Full wwPDB EM Validation Report ⓘ

Nov 12, 2024 – 08:07 AM JST

PDB ID	:	8WXI
EMDB ID	:	EMD-37908
Title	:	human CLC-1 D136G delayed rectification
Authors	:	Zhang, M.F.
Deposited on	:	2023-10-29
Resolution	:	2.57 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:

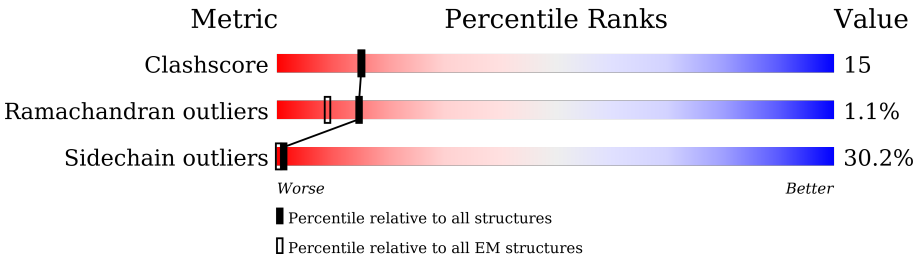
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.57 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	988	29% 14% 53%
1	B	988	29% 14% 5% 53%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SCN	A	1001	-	-	X	-
2	SCN	A	1003	-	-	X	-
2	SCN	B	1001	-	-	X	-
2	SCN	B	1002	-	-	X	-
2	SCN	B	1003	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7194 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.

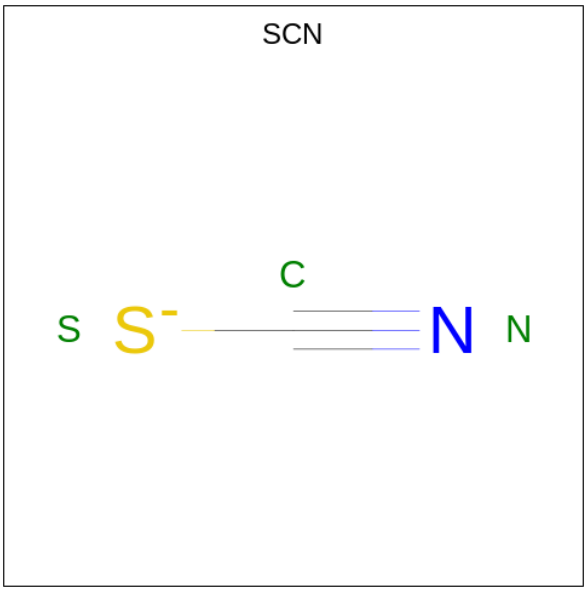
- Molecule 1 is a protein called Chloride channel protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	467	Total	C	N	O	S	0	0
			3585	2394	567	595	29		
1	B	467	Total	C	N	O	S	0	0
			3585	2394	567	595	29		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	GLY	ASP	engineered mutation	UNP P35523
B	136	GLY	ASP	engineered mutation	UNP P35523

- Molecule 2 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	S	0
			3	1	1	1	

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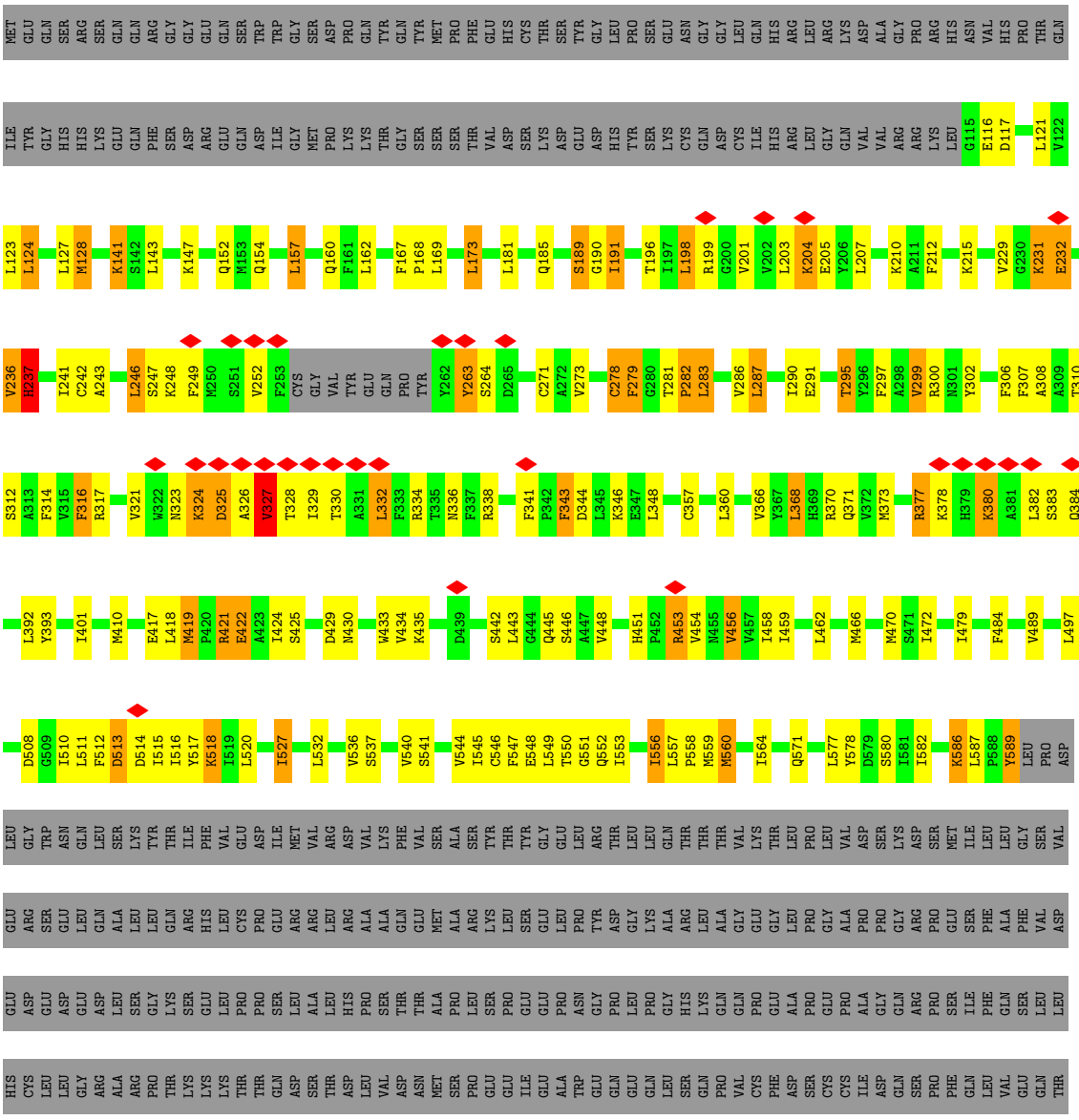
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	S	0
			3	1	1	1	
2	A	1	Total	C	N	S	0
			3	1	1	1	
2	A	1	Total	C	N	S	0
			3	1	1	1	
2	B	1	Total	C	N	S	0
			3	1	1	1	
2	B	1	Total	C	N	S	0
			3	1	1	1	
2	B	1	Total	C	N	S	0
			3	1	1	1	
2	B	1	Total	C	N	S	0
			3	1	1	1	

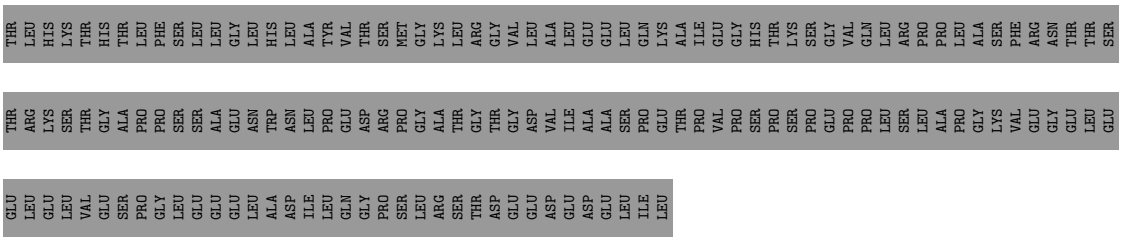
3 Residue-property plots (i)

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: Chloride channel protein 1

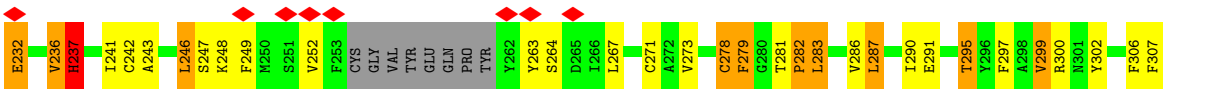
Chain A:

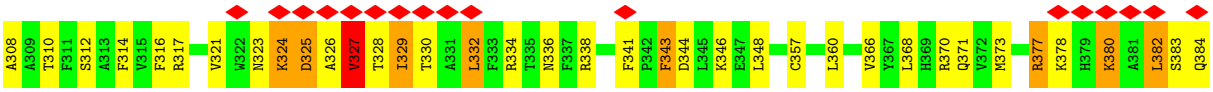


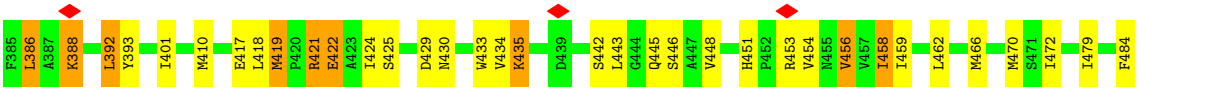


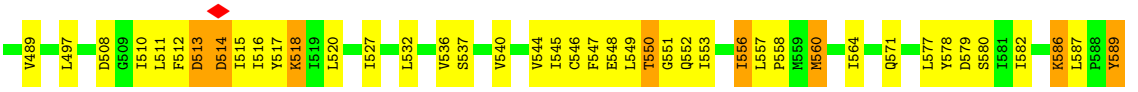
• Molecule 1: Chloride channel protein 1

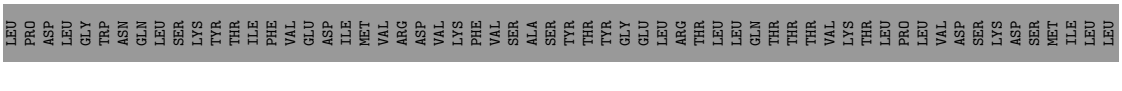
Chain B:

