



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:49 AM UTC

PDB ID : 9J98 / pdb_00009j98
EMDB ID : EMD-61255
Title : Open structure of human XPR1
Authors : Wang, Y.; Wang, Y.; Yang, H.; Shen, H.
Deposited on : 2024-08-22
Resolution : 3.33 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

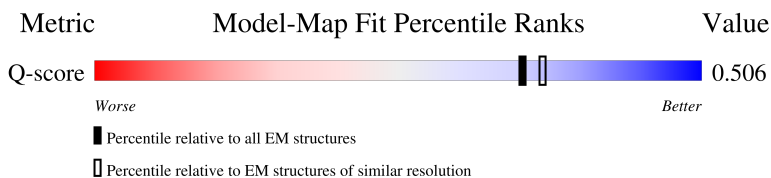
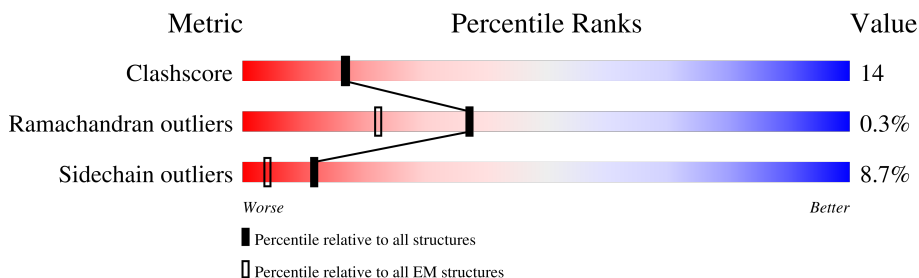
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 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	14484 (2.83 - 3.83)

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	969	
1	B	969	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6752 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 Solute carrier family 53 member 1, Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	397	Total	C	N	O	S	0	0
			3301	2215	530	540	16		
1	B	397	Total	C	N	O	S	0	0
			3301	2215	530	540	16		

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	697	GLY	-	linker	UNP Q9UBH6
A	698	GLY	-	linker	UNP Q9UBH6
A	699	ARG	-	linker	UNP Q9UBH6
A	700	LEU	-	linker	UNP Q9UBH6
A	701	GLU	-	linker	UNP Q9UBH6
A	702	VAL	-	linker	UNP Q9UBH6
A	703	LEU	-	linker	UNP Q9UBH6
A	704	PHE	-	linker	UNP Q9UBH6
A	705	GLN	-	linker	UNP Q9UBH6
A	706	GLY	-	linker	UNP Q9UBH6
A	707	PRO	-	linker	UNP Q9UBH6
A	708	ALA	-	linker	UNP Q9UBH6
A	709	ALA	-	linker	UNP Q9UBH6
A	710	ALA	-	linker	UNP Q9UBH6
A	711	ALA	-	linker	UNP Q9UBH6
A	712	VAL	-	linker	UNP Q9UBH6
A	775	LEU	PHE	conflict	UNP P42212
A	776	THR	SER	conflict	UNP P42212
A	818	THR	LYS	conflict	UNP P42212
A	917	LYS	ALA	conflict	UNP P42212
A	942	LEU	HIS	conflict	UNP P42212
A	950	SER	-	expression tag	UNP P42212
A	951	GLY	-	expression tag	UNP P42212
A	952	LEU	-	expression tag	UNP P42212
A	953	ARG	-	expression tag	UNP P42212
A	954	SER	-	expression tag	UNP P42212

