



Full wwPDB EM Validation Report ⓘ

Sep 8, 2026 – 08:34 PM JST

PDB ID : 22TH / pdb_000022th
EMDB ID : EMD-68657
Title : Cryo-EM structure of Crimean-Congo hemorrhagic fever virus RNA polymerase in complex with suramin
Authors : Ma, J.; Yang, K.; Wu, H.; Liang, Z.
Deposited on : 2026-01-22
Resolution : 2.50 Å(reported)
Based on initial model : .

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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

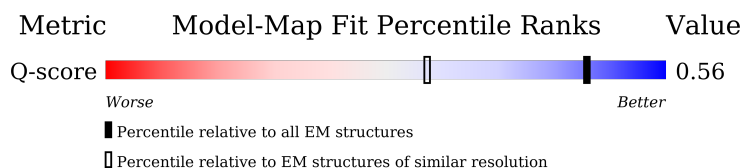
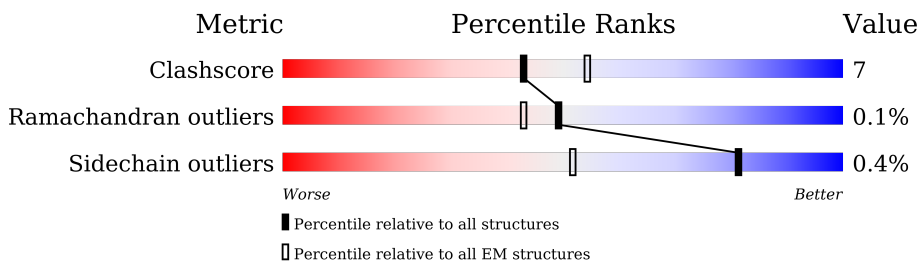
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

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	3974	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11814 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1530	Total	C	N	O	S	0	0
			11563	7323	2007	2153	80		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3946	TRP	-	expression tag	UNP Q6TQR6
A	3947	SER	-	expression tag	UNP Q6TQR6
A	3948	HIS	-	expression tag	UNP Q6TQR6
A	3949	PRO	-	expression tag	UNP Q6TQR6
A	3950	GLN	-	expression tag	UNP Q6TQR6
A	3951	PHE	-	expression tag	UNP Q6TQR6
A	3952	GLU	-	expression tag	UNP Q6TQR6
A	3953	LYS	-	expression tag	UNP Q6TQR6
A	3954	GLY	-	expression tag	UNP Q6TQR6
A	3955	SER	-	expression tag	UNP Q6TQR6
A	3956	SER	-	expression tag	UNP Q6TQR6
A	3957	GLY	-	expression tag	UNP Q6TQR6
A	3958	GLY	-	expression tag	UNP Q6TQR6
A	3959	SER	-	expression tag	UNP Q6TQR6
A	3960	SER	-	expression tag	UNP Q6TQR6
A	3961	GLY	-	expression tag	UNP Q6TQR6
A	3962	SER	-	expression tag	UNP Q6TQR6
A	3963	SER	-	expression tag	UNP Q6TQR6
A	3964	GLY	-	expression tag	UNP Q6TQR6
A	3965	GLY	-	expression tag	UNP Q6TQR6
A	3966	ALA	-	expression tag	UNP Q6TQR6
A	3967	TRP	-	expression tag	UNP Q6TQR6
A	3968	SER	-	expression tag	UNP Q6TQR6
A	3969	HIS	-	expression tag	UNP Q6TQR6
A	3970	PRO	-	expression tag	UNP Q6TQR6
A	3971	GLN	-	expression tag	UNP Q6TQR6
A	3972	PHE	-	expression tag	UNP Q6TQR6
A	3973	GLU	-	expression tag	UNP Q6TQR6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	3974	LYS	-	expression tag	UNP Q6TQR6

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
2	A	2	Total Zn 2 2	0

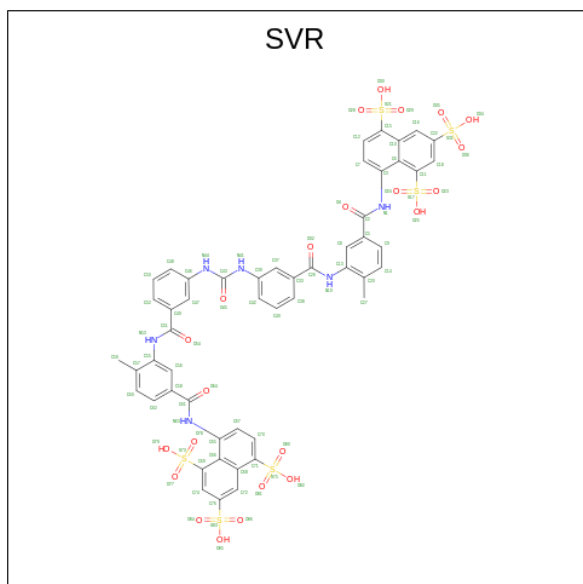
- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Mn 1 1	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Mg 1 1	0

- Molecule 5 is 8,8'-[CARBONYLBIS[IMINO-3,1-PHENYLENECARBONYLIMINO(4-METHYL-3,1-PHENYLENE)CARBONYLIMINO]]BIS-1,3,5-NAPHTHALENETRISULFONIC ACID (CCD ID: SVR) (formula: C₅₁H₄₀N₆O₂₃S₆).

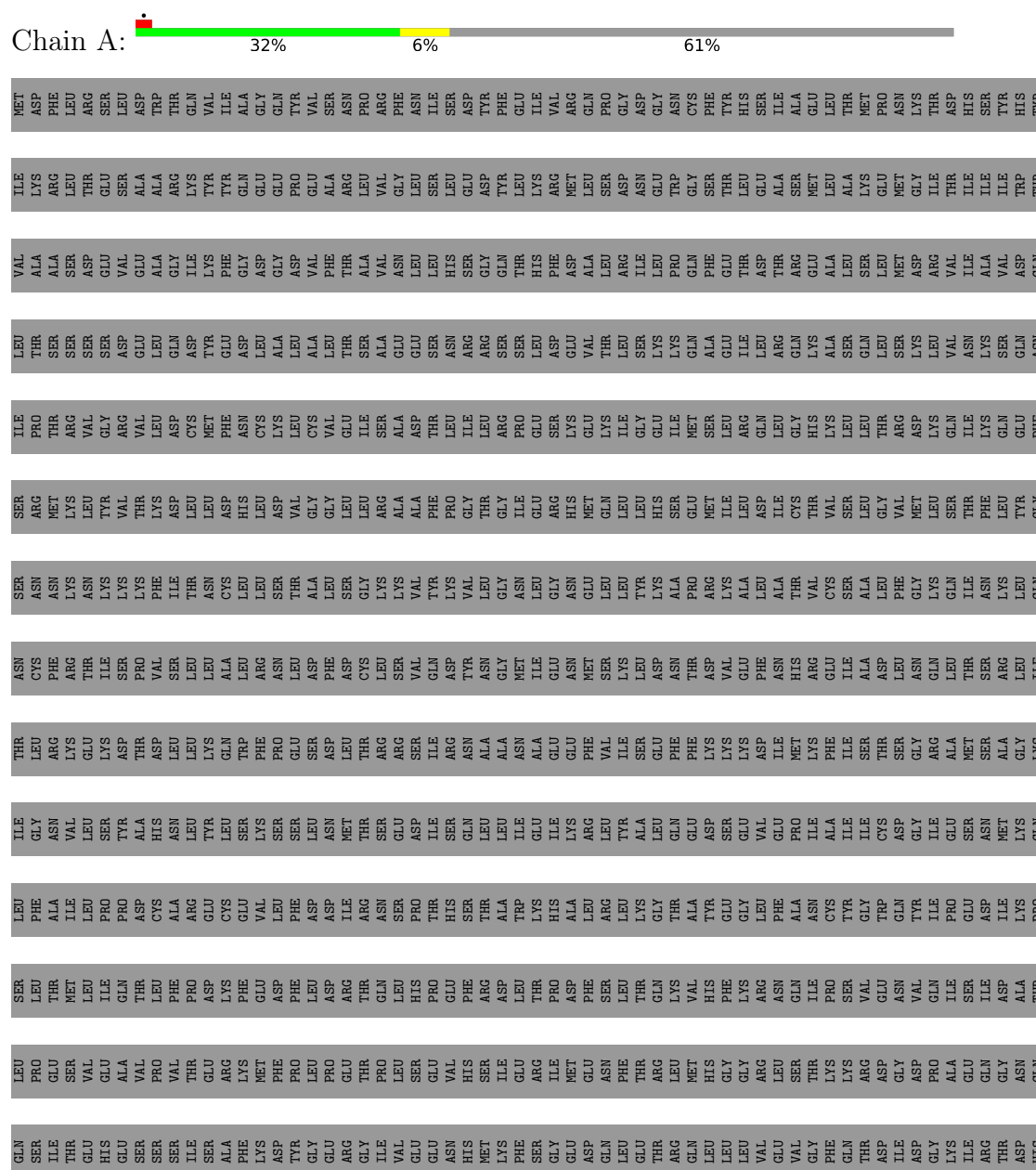


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	S	0
			51	32	4	12	3	
5	A	1	Total	C	N	O	S	0
			86	51	6	23	6	
5	A	1	Total	C	N	O		0
			36	29	4	3		
5	A	1	Total	C	N	O	S	0
			42	25	3	11	3	
5	A	1	Total	C	N	O	S	0
			32	18	1	10	3	

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: RNA-directed RNA polymerase L







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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37822	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.239	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	280.32, 280.32, 280.32	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.73, 0.73, 0.73	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: MN, MG, SVR, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.09	0/11754	0.23	0/15934