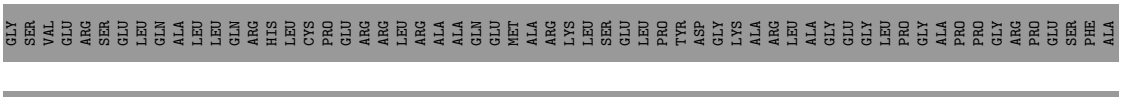


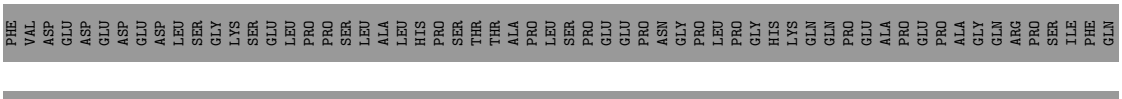


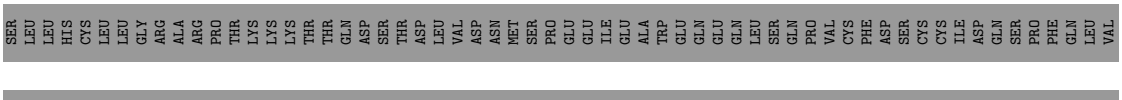


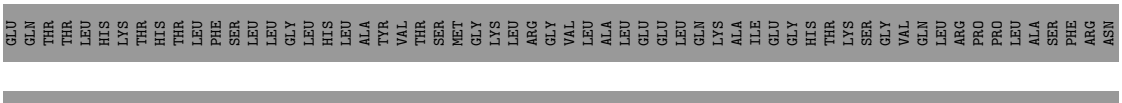












GLU LEU GLU GLU LEU GLU LEU VAL GLU SER PRO GLY LEU GLU GLU GLU LEU ALA ASP ILE LEU GLN GLY PRO SER LEU ARG SER THR ASP GLU GLU ASP GLU ASP GLU LEU ILE LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38321	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.251	Depositor
Minimum map value	-0.141	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	252.0, 252.0, 252.0	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.35, 0.35, 0.35	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.43	0/3685	0.61	4/5013 (0.1%)
1	B	0.43	0/3685	0.61	4/5013 (0.1%)
All	All	0.43	0/7370	0.61	8/10026 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	237	HIS	N-CA-C	-7.98	89.45	111.00
1	B	237	HIS	N-CA-C	-7.98	89.45	111.00
1	A	236	VAL	CA-CB-CG1	7.58	122.28	110.90
1	B	236	VAL	CA-CB-CG1	7.58	122.28	110.90
1	A	236	VAL	N-CA-CB	7.09	127.11	111.50
1	B	236	VAL	N-CA-CB	7.09	127.11	111.50
1	A	236	VAL	CG1-CB-CG2	-5.03	102.85	110.90
1	B	236	VAL	CG1-CB-CG2	-5.03	102.85	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3585	0	3696	144	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3585	0	3696	145	0
2	A	12	0	0	5	0
2	B	12	0	0	6	0
All	All	7194	0	7392	214	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 15.

