



Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 06:45 AM EST

PDB ID : 7UZB
EMDB ID : EMD-26885
Title : Structure of the SARS-CoV-2 S S1 domain in complex with the mouse antibody Fab fragment, HSW-2
Authors : Fan, C.; Bjorkman, P.J.
Deposited on : 2022-05-08
Resolution : 4.10 Å(reported)
Based on initial model : 7SC1

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 : 2022.3.0, CSD as543be (2022)
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

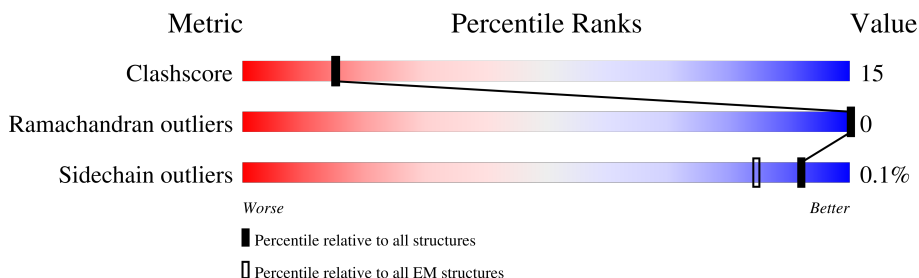
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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 $\leq 5\%$. 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	1256	
2	H	230	
3	L	214	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8392 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	643	Total	C	N	O	S	0	0
			5026	3224	835	946	21		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	814	PRO	PHE	engineered mutation	UNP P0DTC2
A	889	PRO	ALA	engineered mutation	UNP P0DTC2
A	896	PRO	ALA	engineered mutation	UNP P0DTC2
A	939	PRO	ALA	engineered mutation	UNP P0DTC2
A	983	PRO	LYS	engineered mutation	UNP P0DTC2
A	984	PRO	VAL	engineered mutation	UNP P0DTC2
A	1211	SER	-	expression tag	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	ARG	-	expression tag	UNP P0DTC2
A	1214	LEU	-	expression tag	UNP P0DTC2
A	1215	VAL	-	expression tag	UNP P0DTC2
A	1216	PRO	-	expression tag	UNP P0DTC2
A	1217	ARG	-	expression tag	UNP P0DTC2
A	1218	GLY	-	expression tag	UNP P0DTC2
A	1219	SER	-	expression tag	UNP P0DTC2
A	1220	PRO	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	TYR	-	expression tag	UNP P0DTC2
A	1225	ILE	-	expression tag	UNP P0DTC2
A	1226	PRO	-	expression tag	UNP P0DTC2
A	1227	GLU	-	expression tag	UNP P0DTC2
A	1228	ALA	-	expression tag	UNP P0DTC2
A	1229	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1230	ARG	-	expression tag	UNP P0DTC2
A	1231	ASP	-	expression tag	UNP P0DTC2
A	1232	GLY	-	expression tag	UNP P0DTC2
A	1233	GLN	-	expression tag	UNP P0DTC2
A	1234	ALA	-	expression tag	UNP P0DTC2
A	1235	TYR	-	expression tag	UNP P0DTC2
A	1236	VAL	-	expression tag	UNP P0DTC2
A	1237	ARG	-	expression tag	UNP P0DTC2
A	1238	LYS	-	expression tag	UNP P0DTC2
A	1239	ASP	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	TRP	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	LEU	-	expression tag	UNP P0DTC2
A	1246	SER	-	expression tag	UNP P0DTC2
A	1247	THR	-	expression tag	UNP P0DTC2
A	1248	PHE	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	GLY	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called HSW-2 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	220	Total	C	N	O	S	0	0
			1662	1052	276	329	5		

- Molecule 3 is a protein called HSW-2 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	214	Total	C	N	O	S	0	0
			1648	1034	278	330	6		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

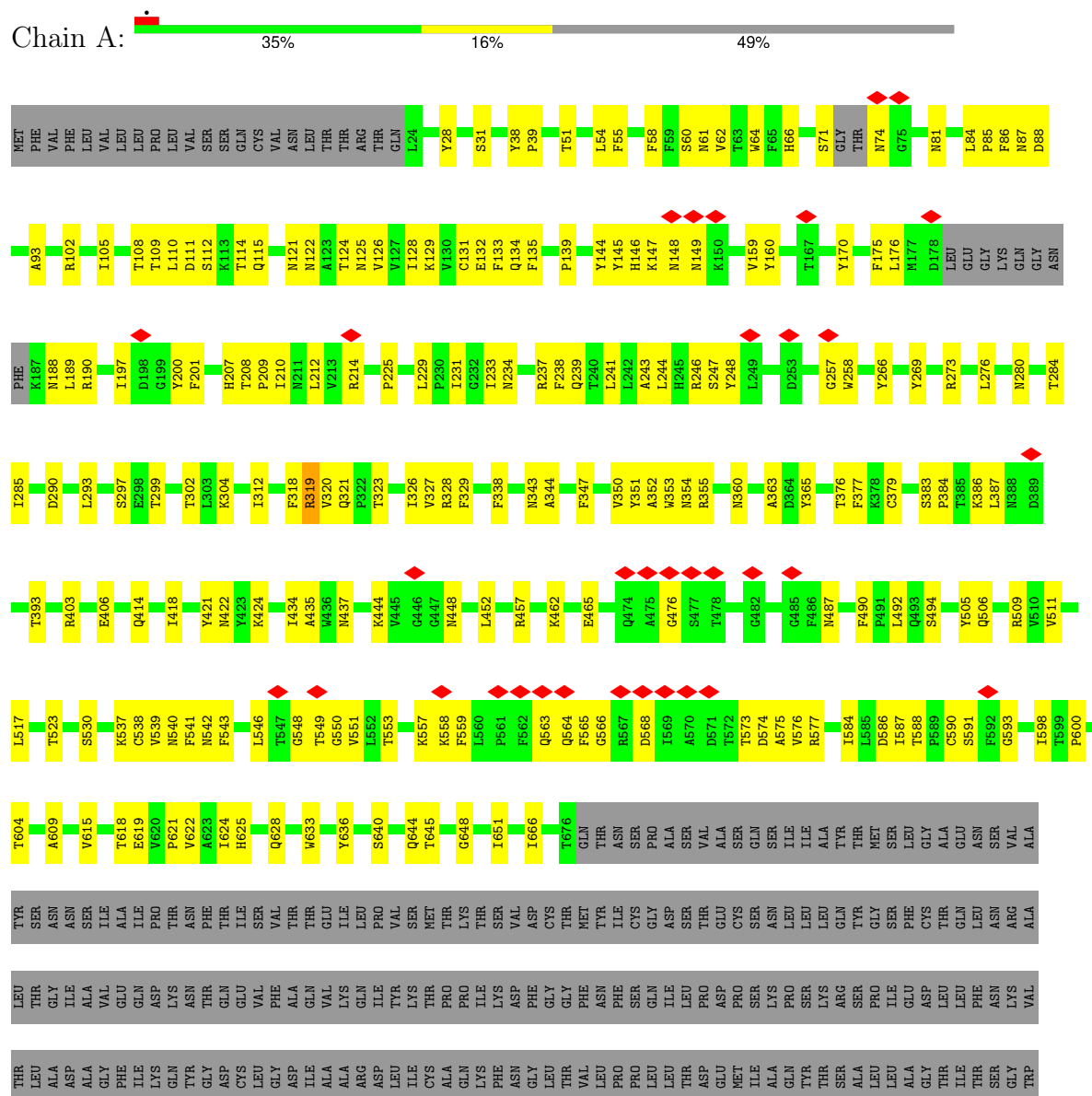


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

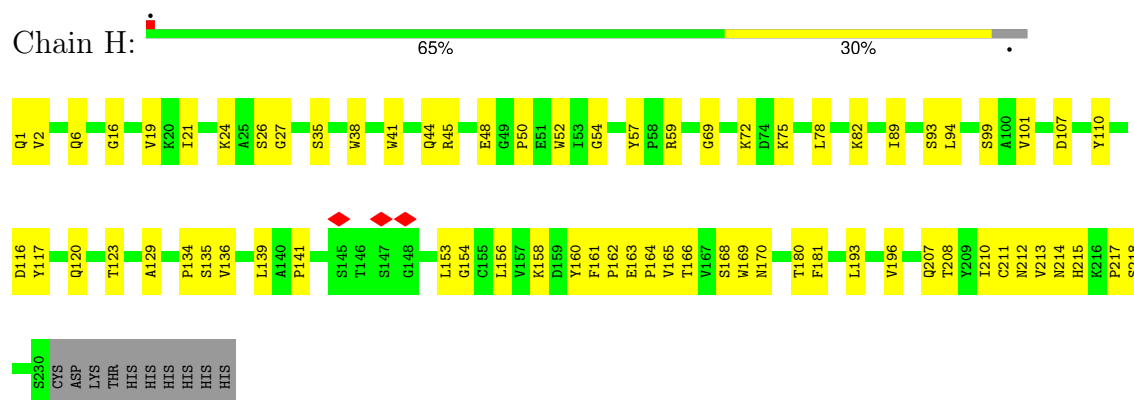
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

