



Full wwPDB EM Validation Report ⓘ

May 19, 2025 – 12:15 PM JST

PDB ID : 8ZVZ / pdb_00008zvz
EMDB ID : EMD-60513
Title : Cryo-EM structure of Prostaglandin D2 Receptor DP1 activated by BW245C
Authors : Xu, J.; Xu, Y.; Wu, C.; Xu, H.E.
Deposited on : 2024-06-12
Resolution : 2.35 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

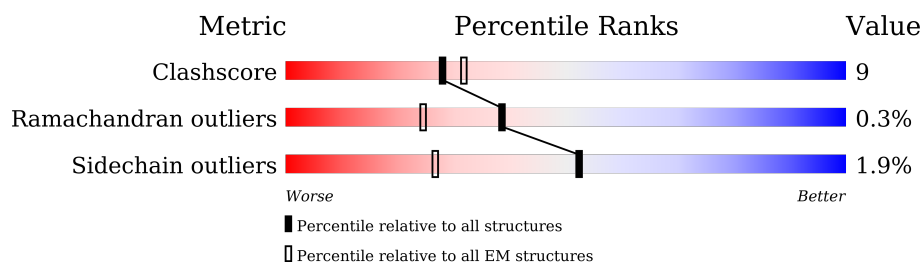
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.35 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	394	 55% 40%
2	B	345	 86% 12%
3	D	468	 49% 14% 35% 20%
4	G	71	 76% 20%
5	N	156	 71% 10% 18%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CLR	D	405	-	-	X	-
7	CLR	D	406	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8532 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 Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	236	Total	C	N	O	S	1	0
			1965	1236	357	365	7		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ASN	SER	engineered mutation	UNP P63092
A	226	ALA	GLY	engineered mutation	UNP P63092
A	268	ALA	GLU	engineered mutation	UNP P63092
A	271	LYS	ASN	engineered mutation	UNP P63092
A	274	ASP	LYS	engineered mutation	UNP P63092
A	280	LYS	ARG	engineered mutation	UNP P63092
A	284	ASP	THR	engineered mutation	UNP P63092
A	285	THR	ILE	engineered mutation	UNP P63092
A	366	SER	ALA	engineered mutation	UNP P63092

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	338	Total	C	N	O	S	0	0
			2600	1604	467	508	21		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	initiating methionine	UNP P62873
B	-3	GLY	-	expression tag	UNP P62873
B	-2	SER	-	expression tag	UNP P62873
B	-1	LEU	-	expression tag	UNP P62873
B	0	LEU	-	expression tag	UNP P62873
B	1	GLN	-	expression tag	UNP P62873

- Molecule 3 is a protein called Soluble cytochrome b562,Prostaglandin D2 receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	306	Total	C	N	O	S	0	0
			2391	1574	394	402	21		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-127	MET	-	initiating methionine	UNP P0ABE7
D	-126	LYS	-	expression tag	UNP P0ABE7
D	-125	THR	-	expression tag	UNP P0ABE7
D	-124	ILE	-	expression tag	UNP P0ABE7
D	-123	ILE	-	expression tag	UNP P0ABE7
D	-122	ALA	-	expression tag	UNP P0ABE7
D	-121	LEU	-	expression tag	UNP P0ABE7
D	-120	SER	-	expression tag	UNP P0ABE7
D	-119	TYR	-	expression tag	UNP P0ABE7
D	-118	ILE	-	expression tag	UNP P0ABE7
D	-117	PHE	-	expression tag	UNP P0ABE7
D	-116	CYS	-	expression tag	UNP P0ABE7
D	-115	LEU	-	expression tag	UNP P0ABE7
D	-114	VAL	-	expression tag	UNP P0ABE7
D	-105	TRP	MET	conflict	UNP P0ABE7
D	-10	ILE	HIS	conflict	UNP P0ABE7
D	-6	LEU	-	linker	UNP P0ABE7
D	-5	GLY	-	linker	UNP P0ABE7
D	-4	GLY	-	linker	UNP P0ABE7
D	-3	SER	-	linker	UNP P0ABE7
D	-2	GLY	-	linker	UNP P0ABE7
D	-1	GLY	-	linker	UNP P0ABE7
D	0	SER	-	linker	UNP P0ABE7

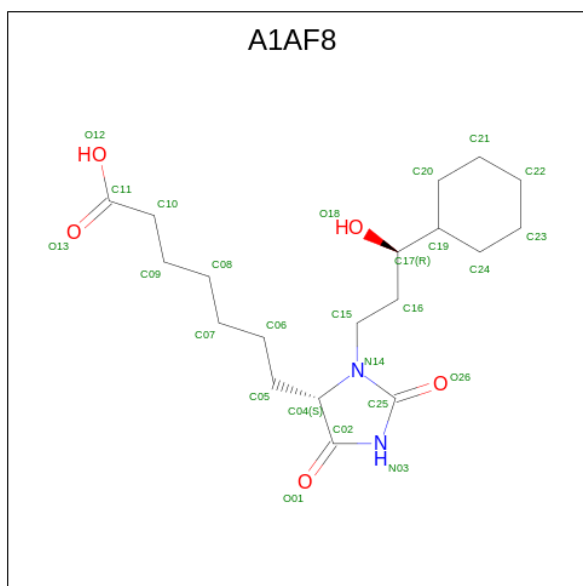
- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	57	Total	C	N	O	S	0	0
			436	273	77	83	3		

- Molecule 5 is a protein called nanobody Nb35.

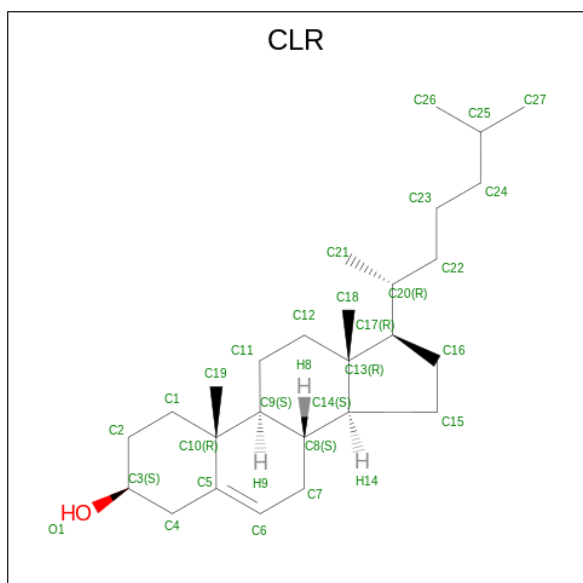
Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	128	Total	C	N	O	S	0	0
			973	605	170	192	6		

- Molecule 6 is 7-[(4S)-3-[(3R)-3-cyclohexyl-3-hydroxypropyl]-2,5-dioxoimidazolidin-4-yl]heptanoic acid (CCD ID: A1AF8) (formula: $C_{19}H_{32}N_2O_5$).



Mol	Chain	Residues	Atoms				AltConf
6	D	1	Total	C	N	O	0
			26	19	2	5	

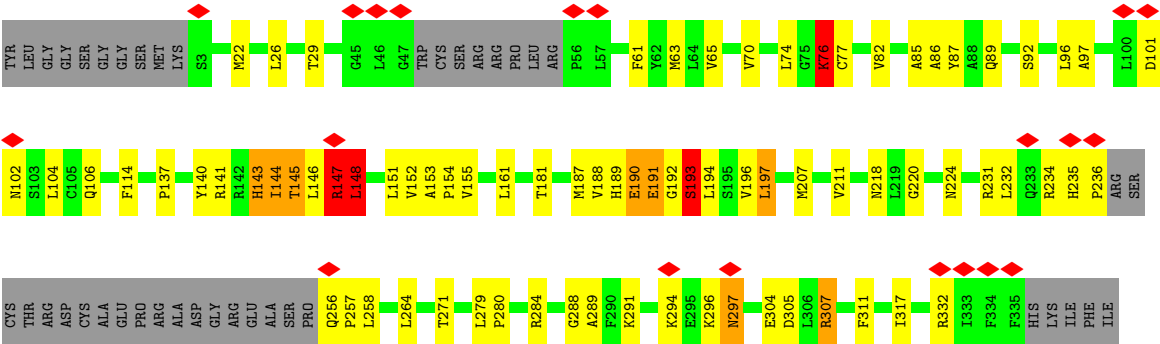
- Molecule 7 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



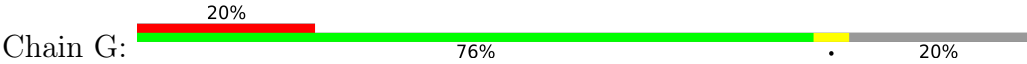
Mol	Chain	Residues	Atoms			AltConf
7	D	1	Total	C	O	0
			28	27	1	
7	D	1	Total	C	O	0
			28	27	1	
7	D	1	Total	C	O	0
			28	27	1	
7	D	1	Total	C	O	0
			28	27	1	
7	D	1	Total	C	O	0
			28	27	1	

- Molecule 8 is water.

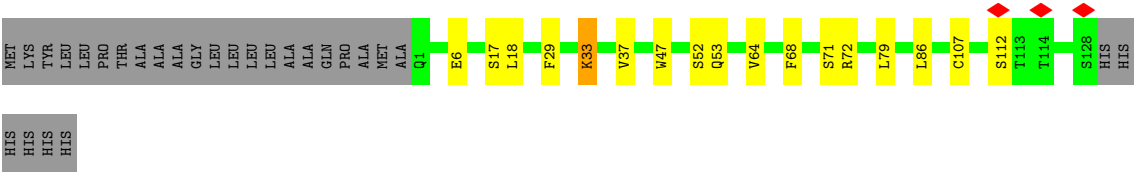
Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	O	0
			1	1	



- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 5: nanobody Nb35



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	224658	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.197	Depositor
Minimum map value	-2.369	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.322	Depositor
Map size (\AA)	263.68, 263.68, 263.68	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.824, 0.824, 0.824	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1AF8, CLR

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	0.45	2/2001 (0.1%)	0.42	1/2690 (0.0%)
2	B	0.09	0/2647	0.28	0/3589
3	D	0.64	6/2449 (0.2%)	0.71	12/3320 (0.4%)
4	G	0.08	0/442	0.22	0/597
5	N	0.10	0/993	0.28	0/1345
All	All	0.41	8/8532 (0.1%)	0.47	13/11541 (0.1%)

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
3	D	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	144	ILE	C-O	15.69	1.42	1.24
3	D	147	ARG	CA-C	-8.39	1.41	1.52
3	D	144	ILE	N-CA	6.94	1.55	1.46
1	A	34	LYS	CA-C	-6.74	1.43	1.52
3	D	144	ILE	CA-C	6.34	1.60	1.52
1	A	384	GLN	C-O	-6.04	1.17	1.24
3	D	307	ARG	C-O	-5.36	1.18	1.24
3	D	77	CYS	C-O	-5.25	1.17	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	143	HIS	O-C-N	-12.35	107.16	122.35
3	D	147	ARG	N-CA-C	-11.65	98.56	113.12
3	D	76	LYS	N-CA-C	-11.44	99.05	113.23
3	D	144	ILE	N-CA-C	10.15	130.45	109.34
3	D	144	ILE	CA-C-O	8.14	130.95	120.78
1	A	34	LYS	N-CA-C	-7.56	103.05	111.82
3	D	148	LEU	N-CA-C	-6.34	104.46	111.82
3	D	291	LYS	N-CA-C	6.24	120.60	112.92
3	D	146	LEU	CA-C-N	-5.90	111.21	122.53
3	D	146	LEU	C-N-CA	-5.90	111.21	122.53
3	D	148	LEU	CB-CG-CD1	-5.78	93.38	110.70
3	D	147	ARG	CA-C-N	-5.58	111.82	120.31
3	D	147	ARG	C-N-CA	-5.58	111.82	120.31

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	143	HIS	Mainchain
3	D	187	MET	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1965	0	1940	14	0
2	B	2600	0	2505	27	0
3	D	2391	0	2455	110	0
4	G	436	0	448	3	0
5	N	973	0	942	11	0
6	D	26	0	0	1	0
7	D	140	0	230	66	0
8	A	1	0	0	2	0
All	All	8532	0	8520	161	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 9.