All (214) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:VAL:HG22	1:B:283:LEU:HD11	1.35	1.08
1:A:295:THR:O	1:B:299:VAL:HG23	1.54	1.06
1:A:299:VAL:HG23	1:B:295:THR:O	1.54	1.05
1:A:302:TYR:OH	1:B:287:LEU:CD1	2.05	1.04
1:A:287:LEU:CD1	1:B:302:TYR:OH	2.05	1.04
1:A:283:LEU:HD11	1:B:544:VAL:HG22	1.35	1.01
1:A:560:MET:HG2	1:B:310:THR:CG2	1.92	1.00
1:A:310:THR:CG2	1:B:560:MET:HG2	1.92	0.99
1:A:560:MET:HG2	1:B:310:THR:HG21	1.51	0.91
1:A:310:THR:HG21	1:B:560:MET:HG2	1.51	0.90
1:A:299:VAL:CG2	1:B:295:THR:O	2.23	0.87
1:A:295:THR:O	1:B:299:VAL:CG2	2.23	0.84
1:A:283:LEU:HD11	1:B:544:VAL:CG2	2.08	0.84
1:A:290:ILE:HG21	1:B:297:PHE:HZ	1.44	0.83
1:A:297:PHE:HZ	1:B:290:ILE:HG21	1.44	0.83
1:A:281:THR:HG21	1:A:545:ILE:HA	1.61	0.83
1:A:544:VAL:CG2	1:B:283:LEU:HD11	2.08	0.83
1:B:281:THR:HG21	1:B:545:ILE:HA	1.61	0.83
1:A:302:TYR:OH	1:B:287:LEU:HD13	1.85	0.77
1:A:553:ILE:HD11	1:B:551:GLY:C	2.05	0.77
1:A:417:GLU:OE2	1:A:448:VAL:HG11	1.85	0.77
1:A:548:GLU:HG2	1:B:556:ILE:HD13	1.67	0.77
1:A:556:ILE:HD13	1:B:548:GLU:HG2	1.67	0.77
1:A:551:GLY:C	1:B:553:ILE:HD11	2.05	0.76
1:A:287:LEU:HD13	1:B:302:TYR:OH	1.85	0.76
1:B:417:GLU:OE2	1:B:448:VAL:HG11	1.85	0.76
1:A:578:TYR:OH	2:A:1002:SCN:N	2.21	0.73
1:B:424:ILE:HD11	1:B:489:VAL:HG12	1.71	0.73
1:A:287:LEU:HD21	1:B:287:LEU:HD21	1.71	0.72
1:B:578:TYR:OH	2:B:1002:SCN:N	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ILE:HD11	1:A:489:VAL:HG12	1.71	0.71
1:A:299:VAL:CG2	1:B:295:THR:HA	2.22	0.69
1:A:295:THR:HA	1:B:299:VAL:CG2	2.22	0.69
1:A:560:MET:HG2	1:B:310:THR:HG22	1.75	0.68
1:A:299:VAL:HG21	1:B:295:THR:HA	1.76	0.67
1:A:232:GLU:HG3	1:A:484:PHE:HB3	1.77	0.67
1:A:310:THR:HG22	1:B:560:MET:HG2	1.75	0.67
1:B:232:GLU:HG3	1:B:484:PHE:HB3	1.77	0.67
1:A:295:THR:HA	1:B:299:VAL:HG21	1.76	0.66
1:A:544:VAL:HG22	1:B:283:LEU:CD1	2.21	0.65
1:B:189:SER:HB2	2:B:1001:SCN:S	2.36	0.65
1:A:299:VAL:HG23	1:B:295:THR:C	2.17	0.65
1:A:189:SER:HB2	2:A:1001:SCN:S	2.36	0.65
1:A:290:ILE:CG2	1:B:297:PHE:HZ	2.10	0.65
1:B:419:MET:H	1:B:422:GLU:HG3	1.62	0.65
1:A:297:PHE:CZ	1:B:290:ILE:HG21	2.30	0.64
1:A:291:GLU:OE1	1:B:302:TYR:CE2	2.51	0.64
1:A:419:MET:H	1:A:422:GLU:HG3	1.62	0.64
1:A:297:PHE:HZ	1:B:290:ILE:CG2	2.10	0.63
1:A:302:TYR:CE2	1:B:291:GLU:OE1	2.51	0.63
1:B:537:SER:O	2:B:1003:SCN:C	2.47	0.63
1:A:537:SER:O	2:A:1003:SCN:C	2.47	0.62
1:A:295:THR:C	1:B:299:VAL:HG23	2.17	0.62
1:A:290:ILE:HG21	1:B:297:PHE:CZ	2.30	0.61
1:A:283:LEU:CD1	1:B:544:VAL:HG22	2.21	0.60
1:A:287:LEU:HD12	1:B:302:TYR:OH	2.01	0.60
1:A:553:ILE:HD11	1:B:552:GLN:N	2.17	0.59
1:A:552:GLN:N	1:B:553:ILE:HD11	2.17	0.58
1:A:299:VAL:CG2	1:B:295:THR:C	2.71	0.58
1:A:295:THR:C	1:B:299:VAL:CG2	2.71	0.58
1:A:279:PHE:CE1	1:A:281:THR:HB	2.39	0.57
1:B:279:PHE:CE1	1:B:281:THR:HB	2.39	0.57
1:A:299:VAL:CG2	1:B:295:THR:CA	2.84	0.56
1:A:291:GLU:OE1	1:B:302:TYR:HE2	1.88	0.56
1:B:582:ILE:HA	1:B:587:LEU:HD12	1.88	0.56
1:A:295:THR:CA	1:B:299:VAL:CG2	2.84	0.55
1:A:560:MET:CG	1:B:310:THR:HG21	2.31	0.55
1:A:582:ILE:HA	1:A:587:LEU:HD12	1.88	0.55
1:A:287:LEU:HD11	1:B:302:TYR:OH	2.01	0.55
1:A:302:TYR:OH	1:B:287:LEU:HD11	2.01	0.55
1:A:302:TYR:OH	1:B:287:LEU:HD12	2.01	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:TYR:HE2	1:B:291:GLU:OE1	1.88	0.55
1:A:287:LEU:HD13	1:B:302:TYR:CZ	2.44	0.53
1:A:307:PHE:HD1	1:B:564:ILE:HG21	1.74	0.53
1:A:302:TYR:CZ	1:B:287:LEU:HD13	2.44	0.53
1:A:564:ILE:HG21	1:B:307:PHE:HD1	1.74	0.52
1:A:279:PHE:HB2	1:A:549:LEU:HD21	1.91	0.52
1:B:279:PHE:HB2	1:B:549:LEU:HD21	1.91	0.51
1:A:366:VAL:HG12	1:A:370:ARG:HH21	1.75	0.51
1:A:299:VAL:HG23	1:B:295:THR:CA	2.41	0.51
1:B:366:VAL:HG12	1:B:370:ARG:HH21	1.75	0.50
1:B:578:TYR:HH	2:B:1002:SCN:C	2.15	0.50
1:A:421:ARG:NH1	1:A:422:GLU:HG2	2.27	0.50
1:B:417:GLU:OE2	1:B:448:VAL:CG1	2.58	0.50
1:A:386:LEU:HG	1:A:393:TYR:HB2	1.94	0.50
1:B:124:LEU:HD21	1:B:243:ALA:HA	1.94	0.49
1:B:433:TRP:HB3	1:B:456:VAL:HG11	1.94	0.49
1:A:295:THR:CA	1:B:299:VAL:HG23	2.41	0.49
1:A:310:THR:HG21	1:B:560:MET:CG	2.31	0.49
1:A:290:ILE:CG2	1:B:297:PHE:CZ	2.93	0.49
1:A:189:SER:CB	2:A:1001:SCN:S	3.01	0.49
1:A:124:LEU:HD21	1:A:243:ALA:HA	1.94	0.49
1:B:189:SER:CB	2:B:1001:SCN:S	3.01	0.49
1:A:324:LYS:HE2	1:B:513:ASP:HB3	1.95	0.49
1:A:513:ASP:HB3	1:B:324:LYS:HE2	1.95	0.49
1:A:417:GLU:OE2	1:A:448:VAL:CG1	2.58	0.49
1:B:386:LEU:HG	1:B:393:TYR:HB2	1.94	0.49
1:B:421:ARG:NH1	1:B:422:GLU:HG2	2.27	0.48
1:B:167:PHE:HB3	1:B:168:PRO:HD3	1.96	0.48
1:A:229:VAL:HG11	1:A:479:ILE:HD11	1.96	0.48
1:A:433:TRP:HB3	1:A:456:VAL:HG11	1.94	0.48
1:A:518:LYS:HA	1:A:518:LYS:HD2	1.63	0.48
1:B:229:VAL:HG11	1:B:479:ILE:HD11	1.96	0.48
1:A:167:PHE:HB3	1:A:168:PRO:HD3	1.96	0.48
1:B:421:ARG:H	1:B:421:ARG:HG3	1.37	0.48
1:A:388:LYS:HE2	1:A:388:LYS:HB2	1.53	0.48
1:A:419:MET:N	1:A:422:GLU:HG3	2.27	0.48
1:A:282:PRO:O	1:A:286:VAL:HG23	2.14	0.47
1:A:324:LYS:HD2	1:A:324:LYS:HA	1.63	0.47
1:A:299:VAL:HG23	1:B:295:THR:HA	1.95	0.47
1:A:418:LEU:HG	1:A:448:VAL:HG21	1.97	0.47
1:A:325:ASP:HB3	1:A:326:ALA:H	1.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:LEU:HG	1:B:448:VAL:HG21	1.97	0.47
1:B:196:THR:HG23	1:B:589:TYR:H	1.80	0.46
1:A:295:THR:HA	1:B:299:VAL:HG23	1.95	0.46
1:A:321:VAL:HG21	1:B:512:PHE:HE2	1.81	0.46
1:A:512:PHE:HE2	1:B:321:VAL:HG21	1.81	0.46
1:B:282:PRO:O	1:B:286:VAL:HG23	2.14	0.46
1:A:196:THR:HG23	1:A:589:TYR:H	1.80	0.46
1:B:154:GLN:HA	1:B:160:GLN:NE2	2.31	0.46
1:A:297:PHE:CZ	1:B:290:ILE:CG2	2.93	0.46
1:A:421:ARG:H	1:A:421:ARG:HG3	1.37	0.46
1:A:154:GLN:HA	1:A:160:GLN:NE2	2.31	0.45
1:A:232:GLU:H	1:A:232:GLU:HG2	1.30	0.45
1:B:377:ARG:HE	1:B:377:ARG:HB3	1.51	0.45
1:B:327:VAL:HB	1:B:328:THR:H	1.61	0.45
1:B:419:MET:N	1:B:422:GLU:HG3	2.27	0.45
1:A:537:SER:O	2:A:1003:SCN:N	2.49	0.45
1:B:191:ILE:HD12	1:B:578:TYR:CZ	2.52	0.45
1:B:537:SER:O	2:B:1003:SCN:N	2.49	0.45
1:A:380:LYS:HD2	1:A:380:LYS:HA	1.37	0.45
1:B:207:LEU:HD21	1:B:267:LEU:HD21	1.97	0.45
1:A:141:LYS:HD2	1:A:141:LYS:HA	1.75	0.45
1:A:191:ILE:HD12	1:A:578:TYR:CZ	2.52	0.45
1:A:377:ARG:HE	1:A:377:ARG:HB3	1.51	0.45
1:A:173:LEU:HD12	1:A:173:LEU:HA	1.73	0.45
1:A:204:LYS:HD2	1:A:204:LYS:HA	1.42	0.45
1:B:332:LEU:C	1:B:334:ARG:H	2.21	0.45
1:B:380:LYS:HA	1:B:380:LYS:HD2	1.37	0.45
1:B:203:LEU:H	1:B:203:LEU:HG	1.60	0.44
1:A:551:GLY:C	1:B:553:ILE:CD1	2.83	0.44
1:A:124:LEU:HD23	1:A:246:LEU:HD23	1.99	0.44
1:A:451:HIS:HD2	1:A:454:VAL:H	1.64	0.44
1:B:210:LYS:H	1:B:210:LYS:HG2	1.42	0.44
1:B:451:HIS:HD2	1:B:454:VAL:H	1.64	0.44
1:B:173:LEU:HD12	1:B:173:LEU:HA	1.73	0.44
1:A:332:LEU:C	1:A:334:ARG:H	2.21	0.44
1:B:212:PHE:HB2	1:B:241:ILE:HG21	2.00	0.44
1:B:215:LYS:HD3	1:B:237:HIS:ND1	2.33	0.44
1:A:212:PHE:HB2	1:A:241:ILE:HG21	2.00	0.43
1:A:287:LEU:CD1	1:B:302:TYR:CZ	2.98	0.43
1:B:128:MET:HG2	1:B:273:VAL:HG23	2.00	0.43
1:B:171:LEU:HD23	1:B:171:LEU:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:MET:HG2	1:A:273:VAL:HG23	2.00	0.43
1:B:124:LEU:HD23	1:B:246:LEU:HD23	1.99	0.43
1:B:388:LYS:HB2	1:B:388:LYS:HE2	1.53	0.43
1:B:547:PHE:CZ	1:B:556:ILE:HA	2.54	0.43
1:A:121:LEU:HB3	1:A:308:ALA:HB2	2.01	0.43
1:B:392:LEU:HD22	1:B:392:LEU:HA	1.77	0.43
1:B:401:ILE:HG12	1:B:470:MET:HG2	2.01	0.43
1:B:329:ILE:H	1:B:329:ILE:HG12	1.80	0.42
1:A:198:LEU:HD12	1:A:198:LEU:HA	1.71	0.42
1:A:215:LYS:HD3	1:A:237:HIS:ND1	2.33	0.42
1:A:547:PHE:CZ	1:A:556:ILE:HA	2.54	0.42
1:B:586:LYS:HE2	1:B:586:LYS:HB2	1.25	0.42
1:A:190:GLY:HA3	1:A:237:HIS:HB2	2.01	0.42
1:A:231:LYS:HB3	1:A:231:LYS:HE2	1.71	0.42
1:A:401:ILE:HG12	1:A:470:MET:HG2	2.01	0.42
1:B:458:ILE:H	1:B:458:ILE:HG13	1.65	0.42
1:B:518:LYS:HA	1:B:518:LYS:HD2	1.63	0.42
1:A:453:ARG:HE	1:A:453:ARG:HB2	1.38	0.42
1:B:143:LEU:HD12	1:B:143:LEU:HA	1.85	0.42
1:B:159:LEU:HD23	1:B:159:LEU:HA	1.85	0.42
1:A:263:TYR:HD1	1:A:263:TYR:HA	1.71	0.42
1:A:287:LEU:CD1	1:B:302:TYR:HH	2.26	0.42
1:A:553:ILE:CD1	1:B:551:GLY:C	2.83	0.42
1:B:190:GLY:HA3	1:B:237:HIS:HB2	2.01	0.42
1:B:343:PHE:CZ	1:B:558:PRO:HG3	2.55	0.42
1:B:382:LEU:HD12	1:B:382:LEU:HA	1.75	0.42
1:A:343:PHE:CZ	1:A:558:PRO:HG3	2.55	0.42
1:B:324:LYS:HA	1:B:324:LYS:HD2	1.63	0.42
1:B:121:LEU:HB3	1:B:308:ALA:HB2	2.01	0.42
1:A:316:PHE:HD1	1:A:316:PHE:HA	1.71	0.41
1:B:141:LYS:HA	1:B:141:LYS:HD2	1.75	0.41
1:B:236:VAL:HG21	1:B:271:CYS:HA	2.03	0.41
1:A:279:PHE:CE2	1:A:545:ILE:HG21	2.56	0.41
1:A:302:TYR:CZ	1:B:287:LEU:CD1	2.98	0.41
1:A:344:ASP:HB2	1:A:517:TYR:CG	2.56	0.41
1:A:527:ILE:HG23	1:A:559:MET:HA	2.03	0.41
1:A:586:LYS:HB2	1:A:586:LYS:HE2	1.25	0.41
1:A:287:LEU:HD22	1:A:287:LEU:HA	1.95	0.41
1:A:236:VAL:HG21	1:A:271:CYS:HA	2.03	0.41
1:A:302:TYR:HE2	1:B:291:GLU:CD	2.24	0.41
1:A:357:CYS:HA	1:A:360:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LEU:HD22	1:A:422:GLU:HB2	2.03	0.41
1:B:513:ASP:HB2	1:B:514:ASP:H	1.70	0.41
1:A:291:GLU:CD	1:B:302:TYR:HE2	2.24	0.40
1:A:327:VAL:HB	1:A:328:THR:H	1.61	0.40
1:A:368:LEU:HD12	1:A:368:LEU:HA	1.93	0.40
1:B:279:PHE:CE2	1:B:545:ILE:HG21	2.56	0.40
1:B:357:CYS:HA	1:B:360:LEU:HD12	2.02	0.40
1:B:435:LYS:HA	1:B:435:LYS:HD3	1.67	0.40
1:A:157:LEU:HD22	1:A:157:LEU:HA	1.88	0.40
1:B:236:VAL:CG2	1:B:271:CYS:HA	2.51	0.40
1:B:325:ASP:HB3	1:B:326:ALA:H	1.55	0.40
1:B:344:ASP:HB2	1:B:517:TYR:CG	2.56	0.40
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.82	0.40
1:A:287:LEU:HB3	1:A:541:SER:HB3	2.04	0.40
1:B:204:LYS:HD2	1:B:204:LYS:HA	1.42	0.40
1:B:550:THR:HG22	1:B:552:GLN:H	1.87	0.40
1:A:117:ASP:O	1:A:121:LEU:HG	2.22	0.40
1:A:236:VAL:CG2	1:A:271:CYS:HA	2.51	0.40
1:A:553:ILE:HD11	1:B:551:GLY:CA	2.51	0.40
1:B:579:ASP:HA	1:B:582:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	463/988 (47%)	423 (91%)	35 (8%)	5 (1%)	12	25
1	B	463/988 (47%)	423 (91%)	35 (8%)	5 (1%)	12	25
All	All	926/1976 (47%)	846 (91%)	70 (8%)	10 (1%)	15	25

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	HIS
1	B	237	HIS
1	A	343	PHE
1	B	343	PHE
1	A	278	CYS
1	B	278	CYS
1	A	282	PRO
1	B	282	PRO
1	A	327	VAL
1	B	327	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	381/837 (46%)	266 (70%)	115 (30%)	0 0
1	B	381/837 (46%)	266 (70%)	115 (30%)	0 0
All	All	762/1674 (46%)	532 (70%)	230 (30%)	1 0

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	GLU
1	A	123	LEU
1	A	124	LEU
1	A	127	LEU
1	A	128	MET
1	A	141	LYS
1	A	143	LEU
1	A	147	LYS
1	A	152	GLN
1	A	157	LEU
1	A	162	LEU
1	A	169	LEU
1	A	173	LEU
1	A	181	LEU