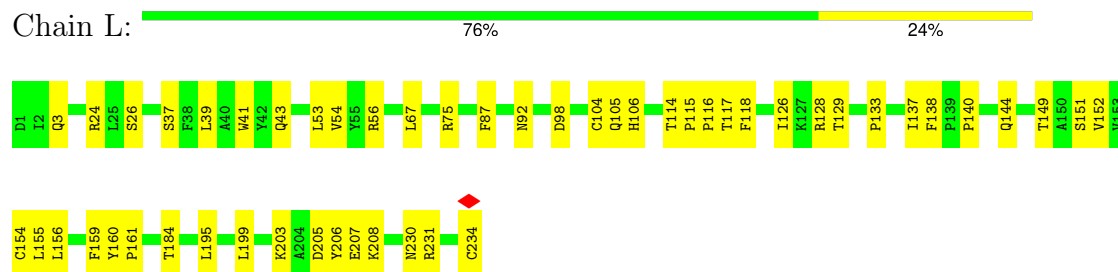


LEU	LEU	ASN	ASP	TYR	TYR	LYS	THR
LEU	LEU	VAL	VAL	VAL	VAL	LEU	PHE
SER	THR	GLY	VAL	PRO	GLN	GLN	GLY
PHE	LEU	ALA	ILE	ALA	GLN	ASP	ALA
LEU	LEU	ASN	ILE	GLU	LEU	VAL	GLY
GLY	LEU	LEU	VAL	LYS	ILE	ASN	PRO
HIS	HIS	ASN	ASN	ASN	ARG	GLN	ALA
HIS	HIS	GLU	ASN	PHE	ALA	ASN	ILE
HIS	HIS	SER	THR	THR	ALA	ALA	GLN
HIS	HIS	LEU	VAL	THR	GLU	GLN	PRO
HIS	HIS	ILE	TYR	ALA	ILE	ALA	PHE
		ASP	ASP	PRO	ARG	LEU	PRO
		PRO	PRO	ALA	ALA	ASN	GLN
		GLN	LEU	ILE	SER	THR	MET
		LEU	GLN	CYS	ALA	LEU	MET
		LEU	PRO	HIS	ASN	VAL	ALA
		GLY	GLU	ASP	LEU	LYS	TYR
		LYS	LEU	GLY	ALA	GLN	ARG
		TYR	ASP	LYS	ALA	LEU	PHE
		GLU	SER	ALA	THR	SER	ASN
		GLN	PHE	HIS	LYS	SER	GLY
		TYR	LYS	PHE	MET	ASN	ILE
		ILE	GLU	PRO	SER	PHE	GLY
		LYS	GLU	ARG	GLU	GLY	VAL
		TRP	LEU	GLY	CYS	THR	GLN
		SER	ASP	VAL	ILE	SER	GLN
		GLY	TYR	PHE	GLY	SER	ASN
		ARG	PHE	VAL	GLN	VAL	LEU
		LEU	LYS	SER	LYS	LEU	TYR
		VAL	ASN	ASN	ASN	GLU	GLY
		PRO	HIS	GLY	VAL	ASP	ASN
		ARG	THR	THR	ARG	ILE	GLN
		GLY	SER	HIS	ASP	LEU	LYS
		SER	PRO	TRP	PHE	SER	LEU
		PRO	ASP	PHE	CYS	ARG	ILE
		GLY	VAL	VAL	GLY	LEU	ALA
		SER	ASP	THR	LYS	ASP	ASN
		GLY	LEU	GLN	GLY	PRO	GLN
		TYR	GLY	ARG	TYR	PRO	PHE
		ILE	ASP	ASN	HIS	GLU	ASN
		PRO	ILE	PHE	LEU	ALA	SER
		GLU	SER	TYR	MET	GLU	ALA
		ALA	GLY	GLU	SER	VAL	ILE
		PRO	ILE	PRO	PHE	GLN	GLY
		ARG	ASN	GLN	PRO	ILE	LYS
		ASP	ALA	ILE	GLN	ASP	ILE
		GLY	SER	ILE	SER	ARG	GLN
		VAL	VAL	THR	ALA	LEU	GLN
		ALA	VAL	THR	PRO	ILE	ASP
		TYR	ASN	ASP	HIS	THR	SER
		VAL	ILE	ASN	GLY	GLY	SER
		ARG	GLN	THR	VAL	ARG	SER
		LYS	LYS	PHE	VAL	LEU	THR
		ASP	GLU	VAL	PHE	GLN	PRO
		GLY	ILE	SER	LEU	LEU	ALA
		GLU	ASP	GLY	HIS	LEU	SER
		TRP	ARG	ASN	VAL	THR	GLY
		VAL	ILE	CYS	THR	THR	ILE

- Molecule 2: HSW-2 Fab heavy chain



- Molecule 3: HSW-2 Fab light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	43362	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.375	Depositor
Minimum map value	-0.147	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	312.84, 312.84, 312.84	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.869, 0.869, 0.869	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: NAG

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	0.27	0/5161	0.48	0/7044
2	H	0.27	0/1708	0.46	0/2327
3	L	0.27	0/1685	0.48	0/2285
All	All	0.27	0/8554	0.48	0/11656

There are no bond length outliers.

There are no bond angle outliers.

