



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 02:50 AM JST

PDB ID : 24VL / pdb_000024vl
EMDB ID : EMD-69843
Title : Cryo-EM structure of the human wild-type KCNQ2/KCNQ3 heterotetramer (3:1 stoichiometry) in apo state (M2223 WT, without symmetry expansion)
Authors : Wang, Y.F.; Yang, H.; Qu, Y.N.; Shen, H.Z.
Deposited on : 2026-03-22
Resolution : 4.05 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.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

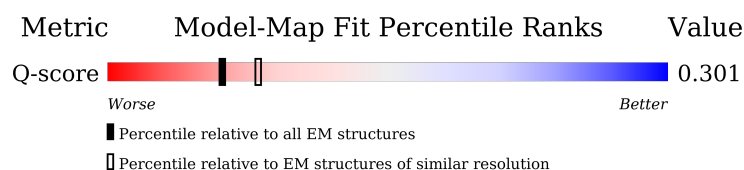
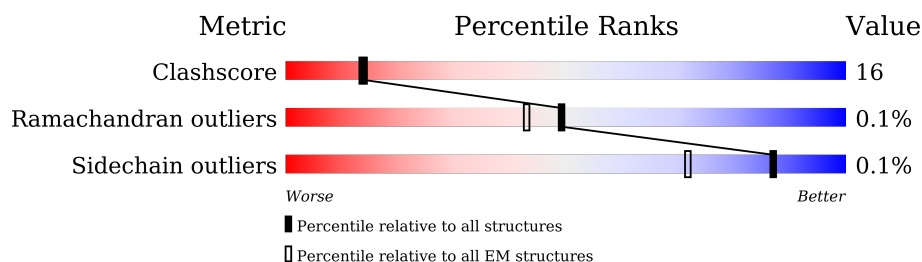
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.05 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	6569 (3.55 - 4.55)

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	892	
2	B	1142	
2	C	1142	
2	D	1142	

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
4	YJ0	B	901	X	-	-	-
4	YJ0	C	901	X	-	-	-
4	YJ0	D	901	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8264 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 Potassium voltage-gated channel subfamily KQT member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	239	Total	C	N	O	S	0	0
			1913	1269	313	321	10		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O43525
A	-18	ALA	-	expression tag	UNP O43525
A	-17	SER	-	expression tag	UNP O43525
A	-16	ASP	-	expression tag	UNP O43525
A	-15	TYR	-	expression tag	UNP O43525
A	-14	LYS	-	expression tag	UNP O43525
A	-13	ASP	-	expression tag	UNP O43525
A	-12	HIS	-	expression tag	UNP O43525
A	-11	ASP	-	expression tag	UNP O43525
A	-10	ILE	-	expression tag	UNP O43525
A	-9	ASP	-	expression tag	UNP O43525
A	-8	TYR	-	expression tag	UNP O43525
A	-7	LYS	-	expression tag	UNP O43525
A	-6	ASP	-	expression tag	UNP O43525
A	-5	ASP	-	expression tag	UNP O43525
A	-4	ASP	-	expression tag	UNP O43525
A	-3	ASP	-	expression tag	UNP O43525
A	-2	LYS	-	expression tag	UNP O43525
A	-1	GLY	-	expression tag	UNP O43525
A	0	THR	-	expression tag	UNP O43525

- Molecule 2 is a protein called Green fluorescent protein,Potassium voltage-gated channel subfamily KQT member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	243	Total	C	N	O	S	0	0
			1982	1318	332	323	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	246	Total	C	N	O	S	0	0
			2000	1330	335	326	9		
2	D	247	Total	C	N	O	S	0	0
			2006	1333	336	328	9		

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-270	MET	-	initiating methionine	UNP P42212
B	-269	ALA	-	expression tag	UNP P42212
B	-268	MET	-	expression tag	UNP P42212
B	-267	HIS	-	expression tag	UNP P42212
B	-266	HIS	-	expression tag	UNP P42212
B	-265	HIS	-	expression tag	UNP P42212
B	-264	HIS	-	expression tag	UNP P42212
B	-263	HIS	-	expression tag	UNP P42212
B	-262	HIS	-	expression tag	UNP P42212
B	-261	HIS	-	expression tag	UNP P42212
B	-260	HIS	-	expression tag	UNP P42212
B	-259	GLY	-	expression tag	UNP P42212
B	-258	GLY	-	expression tag	UNP P42212
B	-257	SER	-	expression tag	UNP P42212
B	-256	MET	-	expression tag	UNP P42212
B	-255	VAL	-	expression tag	UNP P42212
B	-192	LEU	PHE	conflict	UNP P42212
B	-191	THR	SER	conflict	UNP P42212
B	-149	THR	LYS	conflict	UNP P42212
B	-50	LYS	ALA	conflict	UNP P42212
B	-25	LEU	HIS	conflict	UNP P42212
B	-17	SER	-	linker	UNP P42212
B	-16	GLY	-	linker	UNP P42212
B	-15	LEU	-	linker	UNP P42212
B	-14	ARG	-	linker	UNP P42212
B	-13	SER	-	linker	UNP P42212
B	-12	GLY	-	linker	UNP P42212
B	-11	LEU	-	linker	UNP P42212
B	-10	GLU	-	linker	UNP P42212
B	-9	VAL	-	linker	UNP P42212
B	-8	LEU	-	linker	UNP P42212
B	-7	PHE	-	linker	UNP P42212
B	-6	GLN	-	linker	UNP P42212
B	-5	GLY	-	linker	UNP P42212

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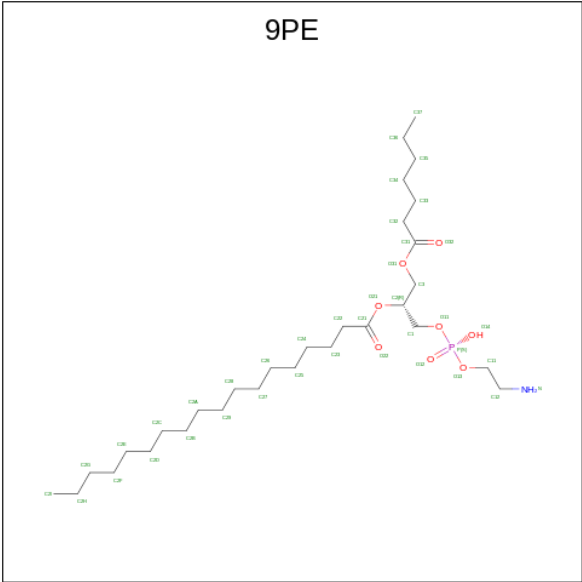
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	PRO	-	linker	UNP P42212
B	-3	GLY	-	linker	UNP P42212
B	-2	GLY	-	linker	UNP P42212
B	-1	ARG	-	linker	UNP P42212
C	-270	MET	-	initiating methionine	UNP P42212
C	-269	ALA	-	expression tag	UNP P42212
C	-268	MET	-	expression tag	UNP P42212
C	-267	HIS	-	expression tag	UNP P42212
C	-266	HIS	-	expression tag	UNP P42212
C	-265	HIS	-	expression tag	UNP P42212
C	-264	HIS	-	expression tag	UNP P42212
C	-263	HIS	-	expression tag	UNP P42212
C	-262	HIS	-	expression tag	UNP P42212
C	-261	HIS	-	expression tag	UNP P42212
C	-260	HIS	-	expression tag	UNP P42212
C	-259	GLY	-	expression tag	UNP P42212
C	-258	GLY	-	expression tag	UNP P42212
C	-257	SER	-	expression tag	UNP P42212
C	-256	MET	-	expression tag	UNP P42212
C	-255	VAL	-	expression tag	UNP P42212
C	-192	LEU	PHE	conflict	UNP P42212
C	-191	THR	SER	conflict	UNP P42212
C	-149	THR	LYS	conflict	UNP P42212
C	-50	LYS	ALA	conflict	UNP P42212
C	-25	LEU	HIS	conflict	UNP P42212
C	-17	SER	-	linker	UNP P42212
C	-16	GLY	-	linker	UNP P42212
C	-15	LEU	-	linker	UNP P42212
C	-14	ARG	-	linker	UNP P42212
C	-13	SER	-	linker	UNP P42212
C	-12	GLY	-	linker	UNP P42212
C	-11	LEU	-	linker	UNP P42212
C	-10	GLU	-	linker	UNP P42212
C	-9	VAL	-	linker	UNP P42212
C	-8	LEU	-	linker	UNP P42212
C	-7	PHE	-	linker	UNP P42212
C	-6	GLN	-	linker	UNP P42212
C	-5	GLY	-	linker	UNP P42212
C	-4	PRO	-	linker	UNP P42212
C	-3	GLY	-	linker	UNP P42212
C	-2	GLY	-	linker	UNP P42212
C	-1	ARG	-	linker	UNP P42212

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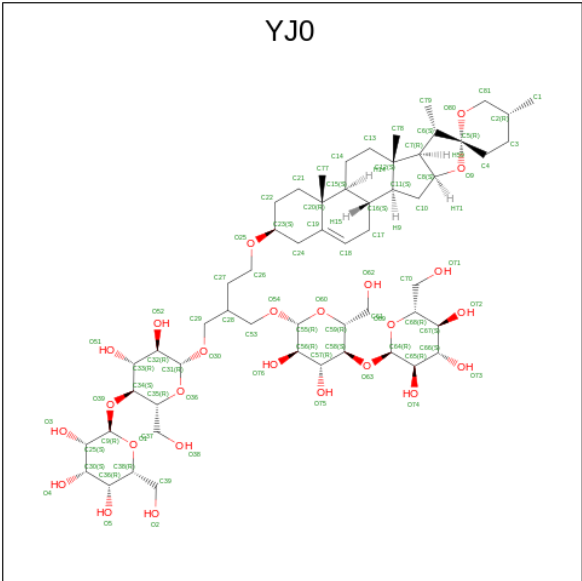
Chain	Residue	Modelled	Actual	Comment	Reference
D	-270	MET	-	initiating methionine	UNP P42212
D	-269	ALA	-	expression tag	UNP P42212
D	-268	MET	-	expression tag	UNP P42212
D	-267	HIS	-	expression tag	UNP P42212
D	-266	HIS	-	expression tag	UNP P42212
D	-265	HIS	-	expression tag	UNP P42212
D	-264	HIS	-	expression tag	UNP P42212
D	-263	HIS	-	expression tag	UNP P42212
D	-262	HIS	-	expression tag	UNP P42212
D	-261	HIS	-	expression tag	UNP P42212
D	-260	HIS	-	expression tag	UNP P42212
D	-259	GLY	-	expression tag	UNP P42212
D	-258	GLY	-	expression tag	UNP P42212
D	-257	SER	-	expression tag	UNP P42212
D	-256	MET	-	expression tag	UNP P42212
D	-255	VAL	-	expression tag	UNP P42212
D	-192	LEU	PHE	conflict	UNP P42212
D	-191	THR	SER	conflict	UNP P42212
D	-149	THR	LYS	conflict	UNP P42212
D	-50	LYS	ALA	conflict	UNP P42212
D	-25	LEU	HIS	conflict	UNP P42212
D	-17	SER	-	linker	UNP P42212
D	-16	GLY	-	linker	UNP P42212
D	-15	LEU	-	linker	UNP P42212
D	-14	ARG	-	linker	UNP P42212
D	-13	SER	-	linker	UNP P42212
D	-12	GLY	-	linker	UNP P42212
D	-11	LEU	-	linker	UNP P42212
D	-10	GLU	-	linker	UNP P42212
D	-9	VAL	-	linker	UNP P42212
D	-8	LEU	-	linker	UNP P42212
D	-7	PHE	-	linker	UNP P42212
D	-6	GLN	-	linker	UNP P42212
D	-5	GLY	-	linker	UNP P42212
D	-4	PRO	-	linker	UNP P42212
D	-3	GLY	-	linker	UNP P42212
D	-2	GLY	-	linker	UNP P42212
D	-1	ARG	-	linker	UNP P42212

- Molecule 3 is (1R)-2-([(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy)-1-[(heptanoyloxy)methyl]ethyl octadecanoate (CCD ID: 9PE) (formula: C₃₀H₆₀NO₈P) (labeled as "Ligand of Interest" by depositor).