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Mol	Chain	Res	Type
1	A	185	GLN
1	A	189	SER
1	A	191	ILE
1	A	198	LEU
1	A	199	ARG
1	A	201	VAL
1	A	203	LEU
1	A	204	LYS
1	A	205	GLU
1	A	207	LEU
1	A	210	LYS
1	A	231	LYS
1	A	232	GLU
1	A	242	CYS
1	A	246	LEU
1	A	247	SER
1	A	248	LYS
1	A	249	PHE
1	A	252	VAL
1	A	263	TYR
1	A	264	SER
1	A	278	CYS
1	A	279	PHE
1	A	283	LEU
1	A	287	LEU
1	A	295	THR
1	A	299	VAL
1	A	300	ARG
1	A	306	PHE
1	A	312	SER
1	A	314	PHE
1	A	316	PHE
1	A	317	ARG
1	A	323	ASN
1	A	324	LYS
1	A	325	ASP
1	A	327	VAL
1	A	329	ILE
1	A	330	THR
1	A	332	LEU
1	A	336	ASN
1	A	338	ARG

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Mol	Chain	Res	Type
1	A	341	PHE
1	A	346	LYS
1	A	348	LEU
1	A	368	LEU
1	A	371	GLN
1	A	373	MET
1	A	377	ARG
1	A	378	LYS
1	A	380	LYS
1	A	382	LEU
1	A	383	SER
1	A	384	GLN
1	A	386	LEU
1	A	388	LYS
1	A	392	LEU
1	A	410	MET
1	A	419	MET
1	A	421	ARG
1	A	422	GLU
1	A	425	SER
1	A	429	ASP
1	A	430	ASN
1	A	434	VAL
1	A	435	LYS
1	A	442	SER
1	A	443	LEU
1	A	445	GLN
1	A	446	SER
1	A	453	ARG
1	A	456	VAL
1	A	458	ILE
1	A	459	ILE
1	A	462	LEU
1	A	466	MET
1	A	472	ILE
1	A	497	LEU
1	A	508	ASP
1	A	510	ILE
1	A	511	LEU
1	A	513	ASP
1	A	514	ASP
1	A	515	ILE

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Mol	Chain	Res	Type
1	A	516	ILE
1	A	518	LYS
1	A	520	LEU
1	A	527	ILE
1	A	532	LEU
1	A	536	VAL
1	A	540	VAL
1	A	546	CYS
1	A	550	THR
1	A	556	ILE
1	A	557	LEU
1	A	560	MET
1	A	571	GLN
1	A	577	LEU
1	A	580	SER
1	A	586	LYS
1	A	589	TYR
1	B	116	GLU
1	B	123	LEU
1	B	124	LEU
1	B	127	LEU
1	B	128	MET
1	B	141	LYS
1	B	143	LEU
1	B	147	LYS
1	B	152	GLN
1	B	157	LEU
1	B	162	LEU
1	B	169	LEU
1	B	173	LEU
1	B	181	LEU
1	B	185	GLN
1	B	189	SER
1	B	191	ILE
1	B	198	LEU
1	B	199	ARG
1	B	201	VAL
1	B	203	LEU
1	B	204	LYS
1	B	205	GLU
1	B	207	LEU
1	B	210	LYS

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Mol	Chain	Res	Type
1	B	231	LYS
1	B	232	GLU
1	B	242	CYS
1	B	246	LEU
1	B	247	SER
1	B	248	LYS
1	B	249	PHE
1	B	252	VAL
1	B	263	TYR
1	B	264	SER
1	B	278	CYS
1	B	279	PHE
1	B	283	LEU
1	B	287	LEU
1	B	295	THR
1	B	299	VAL
1	B	300	ARG
1	B	306	PHE
1	B	312	SER
1	B	314	PHE
1	B	316	PHE
1	B	317	ARG
1	B	323	ASN
1	B	324	LYS
1	B	325	ASP
1	B	327	VAL
1	B	329	ILE
1	B	330	THR
1	B	332	LEU
1	B	336	ASN
1	B	338	ARG
1	B	341	PHE
1	B	346	LYS
1	B	348	LEU
1	B	368	LEU
1	B	371	GLN
1	B	373	MET
1	B	377	ARG
1	B	378	LYS
1	B	380	LYS
1	B	382	LEU
1	B	383	SER

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Mol	Chain	Res	Type
1	B	384	GLN
1	B	386	LEU
1	B	388	LYS
1	B	392	LEU
1	B	410	MET
1	B	419	MET
1	B	421	ARG
1	B	422	GLU
1	B	425	SER
1	B	429	ASP
1	B	430	ASN
1	B	434	VAL
1	B	435	LYS
1	B	442	SER
1	B	443	LEU
1	B	445	GLN
1	B	446	SER
1	B	453	ARG
1	B	456	VAL
1	B	458	ILE
1	B	459	ILE
1	B	462	LEU
1	B	466	MET
1	B	472	ILE
1	B	497	LEU
1	B	508	ASP
1	B	510	ILE
1	B	511	LEU
1	B	513	ASP
1	B	514	ASP
1	B	515	ILE
1	B	516	ILE
1	B	518	LYS
1	B	520	LEU
1	B	527	ILE
1	B	532	LEU
1	B	536	VAL
1	B	540	VAL
1	B	546	CYS
1	B	550	THR
1	B	556	ILE
1	B	557	LEU

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Mol	Chain	Res	Type
1	B	560	MET
1	B	571	GLN
1	B	577	LEU
1	B	580	SER
1	B	586	LYS
1	B	589	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	A	384	GLN
1	A	431	ASN
1	A	451	HIS
1	B	160	GLN
1	B	384	GLN
1	B	431	ASN
1	B	451	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SCN	B	1001	-	1,2,2	0.22	0	0,1,1	-	-
2	SCN	B	1002	-	1,2,2	0.24	0	0,1,1	-	-
2	SCN	A	1004	-	1,2,2	0.21	0	0,1,1	-	-
2	SCN	A	1003	-	1,2,2	0.31	0	0,1,1	-	-
2	SCN	B	1004	-	1,2,2	0.21	0	0,1,1	-	-
2	SCN	B	1003	-	1,2,2	0.31	0	0,1,1	-	-
2	SCN	A	1001	-	1,2,2	0.22	0	0,1,1	-	-
2	SCN	A	1002	-	1,2,2	0.24	0	0,1,1	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

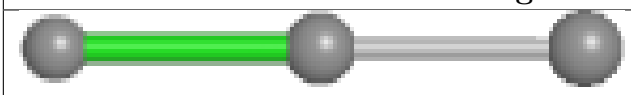
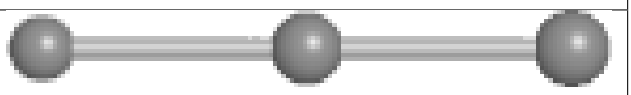
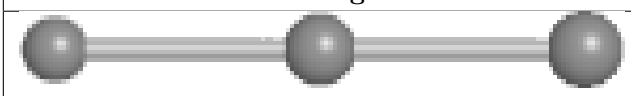
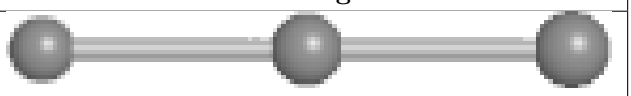
There are no torsion outliers.

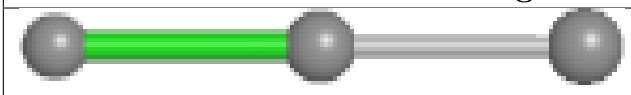
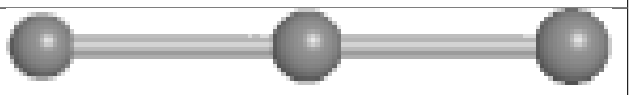
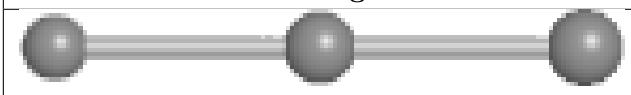
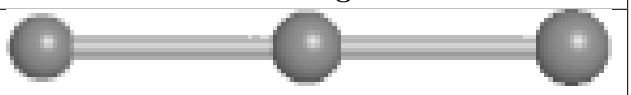
There are no ring outliers.

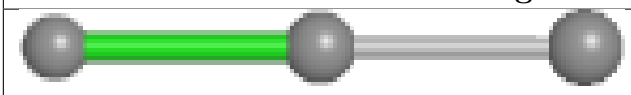
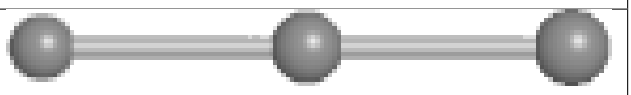
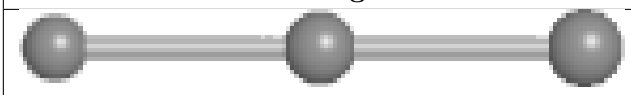
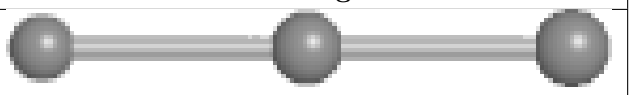
6 monomers are involved in 11 short contacts:

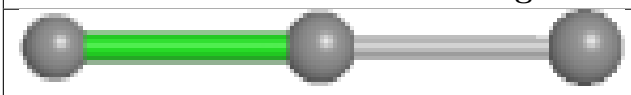
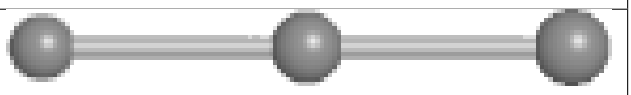
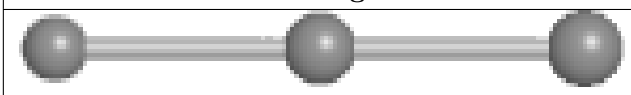
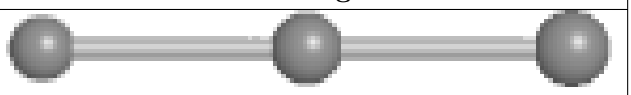
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	SCN	2	0
2	B	1002	SCN	2	0
2	A	1003	SCN	2	0
2	B	1003	SCN	2	0
2	A	1001	SCN	2	0
2	A	1002	SCN	1	0

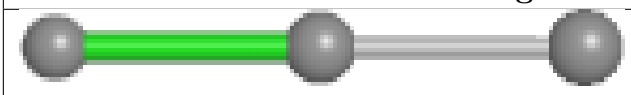
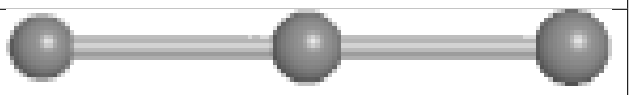
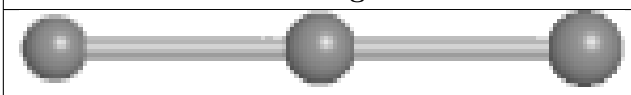
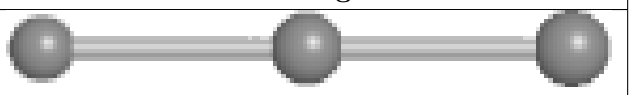
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

