



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 01:01 AM UTC

PDB ID : 8VRT / pdb_00008vrt
EMDB ID : EMD-43487
Title : The structure of LSD1-CoREST-HDAC1 in complex with KBTBD4R313PRR mutant
Authors : Xie, X.; Liao, B.; Zheng, N.
Deposited on : 2024-01-22
Resolution : 3.42 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

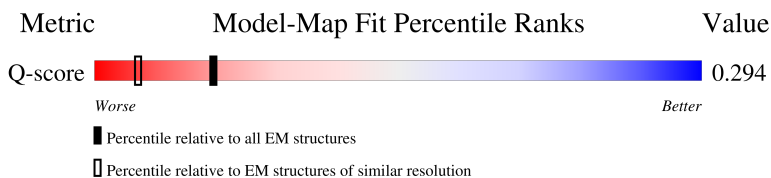
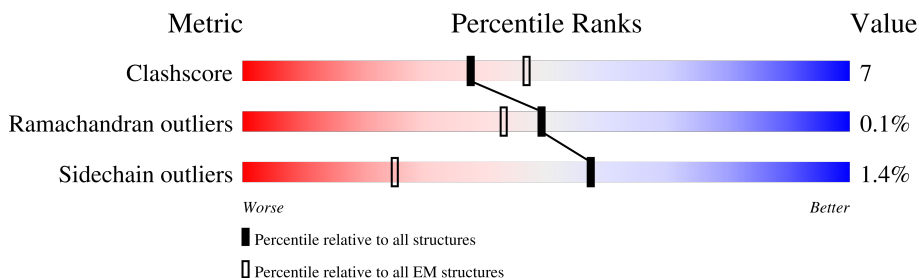
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.42 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	13959 (2.92 - 3.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	520	50% (Poor fit) 78% (0 outliers) 21% (1 outlier) . (2 outliers) . (3+ outliers)
1	B	520	38% (Poor fit) 80% (0 outliers) 17% (1 outlier) .. (2 outliers)
2	C	482	12% (Poor fit) 62% (0 outliers) 14% (1 outlier) . (2 outliers) 23% (3+ outliers)
3	D	401	34% (Poor fit) 27% (0 outliers) 6% (1 outlier) 66% (3+ outliers)

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 12240 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 Kelch repeat and BTB domain-containing protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	514	Total	C	N	O	S	0	0
			4057	2566	699	769	23		
1	B	511	Total	C	N	O	S	0	0
			4041	2556	696	766	23		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	PRO	-	insertion	UNP Q9NVX7
A	312	ARG	-	insertion	UNP Q9NVX7
B	311	PRO	-	insertion	UNP Q9NVX7
B	312	ARG	-	insertion	UNP Q9NVX7

- Molecule 2 is a protein called Histone deacetylase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	369	Total	C	N	O	S	0	0
			2985	1904	507	552	22		

- Molecule 3 is a protein called REST corepressor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	135	Total	C	N	O	S	0	0
			1120	725	190	200	5		

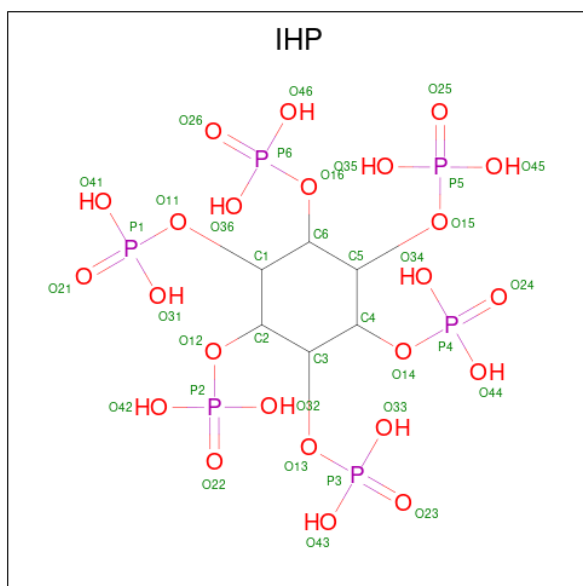
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP Q9UKL0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	Zn	0
			1	1	

- Molecule 5 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).

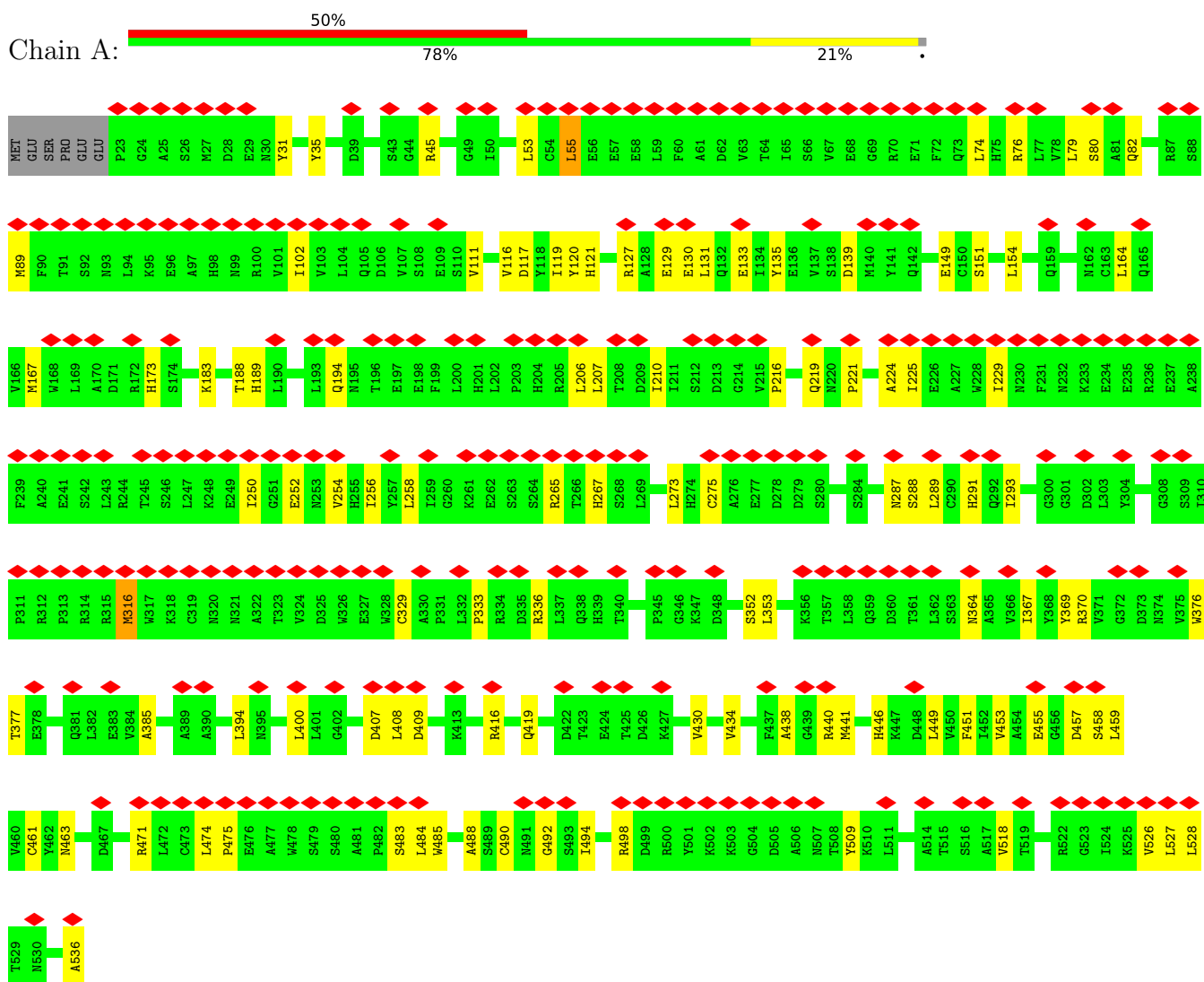


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
5	D	1	36	6	24	6	0

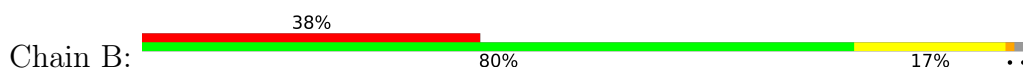
3 Residue-property plots

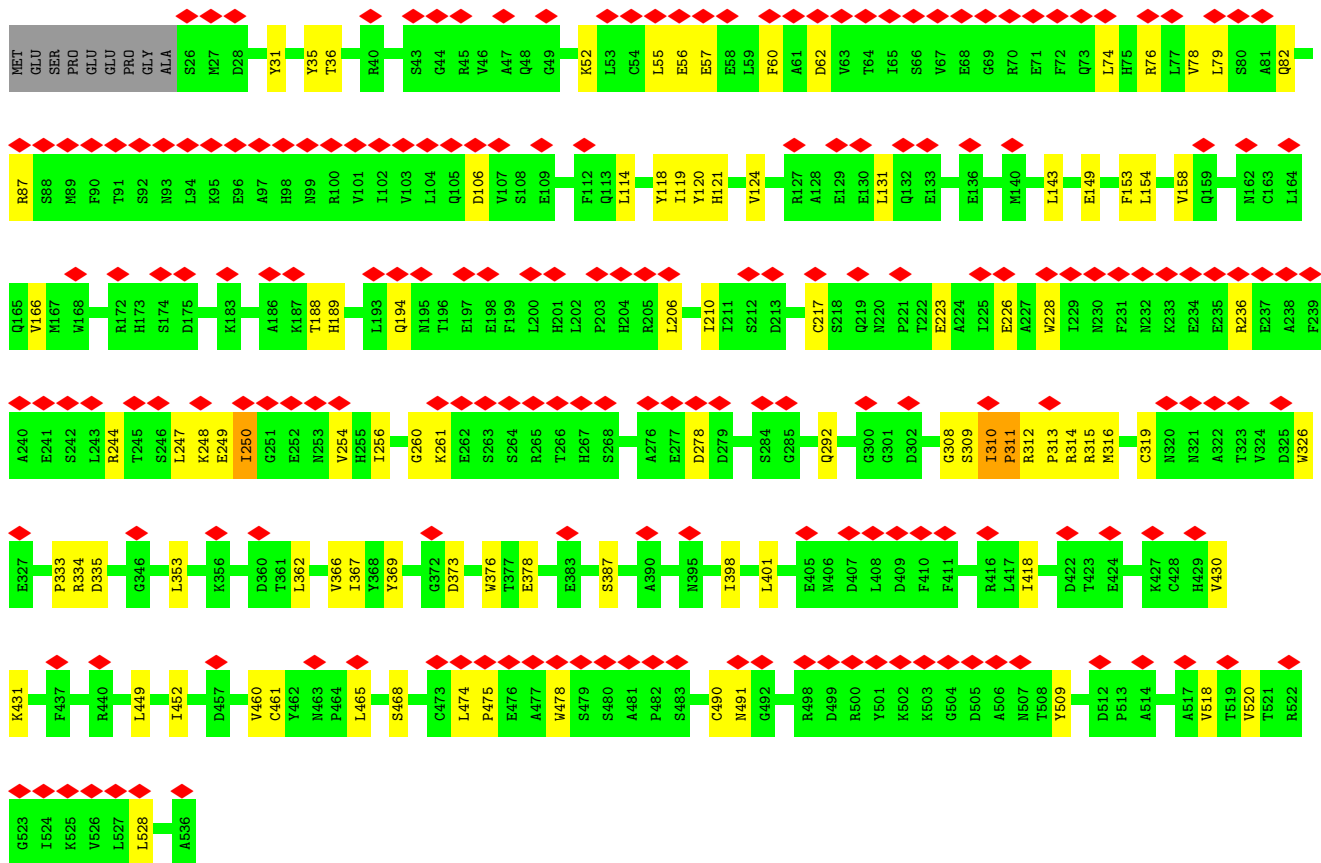
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Kelch repeat and BTB domain-containing protein 4