All (161) 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)
3:D:29:THR:HG21	7:D:405:CLR:C24	1.55	1.34
3:D:22:MET:SD	7:D:405:CLR:H11	1.80	1.20
3:D:29:THR:CG2	7:D:405:CLR:H241	1.86	1.05
3:D:311:PHE:CZ	7:D:405:CLR:H6	1.96	1.01
3:D:189:HIS:CD2	3:D:193:SER:HB3	1.95	1.00
3:D:96:LEU:O	7:D:406:CLR:H42	1.64	0.97
3:D:29:THR:HG21	7:D:405:CLR:H241	0.97	0.96
3:D:29:THR:CG2	7:D:405:CLR:C24	2.47	0.92
3:D:22:MET:SD	7:D:405:CLR:C1	2.58	0.91
3:D:96:LEU:CG	7:D:406:CLR:H192	2.00	0.91
3:D:97:ALA:HB2	7:D:406:CLR:H6	1.52	0.90
3:D:96:LEU:HD21	7:D:406:CLR:C19	2.03	0.89
3:D:26:LEU:HD21	7:D:405:CLR:H122	1.55	0.89
3:D:191:GLU:HG2	3:D:192:GLY:N	1.92	0.84
3:D:96:LEU:CD1	7:D:406:CLR:H192	2.10	0.80
3:D:85:ALA:CB	7:D:406:CLR:H193	2.11	0.80
3:D:152:VAL:HA	7:D:404:CLR:C7	2.12	0.80
3:D:96:LEU:HG	7:D:406:CLR:H192	1.63	0.79
3:D:284:ARG:NH1	3:D:304:GLU:OE1	2.16	0.78
3:D:189:HIS:HD2	3:D:193:SER:HB3	1.47	0.78
3:D:96:LEU:CD2	7:D:406:CLR:C19	2.62	0.77
3:D:96:LEU:HD11	7:D:406:CLR:H192	1.65	0.77
3:D:152:VAL:HA	7:D:404:CLR:C6	2.17	0.75
3:D:152:VAL:HA	7:D:404:CLR:H71	1.68	0.75
3:D:96:LEU:CG	7:D:406:CLR:C19	2.64	0.75
1:A:274:ASP:OD1	1:A:278:ASN:ND2	2.19	0.75
3:D:96:LEU:HG	7:D:406:CLR:C19	2.17	0.74
2:B:218:CYS:O	4:G:18:GLN:NE2	2.21	0.73
2:B:230:ASN:ND2	2:B:246:ASP:OD1	2.23	0.72
3:D:26:LEU:CD2	7:D:405:CLR:H122	2.19	0.71
2:B:260:GLU:OE2	2:B:263:THR:OG1	2.07	0.71
3:D:96:LEU:CD2	7:D:406:CLR:H191	2.22	0.70
5:N:33:LYS:NZ	5:N:107:CYS:SG	2.63	0.70
3:D:29:THR:HG21	7:D:405:CLR:H242	1.70	0.70
3:D:311:PHE:CE1	7:D:405:CLR:H6	2.27	0.69
1:A:385:ARG:NH1	3:D:232:LEU:HB2	2.07	0.69
3:D:85:ALA:HB1	7:D:406:CLR:H193	1.74	0.68
3:D:152:VAL:HA	7:D:404:CLR:H6	1.76	0.68
3:D:232:LEU:HD12	3:D:236:PRO:O	1.94	0.66
2:B:231:ALA:HB1	2:B:276:VAL:HG22	1.78	0.65
3:D:189:HIS:CD2	3:D:193:SER:H	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:189:HIS:HD2	3:D:193:SER:N	1.95	0.65
2:B:74:SER:OG	2:B:76:ASP:OD1	2.12	0.65
3:D:85:ALA:HB3	7:D:406:CLR:H193	1.79	0.64
3:D:96:LEU:HD21	7:D:406:CLR:H191	1.80	0.63
2:B:333:ASP:O	2:B:334:SER:OG	2.14	0.63
4:G:47:GLU:N	4:G:47:GLU:OE1	2.31	0.62
2:B:32:GLN:N	2:B:32:GLN:OE1	2.33	0.62
3:D:189:HIS:HD2	3:D:193:SER:H	1.46	0.62
2:B:31:SER:OG	2:B:32:GLN:OE1	2.15	0.62
3:D:148:LEU:HD11	7:D:404:CLR:H17	1.82	0.61
1:A:229:ASP:OD2	5:N:112:SER:N	2.32	0.61
3:D:63:MET:HE2	7:D:402:CLR:H271	1.83	0.61
3:D:220:GLY:O	3:D:224:ASN:ND2	2.33	0.61
3:D:192:GLY:O	3:D:193:SER:C	2.44	0.61
7:D:405:CLR:H212	7:D:405:CLR:H121	1.82	0.60
3:D:70:VAL:HG12	7:D:402:CLR:H152	1.82	0.60
1:A:381:ASP:O	1:A:385:ARG:HG3	2.00	0.60
3:D:307:ARG:NE	7:D:405:CLR:O1	2.34	0.60
3:D:29:THR:HG21	7:D:405:CLR:C25	2.29	0.59
2:B:44:GLN:N	2:B:44:GLN:OE1	2.35	0.59
3:D:114:PHE:CZ	7:D:402:CLR:H21	2.38	0.59
3:D:191:GLU:HG2	3:D:192:GLY:H	1.68	0.58
5:N:6:GLU:OE1	5:N:6:GLU:N	2.36	0.58
3:D:29:THR:CG2	7:D:405:CLR:H25	2.34	0.57
3:D:192:GLY:O	3:D:194:LEU:N	2.37	0.57
3:D:82:VAL:HG22	7:D:406:CLR:H181	1.85	0.57
7:D:404:CLR:H212	7:D:404:CLR:H121	1.87	0.57
3:D:145:THR:C	3:D:147:ARG:H	2.12	0.57
7:D:406:CLR:H212	7:D:406:CLR:H121	1.86	0.57
3:D:148:LEU:O	3:D:152:VAL:HG23	2.05	0.57
3:D:189:HIS:ND1	3:D:190:GLU:N	2.52	0.57
3:D:76:LYS:HE2	6:D:401:A1AF8:O26	2.05	0.56
3:D:140:TYR:HA	3:D:144:ILE:HD13	1.86	0.56
3:D:29:THR:CG2	7:D:405:CLR:C25	2.83	0.56
3:D:97:ALA:HB2	7:D:406:CLR:C6	2.31	0.56
3:D:70:VAL:CG1	7:D:402:CLR:H152	2.37	0.54
5:N:52:SER:O	5:N:72:ARG:NH2	2.41	0.54
5:N:17:SER:C	5:N:18:LEU:HD22	2.32	0.54
2:B:5:ASP:OD1	2:B:8:ARG:NH1	2.42	0.53
3:D:22:MET:CE	7:D:405:CLR:H11	2.38	0.53
3:D:148:LEU:HD11	7:D:404:CLR:H161	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ARG:HH12	3:D:232:LEU:HB2	1.73	0.53
3:D:114:PHE:CE2	7:D:402:CLR:H3	2.43	0.53
3:D:61:PHE:O	3:D:65:VAL:HG23	2.10	0.52
3:D:207:MET:O	3:D:211:VAL:HG23	2.09	0.52
3:D:307:ARG:CZ	7:D:405:CLR:O1	2.56	0.52
3:D:151:LEU:HB2	7:D:404:CLR:H151	1.91	0.52
3:D:155:VAL:HB	7:D:404:CLR:H72	1.91	0.52
5:N:29:PHE:O	5:N:72:ARG:NH1	2.42	0.52
3:D:70:VAL:HG12	7:D:402:CLR:C15	2.39	0.52
3:D:26:LEU:HD21	7:D:405:CLR:C12	2.33	0.52
2:B:128:THR:OG1	2:B:132:ASN:O	2.20	0.51
3:D:296:LYS:O	3:D:297:ASN:C	2.53	0.51
3:D:101:ASP:OD1	3:D:102:ASN:N	2.44	0.51
3:D:145:THR:C	3:D:147:ARG:N	2.66	0.51
3:D:311:PHE:CE1	7:D:405:CLR:C6	2.94	0.51
3:D:144:ILE:C	3:D:145:THR:HG23	2.36	0.50
3:D:106:GLN:HB2	7:D:403:CLR:H193	1.93	0.50
3:D:148:LEU:HD11	7:D:404:CLR:C17	2.42	0.50
2:B:286:LEU:HG	2:B:296:VAL:HG22	1.94	0.50
8:A:401:HOH:O	3:D:141:ARG:CD	2.60	0.49
2:B:86:THR:O	2:B:87:THR:OG1	2.25	0.49
2:B:61:MET:HE3	2:B:70:LEU:HD13	1.94	0.49
3:D:218:ASN:ND2	3:D:271:THR:OG1	2.43	0.48
2:B:221:THR:N	4:G:22:GLU:OE2	2.45	0.48
3:D:193:SER:O	3:D:194:LEU:C	2.54	0.48
1:A:238:PHE:O	1:A:241:VAL:HG22	2.13	0.48
3:D:144:ILE:HG22	3:D:145:THR:N	2.27	0.48
5:N:37:VAL:HG12	5:N:47:TRP:HA	1.95	0.48
1:A:224:VAL:HG11	1:A:234:TRP:CH2	2.48	0.48
3:D:148:LEU:HD11	7:D:404:CLR:C16	2.44	0.48
2:B:93:ILE:HD12	2:B:93:ILE:N	2.29	0.48
2:B:254:ASP:HB2	2:B:261:LEU:HD11	1.96	0.47
3:D:189:HIS:CG	3:D:190:GLU:N	2.83	0.47
5:N:53:GLN:OE1	5:N:53:GLN:N	2.44	0.47
8:A:401:HOH:O	3:D:141:ARG:HD2	2.13	0.47
2:B:231:ALA:CB	2:B:276:VAL:HG22	2.44	0.47
3:D:29:THR:HG22	7:D:405:CLR:H25	1.96	0.46
2:B:195:ASP:O	2:B:196:THR:OG1	2.25	0.46
3:D:148:LEU:HA	3:D:148:LEU:HD12	0.98	0.46
1:A:263:THR:OG1	1:A:264:ASN:N	2.49	0.46
3:D:193:SER:O	3:D:193:SER:OG	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:92:SER:O	3:D:96:LEU:N	2.48	0.45
3:D:153:ALA:HB3	3:D:154:PRO:HD3	1.99	0.45
3:D:317:ILE:HG22	7:D:405:CLR:H272	1.97	0.45
3:D:197:LEU:HD21	3:D:289:ALA:HA	1.97	0.45
3:D:148:LEU:HD11	7:D:404:CLR:H232	1.98	0.45
3:D:85:ALA:O	3:D:89:GLN:NE2	2.50	0.44
3:D:284:ARG:NE	3:D:305:ASP:OD1	2.46	0.44
3:D:22:MET:CE	7:D:405:CLR:C2	2.95	0.44
3:D:258:LEU:HD21	3:D:332:ARG:CD	2.48	0.44
3:D:96:LEU:HD21	7:D:406:CLR:H193	1.96	0.44
1:A:384:GLN:HG3	3:D:137:PRO:HG3	1.98	0.44
2:B:163:ASP:O	2:B:164:THR:OG1	2.27	0.44
3:D:82:VAL:CG2	7:D:406:CLR:H181	2.47	0.43
3:D:188:VAL:HG22	3:D:288:GLY:HA3	2.00	0.43
3:D:104:LEU:HD21	7:D:406:CLR:H72	2.00	0.43
3:D:87:TYR:CE2	3:D:181:THR:HG21	2.54	0.43
2:B:286:LEU:HD12	2:B:286:LEU:N	2.34	0.43
3:D:97:ALA:CB	7:D:406:CLR:H6	2.36	0.43
3:D:256:GLN:N	3:D:257:PRO:CD	2.82	0.43
5:N:71:SER:O	5:N:79:LEU:HD12	2.18	0.43
3:D:86:ALA:HB1	3:D:181:THR:HG22	2.00	0.43
3:D:22:MET:HE3	7:D:405:CLR:H21	2.01	0.42
3:D:279:LEU:N	3:D:280:PRO:CD	2.82	0.42
3:D:104:LEU:CD2	7:D:406:CLR:H72	2.49	0.42
2:B:307:VAL:C	2:B:308:LEU:HD12	2.45	0.42
2:B:30:LEU:HD23	2:B:262:MET:SD	2.60	0.42
1:A:381:ASP:OD2	3:D:231:ARG:NE	2.53	0.42
3:D:193:SER:OG	3:D:196:VAL:HG23	2.19	0.42
1:A:34:LYS:HZ2	1:A:34:LYS:HG2	1.71	0.41
1:A:32:LYS:HB2	1:A:32:LYS:HE2	1.51	0.41
2:B:65:THR:OG1	2:B:107:PRO:O	2.36	0.41
5:N:64:VAL:HG13	5:N:68:PHE:CD2	2.55	0.41
5:N:86:LEU:HD12	5:N:86:LEU:N	2.35	0.41
1:A:229:ASP:OD1	1:A:229:ASP:N	2.54	0.41
1:A:382:ILE:HG22	1:A:386:MET:HE2	2.02	0.41
2:B:61:MET:HE1	2:B:328:ALA:CB	2.51	0.41
2:B:164:THR:HG22	2:B:185:GLY:C	2.46	0.41
2:B:286:LEU:HD22	2:B:327:VAL:HG21	2.02	0.41

