [starch] synthase, muscle

Chain D: 70% 23% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	322214	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was performed in batch in early steps. CTF correction was performed on per particle bases in the last iterations	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	4.469	Depositor
Minimum map value	-3.439	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.101	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	296.2008, 296.2008, 296.2008	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.9142, 0.9142, 0.9142	Depositor

5 Model quality

5.1 Standard geometry

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	E	0.57	0/299	1.14	0/397
1	F	0.49	0/299	1.10	0/397
1	G	0.49	0/289	1.09	0/385
1	H	0.53	0/289	1.16	0/385
1	I	0.52	0/2158	1.09	4/2945 (0.1%)
1	J	0.50	0/2112	1.06	2/2880 (0.1%)
2	A	0.54	0/4963	1.11	8/6733 (0.1%)
2	B	0.54	0/4937	1.12	11/6701 (0.2%)
2	C	0.59	0/4907	1.17	8/6661 (0.1%)
2	D	0.60	0/4905	1.15	4/6663 (0.1%)
All	All	0.56	0/25158	1.13	37/34147 (0.1%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	112	PRO	CB-CA-C	-9.17	100.36	111.46
2	A	49	THR	CB-CA-C	8.62	124.32	109.24
2	B	49	THR	CB-CA-C	8.34	123.83	109.24
2	D	49	THR	CB-CA-C	8.21	123.61	109.24
2	C	506	PRO	CB-CA-C	-7.80	101.99	111.11
1	J	243	PRO	N-CA-C	-6.81	105.84	114.35
2	A	617	PHE	CB-CA-C	6.80	116.03	111.20
2	C	201	ILE	CA-C-O	-6.68	115.31	121.72
2	B	481	PHE	CA-CB-CG	6.63	120.43	113.80
2	B	617	PHE	CB-CA-C	6.33	115.69	111.20
1	I	57	GLU	CA-C-N	-6.08	115.94	121.65
1	I	57	GLU	C-N-CA	-6.08	115.94	121.65
2	D	568	THR	CA-CB-OG1	5.99	118.59	109.60
2	A	589	THR	CA-CB-OG1	-5.99	100.62	109.60
2	B	589	THR	CA-CB-OG1	-5.98	100.64	109.60
2	B	173	PRO	N-CA-C	-5.82	105.80	113.65
2	A	230	ASP	CA-CB-CG	5.76	118.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	173	PRO	N-CA-C	-5.75	105.89	113.65
2	B	492	ASP	CA-CB-CG	-5.69	106.91	112.60
2	C	174	HIS	CB-CA-C	5.68	118.76	109.90
2	B	230	ASP	CA-CB-CG	5.66	118.26	112.60
2	C	171	GLU	CB-CA-C	5.64	120.34	112.11
2	C	365	PHE	CB-CA-C	-5.63	103.25	112.03
2	C	30	PHE	CA-CB-CG	5.30	119.11	113.80
1	J	126	PRO	N-CA-C	-5.26	103.01	111.38
2	A	232	GLU	CB-CG-CD	5.26	121.55	112.60
1	I	138	VAL	CA-C-O	-5.21	116.23	121.59
2	A	621	PHE	CA-CB-CG	5.15	118.95	113.80
2	C	204	THR	CB-CA-C	-5.14	102.68	111.31
2	B	492	ASP	CB-CA-C	5.13	119.97	109.76
2	B	232	GLU	CB-CG-CD	5.13	121.32	112.60
2	C	178	HIS	CB-CA-C	-5.11	104.34	111.85
2	B	466	PHE	CA-CB-CG	5.10	118.90	113.80
2	D	287	PHE	CA-C-O	-5.07	112.18	120.80
1	I	126	PRO	N-CA-C	-5.02	103.89	111.41
2	B	318	PHE	CB-CA-C	5.01	118.00	109.53
2	A	318	PHE	CB-CA-C	5.01	118.00	109.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	295	0	273	2	0
1	F	295	0	273	3	0
1	G	285	0	265	2	0
1	H	285	0	265	4	0
1	I	2100	0	2057	39	0
1	J	2057	0	2021	29	0
2	A	4834	0	4705	119	0
2	B	4808	0	4653	123	0
2	C	4781	0	4641	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	4777	0	4611	108	0
All	All	24517	0	23764	530	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 11.