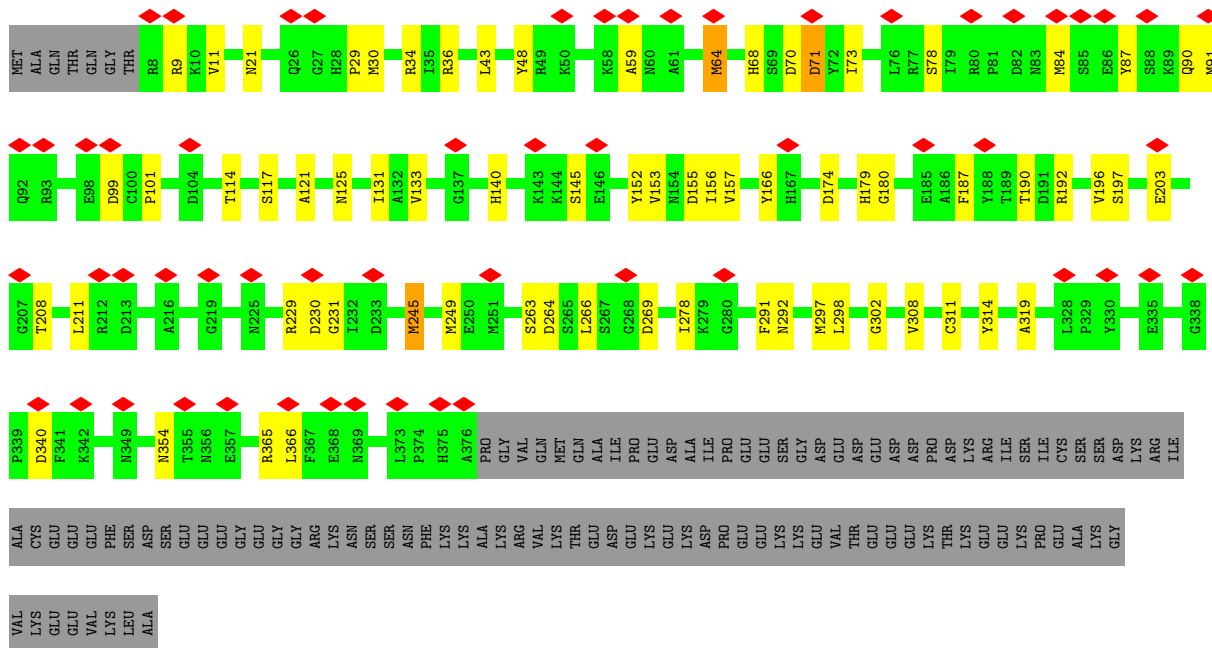


- Molecule 1: Kelch repeat and BTB domain-containing protein 4





• Molecule 2: Histone deacetylase 1



• Molecule 3: REST corepressor 1



MET	S41	Q101	GLU	GLU	ARG	GLY
SER	E42	A102	GLU	ALA	TRP	LYS
TRP	A43	F103	VAL	VAL	THR	GLU
GLU	K44	S104	ALA	ALA	GLU	THR
GLY	L45	F105	ASN	ASN	GLU	ASN
SER	D46	H106	ASN	ALA	GLN	GLY
SER	E47	G107	PRO	THR	LEU	PRO
GLY	Y48	K108	ILE	ALA	SER	SER
SER	I49	T109	ILE	ALA	VAL	ASN
SER	A50	F110	THR	GLN	ALA	LYS
ASP	I51	H111	VAL	LEU	ILE	PRO
GLU	A52	R112	ASP	ARG	ILE	VAL
GLU	K53	T113	GLN	LEU	ARG	VAL
HIS	E54	Q114	ASN	GLN	LYS	LYS
GLY	K55	Q115	LYS	LEU	TYR	ASP
GLY	K56	M116	SER	ASP	ARG	ASN
GLY	H56	L117	LYS	GLU	ASP	SER
GLY	G57	L118	GLU	LEU	PHE	ILE
GLY	Y58	P118	VAL	VAL	GLN	LYS
GLY	M59	D119	VAL	SER	ALA	MET
GLY	M60	K120	LYS	LYS	PRO	PRO
GLY	G61	S121	PRO	ARG	SER	GLU
GLY	Q62	I122	THR	GLM	VAL	GLU
GLY	A63	A123	GLU	ILE	ILE	ASP
GLY	L64	A124	VAL	SER	GLN	GLU
GLY	G65	S124	GLN	ILE	LYS	ALA
GLY	V10	L125	VAL	LYS	SER	VAL
GLY	V11	V126	VAL	GLM	VAL	VAL
GLY	P12	K127	LYS	THR	VAL	ASP
GLY	D13	F128	LYS	ASN	VAL	VAL
GLY	F14	Y129	HIS	ALA	VAL	ARG
GLY	D15	Y130	SER	LEU	ASN	LYS
GLY	P16	S131	THR	LYS	LYS	TYR
GLY	A17	M132	GLN	ALA	GLU	ALA
GLY	K18	K133	LYS	LYS	VAL	ALA
GLY	L19	K134	ASN	ASP	ASN	SER
GLY	A20	T135	ALA	GLY	TYR	ALA
GLY	R21	ARG	LYS	GLY	ARG	ALA
GLY	R22	THR	LYS	ILE	ARG	ALA
GLY	S23	THR	PRO	THR	PHE	ALA
GLY	Q24	L78	PRO	ILE	ASN	ALA
GLY	E25	A79	LYS	ARG	ILE	SER
GLY	R26	D80	VAL	LEU	GLU	GLU
GLY	D27	L81	LYS	PRO	LEU	GLU
GLY	M28	P82	THR	TYR	GLU	GLU
GLY	L29	M83	SER	ARG	TRP	GLU
GLY	G30	F84	ALA	ARG	TRP	GLU
GLY	M31	T85	GLN	LYS	GLU	ALA
GLY	L32	P86	LYS	LYS	ALA	ALA
GLY	V33	F87	LYS	LYS	ASP	ALA
GLY	W34	P88	ARG	ARG	VAL	HIS
GLY	S35	D89	GLU	GLU	VAL	
GLY	P36	E90	GLU	GLU	GLU	
GLY	N37	W91	SER	GLU	LEU	
GLY	Q38	T92	GLU	SER	TRP	
GLY	N39	V93	ASP	GLN	GLU	
GLY	L40	E94	GLU	LYS	GLU	
		D95	LEU	CYS	GLU	
		K96		ASN	ALA	
		V97		ALA	VAL	
		L98				
		F99				
		E100				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110048	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.855	Depositor
Minimum map value	-0.477	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.216	Depositor
Map size (\AA)	389.4, 389.4, 389.4	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.885, 0.885, 0.885	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.19	0/4146	0.35	0/5629
1	B	0.21	0/4129	0.36	0/5606
2	C	0.16	0/3063	0.30	0/4136
3	D	0.09	0/1154	0.27	0/1560
All	All	0.18	0/12492	0.33	0/16931

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	309	SER	Peptide
1	B	310	ILE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4057	0	3978	66	0
1	B	4041	0	3962	67	0
2	C	2985	0	2876	46	0
3	D	1120	0	1092	17	0
4	C	1	0	0	0	0
5	D	36	0	6	0	0
All	All	12240	0	11914	180	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 7.