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	11563	0	11097	149	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	247	0	108	8	0
All	All	11814	0	11205	152	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 (152) 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:1356:SER:HA	1:A:1374:LEU:O	1.76	0.85
1:A:3100:ARG:HE	1:A:3186:GLN:HE21	1.29	0.79
1:A:2610:MET:HE1	1:A:2665:ARG:HD3	1.71	0.73
1:A:1295:ILE:HG12	1:A:1412:LEU:HD21	1.71	0.70
1:A:983:MET:HB2	1:A:1759:LYS:HD2	1.73	0.70
1:A:1307:ARG:NH1	1:A:2666:LEU:O	2.22	0.67
1:A:1671:ARG:NH1	5:A:4006:SVR:O77	2.32	0.63
1:A:2407:SER:O	1:A:2411:ILE:HG12	1.99	0.63
1:A:1773:ASN:OD1	1:A:2562:LYS:NZ	2.33	0.62
1:A:1671:ARG:NH2	5:A:4005:SVR:O4	2.30	0.61
5:A:4005:SVR:O25	5:A:4006:SVR:N41	2.33	0.61
1:A:1550:CYS:SG	1:A:1556:ASN:ND2	2.75	0.60
1:A:2821:ALA:O	1:A:2825:GLN:HB2	2.02	0.60
1:A:1004:LEU:HD21	1:A:2542:TRP:HB3	1.83	0.60
1:A:1809:ASN:OD1	1:A:2302:ASN:ND2	2.34	0.60
1:A:2318:LYS:HD3	1:A:2577:TYR:HB2	1.83	0.60
1:A:1457:GLU:HG3	1:A:1564:THR:HG21	1.84	0.60
1:A:1424:GLN:HE22	1:A:2629:THR:HG1	1.48	0.59
1:A:1006:GLN:HG3	1:A:1009:THR:HB	1.85	0.59
1:A:2603:VAL:HG21	1:A:2609:LEU:HB2	1.84	0.58
1:A:2355:ILE:HG12	1:A:2569:VAL:HG13	1.86	0.58
1:A:1232:LEU:HD13	1:A:1373:LYS:HB2	1.86	0.57
1:A:3105:PRO:O	1:A:3109:MET:HG2	2.05	0.57
1:A:3128:PHE:HA	1:A:3131:LEU:HD13	1.86	0.57
1:A:2535:SER:O	1:A:2539:GLU:HG2	2.04	0.57
1:A:1277:GLN:HG2	1:A:1505:PHE:HB2	1.87	0.56
1:A:2515:SER:OG	1:A:2517:ASP:OD1	2.23	0.56
1:A:1789:GLU:OE1	1:A:2377:GLN:NE2	2.38	0.56
1:A:3143:PRO:O	1:A:3147:THR:HG23	2.06	0.56
1:A:2364:PRO:C	1:A:2366:HIS:H	2.12	0.56
1:A:1800:ILE:HD13	1:A:2303:LEU:HD11	1.87	0.56
1:A:2694:LEU:HD12	1:A:2830:ILE:HG13	1.87	0.56
1:A:2680:ALA:HB1	1:A:2859:ILE:HG12	1.87	0.56
1:A:3026:CYS:HB2	1:A:3045:HIS:HB3	1.86	0.55
1:A:1809:ASN:O	1:A:2294:ALA:N	2.40	0.55
1:A:3199:LYS:NZ	1:A:3200:GLY:O	2.31	0.54
1:A:2503:LEU:O	1:A:2506:THR:OG1	2.25	0.54
1:A:2756:GLU:HG2	1:A:3058:LEU:HD11	1.90	0.54
1:A:1662:ARG:NH1	1:A:1765:ASP:OD2	2.34	0.54
1:A:2440:ASN:O	1:A:2443:SER:OG	2.26	0.53
1:A:1282:LYS:HA	1:A:1444:GLU:HG3	1.91	0.53
1:A:1305:MET:HG2	1:A:1317:VAL:HG11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1323:LEU:HD22	1:A:1420:ILE:HG12	1.90	0.53
1:A:1011:SER:HB3	1:A:1570:VAL:HG23	1.92	0.52
1:A:1534:SER:HA	1:A:2570:SER:HB2	1.91	0.52
1:A:2661:SER:HA	1:A:2665:ARG:HB3	1.91	0.52
1:A:1120:LYS:O	1:A:1124:VAL:HG12	2.10	0.52
1:A:2517:ASP:OD1	1:A:2517:ASP:N	2.43	0.52
1:A:1316:ILE:HD11	1:A:3217:ILE:HG23	1.91	0.51
1:A:996:GLU:OE2	1:A:2550:ASN:ND2	2.41	0.51
1:A:943:GLU:OE2	1:A:943:GLU:N	2.30	0.51
1:A:1462:LEU:HD13	1:A:1560:LEU:HD11	1.91	0.51
1:A:1321:VAL:HG11	1:A:2782:LEU:HB3	1.93	0.51
1:A:1424:GLN:HG3	1:A:1429:LEU:HD22	1.91	0.50
1:A:2364:PRO:O	1:A:2366:HIS:N	2.41	0.50
1:A:1659:ARG:NE	1:A:1765:ASP:OD1	2.39	0.50
1:A:1307:ARG:HH21	1:A:2658:GLY:HA2	1.76	0.50
1:A:1370:LEU:HD11	1:A:1384:CYS:HB3	1.94	0.49
1:A:1537:VAL:HG23	1:A:1539:PRO:HD3	1.95	0.49
1:A:1219:SER:O	1:A:1219:SER:OG	2.28	0.49
1:A:1581:LYS:NZ	1:A:2571:ASP:OD2	2.45	0.49
1:A:1516:GLN:N	5:A:4008:SVR:O34	2.40	0.49
1:A:1001:LYS:HE2	1:A:1003:GLU:HG2	1.94	0.48
1:A:1470:TYR:OH	1:A:1572:ASP:OD2	2.29	0.48
1:A:2355:ILE:HG23	1:A:2569:VAL:HG22	1.95	0.48
1:A:2368:CYS:C	1:A:2370:PHE:H	2.22	0.48
1:A:2621:MET:HE2	1:A:2621:MET:HB3	1.77	0.48
1:A:2581:MET:HE3	1:A:2581:MET:HB3	1.77	0.47
1:A:1388:SER:OG	1:A:1390:ASN:OD1	2.32	0.47
1:A:2603:VAL:HG22	1:A:2641:PHE:CE2	2.49	0.47
1:A:1424:GLN:NE2	1:A:2629:THR:OG1	2.42	0.47
1:A:1567:TYR:O	1:A:1571:ARG:HB2	2.14	0.47
1:A:941:MET:O	1:A:945:ILE:HG12	2.14	0.47
1:A:1271:LYS:HD2	1:A:1455:PHE:CZ	2.50	0.47
1:A:2519:TYR:OH	1:A:2563:ASP:OD2	2.26	0.47
1:A:1345:THR:HG21	1:A:1363:ILE:CD1	2.45	0.46
1:A:1580:TRP:HE3	1:A:1589:VAL:HG11	1.80	0.46
1:A:2357:GLY:HA3	1:A:2519:TYR:CE1	2.50	0.46
1:A:2349:PHE:HB2	1:A:2529:LEU:HD22	1.96	0.46
1:A:2651:ARG:HB3	1:A:2652:TYR:CD2	2.49	0.46
1:A:2808:TRP:CZ2	1:A:2823:ARG:HG2	2.51	0.46
1:A:2687:ILE:HD11	1:A:2860:ILE:HD11	1.97	0.46
1:A:957:SER:OG	5:A:4005:SVR:O36	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1401:ASN:ND2	1:A:1403:ARG:HG2	2.30	0.46
1:A:2831:LEU:HD12	1:A:3027:VAL:HG11	1.97	0.46
1:A:2413:ASN:OD1	1:A:2414:VAL:N	2.49	0.46
1:A:1057:GLN:NE2	1:A:1265:ARG:O	2.46	0.46
1:A:1307:ARG:NH2	1:A:2657:LEU:O	2.49	0.45
1:A:2532:GLU:H	1:A:2532:GLU:CD	2.24	0.45
1:A:1787:ILE:HG13	1:A:2490:LEU:HD22	1.99	0.45
1:A:1428:CYS:HB2	1:A:1492:PHE:HB2	1.99	0.45
1:A:2367:CYS:SG	1:A:2469:ASN:HB3	2.57	0.45
1:A:2532:GLU:O	1:A:2536:GLN:HG3	2.17	0.45
1:A:2630:ASN:HA	1:A:2633:PHE:CE2	2.52	0.45
1:A:2692:GLN:O	1:A:2696:MET:HG3	2.16	0.45
1:A:2698:SER:HB2	1:A:3008:ILE:HG12	1.99	0.45
1:A:3195:PHE:HE1	1:A:3197:MET:HB3	1.81	0.45
1:A:1413:TYR:HD1	1:A:2636:LEU:HD22	1.82	0.45
1:A:1463:GLU:CD	1:A:1465:ARG:HH21	2.24	0.45
1:A:2813:LYS:HB2	1:A:2820:LEU:HD22	1.97	0.45
1:A:2415:LEU:HD22	1:A:2437:LEU:HD13	1.99	0.44
1:A:994:GLU:OE2	1:A:1771:ARG:NH1	2.49	0.44
1:A:2651:ARG:HG2	1:A:2796:VAL:HG21	2.00	0.44
1:A:2298:MET:HA	1:A:2298:MET:HE2	1.98	0.43
1:A:941:MET:HB3	1:A:2398:CYS:SG	2.58	0.43
1:A:1107:ASP:OD2	1:A:1217:LYS:N	2.50	0.43
1:A:3020:PHE:HD2	1:A:3177:HIS:CE1	2.37	0.43
1:A:1524:MET:HE3	1:A:1524:MET:HB3	1.87	0.43
5:A:4005:SVR:H48	5:A:4006:SVR:HN1	1.84	0.43
1:A:1424:GLN:HB3	1:A:3219:GLU:HB3	2.00	0.43
1:A:1604:ASP:HB2	1:A:2582:MET:HG3	1.99	0.43
1:A:2298:MET:O	1:A:2302:ASN:ND2	2.51	0.43
1:A:2354:CYS:HB3	1:A:2574:LEU:HD13	2.00	0.43
1:A:2656:THR:O	1:A:2659:THR:OG1	2.37	0.43
1:A:2857:ASN:OD1	1:A:3184:MET:HA	2.19	0.43
1:A:1305:MET:HE2	1:A:1305:MET:HB3	1.97	0.42
1:A:1445:ASN:O	1:A:1449:THR:HG23	2.19	0.42
1:A:1648:ASN:O	1:A:1652:SER:HB3	2.19	0.42
1:A:1363:ILE:HD11	1:A:1370:LEU:HB2	2.00	0.42
1:A:1072:ILE:HD13	1:A:1072:ILE:HA	1.85	0.42
1:A:2357:GLY:HA2	1:A:2567:THR:HG23	2.01	0.42
1:A:3068:LEU:HD23	1:A:3068:LEU:HA	1.92	0.42
1:A:952:LEU:HD21	1:A:1650:LEU:HD12	2.01	0.42
1:A:1605:ARG:NH2	1:A:2590:VAL:HG11	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1656:LYS:NZ	5:A:4006:SVR:O35	2.48	0.42
1:A:2335:LEU:HB3	1:A:2348:ASN:HD21	1.83	0.42
1:A:2557:ARG:HA	1:A:2557:ARG:HD2	1.87	0.42
1:A:2904:ALA:HB2	1:A:3113:LEU:HD23	2.01	0.42
1:A:992:THR:O	1:A:996:GLU:HG3	2.19	0.42
1:A:1027:ARG:NH1	1:A:1031:CYS:SG	2.93	0.42
1:A:1141:ILE:HD12	1:A:1219:SER:HB2	2.02	0.42
1:A:1606:GLN:NE2	1:A:1610:ASP:OD1	2.47	0.42
1:A:2454:VAL:HA	1:A:2458:ILE:HB	2.02	0.42
1:A:3101:LEU:HD12	1:A:3101:LEU:HA	1.92	0.42
1:A:2585:ARG:HD2	1:A:3087:ILE:HB	2.01	0.41
1:A:2678:ALA:O	1:A:2682:GLU:HG3	2.20	0.41
1:A:1319:THR:HG23	1:A:1432:ILE:HG21	2.01	0.41
1:A:1333:PHE:O	1:A:1337:VAL:HG23	2.20	0.41
1:A:2452:PHE:HA	1:A:2455:THR:HG22	2.02	0.41
1:A:1543:GLY:HA2	1:A:1546:PHE:HD2	1.85	0.41
1:A:1532:GLY:N	1:A:1570:VAL:HG12	2.36	0.41
1:A:3009:ASN:N	1:A:3041:VAL:O	2.50	0.41
5:A:4006:SVR:O25	5:A:4006:SVR:N1	2.54	0.41
1:A:1338:LEU:HD11	1:A:1368:ILE:HD11	2.02	0.41
1:A:1787:ILE:CG1	1:A:2490:LEU:HD22	2.51	0.41
1:A:2621:MET:HG3	1:A:2671:TYR:HE1	1.86	0.41
1:A:2691:ALA:HB2	1:A:2830:ILE:HD11	2.02	0.41
1:A:2520:ALA:HB1	1:A:2574:LEU:HD11	2.03	0.40
1:A:2312:LEU:HD11	1:A:2477:HIS:ND1	2.36	0.40
1:A:2633:PHE:CD1	1:A:2633:PHE:C	2.98	0.40
1:A:3109:MET:HG2	1:A:3109:MET:H	1.71	0.40
1:A:3025:ARG:C	1:A:3027:VAL:H	2.30	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	1498/3974 (38%)	1465 (98%)	32 (2%)	1 (0%)	48 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2365	ILE