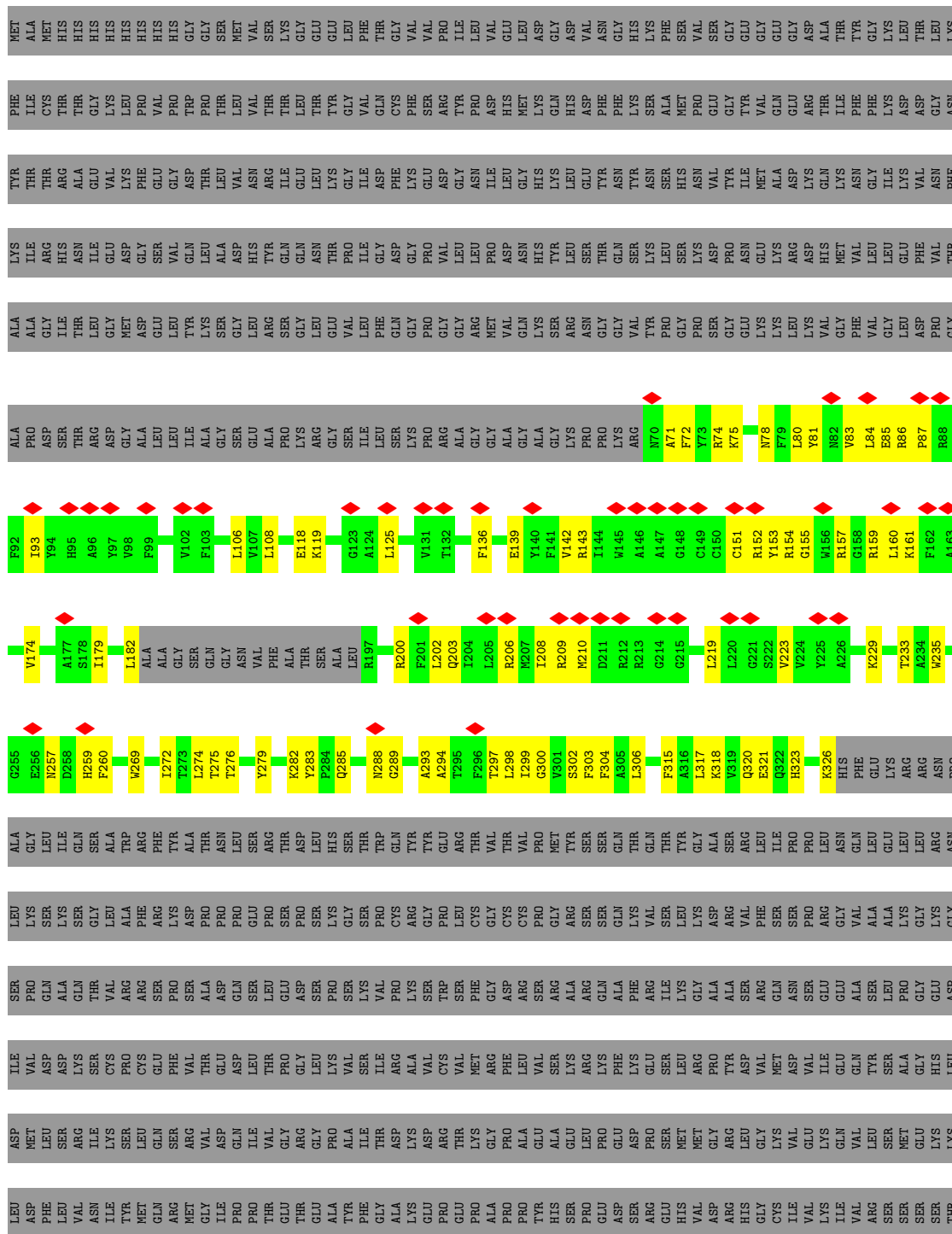


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
3	B	1	Total	C	N	O	P	0
			40	30	1	8	1	
3	C	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 4 is (2R)-2-{[(4-O-hexopyranosyl-beta-D-glucopyranosyl)oxy]methyl}-4-{[(25R)-5beta,14beta,17beta-spirostan-3beta-yl]oxy}butyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (CCD ID: YJ0) (formula: C₅₆H₉₂O₂₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	B	1	Total 81	C 56	O 25	0
4	C	1	Total 81	C 56	O 25	0
4	D	1	Total 81	C 56	O 25	0

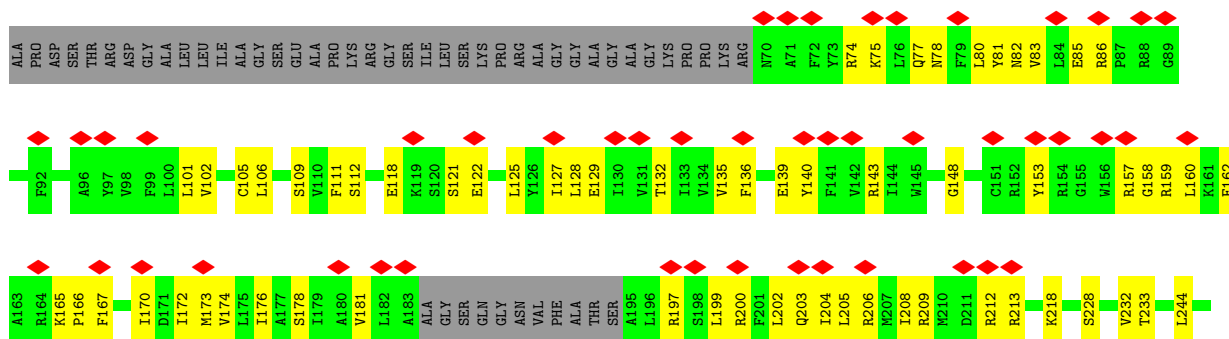


LEU	ASN	SER	CYS	TYR	ALA	ALA	VAL	ALA	PRO	CYS	ALA	LYS	VAL	ARG	PRO	TYR	THR	ASP	SER	ASP	ASP	LEU	CYS	THR	PRO	CYS	GLY	PRO	PRO	PRO	ARG	SER	ALA	ALA	THR	GLY	GLY	GLY	PRO	PHE	GLY	ASP	VAL	GLY	TRP	ALA	GLY	PRO	GLY	ARG	LYS
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● Molecule 2: Green fluorescent protein, Potassium voltage-gated channel subfamily KQT member 2



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



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

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14542	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)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.874	Depositor
Minimum map value	-0.911	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.424	Depositor
Map size ($\text{\AA}$)	260.88, 260.88, 260.88	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	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: 9PE, YJ0

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	0.18	0/1960	0.40	0/2653
2	B	0.23	0/2036	0.42	0/2757
2	C	0.17	0/2054	0.38	0/2782
2	D	0.27	0/2060	0.46	0/2790
All	All	0.22	0/8110	0.41	0/10982

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	1913	0	1970	54	0
2	B	1982	0	2020	68	0
2	C	2000	0	2041	65	0
2	D	2006	0	2046	83	0
3	A	40	0	59	2	0
3	B	40	0	59	4	0
3	C	40	0	59	4	0
4	B	81	0	0	3	0
4	C	81	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	81	0	0	3	0
All	All	8264	0	8254	260	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 16.