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	231/394 (59%)	225 (97%)	6 (3%)	0	100	100
2	B	336/345 (97%)	334 (99%)	2 (1%)	0	100	100
3	D	300/468 (64%)	289 (96%)	8 (3%)	3 (1%)	13	13
4	G	55/71 (78%)	55 (100%)	0	0	100	100
5	N	126/156 (81%)	126 (100%)	0	0	100	100
All	All	1048/1434 (73%)	1029 (98%)	16 (2%)	3 (0%)	38	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	193	SER
3	D	297	ASN
3	D	234	ARG

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	213/350 (61%)	209 (98%)	4 (2%)	52	65
2	B	281/287 (98%)	281 (100%)	0	100	100
3	D	260/392 (66%)	247 (95%)	13 (5%)	20	25
4	G	46/58 (79%)	46 (100%)	0	100	100
5	N	106/126 (84%)	105 (99%)	1 (1%)	75	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	906/1213 (75%)	888 (98%)	18 (2%)	52 63

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	357	HIS
1	A	390[A]	GLN
1	A	390[B]	GLN
3	D	74	LEU
3	D	76	LYS
3	D	145	THR
3	D	147	ARG
3	D	148	LEU
3	D	161	LEU
3	D	190	GLU
3	D	191	GLU
3	D	193	SER
3	D	197	LEU
3	D	235	HIS
3	D	264	LEU
3	D	294	LYS
5	N	33	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	220	HIS
1	A	267	GLN
1	A	278	ASN
1	A	279	ASN
2	B	175	GLN
3	D	89	GLN
3	D	189	HIS
3	D	229	HIS
3	D	233	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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
7	CLR	D	404	-	31,31,31	1.05	3 (9%)	48,48,48	1.59	9 (18%)
7	CLR	D	403	-	31,31,31	0.56	0	48,48,48	1.22	5 (10%)
7	CLR	D	402	-	31,31,31	0.61	0	48,48,48	1.56	9 (18%)
7	CLR	D	406	-	31,31,31	1.00	2 (6%)	48,48,48	1.62	8 (16%)
7	CLR	D	405	-	31,31,31	1.04	2 (6%)	48,48,48	1.40	7 (14%)
6	A1AF8	D	401	-	27,27,27	1.89	5 (18%)	29,35,35	1.24	4 (13%)

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
7	CLR	D	404	-	-	1/10/68/68	0/4/4/4
7	CLR	D	403	-	-	3/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CLR	D	402	-	-	4/10/68/68	0/4/4/4
7	CLR	D	406	-	-	4/10/68/68	0/4/4/4
7	CLR	D	405	-	-	2/10/68/68	0/4/4/4
6	A1AF8	D	401	-	-	4/18/42/42	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	401	A1AF8	C25-N14	6.27	1.47	1.36
6	D	401	A1AF8	C02-N03	3.53	1.42	1.37
6	D	401	A1AF8	C25-N03	3.53	1.45	1.38
6	D	401	A1AF8	O26-C25	-3.52	1.16	1.23
6	D	401	A1AF8	O01-C02	-2.94	1.17	1.23
7	D	404	CLR	C10-C9	-2.71	1.51	1.56
7	D	406	CLR	C10-C9	-2.35	1.52	1.56
7	D	405	CLR	C13-C14	-2.24	1.50	1.55
7	D	404	CLR	C12-C13	-2.19	1.50	1.54
7	D	405	CLR	C10-C9	-2.15	1.52	1.56
7	D	406	CLR	C13-C14	-2.03	1.51	1.55
7	D	404	CLR	C13-C14	-2.02	1.51	1.55

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	406	CLR	C4-C5-C10	5.51	123.74	116.42
7	D	402	CLR	C3-C4-C5	-4.01	105.22	112.03
7	D	402	CLR	C12-C11-C9	3.97	120.00	113.11
7	D	404	CLR	C7-C8-C9	3.95	114.50	109.71
7	D	404	CLR	C14-C8-C9	-3.73	104.10	109.09
7	D	404	CLR	C4-C5-C10	3.44	120.99	116.42
7	D	405	CLR	C3-C4-C5	-3.37	106.30	112.03
7	D	403	CLR	C19-C10-C5	-3.37	102.89	108.34
7	D	406	CLR	C9-C10-C5	-3.26	104.54	109.65
7	D	402	CLR	C19-C10-C5	-3.22	103.13	108.34
7	D	406	CLR	C7-C8-C9	3.21	113.60	109.71
7	D	405	CLR	C8-C7-C6	-2.97	108.46	112.73
6	D	401	A1AF8	C15-N14-C25	2.90	127.69	121.51
7	D	404	CLR	C2-C3-C4	-2.88	106.36	110.31
7	D	406	CLR	C4-C5-C6	-2.86	116.49	120.61
7	D	405	CLR	C10-C9-C8	-2.81	108.51	112.73
7	D	402	CLR	C1-C2-C3	2.73	113.97	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	402	CLR	C1-C10-C9	2.73	112.54	108.73
7	D	406	CLR	C1-C2-C3	-2.73	106.97	110.47
7	D	405	CLR	C21-C20-C17	-2.65	108.86	112.92
7	D	404	CLR	C15-C14-C8	-2.65	114.71	119.08
7	D	405	CLR	C15-C14-C8	-2.59	114.82	119.08
7	D	402	CLR	C15-C14-C8	-2.57	114.86	119.08
7	D	405	CLR	C21-C20-C22	2.55	114.36	110.36
6	D	401	A1AF8	C15-N14-C04	2.52	126.39	122.19
7	D	404	CLR	C10-C9-C8	-2.51	108.98	112.73
7	D	403	CLR	C21-C20-C22	-2.46	106.51	110.36
7	D	406	CLR	C14-C8-C9	-2.42	105.86	109.09
7	D	403	CLR	C19-C10-C9	2.38	114.52	111.68
7	D	404	CLR	C9-C10-C5	-2.37	105.93	109.65
6	D	401	A1AF8	C05-C04-N14	-2.25	110.20	114.35
7	D	403	CLR	C2-C1-C10	2.25	117.61	112.74
7	D	403	CLR	C12-C11-C9	2.21	116.94	113.11
7	D	402	CLR	C19-C10-C1	2.19	112.89	109.43
7	D	404	CLR	C1-C10-C5	2.17	112.73	108.75
7	D	404	CLR	C1-C2-C3	-2.16	107.70	110.47
7	D	402	CLR	C11-C9-C10	2.12	115.87	113.08
7	D	405	CLR	C4-C5-C6	-2.08	117.61	120.61
6	D	401	A1AF8	O12-C11-C10	2.07	120.67	114.03
7	D	406	CLR	C10-C5-C6	-2.05	119.77	122.90
7	D	406	CLR	C1-C10-C5	2.03	112.47	108.75
7	D	402	CLR	C11-C9-C8	2.02	114.66	111.75