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	1218/3623 (34%)	1213 (100%)	5 (0%)	84 93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1390	ASN
1	A	1657	ASP
1	A	2596	THR
1	A	2755	THR
1	A	3038	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	960	GLN
1	A	1068	ASN
1	A	1433	ASN
1	A	1510	ASN
1	A	1519	ASN
1	A	1521	GLN
1	A	1523	GLN
1	A	1556	ASN
1	A	2302	ASN
1	A	2345	ASN

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Mol	Chain	Res	Type
1	A	2359	ASN
1	A	2505	GLN
1	A	2770	GLN
1	A	2787	ASN
1	A	2817	ASN
1	A	2825	GLN
1	A	3057	ASN
1	A	3177	HIS
1	A	3201	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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	SVR	A	4008	-	43,45,93	0.46	0	62,70,145	0.88	2 (3%)
5	SVR	A	4006	-	89,93,93	0.50	0	129,145,145	0.82	4 (3%)
5	SVR	A	4007	-	39,39,93	0.35	0	53,53,145	0.61	0
5	SVR	A	4009	-	32,34,93	0.55	0	46,54,145	0.85	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SVR	A	4005	-	53,55,93	0.49	0	75,83,145	0.77	2 (2%)

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	SVR	A	4008	-	-	3/34/34/76	0/4/4/8
5	SVR	A	4006	-	-	10/76/76/76	0/8/8/8
5	SVR	A	4007	-	-	6/24/24/76	0/4/4/8
5	SVR	A	4009	-	-	7/26/26/76	0/3/3/8
5	SVR	A	4005	-	-	5/42/42/76	0/5/5/8

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	4008	SVR	C7-C3-N1	-2.81	115.53	123.29
5	A	4006	SVR	C67-C65-N63	-2.56	116.22	123.29
5	A	4005	SVR	C7-C3-N1	-2.51	116.36	123.29
5	A	4008	SVR	C6-C3-N1	2.46	124.25	120.58
5	A	4009	SVR	C58-C61-N63	2.33	121.06	115.92
5	A	4006	SVR	C7-C3-N1	-2.18	117.26	123.29
5	A	4009	SVR	C67-C65-N63	-2.16	117.33	123.29
5	A	4006	SVR	C66-C65-N63	2.15	123.79	120.58
5	A	4005	SVR	C3-N1-C2	-2.06	122.54	128.64
5	A	4006	SVR	C3-N1-C2	-2.04	122.61	128.64

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	4009	SVR	C58-C61-N63-C65
5	A	4009	SVR	O64-C61-N63-C65
5	A	4005	SVR	C47-C46-N44-C43
5	A	4006	SVR	N1-C2-C5-C8
5	A	4006	SVR	O4-C2-C5-C8
5	A	4005	SVR	C48-C46-N44-C43
5	A	4006	SVR	N1-C2-C5-C9

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Mol	Chain	Res	Type	Atoms
5	A	4006	SVR	O4-C2-C5-C9
5	A	4007	SVR	C37-C39-N41-C43
5	A	4007	SVR	C42-C39-N41-C43
5	A	4009	SVR	C62-C58-C61-N63
5	A	4009	SVR	C62-C58-C61-O64
5	A	4009	SVR	C56-C58-C61-N63
5	A	4009	SVR	C56-C58-C61-O64
5	A	4006	SVR	C56-C55-N53-C51
5	A	4007	SVR	C8-C13-N19-C26
5	A	4006	SVR	C57-C55-N53-C51
5	A	4007	SVR	C20-C13-N19-C26
5	A	4006	SVR	C7-C3-N1-C2
5	A	4005	SVR	C7-C3-N1-C2
5	A	4008	SVR	C7-C3-N1-C2
5	A	4005	SVR	C37-C39-N41-C43
5	A	4006	SVR	C20-C13-N19-C26
5	A	4009	SVR	C67-C65-N63-C61
5	A	4005	SVR	C42-C39-N41-C43
5	A	4006	SVR	C8-C13-N19-C26
5	A	4007	SVR	C57-C55-N53-C51
5	A	4007	SVR	C56-C55-N53-C51
5	A	4006	SVR	C67-C65-N63-C61
5	A	4008	SVR	C20-C13-N19-C26
5	A	4008	SVR	C8-C13-N19-C26

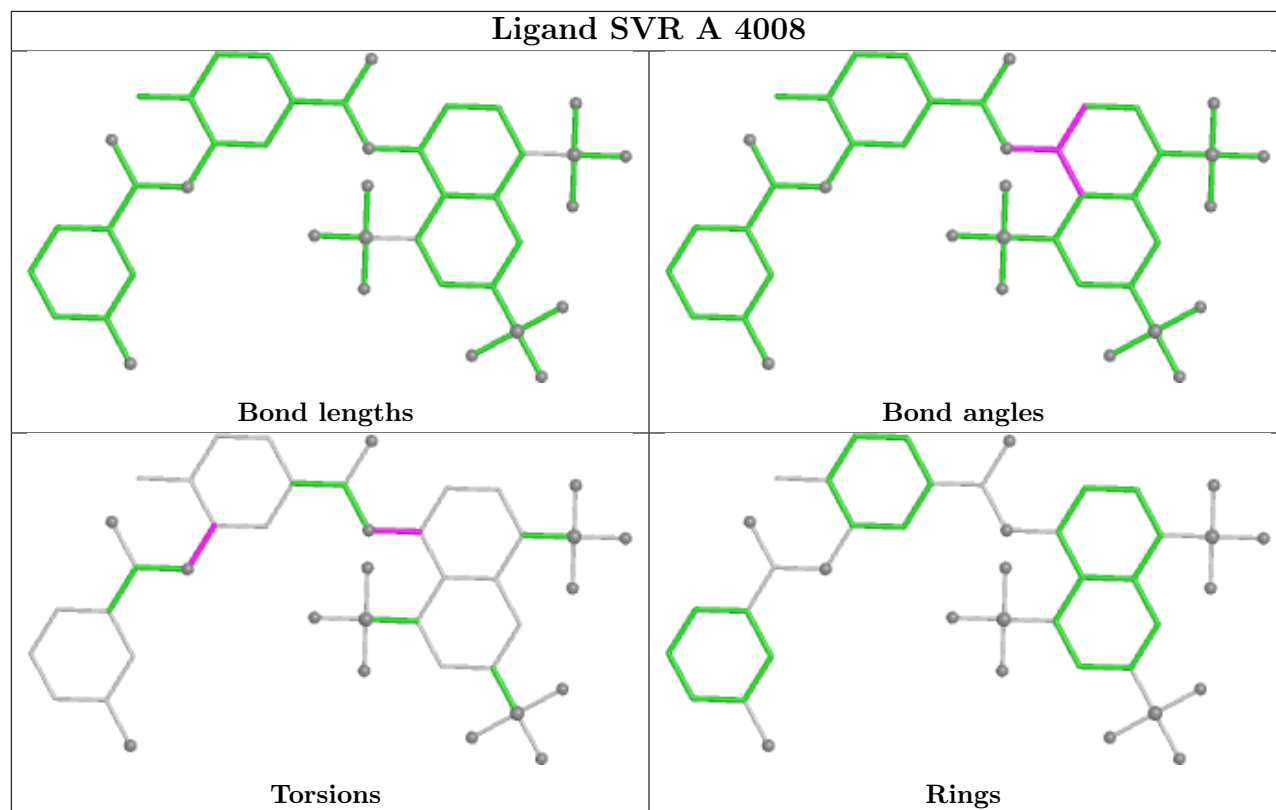
There are no ring outliers.