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	A	5026	0	4769	153	0
2	H	1662	0	1616	54	0
3	L	1648	0	1601	38	0
4	A	56	0	52	1	0
All	All	8392	0	8038	239	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 (239) 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:H:168:SER:HB2	2:H:212:ASN:HB2	1.58	0.83
1:A:452:LEU:HD21	1:A:492:LEU:HB3	1.60	0.81
1:A:328:ARG:NH2	1:A:530:SER:O	2.15	0.79
1:A:273:ARG:HA	1:A:320:VAL:HG11	1.65	0.77
2:H:134:PRO:HB3	2:H:160:TYR:HE1	1.50	0.77
2:H:135:SER:HB2	2:H:158:LYS:HB3	1.69	0.75
1:A:393:THR:OG1	2:H:110:TYR:OH	2.04	0.75
1:A:319:ARG:NH2	1:A:590:CYS:SG	2.63	0.72
3:L:43:GLN:HB2	3:L:53:LEU:HD11	1.72	0.72
1:A:326:ILE:O	1:A:542:ASN:N	2.22	0.72
2:H:196:VAL:HG21	3:L:155:LEU:HD11	1.73	0.71
1:A:93:ALA:HB3	1:A:266:TYR:HB2	1.71	0.70
1:A:135:PHE:HA	1:A:160:TYR:HA	1.74	0.69
2:H:75:LYS:NZ	2:H:93:SER:O	2.27	0.68
1:A:244:LEU:HD22	1:A:248:TYR:HD2	1.58	0.67
1:A:144:TYR:HA	1:A:246:ARG:HB2	1.78	0.65
1:A:327:VAL:HG22	1:A:542:ASN:HB2	1.79	0.65
1:A:109:THR:OG1	1:A:111:ASP:OD1	2.14	0.64
3:L:128:ARG:NH2	3:L:129:THR:OG1	2.31	0.63
1:A:121:ASN:ND2	1:A:176:LEU:HB3	2.14	0.63
2:H:45:ARG:NH1	2:H:99:SER:O	2.32	0.62
2:H:16:GLY:N	2:H:94:LEU:O	2.30	0.61
2:H:139:LEU:HD21	2:H:156:LEU:HB2	1.82	0.61
1:A:110:LEU:HD23	1:A:237:ARG:HH11	1.65	0.60
1:A:188:ASN:HA	1:A:209:PRO:HA	1.83	0.60
1:A:403:ARG:HD2	1:A:505:TYR:HA	1.82	0.60
1:A:577:ARG:HG3	1:A:584:ILE:HG13	1.82	0.60
1:A:559:PHE:HE2	1:A:575:ALA:HB3	1.65	0.60
1:A:621:PRO:O	1:A:625:HIS:ND1	2.35	0.59
2:H:161:PHE:HB3	2:H:162:PRO:HD3	1.84	0.59
1:A:86:PHE:H	1:A:237:ARG:HA	1.66	0.59
1:A:54:LEU:HD13	1:A:88:ASP:HB3	1.83	0.59
3:L:205:ASP:HA	3:L:208:LYS:HD2	1.86	0.58
3:L:137:ILE:HD12	3:L:154:CYS:HB3	1.86	0.58
1:A:353:TRP:HZ3	1:A:355:ARG:HB2	1.68	0.58
1:A:31:SER:OG	1:A:60:SER:N	2.37	0.58
1:A:210:ILE:HG13	1:A:212:LEU:H	1.69	0.57
1:A:276:LEU:HD11	1:A:304:LYS:HA	1.86	0.57
2:H:35:SER:HB2	2:H:59:ARG:HB3	1.85	0.57
1:A:539:VAL:HG22	1:A:540:ASN:H	1.70	0.57
1:A:318:PHE:CE1	1:A:591:SER:HB2	2.40	0.57
1:A:328:ARG:HG3	1:A:543:PHE:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:69:GLY:HA2	2:H:72:LYS:HE2	1.86	0.56
2:H:170:ASN:OD1	2:H:210:ILE:N	2.34	0.56
1:A:452:LEU:HA	1:A:494:SER:HA	1.87	0.56
1:A:112:SER:HB3	1:A:134:GLN:HB2	1.88	0.56
1:A:280:ASN:OD1	1:A:284:THR:N	2.38	0.55
1:A:201:PHE:HB3	1:A:229:LEU:HB2	1.88	0.55
2:H:162:PRO:HD2	2:H:215:HIS:CE1	2.41	0.55
1:A:39:PRO:HG3	1:A:51:THR:HG21	1.88	0.55
2:H:141:PRO:HG3	2:H:153:LEU:HB3	1.88	0.55
1:A:108:THR:OG1	1:A:234:ASN:O	2.25	0.55
1:A:145:TYR:HE2	1:A:147:LYS:HD3	1.71	0.55
1:A:319:ARG:NH2	1:A:538:CYS:HB3	2.21	0.55
2:H:6:GLN:H	2:H:120:GLN:NE2	2.05	0.55
1:A:622:VAL:HA	1:A:625:HIS:HD1	1.72	0.55
1:A:574:ASP:O	1:A:587:ILE:N	2.35	0.55
1:A:344:ALA:HB3	1:A:347:PHE:HE1	1.71	0.54
1:A:365:TYR:CD2	1:A:387:LEU:HB3	2.42	0.54
2:H:6:GLN:H	2:H:120:GLN:HE22	1.56	0.54
1:A:290:ASP:HB3	1:A:293:LEU:HB2	1.90	0.54
1:A:568:ASP:H	1:A:573:THR:HG22	1.71	0.54
3:L:105:GLN:NE2	3:L:106:HIS:O	2.39	0.54
1:A:365:TYR:HD2	1:A:387:LEU:HB3	1.73	0.54
1:A:645:THR:OG1	1:A:648:GLY:O	2.15	0.54
1:A:189:LEU:N	1:A:208:THR:O	2.38	0.53
1:A:598:ILE:HB	1:A:609:ALA:HB3	1.89	0.53
1:A:273:ARG:HD3	1:A:320:VAL:HG11	1.88	0.53
1:A:444:LYS:HE2	1:A:448:ASN:HA	1.90	0.53
1:A:71:SER:O	1:A:74:ASN:N	2.42	0.53
3:L:140:PRO:HD3	3:L:152:VAL:HG22	1.91	0.53
1:A:621:PRO:HA	1:A:624:ILE:HB	1.91	0.53
3:L:128:ARG:NE	3:L:129:THR:O	2.41	0.53
2:H:1:GLN:NE2	2:H:2:VAL:HG23	2.24	0.53
1:A:190:ARG:HH21	1:A:207:HIS:CE1	2.26	0.52
3:L:144:GLN:HG2	3:L:149:THR:O	2.09	0.52
1:A:644:GLN:NE2	1:A:645:THR:O	2.43	0.52
1:A:84:LEU:O	1:A:238:PHE:N	2.37	0.52
1:A:109:THR:OG1	1:A:114:THR:OG1	2.22	0.52
2:H:136:VAL:HG21	2:H:213:VAL:HG11	1.91	0.52
1:A:437:ASN:ND2	1:A:506:GLN:OE1	2.38	0.52
1:A:126:VAL:HG21	1:A:175:PHE:HE1	1.75	0.51
1:A:551:VAL:HG12	1:A:588:THR:HB	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:PHE:CE1	1:A:587:ILE:HG12	2.45	0.51
1:A:360:ASN:H	1:A:523:THR:HB	1.75	0.51
1:A:55:PHE:HB2	1:A:273:ARG:HB2	1.93	0.51
3:L:75:ARG:NH1	3:L:98:ASP:OD2	2.44	0.51
1:A:565:PHE:HB2	1:A:576:VAL:HG13	1.92	0.51
1:A:625:HIS:O	1:A:628:GLN:HG2	2.12	0.50
1:A:403:ARG:HG2	1:A:406:GLU:CD	2.31	0.50
1:A:115:GLN:HA	1:A:132:GLU:HG2	1.92	0.50
2:H:134:PRO:HB3	2:H:160:TYR:CE1	2.38	0.50
1:A:231:ILE:HG12	1:A:233:ILE:HG12	1.94	0.50
1:A:517:LEU:HD23	3:L:56:ARG:HD2	1.92	0.50
1:A:28:TYR:HD2	1:A:61:ASN:HB3	1.77	0.49
1:A:247:SER:OG	1:A:258:TRP:HB3	2.12	0.49
2:H:52:TRP:CD2	3:L:116:PRO:HD2	2.47	0.49
1:A:591:SER:OG	1:A:593:GLY:O	2.28	0.49
3:L:152:VAL:O	3:L:199:LEU:N	2.39	0.49
2:H:101:VAL:HG22	2:H:123:THR:HG22	1.95	0.49
1:A:326:ILE:HB	1:A:541:PHE:HA	1.93	0.49
2:H:162:PRO:HD2	2:H:215:HIS:HE1	1.78	0.49
1:A:323:THR:HG21	1:A:537:LYS:HG3	1.95	0.49
1:A:347:PHE:CE2	1:A:509:ARG:HD3	2.47	0.49
3:L:160:TYR:CG	3:L:161:PRO:HA	2.47	0.49
1:A:146:HIS:CD2	1:A:149:ASN:H	2.31	0.49
1:A:146:HIS:HD2	1:A:149:ASN:H	1.60	0.49
1:A:376:THR:HB	1:A:435:ALA:HB3	1.95	0.49
1:A:58:PHE:HB2	1:A:293:LEU:HD13	1.95	0.48
2:H:59:ARG:HA	2:H:82:LYS:HD2	1.94	0.48
3:L:39:LEU:HD13	3:L:87:PHE:CD2	2.47	0.48
1:A:565:PHE:HA	1:A:577:ARG:HB3	1.94	0.48
2:H:207:GLN:NE2	2:H:208:THR:O	2.46	0.48
1:A:541:PHE:CD1	1:A:587:ILE:HG12	2.49	0.48
1:A:577:ARG:HA	1:A:584:ILE:HA	1.95	0.48
1:A:598:ILE:HD13	1:A:666:ILE:HG12	1.96	0.48
2:H:215:HIS:CD2	2:H:217:PRO:HD2	2.49	0.48
1:A:354:ASN:OD1	1:A:355:ARG:N	2.47	0.48
2:H:41:TRP:CE2	2:H:89:ILE:HB	2.48	0.47
1:A:139:PRO:HA	1:A:159:VAL:HA	1.96	0.47
1:A:550:GLY:HA3	1:A:587:ILE:HG13	1.96	0.47
1:A:575:ALA:HA	1:A:586:ASP:HA	1.97	0.47
2:H:57:TYR:CE2	2:H:59:ARG:HG2	2.50	0.47
3:L:37:SER:OG	3:L:56:ARG:NH2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:NZ	1:A:246:ARG:HH22	2.12	0.47
3:L:24:ARG:HG3	3:L:24:ARG:HH11	1.80	0.46
1:A:462:LYS:N	1:A:465:GLU:OE1	2.39	0.46
3:L:106:HIS:HE2	3:L:117:THR:HG23	1.81	0.46
1:A:105:ILE:HD11	1:A:241:LEU:HD12	1.97	0.46
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.96	0.46
1:A:563:GLN:O	1:A:577:ARG:HD3	2.15	0.46
2:H:129:ALA:HB3	2:H:161:PHE:CE1	2.51	0.46
1:A:62:VAL:HG11	1:A:266:TYR:HB3	1.98	0.46
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.51	0.46
1:A:110:LEU:HD23	1:A:237:ARG:NH1	2.30	0.46
3:L:206:TYR:O	3:L:231:ARG:NE	2.49	0.46
1:A:319:ARG:HH21	1:A:538:CYS:HB3	1.80	0.45
2:H:19:VAL:HG12	2:H:94:LEU:HD21	1.98	0.45
1:A:84:LEU:HB3	1:A:269:TYR:OH	2.17	0.45
2:H:165:VAL:HG21	2:H:193:LEU:HD13	1.99	0.45
1:A:414:GLN:O	1:A:424:LYS:NZ	2.40	0.45
3:L:3:GLN:HB2	3:L:26:SER:OG	2.16	0.45
3:L:126:ILE:O	3:L:126:ILE:HG13	2.16	0.45
1:A:122:ASN:OD1	1:A:124:THR:OG1	2.19	0.45
1:A:418:ILE:HD12	1:A:418:ILE:H	1.82	0.45
3:L:39:LEU:HA	3:L:106:HIS:HA	1.98	0.45
1:A:85:PRO:HB2	1:A:87:ASN:OD1	2.17	0.45
1:A:338:PHE:CE2	1:A:363:ALA:HB1	2.52	0.45
1:A:201:PHE:HB2	1:A:231:ILE:HG22	1.99	0.45
1:A:319:ARG:NH1	1:A:321:GLN:OE1	2.50	0.45
1:A:328:ARG:HE	1:A:530:SER:HB3	1.83	0.44
1:A:551:VAL:O	1:A:587:ILE:HA	2.17	0.44
1:A:600:PRO:HB2	1:A:604:THR:HB	1.99	0.44
1:A:146:HIS:NE2	1:A:148:ASN:HB2	2.33	0.44
1:A:377:PHE:CD1	1:A:434:ILE:HG12	2.51	0.44
2:H:181:PHE:CD1	3:L:184:THR:HG23	2.53	0.44
1:A:353:TRP:CZ3	1:A:355:ARG:HB2	2.51	0.44
1:A:640:SER:HA	1:A:651:ILE:HD13	2.00	0.44
3:L:105:GLN:HG3	3:L:118:PHE:CD2	2.53	0.44
1:A:38:TYR:CZ	1:A:285:ILE:HG13	2.53	0.44
3:L:207:GLU:O	3:L:231:ARG:NH2	2.51	0.44
2:H:154:GLY:HA3	2:H:196:VAL:HG12	1.99	0.44
1:A:64:TRP:CZ3	1:A:66:HIS:HB2	2.52	0.44
1:A:553:THR:O	1:A:586:ASP:N	2.50	0.44
2:H:169:TRP:CZ3	2:H:211:CYS:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:PHE:HB2	1:A:546:LEU:HD12	2.00	0.44
3:L:114:THR:HA	3:L:115:PRO:HA	1.75	0.44
3:L:230:ASN:HB3	3:L:234:CYS:HB2	1.98	0.44
1:A:319:ARG:HH12	1:A:321:GLN:CD	2.21	0.43
2:H:139:LEU:HB3	3:L:138:PHE:CD2	2.53	0.43
3:L:160:TYR:CD1	3:L:161:PRO:HA	2.53	0.43
1:A:214:ARG:O	1:A:214:ARG:HG2	2.18	0.43
3:L:114:THR:HA	3:L:116:PRO:HD3	2.00	0.43
1:A:551:VAL:O	1:A:587:ILE:HD12	2.18	0.43
1:A:557:LYS:HE3	1:A:557:LYS:HB2	1.82	0.43
3:L:140:PRO:HB3	3:L:151:SER:O	2.17	0.43
2:H:38:TRP:HB2	2:H:107:ASP:HB3	2.00	0.43
1:A:379:CYS:SG	1:A:384:PRO:HG3	2.59	0.43
2:H:82:LYS:HE2	2:H:82:LYS:HB3	1.82	0.43
2:H:165:VAL:HG11	2:H:193:LEU:HD13	1.99	0.43
3:L:75:ARG:O	3:L:92:ASN:ND2	2.52	0.43
2:H:52:TRP:CH2	2:H:54:GLY:HA2	2.54	0.43
1:A:122:ASN:ND2	1:A:125:ASN:O	2.52	0.42
2:H:44:GLN:HA	2:H:50:PRO:HA	2.00	0.42
1:A:566:GLY:H	1:A:577:ARG:H	1.66	0.42
1:A:633:TRP:HA	1:A:636:TYR:HB2	2.02	0.42
2:H:24:LYS:NZ	2:H:26:SER:HB3	2.34	0.42
1:A:238:PHE:CD1	1:A:239:GLN:N	2.87	0.42
2:H:38:TRP:CD1	2:H:57:TYR:HB2	2.53	0.42
1:A:247:SER:HB3	1:A:257:GLY:H	1.85	0.42
3:L:41:TRP:CZ3	3:L:104:CYS:HB3	2.54	0.42
1:A:541:PHE:CZ	1:A:548:GLY:HA3	2.55	0.42
3:L:54:VAL:HG22	3:L:67:LEU:HD12	2.02	0.42
1:A:434:ILE:HB	1:A:511:VAL:HG13	2.01	0.42
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.54	0.42
3:L:156:LEU:HB2	3:L:195:LEU:HB3	2.02	0.42
1:A:86:PHE:N	1:A:237:ARG:HA	2.34	0.42
1:A:273:ARG:HA	1:A:273:ARG:HD3	1.91	0.42
1:A:38:TYR:HB2	1:A:225:PRO:HD3	2.02	0.42
1:A:128:ILE:HD13	1:A:170:TYR:HD2	1.85	0.42
1:A:343:ASN:HD22	4:A:1302:NAG:H62	1.83	0.42
1:A:564:GLN:HG3	1:A:565:PHE:HD1	1.85	0.42
2:H:1:GLN:O	2:H:27:GLY:HA3	2.19	0.42
1:A:81:ASN:OD1	1:A:81:ASN:N	2.52	0.41
2:H:44:GLN:HB2	2:H:50:PRO:HB3	2.02	0.41
2:H:180:THR:HG23	2:H:193:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:CYS:HB2	1:A:133:PHE:CZ	2.55	0.41
1:A:304:LYS:HA	1:A:304:LYS:HD3	1.94	0.41
1:A:618:THR:O	1:A:621:PRO:HD2	2.20	0.41
1:A:197:ILE:O	1:A:200:TYR:N	2.45	0.41
1:A:383:SER:HB3	1:A:386:LYS:HE2	2.02	0.41
2:H:2:VAL:HB	2:H:117:TYR:CE2	2.54	0.41
2:H:45:ARG:HB2	2:H:48:GLU:HB3	2.02	0.41
1:A:540:ASN:HA	1:A:549:THR:HA	2.03	0.41
1:A:328:ARG:HA	1:A:328:ARG:NE	2.36	0.41
3:L:133:PRO:HB3	3:L:159:PHE:HB3	2.02	0.41
1:A:121:ASN:HD22	1:A:176:LEU:HB3	1.85	0.41
1:A:290:ASP:O	1:A:297:SER:HB3	2.20	0.41
2:H:116:ASP:OD1	2:H:117:TYR:N	2.54	0.41
3:L:203:LYS:O	3:L:207:GLU:HG2	2.21	0.41
1:A:540:ASN:OD1	1:A:549:THR:HG22	2.20	0.41
2:H:78:LEU:HG	2:H:89:ILE:HD13	2.02	0.41
2:H:163:GLU:N	2:H:164:PRO:HD2	2.35	0.41
1:A:126:VAL:HG21	1:A:175:PHE:CE1	2.55	0.41
1:A:312:ILE:HD12	1:A:598:ILE:HD11	2.03	0.41
1:A:476:GLY:HA3	1:A:487:ASN:HB3	2.02	0.41
2:H:21:ILE:HB	2:H:89:ILE:HG22	2.02	0.41
2:H:166:THR:HB	2:H:214:ASN:HB3	2.03	0.41
1:A:129:LYS:HG2	1:A:131:CYS:SG	2.60	0.40
1:A:102:ARG:HG3	1:A:243:ALA:HB2	2.03	0.40
2:H:215:HIS:HB3	2:H:218:SER:OG	2.21	0.40
1:A:299:THR:HA	1:A:302:THR:HG22	2.02	0.40
1:A:329:PHE:O	1:A:530:SER:OG	2.39	0.40
1:A:558:LYS:HD3	1:A:584:ILE:HD13	2.04	0.40
1:A:351:TYR:CG	1:A:352:ALA:N	2.89	0.40
3:L:206:TYR:CD1	3:L:231:ARG:HD3	2.55	0.40
1:A:344:ALA:HB3	1:A:347:PHE:CE1	2.55	0.40
1:A:615:VAL:HG13	1:A:619:GLU:HB2	2.04	0.40
2:H:160:TYR:CD2	2:H:165:VAL:HG22	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	637/1256 (51%)	608 (95%)	29 (5%)	0	100	100
2	H	218/230 (95%)	213 (98%)	5 (2%)	0	100	100
3	L	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
All	All	1067/1700 (63%)	1029 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	547/1096 (50%)	546 (100%)	1 (0%)	92	94
2	H	188/198 (95%)	188 (100%)	0	100	100
3	L	186/186 (100%)	186 (100%)	0	100	100
All	All	921/1480 (62%)	920 (100%)	1 (0%)	92	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	HIS
2	H	215	HIS