All (530) 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:C:313:TYR:HD1	2:C:382:GLY:HA2	1.49	0.75
1:I:194:ILE:HG13	1:I:241:THR:HB	1.68	0.74
2:B:105:ARG:HD3	2:B:113:LEU:HD23	1.72	0.72
2:A:105:ARG:HD3	2:A:113:LEU:HD23	1.71	0.72
2:C:295:ASN:HD21	2:A:293:PHE:H	1.38	0.71
2:B:229:VAL:HG11	2:B:269:LEU:HA	1.73	0.71
2:A:229:VAL:HG11	2:A:269:LEU:HA	1.71	0.71
2:C:538:MET:HE1	2:C:592:LEU:HD13	1.71	0.70
2:C:90:THR:HG21	2:C:165:PHE:HA	1.73	0.70
2:A:296:LEU:HD13	2:A:498:ARG:HH21	1.56	0.70
1:I:122:ALA:HB3	1:I:132:PHE:HB2	1.74	0.69
2:D:31:GLU:HB2	2:D:64:LEU:HD23	1.73	0.69
2:D:389:LEU:HD23	2:D:431:ALA:HB1	1.74	0.69
2:A:301:LYS:HG3	2:A:325:TYR:HE2	1.57	0.69
2:C:36:VAL:HB	2:C:66:GLY:HA3	1.74	0.68
2:B:397:LYS:HG3	2:C:397:LYS:HG3	1.74	0.68
2:C:107:LEU:O	2:D:426:THR:HB	1.93	0.68
2:A:389:LEU:HD23	2:A:431:ALA:HB1	1.76	0.67
2:D:389:LEU:HD22	2:A:408:LEU:HB3	1.77	0.67
2:D:446:HIS:HB2	2:D:479:PRO:HG2	1.77	0.67
2:A:65:VAL:HG11	2:A:158:THR:HG22	1.75	0.67
2:A:99:CYS:HG	2:A:160:TRP:HZ3	1.43	0.67
2:D:408:LEU:HB3	2:A:389:LEU:HD22	1.78	0.66
1:J:179:ILE:HB	1:I:179:ILE:HB	1.76	0.66
2:A:36:VAL:HB	2:A:66:GLY:HA3	1.77	0.66
2:D:36:VAL:HB	2:D:66:GLY:HA3	1.77	0.66
2:B:175:VAL:HB	2:B:198:VAL:CG1	2.27	0.65
2:B:312:PHE:HE1	2:B:476:ILE:HD11	1.61	0.64
2:D:229:VAL:HG11	2:D:269:LEU:HA	1.78	0.64
2:C:538:MET:HG3	2:C:550:ILE:HG21	1.78	0.64
2:C:91:LEU:HD13	2:C:101:VAL:HG13	1.80	0.64
2:A:151:ALA:HB2	2:A:183:LEU:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ALA:HB2	2:B:183:LEU:HB2	1.79	0.63
2:D:305:GLN:HE21	2:D:320:LEU:HB3	1.62	0.63
2:B:331:ARG:HH21	2:B:336:ASN:HD22	1.47	0.63
2:A:524:ILE:HD12	2:A:586:ARG:HH22	1.63	0.63
1:I:61:VAL:HG12	1:I:85:THR:HG23	1.81	0.63
2:D:51:ALA:HB1	2:D:112:PRO:HG3	1.79	0.63
2:D:141:VAL:HG21	2:D:152:VAL:HG21	1.81	0.63
2:D:550:ILE:HD13	2:D:592:LEU:HD23	1.80	0.63
2:C:301:LYS:HG3	2:C:325:TYR:HE2	1.64	0.62
2:D:201:ILE:HD11	2:D:609:ARG:HA	1.81	0.62
2:C:125:ALA:HA	2:C:129:TRP:HB2	1.79	0.62
2:B:32:VAL:N	2:B:178:HIS:O	2.32	0.62
2:B:377:VAL:HG21	1:I:145:THR:OG1	1.99	0.61
2:B:524:ILE:HD12	2:B:586:ARG:HH22	1.65	0.61
2:C:208:LEU:HG	2:C:238:ILE:HD11	1.82	0.61
1:J:9:LEU:HD11	1:J:85:THR:HG22	1.83	0.61
2:C:596:LEU:HA	2:C:601:LEU:HD11	1.82	0.61
2:A:106:TRP:HB2	2:A:114:VAL:HG21	1.83	0.61
1:I:9:LEU:HD11	1:I:85:THR:HG22	1.83	0.60
2:C:379:THR:HG21	2:C:445:THR:HA	1.84	0.60
2:A:132:GLU:CD	2:A:156:PHE:HE1	2.09	0.60
2:A:236:ARG:O	2:A:238:ILE:HG12	2.01	0.60
2:A:396:VAL:HG22	2:A:424:ASP:HB2	1.84	0.60
2:B:132:GLU:CD	2:B:156:PHE:HE1	2.09	0.60
2:B:236:ARG:O	2:B:238:ILE:HG12	2.01	0.60
2:B:83:PRO:HD2	2:B:87:LEU:HD23	1.83	0.60
1:J:122:ALA:HB3	1:J:132:PHE:HB2	1.83	0.59
2:B:50:LYS:HE2	2:B:180:HIS:HE1	1.66	0.59
2:A:83:PRO:HD2	2:A:87:LEU:HD23	1.83	0.59
2:C:279:PRO:HG2	2:C:601:LEU:HD22	1.84	0.59
2:D:94:MET:HE1	2:D:117:LEU:HD11	1.84	0.59
2:D:34:TRP:HH2	2:D:150:ASP:HB3	1.67	0.59
2:C:201:ILE:HD11	2:C:609:ARG:HA	1.85	0.59
2:B:175:VAL:HB	2:B:198:VAL:HG11	1.84	0.59
2:B:263:ALA:HB1	2:B:274:PRO:HG3	1.85	0.59
2:A:124:TRP:O	2:A:128:ARG:HB3	2.03	0.59
2:B:558:ARG:HG2	2:B:562:ASP:HB2	1.86	0.58
2:A:263:ALA:HB1	2:A:274:PRO:HG3	1.85	0.58
2:A:558:ARG:HG2	2:A:562:ASP:HB2	1.86	0.58
2:C:347:ALA:HB2	2:C:463:ILE:HB	1.86	0.58
2:B:550:ILE:HD13	2:B:592:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:550:ILE:HD13	2:A:592:LEU:HD12	1.85	0.57
2:B:31:GLU:HB2	2:B:64:LEU:HD23	1.86	0.57
2:B:106:TRP:HB2	2:B:114:VAL:HG21	1.86	0.57
2:C:51:ALA:HB1	2:C:112:PRO:HG3	1.85	0.57
2:A:276:ILE:HD11	2:A:611:MET:HG3	1.86	0.57
2:D:166:LEU:HD13	2:D:197:PRO:HD2	1.87	0.57
1:I:40:THR:HB	1:I:41:PRO:HD2	1.85	0.57
2:C:208:LEU:HD21	2:C:241:ARG:HB3	1.86	0.57
2:B:564:CYS:O	2:B:568:THR:HG23	2.05	0.56
2:A:34:TRP:CH2	2:A:150:ASP:HB3	2.39	0.56
2:A:564:CYS:O	2:A:568:THR:HG23	2.05	0.56
2:B:117:LEU:HD11	2:B:154:PHE:HD1	1.70	0.56
2:A:372:THR:HG21	2:A:479:PRO:HG2	1.87	0.56
2:D:307:PHE:CD1	2:D:488:LEU:HD21	2.40	0.56
2:B:174:HIS:CE1	2:B:620:HIS:HB3	2.41	0.56
2:A:174:HIS:CE1	2:A:620:HIS:HB3	2.40	0.56
2:B:188:LEU:HD13	2:B:202:PHE:HB2	1.87	0.56
2:C:34:TRP:HH2	2:C:150:ASP:HB3	1.71	0.56
2:A:456:ILE:O	2:A:460:ILE:HG13	2.06	0.56
2:D:65:VAL:HG11	2:D:158:THR:HG22	1.87	0.56
2:D:312:PHE:HE1	2:D:474:LYS:HE3	1.71	0.56
2:C:263:ALA:HB1	2:C:274:PRO:HG3	1.88	0.56
2:C:46:VAL:HG11	2:C:205:HIS:HE1	1.69	0.55
2:A:174:HIS:CD2	2:A:617:PHE:HE2	2.24	0.55
2:C:204:THR:O	2:C:204:THR:OG1	2.12	0.55
2:C:527:ILE:HG23	2:C:551:TYR:HB2	1.87	0.55
2:A:188:LEU:HD13	2:A:202:PHE:HB2	1.89	0.55
1:J:159:PHE:HB2	1:I:203:VAL:HG21	1.88	0.55
2:C:564:CYS:O	2:C:568:THR:HG23	2.06	0.55
2:B:50:LYS:NZ	2:B:180:HIS:CE1	2.74	0.55
2:B:149:ASN:O	2:B:153:LEU:HG	2.07	0.55
2:B:212:TYR:HB3	2:B:236:ARG:HD3	1.89	0.55
2:B:534:PHE:CE1	2:B:596:LEU:HD11	2.42	0.55
2:C:28:VAL:HA	2:C:61:ASN:HB3	1.88	0.55
2:C:538:MET:O	2:C:542:ILE:HG22	2.07	0.55
2:D:513:GLY:C	2:D:516:PRO:HD2	2.32	0.55
2:B:174:HIS:CD2	2:B:617:PHE:HE2	2.25	0.55
2:D:539:GLU:HG3	2:D:552:ILE:HG13	1.88	0.55
2:A:460:ILE:HG22	2:A:465:LEU:O	2.07	0.55
2:A:534:PHE:CE1	2:A:596:LEU:HD11	2.42	0.55
2:C:62:TYR:CE2	2:C:64:LEU:HD11	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:367:ILE:HD11	2:C:496:PHE:CE1	2.43	0.54
1:J:40:THR:HB	1:J:41:PRO:HD2	1.89	0.54
2:B:37:ALA:HB2	2:B:116:LEU:HD23	1.88	0.54
2:D:27:ALA:HA	2:D:174:HIS:O	2.07	0.54
2:A:149:ASN:O	2:A:153:LEU:HG	2.08	0.54
2:C:26:ASN:HB3	2:C:173:PRO:HB3	1.90	0.54
2:C:295:ASN:ND2	2:A:293:PHE:H	2.03	0.54
2:C:238:ILE:HG13	2:C:241:ARG:HH11	1.72	0.54
2:C:376:ASN:HB3	2:C:379:THR:HG23	1.89	0.54
2:D:307:PHE:HA	2:D:383:GLN:HE21	1.71	0.54
2:B:258:VAL:HG21	2:B:512:TRP:HB2	1.90	0.54
2:D:251:CYS:HA	1:H:349:LEU:HD11	1.90	0.54
2:B:34:TRP:CH2	2:B:150:ASP:HB3	2.43	0.54
2:C:219:ASP:OD2	2:C:222:ASN:HB2	2.07	0.54
2:C:307:PHE:HE2	2:C:476:ILE:HG21	1.73	0.54
2:A:538:MET:O	2:A:542:ILE:HG22	2.07	0.54
2:C:463:ILE:HD11	2:C:465:LEU:HD12	1.88	0.54
1:E:322:LYS:O	1:E:326:GLU:HG2	2.07	0.54
1:I:36:VAL:HG21	1:I:95:TYR:CZ	2.42	0.54
2:B:538:MET:O	2:B:542:ILE:HG22	2.07	0.54
2:C:507:SER:H	2:C:529:THR:HG21	1.72	0.54
2:D:33:ALA:HB3	2:D:36:VAL:HG23	1.91	0.53
2:D:141:VAL:HG21	2:D:152:VAL:CG2	2.39	0.53
2:D:64:LEU:HB2	2:D:114:VAL:HG22	1.90	0.53
1:I:212:HIS:CE1	1:I:214:LEU:HD21	2.43	0.53
2:D:420:LEU:HD11	2:A:400:PHE:HZ	1.74	0.53
2:C:62:TYR:CZ	2:C:64:LEU:HD11	2.44	0.53
1:I:117:ARG:HG3	1:I:183:LEU:HD21	1.91	0.53
2:D:376:ASN:HA	2:D:447:ASN:HD22	1.74	0.53
2:B:263:ALA:CB	2:B:274:PRO:HG3	2.39	0.53
2:D:34:TRP:CH2	2:D:150:ASP:HB3	2.44	0.53
2:D:389:LEU:HD11	2:D:435:THR:HG22	1.91	0.53
2:A:211:ARG:HG3	2:A:509:TYR:CE2	2.44	0.53
2:A:498:ARG:HA	2:A:524:ILE:HD11	1.91	0.53
2:A:65:VAL:CG1	2:A:158:THR:HG22	2.39	0.52
2:C:142:PRO:HA	1:G:326:GLU:HA	1.92	0.52
2:C:519:CYS:SG	2:C:526:SER:HB3	2.48	0.52
2:D:263:ALA:CB	2:D:274:PRO:HG2	2.39	0.52
2:A:31:GLU:HB2	2:A:64:LEU:HD23	1.90	0.52
1:J:129:PRO:HB2	1:I:124:PRO:HB2	1.91	0.52
2:B:331:ARG:NH2	2:B:336:ASN:HD22	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:513:GLY:C	2:A:516:PRO:HD2	2.34	0.52
2:A:524:ILE:HD12	2:A:586:ARG:NH2	2.24	0.52
1:H:322:LYS:O	1:H:326:GLU:HG2	2.10	0.52
2:B:152:VAL:HG12	2:B:244:MET:HE1	1.91	0.52
2:C:22:PHE:HB2	2:C:623:TYR:HB3	1.90	0.52
2:A:350:ASN:O	2:A:354:ARG:HG2	2.10	0.52
2:D:114:VAL:HG12	2:D:116:LEU:HG	1.92	0.52
2:A:456:ILE:HG22	2:A:460:ILE:HD11	1.92	0.52
2:B:524:ILE:HD12	2:B:586:ARG:NH2	2.25	0.52
2:C:263:ALA:CB	2:C:274:PRO:HG3	2.40	0.52
2:A:35:GLU:HB3	2:A:44:TYR:HB2	1.90	0.52
2:A:99:CYS:SG	2:A:160:TRP:HZ3	2.32	0.52
2:A:332:TYR:HB2	2:A:369:PRO:O	2.10	0.52
1:F:322:LYS:O	1:F:326:GLU:HG2	2.10	0.52
2:B:138:ASN:HD21	1:F:321:ARG:HH22	1.56	0.52
2:B:284:VAL:HG23	2:B:597:ASP:OD1	2.09	0.52
2:C:312:PHE:HD1	2:C:441:PRO:HG2	1.75	0.52
1:G:322:LYS:O	1:G:326:GLU:HG2	2.10	0.52
2:C:513:GLY:C	2:C:516:PRO:HD2	2.35	0.52
2:D:106:TRP:HB2	2:D:114:VAL:HG21	1.92	0.52
2:A:509:TYR:O	2:A:510:GLU:C	2.53	0.52
2:D:456:ILE:O	2:D:460:ILE:HG13	2.09	0.51
2:B:513:GLY:C	2:B:516:PRO:HD2	2.36	0.51
2:C:33:ALA:HB3	2:C:36:VAL:HG23	1.93	0.51