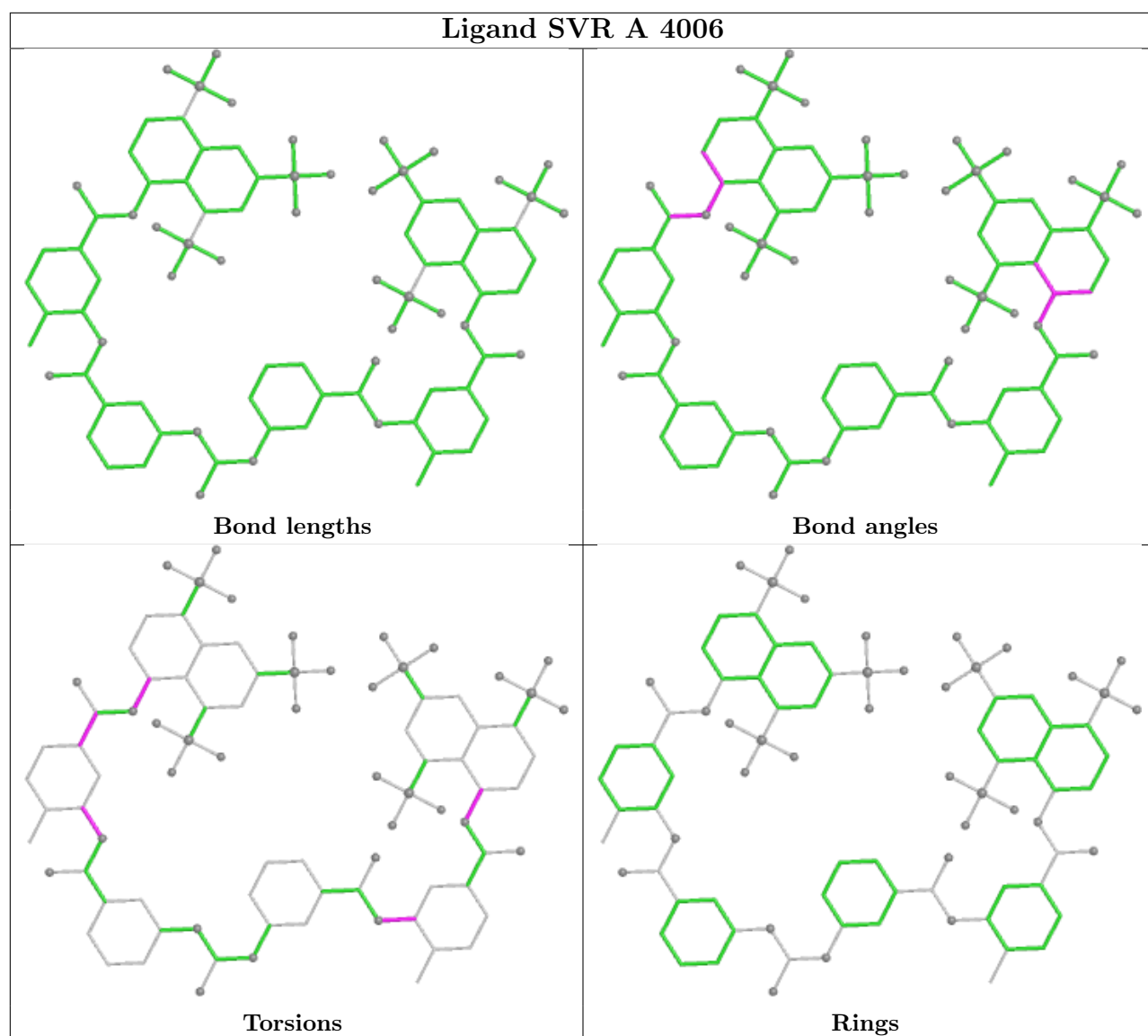
3 monomers are involved in 8 short contacts:

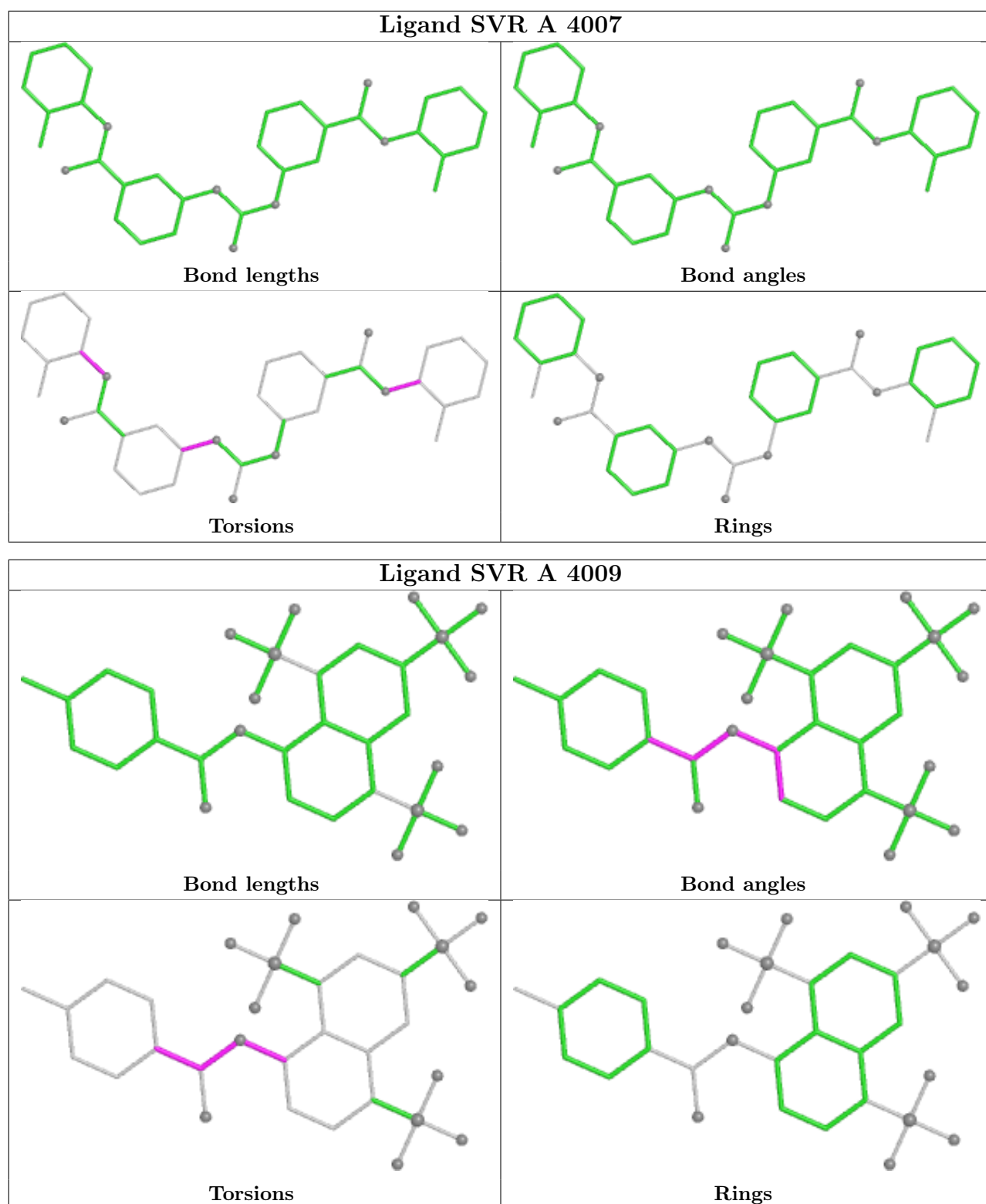
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	4008	SVR	1	0
5	A	4006	SVR	5	0
5	A	4005	SVR	4	0

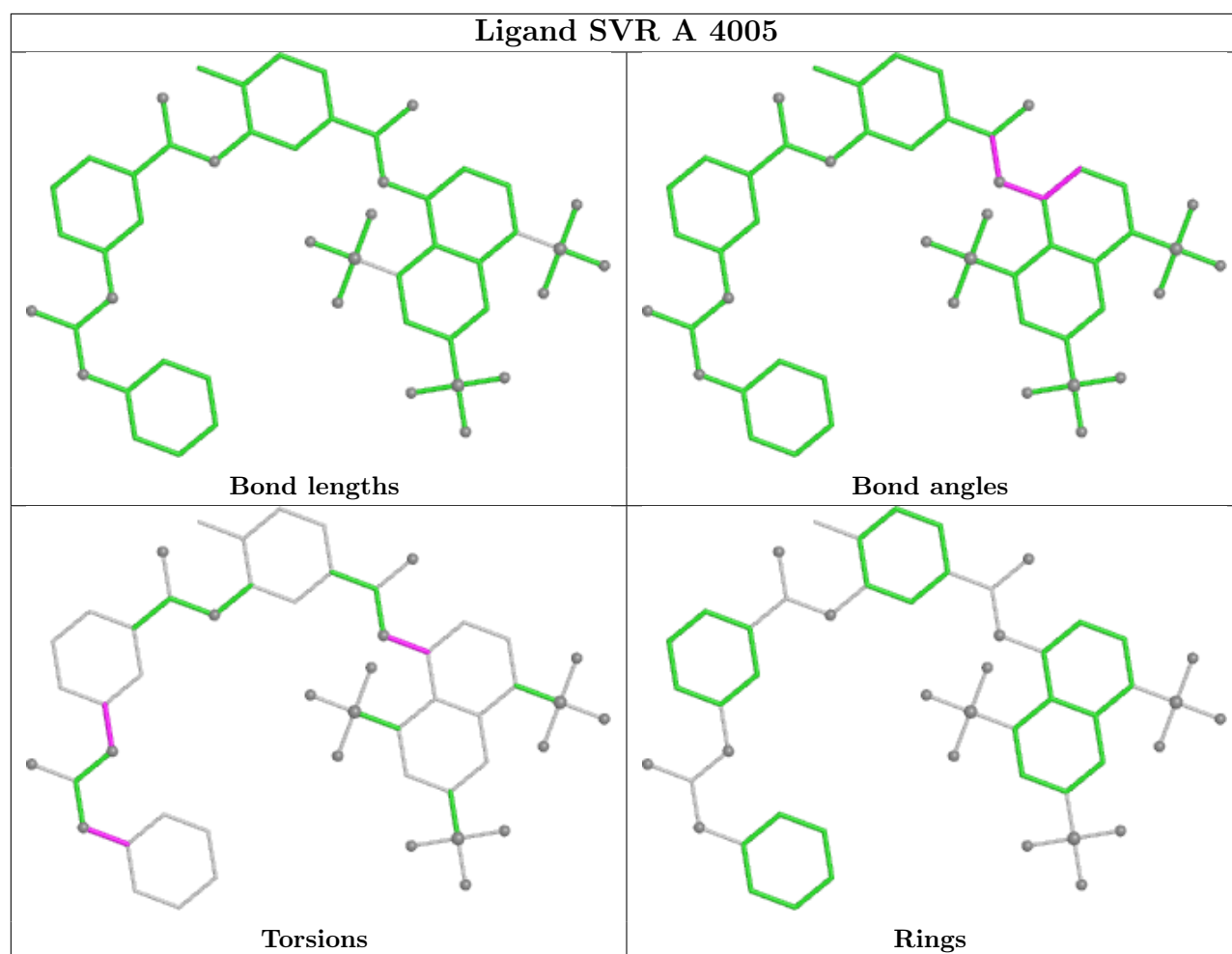
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