All (180) 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:264:ASP:HB3	2:C:302:GLY:H	1.48	0.78
1:B:114:LEU:HD22	1:B:124:VAL:HG23	1.66	0.77
1:B:313:PRO:HD2	1:B:335:ASP:HB2	1.65	0.77
2:C:30:MET:SD	2:C:34:ARG:NH2	2.60	0.74
2:C:64:MET:HE3	2:C:153:VAL:HG21	1.70	0.74
1:B:316:MET:HE1	1:B:376:TRP:HZ2	1.55	0.71
2:C:190:THR:HG22	2:C:192:ARG:H	1.56	0.71
1:B:475:PRO:HG3	1:B:518:VAL:HG21	1.73	0.70
1:A:31:TYR:HH	1:B:468:SER:HG	1.34	0.69
1:B:314:ARG:NH1	1:B:335:ASP:OD2	2.26	0.68
1:A:45:ARG:NH1	1:B:82:GLN:OE1	2.27	0.68
1:A:458:SER:OG	1:A:471:ARG:NH1	2.27	0.67
1:A:474:LEU:HD23	1:A:475:PRO:HD2	1.75	0.67
1:A:289:LEU:HD23	1:A:291:HIS:H	1.62	0.65
1:A:316:MET:HB3	1:A:329:CYS:HB2	1.77	0.65
1:A:82:GLN:NE2	1:A:119:ILE:O	2.30	0.64
1:A:265:ARG:HE	1:A:267:HIS:HB2	1.61	0.64
1:A:167:MET:HE2	1:A:183:LYS:HA	1.79	0.63
2:C:121:ALA:O	2:C:125:ASN:HB2	1.98	0.63
2:C:192:ARG:NH1	3:D:12:PRO:O	2.32	0.63
1:A:35:TYR:OH	1:B:149:GLU:OE2	2.18	0.62
2:C:71:ASP:N	2:C:71:ASP:OD1	2.31	0.62
1:A:53:LEU:HD21	1:B:87:ARG:HH11	1.64	0.61
1:A:370:ARG:NH2	1:A:377:THR:OG1	2.33	0.61
2:C:145:SER:O	2:C:145:SER:OG	2.19	0.61
2:C:68:HIS:HB2	2:C:73:ILE:HD11	1.83	0.61
1:A:483:SER:OG	1:A:498:ARG:NH2	2.34	0.60
1:B:333:PRO:HD2	1:B:367:ILE:HD12	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HH21	1:B:60:PHE:HD1	1.50	0.60
2:C:84:MET:HG3	2:C:91:MET:HE1	1.84	0.59
2:C:196:VAL:HG11	2:C:245:MET:HE1	1.84	0.58
1:A:458:SER:HG	1:A:471:ARG:NH1	2.00	0.58
2:C:297:MET:HE1	2:C:319:ALA:HB2	1.84	0.58
2:C:21:ASN:OD1	2:C:36:ARG:NH2	2.34	0.58
1:A:149:GLU:OE2	1:B:35:TYR:OH	2.21	0.58
1:B:401:LEU:HD23	1:B:418:ILE:HD12	1.86	0.58
1:A:419:GLN:HG2	1:A:430:VAL:HG22	1.86	0.57
2:C:156:ILE:HD12	2:C:298:LEU:HD12	1.85	0.57
1:B:194:GLN:HE22	1:B:223:GLU:C	2.12	0.57
2:C:101:PRO:O	2:C:152:TYR:OH	2.23	0.57
1:B:418:ILE:HB	1:B:431:LYS:HB2	1.87	0.57
3:D:131:SER:HA	3:D:134:LYS:HE3	1.85	0.56
1:B:188:THR:HG23	1:B:189:HIS:CD2	2.39	0.56
2:C:166:TYR:OH	3:D:23:SER:N	2.38	0.56
1:A:55:LEU:HD21	1:A:120:TYR:HB3	1.87	0.56
1:A:127:ARG:HG3	1:A:129:GLU:HG2	1.87	0.56
1:A:440:ARG:NH2	1:A:484:LEU:HB3	2.20	0.56
3:D:58:TYR:OH	3:D:84:PHE:O	2.20	0.55
3:D:1:MET:HA	3:D:1:MET:HE3	1.88	0.55
1:B:334:ARG:HB2	2:C:203:GLU:HB2	1.88	0.55
2:C:266:LEU:HD11	2:C:311:CYS:HB2	1.88	0.55
1:B:256:ILE:HD11	1:B:490:CYS:HB2	1.88	0.54
1:B:57:GLU:OE1	1:B:57:GLU:N	2.41	0.54
2:C:264:ASP:HB3	2:C:302:GLY:N	2.21	0.54
1:B:474:LEU:HD21	1:B:478:TRP:CE3	2.43	0.54
1:A:117:ASP:OD1	1:A:121:HIS:ND1	2.41	0.53
1:A:287:ASN:OD1	1:A:288:SER:N	2.42	0.53
1:A:451:PHE:HD2	1:A:459:LEU:HD21	1.73	0.53
1:B:260:GLY:HA3	1:B:528:LEU:HD22	1.90	0.53
2:C:190:THR:HG21	3:D:11:VAL:HG11	1.89	0.53
2:C:43:LEU:HD13	3:D:60:MET:HG3	1.90	0.52
1:B:319:CYS:HB2	1:B:326:TRP:CZ3	2.43	0.52
1:B:247:LEU:HD12	1:B:248:LYS:N	2.25	0.52
1:A:129:GLU:HG3	1:A:130:GLU:HG3	1.90	0.52
1:A:216:PRO:HG2	1:A:219:GLN:HG2	1.91	0.52
2:C:34:ARG:HD2	2:C:308:VAL:HG11	1.92	0.52
1:A:526:VAL:HG13	1:A:528:LEU:HD23	1.92	0.51
1:A:139:ASP:OD2	1:A:173:HIS:ND1	2.42	0.51
1:B:491:ASN:O	1:B:491:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LEU:O	1:B:158:VAL:HG13	2.10	0.51
1:A:509:TYR:HB3	1:A:518:VAL:HG13	1.93	0.51
3:D:99:PHE:HZ	3:D:129:TYR:HB2	1.75	0.51
2:C:133:VAL:HG22	2:C:297:MET:HE3	1.93	0.51
1:A:369:TYR:HB2	1:A:376:TRP:CE2	2.46	0.50
1:A:254:VAL:HG13	1:A:490:CYS:SG	2.52	0.50
1:A:408:LEU:HD23	1:A:408:LEU:O	2.11	0.50
1:B:56:GLU:HB2	1:B:57:GLU:OE1	2.12	0.49
1:A:89:MET:HE3	1:A:102:ILE:HG21	1.93	0.49
1:A:131:LEU:HD23	1:A:154:LEU:HD13	1.95	0.49
2:C:263:SER:O	2:C:263:SER:OG	2.28	0.49
1:A:188:THR:HG23	1:A:189:HIS:ND1	2.27	0.49
2:C:70:ASP:OD1	2:C:70:ASP:N	2.44	0.49
1:A:527:LEU:HD23	1:A:527:LEU:H	1.77	0.49
1:A:449:LEU:HD13	1:A:461:CYS:SG	2.53	0.48
1:B:158:VAL:HG12	1:B:166:VAL:HG21	1.94	0.48
1:A:446:HIS:HE2	1:A:492:GLY:C	2.21	0.48
1:A:364:ASN:HB3	1:A:385:ALA:HB2	1.96	0.48
2:C:179:HIS:ND1	2:C:208:THR:OG1	2.44	0.47
3:D:16:PRO:HA	3:D:19:LEU:HD13	1.97	0.47
1:B:367:ILE:HG22	1:B:378:GLU:HG2	1.97	0.47
1:B:316:MET:HE1	1:B:376:TRP:CZ2	2.44	0.47
1:A:207:LEU:HA	1:A:210:ILE:HG22	1.95	0.47
1:A:225:ILE:O	1:A:229:ILE:HG13	2.14	0.47
2:C:249:MET:HG3	2:C:291:PHE:CE2	2.49	0.47
1:A:416:ARG:HB3	1:A:438:ALA:HB2	1.96	0.47
2:C:211:LEU:HD21	2:C:365:ARG:HG2	1.96	0.47
1:B:334:ARG:NH2	1:B:378:GLU:OE2	2.48	0.47
1:B:79:LEU:HD23	1:B:119:ILE:HG21	1.97	0.47
1:B:206:LEU:O	1:B:210:ILE:HG23	2.15	0.47
3:D:3:VAL:HA	3:D:8:GLN:HE22	1.80	0.47
1:B:475:PRO:HG2	1:B:478:TRP:NE1	2.30	0.46
2:C:117:SER:OG	2:C:155:ASP:OD2	2.17	0.46
1:A:74:LEU:HD22	1:A:79:LEU:HD11	1.97	0.46
2:C:278:ILE:HD11	2:C:314:TYR:HB2	1.97	0.46
1:B:131:LEU:HD22	1:B:153:PHE:CD2	2.51	0.46
1:A:111:VAL:HG21	1:A:133:GLU:HG2	1.96	0.46
1:A:333:PRO:HD2	1:A:367:ILE:HD12	1.97	0.46
3:D:78:LEU:HD23	3:D:81:LEU:HD12	1.98	0.46
1:A:453:VAL:HG11	1:A:485:TRP:HB2	1.97	0.46
1:B:315:ARG:NH1	2:C:29:PRO:HG3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LYS:HE3	1:B:52:LYS:HB2	1.69	0.46
1:B:217:CYS:SG	1:B:250:ILE:O	2.68	0.45
1:B:310:ILE:CG2	1:B:313:PRO:HG3	2.47	0.45
2:C:87:TYR:O	2:C:91:MET:HG3	2.16	0.45
2:C:157:VAL:HG23	2:C:187:PHE:CE2	2.52	0.45
1:A:408:LEU:N	1:A:409:ASP:HA	2.32	0.45
1:B:55:LEU:HD22	1:B:121:HIS:NE2	2.32	0.45
1:B:223:GLU:O	1:B:226:GLU:HG3	2.16	0.45
1:B:353:LEU:HD23	1:B:366:VAL:HG22	1.99	0.45
1:A:74:LEU:HD21	1:A:116:VAL:HG22	1.97	0.45
1:A:221:PRO:O	1:A:225:ILE:HG13	2.16	0.45
1:B:369:TYR:HB2	1:B:376:TRP:CE2	2.52	0.45
1:B:247:LEU:HD12	1:B:248:LYS:H	1.81	0.45
2:C:340:ASP:N	2:C:340:ASP:OD1	2.45	0.44
1:B:228:TRP:CD2	1:B:236:ARG:HD3	2.52	0.44
1:B:74:LEU:HD13	1:B:79:LEU:HD11	1.99	0.44
3:D:102:ALA:HB1	3:D:113:ILE:HG12	2.00	0.44
1:B:118:TYR:HE2	1:B:143:LEU:HD22	1.83	0.44
1:B:311:PRO:HG2	2:C:99:ASP:OD1	2.16	0.44
3:D:66:MET:HE3	3:D:77:SER:HA	1.98	0.44
1:A:336:ARG:NH2	1:A:352:SER:OG	2.46	0.44
1:A:164:LEU:O	1:A:167:MET:HB2	2.17	0.44
1:B:154:LEU:HD23	1:B:154:LEU:HA	1.83	0.44
2:C:174:ASP:HB3	2:C:197:SER:HA	2.00	0.43
2:C:11:VAL:HG22	2:C:131:ILE:HB	1.99	0.43
1:A:206:LEU:HD23	1:A:206:LEU:HA	1.88	0.43
1:A:494:ILE:HD13	1:A:494:ILE:HA	1.86	0.43
1:B:308:GLY:H	1:B:310:ILE:HG13	1.83	0.43
1:A:488:ALA:HB1	1:A:536:ALA:HB2	2.00	0.43
1:A:440:ARG:HG2	1:A:441:MET:N	2.34	0.42
1:B:292:GLN:H	1:B:292:GLN:HG3	1.66	0.42
1:B:475:PRO:HG2	1:B:478:TRP:CD1	2.54	0.42
1:A:353:LEU:HD12	1:A:400:LEU:HD11	2.02	0.42
2:C:230:ASP:OD1	2:C:231:GLY:N	2.53	0.42
1:B:131:LEU:HD13	1:B:153:PHE:HD2	1.84	0.42
1:B:353:LEU:HD11	1:B:398:ILE:HG21	2.01	0.42
2:C:59:ALA:HB3	2:C:114:THR:HG23	2.01	0.42
2:C:140:HIS:ND1	2:C:180:GLY:HA2	2.34	0.42
1:A:455:GLU:OE2	1:A:455:GLU:N	2.51	0.42
1:A:394:LEU:HD12	1:A:394:LEU:HA	1.75	0.42
2:C:366:LEU:HD23	2:C:366:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ARG:HH12	2:C:29:PRO:HG3	1.84	0.42
3:D:96:LYS:HG2	3:D:128:PHE:HZ	1.84	0.41
1:A:135:TYR:HE1	1:A:151:SER:HB2	1.86	0.41
1:A:254:VAL:CG1	1:A:275:CYS:HB3	2.51	0.41
1:B:452:ILE:HG13	1:B:460:VAL:HB	2.02	0.41
1:A:207:LEU:O	1:A:210:ILE:HG22	2.21	0.41
1:B:278:ASP:O	1:B:278:ASP:OD1	2.39	0.41
2:C:229:ARG:HB2	2:C:354:ASN:ND2	2.35	0.41
3:D:14:PHE:CE1	3:D:19:LEU:HD11	2.55	0.41
1:B:261:LYS:HB3	1:B:261:LYS:HE3	1.83	0.41
1:B:362:LEU:HD22	1:B:387:SER:HB3	2.01	0.41
1:A:407:ASP:OD1	1:A:407:ASP:C	2.63	0.41
1:B:62:ASP:OD1	1:B:76:ARG:HD2	2.20	0.41
1:B:313:PRO:CD	1:B:335:ASP:HB2	2.44	0.41
1:B:449:LEU:HD13	1:B:461:CYS:SG	2.61	0.41
1:B:478:TRP:CZ2	1:B:509:TYR:HD2	2.38	0.41
1:A:76:ARG:O	1:A:80:SER:OG	2.36	0.41
1:B:244:ARG:HD3	1:B:244:ARG:HA	1.98	0.40
2:C:9:ARG:NH2	2:C:292:ASN:OD1	2.54	0.40
1:A:416:ARG:HG3	1:A:434:VAL:HB	2.03	0.40
2:C:87:TYR:HB3	2:C:90:GLN:HB2	2.02	0.40
1:A:194:GLN:HE22	1:A:224:ALA:N	2.19	0.40
1:B:78:VAL:HG11	1:B:120:TYR:CE1	2.56	0.40
1:B:312:ARG:HE	1:B:314:ARG:NH2	2.20	0.40
1:B:509:TYR:CE1	1:B:520:VAL:HG12	2.56	0.40
1:A:463:ASN:HB2	1:B:31:TYR:CE2	2.57	0.40
2:C:48:TYR:HE2	3:D:64:LEU:HG	1.87	0.40
3:D:96:LYS:HG2	3:D:128:PHE:CZ	2.57	0.40
1:A:258:LEU:HD13	1:A:273:LEU:HD12	2.02	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	512/520 (98%)	495 (97%)	17 (3%)	0	100	100
1	B	509/520 (98%)	490 (96%)	17 (3%)	2 (0%)	30	59
2	C	367/482 (76%)	360 (98%)	7 (2%)	0	100	100
3	D	133/401 (33%)	129 (97%)	4 (3%)	0	100	100
All	All	1521/1923 (79%)	1474 (97%)	45 (3%)	2 (0%)	49	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	254	VAL
1	B	311	PRO