2:C:267:GLN:HG2	2:C:273:LYS:HD2	1.91	0.51
2:D:362:VAL:HG12	2:D:473:VAL:HG13	1.92	0.51
2:B:416:MET:HG3	2:C:416:MET:HE3	1.92	0.51
2:B:350:ASN:O	2:B:354:ARG:HG2	2.10	0.51
2:C:484:SER:HA	2:C:490:PRO:O	2.10	0.51
2:C:404:LEU:HD12	2:C:414:PRO:HB3	1.91	0.51
2:C:456:ILE:O	2:C:460:ILE:HG13	2.10	0.51
2:B:183:LEU:HD23	2:B:183:LEU:H	1.75	0.51
2:A:94:MET:HB3	2:A:101:VAL:HG11	1.93	0.51
2:A:183:LEU:HD23	2:A:183:LEU:H	1.74	0.51
1:I:61:VAL:CG1	1:I:85:THR:HG23	2.40	0.51
2:B:498:ARG:HA	2:B:524:ILE:HD11	1.92	0.51
2:A:238:ILE:O	2:A:238:ILE:HG22	2.11	0.51
2:B:456:ILE:O	2:B:460:ILE:HG13	2.11	0.51
2:D:534:PHE:HE1	2:D:596:LEU:HD11	1.76	0.51
1:J:101:MET:HA	1:J:135:GLY:O	2.11	0.51
1:J:211:VAL:HG11	1:J:245:PHE:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:HIS:CD2	2:B:201:ILE:HB	2.46	0.51
2:C:507:SER:O	2:C:529:THR:HG21	2.11	0.51
2:D:534:PHE:CE1	2:D:596:LEU:HD11	2.46	0.51
2:A:263:ALA:CB	2:A:274:PRO:HG3	2.40	0.50
2:B:369:PRO:HA	2:B:479:PRO:O	2.12	0.50
2:A:97:LYS:HB3	2:A:160:TRP:HH2	1.76	0.50
2:A:117:LEU:HD11	2:A:154:PHE:HD1	1.76	0.50
2:A:133:LEU:HB2	2:A:156:PHE:HE2	1.76	0.50
2:B:94:MET:HB3	2:B:101:VAL:HG11	1.92	0.50
2:C:332:TYR:HA	2:C:368:MET:HE2	1.94	0.50
2:C:312:PHE:CE1	2:C:474:LYS:HD2	2.47	0.50
2:D:527:ILE:HG12	2:D:551:TYR:HB2	1.94	0.50
2:B:276:ILE:HD12	2:B:608:ALA:HA	1.94	0.50
2:C:34:TRP:CH2	2:C:150:ASP:HB3	2.46	0.50
2:D:313:TYR:CE1	2:D:385:VAL:HG11	2.46	0.50
2:D:416:MET:HE1	2:A:428:MET:HE1	1.93	0.50
2:C:389:LEU:HD22	2:C:431:ALA:HB1	1.94	0.49
2:D:602:GLY:HA2	2:D:605:TYR:CE2	2.48	0.49
1:I:222:TYR:HB2	1:I:250:TRP:HE1	1.77	0.49
2:B:389:LEU:HD11	2:B:435:THR:HG22	1.95	0.49
2:B:527:ILE:HG13	2:B:551:TYR:HB2	1.95	0.49
2:C:375:PHE:CD1	2:C:488:LEU:HD12	2.48	0.49
2:A:124:TRP:CB	2:A:128:ARG:HE	2.26	0.49
1:I:101:MET:HA	1:I:135:GLY:O	2.11	0.49
1:I:8:THR:HG23	1:I:37:VAL:HG23	1.94	0.49
2:B:238:ILE:HG22	2:B:238:ILE:O	2.12	0.49
2:A:106:TRP:HB2	2:A:114:VAL:CG2	2.41	0.49
2:B:389:LEU:HD23	2:B:431:ALA:HB1	1.94	0.49
1:J:36:VAL:HG13	1:J:57:GLU:HB2	1.95	0.49
2:A:200:THR:H	2:A:253:HIS:CD2	2.31	0.49
2:B:133:LEU:HB2	2:B:156:PHE:HE2	1.76	0.49
2:C:385:VAL:HG22	2:C:434:ALA:HB1	1.95	0.49
2:A:132:GLU:CD	2:A:156:PHE:CE1	2.91	0.49
2:B:534:PHE:HE1	2:B:596:LEU:HD11	1.77	0.49
2:C:352:LEU:HD23	2:C:572:TYR:CG	2.48	0.49
2:A:527:ILE:HG13	2:A:551:TYR:HB2	1.95	0.49
2:B:50:LYS:HE2	2:B:180:HIS:CE1	2.47	0.49
2:C:509:TYR:O	2:C:510:GLU:C	2.56	0.49
2:D:73:VAL:HA	2:D:77:VAL:HB	1.95	0.49
2:A:258:VAL:HG21	2:A:512:TRP:HB2	1.95	0.49
2:A:345:ALA:HA	2:A:568:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:GLN:HA	2:D:108:ILE:HD13	1.94	0.48
2:B:393:ALA:O	2:B:397:LYS:HB3	2.13	0.48
1:I:36:VAL:HG21	1:I:95:TYR:OH	2.12	0.48
1:J:153:ALA:HB2	1:J:166:ILE:CD1	2.43	0.48
2:B:106:TRP:HB2	2:B:114:VAL:CG2	2.42	0.48
2:B:345:ALA:HA	2:B:568:THR:HG22	1.96	0.48
2:D:369:PRO:HA	2:D:479:PRO:O	2.13	0.48
2:B:175:VAL:HB	2:B:198:VAL:HG13	1.96	0.48
2:D:137:CYS:SG	2:D:189:CYS:HB3	2.53	0.48
2:A:297:HIS:HB2	2:A:586:ARG:NH1	2.28	0.48
2:B:38:ASN:HB3	2:B:69:THR:HG21	1.95	0.48
2:C:30:PHE:HE2	2:C:162:LEU:HB3	1.79	0.48
2:B:24:LEU:HB2	2:B:27:ALA:HB3	1.95	0.48
2:C:27:ALA:HA	2:C:174:HIS:O	2.12	0.48
2:D:601:LEU:HA	2:D:601:LEU:HD23	1.68	0.48
2:A:534:PHE:HE1	2:A:596:LEU:HD11	1.79	0.48
2:A:174:HIS:HD2	2:A:617:PHE:HE2	1.60	0.48
2:B:276:ILE:HD11	2:B:611:MET:HG3	1.95	0.48
2:D:258:VAL:HG21	2:D:512:TRP:HB2	1.96	0.48
2:D:375:PHE:CE1	2:D:487:PRO:HD2	2.49	0.47
2:A:413:LEU:HD23	2:A:414:PRO:HD2	1.94	0.47
2:A:598:TRP:CZ3	2:A:605:TYR:CE2	3.02	0.47
2:B:32:VAL:O	2:B:179:PHE:HA	2.14	0.47
2:B:509:TYR:O	2:B:510:GLU:C	2.57	0.47
2:B:598:TRP:CZ3	2:B:605:TYR:CE2	3.02	0.47
2:D:65:VAL:CG1	2:D:158:THR:HG22	2.44	0.47
2:D:209:LEU:HD23	2:D:229:VAL:HG12	1.96	0.47
2:D:307:PHE:HD1	2:D:488:LEU:HD21	1.77	0.47
1:I:50:VAL:HG21	1:I:261:LEU:HD23	1.95	0.47
2:B:28:VAL:HA	2:B:61:ASN:HB3	1.97	0.47
2:C:313:TYR:HD2	2:C:437:ARG:HB3	1.78	0.47
2:D:188:LEU:HD11	2:D:252:ALA:HA	1.96	0.47
2:D:332:TYR:HB2	2:D:369:PRO:O	2.13	0.47
2:A:211:ARG:HG3	2:A:509:TYR:HE2	1.78	0.47
2:C:258:VAL:HG21	2:C:512:TRP:HB2	1.96	0.47
2:D:375:PHE:CE2	2:D:488:LEU:HB2	2.50	0.47
1:J:10:THR:HG22	1:J:15:TYR:O	2.14	0.47
2:C:313:TYR:CD1	2:C:382:GLY:HA2	2.40	0.47
2:C:345:ALA:HA	2:C:568:THR:HG22	1.96	0.47
2:D:238:ILE:HG13	2:D:241:ARG:HD2	1.96	0.47
2:C:86:ALA:O	2:C:90:THR:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:LEU:CB	2:B:27:ALA:HB3	2.45	0.47
2:B:36:VAL:HB	2:B:66:GLY:HA3	1.96	0.47
2:B:114:VAL:HG12	2:B:116:LEU:HG	1.97	0.47
2:B:124:TRP:CB	2:B:128:ARG:HE	2.27	0.47
2:B:365:PHE:HB3	2:B:367:ILE:HD11	1.97	0.47
2:A:178:HIS:CD2	2:A:201:ILE:HB	2.50	0.47
2:B:420:LEU:HD13	2:B:428:MET:HE1	1.97	0.47
2:D:209:LEU:HD12	2:D:209:LEU:HA	1.79	0.47
2:A:369:PRO:HA	2:A:479:PRO:O	2.14	0.47
2:B:30:PHE:N	2:B:176:VAL:O	2.41	0.47
2:B:495:GLU:HA	2:B:495:GLU:OE1	2.15	0.47
1:J:9:LEU:HD22	1:J:86:LYS:HB2	1.97	0.47
2:C:394:ASN:HA	2:C:397:LYS:HE2	1.96	0.47
1:I:31:THR:HG21	1:I:35:LEU:HD21	1.97	0.47
2:C:30:PHE:CE2	2:C:162:LEU:HB3	2.50	0.46
2:C:332:TYR:HE1	2:C:477:PHE:CZ	2.34	0.46
2:A:114:VAL:HG12	2:A:116:LEU:HG	1.97	0.46
1:I:36:VAL:HG13	1:I:57:GLU:HB2	1.97	0.46
2:C:368:MET:O	2:C:369:PRO:C	2.59	0.46
2:A:27:ALA:HA	2:A:174:HIS:O	2.14	0.46
1:I:117:ARG:HG3	1:I:183:LEU:CD2	2.45	0.46
2:A:378:GLU:HG2	2:A:442:PRO:HD3	1.98	0.46
2:B:174:HIS:HD2	2:B:617:PHE:HE2	1.62	0.46
2:C:202:PHE:O	2:C:202:PHE:CG	2.68	0.46
2:D:106:TRP:HB2	2:D:114:VAL:CG2	2.45	0.46
2:A:495:GLU:OE1	2:A:495:GLU:HA	2.16	0.46
2:B:36:VAL:HG11	2:B:64:LEU:HB3	1.97	0.46
2:D:28:VAL:HA	2:D:61:ASN:HB3	1.97	0.46
2:D:152:VAL:HA	2:D:186:VAL:HG21	1.98	0.46
2:D:548:TYR:HB3	2:D:592:LEU:HD22	1.98	0.46
1:I:10:THR:HG22	1:I:15:TYR:O	2.16	0.46
2:B:125:ALA:HA	2:B:129:TRP:HB2	1.96	0.46
2:B:177:ALA:HB3	2:B:200:THR:HG22	1.98	0.46
1:I:63:VAL:HG12	1:I:70:ALA:HB3	1.97	0.46
2:B:200:THR:H	2:B:253:HIS:HD2	1.62	0.46
2:B:132:GLU:CD	2:B:156:PHE:CE1	2.91	0.46
2:B:310:GLY:HA2	2:B:386:ARG:HB2	1.98	0.46
2:C:188:LEU:CD1	2:C:202:PHE:HB2	2.46	0.46
2:D:38:ASN:HB3	2:D:69:THR:HG21	1.98	0.46
2:B:416:MET:HG2	2:C:417:ASN:H	1.81	0.45
2:C:307:PHE:CE2	2:C:476:ILE:HG21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:ALA:HB1	2:D:112:PRO:CG	2.46	0.45
2:A:68:TYR:HD1	2:A:73:VAL:HG21	1.82	0.45
2:B:124:TRP:HB3	2:B:128:ARG:HE	1.81	0.45
2:A:125:ALA:HA	2:A:129:TRP:HB2	1.97	0.45
2:A:343:LEU:HD11	2:A:456:ILE:HG23	1.98	0.45
2:A:372:THR:HG22	2:A:448:MET:HA	1.99	0.45
2:C:258:VAL:HA	2:C:278:THR:O	2.16	0.45
2:C:327:PHE:CZ	2:C:505:PHE:HZ	2.34	0.45
2:D:308:VAL:O	2:D:312:PHE:HD2	2.00	0.45
2:A:28:VAL:HA	2:A:61:ASN:HB3	1.97	0.45
2:A:212:TYR:HB3	2:A:236:ARG:HD3	1.98	0.45
2:A:348:ARG:HD2	2:A:568:THR:HG21	1.98	0.45
2:B:27:ALA:HA	2:B:174:HIS:O	2.16	0.45
2:B:77:VAL:HG11	2:B:116:LEU:HD11	1.98	0.45
2:C:313:TYR:CD2	2:C:437:ARG:HB3	2.51	0.45
2:C:368:MET:HB2	2:C:477:PHE:HE1	1.82	0.45
2:D:115:VAL:HG21	2:D:161:PHE:CE2	2.51	0.45
2:D:231:LYS:O	2:D:235:GLU:HG2	2.17	0.45
2:D:488:LEU:C	2:D:488:LEU:HD23	2.41	0.45
2:C:519:CYS:SG	2:C:524:ILE:HB	2.56	0.45
2:D:607:SER:O	2:D:611:MET:HG2	2.17	0.45
2:B:286:LYS:HG3	2:B:521:VAL:HG12	1.99	0.45
2:C:117:LEU:HD11	2:C:154:PHE:CD1	2.51	0.45
2:B:68:TYR:HD1	2:B:73:VAL:HG21	1.82	0.45
2:C:119:VAL:HG12	2:C:119:VAL:O	2.16	0.45
2:A:312:PHE:HD2	2:A:318:PHE:CZ	2.34	0.45
2:D:401:GLY:HA3	2:A:397:LYS:HD2	1.99	0.45
2:D:489:LEU:HD12	2:D:489:LEU:HA	1.88	0.45
2:B:117:LEU:HD11	2:B:154:PHE:CD1	2.51	0.45
2:C:467:ASN:HB3	2:C:474:LYS:HD3	1.99	0.45
2:D:414:PRO:HG2	2:D:416:MET:HE1	1.98	0.45
2:A:310:GLY:HA2	2:A:386:ARG:HB2	1.99	0.45
2:C:446:HIS:HB2	2:C:479:PRO:HD2	1.99	0.45
2:A:525:PRO:HD3	2:A:586:ARG:HD2	1.99	0.45
1:I:9:LEU:HD22	1:I:86:LYS:HB2	1.98	0.45
2:D:327:PHE:HZ	2:D:519:CYS:HG	1.65	0.44
2:C:574:PHE:O	2:C:577:GLN:HB2	2.17	0.44
2:A:147:GLU:HG3	2:A:183:LEU:HD13	1.98	0.44
1:J:159:PHE:CB	1:I:203:VAL:HG21	2.48	0.44
2:C:416:MET:O	2:C:417:ASN:HB2	2.18	0.44
2:D:23:ASP:OD2	2:D:621:PHE:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:TYR:CD1	2:B:73:VAL:HG21	2.52	0.44
1:I:151:HIS:CE1	1:I:155:GLU:HG3	2.52	0.44