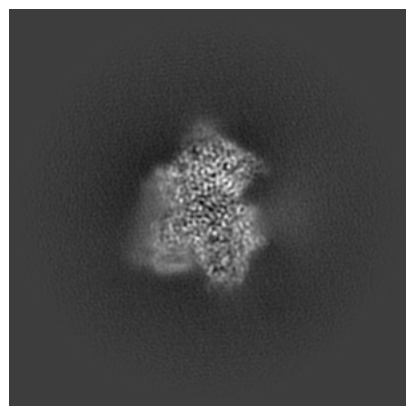
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68657. These allow visual inspection of the internal detail of the map and identification of artifacts.

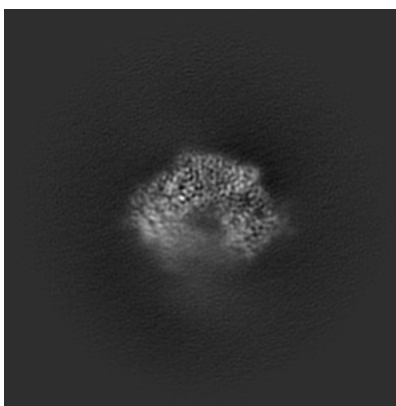
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

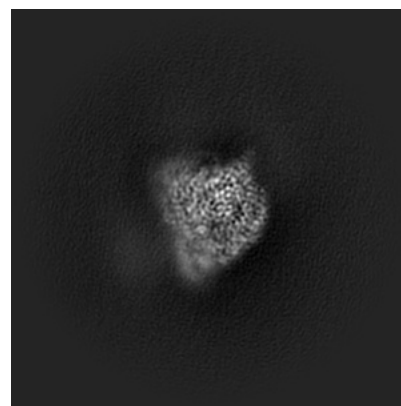
6.1.1 Primary map



X

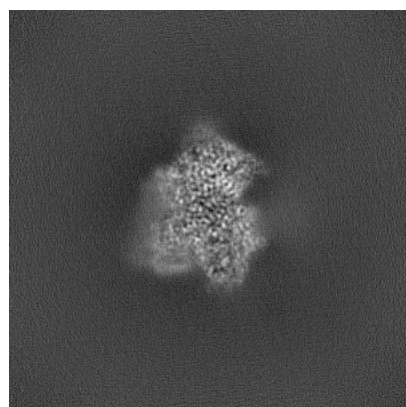


Y

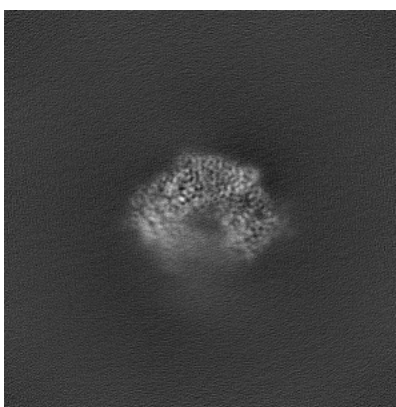


Z

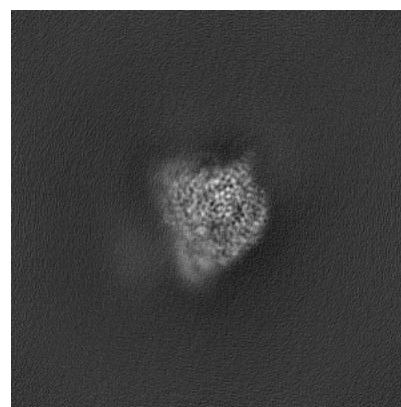
6.1.2 Raw map



X



Y

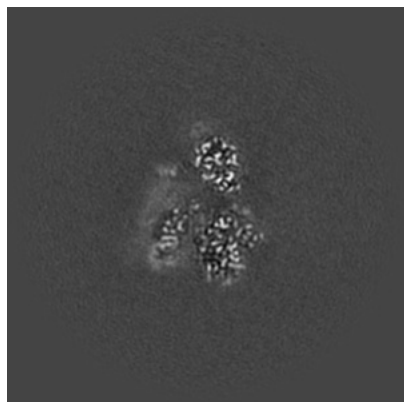


Z

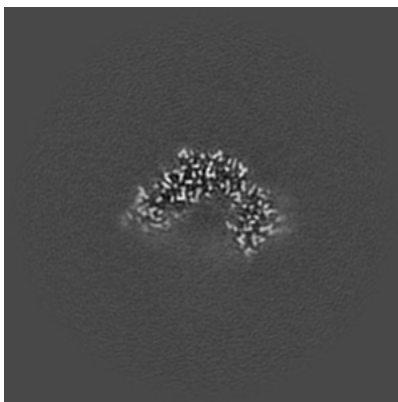
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

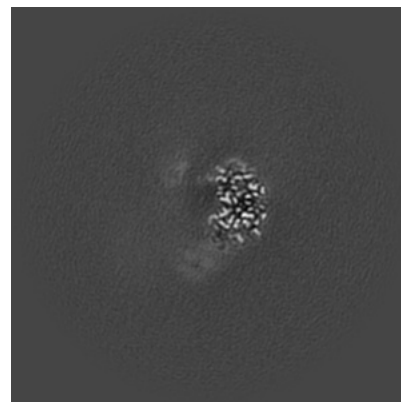
6.2.1 Primary map



X Index: 192

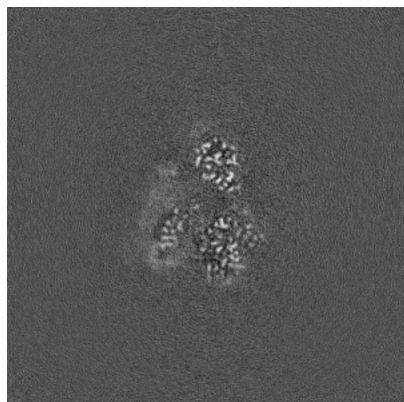


Y Index: 192

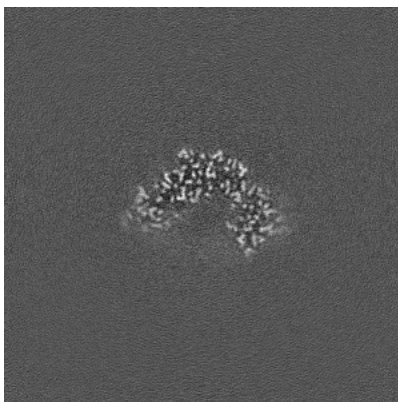


Z Index: 192

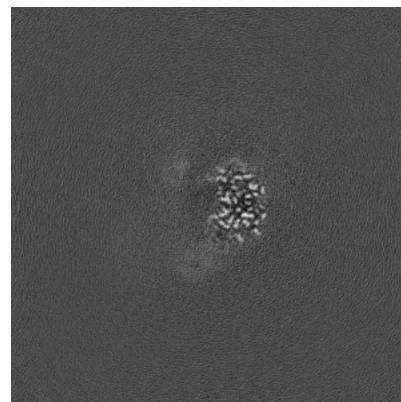
6.2.2 Raw map



X Index: 192



Y Index: 192

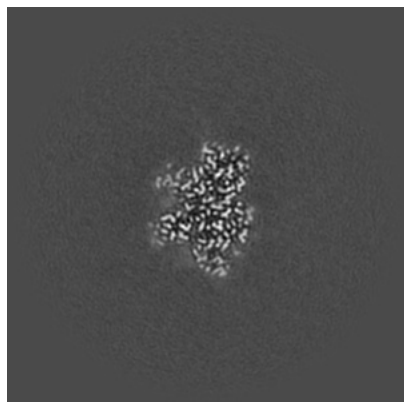


Z Index: 192

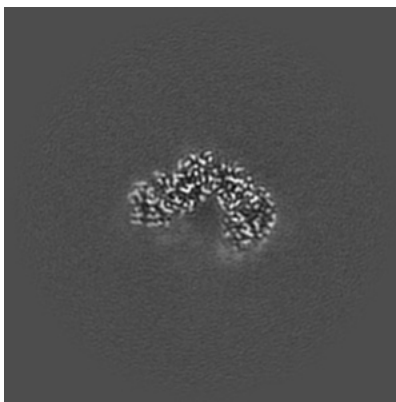
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