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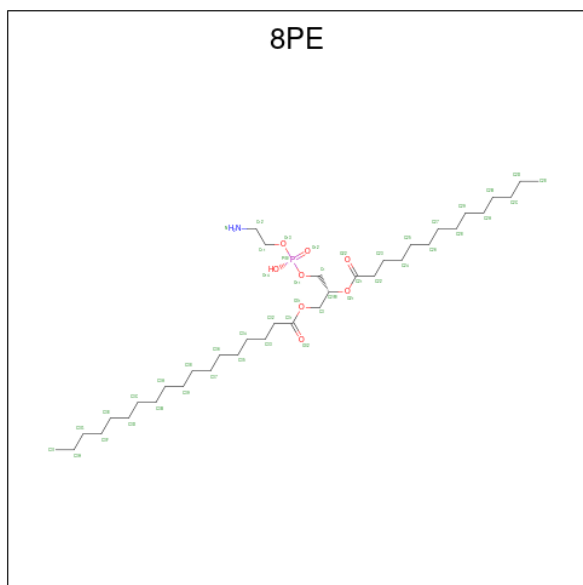
Chain	Residue	Modelled	Actual	Comment	Reference
A	955	ASP	-	expression tag	UNP P42212
A	956	TYR	-	expression tag	UNP P42212
A	957	LYS	-	expression tag	UNP P42212
A	958	ASP	-	expression tag	UNP P42212
A	959	HIS	-	expression tag	UNP P42212
A	960	ASP	-	expression tag	UNP P42212
A	961	ILE	-	expression tag	UNP P42212
A	962	ASP	-	expression tag	UNP P42212
A	963	TYR	-	expression tag	UNP P42212
A	964	LYS	-	expression tag	UNP P42212
A	965	ASP	-	expression tag	UNP P42212
A	966	ASP	-	expression tag	UNP P42212
A	967	ASP	-	expression tag	UNP P42212
A	968	ASP	-	expression tag	UNP P42212
A	969	LYS	-	expression tag	UNP P42212
B	697	GLY	-	linker	UNP Q9UBH6
B	698	GLY	-	linker	UNP Q9UBH6
B	699	ARG	-	linker	UNP Q9UBH6
B	700	LEU	-	linker	UNP Q9UBH6
B	701	GLU	-	linker	UNP Q9UBH6
B	702	VAL	-	linker	UNP Q9UBH6
B	703	LEU	-	linker	UNP Q9UBH6
B	704	PHE	-	linker	UNP Q9UBH6
B	705	GLN	-	linker	UNP Q9UBH6
B	706	GLY	-	linker	UNP Q9UBH6
B	707	PRO	-	linker	UNP Q9UBH6
B	708	ALA	-	linker	UNP Q9UBH6
B	709	ALA	-	linker	UNP Q9UBH6
B	710	ALA	-	linker	UNP Q9UBH6
B	711	ALA	-	linker	UNP Q9UBH6
B	712	VAL	-	linker	UNP Q9UBH6
B	775	LEU	PHE	conflict	UNP P42212
B	776	THR	SER	conflict	UNP P42212
B	818	THR	LYS	conflict	UNP P42212
B	917	LYS	ALA	conflict	UNP P42212
B	942	LEU	HIS	conflict	UNP P42212
B	950	SER	-	expression tag	UNP P42212
B	951	GLY	-	expression tag	UNP P42212
B	952	LEU	-	expression tag	UNP P42212
B	953	ARG	-	expression tag	UNP P42212
B	954	SER	-	expression tag	UNP P42212
B	955	ASP	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	956	TYR	-	expression tag	UNP P42212
B	957	LYS	-	expression tag	UNP P42212
B	958	ASP	-	expression tag	UNP P42212
B	959	HIS	-	expression tag	UNP P42212
B	960	ASP	-	expression tag	UNP P42212
B	961	ILE	-	expression tag	UNP P42212
B	962	ASP	-	expression tag	UNP P42212
B	963	TYR	-	expression tag	UNP P42212
B	964	LYS	-	expression tag	UNP P42212
B	965	ASP	-	expression tag	UNP P42212
B	966	ASP	-	expression tag	UNP P42212
B	967	ASP	-	expression tag	UNP P42212
B	968	ASP	-	expression tag	UNP P42212
B	969	LYS	-	expression tag	UNP P42212

- Molecule 2 is (2R)-3-[[[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-2-(tetradecanoyloxy)propyl octadecanoate (CCD ID: 8PE) (formula: C₃₇H₇₄NO₈P).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
2	B	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	