All (260) 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:192:LYS:HA	1:A:195:ARG:HE	1.45	0.80
2:C:170:ILE:HA	2:C:173:MET:HE2	1.62	0.79
2:B:298:LEU:HD21	2:C:271:LEU:HD11	1.63	0.79
2:C:174:VAL:HB	2:C:202:LEU:HD21	1.63	0.79
1:A:314:LEU:HD12	1:A:340:GLY:HA3	1.65	0.78
1:A:233:GLN:HG3	1:A:236:ARG:HH21	1.49	0.78
2:B:139:GLU:HG3	2:B:143:ARG:HH12	1.49	0.77
1:A:183:ARG:HG3	1:A:192:LYS:HE2	1.66	0.76
1:A:117:ARG:HH12	1:A:124:LEU:HB2	1.54	0.72
2:B:229:LYS:NZ	4:C:901:YJ0:O73	2.23	0.72
1:A:265:TRP:HB3	3:A:1001:9PE:H2EA	1.72	0.71
2:D:274:LEU:HD22	2:D:300:GLY:HA3	1.71	0.70
1:A:309:TRP:NE1	2:B:279:TYR:OH	2.25	0.69
2:D:84:LEU:HD23	2:D:143:ARG:HE	1.57	0.69
2:D:170:ILE:HA	2:D:173:MET:HG2	1.76	0.68
2:B:108:LEU:HG	2:B:125:LEU:HD22	1.76	0.67
2:C:153:TYR:O	2:C:159:ARG:NH1	2.27	0.67
2:D:257:ASN:ND2	2:D:285:GLN:OE1	2.28	0.67
2:D:209:ARG:O	2:D:209:ARG:NH1	2.27	0.66
2:C:78:ASN:O	2:C:82:ASN:ND2	2.29	0.66
1:A:192:LYS:HA	1:A:195:ARG:NE	2.11	0.66
2:B:157:ARG:HA	2:B:160:LEU:HD12	1.79	0.65
3:C:902:9PE:H25A	2:D:210:MET:HG3	1.77	0.65
2:B:288:ASN:OD1	2:B:289:GLY:N	2.30	0.64
2:B:179:ILE:HD12	2:B:182:LEU:HD21	1.79	0.64
1:A:182:CYS:SG	1:A:183:ARG:N	2.71	0.64
2:C:85:GLU:OE2	2:C:86:ARG:NH1	2.31	0.64
2:B:200:ARG:HB3	2:B:203:GLN:NE2	2.13	0.63
2:D:233:THR:OG1	2:D:234:ALA:N	2.26	0.63
2:D:250:TYR:OH	2:D:254:LYS:NZ	2.27	0.63
2:D:148:GLY:HA2	2:D:154:ARG:HH22	1.64	0.62
2:D:154:ARG:H	2:D:158:GLY:HA3	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:74:ARG:O	2:C:78:ASN:ND2	2.33	0.62
2:C:213:ARG:O	2:C:218:LYS:NZ	2.32	0.62
1:A:296:MET:SD	1:A:298:GLU:N	2.73	0.62
2:B:274:LEU:HD12	2:B:300:GLY:HA3	1.81	0.61
1:A:129:VAL:HA	1:A:132:ILE:HG12	1.82	0.61
2:D:265:ASP:OD1	2:D:266:ALA:N	2.33	0.61
2:B:274:LEU:HB3	2:B:304:PHE:CE2	2.37	0.59
2:B:74:ARG:O	2:B:78:ASN:ND2	2.35	0.59
2:C:259:HIS:HB3	2:C:282:LYS:HG2	1.82	0.59
1:A:357:LEU:HD21	2:B:320:GLN:HG3	1.84	0.59
2:D:230:GLU:HA	2:D:233:THR:HG23	1.83	0.58
2:B:200:ARG:HB3	2:B:203:GLN:HE22	1.68	0.58
1:A:321:ASP:OD1	1:A:322:LYS:N	2.36	0.58
2:B:223:VAL:HG21	2:B:315:PHE:CE1	2.38	0.58
2:B:75:LYS:HA	2:B:78:ASN:HD21	1.69	0.58
2:B:206:ARG:HA	2:B:209:ARG:HD3	1.85	0.57
1:A:326:THR:HG23	1:A:329:GLY:H	1.68	0.57
2:D:158:GLY:HA2	2:D:161:LYS:HE3	1.87	0.57
2:D:198:SER:HA	2:D:201:PHE:HD2	1.70	0.56
2:D:148:GLY:HA2	2:D:154:ARG:NH2	2.21	0.56
2:D:196:LEU:HA	2:D:199:LEU:HD12	1.88	0.56
2:D:118:GLU:OE1	2:D:118:GLU:N	2.37	0.56
2:D:206:ARG:HH12	2:D:209:ARG:HD3	1.70	0.56
2:C:250:TYR:OH	2:C:254:LYS:NZ	2.36	0.55
2:C:81:TYR:HE1	2:C:143:ARG:HH12	1.54	0.55
2:C:129:GLU:HA	2:C:132:THR:HG22	1.88	0.55
2:C:102:VAL:O	2:C:106:LEU:HG	2.06	0.55
1:A:239:ARG:O	1:A:239:ARG:NH1	2.40	0.55
2:C:157:ARG:O	2:C:157:ARG:NH1	2.39	0.55
2:D:206:ARG:HH22	2:D:209:ARG:HD3	1.71	0.55
2:D:154:ARG:N	2:D:158:GLY:HA3	2.22	0.54
1:A:146:LYS:NZ	2:D:261:ASP:O	2.41	0.54
2:C:197:ARG:HA	2:C:200:ARG:HH12	1.72	0.54
2:D:293:ALA:O	2:D:297:THR:OG1	2.21	0.54
2:D:140:TYR:CZ	2:D:172:ILE:HD11	2.42	0.54
2:D:135:VAL:O	2:D:138:VAL:HG22	2.08	0.54
2:D:115:LYS:O	2:D:116:GLU:HG3	2.08	0.53
2:C:286:THR:HG23	2:C:288:ASN:H	1.72	0.53
2:B:250:TYR:OH	2:B:254:LYS:NZ	2.36	0.53
2:B:84:LEU:HD12	2:B:143:ARG:HE	1.72	0.53
2:D:83:VAL:HG23	2:D:84:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:153:TYR:HA	2:C:158:GLY:HA3	1.91	0.53
2:D:288:ASN:OD1	2:D:289:GLY:N	2.41	0.53
2:D:297:THR:O	2:D:301:VAL:HG12	2.09	0.53
2:B:118:GLU:HG2	2:B:119:LYS:N	2.23	0.52
2:B:151:CYS:N	2:B:154:ARG:HH12	2.08	0.52
2:C:109:SER:O	2:C:112:SER:OG	2.23	0.52
2:D:287:TRP:H	2:D:287:TRP:CD1	2.27	0.52
1:A:299:GLU:OE1	1:A:322:LYS:HA	2.09	0.52
2:B:85:GLU:HG2	2:B:86:ARG:HG3	1.92	0.52
2:B:167:PHE:HA	2:B:170:ILE:HG12	1.91	0.52
2:C:310:ILE:HD13	2:D:312:GLY:HA2	1.92	0.52
2:C:74:ARG:O	2:C:77:GLN:HG3	2.10	0.51
2:C:232:VAL:HG11	3:C:902:9PE:H22A	1.91	0.51
2:B:139:GLU:HA	2:B:142:VAL:HG22	1.92	0.51
2:B:71:ALA:O	2:B:75:LYS:HG2	2.09	0.51
2:B:153:TYR:O	2:B:154:ARG:NH1	2.34	0.51
2:D:130:ILE:HG13	2:D:131:VAL:N	2.26	0.51
2:D:198:SER:HA	2:D:201:PHE:CD2	2.45	0.51
2:D:154:ARG:CZ	2:D:154:ARG:HA	2.41	0.51
2:D:225:TYR:O	2:D:228:SER:OG	2.29	0.51
1:A:156:LEU:O	1:A:159:LEU:N	2.44	0.51
2:C:173:MET:HA	2:C:176:ILE:HG22	1.93	0.51
2:D:143:ARG:NH1	4:D:901:YJ0:O2	2.44	0.50
1:A:200:MET:O	1:A:203:ILE:HG22	2.11	0.50
2:C:80:LEU:HA	2:C:83:VAL:HG12	1.93	0.50
2:C:140:TYR:HE2	2:C:172:ILE:HD13	1.76	0.50
2:C:274:LEU:HD22	2:C:300:GLY:HA3	1.93	0.50
3:C:902:9PE:O11	4:D:901:YJ0:O62	2.29	0.50
1:A:320:GLY:HA2	2:B:279:TYR:HD1	1.75	0.50
2:B:203:GLN:HB3	2:B:206:ARG:NH2	2.27	0.50
2:B:306:LEU:HD11	2:C:311:LEU:HB3	1.93	0.50
2:C:205:LEU:HD13	2:C:208:ILE:HD12	1.94	0.50
2:D:88:ARG:HD3	2:D:89:GLY:N	2.27	0.50
2:D:211:ASP:OD1	2:D:212:ARG:N	2.45	0.50
2:C:75:LYS:HA	2:C:78:ASN:HD21	1.76	0.50
1:A:233:GLN:HG3	1:A:236:ARG:NH2	2.23	0.50
4:B:901:YJ0:O39	4:B:901:YJ0:O2	2.30	0.50
2:B:235:TRP:HB3	3:B:902:9PE:H2F	1.94	0.50
2:C:204:ILE:O	2:C:208:ILE:HG13	2.11	0.50
1:A:331:LEU:HD21	2:C:111:PHE:CZ	2.47	0.49
2:B:274:LEU:HD11	2:B:297:THR:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LEU:O	1:A:161:THR:OG1	2.25	0.49
1:A:277:PHE:HA	1:A:303:TYR:HE1	1.77	0.49
2:C:165:LYS:HZ2	2:C:167:PHE:HB2	1.75	0.49
2:B:269:TRP:HE1	2:B:283:TYR:HA	1.78	0.49
2:D:230:GLU:HA	2:D:233:THR:CG2	2.43	0.49
2:D:153:TYR:O	2:D:154:ARG:NH1	2.46	0.49
2:D:231:LEU:HD21	2:D:311:LEU:HD21	1.94	0.49
2:C:85:GLU:O	2:C:86:ARG:HG2	2.12	0.49
2:C:203:GLN:HA	2:C:206:ARG:HG2	1.94	0.49
1:A:187:TRP:CD1	1:A:188:ARG:HG2	2.48	0.49
2:B:81:TYR:HB3	2:B:86:ARG:NH2	2.28	0.49
2:D:262:THR:HG23	2:D:265:ASP:H	1.78	0.48
1:A:184:TYR:HA	1:A:192:LYS:HE3	1.95	0.48
2:D:124:ALA:O	2:D:128:LEU:HD23	2.13	0.48
2:C:204:ILE:HD12	2:C:204:ILE:H	1.79	0.48
2:B:136:PHE:CE2	2:B:206:ARG:HD2	2.48	0.48
2:D:106:LEU:O	2:D:109:SER:OG	2.28	0.48
2:B:152:ARG:HH22	2:B:161:LYS:HG3	1.77	0.48
2:C:157:ARG:HH11	2:C:160:LEU:HB3	1.78	0.48
1:A:263:THR:HG21	2:B:219:LEU:HD21	1.96	0.48
2:C:203:GLN:O	2:C:206:ARG:HG2	2.13	0.48
1:A:161:THR:O	1:A:164:ILE:HG22	2.14	0.48
2:D:269:TRP:HD1	2:D:282:LYS:HB2	1.78	0.48
1:A:140:ALA:O	1:A:143:THR:HG22	2.15	0.47
2:D:168:CYS:O	2:D:172:ILE:HG12	2.13	0.47
1:A:346:LEU:O	1:A:350:ILE:HG12	2.15	0.47
2:B:75:LYS:HA	2:B:78:ASN:ND2	2.29	0.47
2:B:87:PRO:HB3	2:B:91:ALA:HB3	1.97	0.47
2:D:119:LYS:O	2:D:122:GLU:HG2	2.14	0.47
1:A:296:MET:SD	1:A:297:LYS:N	2.87	0.47
2:B:223:VAL:HG21	2:B:315:PHE:HE1	1.78	0.47
2:C:166:PRO:O	2:C:170:ILE:HG23	2.15	0.47
2:C:125:LEU:HA	2:C:128:LEU:HG	1.96	0.47
2:C:167:PHE:HA	2:C:170:ILE:HG12	1.97	0.47
2:C:209:ARG:O	4:C:901:YJ0:O3	2.31	0.47
2:B:139:GLU:CG	2:B:143:ARG:HH12	2.23	0.47
2:B:139:GLU:HG3	2:B:143:ARG:NH1	2.26	0.46
2:D:80:LEU:HA	2:D:83:VAL:HG22	1.97	0.46
2:B:106:LEU:HD23	2:B:203:GLN:HG3	1.97	0.46
1:A:180:CYS:SG	1:A:181:CYS:N	2.88	0.46
4:B:901:YJ0:O2	4:B:901:YJ0:O4	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:ARG:O	2:D:161:LYS:NZ	2.38	0.46
2:C:136:PHE:O	2:C:139:GLU:HG3	2.16	0.46
2:D:230:GLU:N	2:D:230:GLU:OE1	2.48	0.46
2:C:233:THR:HG23	2:D:216:THR:HB	1.97	0.46
2:D:116:GLU:N	2:D:118:GLU:OE1	2.49	0.46
2:D:296:PHE:HA	2:D:299:ILE:HG22	1.97	0.46
2:D:287:TRP:O	2:D:291:LEU:HG	2.16	0.45
2:D:81:TYR:CD1	2:D:147:ALA:HB2	2.51	0.45
2:D:135:VAL:O	2:D:138:VAL:N	2.50	0.45
1:A:137:LEU:O	1:A:141:VAL:HG23	2.16	0.45
2:B:83:VAL:HG23	2:B:84:LEU:HD22	1.98	0.45
2:D:209:ARG:HG2	2:D:209:ARG:HH11	1.80	0.45
1:A:148:TYR:O	1:A:152:SER:HB2	2.16	0.45
1:A:197:PRO:HA	1:A:200:MET:HG2	1.98	0.45
2:D:248:LEU:HD12	2:D:296:PHE:HE2	1.82	0.45
2:B:299:ILE:O	2:B:303:PHE:HD1	2.00	0.45
1:A:288:GLU:HB3	1:A:298:GLU:OE1	2.17	0.45
1:A:232:LEU:O	1:A:236:ARG:HG3	2.16	0.45
2:B:80:LEU:HA	2:B:83:VAL:HG22	1.98	0.45
2:D:109:SER:O	2:D:113:THR:HG23	2.17	0.45
2:D:81:TYR:CG	2:D:147:ALA:HB2	2.51	0.45
2:B:275:THR:O	2:B:276:THR:OG1	2.34	0.44
2:B:210:MET:O	4:B:901:YJ0:O75	2.35	0.44
2:B:171:ASP:O	2:B:174:VAL:HG12	2.18	0.44
2:B:317:LEU:O	2:B:321:GLU:OE1	2.36	0.44
1:A:317:ILE:HD13	2:D:276:THR:HA	1.99	0.44
2:B:72:PHE:HA	2:B:75:LYS:HE2	1.99	0.44
2:B:259:HIS:O	2:B:282:LYS:NZ	2.35	0.44
1:A:262:ILE:HG21	3:A:1001:9PE:H24	2.00	0.44
2:D:136:PHE:HA	2:D:139:GLU:OE2	2.18	0.44
3:B:902:9PE:O12	4:C:901:YJ0:O75	2.36	0.44
3:B:902:9PE:O12	4:C:901:YJ0:O72	2.36	0.44
2:D:75:LYS:HB3	2:D:79:PHE:CZ	2.53	0.44
1:A:332:ILE:HG13	1:A:333:ALA:N	2.33	0.43
2:D:161:LYS:O	2:D:164:ARG:HG2	2.18	0.43
1:A:200:MET:O	1:A:204:PHE:CD2	2.71	0.43
2:B:293:ALA:O	2:B:294:ALA:C	2.61	0.43
2:C:122:GLU:H	2:C:122:GLU:CD	2.24	0.43
2:C:206:ARG:O	2:C:209:ARG:HG2	2.17	0.43
2:C:212:ARG:NH2	4:C:901:YJ0:O52	2.51	0.43
2:D:175:LEU:O	2:D:179:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:PHE:O	1:A:170:GLU:HG3	2.19	0.43
2:B:229:LYS:O	2:B:233:THR:HG23	2.19	0.43
2:D:286:THR:O	2:D:290:ARG:HG3	2.18	0.43
1:A:266:TYR:OH	2:B:208:ILE:HG13	2.19	0.43
1:A:359:VAL:HG21	2:D:230:GLU:OE2	2.17	0.43
2:C:132:THR:HA	2:C:135:VAL:HG22	2.00	0.42
1:A:188:ARG:HD3	1:A:191:LEU:HD12	2.01	0.42
1:A:309:TRP:O	1:A:313:THR:HG22	2.18	0.42
2:B:200:ARG:HA	2:B:200:ARG:HD3	1.86	0.42
2:C:199:LEU:H	2:C:200:ARG:NH1	2.17	0.42
2:D:95:HIS:HA	2:D:98:VAL:HG22	2.00	0.42
2:D:172:ILE:O	2:D:175:LEU:HG	2.19	0.42
2:B:202:LEU:HD12	2:B:206:ARG:HH21	1.84	0.42
2:B:253:GLU:OE1	2:B:260:PHE:HB2	2.20	0.42
2:B:303:PHE:HA	2:B:306:LEU:HD23	2.01	0.42
3:B:902:9PE:H27	3:B:902:9PE:H24	1.79	0.42
2:D:128:LEU:HA	2:D:131:VAL:HG22	2.01	0.42
1:A:156:LEU:O	1:A:157:LEU:C	2.62	0.42
2:C:153:TYR:CD1	2:C:162:PHE:HB2	2.55	0.42
1:A:144:THR:HG21	2:D:263:TYR:HB2	2.01	0.42
2:C:101:LEU:HD21	2:C:132:THR:HB	2.01	0.42
2:B:83:VAL:HG23	2:B:84:LEU:CD2	2.50	0.42
2:C:167:PHE:O	2:C:170:ILE:HG12	2.20	0.42
2:C:174:VAL:HA	2:C:202:LEU:HD11	2.01	0.42
2:D:223:VAL:HG21	2:D:315:PHE:CE1	2.55	0.42
2:C:228:SER:O	3:C:902:9PE:H3	2.19	0.42
2:C:306:LEU:O	2:C:310:ILE:HG12	2.19	0.42
2:D:227:HIS:O	2:D:231:LEU:HD13	2.20	0.42
1:A:115:LEU:O	1:A:118:PRO:HD2	2.19	0.42
1:A:142:LEU:HD13	1:A:145:PHE:CD2	2.55	0.42
2:D:150:CYS:HB3	2:D:153:TYR:CE1	2.55	0.42
2:C:118:GLU:OE1	2:C:121:SER:OG	2.35	0.41
2:D:275:THR:O	2:D:277:ILE:HG13	2.20	0.41
1:A:323:THR:HG22	2:B:279:TYR:CD1	2.55	0.41
1:A:361:GLU:O	1:A:364:ARG:HG2	2.20	0.41
2:C:125:LEU:HD23	2:C:128:LEU:HD21	2.02	0.41
2:C:244:LEU:O	2:C:248:LEU:HD23	2.20	0.41
2:B:136:PHE:CZ	2:B:206:ARG:HD2	2.56	0.41
2:B:272:ILE:HD13	2:B:272:ILE:HA	1.86	0.41
2:D:113:THR:OG1	2:D:114:ILE:N	2.50	0.41
2:D:324:ARG:HG2	2:D:324:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:MET:HA	1:A:203:ILE:HG22	2.02	0.41
2:C:102:VAL:HA	2:C:206:ARG:HH21	1.84	0.41
2:D:292:LEU:HD23	2:D:292:LEU:HA	1.93	0.41
2:C:148:GLY:HA3	2:C:159:ARG:HH22	1.86	0.41
2:D:144:ILE:O	2:D:159:ARG:NH1	2.53	0.41
2:B:257:ASN:OD1	2:B:285:GLN:HB2	2.21	0.41
2:B:318:LYS:HA	2:B:321:GLU:OE2	2.20	0.41
2:C:178:SER:O	2:C:181:VAL:HG12	2.21	0.41
2:D:84:LEU:O	4:D:901:YJ0:O52	2.38	0.41
2:D:135:VAL:O	2:D:139:GLU:OE1	2.38	0.41
2:D:207:MET:HE2	2:D:207:MET:HB3	1.88	0.41
2:B:81:TYR:HB3	2:B:86:ARG:HH21	1.86	0.41
2:B:93:ILE:HD12	2:B:93:ILE:H	1.86	0.41
2:D:115:LYS:C	2:D:117:TYR:H	2.29	0.41
2:C:74:ARG:CZ	2:C:77:GLN:HG2	2.51	0.40
2:C:127:ILE:HD12	2:C:127:ILE:HA	1.99	0.40
2:C:317:LEU:HD13	2:D:320:GLN:OE1	2.21	0.40
1:A:198:LEU:O	1:A:201:LEU:HG	2.22	0.40
2:B:323:HIS:HA	2:B:326:LYS:NZ	2.36	0.40
2:C:102:VAL:HG13	2:C:206:ARG:HE	1.87	0.40
2:B:155:GLY:HA2	2:B:159:ARG:HD3	2.03	0.40
2:C:86:ARG:HA	2:C:212:ARG:HH22	1.87	0.40
2:C:105:CYS:SG	2:C:128:LEU:HD13	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/892 (26%)	219 (93%)	15 (6%)	1 (0%)	30	65
2	B	239/1142 (21%)	219 (92%)	20 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	242/1142 (21%)	236 (98%)	6 (2%)	0	100	100
2	D	243/1142 (21%)	228 (94%)	15 (6%)	0	100	100
All	All	959/4318 (22%)	902 (94%)	56 (6%)	1 (0%)	49	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/743 (26%)	196 (100%)	0	100	100
2	B	204/961 (21%)	203 (100%)	1 (0%)	81	82
2	C	205/961 (21%)	205 (100%)	0	100	100
2	D	206/961 (21%)	206 (100%)	0	100	100
All	All	811/3626 (22%)	810 (100%)	1 (0%)	87	89