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](#)

4 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	$\# Z > 2$
4	NAG	A	1302	1	14,14,15	0.41	0	17,19,21	1.26	1 (5%)
4	NAG	A	1304	1	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	A	1301	1	14,14,15	0.19	0	17,19,21	0.43	0
4	NAG	A	1303	1	14,14,15	0.25	0	17,19,21	0.54	0

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
4	NAG	A	1302	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1302	NAG	C1-O5-C5	4.79	118.61	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

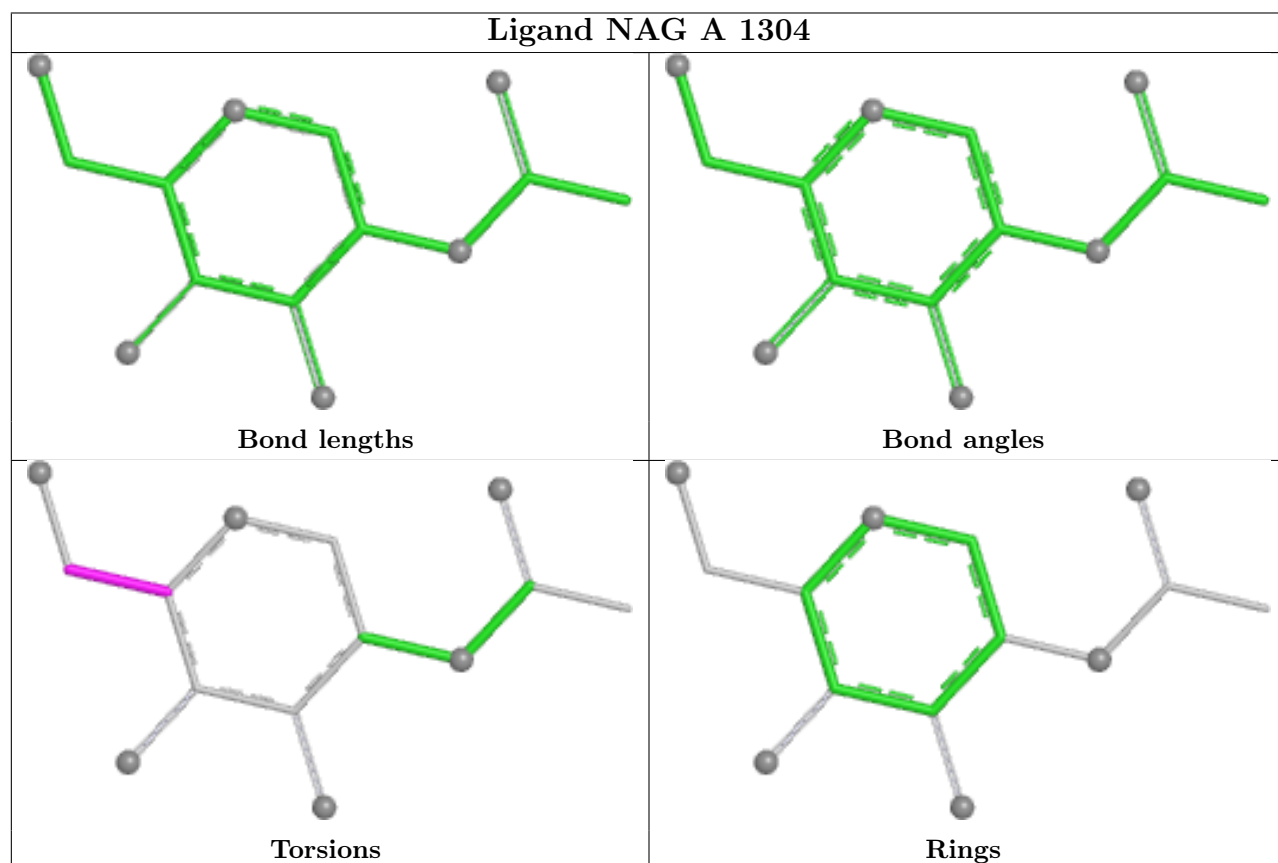
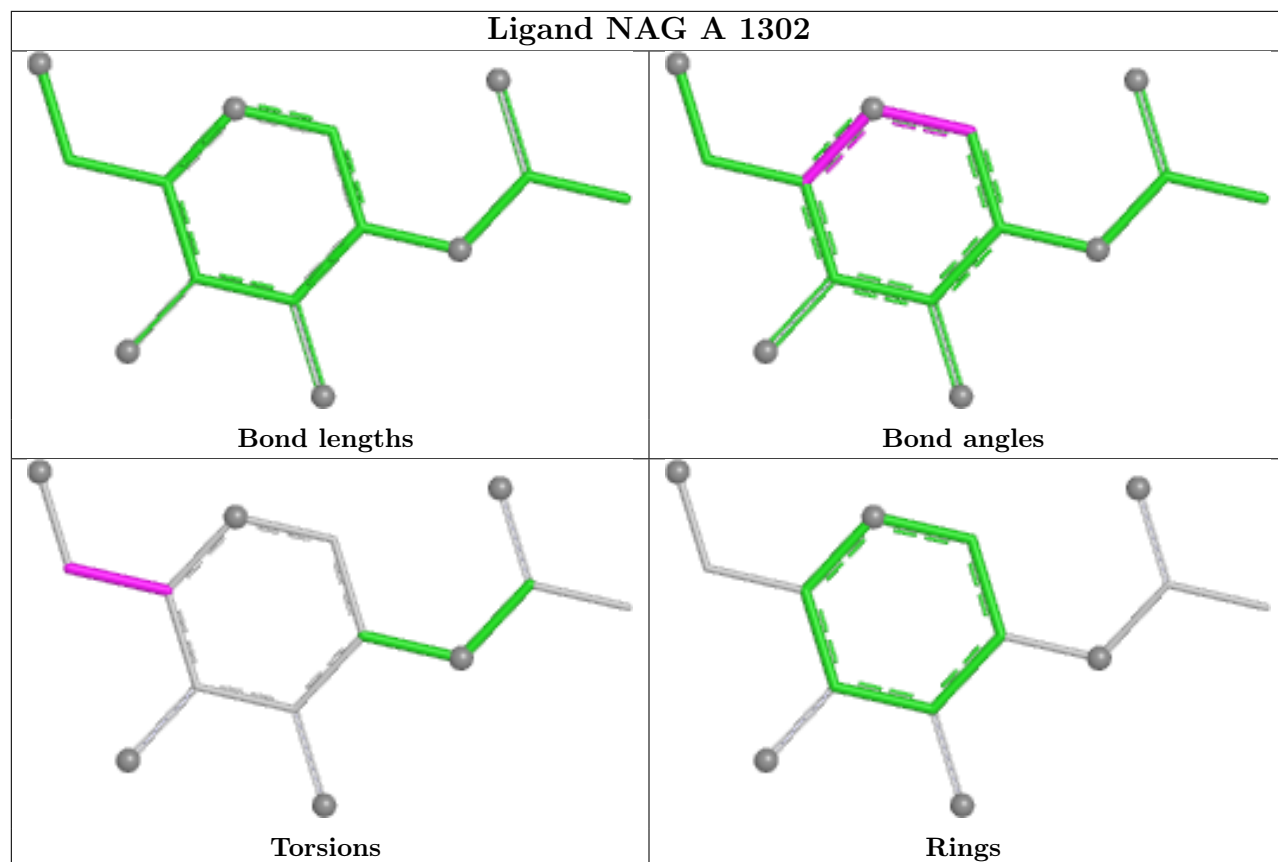
Mol	Chain	Res	Type	Atoms
4	A	1304	NAG	C4-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	A	1301	NAG	C4-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	A	1303	NAG	C1-C2-N2-C7
4	A	1303	NAG	C3-C2-N2-C7