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	406	CLR	C17-C20-C22-C23
7	D	406	CLR	C21-C20-C22-C23
7	D	402	CLR	C17-C20-C22-C23
7	D	402	CLR	C21-C20-C22-C23
7	D	402	CLR	C22-C23-C24-C25
7	D	403	CLR	C17-C20-C22-C23
7	D	405	CLR	C20-C22-C23-C24
7	D	405	CLR	C22-C23-C24-C25
6	D	401	A1AF8	C07-C08-C09-C10
6	D	401	A1AF8	C08-C09-C10-C11
7	D	406	CLR	C22-C23-C24-C25
7	D	403	CLR	C22-C23-C24-C25

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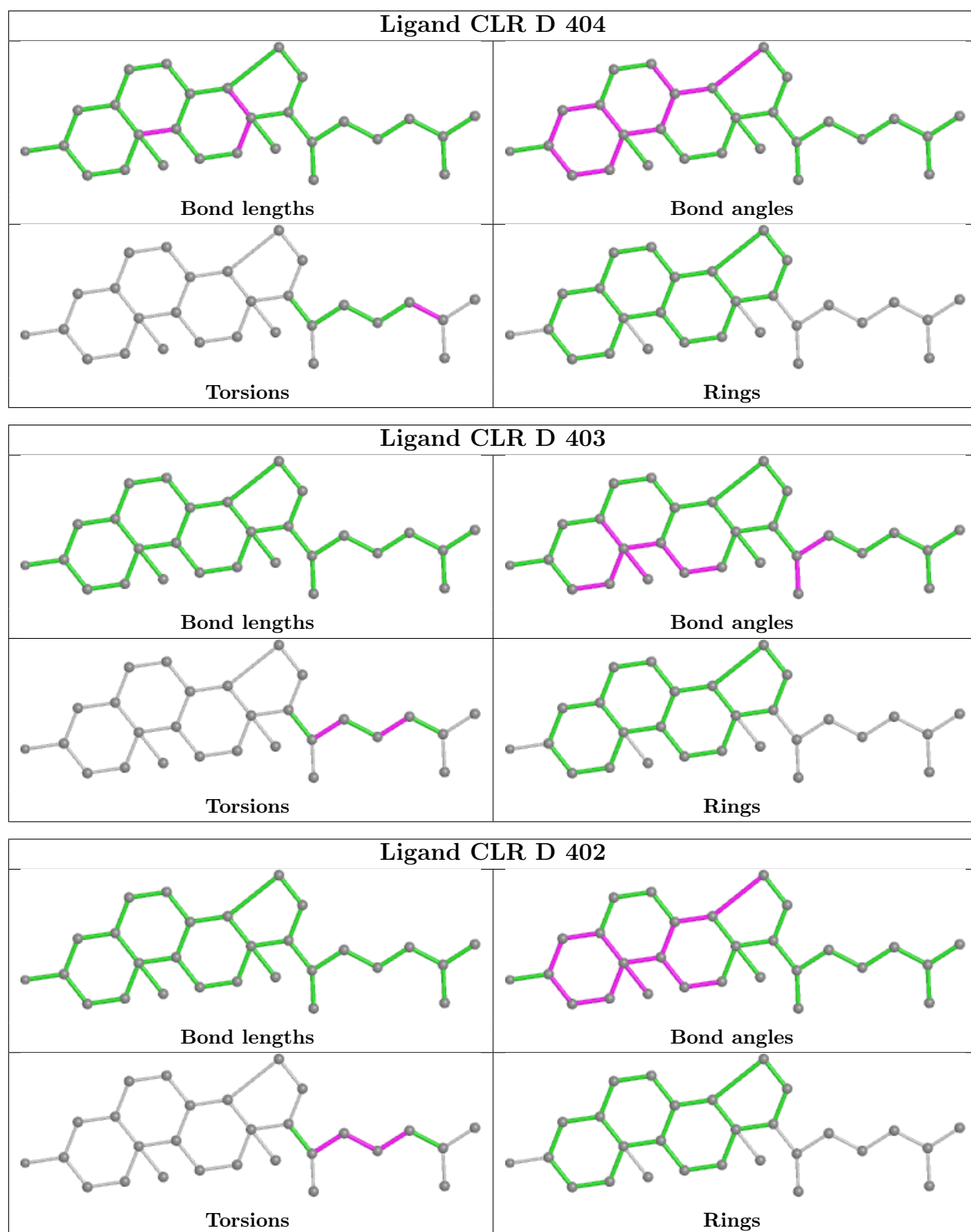
Mol	Chain	Res	Type	Atoms
7	D	403	CLR	C21-C20-C22-C23
7	D	402	CLR	C20-C22-C23-C24
7	D	406	CLR	C20-C22-C23-C24
6	D	401	A1AF8	C09-C10-C11-O13
6	D	401	A1AF8	C09-C10-C11-O12
7	D	404	CLR	C23-C24-C25-C27

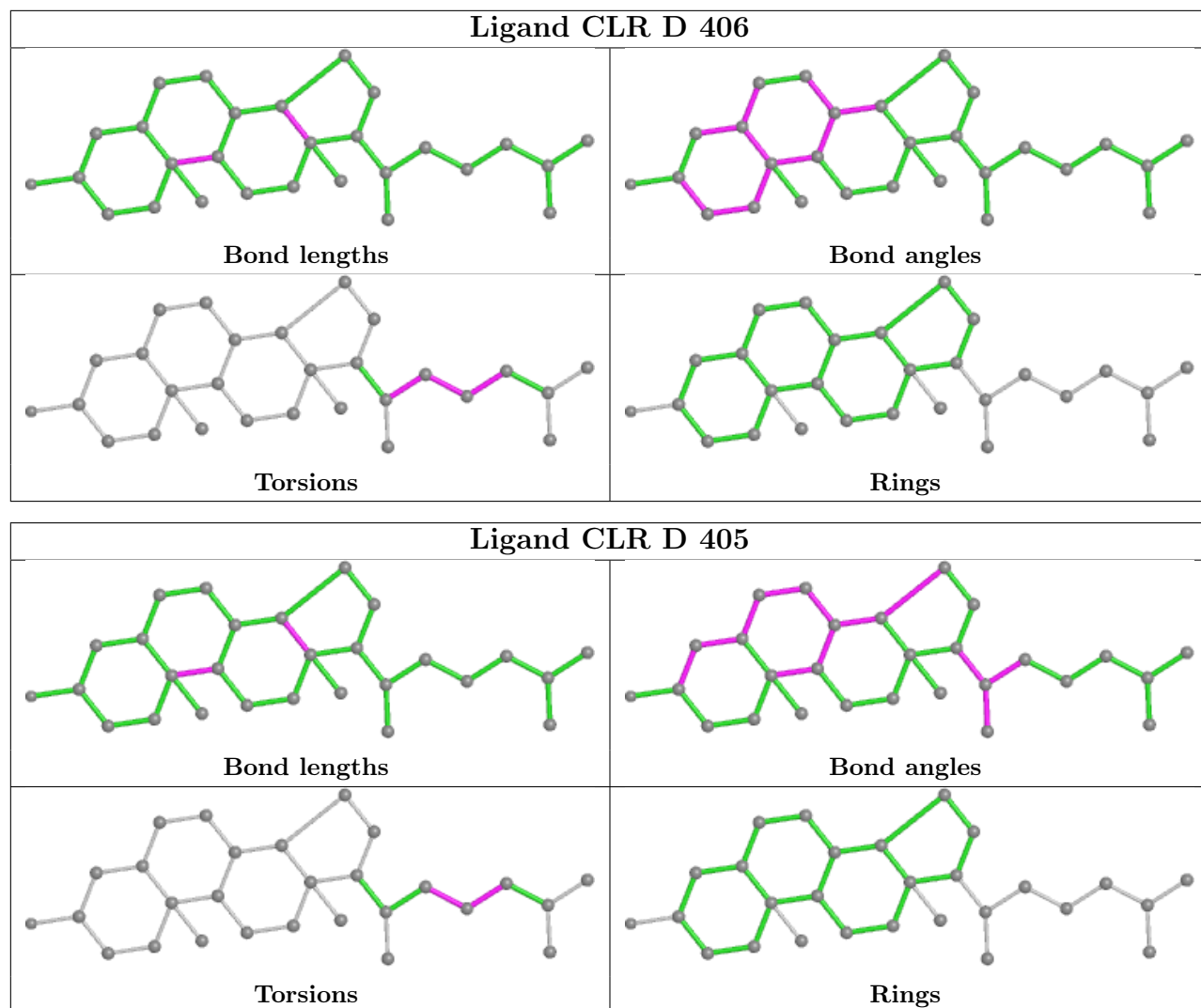
There are no ring outliers.