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	447/453 (99%)	440 (98%)	7 (2%)	55	68
1	B	446/453 (98%)	439 (98%)	7 (2%)	55	68
2	C	320/419 (76%)	315 (98%)	5 (2%)	55	68
3	D	120/354 (34%)	120 (100%)	0	100	100
All	All	1333/1679 (79%)	1314 (99%)	19 (1%)	57	69

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	250	ILE
1	A	252	GLU
1	A	256	ILE
1	A	293	ILE
1	A	316	MET
1	A	457	ASP
1	B	36	THR
1	B	106	ASP

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Mol	Chain	Res	Type
1	B	249	GLU
1	B	250	ILE
1	B	373	ASP
1	B	430	VAL
1	B	465	LEU
2	C	64	MET
2	C	71	ASP
2	C	78	SER
2	C	245	MET
2	C	269	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	321	ASN
1	A	429	HIS
1	B	189	HIS
1	B	204	HIS
1	B	232	ASN
1	B	287	ASN
2	C	28	HIS
2	C	225	ASN
2	C	344	HIS
2	C	354	ASN
3	D	28	ASN
3	D	83	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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
5	IHP	D	701	-	36,36,36	0.95	5 (13%)	60,60,60	0.89	2 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IHP	D	701	-	-	8/30/54/54	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	701	IHP	P4-O14	2.06	1.63	1.59
5	D	701	IHP	P2-O12	2.03	1.63	1.59
5	D	701	IHP	P1-O11	2.02	1.63	1.59
5	D	701	IHP	P6-O16	2.01	1.63	1.59
5	D	701	IHP	P3-O13	2.00	1.63	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	701	IHP	P2-O12-C2	2.71	130.67	123.43
5	D	701	IHP	P3-O13-C3	2.55	130.23	123.43

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	701	IHP	C1-O11-P1-O41

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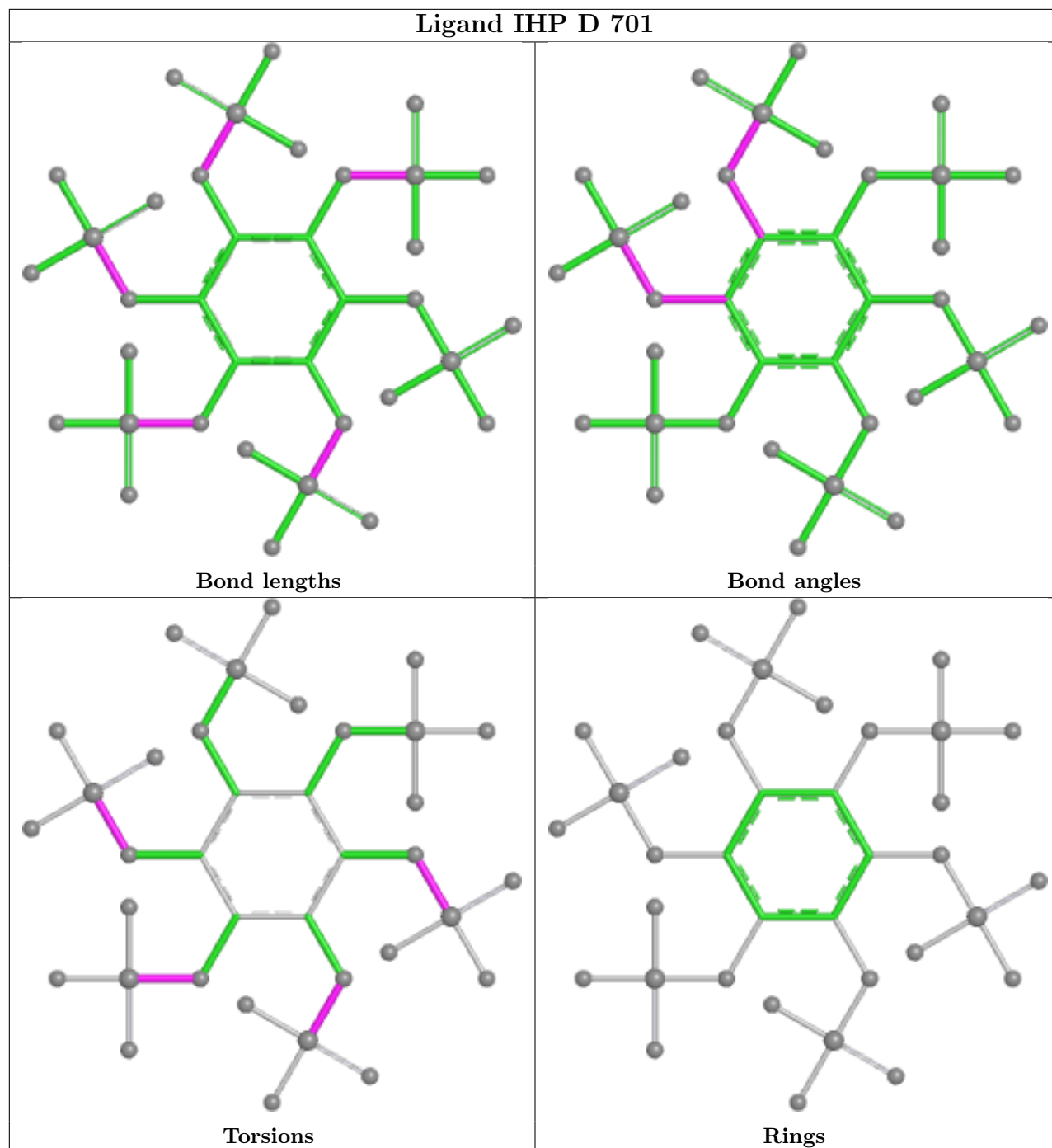
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Mol	Chain	Res	Type	Atoms
5	D	701	IHP	C5-O15-P5-O35
5	D	701	IHP	C6-O16-P6-O46
5	D	701	IHP	C1-O11-P1-O21
5	D	701	IHP	C2-O12-P2-O22
5	D	701	IHP	C1-O11-P1-O31
5	D	701	IHP	C2-O12-P2-O32
5	D	701	IHP	C2-O12-P2-O42

There are no ring outliers.

No monomer is involved in short contacts.

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 than 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.



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.