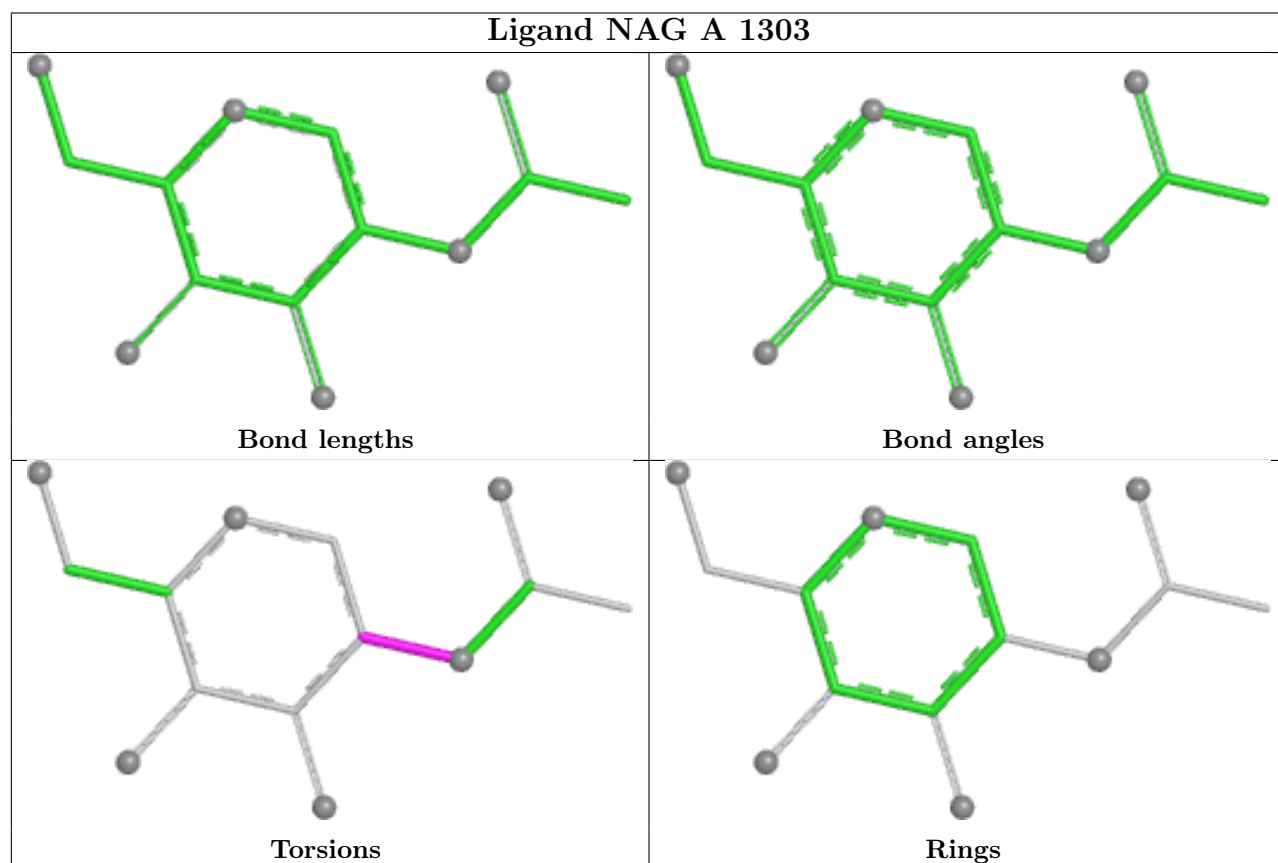
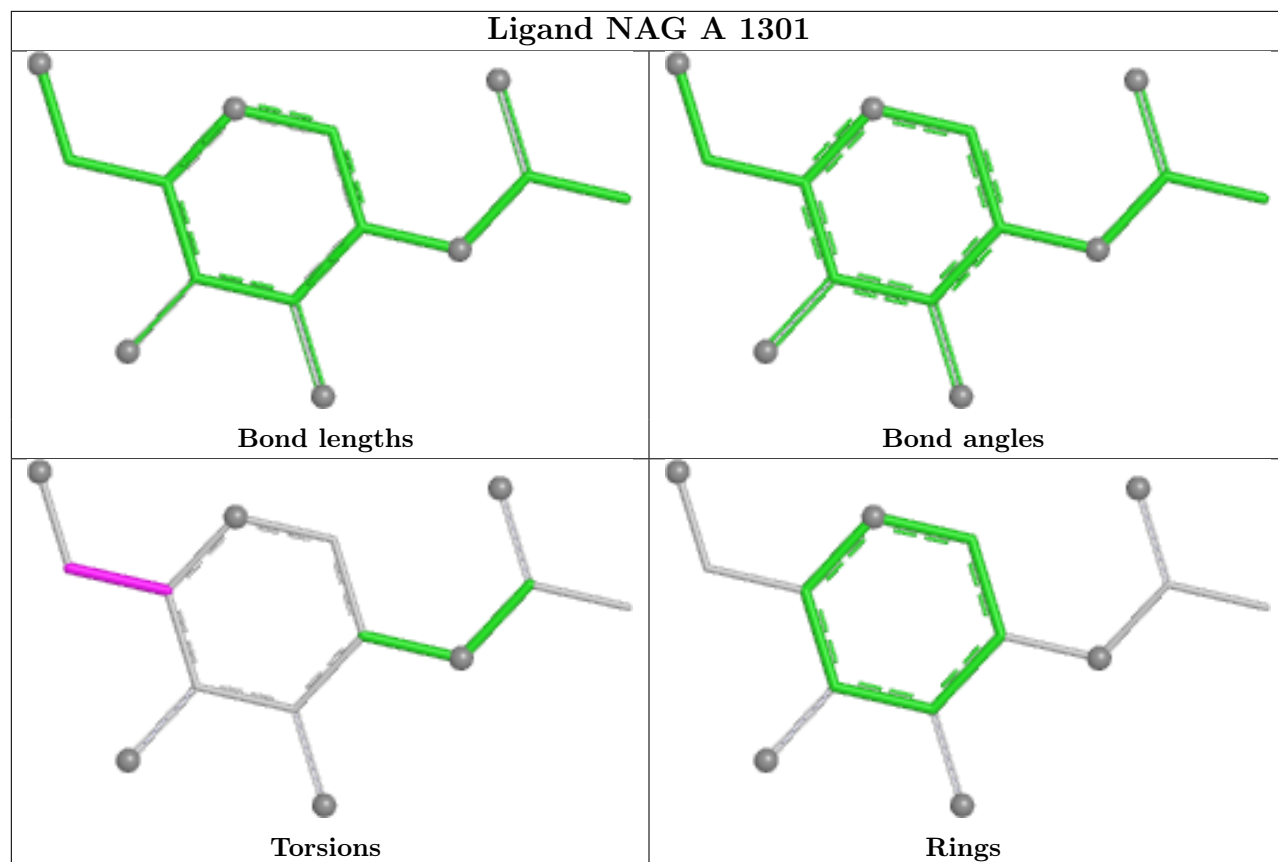
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1302	NAG	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 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.

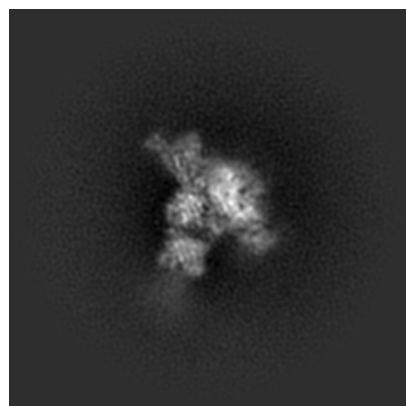
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26885. These allow visual inspection of the internal detail of the map and identification of artifacts.

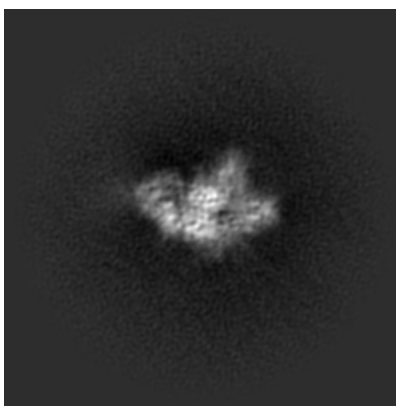
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

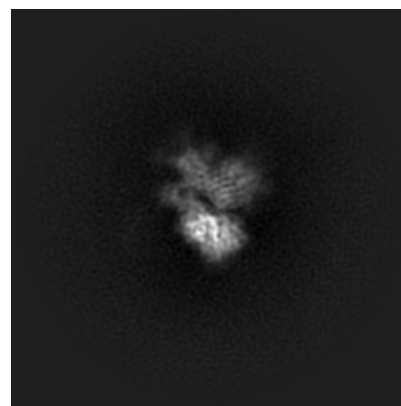
6.1.1 Primary map



X

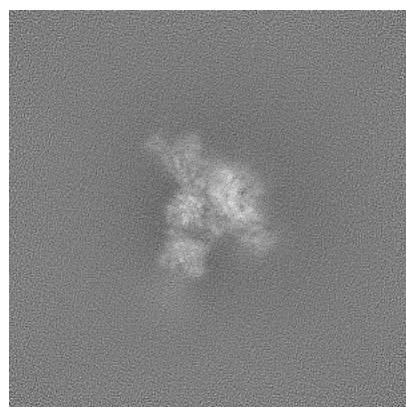


Y

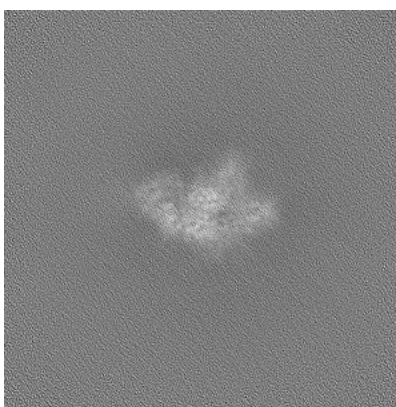


Z

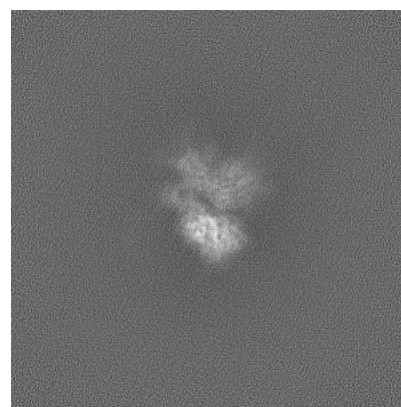
6.1.2 Raw map



X



Y

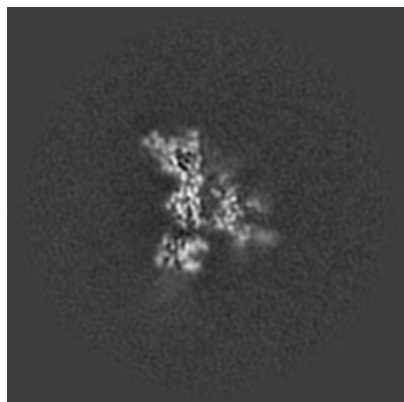


Z

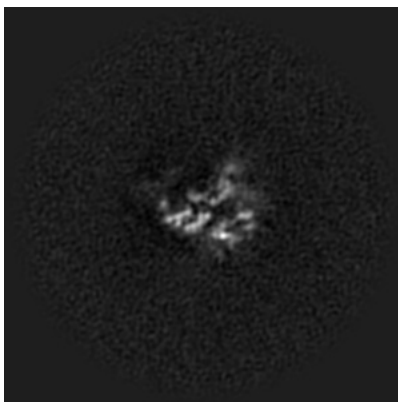
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

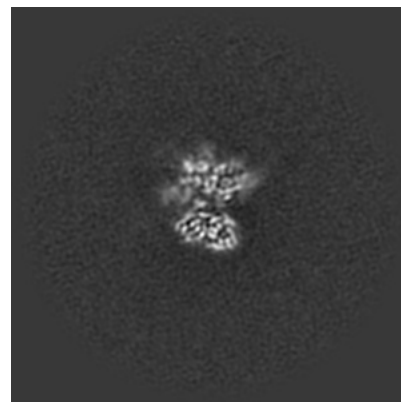
6.2.1 Primary map



X Index: 180

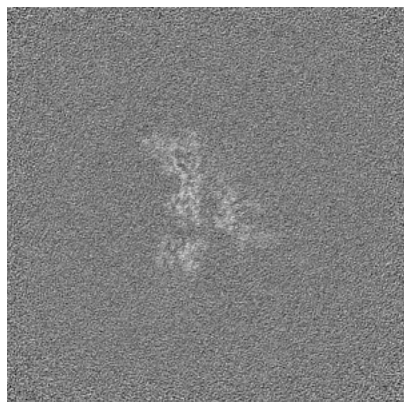


Y Index: 180

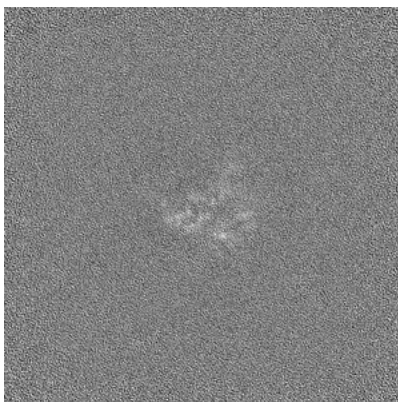


Z Index: 180

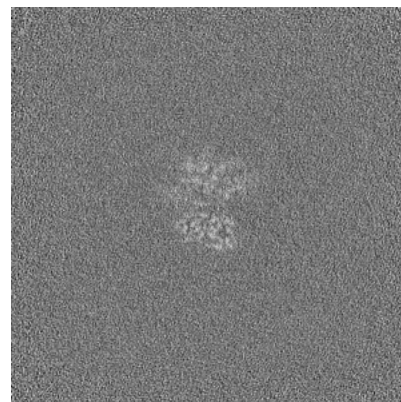
6.2.2 Raw map



X Index: 180



Y Index: 180

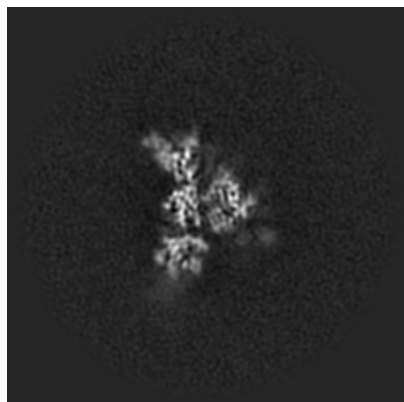


Z Index: 180

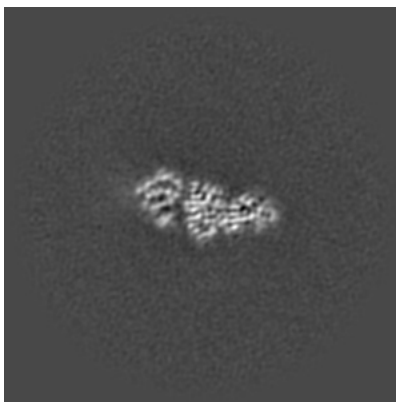
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