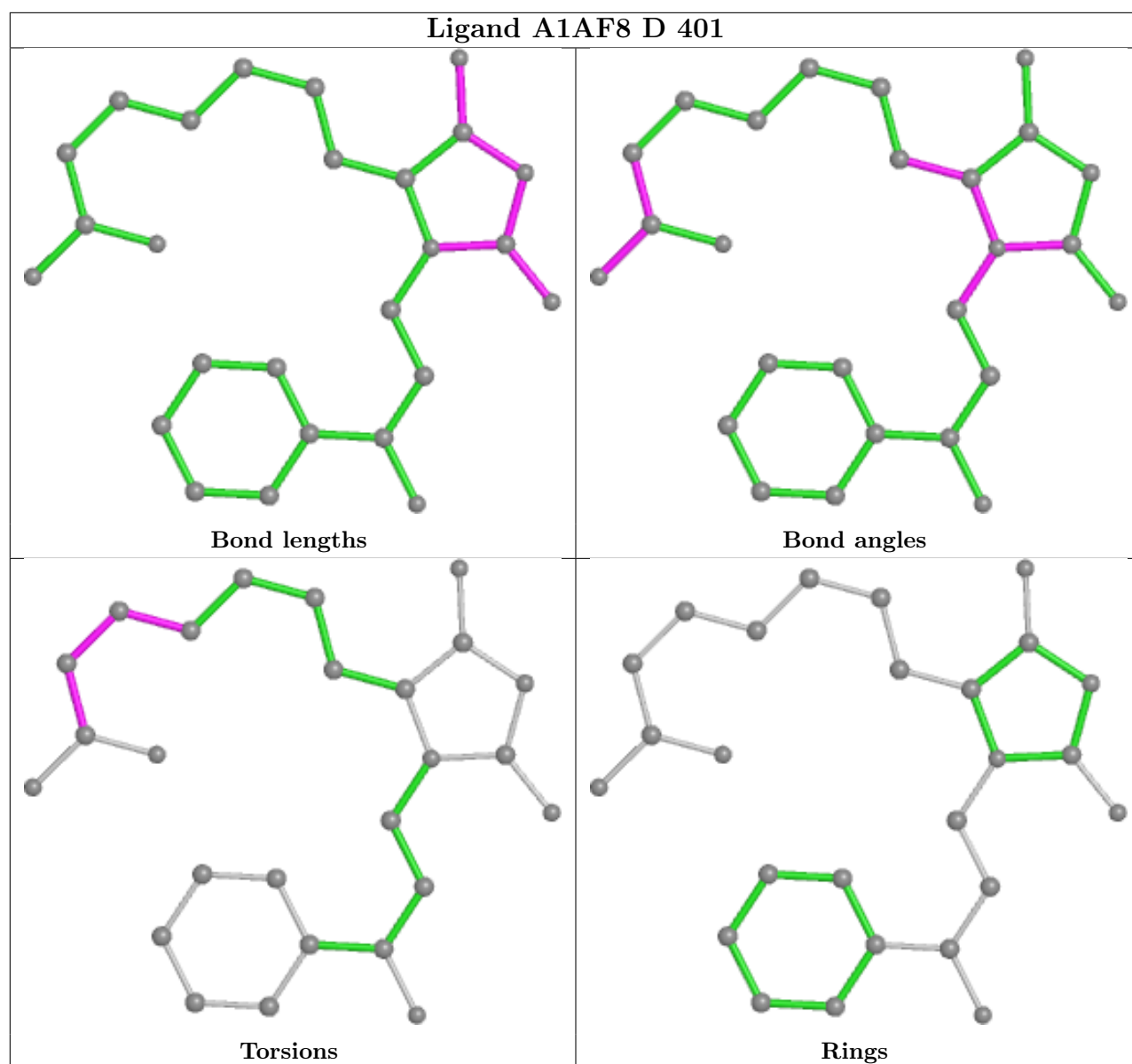
6 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	404	CLR	12	0
7	D	403	CLR	1	0
7	D	402	CLR	6	0
7	D	406	CLR	23	0
7	D	405	CLR	24	0
6	D	401	A1AF8	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.

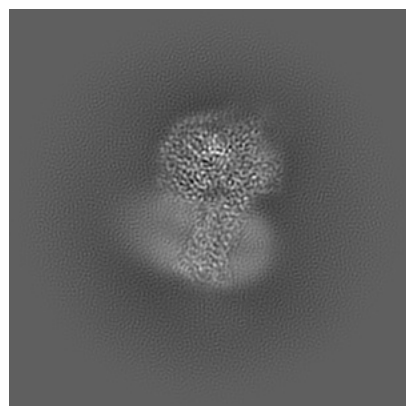
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60513. These allow visual inspection of the internal detail of the map and identification of artifacts.

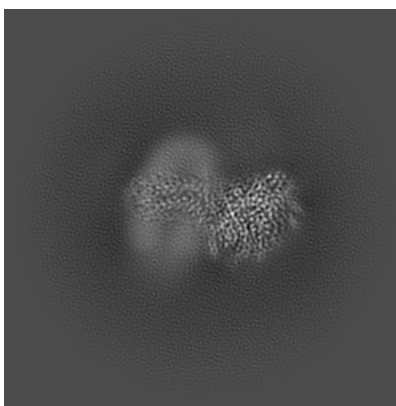
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

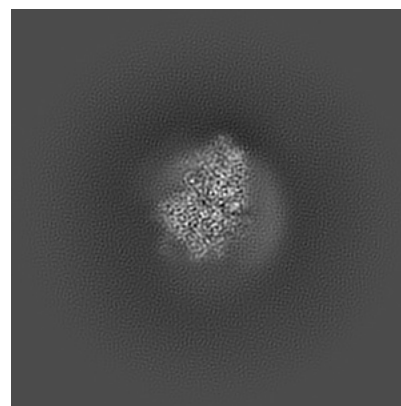
6.1.1 Primary map



X

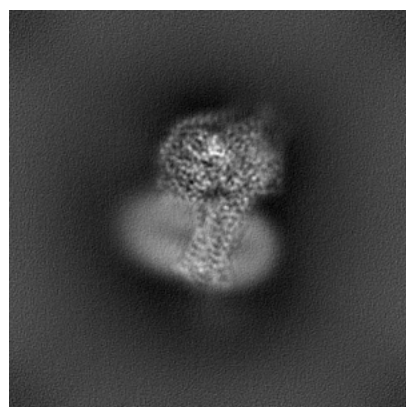


Y

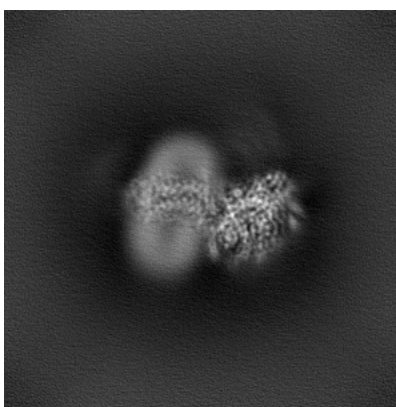


Z

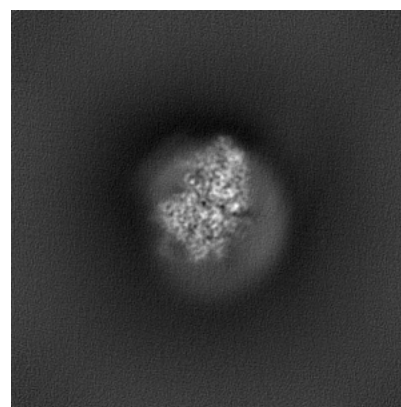
6.1.2 Raw map



X



Y

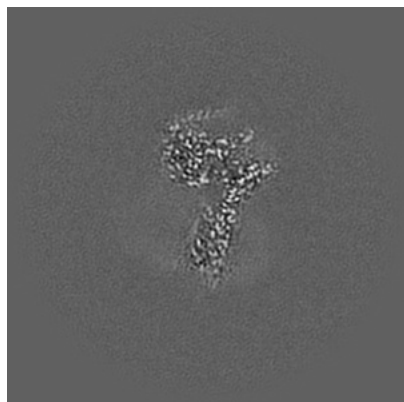


Z

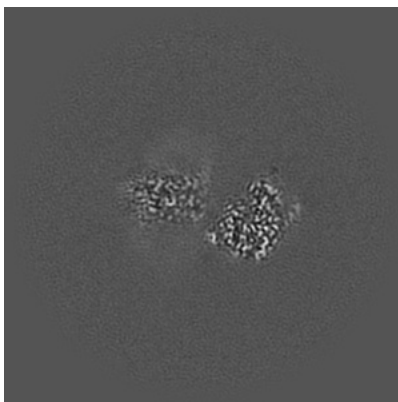
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

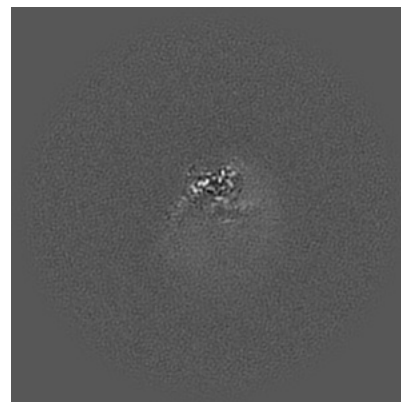
6.2.1 Primary map



X Index: 160

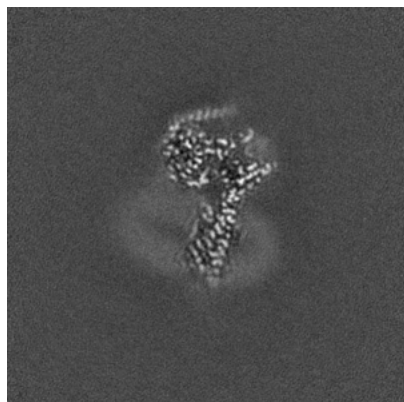


Y Index: 160

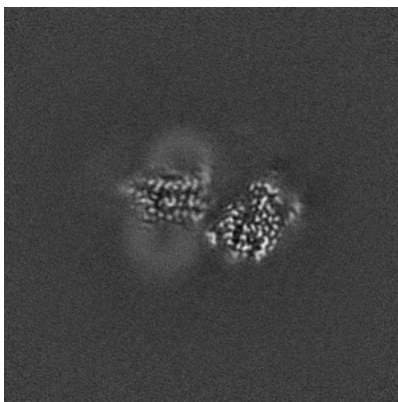


Z Index: 160

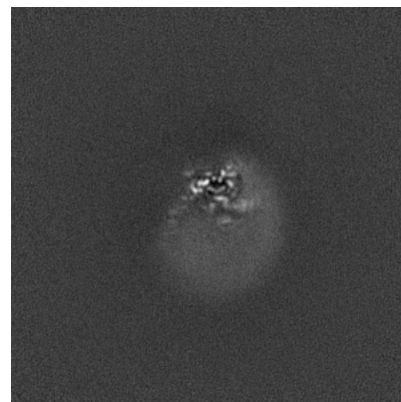
6.2.2 Raw map



X Index: 160



Y Index: 160

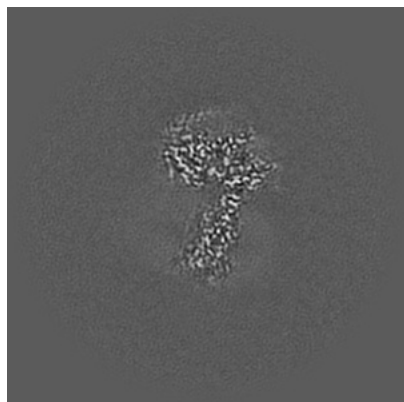


Z Index: 160

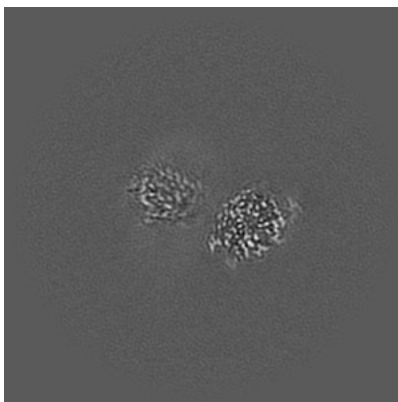
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