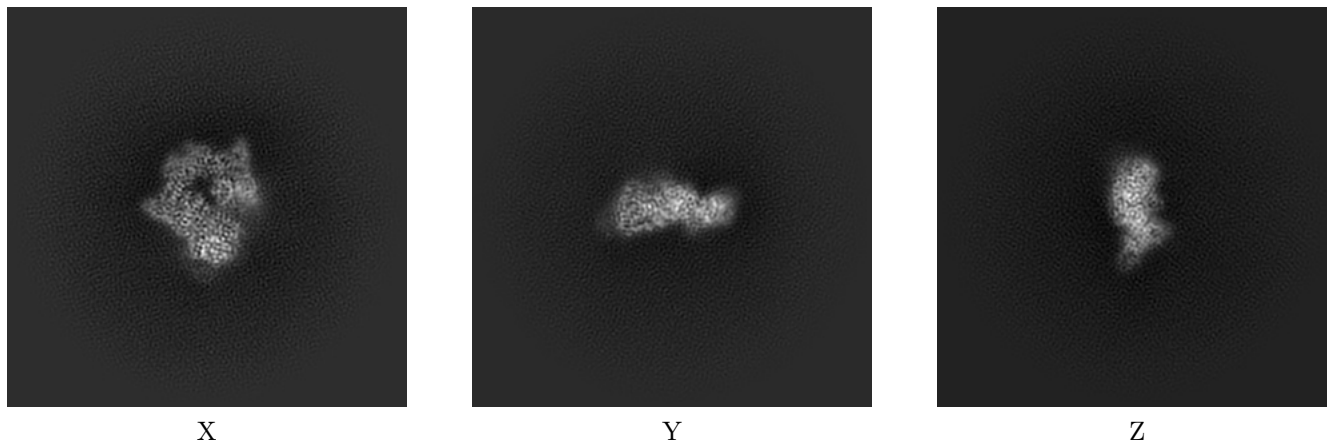
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43487. These allow visual inspection of the internal detail of the map and identification of artifacts.

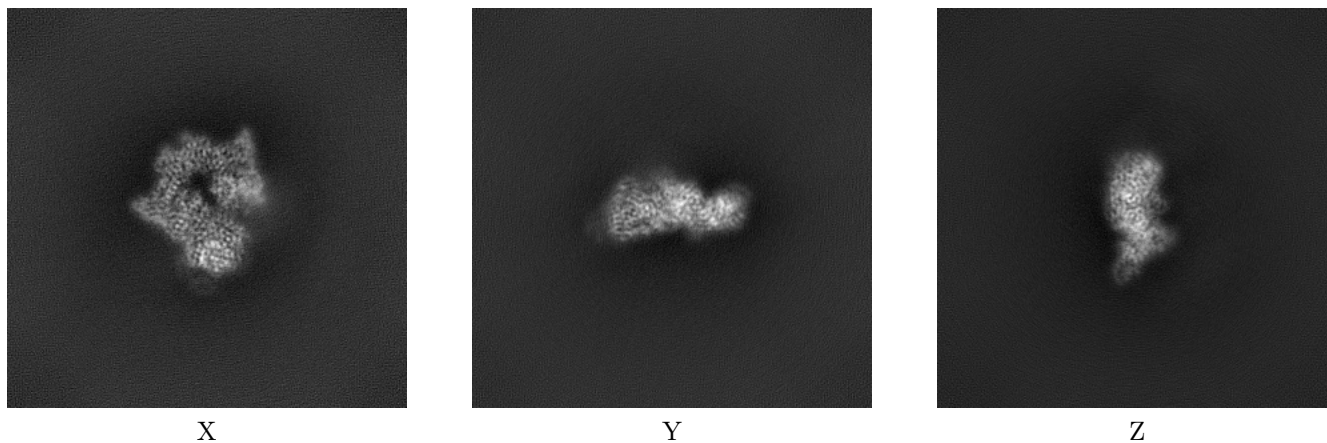
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



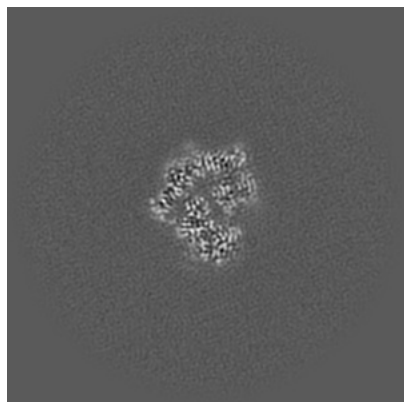
6.1.2 Raw map



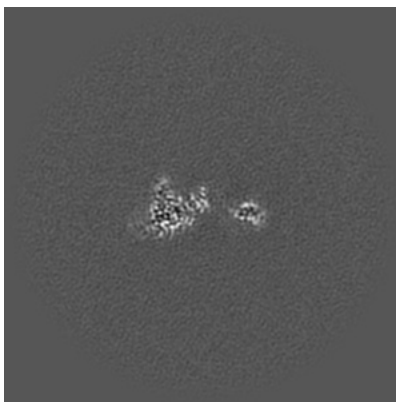
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

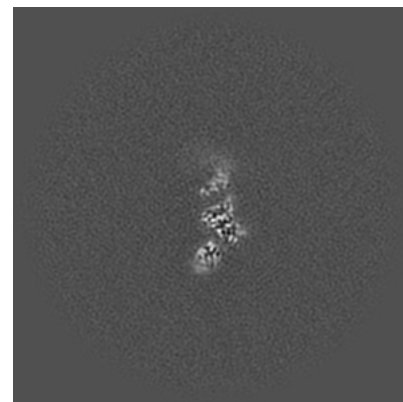
6.2.1 Primary map



X Index: 220

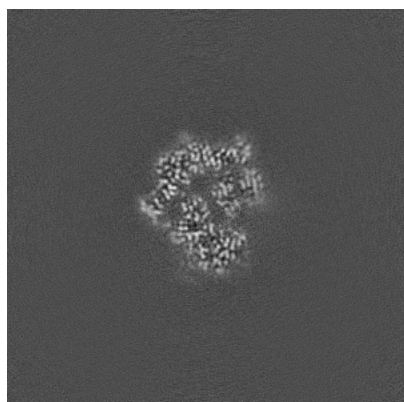


Y Index: 220



Z Index: 220

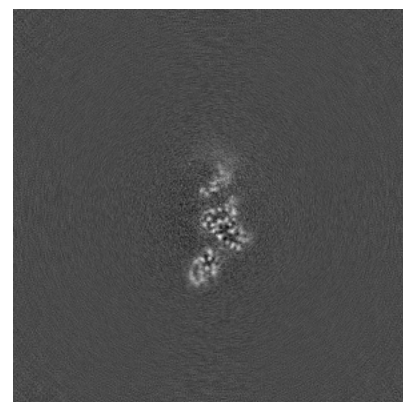
6.2.2 Raw map



X Index: 192



Y Index: 192

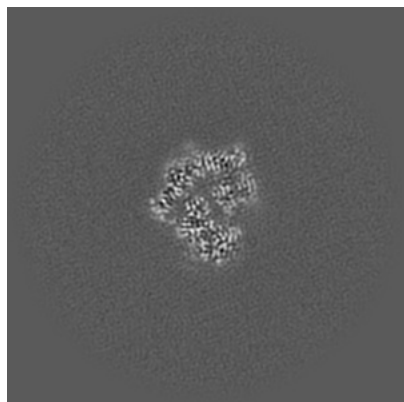


Z Index: 192

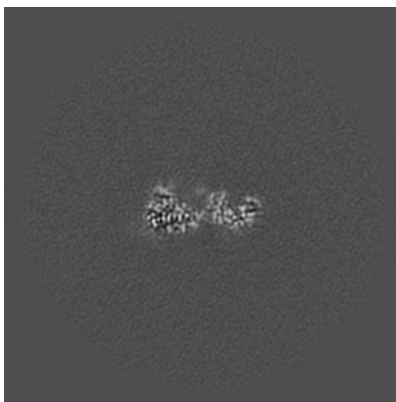
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

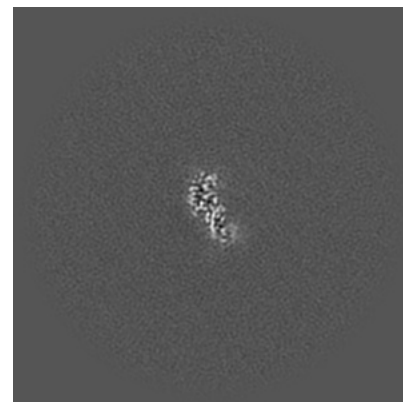
6.3.1 Primary map



X Index: 220

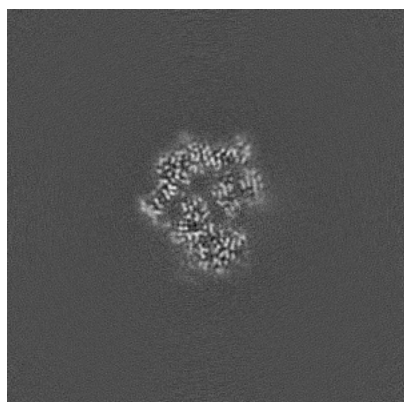


Y Index: 233

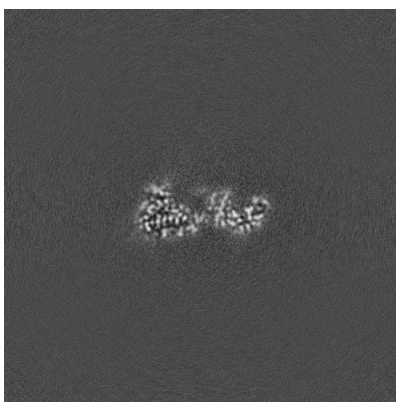


Z Index: 195

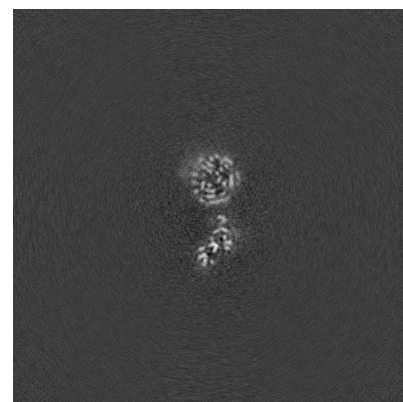
6.3.2 Raw map



X Index: 192



Y Index: 204

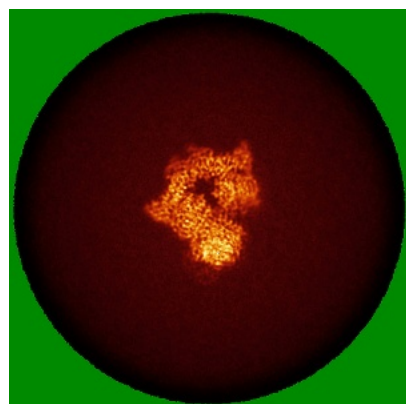


Z Index: 207

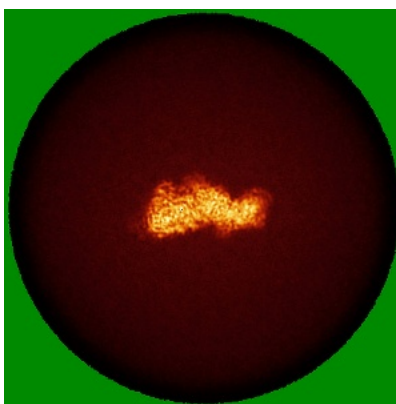
The images above show the largest variance slices of the map in three orthogonal directions.