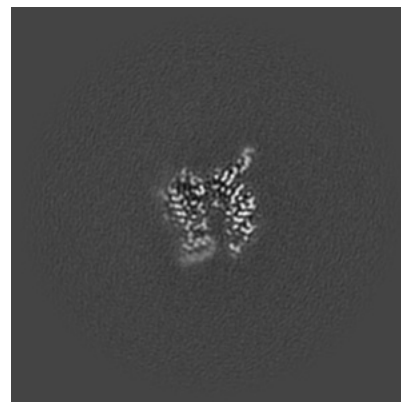
6.3.1 Primary map



X Index: 208

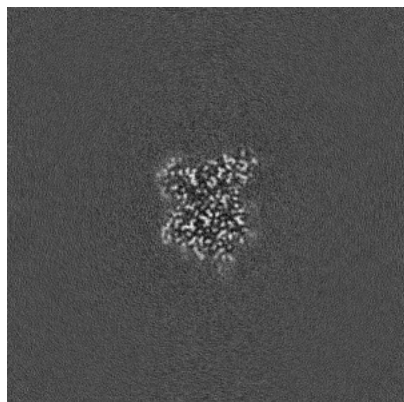


Y Index: 204

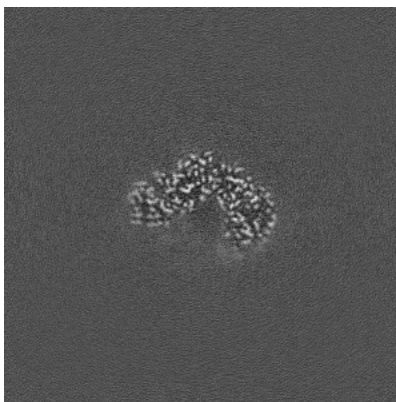


Z Index: 227

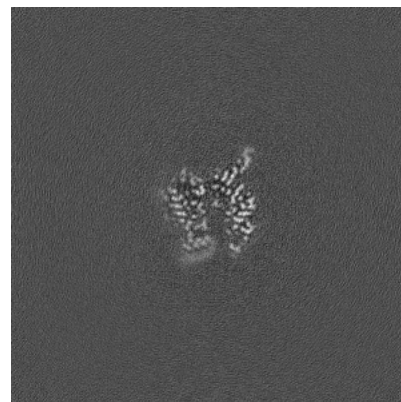
6.3.2 Raw map



X Index: 216



Y Index: 204

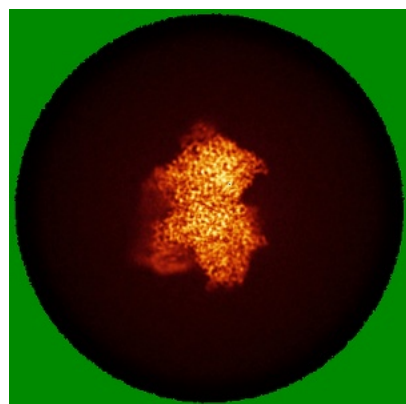


Z Index: 227

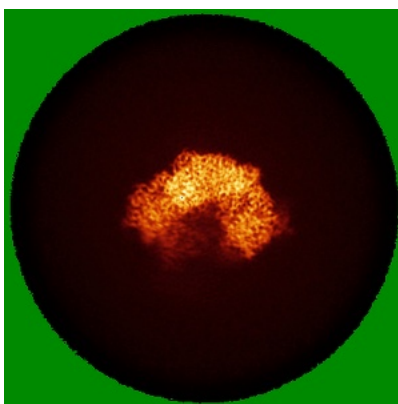
The images above show the largest variance slices of the map in three orthogonal directions.

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

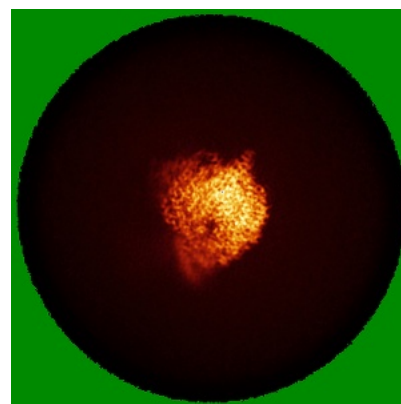
6.4.1 Primary map



X

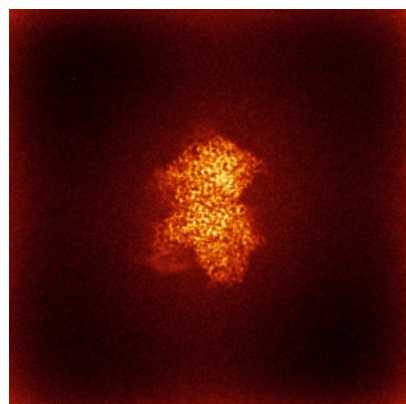


Y

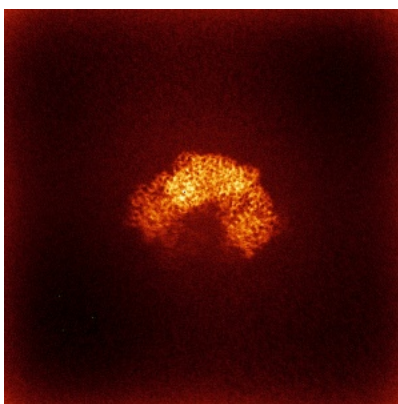


Z

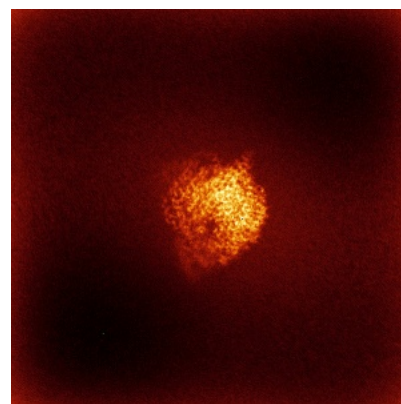
6.4.2 Raw map



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.

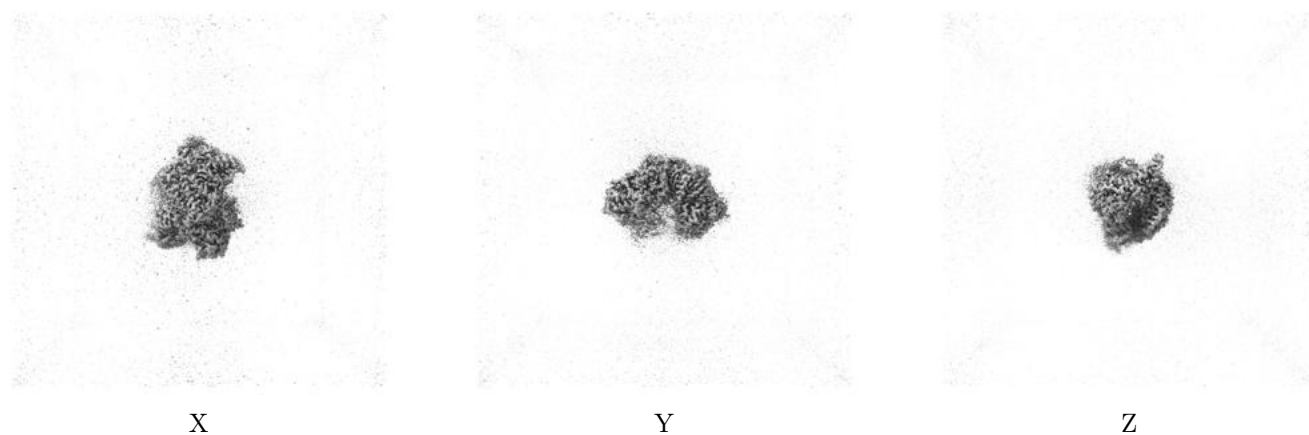
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

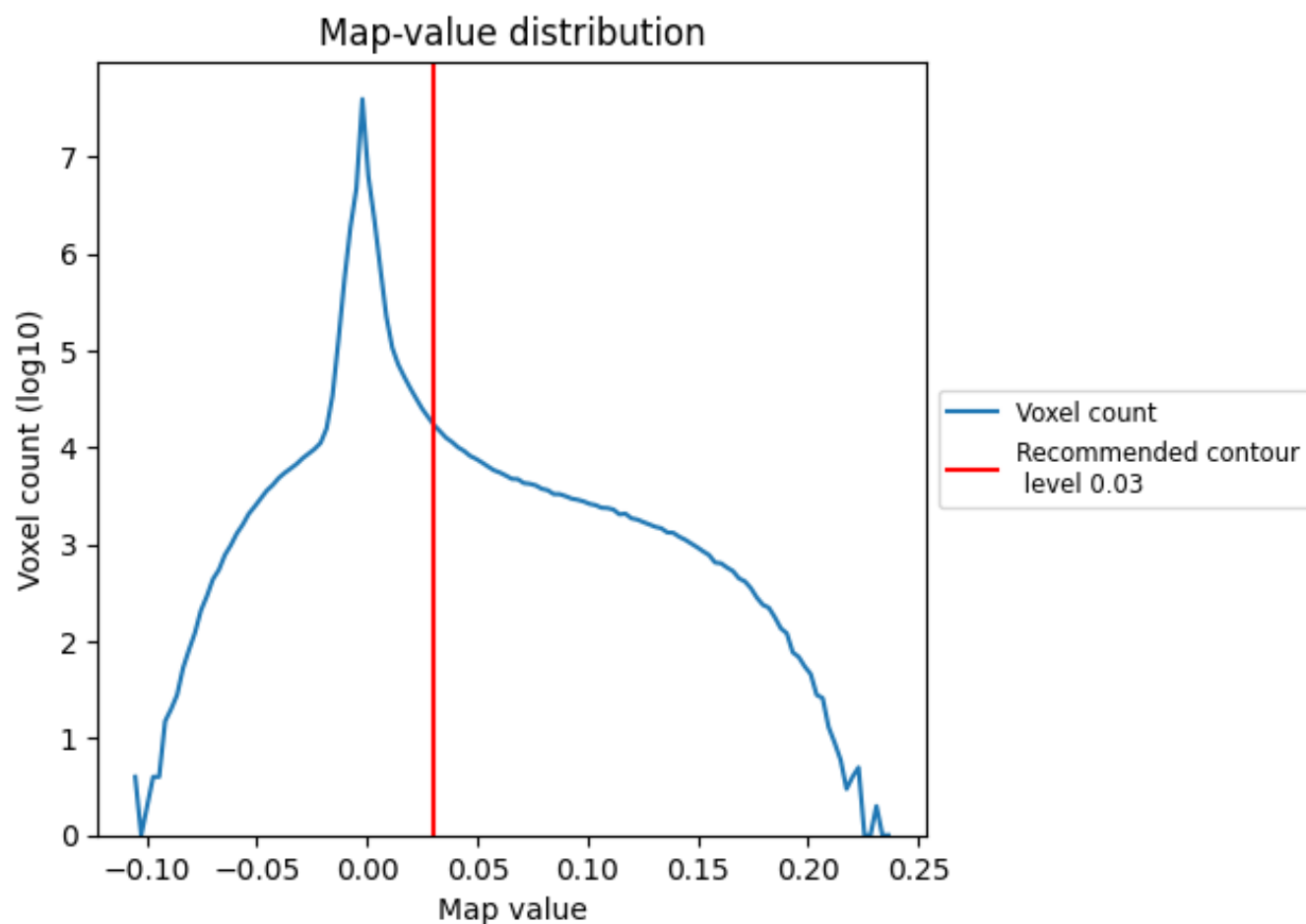
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