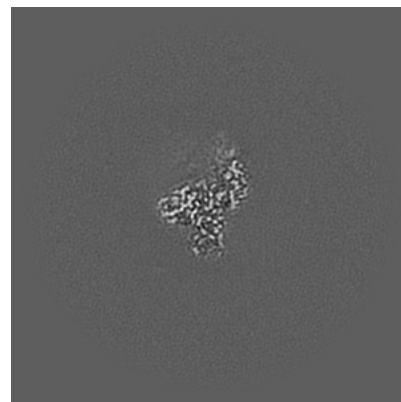
6.3.1 Primary map



X Index: 162

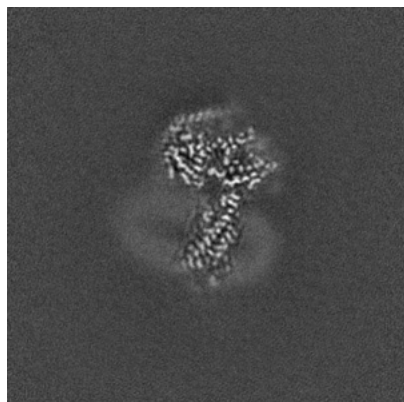


Y Index: 153

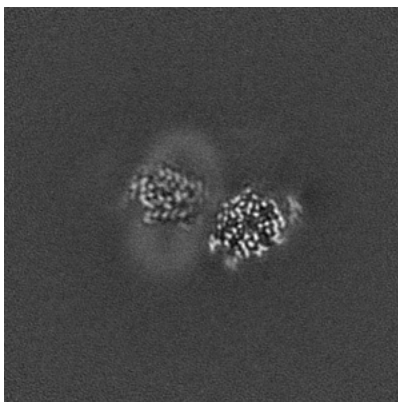


Z Index: 204

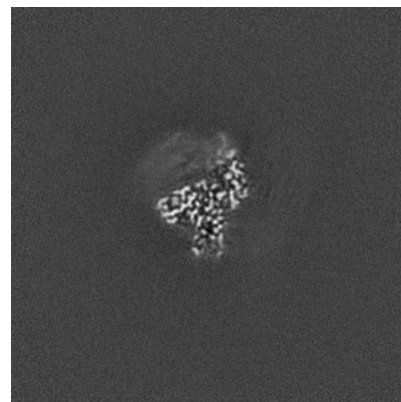
6.3.2 Raw map



X Index: 162



Y Index: 153

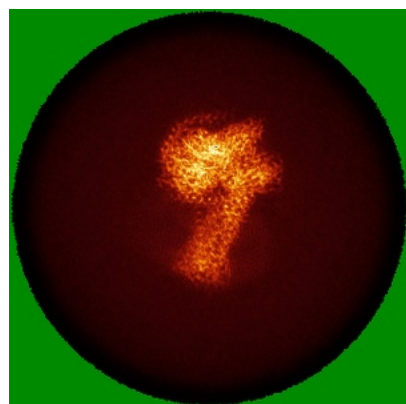


Z Index: 204

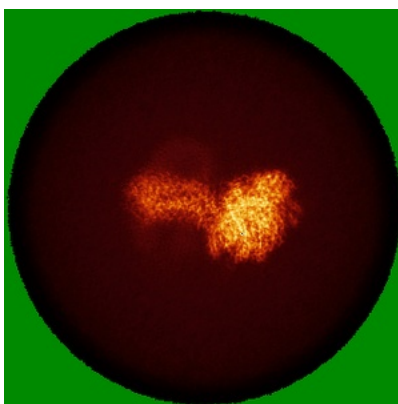
The images above show the largest variance slices of the map in three orthogonal directions.

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

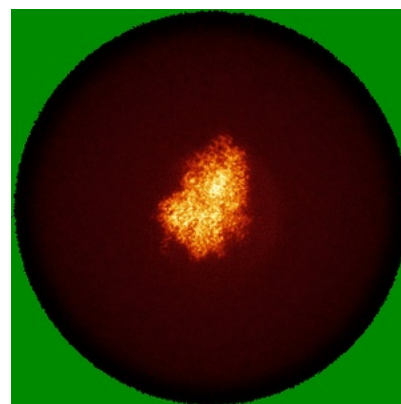
6.4.1 Primary map



X

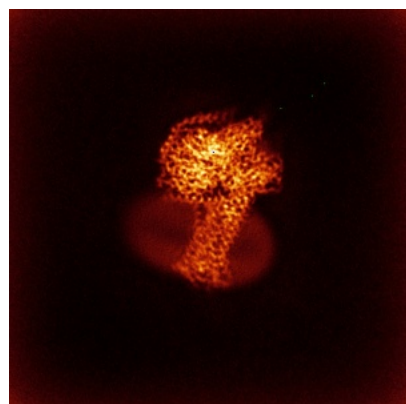


Y

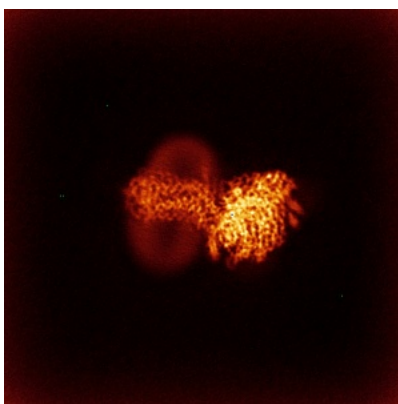


Z

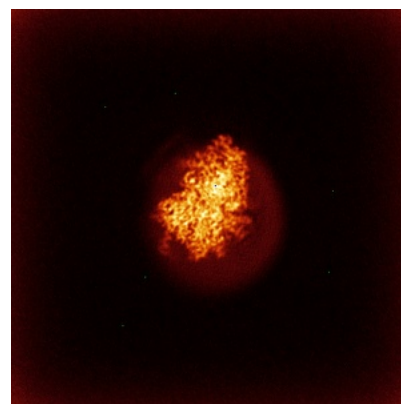
6.4.2 Raw map



X



Y

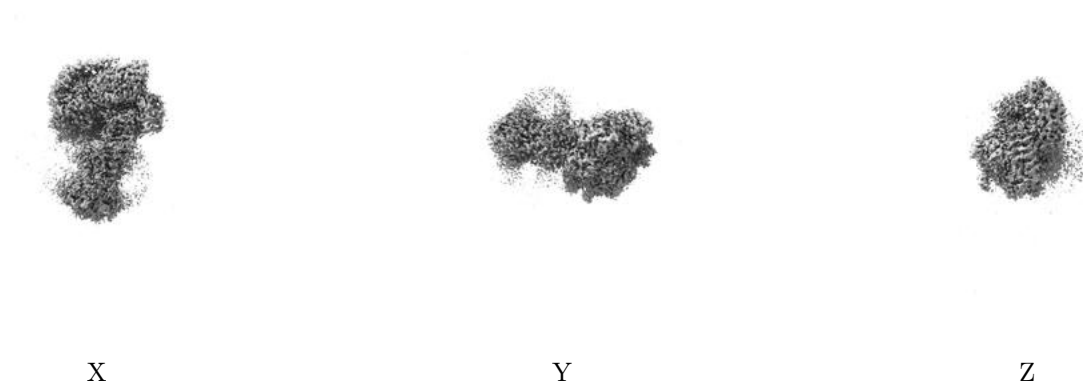


Z

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.

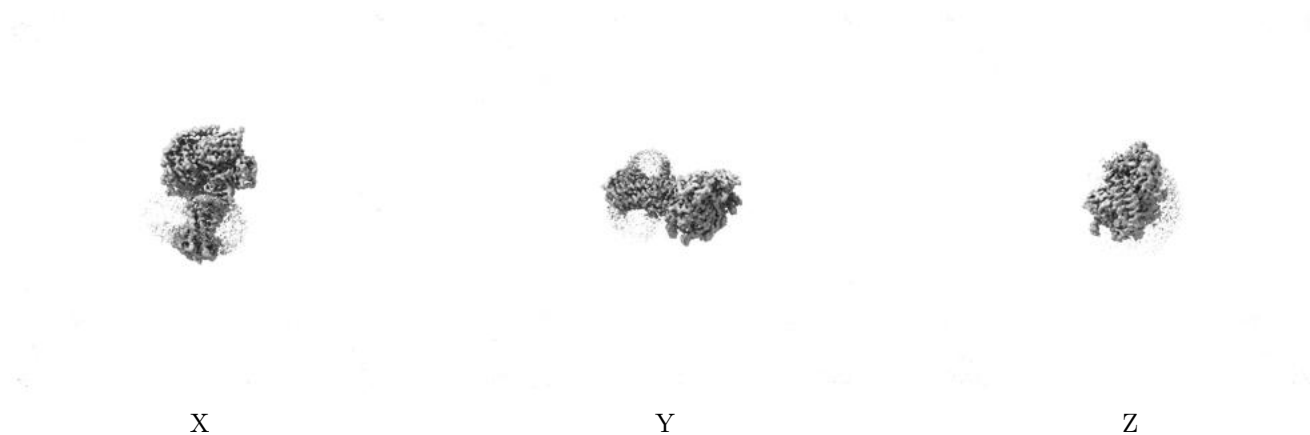
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.322. 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.

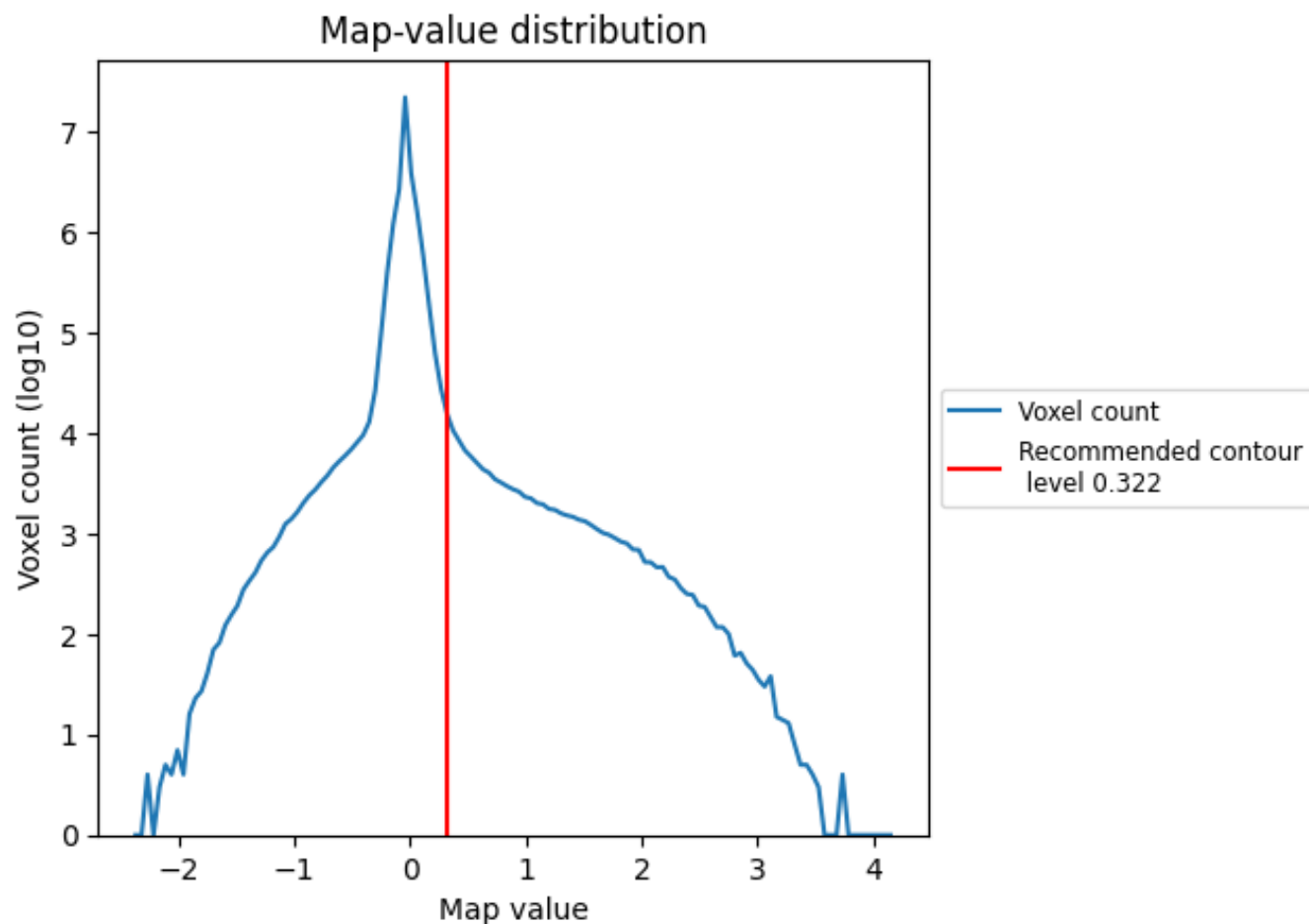
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