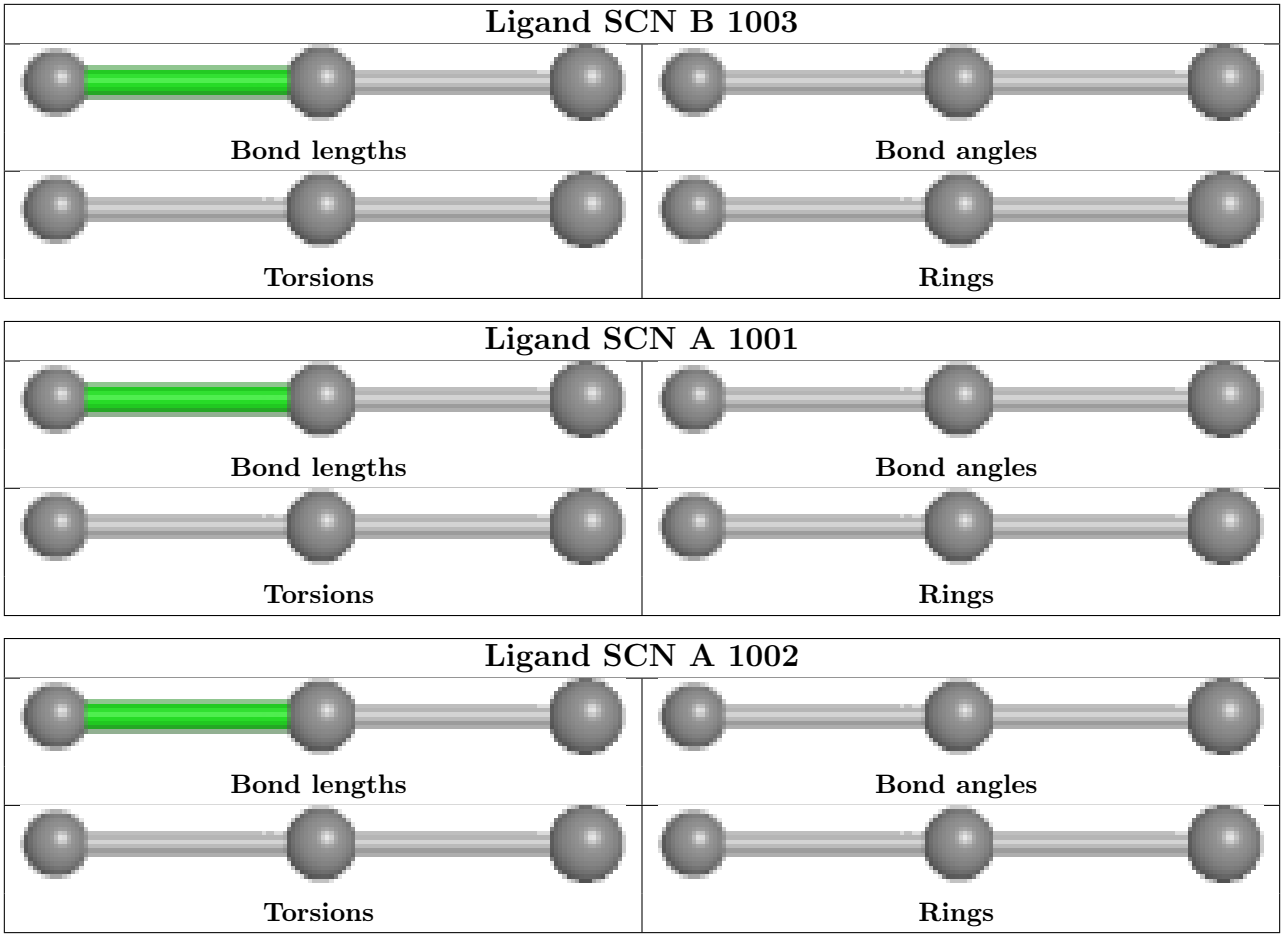
Ligand SCN B 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SCN B 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SCN A 1004	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SCN A 1003	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SCN B 1004	
 Bond lengths	 Bond angles
 Torsions	 Rings



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.

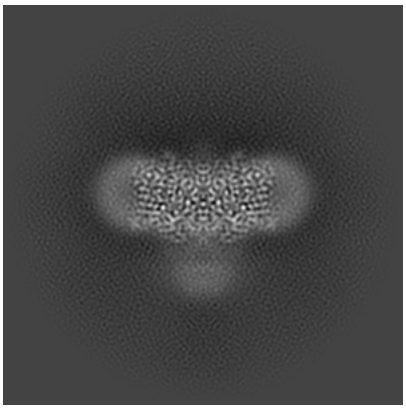
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37908. These allow visual inspection of the internal detail of the map and identification of artifacts.

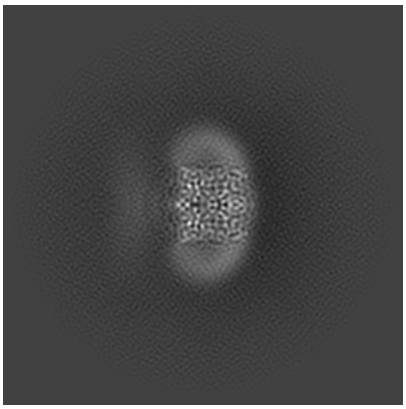
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

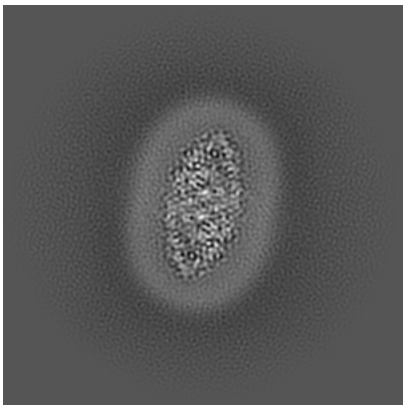
6.1.1 Primary map



X

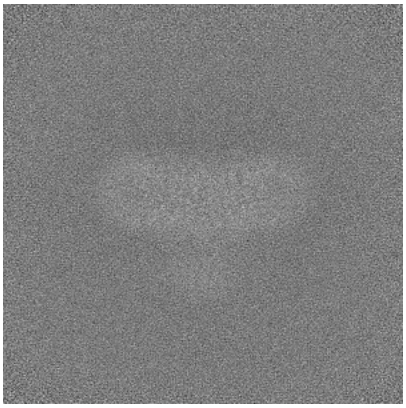


Y

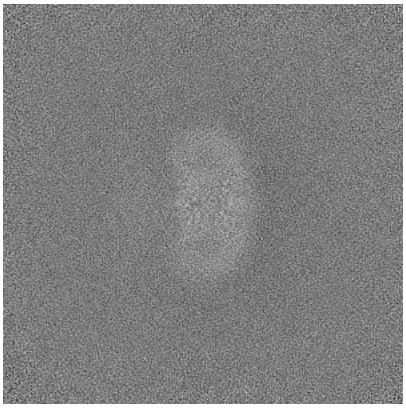


Z

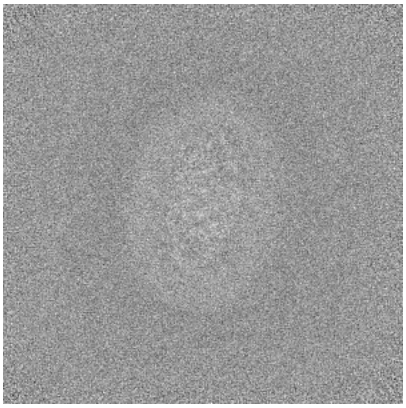
6.1.2 Raw map



X



Y



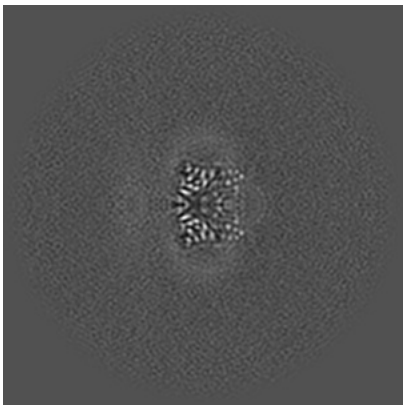
Z

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

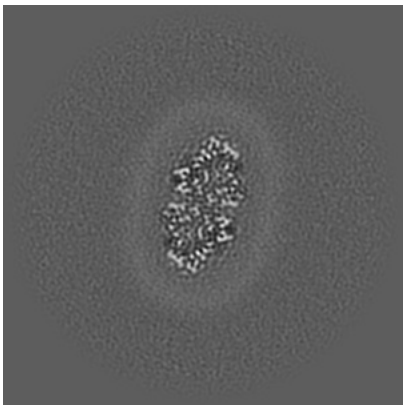
6.2 Central slices (i)

6.2.1 Primary map

X Index: 360

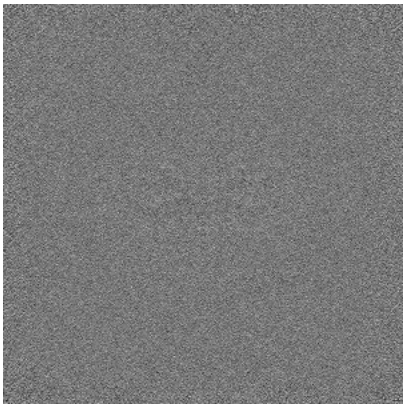


Y Index: 360

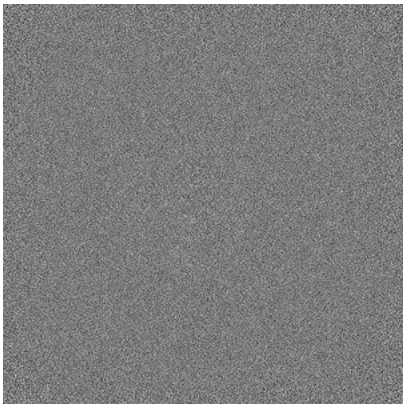


Z Index: 360

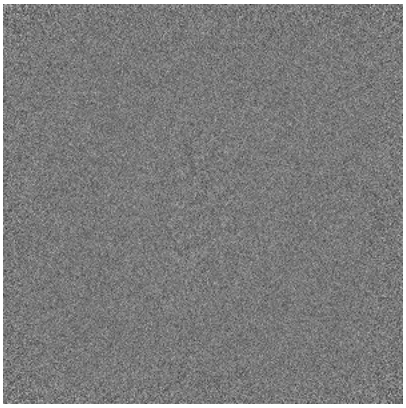
6.2.2 Raw map



X Index: 360



Y Index: 360



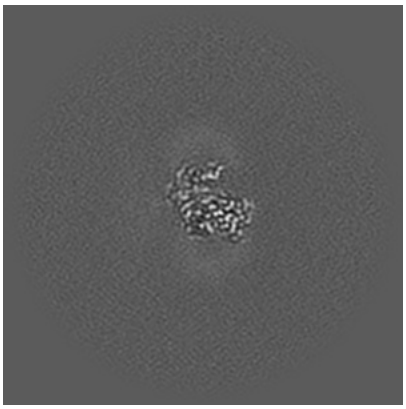
Z Index: 360

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

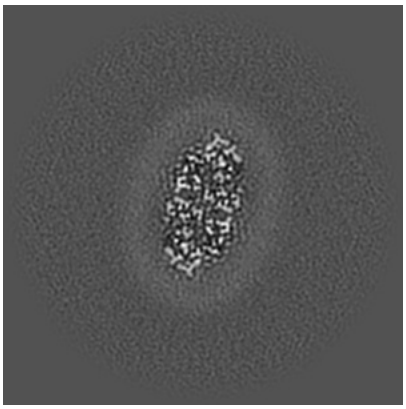
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 360