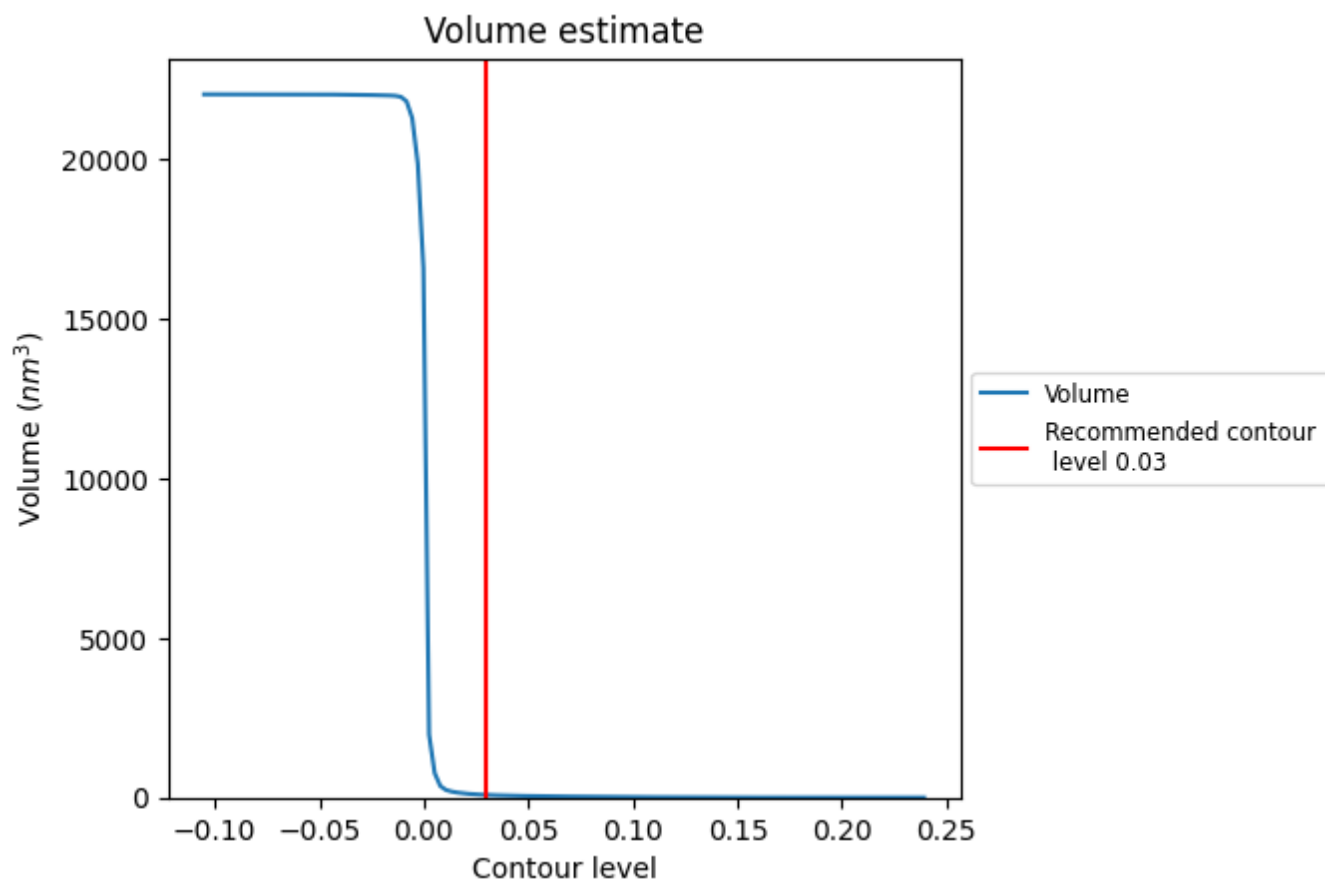
This section contains the results of statistical analysis of the map.

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.

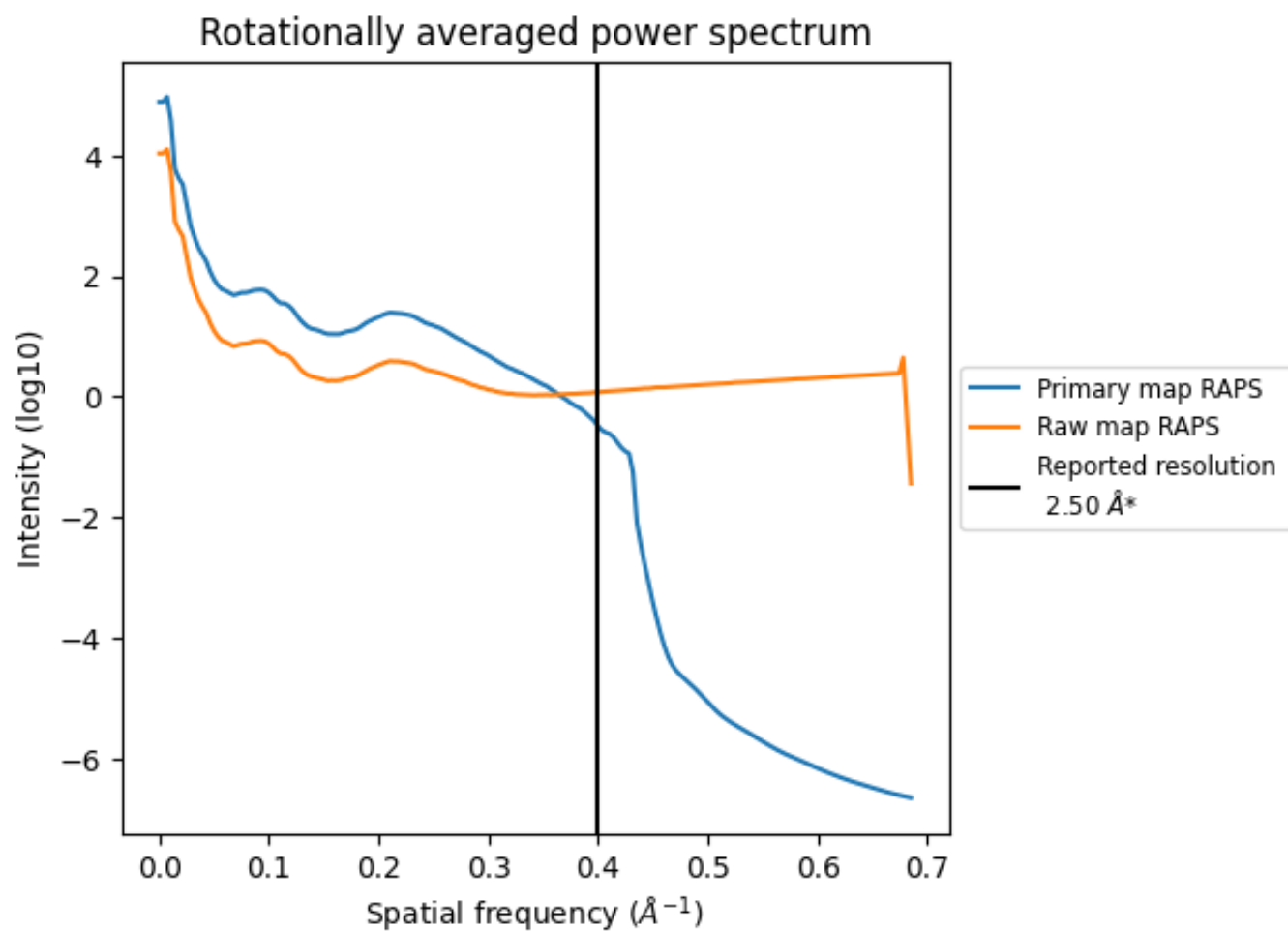
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82 nm^3 ; this corresponds to an approximate mass of 74 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 ⓘ

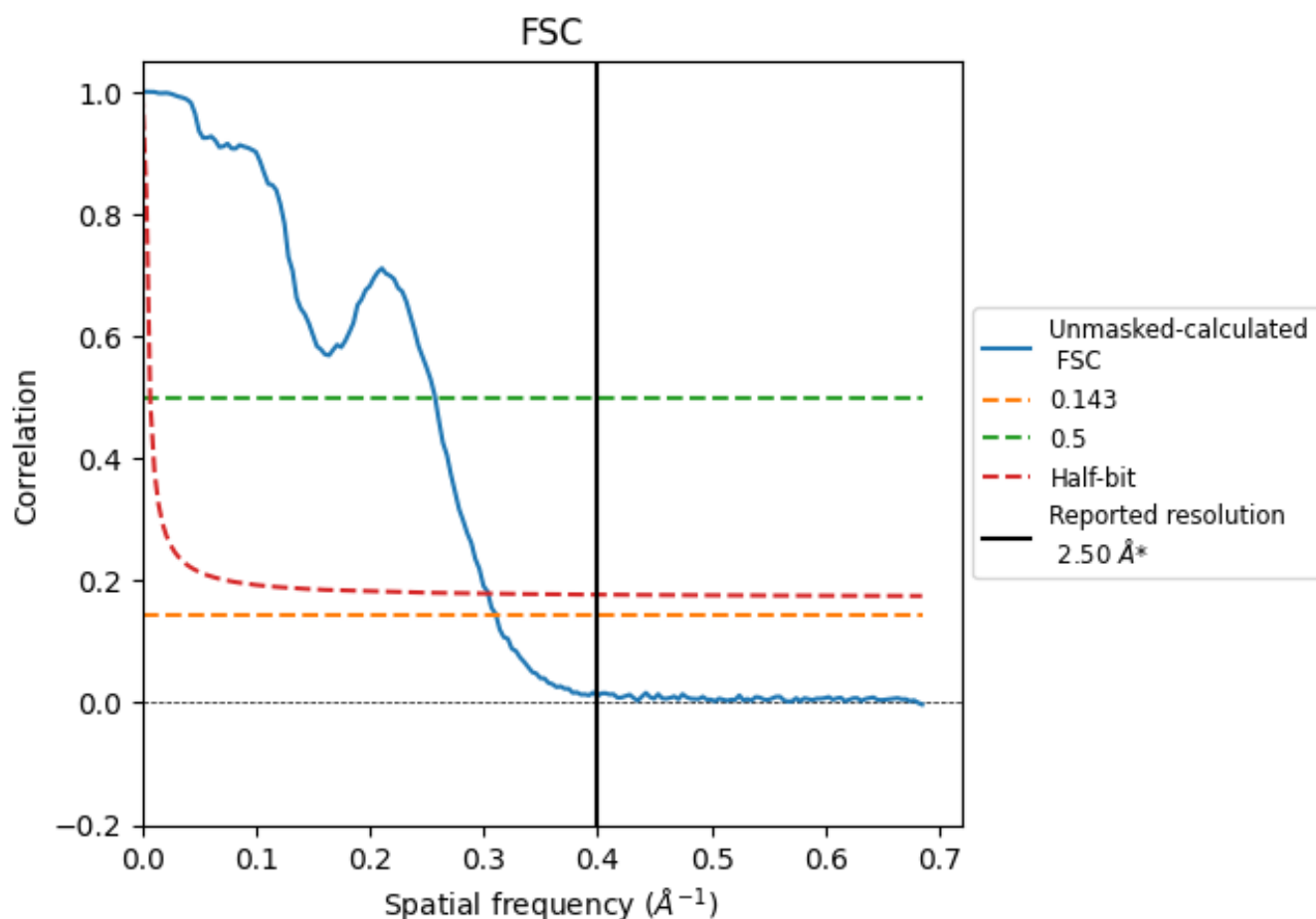


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 $0.400 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