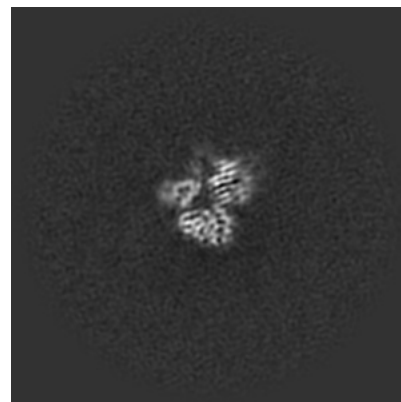
6.3.1 Primary map



X Index: 184

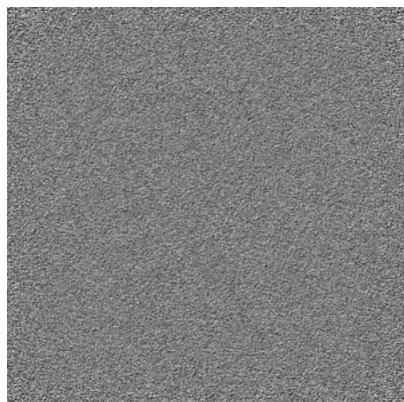


Y Index: 158

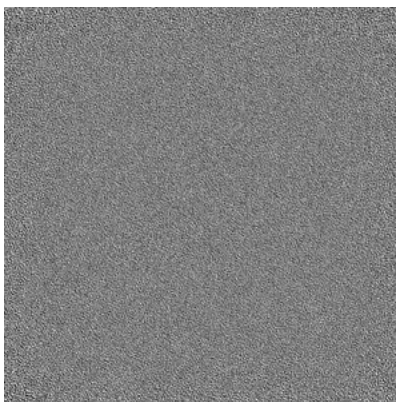


Z Index: 188

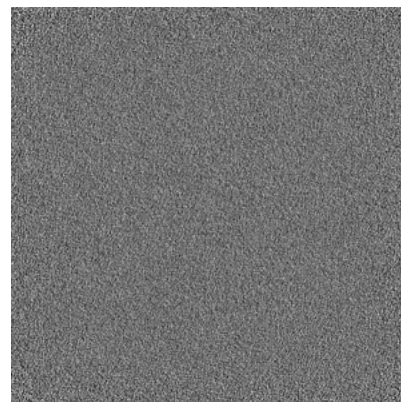
6.3.2 Raw map



X Index: 0



Y Index: 0

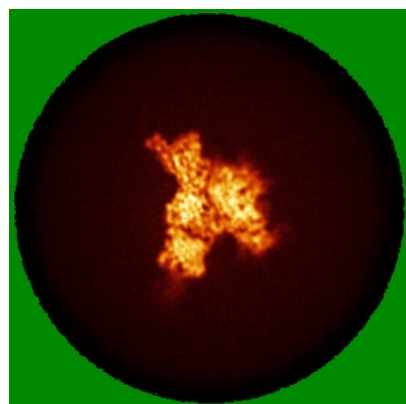


Z Index: 0

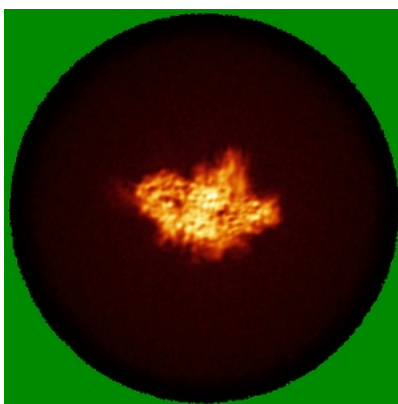
The images above show the largest variance slices of the map in three orthogonal directions.

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

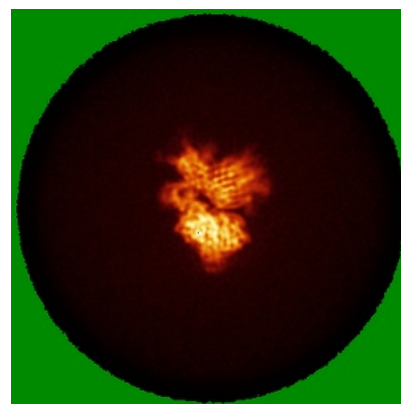
6.4.1 Primary map



X

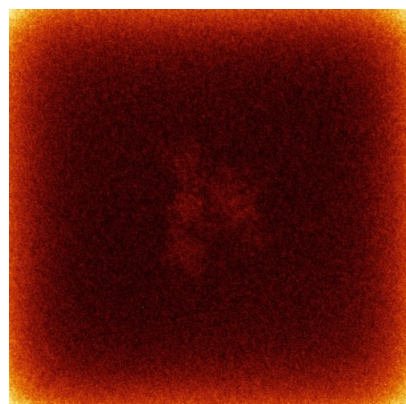


Y

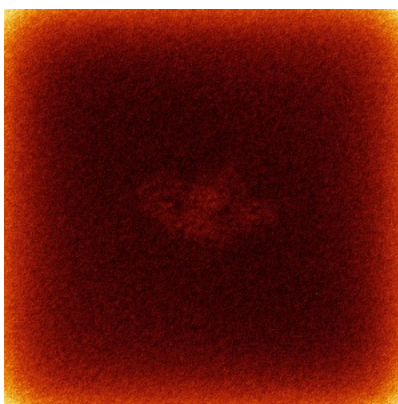


Z

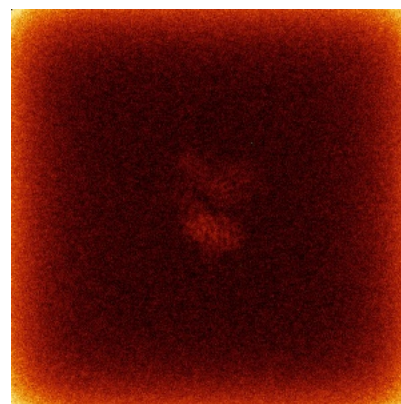
6.4.2 Raw map



X



Y

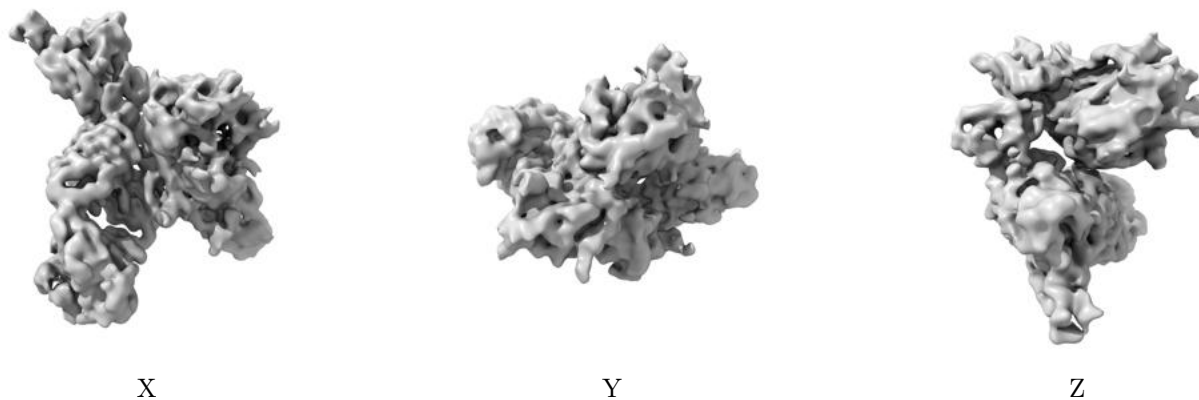


Z

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.

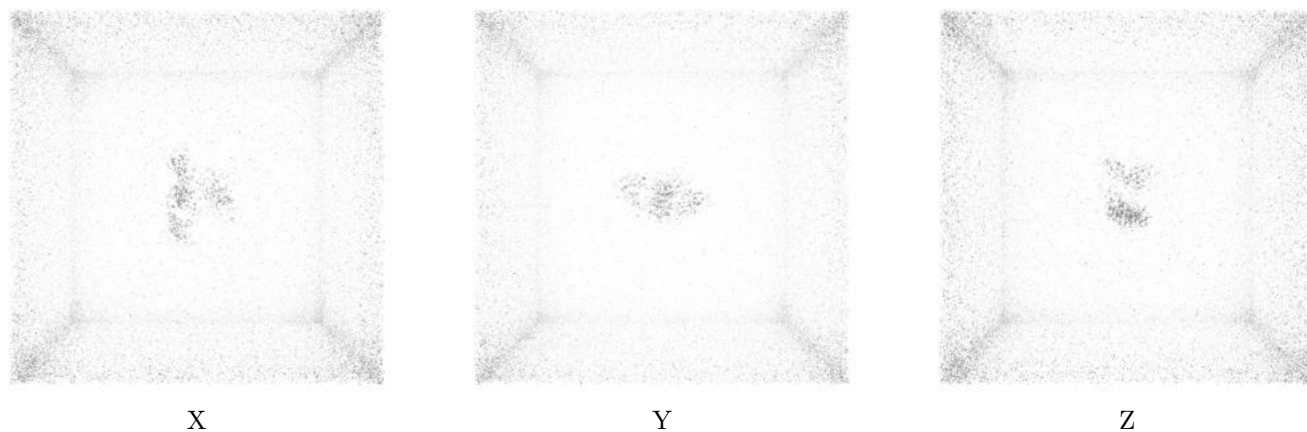
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