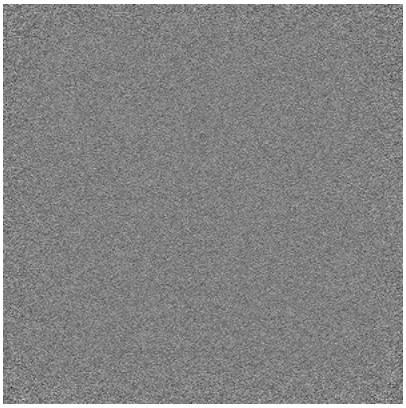


Y Index: 413

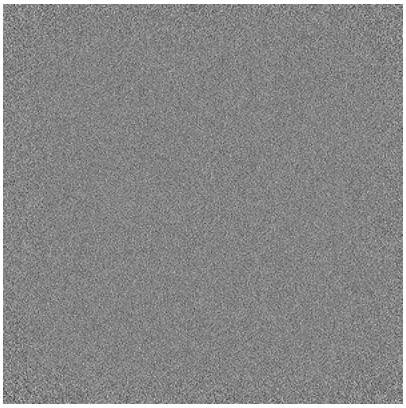


Z Index: 347

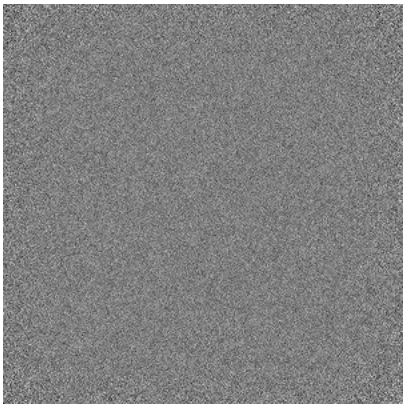
6.3.2 Raw map



X Index: 0



Y Index: 0

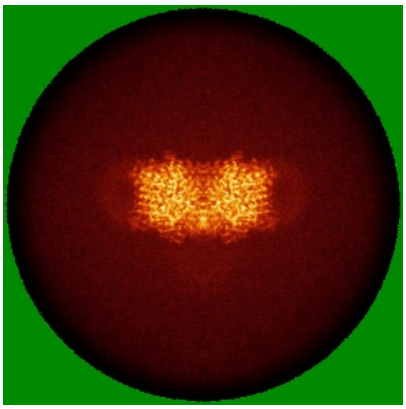


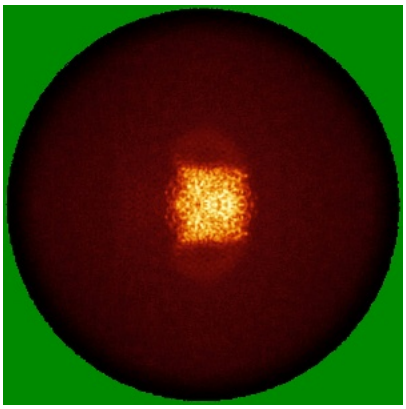
Z Index: 0

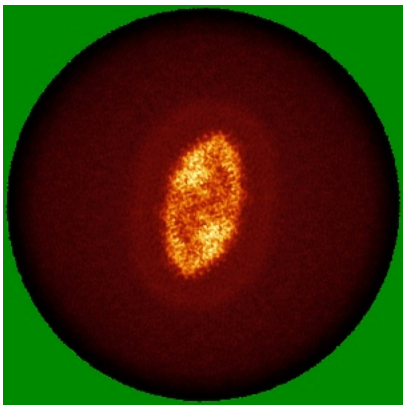
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

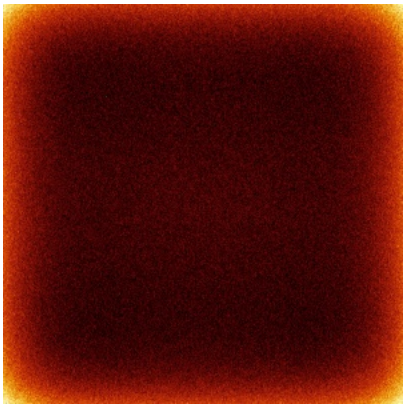
6.4.1 Primary map

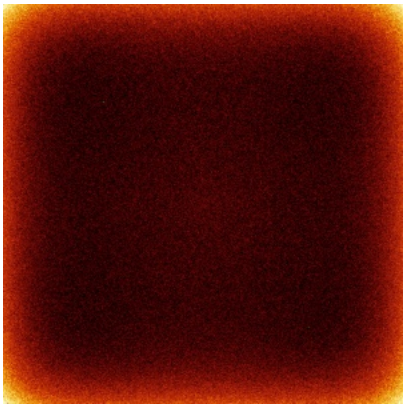

X

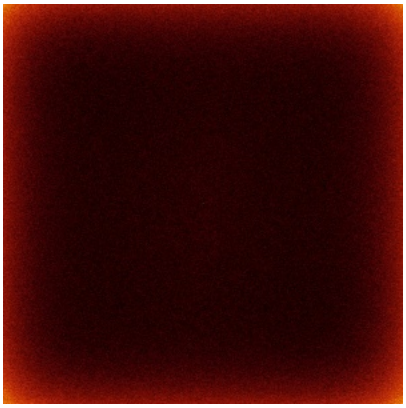

Y


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.

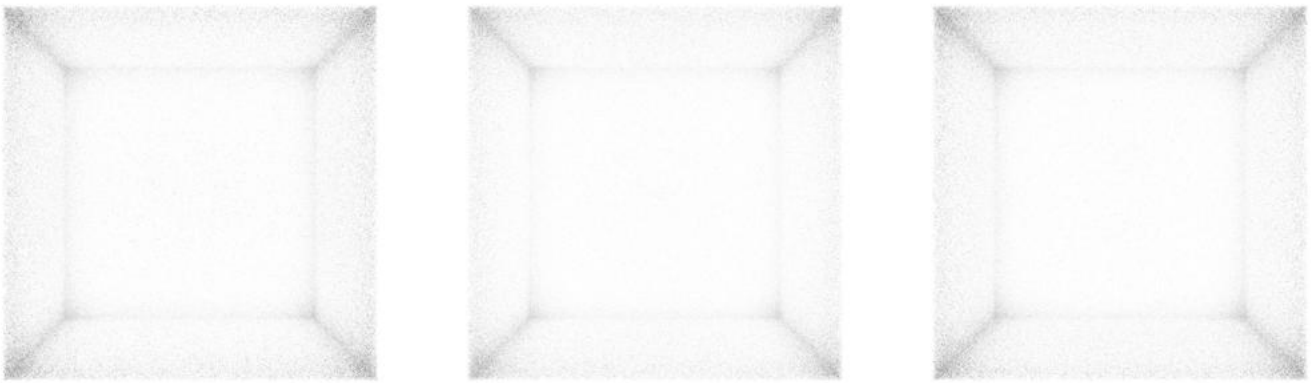
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

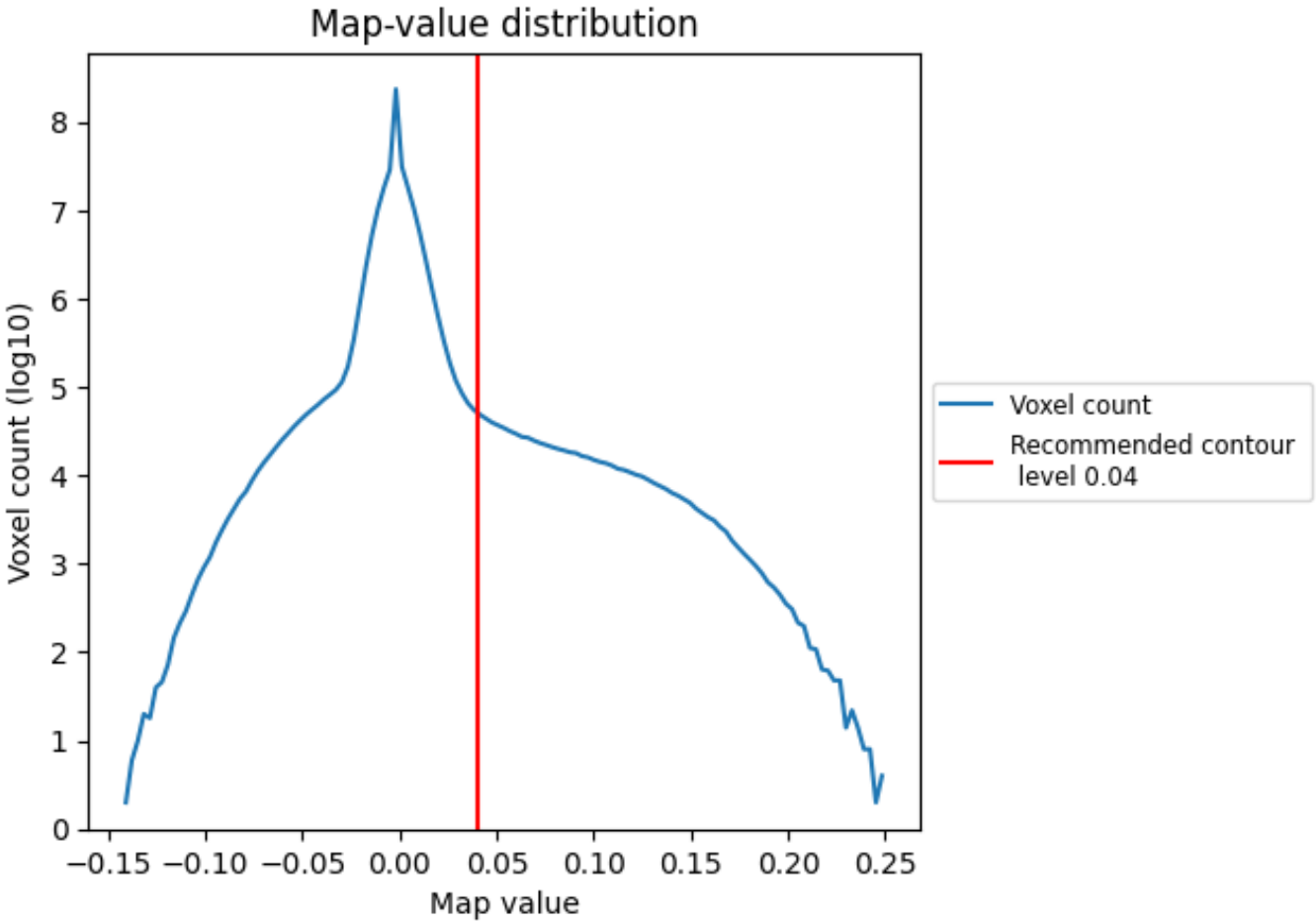
6.6 Mask visualisation (i)