1:J:8:THR:HG23	1:J:37:VAL:HG23	1.98	0.44
2:D:33:ALA:O	2:D:67:PRO:HD3	2.18	0.44
2:D:332:TYR:CE2	2:D:456:ILE:HG12	2.52	0.44
2:A:489:LEU:HD23	2:A:489:LEU:HA	1.87	0.44
1:J:117:ARG:HG3	1:J:183:LEU:CD2	2.48	0.44
2:B:50:LYS:HZ1	2:B:180:HIS:CE1	2.36	0.44
2:D:502:LEU:HD12	2:D:525:PRO:HB2	2.00	0.44
2:A:393:ALA:O	2:A:397:LYS:HB3	2.17	0.44
1:J:194:ILE:HB	1:J:201:PHE:HB2	2.00	0.44
2:C:296:LEU:HD13	2:C:296:LEU:HA	1.81	0.44
2:C:448:MET:HE2	2:C:454:ASP:OD2	2.17	0.44
2:D:258:VAL:O	2:D:279:PRO:HA	2.17	0.44
2:B:348:ARG:HD2	2:B:568:THR:HG21	2.00	0.43
2:C:273:LYS:HE3	2:C:273:LYS:HB3	1.75	0.43
2:D:138:ASN:HB3	1:H:341:ILE:HD12	2.00	0.43
2:D:488:LEU:HD22	2:D:489:LEU:HB2	2.00	0.43
2:A:68:TYR:CD1	2:A:73:VAL:HG21	2.53	0.43
2:A:77:VAL:HG11	2:A:116:LEU:HD11	2.00	0.43
1:E:349:LEU:O	1:E:350:GLN:C	2.61	0.43
2:D:47:LEU:HD23	2:D:64:LEU:HD22	2.00	0.43
2:D:176:VAL:HA	2:D:199:ALA:O	2.19	0.43
2:A:334:PHE:CE2	2:A:340:ASP:HB3	2.53	0.43
2:C:224:LEU:HD21	2:C:265:GLU:HA	2.00	0.43
1:I:60:MET:HB3	1:I:60:MET:HE3	1.67	0.43
2:C:343:LEU:HG	2:C:366:PHE:CZ	2.54	0.43
1:J:120:LEU:HD23	1:J:171:PHE:CZ	2.53	0.43
2:B:200:THR:H	2:B:253:HIS:CD2	2.35	0.43
2:A:400:PHE:CE2	2:A:404:LEU:HD13	2.53	0.43
2:A:515:THR:HG23	2:A:516:PRO:HD3	1.99	0.43
2:B:404:LEU:HD12	2:B:408:LEU:HD13	2.00	0.43
2:D:43:ILE:HD12	2:D:43:ILE:H	1.83	0.43
2:A:375:PHE:CE2	2:A:488:LEU:HB2	2.53	0.43
2:C:84:THR:HB	2:C:87:LEU:HB3	2.00	0.43
2:D:117:LEU:HG	2:D:157:LEU:HB3	2.01	0.43
2:D:119:VAL:O	2:D:153:LEU:HD13	2.19	0.43
2:A:152:VAL:HG12	2:A:244:MET:HE1	2.00	0.43
2:C:573:SER:O	2:C:577:GLN:HG3	2.19	0.43
1:I:37:VAL:HG13	1:I:58:VAL:HG13	2.00	0.43
2:B:151:ALA:HB1	2:B:183:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:404:LEU:HD13	2:B:414:PRO:HG3	2.01	0.42
2:C:28:VAL:O	2:C:175:VAL:HG13	2.19	0.42
2:C:366:PHE:HD1	2:C:366:PHE:H	1.67	0.42
2:D:394:ASN:O	2:D:398:GLU:HG3	2.19	0.42
1:F:349:LEU:O	1:F:350:GLN:C	2.61	0.42
1:H:316:VAL:HB	1:H:317:SER:H	1.71	0.42
2:B:258:VAL:CG2	2:B:512:TRP:HB2	2.49	0.42
2:B:525:PRO:HD3	2:B:586:ARG:HD2	2.01	0.42
2:D:581:GLN:HA	2:D:584:ILE:HD12	2.01	0.42
1:J:90:TRP:CZ2	1:J:120:LEU:HD21	2.54	0.42
2:B:393:ALA:HA	2:C:404:LEU:HD23	2.02	0.42
2:C:209:LEU:HD21	2:C:232:GLU:HB2	2.01	0.42
2:C:301:LYS:HG3	2:C:325:TYR:CE2	2.51	0.42
2:C:329:ALA:HA	2:C:367:ILE:O	2.19	0.42
2:C:348:ARG:HD2	2:C:568:THR:HG21	2.01	0.42
2:C:393:ALA:O	2:C:397:LYS:HB3	2.18	0.42
2:C:554:ASP:O	2:C:558:ARG:HD2	2.19	0.42
1:I:185:PHE:HZ	1:I:193:SER:HB3	1.84	0.42
2:B:296:LEU:HD22	2:B:498:ARG:NH2	2.34	0.42
2:C:29:LEU:HD12	2:C:176:VAL:O	2.19	0.42
2:C:498:ARG:HA	2:C:524:ILE:HD11	2.01	0.42
2:C:595:LEU:HD13	2:C:595:LEU:HA	1.93	0.42
2:A:132:GLU:OE2	2:A:156:PHE:HE1	2.03	0.42
2:A:174:HIS:CD2	2:A:613:LEU:HG	2.55	0.42
1:J:128:TRP:CH2	1:I:189:LEU:HD11	2.54	0.42
2:D:448:MET:HE2	2:D:454:ASP:OD2	2.20	0.42
1:J:40:THR:HA	1:J:61:VAL:O	2.20	0.42
1:J:218:LYS:HD3	1:J:218:LYS:HA	1.78	0.42
2:B:511:PRO:HB2	2:B:512:TRP:H	1.58	0.42
2:C:372:THR:OG1	2:C:446:HIS:HB3	2.20	0.42
2:D:263:ALA:HB1	2:D:274:PRO:HG2	2.00	0.42
1:I:21:VAL:HG11	1:I:249:TRP:CD1	2.55	0.42
1:J:21:VAL:HG11	1:J:249:TRP:CD1	2.55	0.42
2:D:224:LEU:HD12	2:D:224:LEU:HA	1.79	0.42
2:D:246:ARG:HG3	2:D:270:LEU:O	2.19	0.42
2:D:301:LYS:HG3	2:D:325:TYR:HE2	1.84	0.42
2:A:24:LEU:H	2:A:24:LEU:HG	1.69	0.42
2:A:137:CYS:HB2	2:A:139:ILE:HG22	2.02	0.42
2:B:43:ILE:HD12	2:B:43:ILE:H	1.85	0.42
2:C:175:VAL:C	2:C:198:VAL:HG23	2.44	0.42
2:C:343:LEU:HD23	2:C:343:LEU:HA	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:279:PRO:HD2	2:D:601:LEU:HD22	2.02	0.42
2:B:33:ALA:HB2	2:B:180:HIS:HB2	2.01	0.42
2:C:362:VAL:HB	2:C:473:VAL:HG22	2.02	0.42
2:C:580:ARG:HA	2:C:583:ILE:HD12	2.01	0.42
1:I:34:ARG:HE	1:I:34:ARG:HB3	1.65	0.42
1:J:120:LEU:N	1:J:138:VAL:O	2.52	0.41
2:B:375:PHE:HB3	2:B:380:LEU:HG	2.02	0.41
2:A:154:PHE:O	2:A:158:THR:HG23	2.20	0.41
2:A:258:VAL:CG2	2:A:512:TRP:HB2	2.49	0.41
2:A:598:TRP:HZ3	2:A:605:TYR:CE2	2.38	0.41
1:I:50:VAL:HG22	1:I:264:PHE:HB2	2.01	0.41
2:B:24:LEU:H	2:B:24:LEU:HG	1.72	0.41
2:B:31:GLU:HG3	2:B:62:TYR:HE1	1.85	0.41
2:B:132:GLU:OE2	2:B:156:PHE:HE1	2.02	0.41
2:B:137:CYS:HB2	2:B:139:ILE:HG22	2.02	0.41
2:B:151:ALA:CB	2:B:183:LEU:HB2	2.47	0.41
2:C:166:LEU:HD21	2:C:175:VAL:HG23	2.02	0.41
2:C:507:SER:H	2:C:529:THR:CG2	2.32	0.41
1:I:133:ASN:HB3	1:I:188:ASN:ND2	2.35	0.41
2:C:332:TYR:CE1	2:C:456:ILE:HD13	2.55	0.41
2:C:472:ARG:HE	2:C:472:ARG:HA	1.85	0.41
2:C:588:ARG:HH21	2:A:591:ARG:NH2	2.18	0.41
2:D:579:ARG:HD2	2:D:582:ARG:HH21	1.85	0.41
2:B:347:ALA:HB2	2:B:463:ILE:HG13	2.02	0.41
2:B:379:THR:HG22	2:B:488:LEU:HD22	2.01	0.41
2:C:106:TRP:CD2	2:C:108:ILE:HG12	2.55	0.41
2:A:43:ILE:HD12	2:A:43:ILE:H	1.85	0.41
2:A:51:ALA:HB3	2:A:108:ILE:CD1	2.51	0.41
2:A:595:LEU:HD13	2:A:595:LEU:HA	1.92	0.41
1:I:218:LYS:HB3	1:I:219:PRO:HD2	2.02	0.41
1:J:194:ILE:HG12	1:J:195:PHE:N	2.35	0.41
1:J:198:LEU:O	1:J:199:PRO:C	2.63	0.41
2:B:51:ALA:HB3	2:B:108:ILE:CD1	2.50	0.41
2:B:284:VAL:HG12	2:B:287:PHE:CD2	2.56	0.41
2:C:258:VAL:CG2	2:C:512:TRP:HB2	2.50	0.41
2:C:276:ILE:HD13	2:C:608:ALA:HA	2.02	0.41
2:D:258:VAL:CG2	2:D:512:TRP:HB2	2.51	0.41
2:B:36:VAL:HG22	2:B:47:LEU:HD22	2.03	0.41
2:D:375:PHE:CE2	2:D:488:LEU:CB	3.04	0.41
2:D:537:PHE:CE2	2:D:595:LEU:HD23	2.56	0.41
2:A:200:THR:H	2:A:253:HIS:HD2	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:257:VAL:O	1:I:260:LEU:N	2.54	0.41
2:D:313:TYR:CD1	2:D:385:VAL:HG21	2.55	0.41
2:B:489:LEU:HD12	2:B:489:LEU:HA	1.94	0.41
2:C:122:SER:HA	2:C:153:LEU:HD11	2.03	0.41
2:C:343:LEU:HD13	2:C:459:THR:HB	2.02	0.41
2:D:36:VAL:HG11	2:D:64:LEU:O	2.21	0.41
2:D:592:LEU:HD12	2:D:592:LEU:HA	1.69	0.41
2:B:30:PHE:O	2:B:178:HIS:N	2.37	0.41
2:B:106:TRP:CD2	2:B:108:ILE:HG12	2.56	0.41
2:B:320:LEU:HD23	2:B:323:THR:HG21	2.02	0.41
2:C:34:TRP:CD2	2:C:67:PRO:HG3	2.55	0.41
2:C:70:GLU:HG3	2:C:71:GLN:N	2.35	0.41
2:D:78:GLU:HB2	2:D:107:LEU:HD21	2.02	0.41
2:D:515:THR:OG1	2:D:516:PRO:HD3	2.20	0.41
2:A:31:GLU:HG2	2:A:178:HIS:HB3	2.03	0.41
2:A:117:LEU:HD11	2:A:154:PHE:CD1	2.54	0.41
1:I:235:ALA:O	1:I:236:HIS:C	2.64	0.41
1:J:189:LEU:O	1:J:190:SER:C	2.64	0.41
2:B:174:HIS:CD2	2:B:613:LEU:HG	2.56	0.41
2:C:99:CYS:SG	2:C:160:TRP:HZ3	2.44	0.41
2:D:361:THR:HG23	2:D:472:ARG:O	2.21	0.41
2:A:106:TRP:CD2	2:A:108:ILE:HG12	2.56	0.41
2:D:313:TYR:HD1	2:D:385:VAL:HG21	1.86	0.40
1:I:194:ILE:HD12	1:I:242:HIS:HB2	2.02	0.40
1:J:224:TYR:CE1	1:J:254:THR:HG21	2.56	0.40
2:B:267:GLN:HG2	2:B:273:LYS:HG2	2.03	0.40
2:C:580:ARG:HH22	2:A:284:VAL:HG21	1.86	0.40
2:A:32:VAL:N	2:A:178:HIS:O	2.50	0.40
2:A:149:ASN:O	2:A:152:VAL:HG22	2.21	0.40
2:A:333:GLU:HG2	2:A:336:ASN:HB2	2.02	0.40
2:C:64:LEU:HD12	2:C:64:LEU:N	2.36	0.40
2:C:258:VAL:O	2:C:279:PRO:HA	2.21	0.40
2:D:35:GLU:HB3	2:D:44:TYR:HB2	2.04	0.40
2:A:30:PHE:HA	2:A:63:PHE:O	2.22	0.40
2:A:463:ILE:CG2	2:A:465:LEU:HG	2.51	0.40
1:J:201:PHE:O	1:J:205:GLY:N	2.54	0.40
1:J:203:VAL:HG21	1:I:159:PHE:HB3	2.03	0.40
2:B:154:PHE:O	2:B:158:THR:HG23	2.22	0.40
2:B:595:LEU:HD13	2:B:595:LEU:HA	1.93	0.40
2:D:106:TRP:CD2	2:D:108:ILE:HG12	2.56	0.40
2:D:155:GLY:HA3	2:D:186:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:393:ALA:HA	2:A:404:LEU:HD23	2.03	0.40
2:A:320:LEU:HD23	2:A:323:THR:HG21	2.03	0.40
2:B:296:LEU:HD22	2:B:498:ARG:HH21	1.85	0.40
2:C:43:ILE:HD12	2:C:43:ILE:H	1.86	0.40
2:C:192:ARG:HD2	2:C:192:ARG:HA	1.77	0.40
2:D:154:PHE:O	2:D:158:THR:HG23	2.21	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	E	33/352 (9%)	31 (94%)	2 (6%)	0	100	100
1	F	33/352 (9%)	30 (91%)	3 (9%)	0	100	100
1	G	32/352 (9%)	29 (91%)	3 (9%)	0	100	100
1	H	32/352 (9%)	28 (88%)	4 (12%)	0	100	100
1	I	265/352 (75%)	253 (96%)	12 (4%)	0	100	100
1	J	257/352 (73%)	247 (96%)	10 (4%)	0	100	100
2	A	597/634 (94%)	587 (98%)	10 (2%)	0	100	100
2	B	598/634 (94%)	583 (98%)	14 (2%)	1 (0%)	43	74
2	C	596/634 (94%)	572 (96%)	23 (4%)	1 (0%)	43	74
2	D	597/634 (94%)	587 (98%)	10 (2%)	0	100	100
All	All	3040/4648 (65%)	2947 (97%)	91 (3%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	511	PRO