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

Mol	Chain	Res	Type
2	B	302	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	78	ASN
2	C	70	ASN
2	C	78	ASN

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	$\# Z > 2$
3	9PE	B	902	-	39,39,39	0.97	4 (10%)	42,44,44	0.92	2 (4%)
4	YJ0	B	901	-	90,90,90	0.32	0	136,138,138	1.16	11 (8%)
3	9PE	C	902	-	39,39,39	0.98	4 (10%)	42,44,44	0.98	2 (4%)
4	YJ0	C	901	-	90,90,90	0.25	0	136,138,138	0.73	2 (1%)
3	9PE	A	1001	-	39,39,39	0.97	4 (10%)	42,44,44	0.95	2 (4%)
4	YJ0	D	901	-	90,90,90	0.21	0	136,138,138	0.55	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
3	9PE	B	902	-	-	28/43/43/43	-
4	YJ0	B	901	-	13/13/33/34	14/32/200/200	1/10/10/10

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	9PE	C	902	-	-	24/43/43/43	-
4	YJ0	C	901	-	8/8/33/34	16/32/200/200	1/10/10/10
3	9PE	A	1001	-	-	27/43/43/43	-
4	YJ0	D	901	-	9/9/33/34	12/32/200/200	1/10/10/10

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	902	9PE	O21-C2	-2.51	1.40	1.46
3	A	1001	9PE	O21-C2	-2.50	1.40	1.46
3	B	902	9PE	O21-C2	-2.42	1.40	1.46
3	B	902	9PE	O31-C31	2.42	1.40	1.33
3	A	1001	9PE	O31-C31	2.42	1.40	1.33
3	C	902	9PE	O31-C31	2.38	1.40	1.33
3	B	902	9PE	O21-C21	2.29	1.40	1.34
3	C	902	9PE	O31-C3	-2.21	1.40	1.45
3	C	902	9PE	O21-C21	2.19	1.40	1.34
3	A	1001	9PE	O31-C3	-2.16	1.40	1.45
3	B	902	9PE	O31-C3	-2.12	1.40	1.45
3	A	1001	9PE	O21-C21	2.10	1.40	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	901	YJ0	C12-C7-C8	-5.17	97.87	104.13
3	C	902	9PE	O21-C21-C22	4.20	120.55	111.50
4	B	901	YJ0	C26-C27-C28	-4.01	108.81	113.88
3	A	1001	9PE	O21-C21-C22	3.98	120.07	111.50
3	B	902	9PE	O21-C21-C22	3.91	119.92	111.50
4	B	901	YJ0	O9-C8-C7	-3.57	99.80	105.07
4	B	901	YJ0	C10-C8-C7	-3.36	100.50	107.52
4	B	901	YJ0	C17-C16-C15	3.18	113.57	109.71
4	B	901	YJ0	C12-C7-C6	2.72	129.81	120.56
3	B	902	9PE	O31-C31-C32	2.66	120.26	111.91
4	B	901	YJ0	C10-C11-C12	2.62	107.40	103.91
4	B	901	YJ0	O9-C8-C10	2.60	118.59	112.36
3	C	902	9PE	O31-C31-C32	2.60	120.07	111.91
3	A	1001	9PE	O31-C31-C32	2.52	119.82	111.91
4	B	901	YJ0	C53-C28-C29	2.51	115.02	111.00
4	B	901	YJ0	C20-C15-C16	2.39	116.32	112.73
4	C	901	YJ0	C12-C11-C16	2.16	117.58	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	901	YJ0	C16-C17-C18	2.02	115.64	112.73
4	C	901	YJ0	C14-C15-C20	2.00	115.71	113.08

All (30) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	901	YJ0	C23
4	B	901	YJ0	C6
4	B	901	YJ0	C11
4	B	901	YJ0	C58
4	B	901	YJ0	C59
4	B	901	YJ0	C68
4	B	901	YJ0	C34
4	B	901	YJ0	C16
4	B	901	YJ0	C35
4	B	901	YJ0	C55
4	B	901	YJ0	C8
4	B	901	YJ0	C5
4	B	901	YJ0	C31
4	C	901	YJ0	C12
4	C	901	YJ0	C33
4	C	901	YJ0	C11
4	C	901	YJ0	C34
4	C	901	YJ0	C66
4	C	901	YJ0	C56
4	C	901	YJ0	C35
4	C	901	YJ0	C5
4	D	901	YJ0	C6
4	D	901	YJ0	C12
4	D	901	YJ0	C59
4	D	901	YJ0	C32
4	D	901	YJ0	C16
4	D	901	YJ0	C65
4	D	901	YJ0	C57
4	D	901	YJ0	C15
4	D	901	YJ0	C5

All (121) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	9PE	C1-O11-P-O12
3	A	1001	9PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
3	A	1001	9PE	O13-C11-C12-N
3	A	1001	9PE	C22-C21-O21-C2
3	B	902	9PE	C11-O13-P-O14
3	B	902	9PE	C12-C11-O13-P
3	B	902	9PE	O21-C2-C3-O31
3	C	902	9PE	C1-O11-P-O12
3	C	902	9PE	O13-C11-C12-N
4	B	901	YJ0	C29-C28-C53-O54
4	B	901	YJ0	C28-C29-O30-C31
4	B	901	YJ0	C28-C53-O54-C55
4	C	901	YJ0	O60-C55-O54-C53
4	D	901	YJ0	C27-C28-C53-O54
4	D	901	YJ0	C29-C28-C53-O54
4	D	901	YJ0	O36-C31-O30-C29
4	D	901	YJ0	C28-C53-O54-C55
4	B	901	YJ0	O69-C64-O63-C58
4	C	901	YJ0	C59-C58-O63-C64
3	A	1001	9PE	O22-C21-O21-C2
4	B	901	YJ0	O1-C9-O39-C34
3	B	902	9PE	C32-C31-O31-C3
4	B	901	YJ0	C65-C64-O63-C58
3	C	902	9PE	C22-C21-O21-C2
3	B	902	9PE	C27-C28-C29-C2A
3	A	1001	9PE	C27-C28-C29-C2A
4	B	901	YJ0	C25-C9-O39-C34
3	A	1001	9PE	C32-C33-C34-C35
4	C	901	YJ0	C33-C34-O39-C9
3	B	902	9PE	O32-C31-O31-C3
3	C	902	9PE	O22-C21-O21-C2
3	C	902	9PE	C32-C31-O31-C3
4	C	901	YJ0	C32-C31-O30-C29
4	D	901	YJ0	C32-C31-O30-C29
3	C	902	9PE	O32-C31-O31-C3
3	A	1001	9PE	C21-C22-C23-C24
4	B	901	YJ0	C35-C34-O39-C9
3	C	902	9PE	C33-C34-C35-C36
3	B	902	9PE	C21-C22-C23-C24
3	B	902	9PE	C31-C32-C33-C34
4	B	901	YJ0	C33-C34-O39-C9
4	B	901	YJ0	C27-C28-C53-O54
4	C	901	YJ0	C25-C9-O39-C34
3	B	902	9PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
4	D	901	YJ0	C59-C58-O63-C64
3	A	1001	9PE	C2C-C2D-C2E-C2F
4	B	901	YJ0	C32-C31-O30-C29
4	C	901	YJ0	O1-C9-O39-C34
3	C	902	9PE	C2D-C2E-C2F-C2G
4	B	901	YJ0	O36-C31-O30-C29
3	C	902	9PE	C21-C22-C23-C24
3	B	902	9PE	C29-C2A-C2B-C2C
4	D	901	YJ0	C57-C58-O63-C64
3	C	902	9PE	C2B-C2C-C2D-C2E
3	A	1001	9PE	O11-C1-C2-O21
3	B	902	9PE	C2A-C2B-C2C-C2D
3	C	902	9PE	C1-O11-P-O13
3	C	902	9PE	C2A-C2B-C2C-C2D
3	A	1001	9PE	C2B-C2C-C2D-C2E
3	B	902	9PE	C1-C2-C3-O31
3	B	902	9PE	C34-C35-C36-C37
3	C	902	9PE	C2F-C2G-C2H-C2I
4	C	901	YJ0	O36-C31-O30-C29
4	C	901	YJ0	O36-C35-C37-O38
3	A	1001	9PE	C31-C32-C33-C34
3	A	1001	9PE	C2F-C2G-C2H-C2I
3	B	902	9PE	C2F-C2G-C2H-C2I
4	C	901	YJ0	C56-C55-O54-C53
3	A	1001	9PE	O11-C1-C2-C3
3	C	902	9PE	O11-C1-C2-C3
3	A	1001	9PE	C33-C34-C35-C36
3	A	1001	9PE	C34-C35-C36-C37
4	C	901	YJ0	C35-C34-O39-C9
3	A	1001	9PE	C1-C2-C3-O31
3	C	902	9PE	C29-C2A-C2B-C2C
3	A	1001	9PE	C1-O11-P-O13
3	A	1001	9PE	O21-C2-C3-O31
3	C	902	9PE	C22-C23-C24-C25
3	C	902	9PE	C2-C1-O11-P
3	A	1001	9PE	C29-C2A-C2B-C2C
3	C	902	9PE	C2C-C2D-C2E-C2F
3	A	1001	9PE	C2A-C2B-C2C-C2D
3	B	902	9PE	O11-C1-C2-O21
3	C	902	9PE	O11-C1-C2-O21
4	C	901	YJ0	O69-C64-O63-C58
3	A	1001	9PE	C2D-C2E-C2F-C2G

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Mol	Chain	Res	Type	Atoms
4	C	901	YJ0	O25-C26-C27-C28
3	A	1001	9PE	C1-O11-P-O14
3	B	902	9PE	C11-O13-P-O12
3	C	902	9PE	C1-O11-P-O14
3	B	902	9PE	O11-C1-C2-C3
3	A	1001	9PE	C12-C11-O13-P
4	D	901	YJ0	C28-C29-O30-C31
3	B	902	9PE	C2D-C2E-C2F-C2G
3	C	902	9PE	C1-C2-C3-O31
3	C	902	9PE	O21-C2-C3-O31
3	A	1001	9PE	C11-O13-P-O11
3	B	902	9PE	C1-O11-P-O13
4	D	901	YJ0	C27-C28-C29-O30
3	B	902	9PE	C23-C24-C25-C26
4	C	901	YJ0	C27-C26-O25-C23
3	B	902	9PE	O22-C21-O21-C2
4	D	901	YJ0	O1-C9-O39-C34
4	C	901	YJ0	C57-C58-O63-C64
4	B	901	YJ0	C27-C26-O25-C23
3	B	902	9PE	C2C-C2D-C2E-C2F
4	D	901	YJ0	C25-C9-O39-C34
4	C	901	YJ0	C65-C64-O63-C58
4	D	901	YJ0	O25-C26-C27-C28
3	B	902	9PE	C24-C25-C26-C27
3	B	902	9PE	O31-C31-C32-C33
3	C	902	9PE	O21-C21-C22-C23
3	B	902	9PE	C22-C21-O21-C2
3	B	902	9PE	C22-C23-C24-C25
4	B	901	YJ0	O60-C55-O54-C53
4	C	901	YJ0	C24-C23-O25-C26
3	B	902	9PE	O32-C31-C32-C33
3	B	902	9PE	C1-O11-P-O12
3	C	902	9PE	O22-C21-C22-C23
3	A	1001	9PE	O21-C21-C22-C23
3	A	1001	9PE	O22-C21-C22-C23

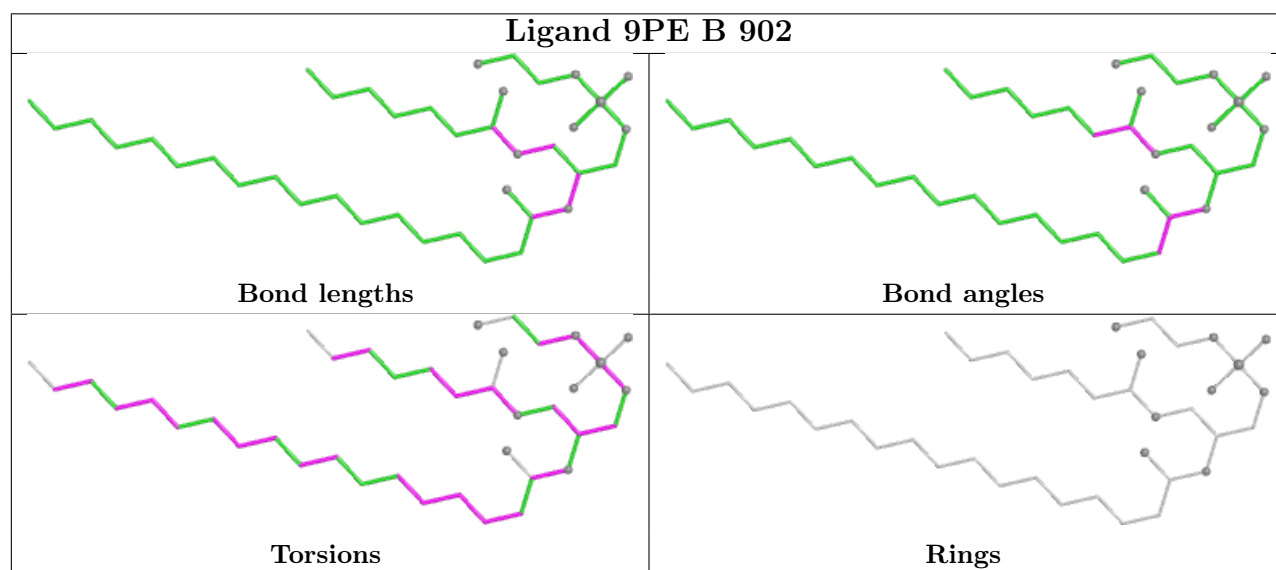
All (3) ring outliers are listed below:

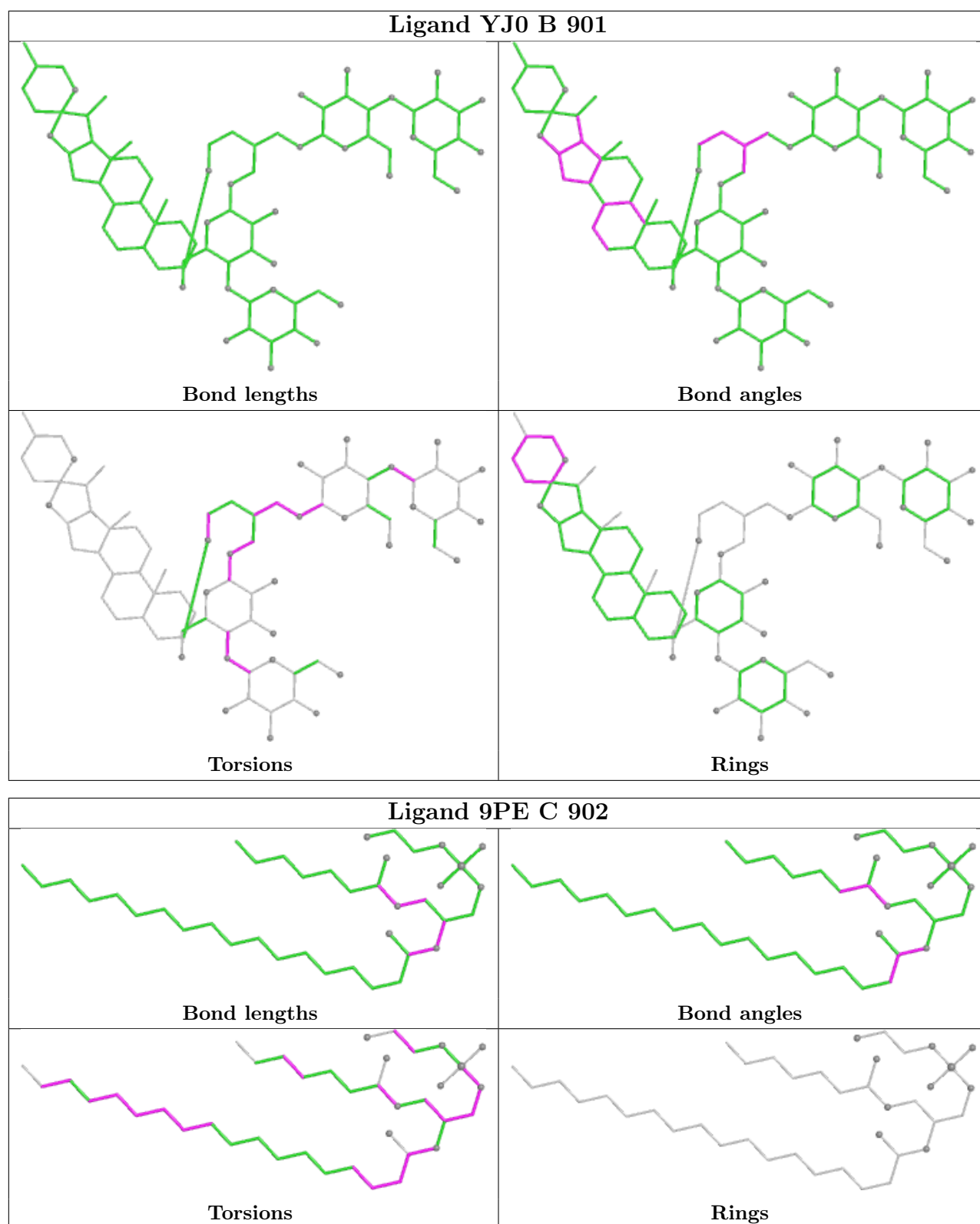
Mol	Chain	Res	Type	Atoms
4	C	901	YJ0	C2-C3-C4-C5-C81-O80
4	D	901	YJ0	C2-C3-C4-C5-C81-O80
4	B	901	YJ0	C2-C3-C4-C5-C81-O80

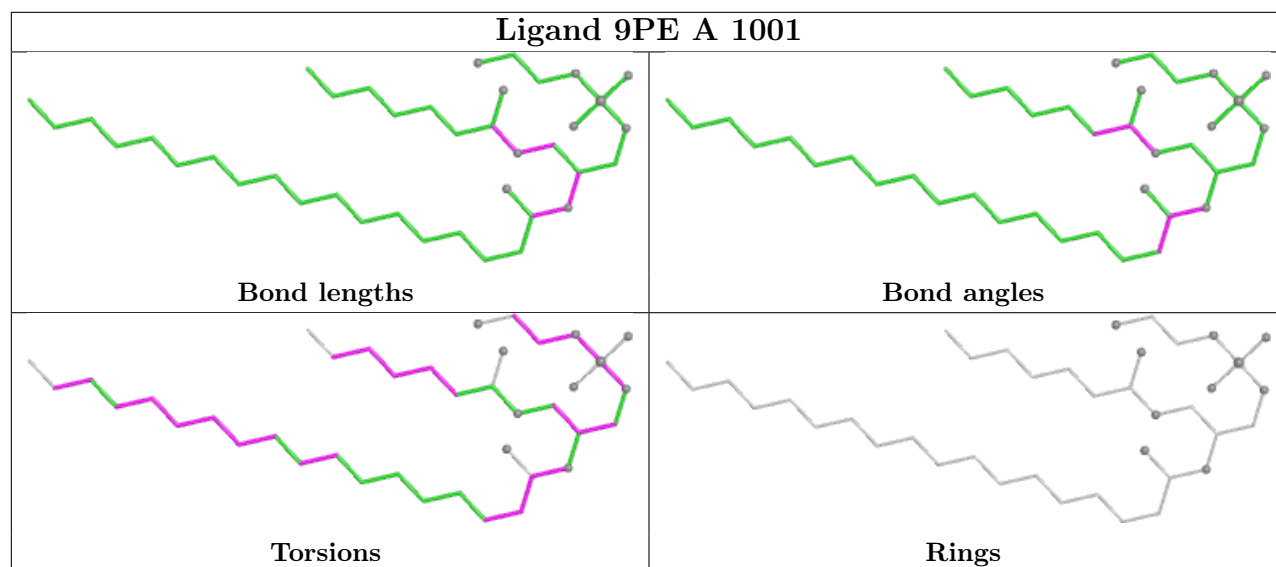
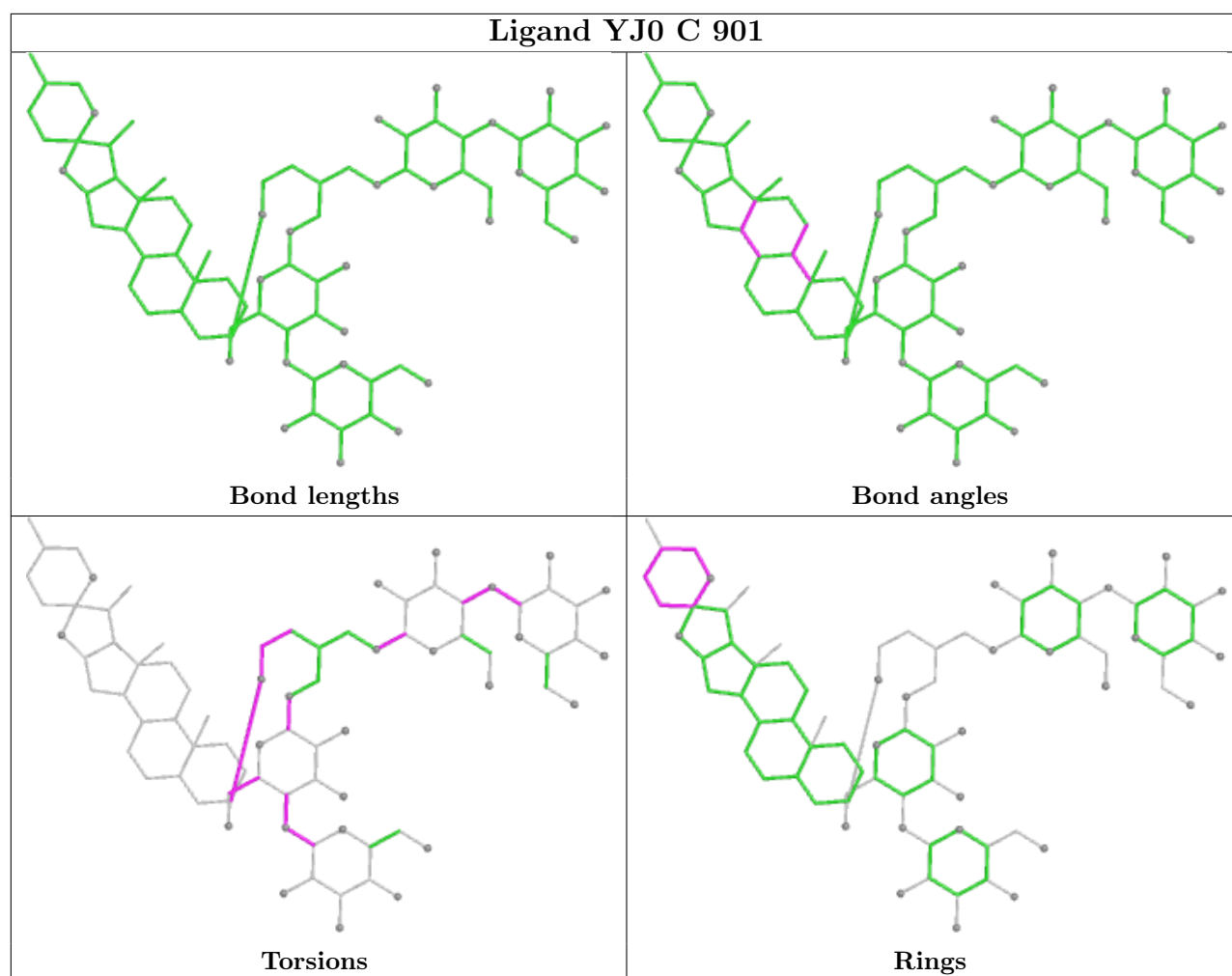
6 monomers are involved in 18 short contacts:

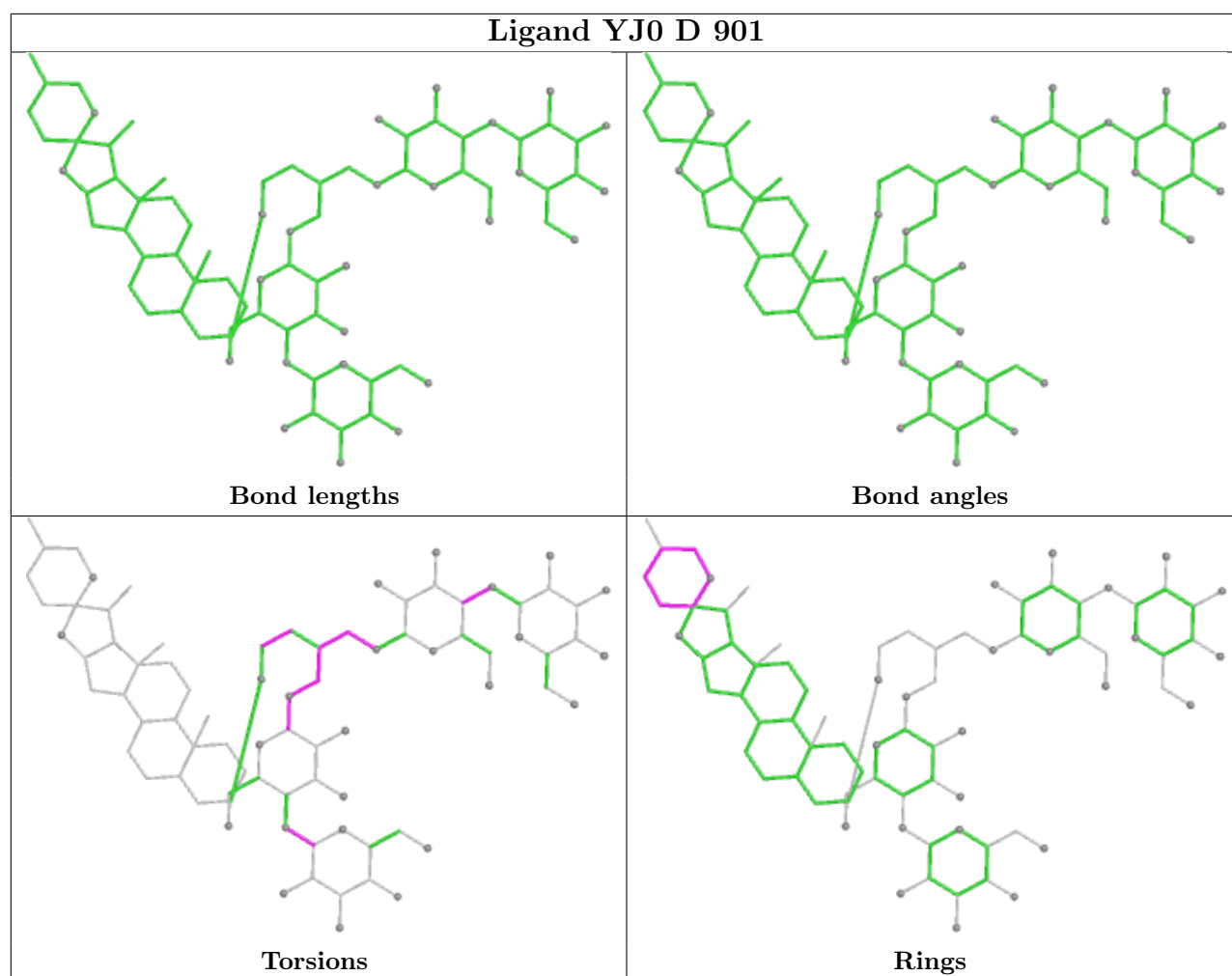
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	9PE	4	0
4	B	901	YJ0	3	0
3	C	902	9PE	4	0
4	C	901	YJ0	5	0
3	A	1001	9PE	2	0
4	D	901	YJ0	3	0

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.