LYS
ASP
HIS
ASP
ILE
ASP
TYR
LYS
ASP
ASP
ASP
ASP
LYS

- Molecule 1: Solute carrier family 53 member 1, Green fluorescent protein

Chain B: 27% 11% 59%

GLU	ARG	VAL	GLN	HIS	ARG	ASN	ILE	ASP	LYS	LEU	LYS	LEU	LEU	ALA	PHE	SER	GLU	PHE	TYR	LEU	SER	LEU	ILE	LEU	GLN	ASN	ASN	ASN	PHE	THR	GLY	PHE	ARG	LYS	ILE	ILE	LEU	LYS	LYS	HIS	ASP	LYS	ARG	SER	GLY	ALA	ASP	TRP	ARG	VAL	ALA	HIS	VAL
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GLU	VAL	ALA	VAL	PRO	PHE	TYR	THR	CYS	LYS	LYS	ILE	ASN	GLN	LEU	ILE	SER	GLU	THR	GLU	ALA	VAL	VAL	THR	ASN	GLU	LEU	GLU	ASP	GLY	ASP	ARG	GLN	LYS	ALA	ALA	MET	LYS	ARG	LEU	ARG	VAL	PRO	PRO	GLY	GLY	ALA	ALA	ALA	GLN	A228	P228	P230	T233	V246	L251	V252	V256
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◆ L259 ◆ E260 ◆ T261 ◆ T262 ◆ T263 ◆ S264 ◆ T265 ◆ T266 ◆ R270 ◆ T271 ◆ V272 ◆ T273 ◆ L278 ◆ T279 ◆ E280 ◆ L285 ◆ V300 ◆ L305 ◆ N306 ◆ P307 ◆ R308 ◆ N309 ◆ N310 ◆ Q314 ◆ G324 ◆ L331 ◆ L332 ◆ V341 ◆ L342 ◆ Y352 ◆ N361 ◆ P362 ◆ T363 ◆ K364 ◆ T365 ◆ Y368 ◆ K369 ◆ S370 ◆ R371 ◆ L378 ◆ F382 ◆ T383 ◆ A384 ◆ P385

[illegible][illegible]

D590	I591	I592	A593	T594	V595	F596	A597	P598	L599	R604	N608	R611	L612	E613	N614	E615	N618	N619	C620	G621	E622	F623	R624	A625	V626	ARG	ASP	ILE	SER	VAL	ALA	PRO	LEU	ASN	ALA	ASP	ASP	GLN	THR	LEU	LEU	GLU	GLN	MET	MET	ASP	GLN	ASP	ASP	GLY	VAL	ARG	ASN	ARG
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LYS ASN ARC SEF TRP LYS TYR ASN GLN ILE LEU ARC ARC PRP ARC LEU ALA ALA ARG ASN THH LYS VAL VAL LEU ILE GLU ASH THH ASH ASH GLU ALA ASN THH GLN GLY ARC LEU GLU VAL LEU PHH GLN GLY PRP ALA ALA ALA VAL SEF LYS GLN

GLU	LEU	PHE	THR	GLY	VAL	VAL	PRO	ILE	LEU	VAL	GLU	LEU	ASP	GLY	ASN	HIS	LYS	PHE	SER	VAL	VAL	SER	GLY	GLU	GLY	GLY	ASP	ALA	THR	TYR	GLY	LYS	LEU	THR	THR	LEU	LEU	PHE	ILE	CYS	THR	THR	GLY	GLY	LEU	PRO	VAL	PRO	TRP	PRO	THR	LEU	THR	THR	LEU
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[illegible]

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46087	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.769	Depositor
Minimum map value	-2.307	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.641	Depositor
Map size ($\text{\AA}$)	278.272, 278.272, 278.272	wwPDB
Map dimensions	256, 256, 256	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8PE, 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	0.47	3/3411 (0.1%)	0.70	13/4641 (0.3%)
1	B	0.58	9/3411 (0.3%)	0.72	16/4641 (0.3%)
All	All	0.53	12/6822 (0.2%)	0.71	29/9282 (0.3%)

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

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	597	ALA	C-O	-9.82	1.15	1.24
1	B	598	PRO	C-O	-8.30	1.13	1.24
1	B	578	SER	C-N	7.96	1.42	1.34
1	B	599	LEU	C-O	-6.78	1.15	1.24
1	A	409	ASP	C-O	-6.69	1.15	1.24
1	B	409	ASP	C-O	-6.68	1.15	1.24
1	A	593	ALA	C-O	-6.61	1.16	1.24
1	B	593	ALA	C-O	-6.59	1.16	1.24
1	B	590	ASP	C-O	-5.87	1.17	1.24
1	A	590	ASP	C-O	-5.82	1.17	1.24
1	B	597	ALA	CA-CB	-5.63	1.46	1.53
1	B	595	VAL	C-O	-5.16	1.18	1.24