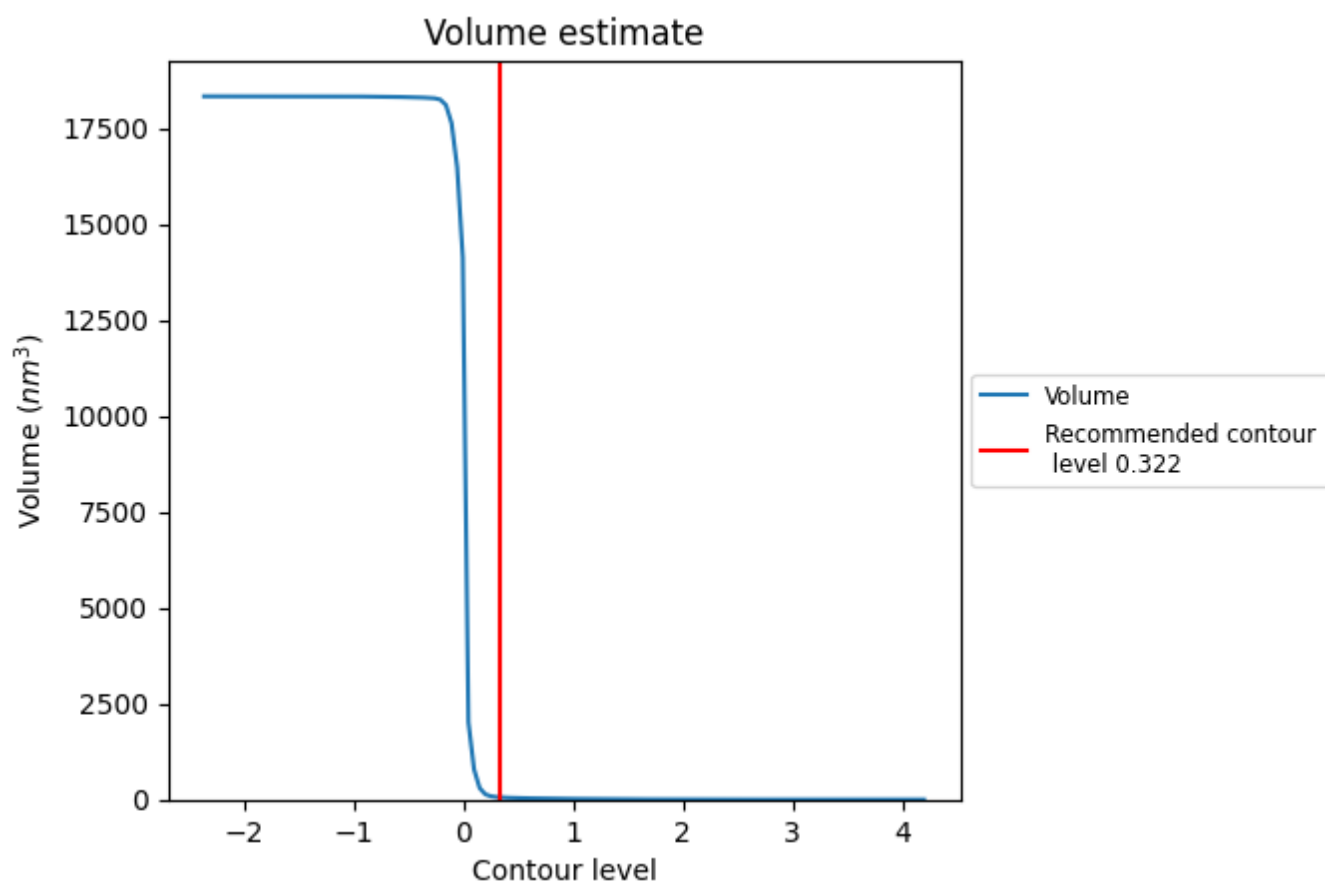
This section contains the results of statistical analysis of the map.

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.

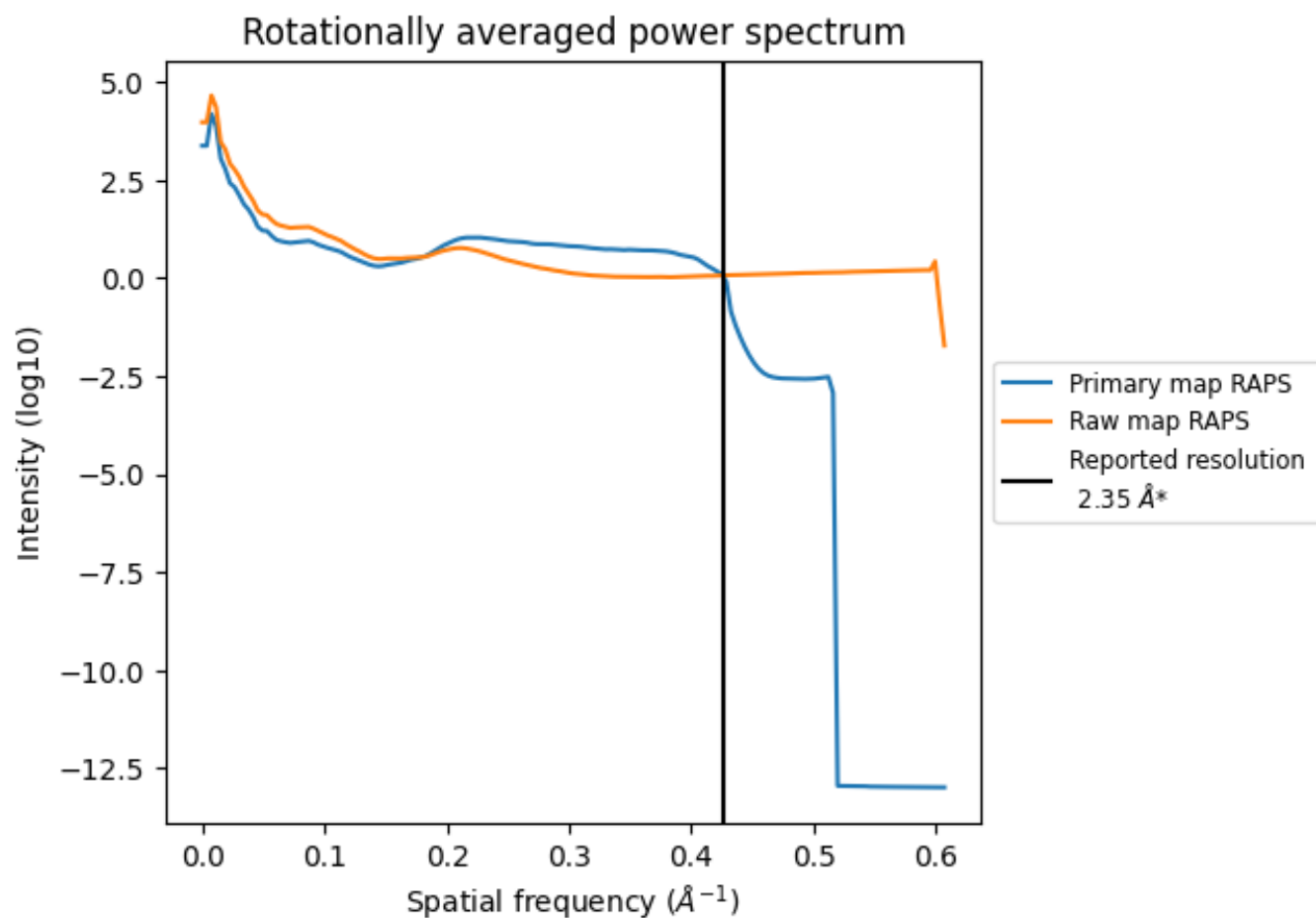
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60 nm³; this corresponds to an approximate mass of 55 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 ⓘ