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Mol	Chain	Res	Type
2	C	369	PRO

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	E	31/311 (10%)	28 (90%)	3 (10%)	8	31
1	F	31/311 (10%)	28 (90%)	3 (10%)	8	31
1	G	30/311 (10%)	27 (90%)	3 (10%)	7	29
1	H	30/311 (10%)	26 (87%)	4 (13%)	4	21
1	I	233/311 (75%)	226 (97%)	7 (3%)	36	60
1	J	229/311 (74%)	220 (96%)	9 (4%)	28	55
2	A	511/545 (94%)	478 (94%)	33 (6%)	15	42
2	B	505/545 (93%)	476 (94%)	29 (6%)	18	46
2	C	501/545 (92%)	472 (94%)	29 (6%)	18	45
2	D	499/545 (92%)	468 (94%)	31 (6%)	16	44
All	All	2600/4046 (64%)	2449 (94%)	151 (6%)	20	45

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	113	ASP
1	J	120	LEU
1	J	163	ASP
1	J	189	LEU
1	J	194	ILE
1	J	198	LEU
1	J	241	THR
1	J	242	HIS
1	J	261	LEU
2	B	24	LEU
2	B	28	VAL
2	B	47	LEU

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Mol	Chain	Res	Type
2	B	50	LYS
2	B	53	VAL
2	B	65	VAL
2	B	71	GLN
2	B	79	LEU
2	B	80	LEU
2	B	108	ILE
2	B	115	VAL
2	B	116	LEU
2	B	171	GLU
2	B	201	ILE
2	B	214	CYS
2	B	292	GLU
2	B	319	ASN
2	B	320	LEU
2	B	367	ILE
2	B	408	LEU
2	B	429	LYS
2	B	432	ILE
2	B	445	THR
2	B	463	ILE
2	B	515	THR
2	B	553	LEU
2	B	581	GLN
2	B	592	LEU
2	B	595	LEU
2	C	24	LEU
2	C	36	VAL
2	C	47	LEU
2	C	50	LYS
2	C	53	VAL
2	C	80	LEU
2	C	87	LEU
2	C	91	LEU
2	C	108	ILE
2	C	115	VAL
2	C	141	VAL
2	C	153	LEU
2	C	214	CYS
2	C	242	TYR
2	C	296	LEU
2	C	308	VAL

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Mol	Chain	Res	Type
2	C	315	HIS
2	C	316	LEU
2	C	323	THR
2	C	350	ASN
2	C	372	THR
2	C	385	VAL
2	C	420	LEU
2	C	432	ILE
2	C	457	LEU
2	C	491	VAL
2	C	595	LEU
2	C	617	PHE
2	C	619	GLU
2	D	24	LEU
2	D	28	VAL
2	D	36	VAL
2	D	38	ASN
2	D	47	LEU
2	D	50	LYS
2	D	53	VAL
2	D	108	ILE
2	D	115	VAL
2	D	117	LEU
2	D	138	ASN
2	D	188	LEU
2	D	204	THR
2	D	208	LEU
2	D	224	LEU
2	D	230	ASP
2	D	323	THR
2	D	362	VAL
2	D	372	THR
2	D	449	LEU
2	D	457	LEU
2	D	463	ILE
2	D	491	VAL
2	D	495	GLU
2	D	529	THR
2	D	540	GLU
2	D	542	ILE
2	D	592	LEU
2	D	595	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	599	LYS
2	D	609	ARG
2	A	24	LEU
2	A	28	VAL
2	A	36	VAL
2	A	47	LEU
2	A	50	LYS
2	A	53	VAL
2	A	71	GLN
2	A	79	LEU
2	A	80	LEU
2	A	108	ILE
2	A	115	VAL
2	A	116	LEU
2	A	141	VAL
2	A	171	GLU
2	A	176	VAL
2	A	214	CYS
2	A	287	PHE
2	A	295	ASN
2	A	319	ASN
2	A	320	LEU
2	A	380	LEU
2	A	404	LEU
2	A	413	LEU
2	A	420	LEU
2	A	429	LYS
2	A	449	LEU
2	A	463	ILE
2	A	489	LEU
2	A	515	THR
2	A	553	LEU
2	A	581	GLN
2	A	592	LEU
2	A	595	LEU
1	E	316	VAL
1	E	317	SER
1	E	348	TYR
1	I	35	LEU
1	I	60	MET
1	I	120	LEU
1	I	189	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	193	SER
1	I	194	ILE
1	I	233	SER
1	F	316	VAL
1	F	317	SER
1	F	348	TYR
1	G	316	VAL
1	G	317	SER
1	G	348	TYR
1	H	316	VAL
1	H	317	SER
1	H	348	TYR
1	H	349	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	28	GLN
1	J	140	GLN
1	J	151	HIS
1	J	164	GLN
1	J	251	ASN
2	B	71	GLN
2	B	138	ASN
2	B	174	HIS
2	B	178	HIS
2	B	180	HIS
2	B	253	HIS
2	B	260	GLN
2	B	336	ASN
2	B	388	GLN
2	B	438	GLN
2	B	530	ASN
2	B	541	HIS
2	B	587	ASN
2	C	138	ASN
2	C	168	GLN
2	C	205	HIS
2	C	240	HIS
2	C	280	ASN
2	C	283	ASN
2	C	295	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	299	GLN
2	C	388	GLN
2	C	436	GLN
2	C	446	HIS
2	C	577	GLN
2	D	138	ASN
2	D	280	ASN
2	D	305	GLN
2	D	315	HIS
2	D	360	GLN
2	D	436	GLN
2	D	447	ASN
2	D	581	GLN
2	D	620	HIS
2	A	71	GLN
2	A	138	ASN
2	A	174	HIS
2	A	178	HIS
2	A	253	HIS
2	A	260	GLN
2	A	297	HIS
2	A	299	GLN
2	A	315	HIS
2	A	388	GLN
2	A	417	ASN
2	A	446	HIS
2	A	530	ASN
2	A	541	HIS
2	A	587	ASN
2	A	620	HIS
1	I	28	GLN
1	I	133	ASN
1	I	140	GLN
1	I	164	GLN
1	I	188	ASN
1	I	212	HIS
1	I	239	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](#)

There are no chain breaks in this entry.

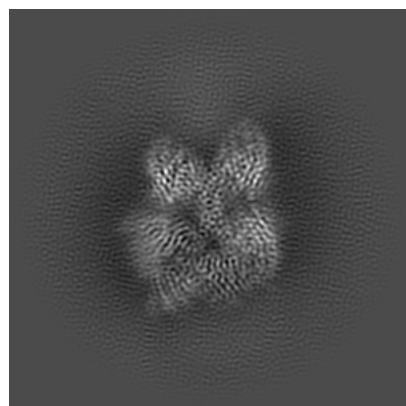
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27022. These allow visual inspection of the internal detail of the map and identification of artifacts.

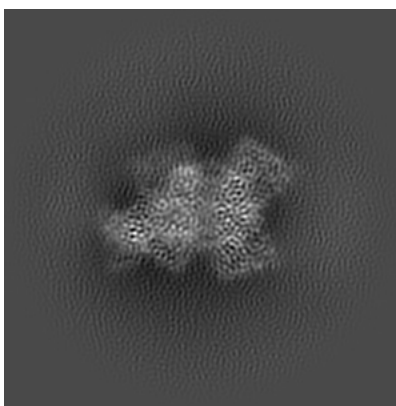
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

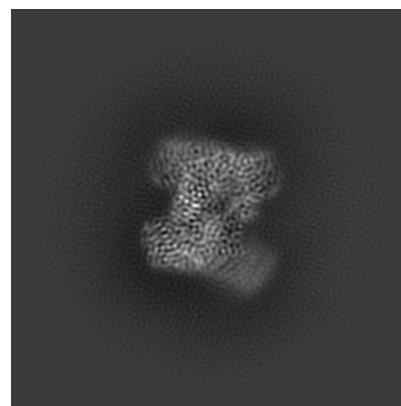
6.1.1 Primary map



X

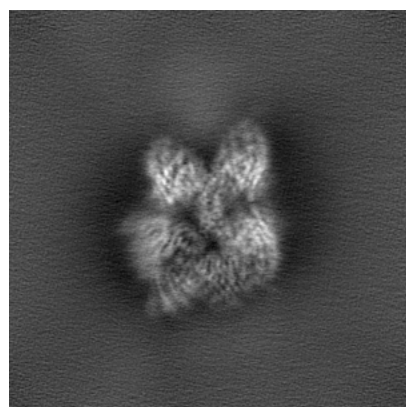


Y

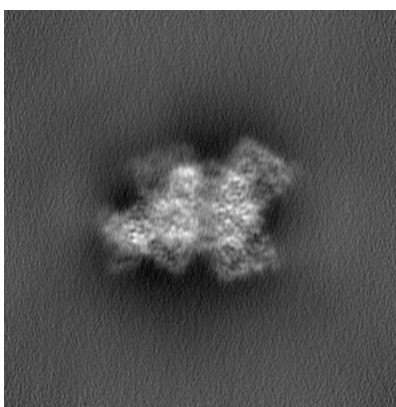


Z

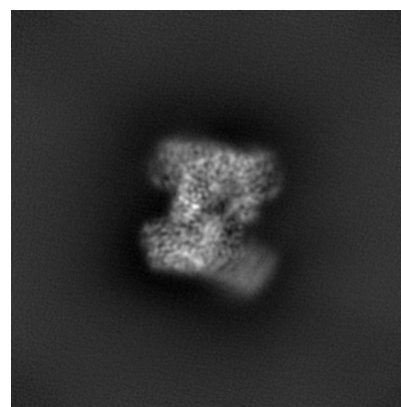
6.1.2 Raw map



X



Y

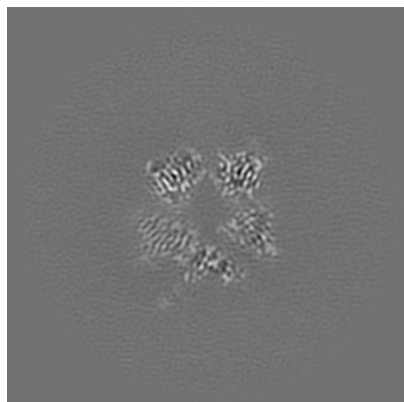


Z

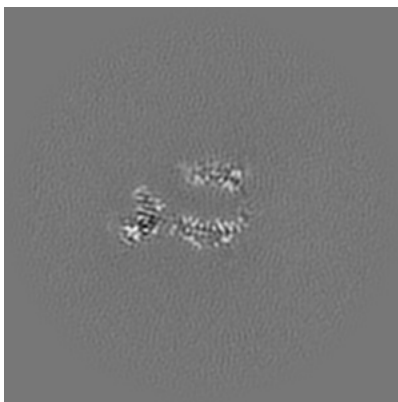
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