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	574	THR	CA-CB-OG1	-8.02	97.56	109.60
1	A	574	THR	CA-CB-OG1	-8.01	97.59	109.60
1	B	571	PHE	CA-CB-CG	-7.14	106.66	113.80
1	A	571	PHE	CA-CB-CG	-7.09	106.71	113.80
1	B	578	SER	CA-C-N	-6.54	109.78	120.64
1	B	578	SER	C-N-CA	-6.54	109.78	120.64
1	A	587	HIS	CA-C-N	6.28	129.21	120.29
1	A	587	HIS	C-N-CA	6.28	129.21	120.29
1	A	576	GLN	CA-C-O	-5.95	114.24	120.55
1	B	620	CYS	CB-CA-C	-5.83	98.95	110.27
1	A	620	CYS	CB-CA-C	-5.83	98.97	110.27
1	B	622	GLU	CB-CA-C	5.81	120.40	111.39
1	B	623	PHE	N-CA-C	-5.81	104.32	111.40
1	A	576	GLN	CA-C-N	-5.78	112.21	120.42
1	A	576	GLN	C-N-CA	-5.78	112.21	120.42
1	A	576	GLN	N-CA-CB	5.62	118.38	110.12
1	B	409	ASP	CB-CA-C	5.41	120.17	110.81
1	B	570	ARG	O-C-N	5.37	129.82	122.46
1	A	623	PHE	N-CA-C	-5.37	104.31	111.24
1	A	409	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	409	ASP	CB-CA-C	5.36	120.09	110.81
1	B	598	PRO	CB-CA-C	-5.36	104.24	111.85
1	B	409	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	588	SER	N-CA-C	-5.30	105.08	112.45
1	B	623	PHE	CA-CB-CG	-5.12	108.67	113.80
1	B	588	SER	CA-C-N	-5.08	114.40	119.94
1	B	588	SER	C-N-CA	-5.08	114.40	119.94
1	B	596	PHE	CB-CA-C	-5.08	101.60	110.09
1	A	623	PHE	CA-CB-CG	-5.02	108.78	113.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	ARG	Sidechain
1	B	273	ARG	Sidechain

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	3301	0	3294	92	0
1	B	3301	0	3294	90	0
2	A	47	0	73	5	0
2	B	47	0	73	6	0
3	A	28	0	46	7	0
3	B	28	0	46	4	0
All	All	6752	0	6826	189	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 14.