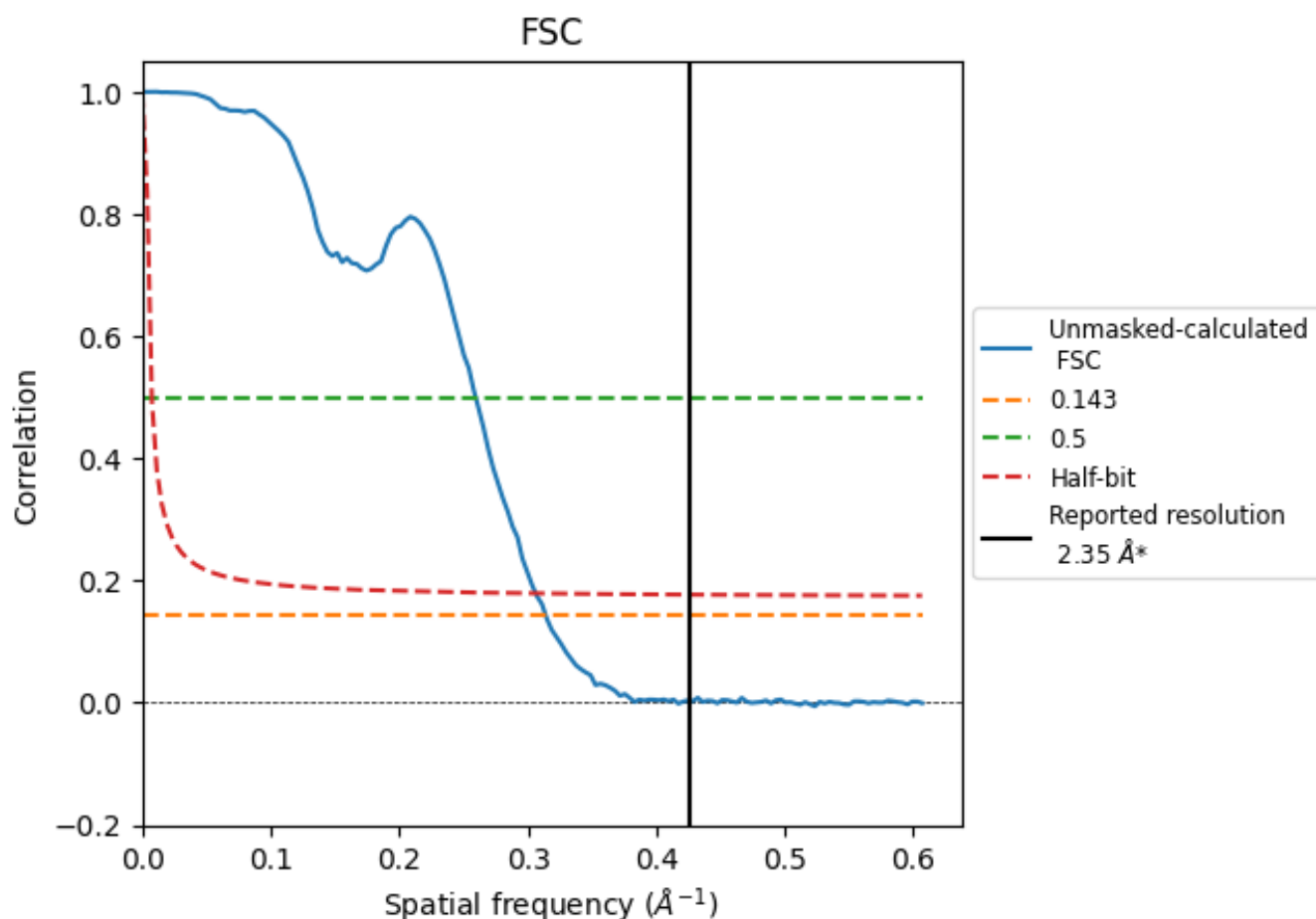


*Reported resolution corresponds to spatial frequency of 0.426 Å⁻¹

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 0.426 \AA^{-1}

8.2 Resolution estimates [i](#)

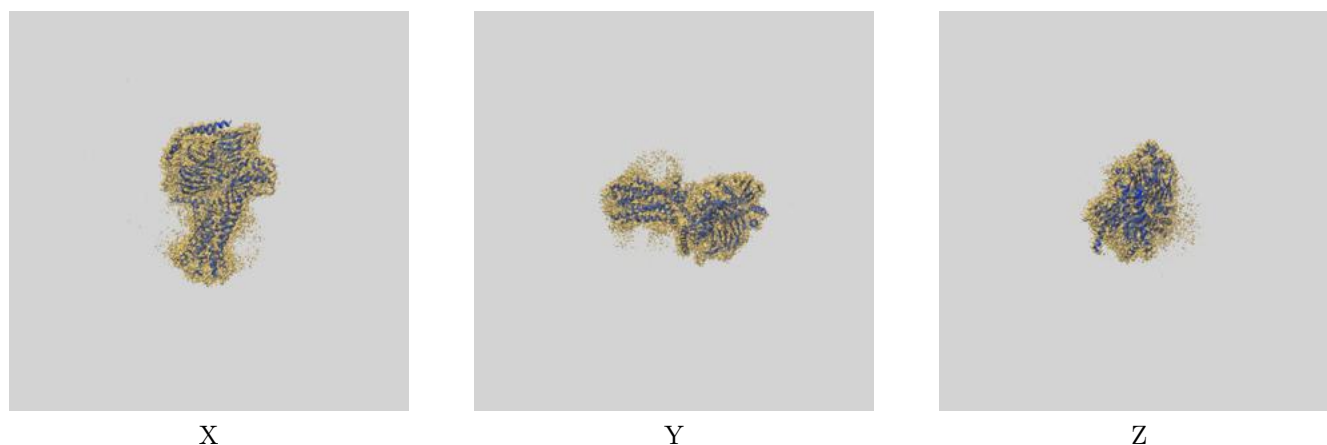
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.19	3.86	3.27

*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 3.19 differs from the reported value 2.35 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60513 and PDB model 8ZVZ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



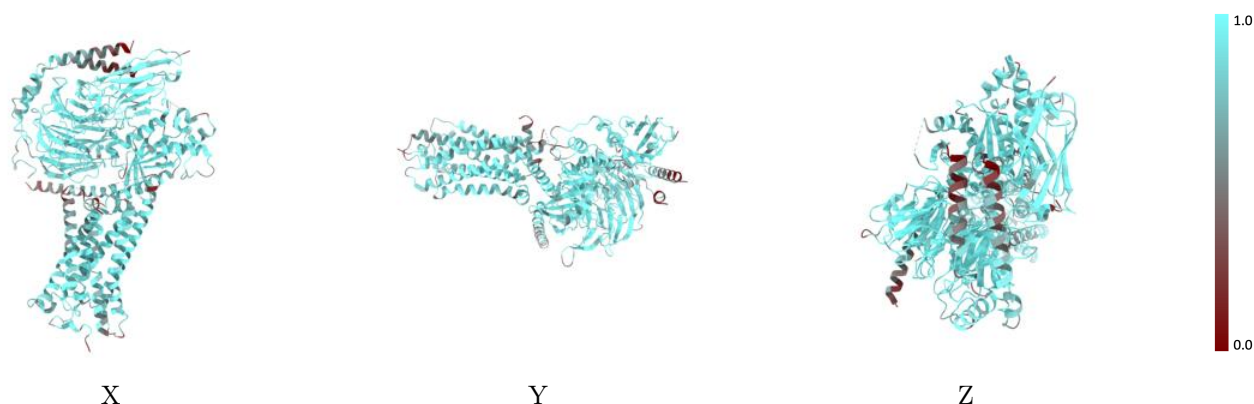
The images above show the 3D surface view of the map at the recommended contour level 0.322 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



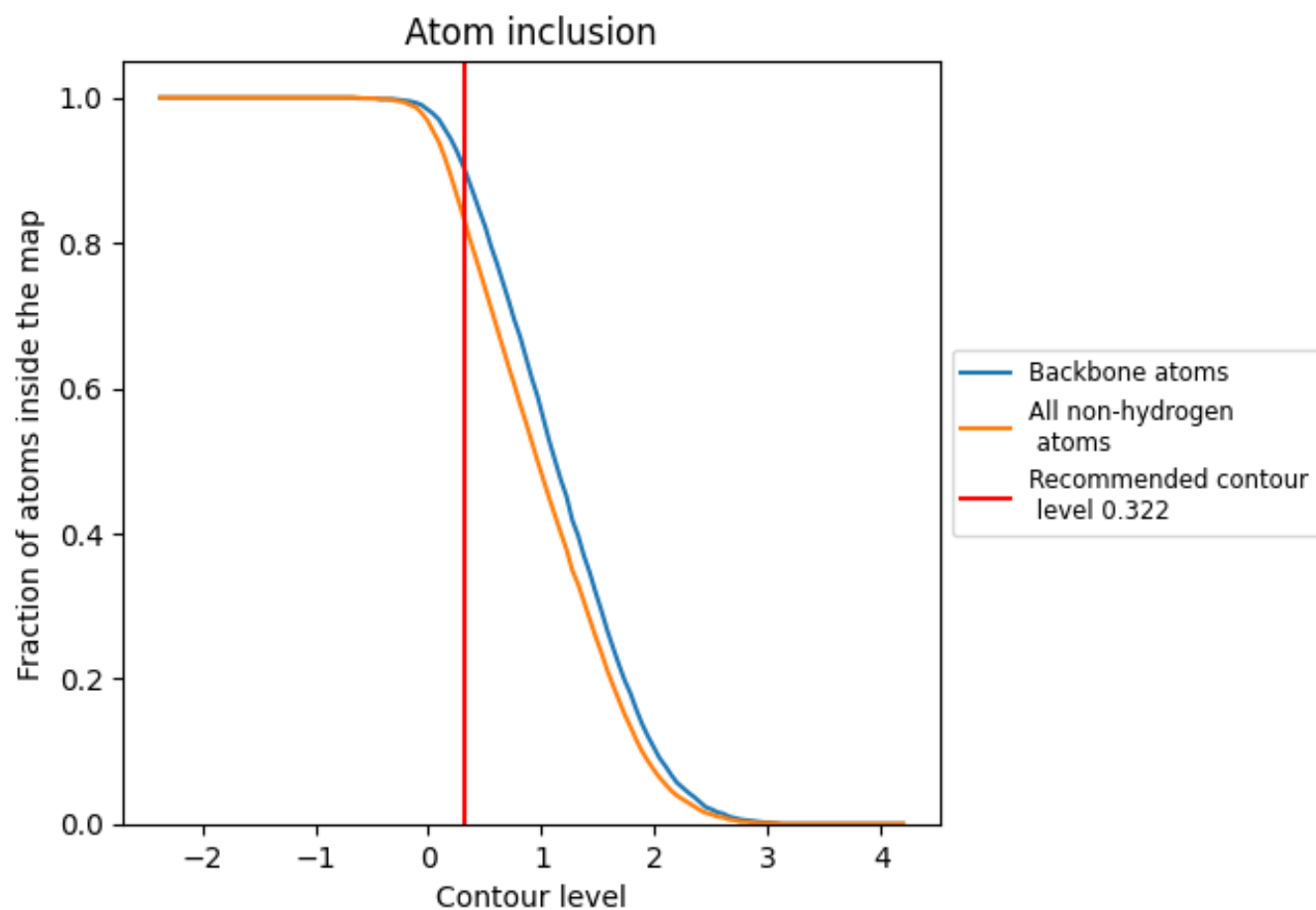
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.322).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 83% 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 (0.322) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8300	<div></div> 0.5230
A	<div></div> 0.8430	<div></div> 0.5300
B	<div></div> 0.8930	<div></div> 0.5630
D	<div></div> 0.7820	<div></div> 0.4820
G	<div></div> 0.6500	<div></div> 0.4310
N	<div></div> 0.8790	<div></div> 0.5510