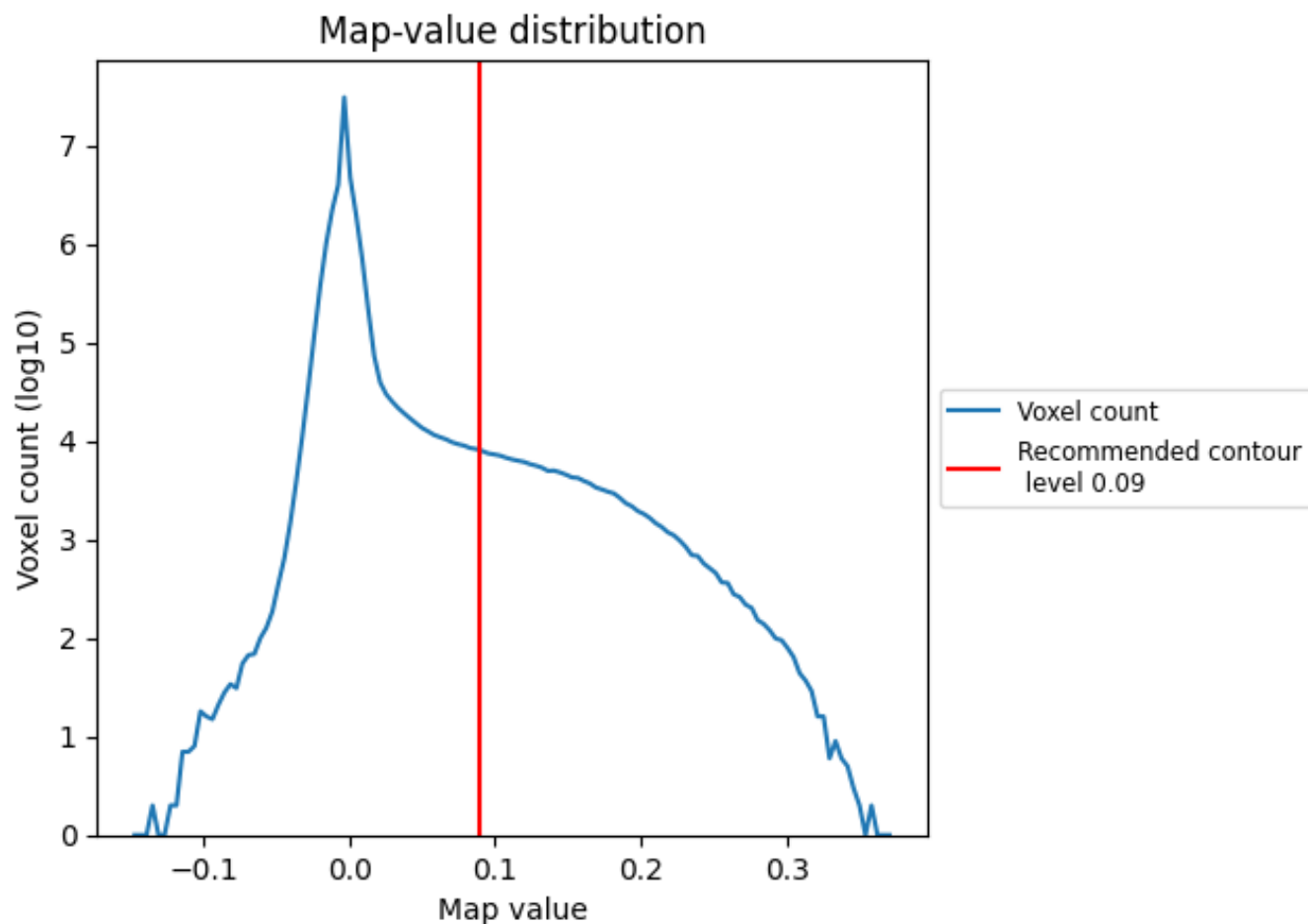
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

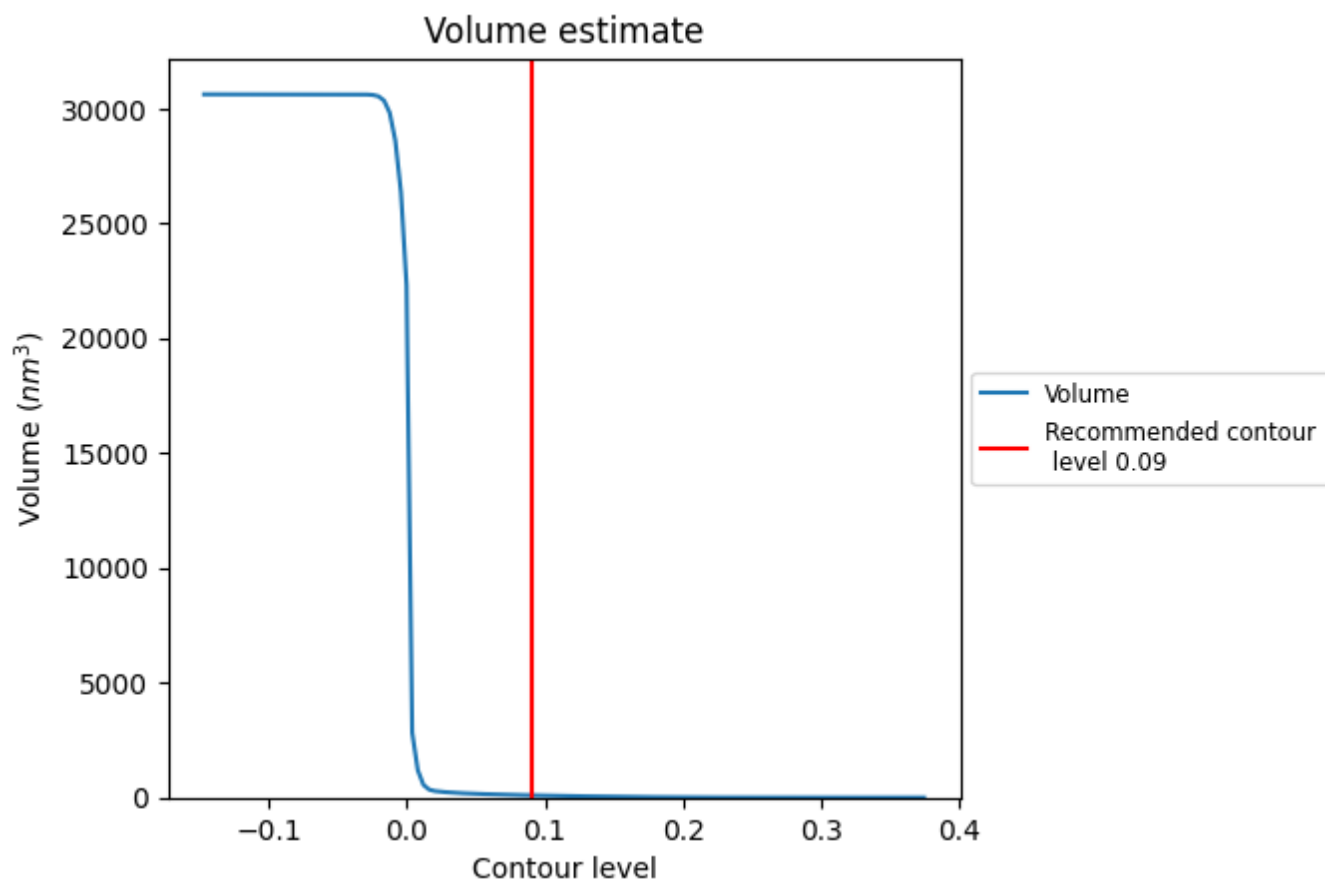
This section contains the results of statistical analysis of the map.

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.

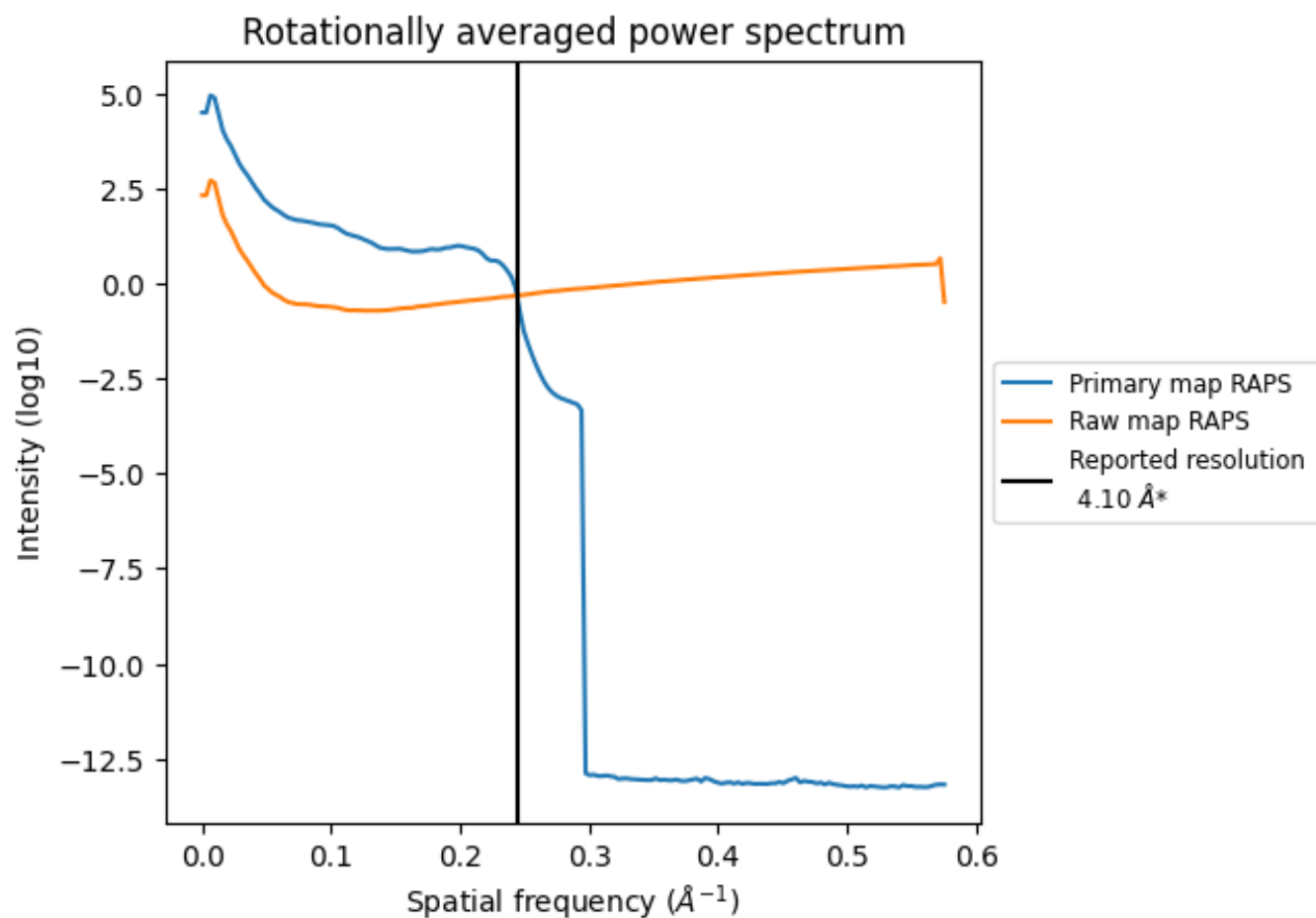
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 97 nm^3 ; this corresponds to an approximate mass of 88 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 ⓘ