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

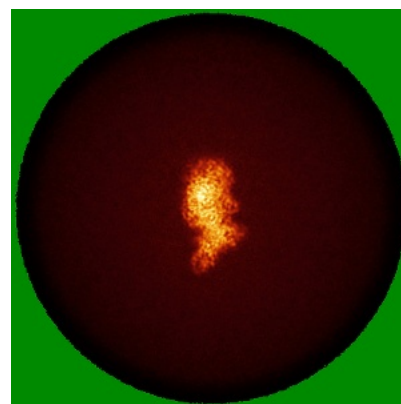
6.4.1 Primary map



X

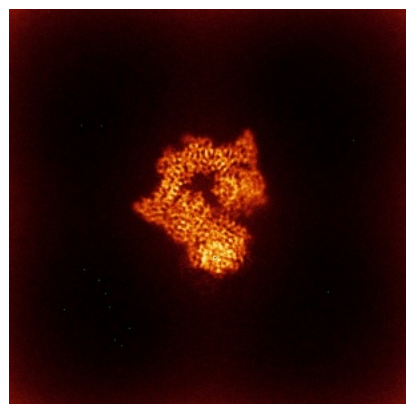


Y

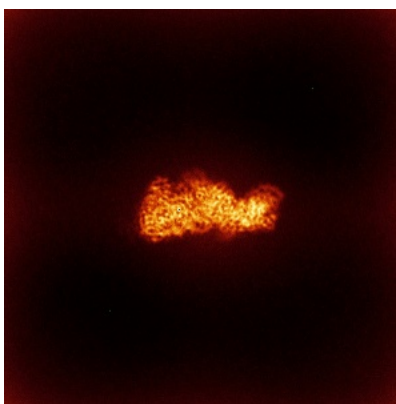


Z

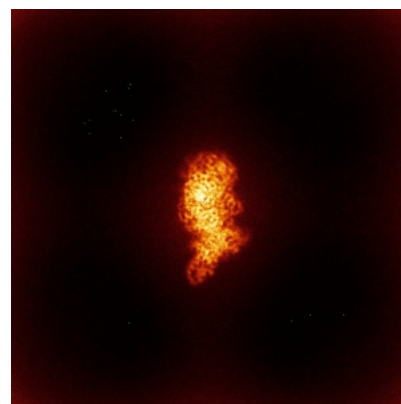
6.4.2 Raw map



X



Y

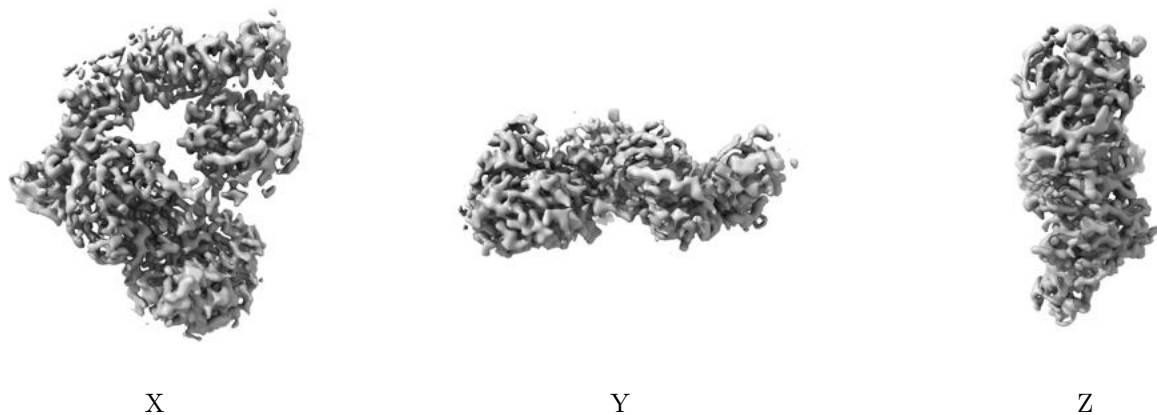


Z

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

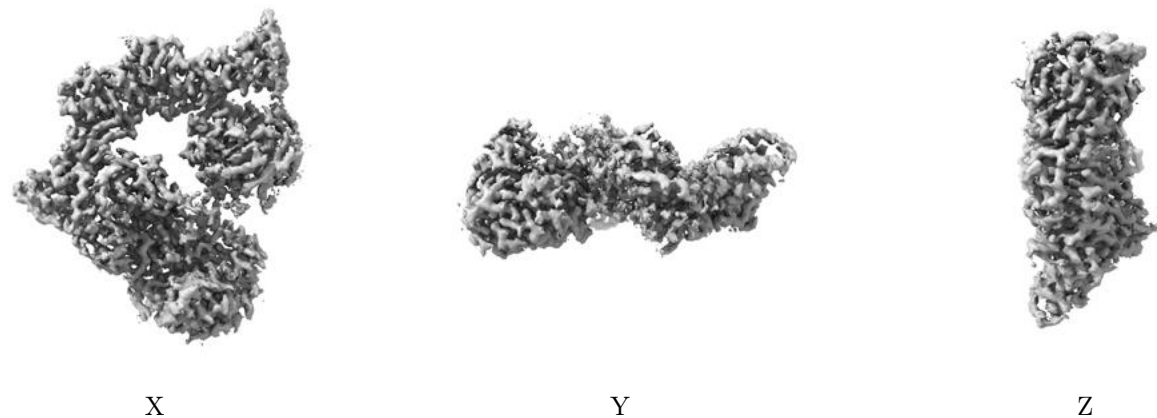
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.216. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

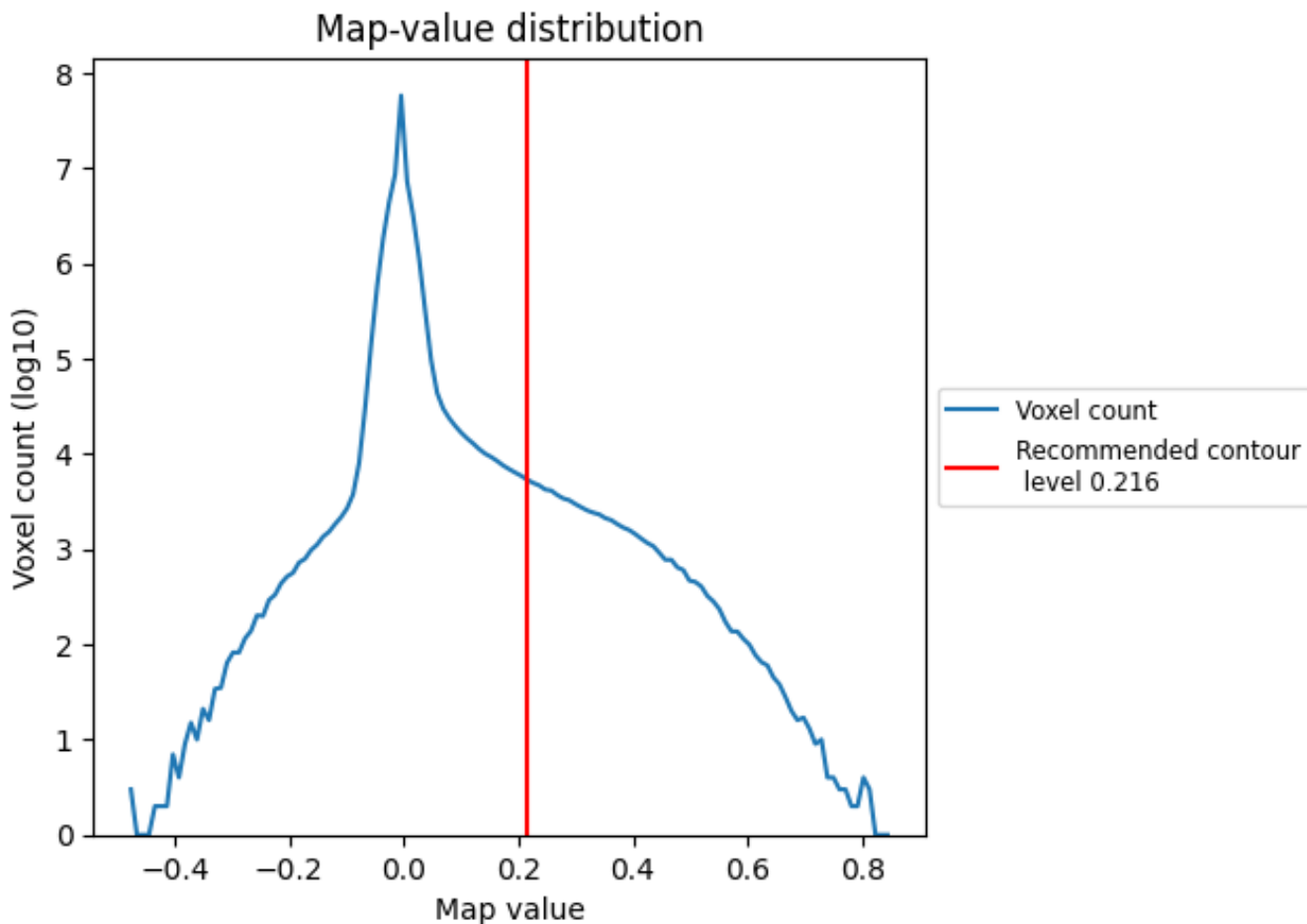
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