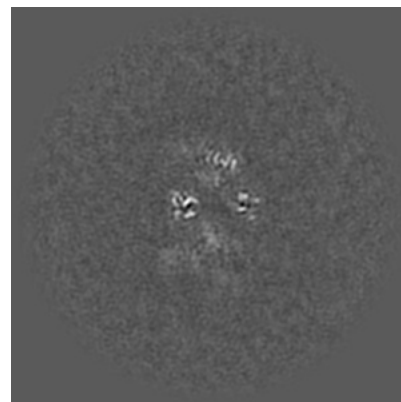
6.2.1 Primary map



X Index: 162

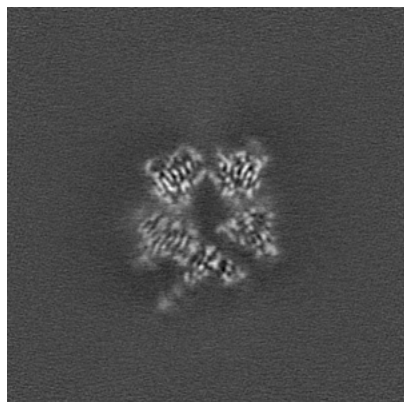


Y Index: 162

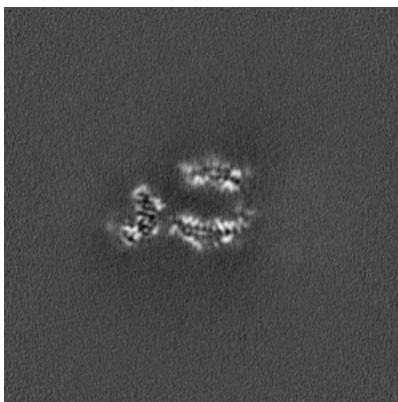


Z Index: 162

6.2.2 Raw map



X Index: 162



Y Index: 162

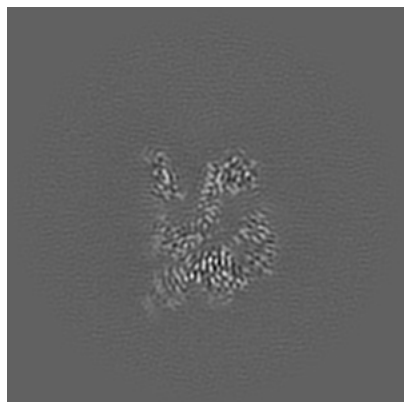


Z Index: 162

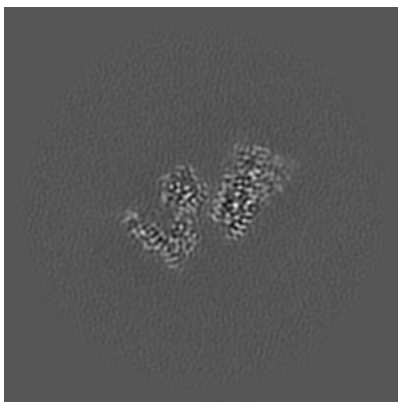
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

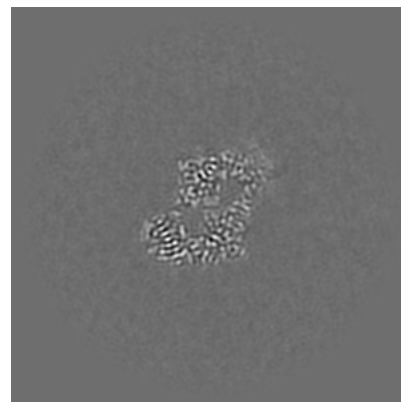
6.3.1 Primary map



X Index: 147

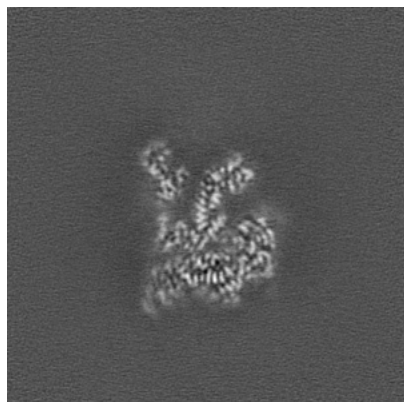


Y Index: 195

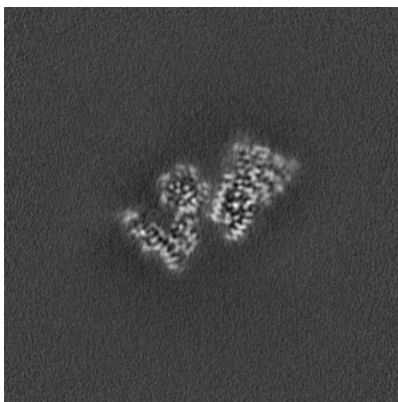


Z Index: 186

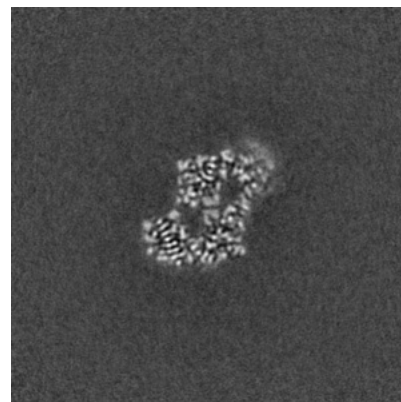
6.3.2 Raw map



X Index: 142



Y Index: 195

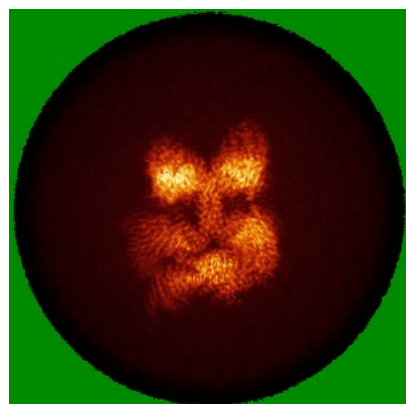


Z Index: 187

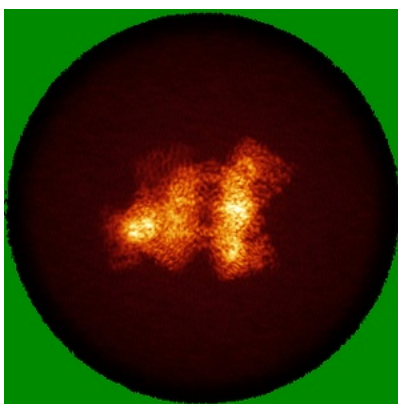
The images above show the largest variance slices of the map in three orthogonal directions.

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

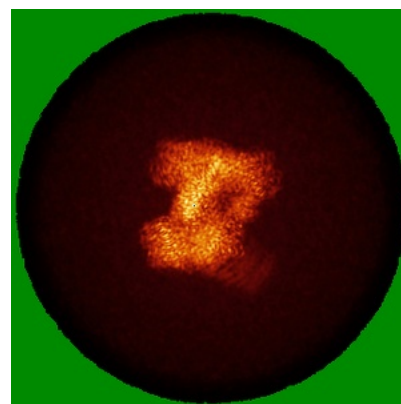
6.4.1 Primary map



X

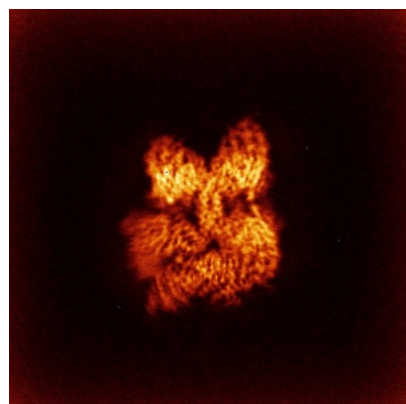


Y

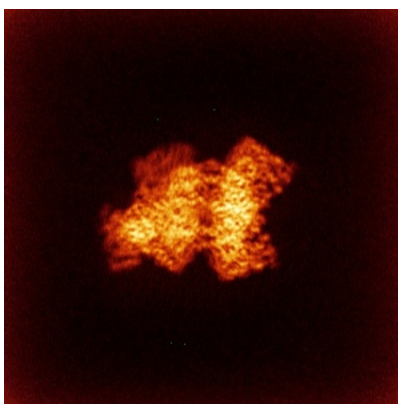


Z

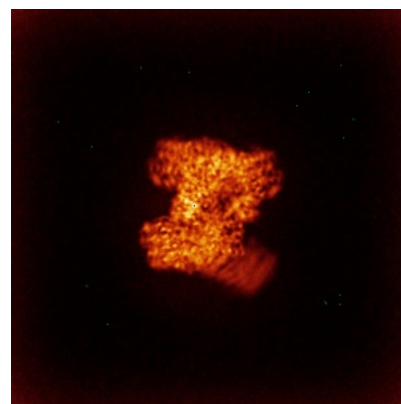
6.4.2 Raw map



X



Y

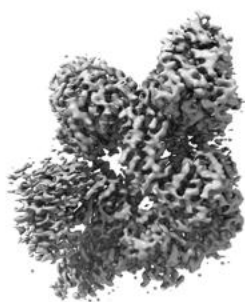


Z

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](#)

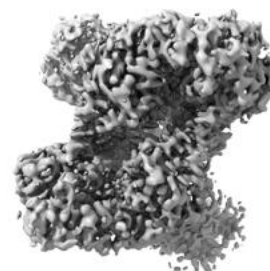
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

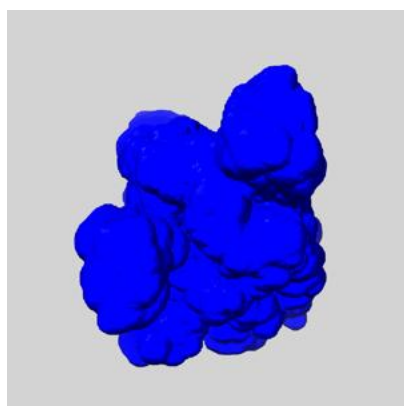
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

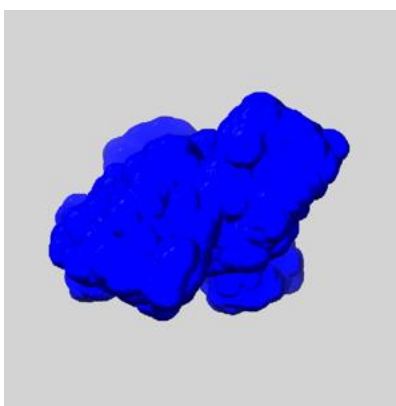
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

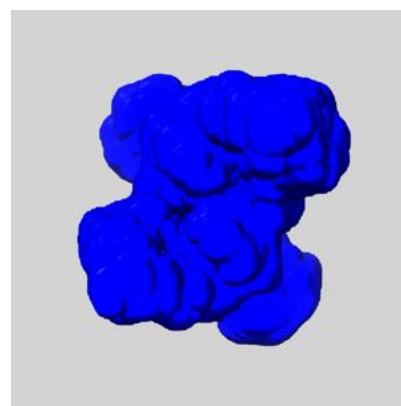
6.6.1 emd_27022_msk_1.map [i](#)