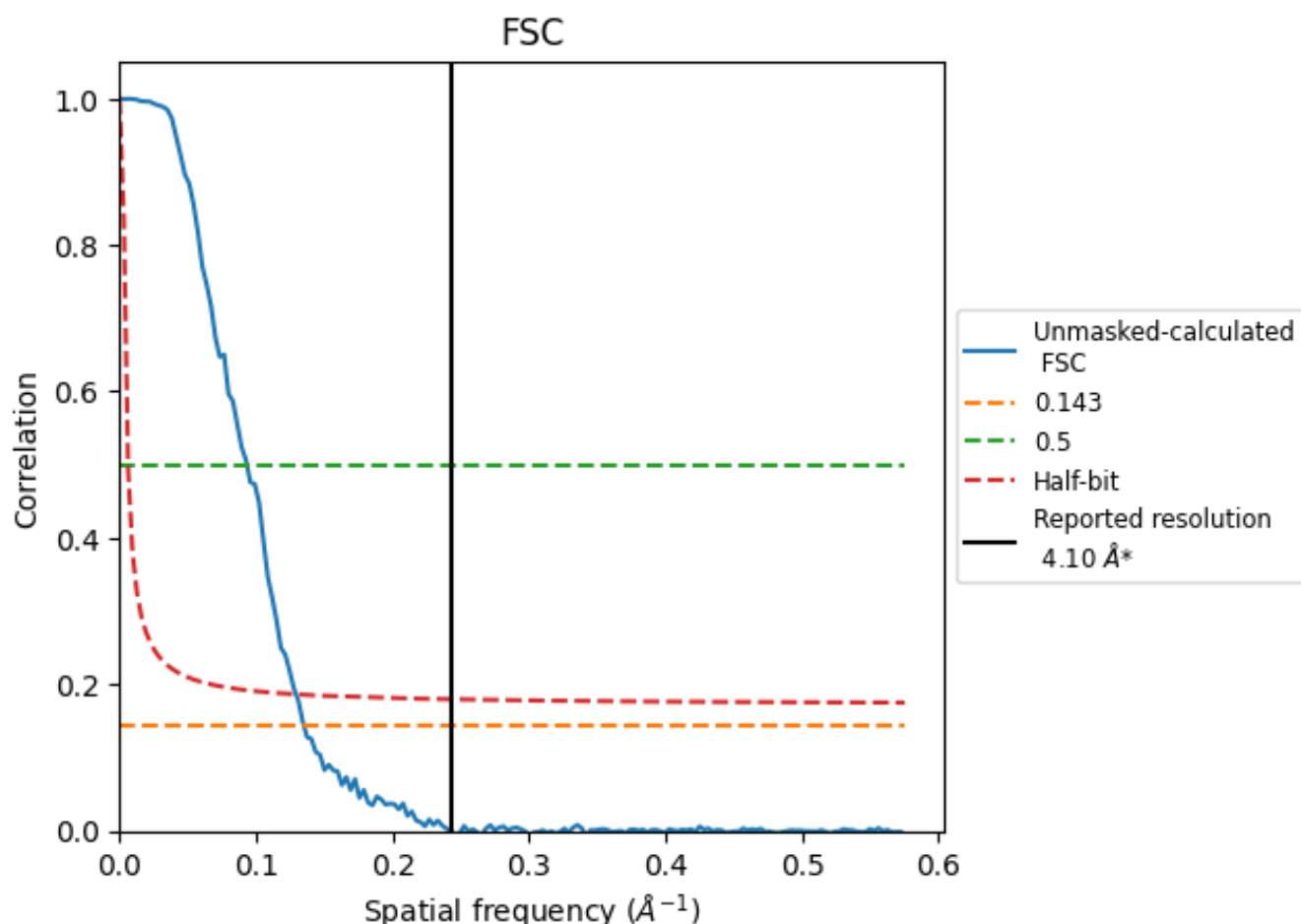


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 \AA^{-1}

8.2 Resolution estimates [i](#)

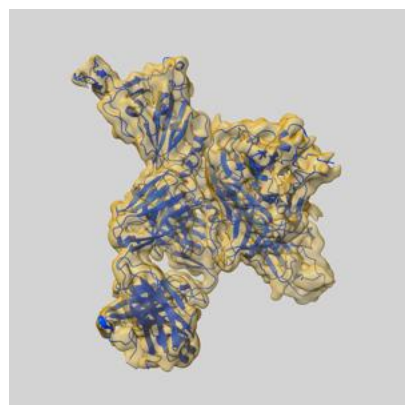
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.40	10.71	7.73

*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 7.40 differs from the reported value 4.1 by more than 10 %

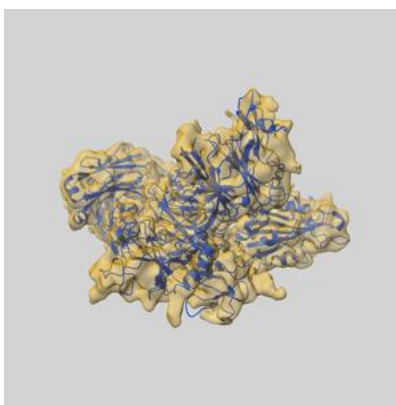
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26885 and PDB model 7UZB. Per-residue inclusion information can be found in section 3 on page 6.

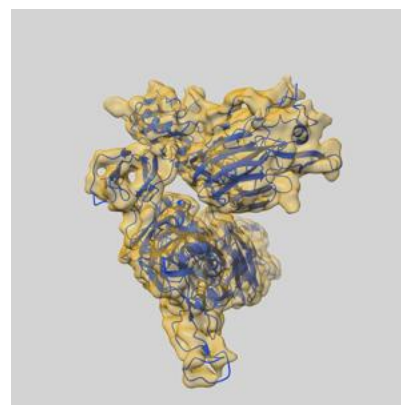
9.1 Map-model overlay [i](#)



X



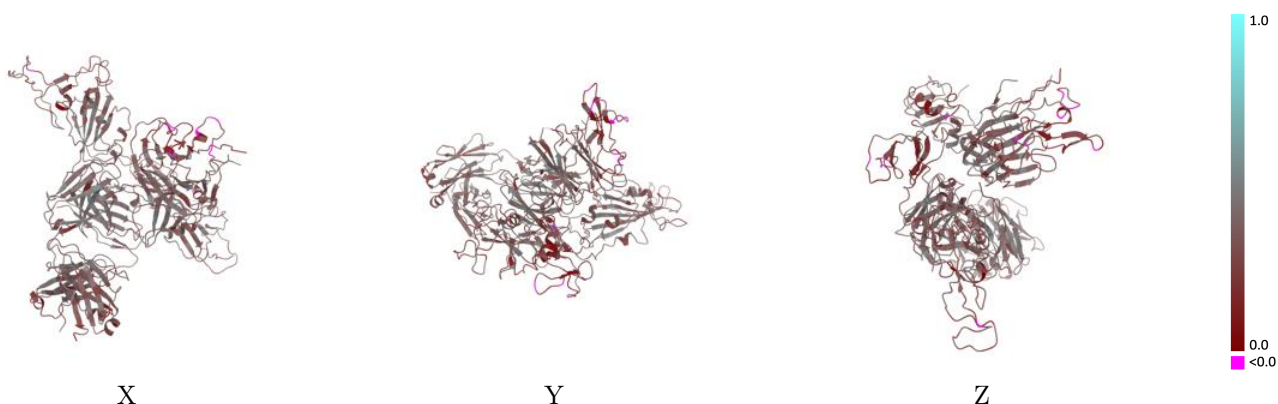
Y



Z

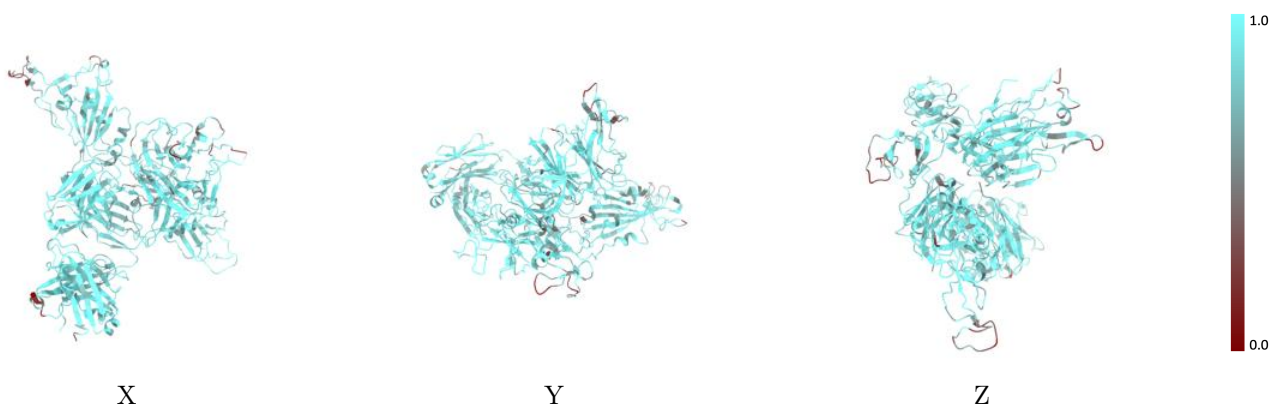
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



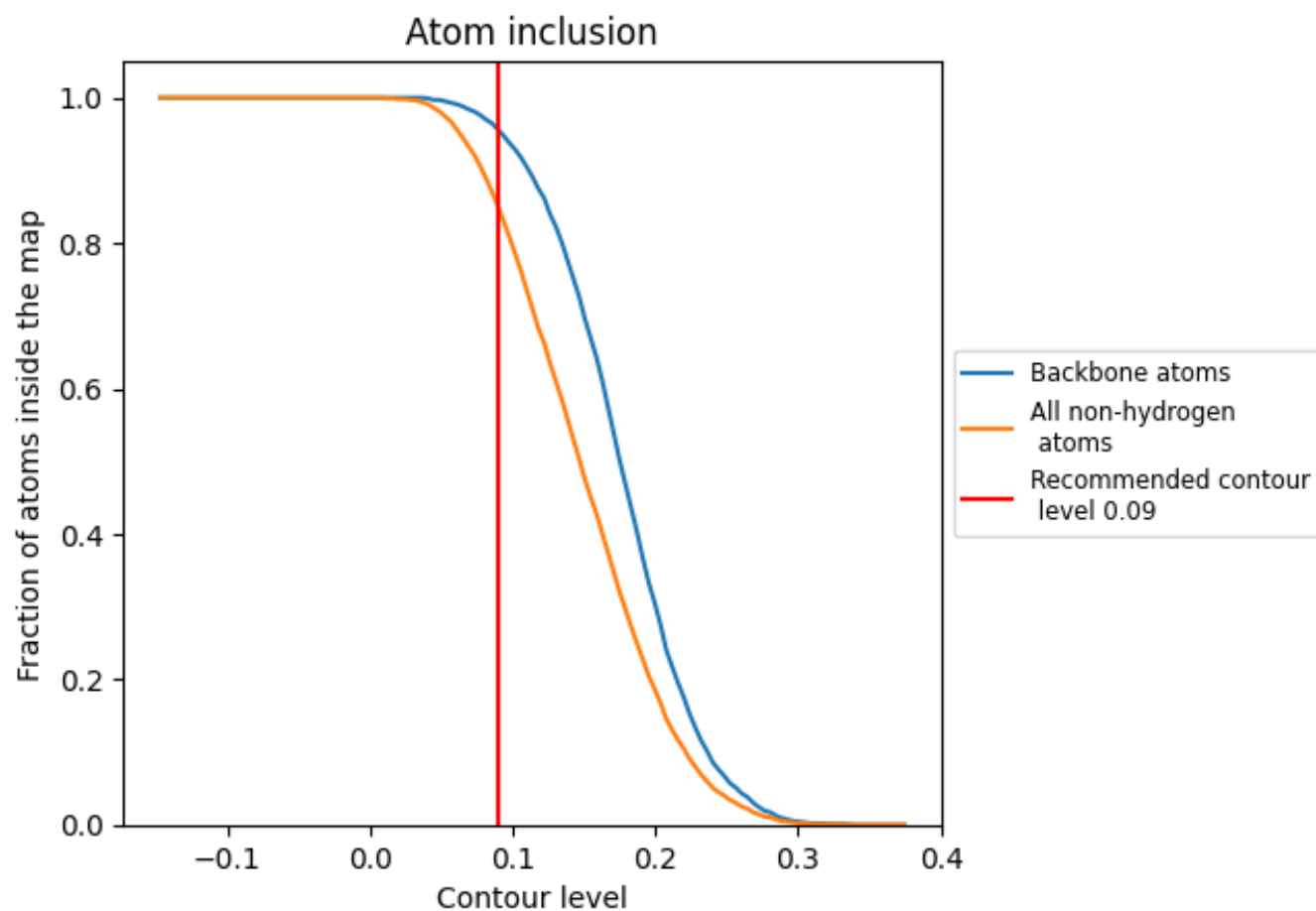
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 85% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8490	<div></div> 0.3340
A	<div></div> 0.8280	<div></div> 0.3150
H	<div></div> 0.8810	<div></div> 0.3580
L	<div></div> 0.8790	<div></div> 0.3700