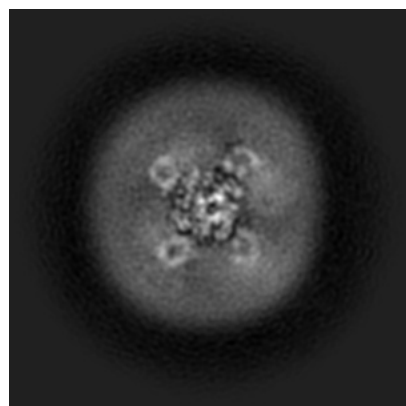
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-69843. These allow visual inspection of the internal detail of the map and identification of artifacts.

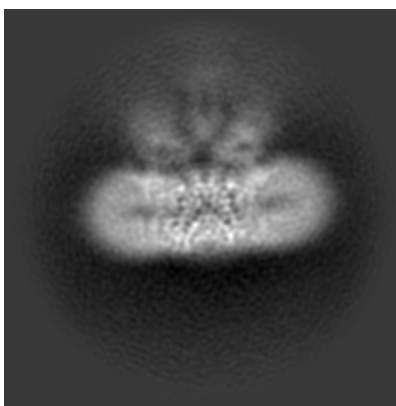
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

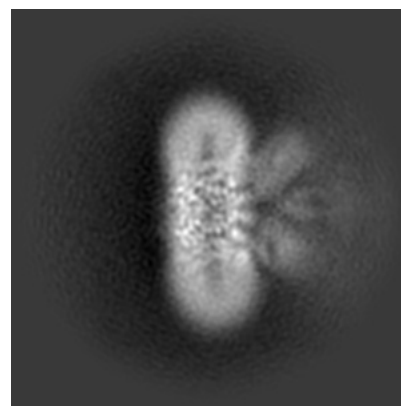
6.1.1 Primary map



X

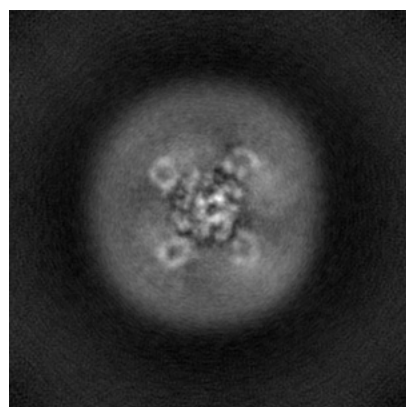


Y

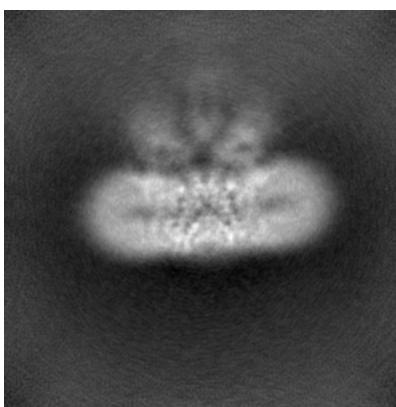


Z

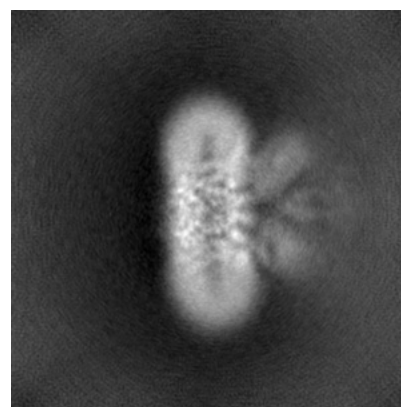
6.1.2 Raw map



X



Y

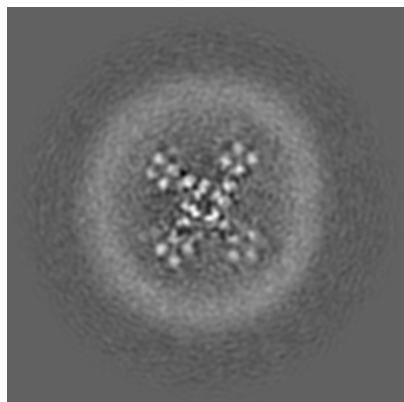


Z

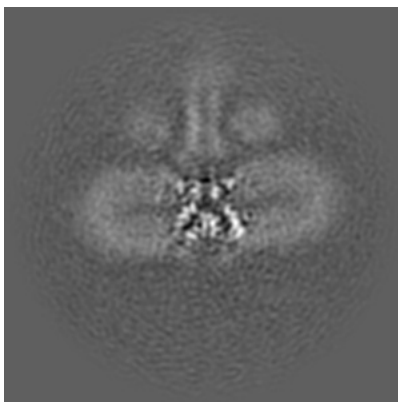
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

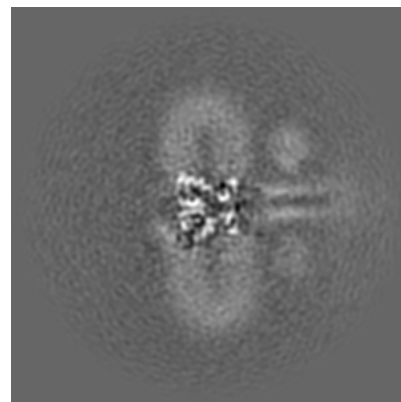
6.2.1 Primary map



X Index: 120

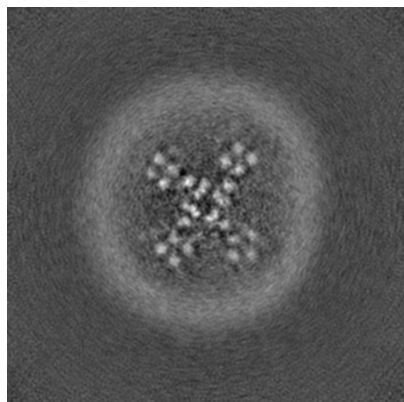


Y Index: 120

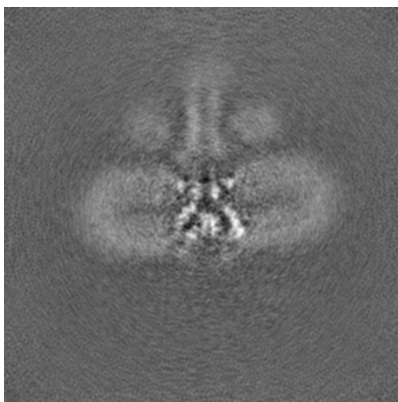


Z Index: 120

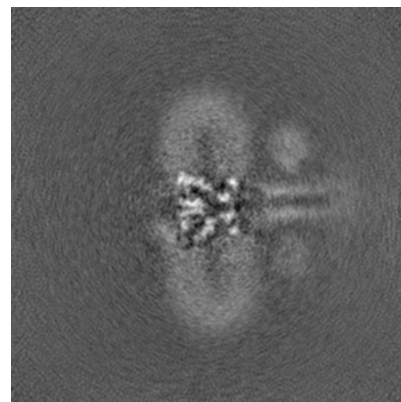
6.2.2 Raw map



X Index: 120



Y Index: 120

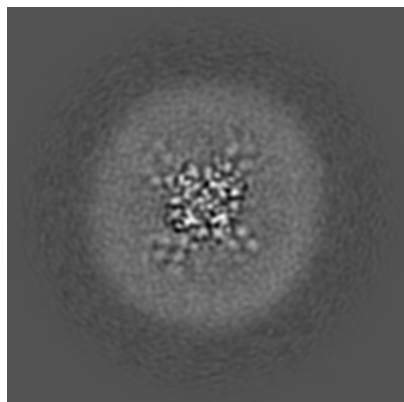


Z Index: 120

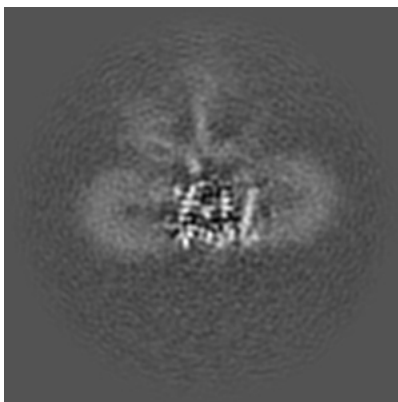
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

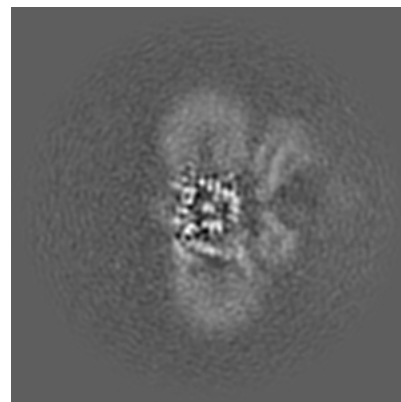
6.3.1 Primary map



X Index: 107

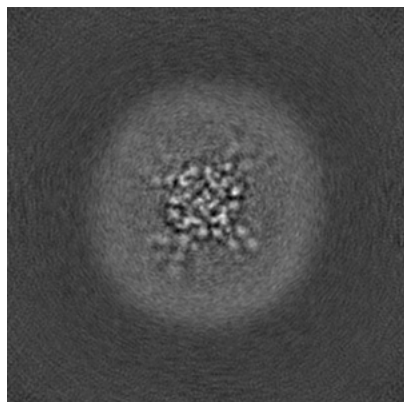


Y Index: 131

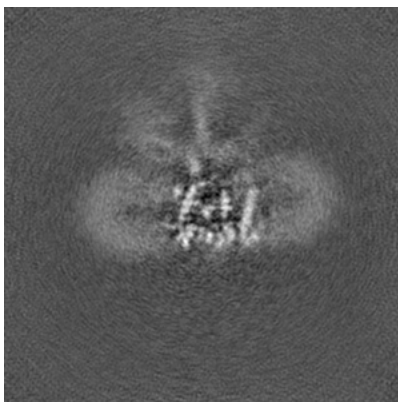


Z Index: 134

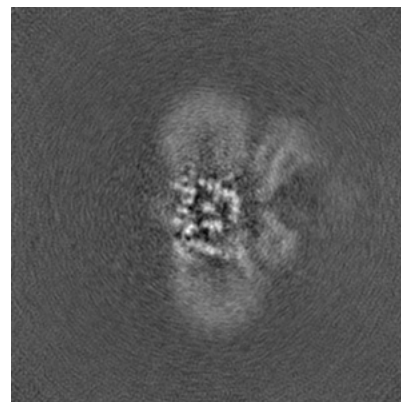
6.3.2 Raw map



X Index: 106



Y Index: 131

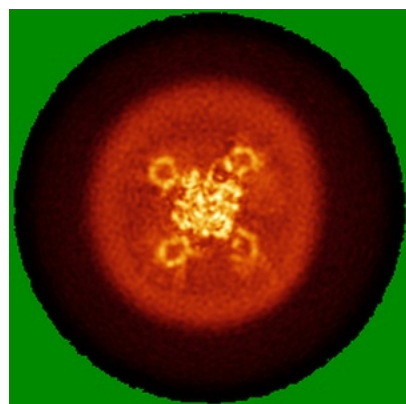


Z Index: 134

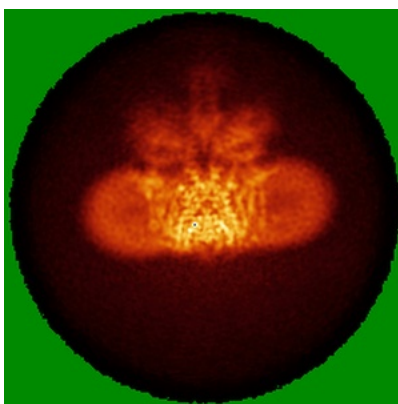
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

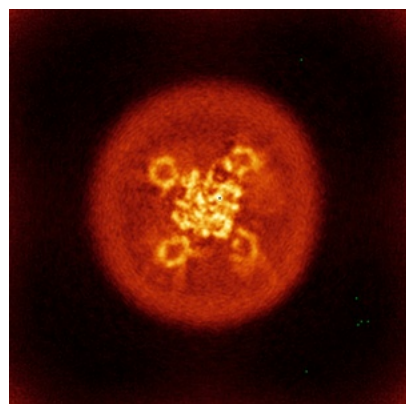


Y

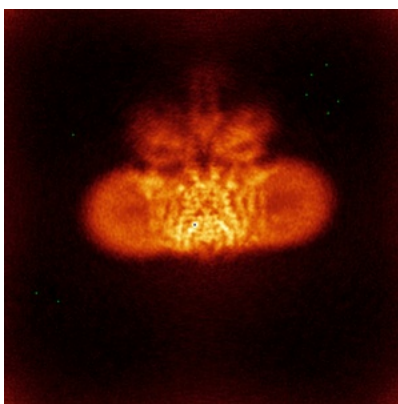


Z

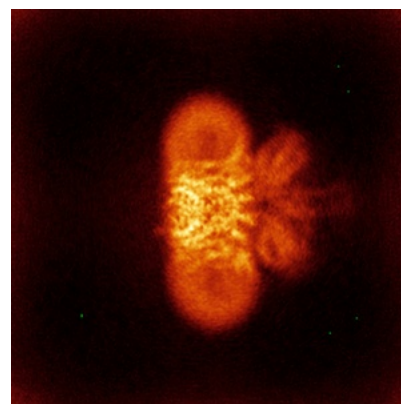
6.4.2 Raw map



X



Y

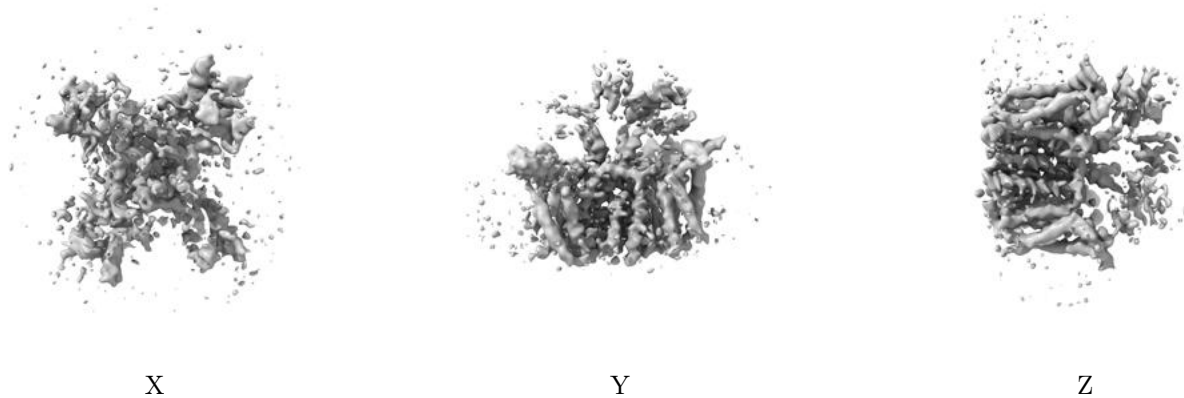


Z

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.