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

7 Map analysis

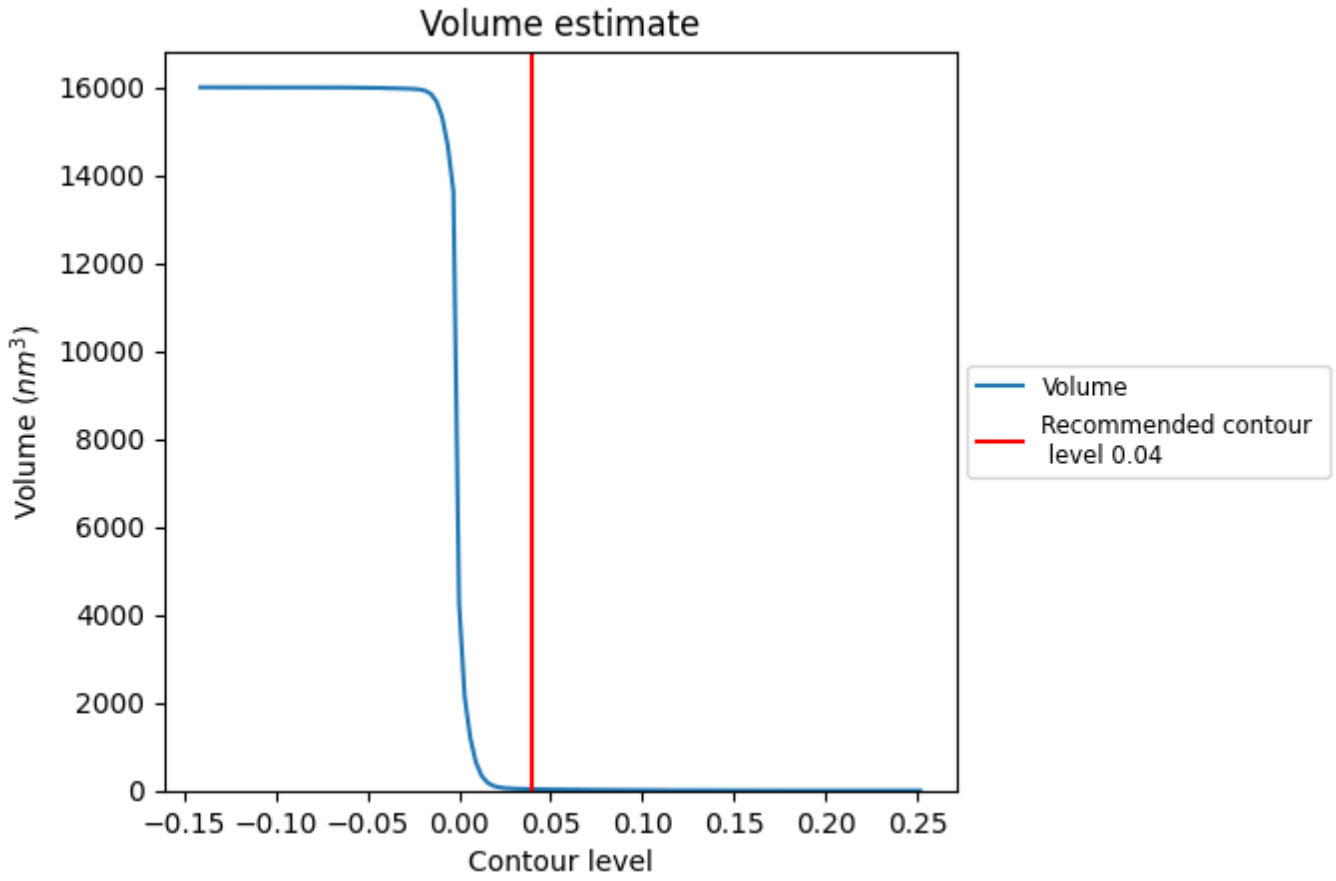
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

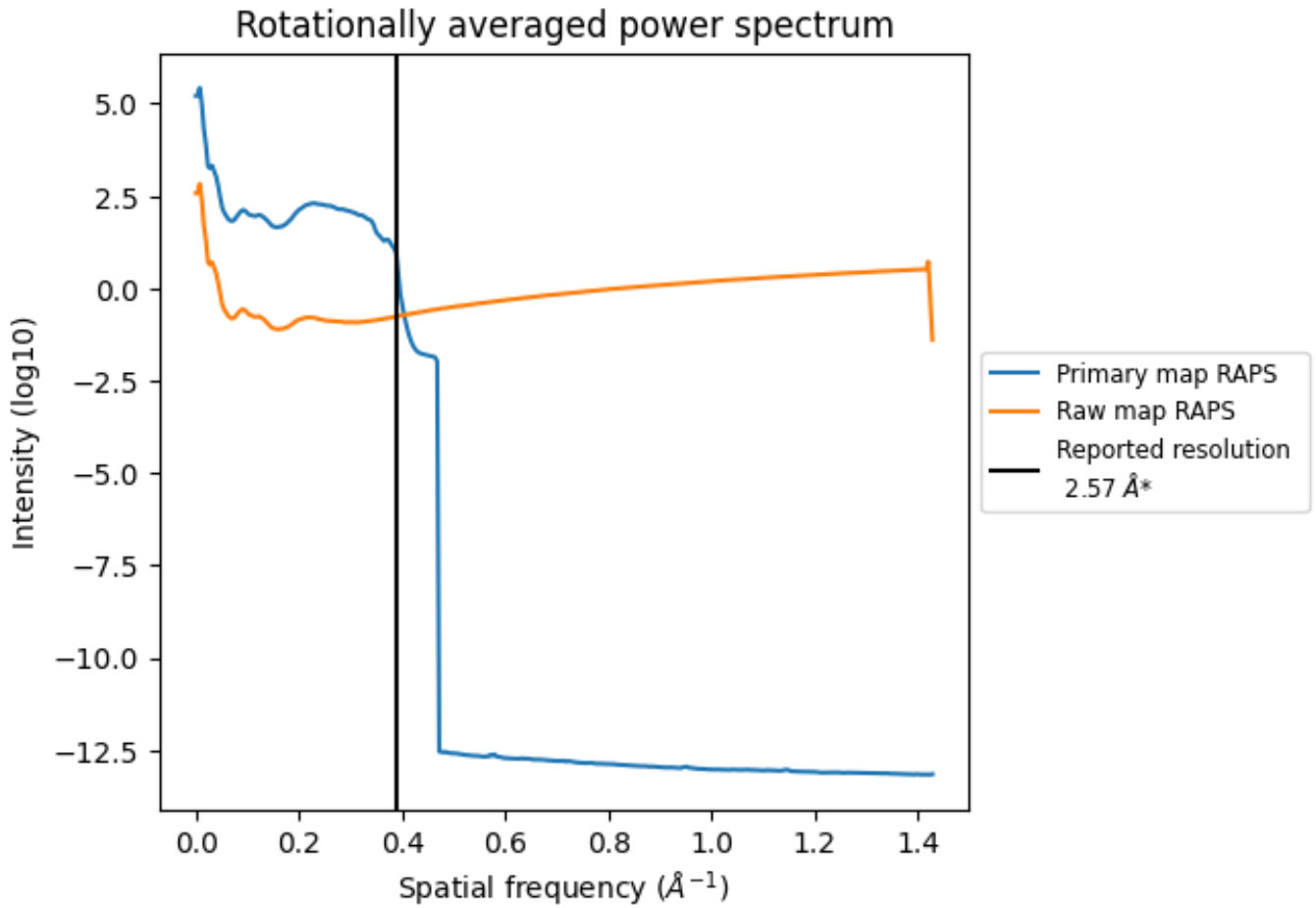
7.2 Volume estimate (i)



The volume at the recommended contour level is 32 nm^3; this corresponds to an approximate mass of 29 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