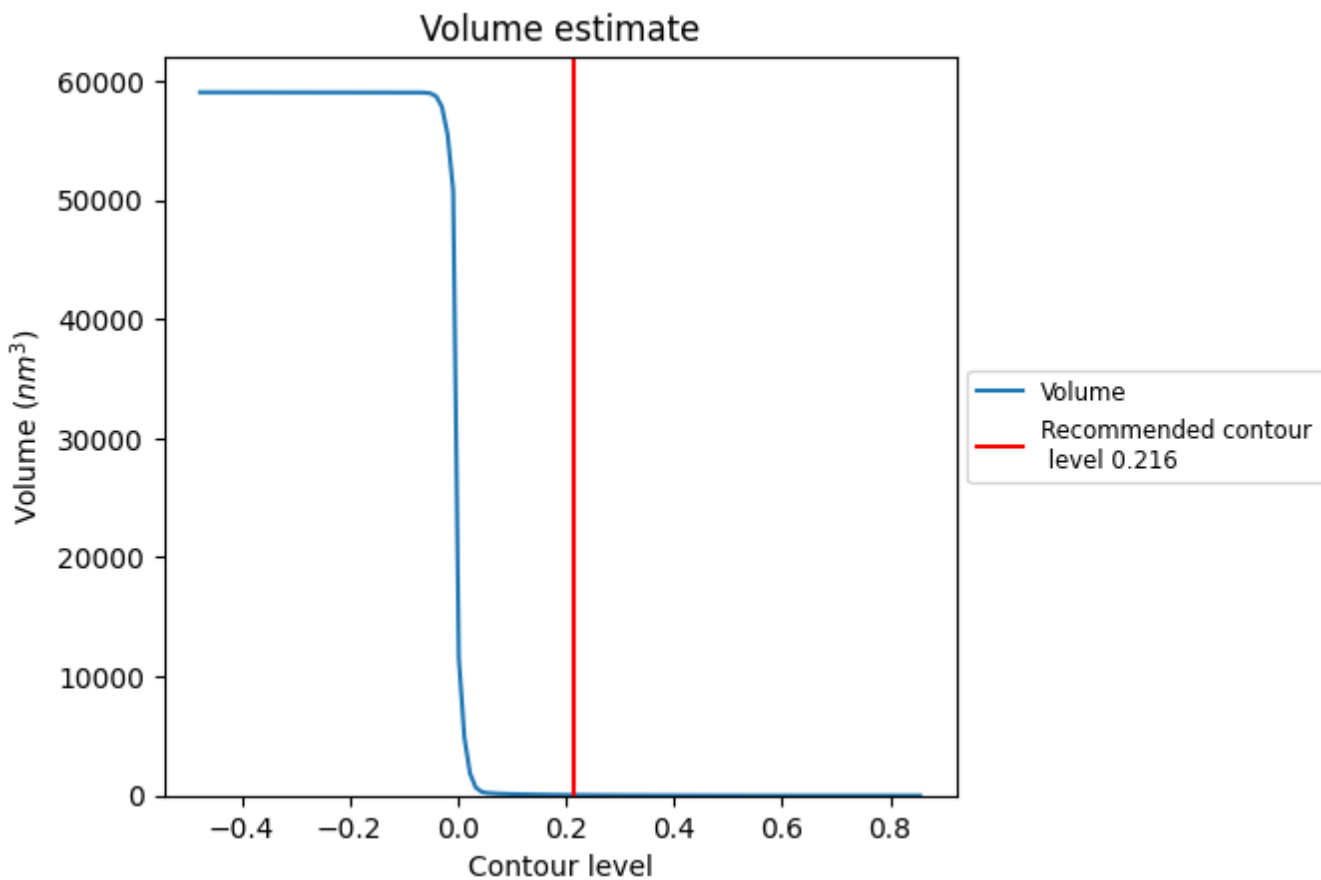
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

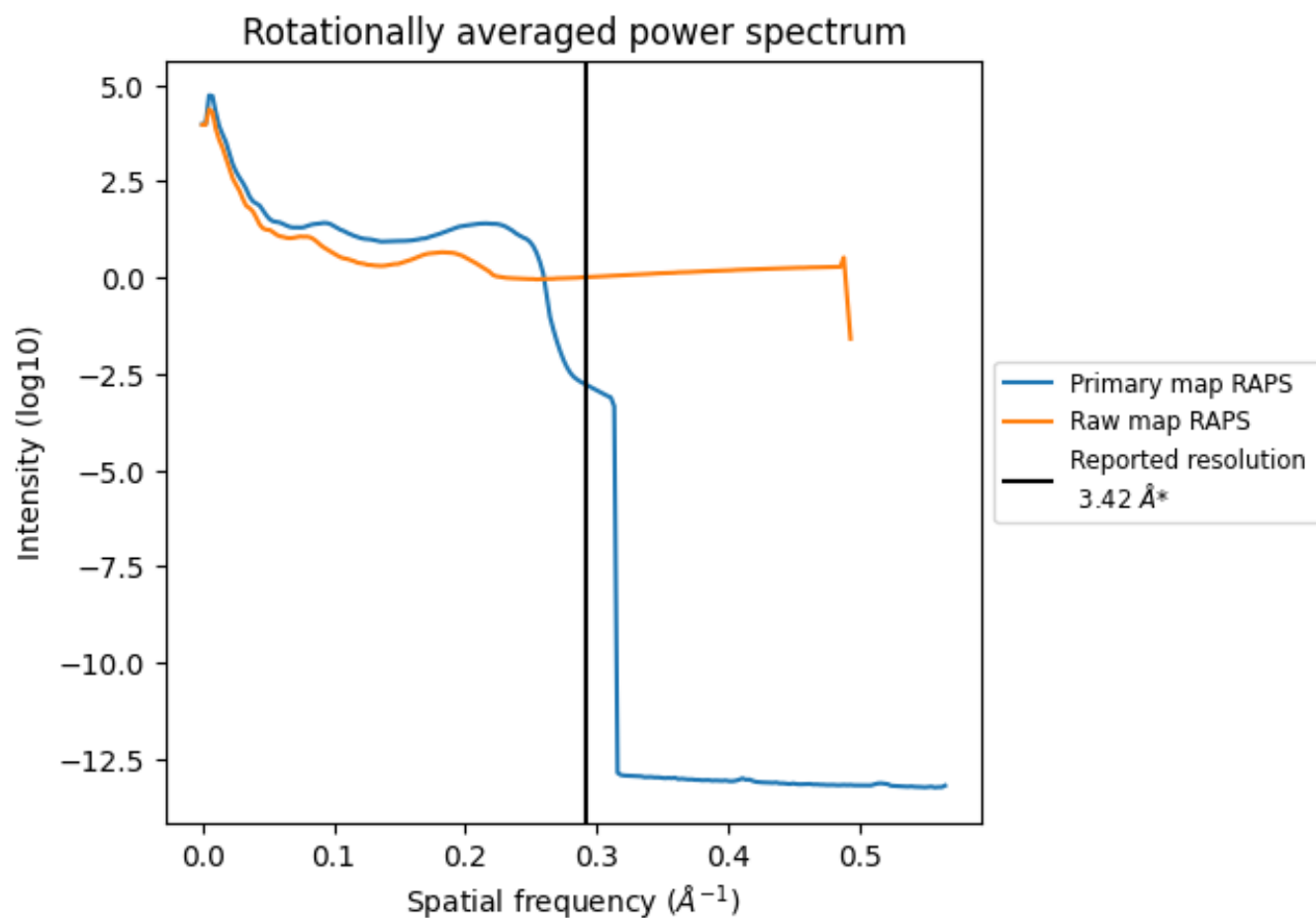
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 47 nm^3 ; this corresponds to an approximate mass of 42 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