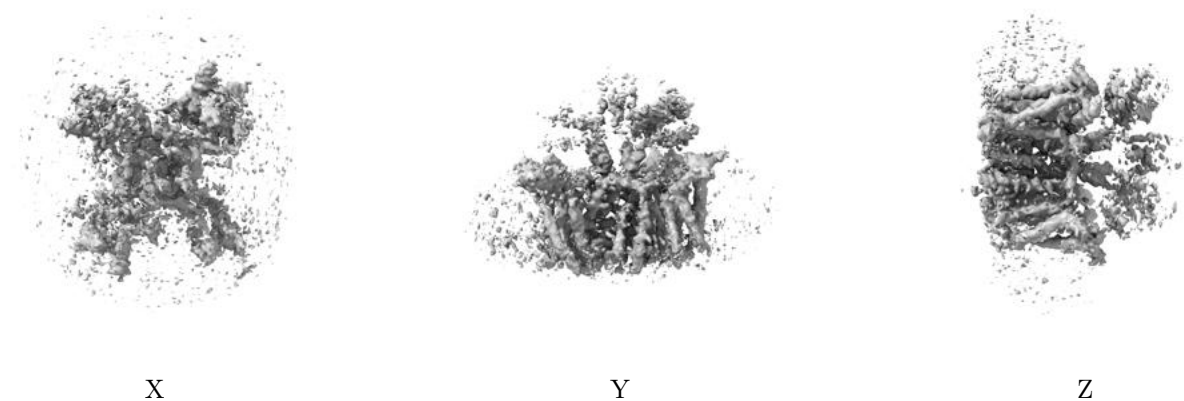
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.424. 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.

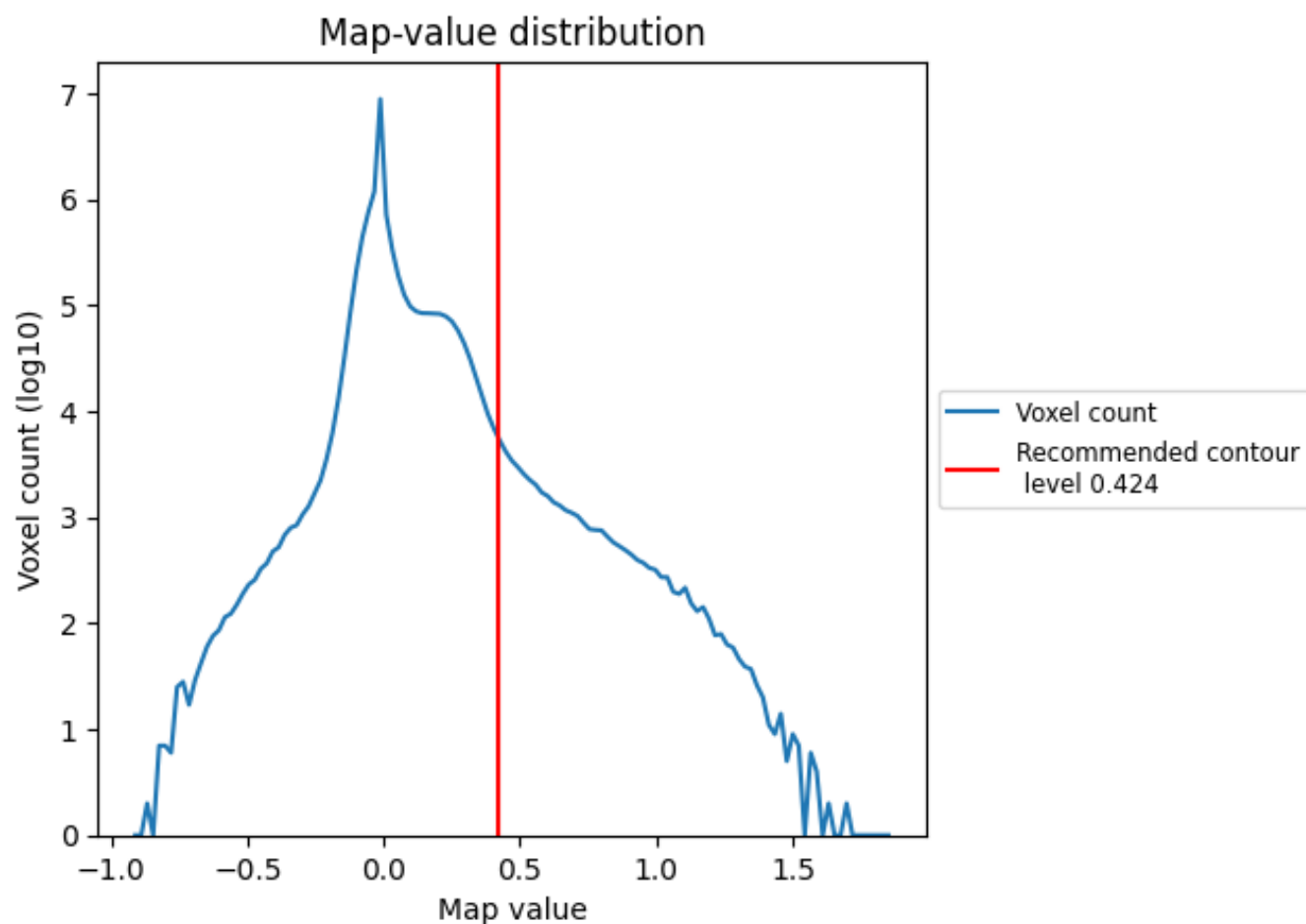
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

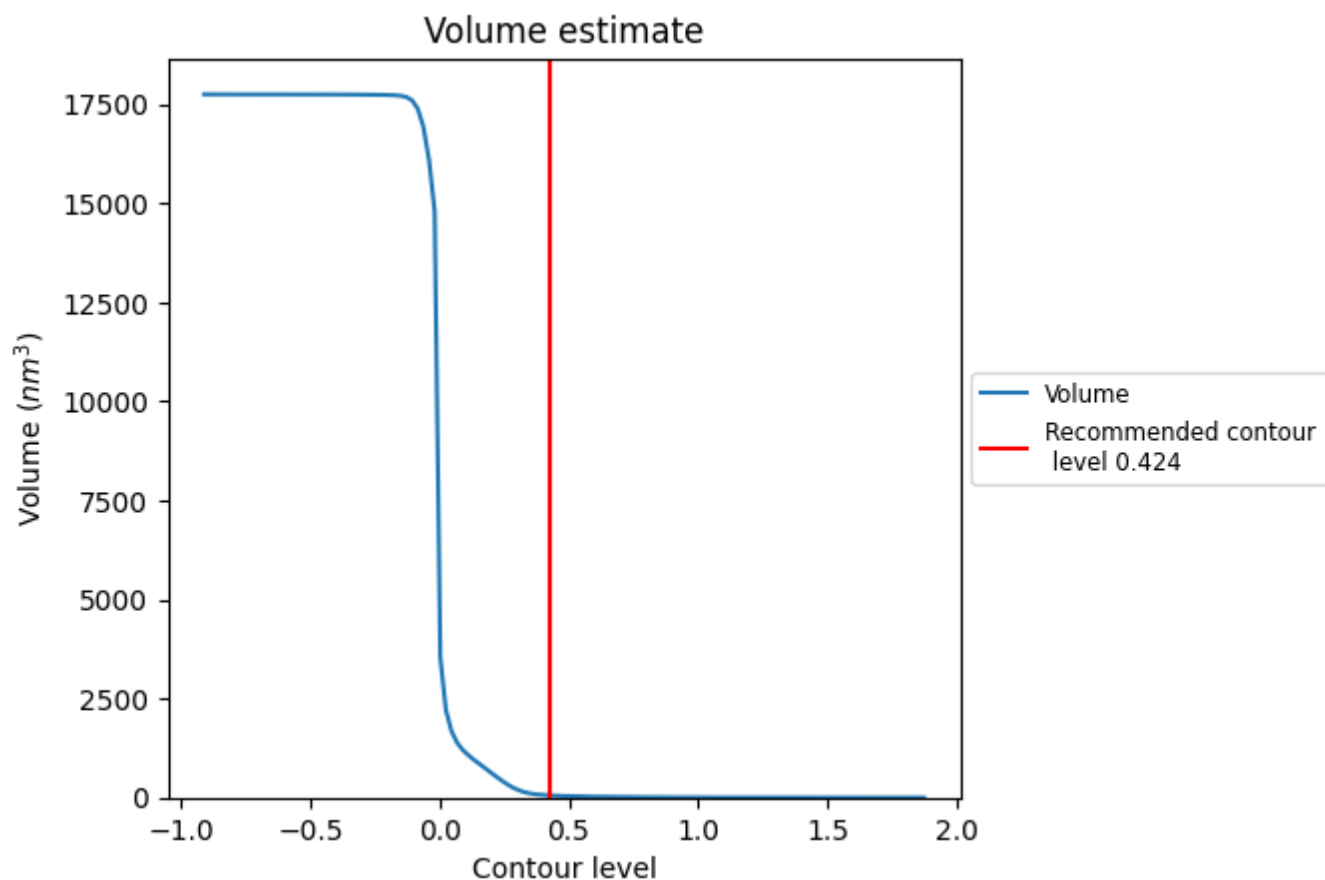
This section contains the results of statistical analysis of the map.

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.

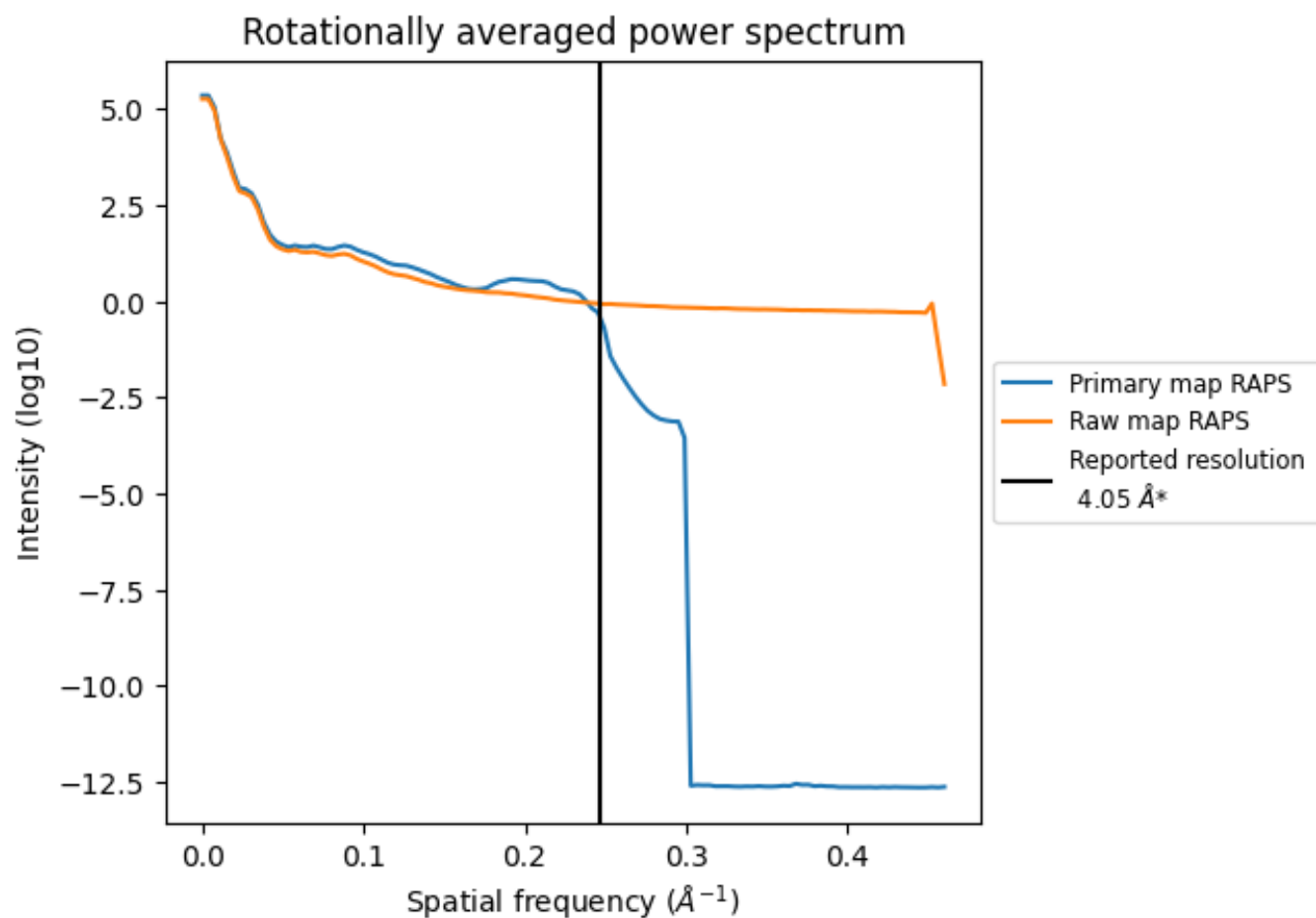
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 54 nm³; this corresponds to an approximate mass of 49 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 ⓘ