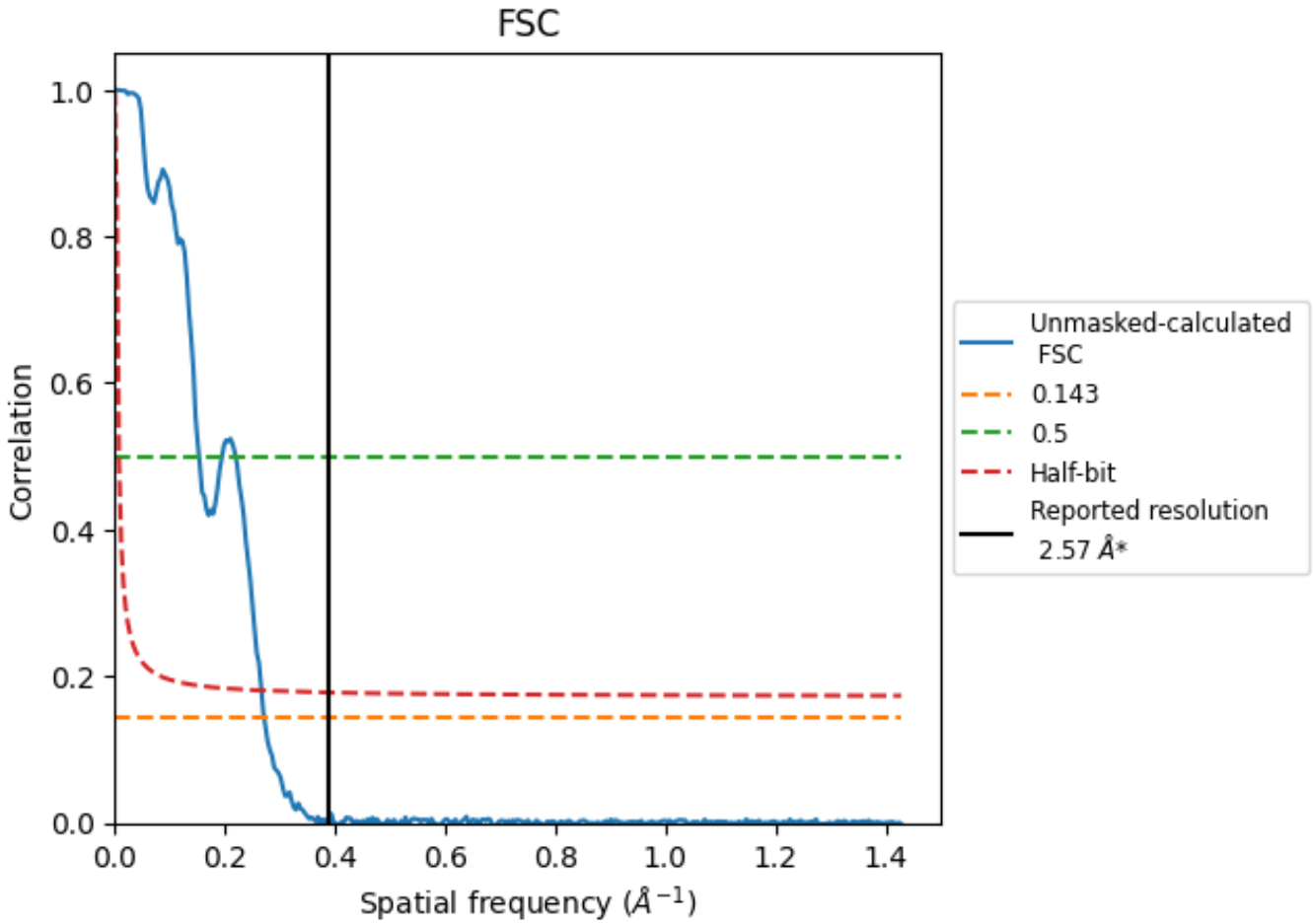


*Reported resolution corresponds to spatial frequency of 0.389 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.389 Å^{-1}

8.2 Resolution estimates (i)

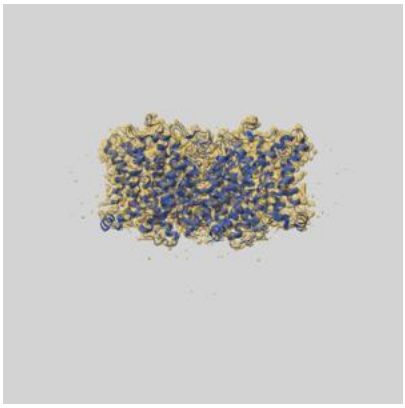
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.57	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.69	6.53	3.75

*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 3.69 differs from the reported value 2.57 by more than 10 %

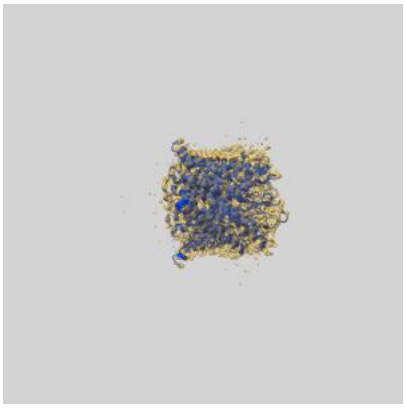
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37908 and PDB model 8WXI. Per-residue inclusion information can be found in section 3 on page 5.

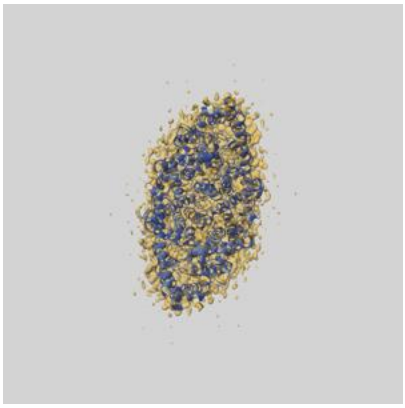
9.1 Map-model overlay



X



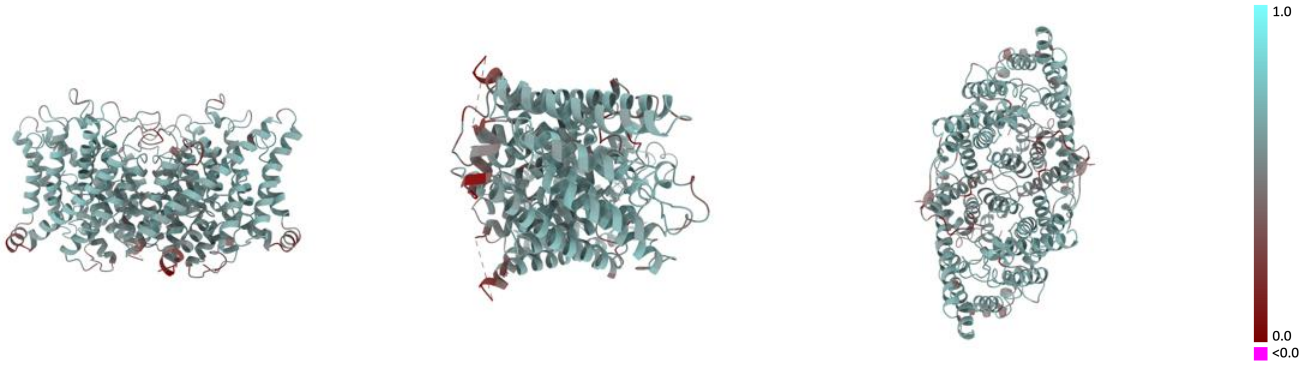
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

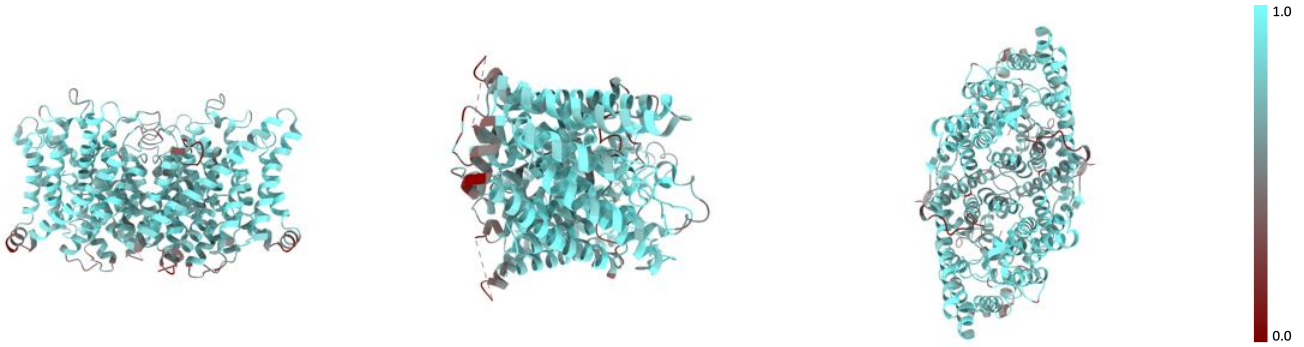
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

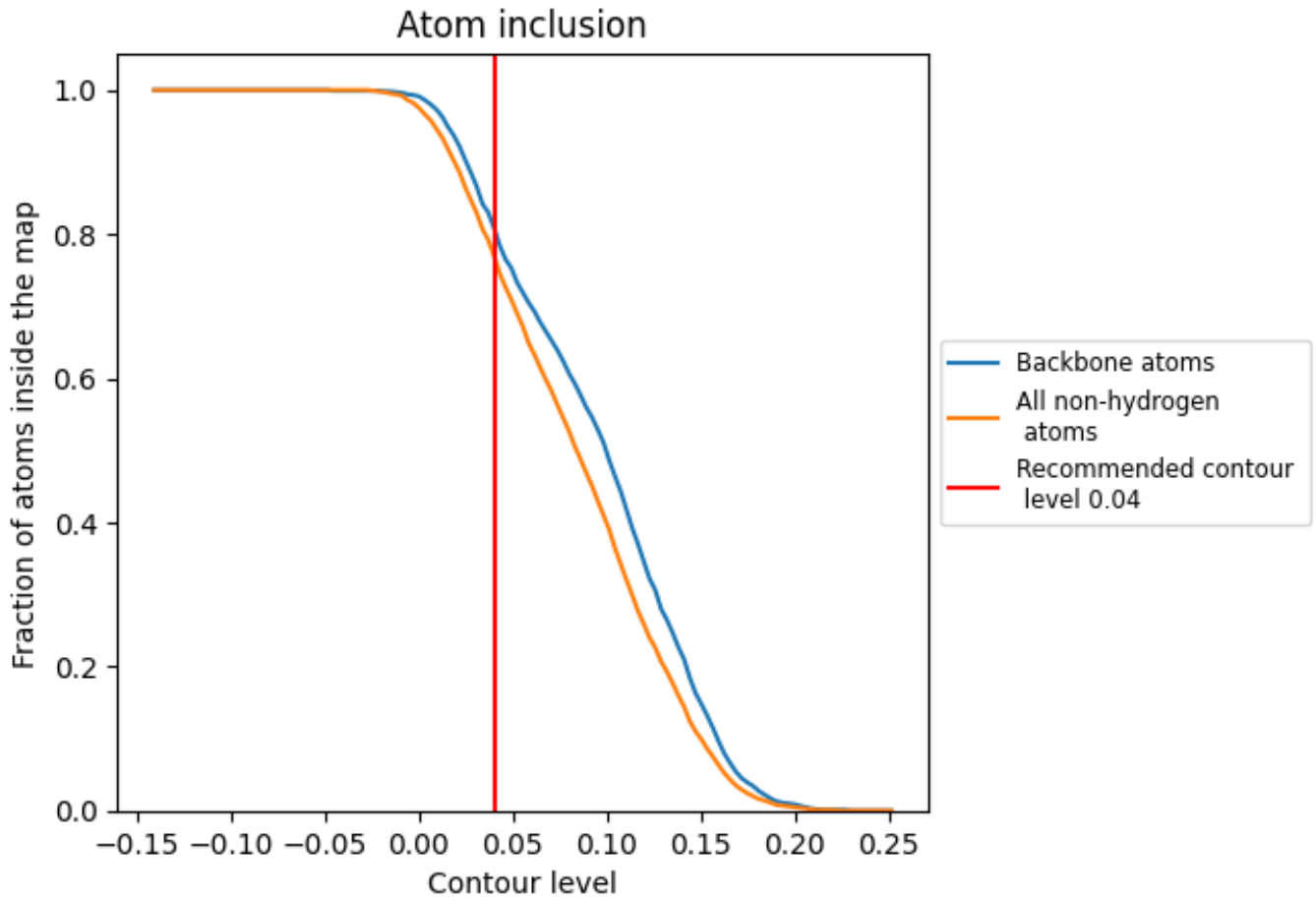
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7690	0.5640
A	0.7690	0.5640
B	0.7690	0.5650