X



Y

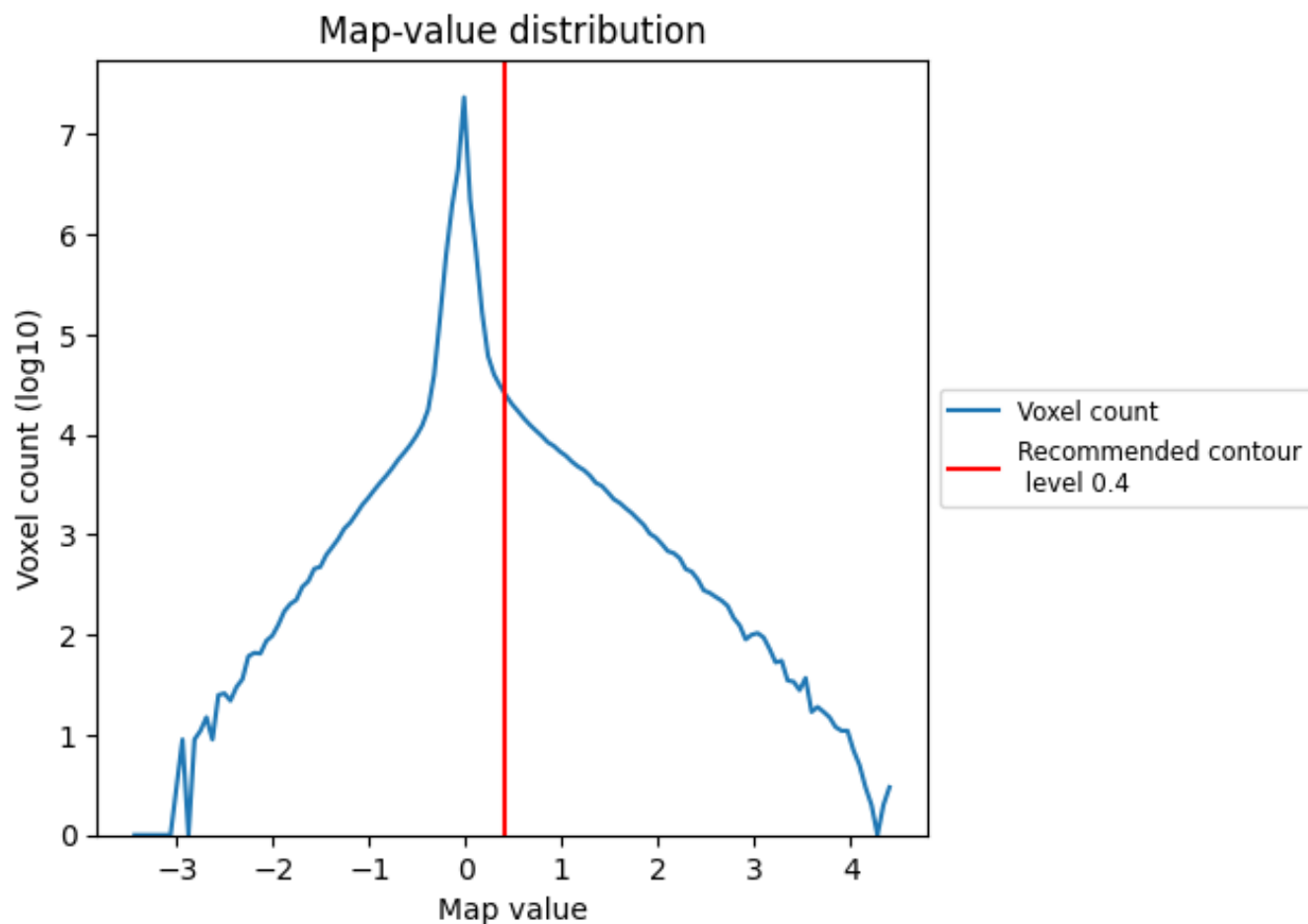


Z

7 Map analysis [i](#)

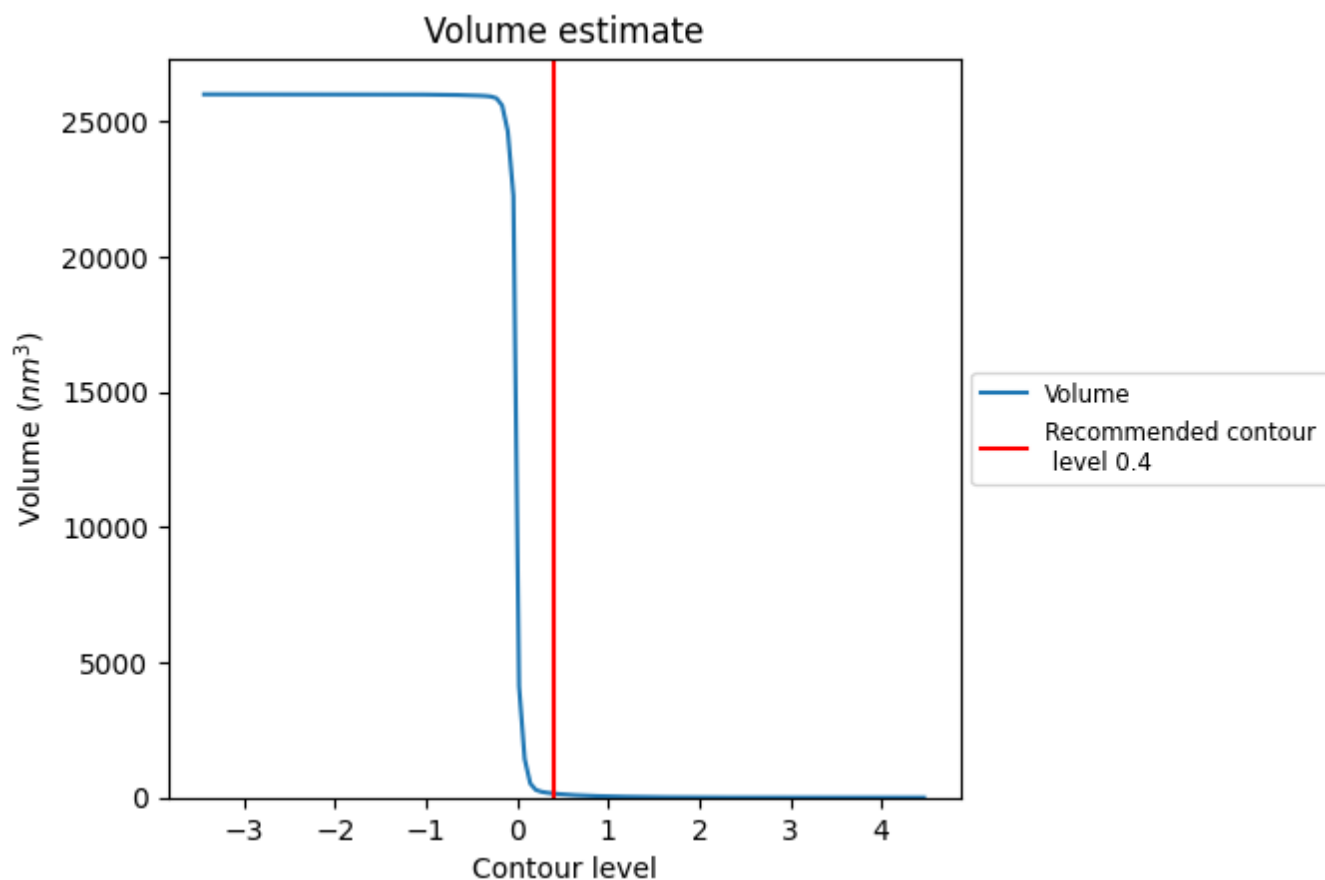
This section contains the results of statistical analysis of the map.

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.

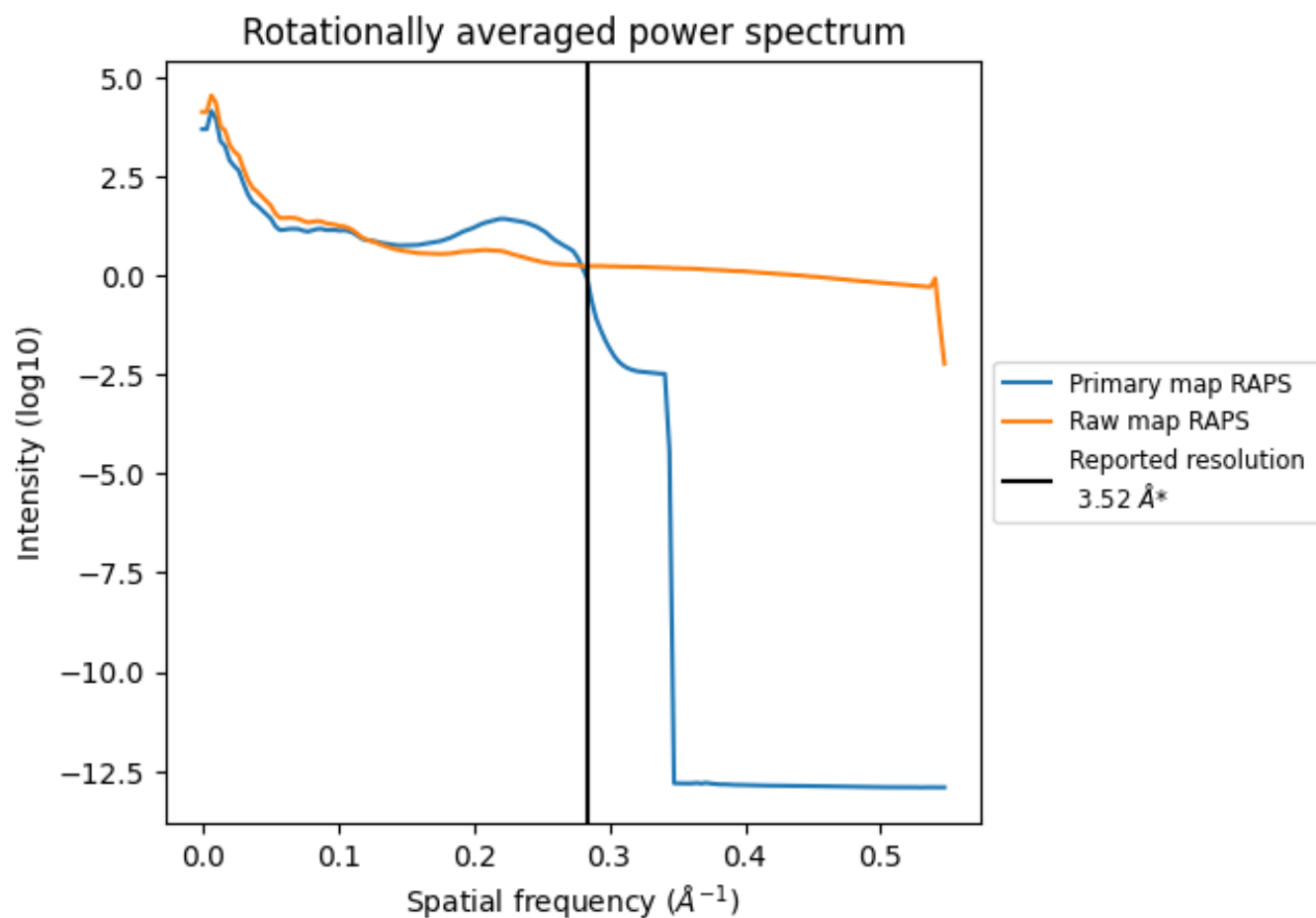
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 149 nm³; this corresponds to an approximate mass of 134 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 ⓘ