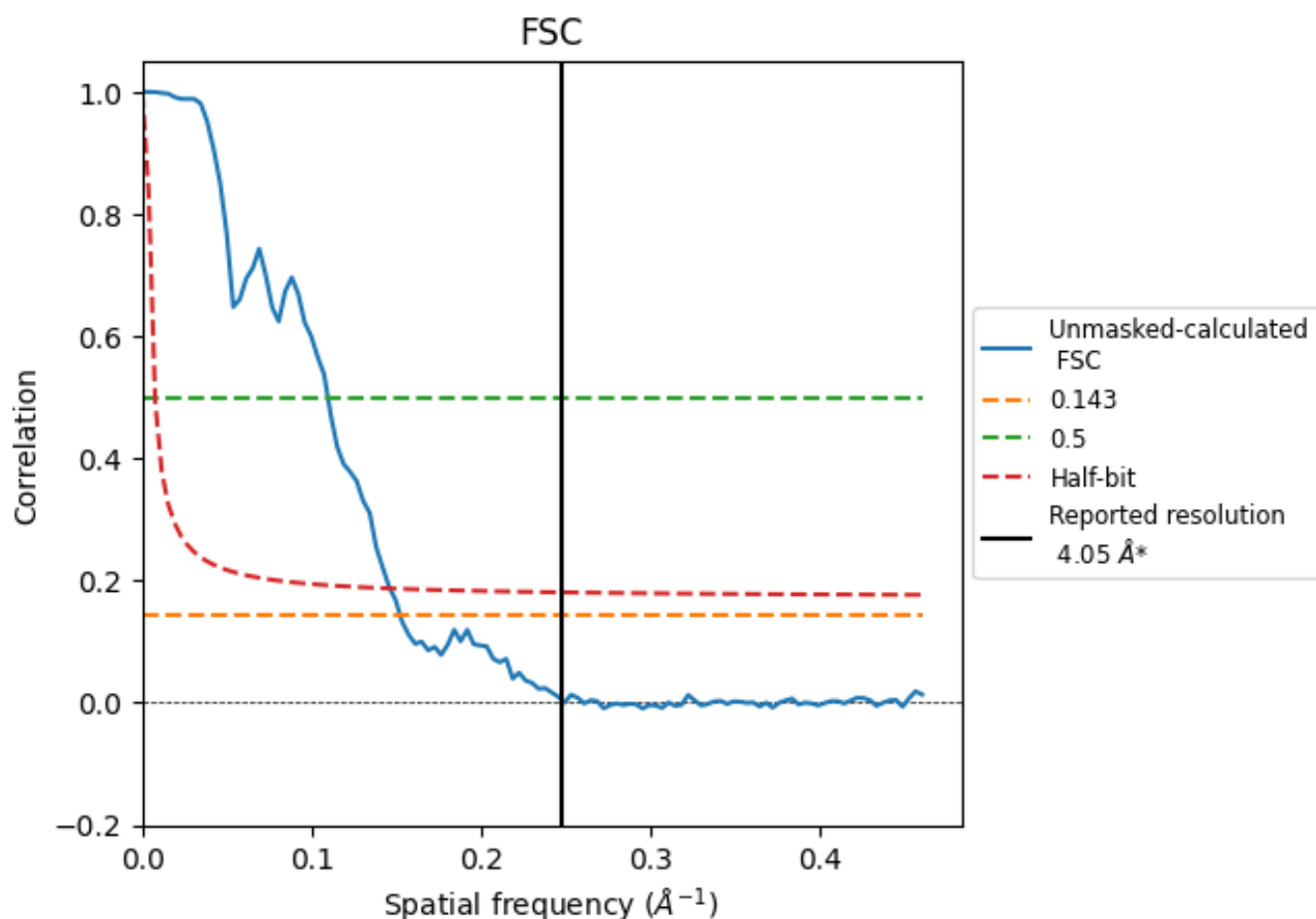


*Reported resolution corresponds to spatial frequency of 0.247 Å⁻¹

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 $0.247 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

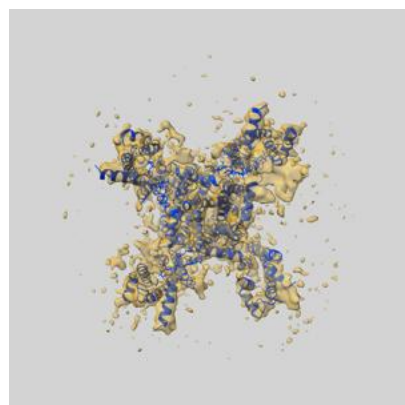
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.05	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.57	9.13	6.85

*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 6.57 differs from the reported value 4.05 by more than 10 %

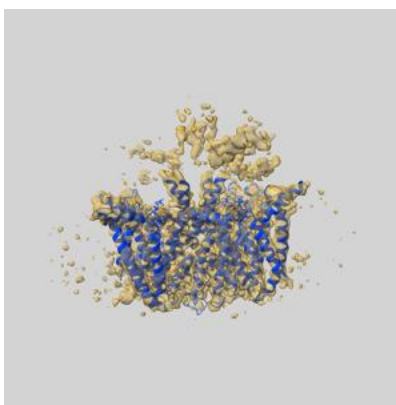
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-69843 and PDB model 24VL. Per-residue inclusion information can be found in section [3](#) on page [10](#).

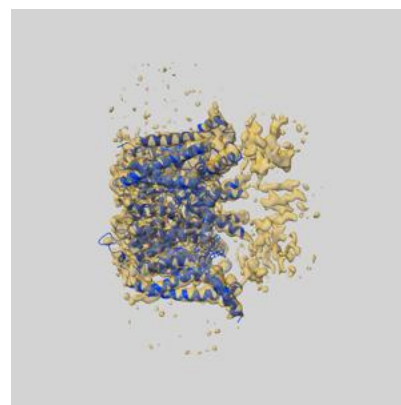
9.1 Map-model overlay [i](#)



X



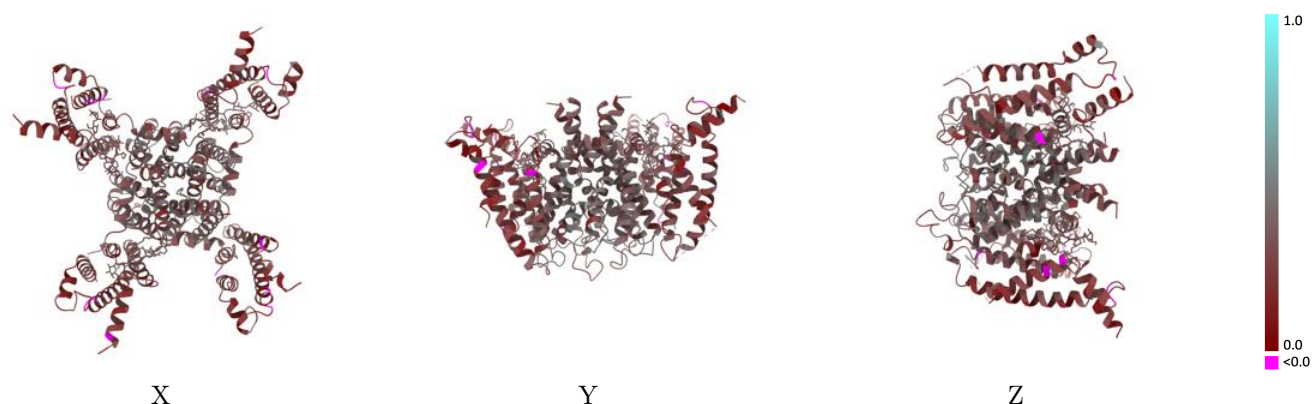
Y



Z

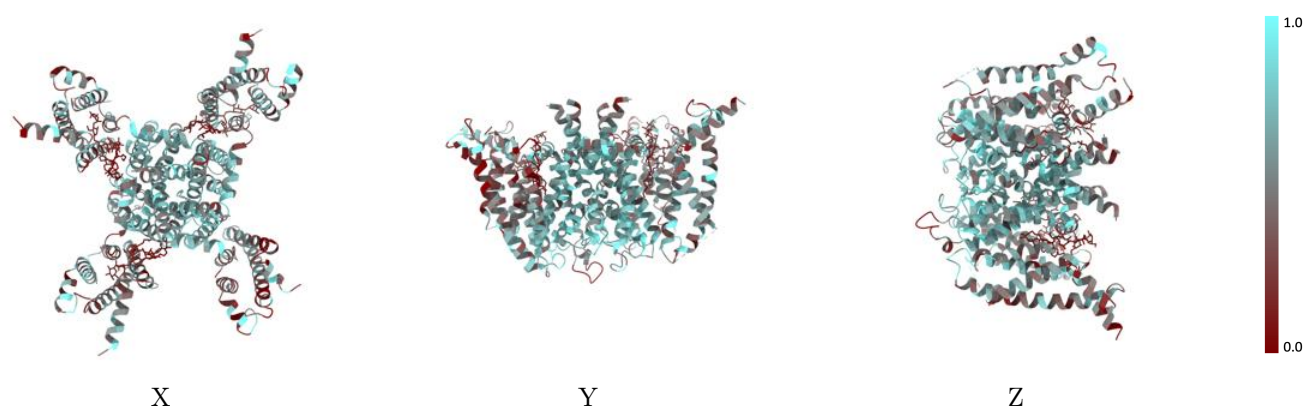
The images above show the 3D surface view of the map at the recommended contour level 0.424 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



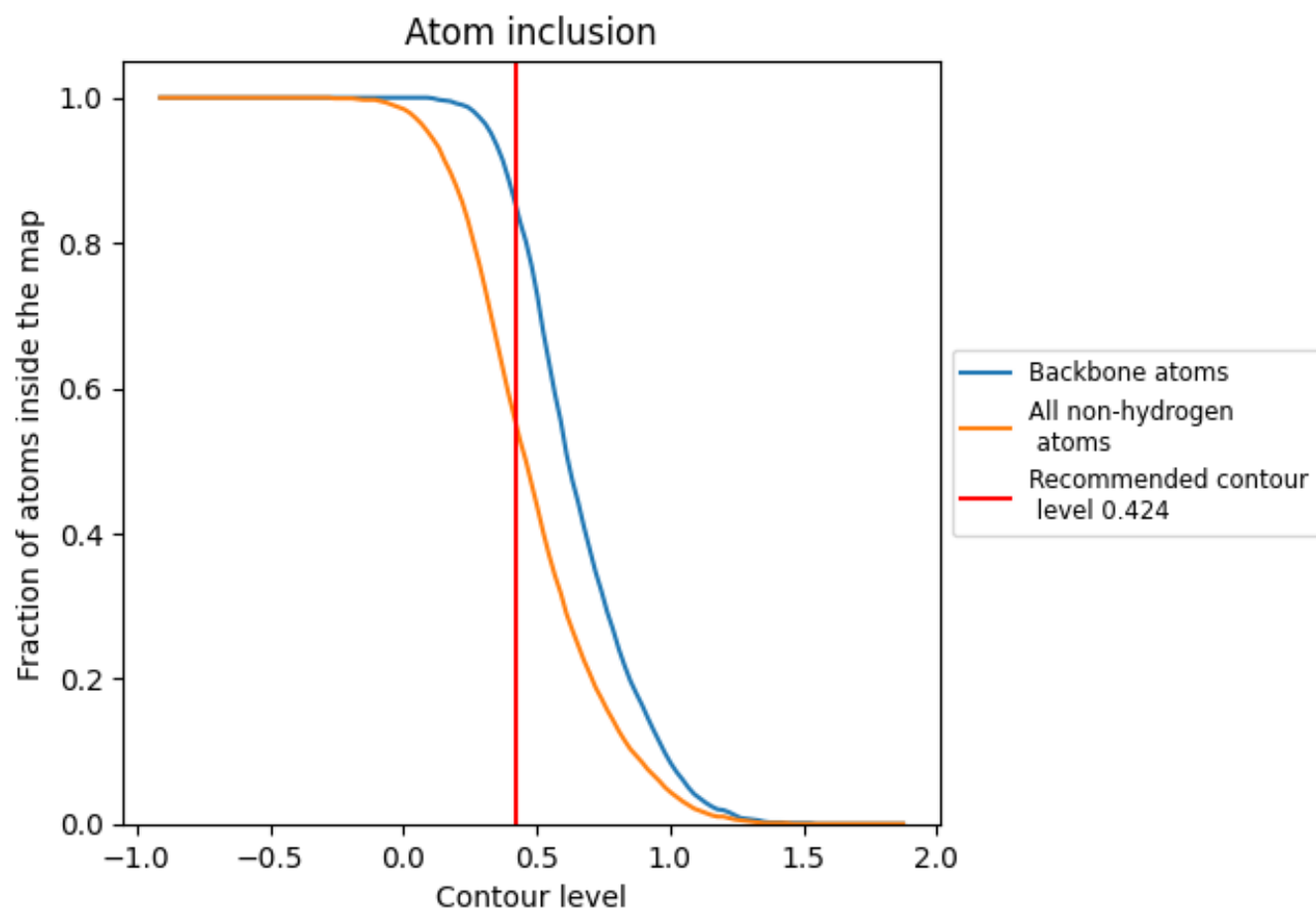
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.424).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 55% 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 (0.424) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5490	0.3010
A	0.5070	0.2940
B	0.5510	0.3030
C	0.5500	0.2990
D	0.5840	0.3100