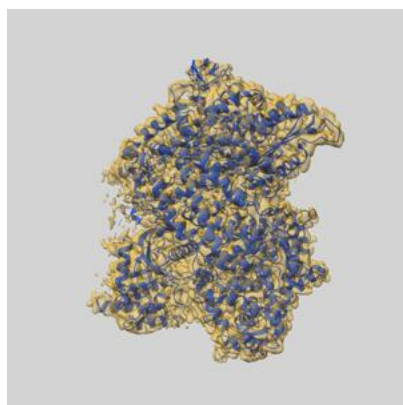
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.22	3.89	3.29

*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 3.22 differs from the reported value 2.5 by more than 10 %

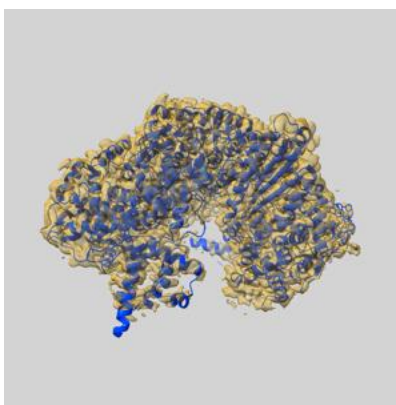
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-68657 and PDB model 22TH. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

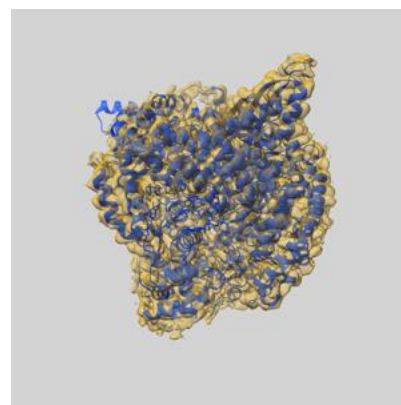
9.1 Map-model overlay [i](#)



X



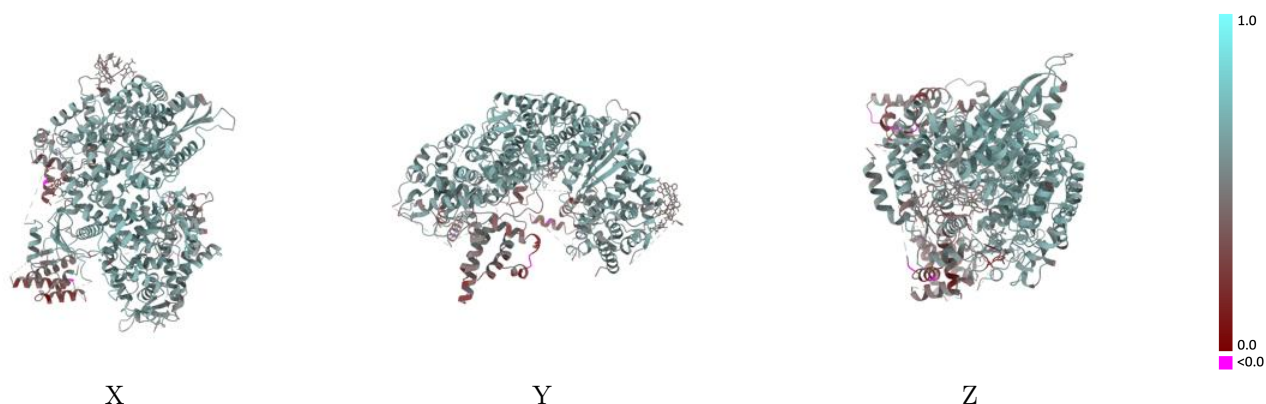
Y



Z

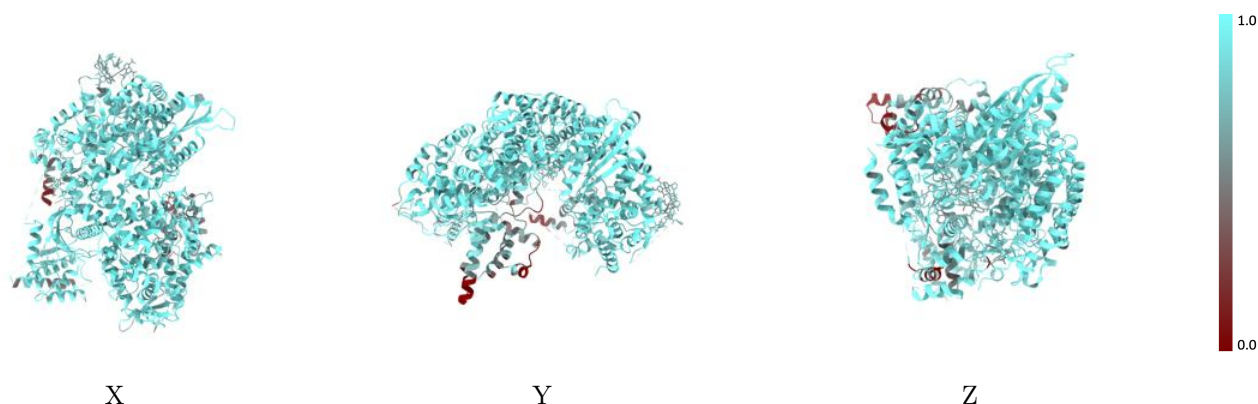
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



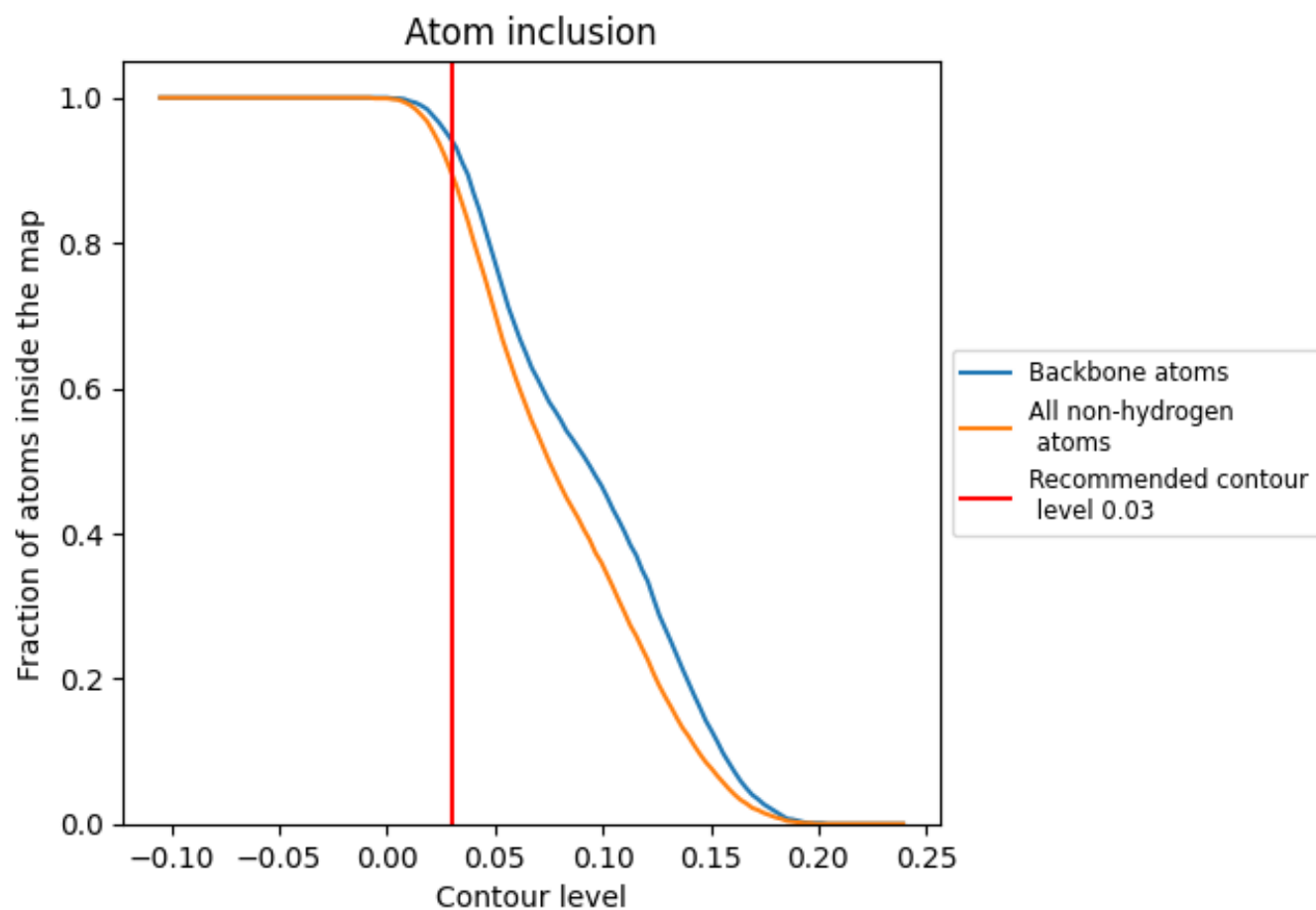
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8950	0.5600
A	0.8950	0.5600