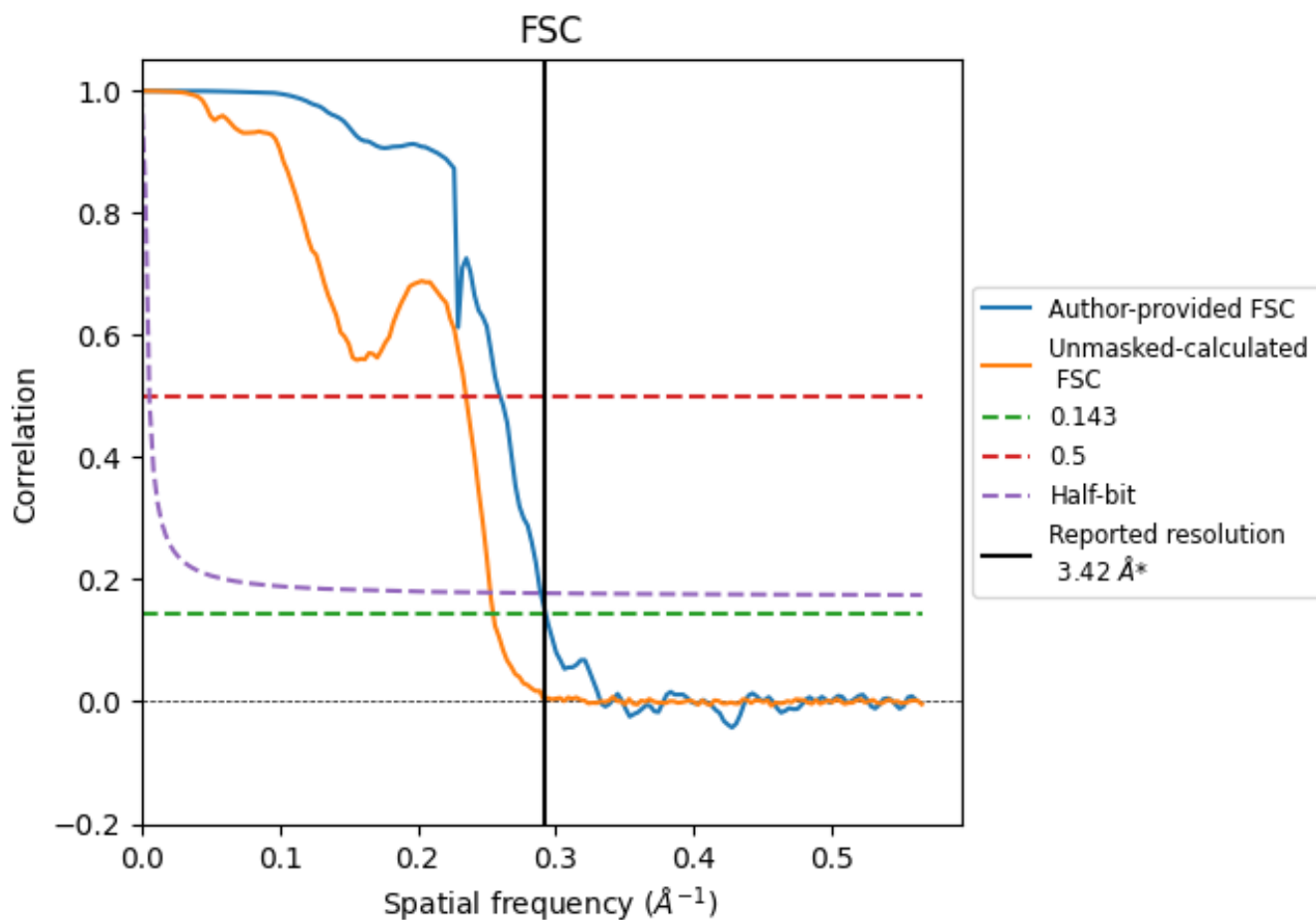


*Reported resolution corresponds to spatial frequency of 0.292 \AA^{-1}

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 0.292 Å⁻¹

8.2 Resolution estimates [i](#)

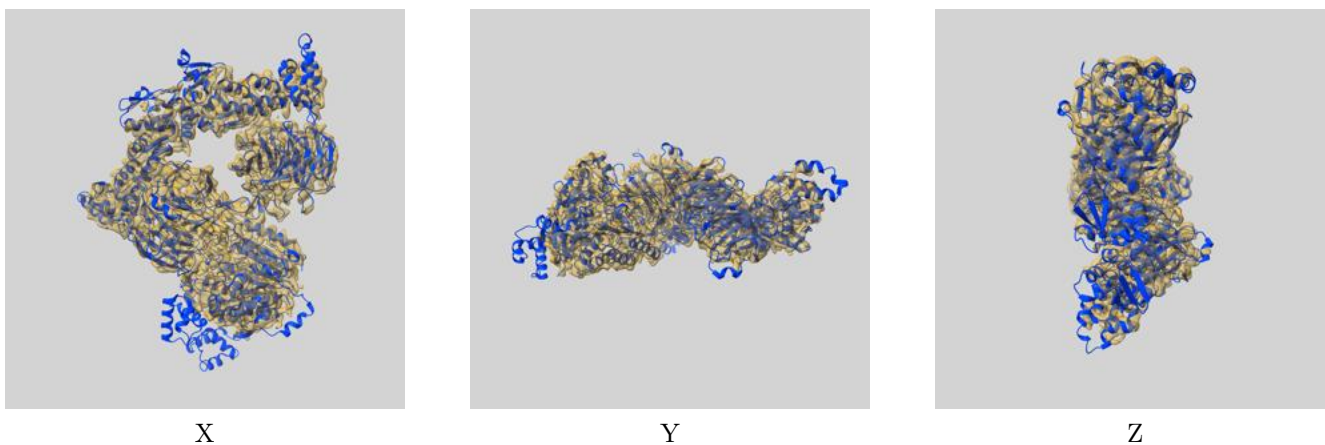
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.42	3.85	3.46
Unmasked-calculated*	3.92	4.25	3.96

*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 3.92 differs from the reported value 3.42 by more than 10 %

9 Map-model fit [i](#)

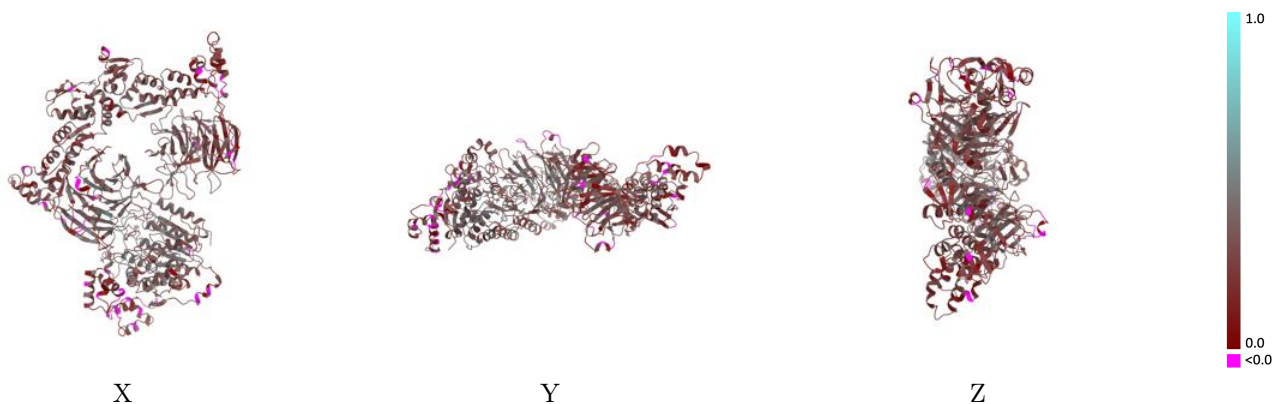
This section contains information regarding the fit between EMDB map EMD-43487 and PDB model 8VRT. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



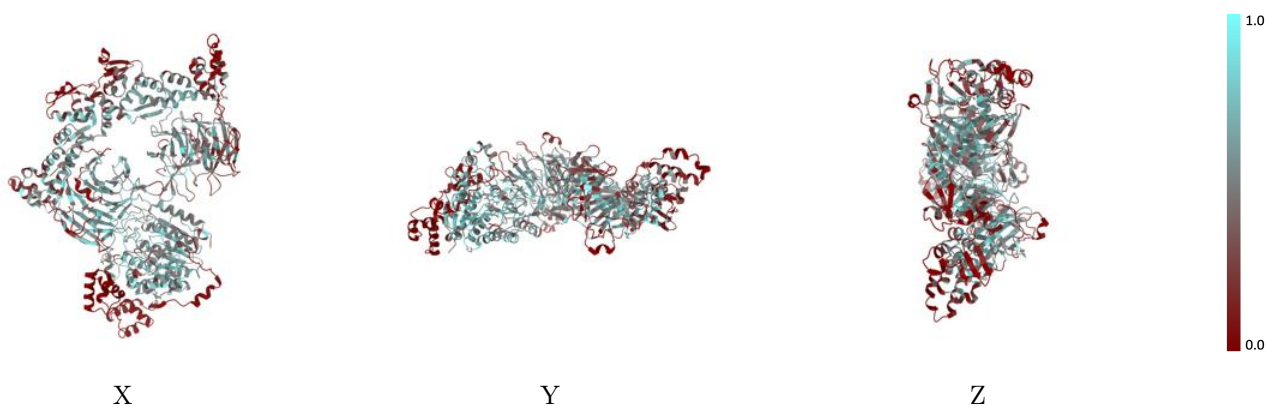
The images above show the 3D surface view of the map at the recommended contour level 0.216 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



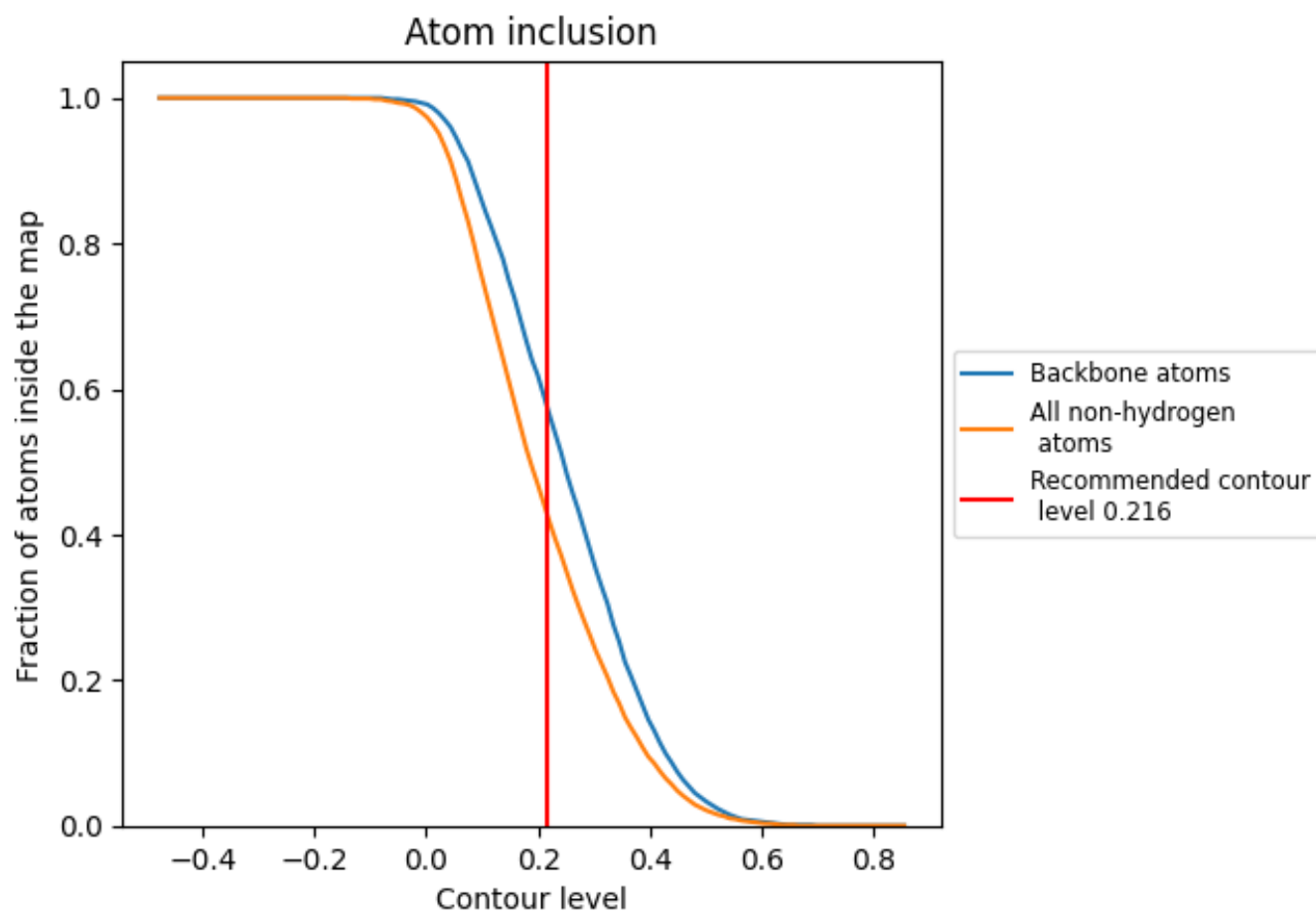
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.216).











9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 43% 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 (0.216) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4290	 0.2940
A	 0.3860	 0.2670
B	 0.4590	 0.3030
C	 0.6090	 0.3690
D	 0.0180	 0.1620