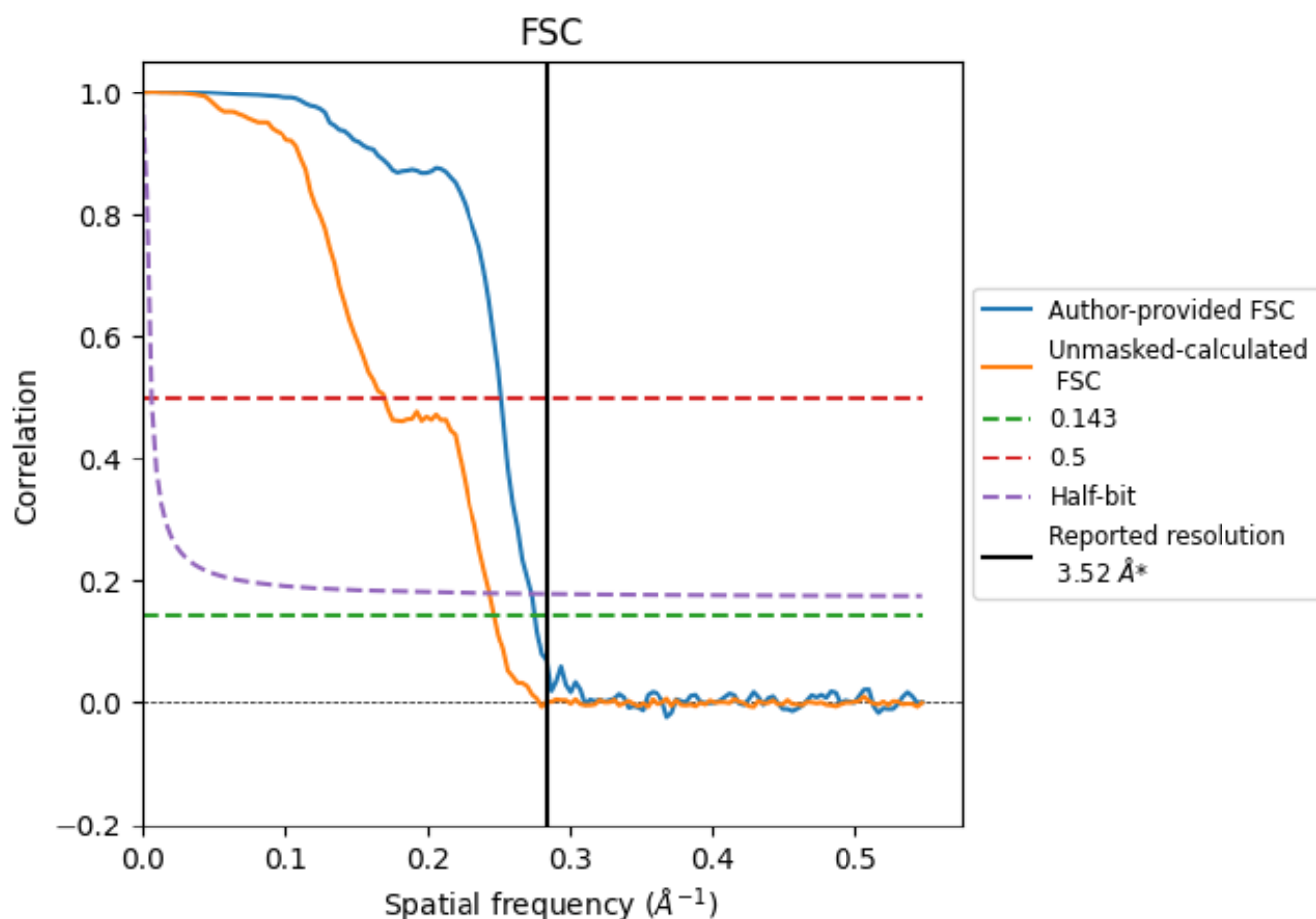


*Reported resolution corresponds to spatial frequency of 0.284 Å⁻¹

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 0.284 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

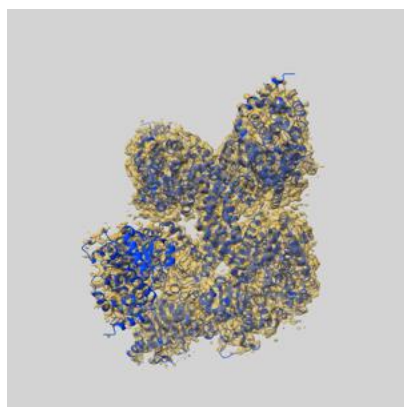
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.52	-	-
Author-provided FSC curve	3.63	3.97	3.66
Unmasked-calculated*	4.05	5.89	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.05 differs from the reported value 3.52 by more than 10 %

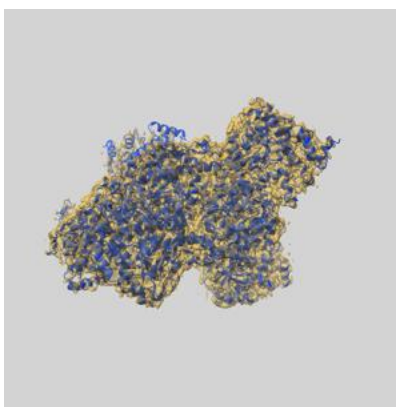
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27022 and PDB model 8CVZ. Per-residue inclusion information can be found in section 3 on page 6.

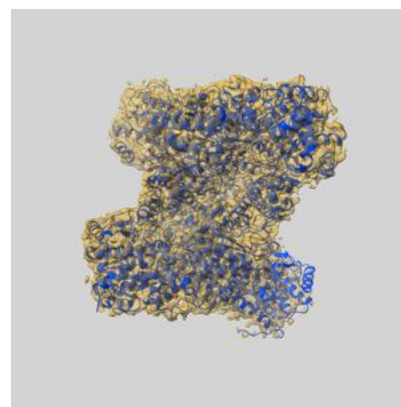
9.1 Map-model overlay [i](#)



X



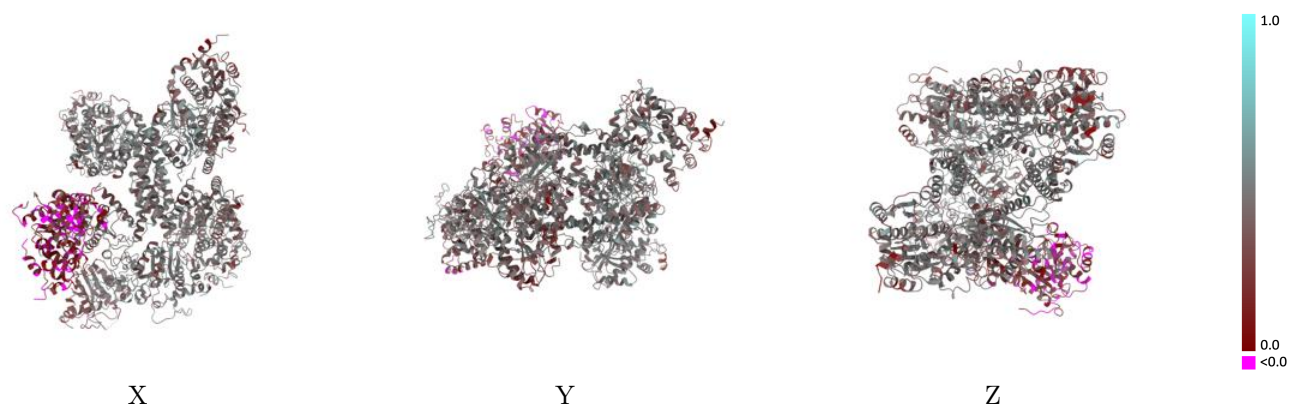
Y



Z

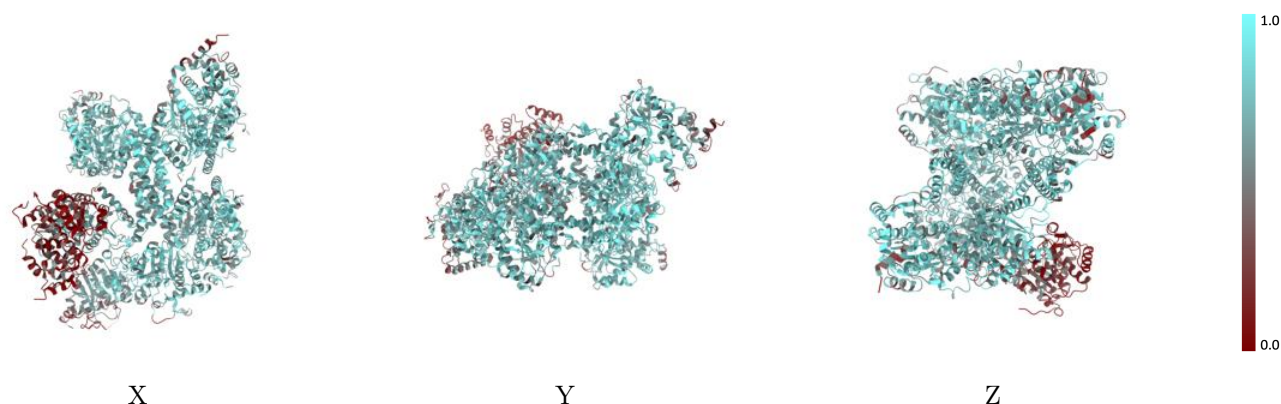
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



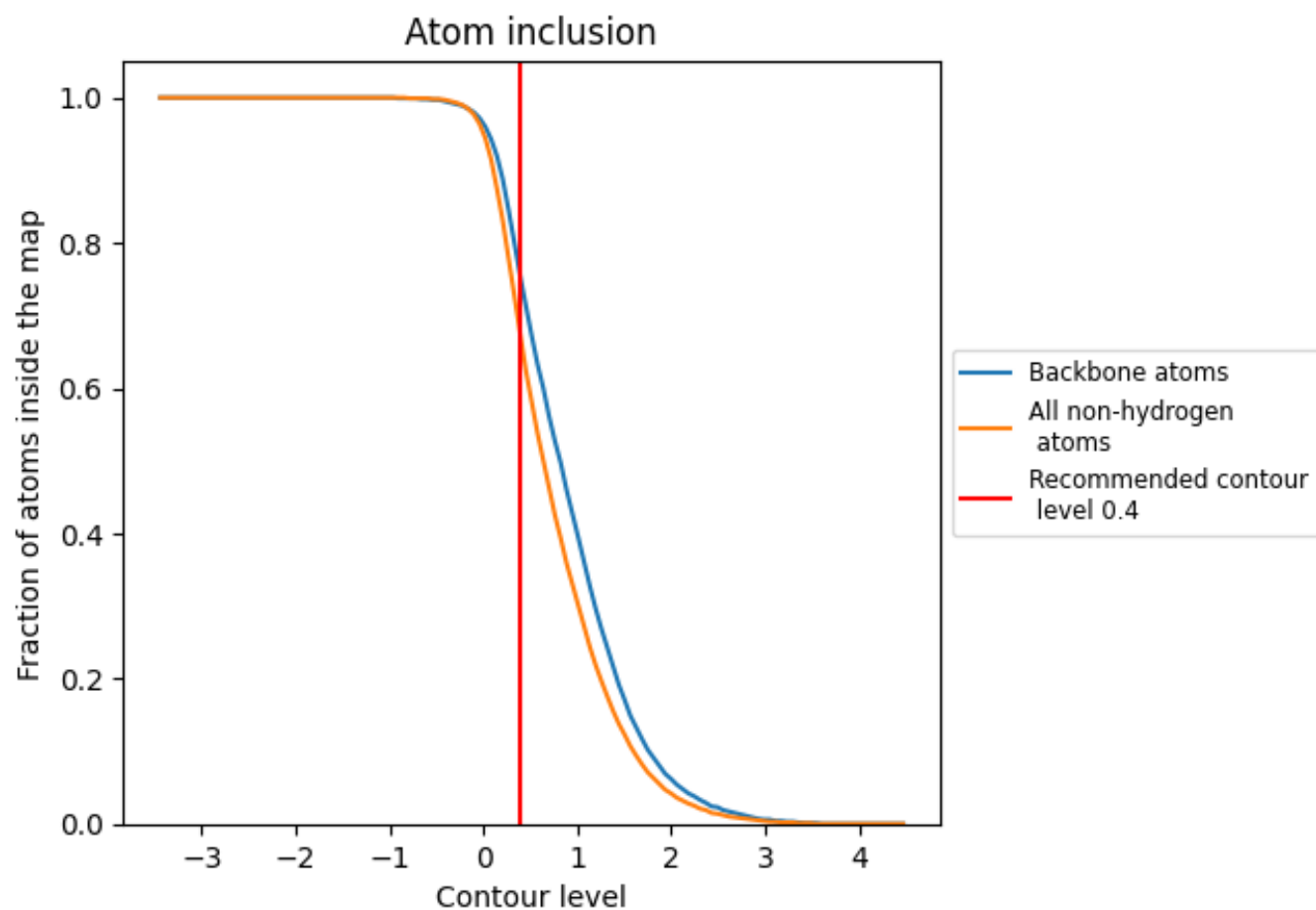
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 67% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6670	0.3830
A	0.7330	0.4090
B	0.4570	0.2430
C	0.7590	0.4390
D	0.7820	0.4470
E	0.6850	0.4090
F	0.1500	0.0810
G	0.4310	0.2730
H	0.5430	0.3190
I	0.7510	0.4560
J	0.5580	0.3550

1.0

0.0

<0.0