All (189) 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:B:597:ALA:HB3	1:B:598:PRO:HD3	1.24	1.09
3:A:1002:CLR:H242	3:A:1002:CLR:H211	1.41	1.02
3:B:1002:CLR:H242	3:B:1002:CLR:H211	1.41	0.99
1:B:576:GLN:NE2	1:B:596:PHE:CD1	2.33	0.96
1:B:571:PHE:O	1:B:573:TRP:CD1	2.24	0.91
1:A:571:PHE:O	1:A:573:TRP:CD1	2.24	0.91
1:B:571:PHE:O	1:B:573:TRP:HD1	1.59	0.85
1:A:571:PHE:O	1:A:573:TRP:HD1	1.59	0.83
1:B:597:ALA:HB3	1:B:598:PRO:CD	2.07	0.82
1:A:553:TYR:CD2	3:A:1002:CLR:H6	2.15	0.80
1:B:553:TYR:CD2	3:B:1002:CLR:H6	2.16	0.80
1:B:259:LEU:HD13	1:B:261:THR:H	1.48	0.78
1:B:576:GLN:NE2	1:B:596:PHE:CG	2.52	0.78
1:A:266:TRP:NE1	1:A:587:HIS:CD2	2.51	0.78
1:A:259:LEU:HD13	1:A:261:THR:H	1.48	0.76
1:A:266:TRP:CD1	1:A:587:HIS:CD2	2.74	0.76
1:B:591:ILE:O	1:B:595:VAL:HG23	1.86	0.75
3:B:1002:CLR:H211	3:B:1002:CLR:C24	2.16	0.75
1:B:622:GLU:HG2	1:B:622:GLU:O	1.86	0.74
1:B:473:ALA:O	1:B:477:LEU:HB2	1.88	0.74
1:B:576:GLN:HE22	1:B:596:PHE:HB2	1.53	0.73
1:B:273:ARG:CZ	1:B:594:THR:OG1	2.36	0.73
1:A:473:ALA:O	1:A:477:LEU:HB2	1.88	0.72
1:A:615:GLU:OE1	1:A:620:CYS:SG	2.47	0.71
1:A:399:GLN:HE22	1:A:608:ASN:HD21	1.38	0.71
1:B:615:GLU:OE1	1:B:620:CYS:SG	2.48	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:GLU:O	1:A:622:GLU:HG3	1.89	0.70
1:B:399:GLN:HE22	1:B:608:ASN:HD21	1.38	0.69
1:A:273:ARG:CZ	1:A:594:THR:OG1	2.42	0.68
1:A:576:GLN:H	1:A:576:GLN:NE2	1.94	0.65
1:A:575:ILE:HD13	1:A:575:ILE:N	2.11	0.65
1:B:465:ARG:NH1	1:B:469:ASP:OD2	2.31	0.64
1:A:370:SER:HB3	2:A:1001:8PE:O32	1.98	0.64
1:A:251:LEU:HD21	1:A:331:LEU:HD23	1.80	0.63
1:A:529:ASP:OD2	1:A:570:ARG:NH1	2.31	0.63
1:A:465:ARG:NH1	1:A:469:ASP:OD2	2.31	0.63
1:B:251:LEU:HD21	1:B:331:LEU:HD23	1.80	0.63
1:B:575:ILE:HD13	1:B:575:ILE:N	2.11	0.63
1:B:529:ASP:OD2	1:B:570:ARG:NH1	2.31	0.63
1:B:266:TRP:CD1	1:B:587:HIS:CD2	2.87	0.63
1:B:229:ALA:HB1	1:B:233:THR:HB	1.80	0.62
1:B:266:TRP:NE1	1:B:587:HIS:CD2	2.67	0.62
1:B:370:SER:HB3	2:B:1001:8PE:O32	1.99	0.62
1:B:279:ILE:HD13	1:B:324:GLY:HA2	1.83	0.61
1:A:266:TRP:HE1	1:A:587:HIS:CD2	2.17	0.61
1:A:229:ALA:HB1	1:A:233:THR:HB	1.81	0.61
1:B:583:THR:O	1:B:583:THR:HG23	2.01	0.60
1:A:583:THR:HG23	1:A:583:THR:O	2.02	0.60
1:A:279:ILE:HD13	1:A:324:GLY:HA2	1.83	0.60
1:A:576:GLN:HB2	1:A:592:ILE:HD12	1.82	0.60
3:A:1002:CLR:H211	3:A:1002:CLR:C24	2.16	0.59
1:B:597:ALA:N	1:B:598:PRO:CD	2.64	0.59
1:B:597:ALA:CB	1:B:598:PRO:HD3	2.10	0.59
1:A:573:TRP:HA	1:A:576:GLN:HE22	1.68	0.59
1:A:576:GLN:H	1:A:576:GLN:HE21	1.52	0.58
1:A:580:THR:HG22	1:A:580:THR:O	2.04	0.58
1:A:614:ASN:HD21	1:A:620:CYS:HB3	1.69	0.57
1:B:580:THR:HG22	1:B:580:THR:O	2.04	0.57
1:B:595:VAL:HG12	1:B:595:VAL:O	2.04	0.57
1:B:614:ASN:HD21	1:B:620:CYS:HB3	1.69	0.57
1:A:553:TYR:CE2	3:A:1002:CLR:H6	2.41	0.56
1:A:270:ARG:O	1:A:409:ASP:OD1	2.25	0.55
1:A:266:TRP:HE1	1:A:587:HIS:HD2	1.55	0.55
1:B:576:GLN:NE2	1:B:596:PHE:HB2	2.19	0.55
3:A:1002:CLR:C24	3:A:1002:CLR:C21	2.84	0.54
1:B:300:VAL:HG23	1:B:305:LEU:HB2	1.88	0.54
1:B:553:TYR:CE2	3:B:1002:CLR:H6	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ARG:NH1	1:A:594:THR:OG1	2.40	0.54
1:B:455:PRO:HA	1:B:458:LEU:HD12	1.88	0.54
1:A:363:THR:OG1	1:A:365:THR:OG1	2.26	0.54
1:A:300:VAL:HG23	1:A:305:LEU:HB2	1.88	0.54
1:A:246:VAL:HG11	1:B:246:VAL:HG11	1.89	0.53
1:A:455:PRO:HA	1:A:458:LEU:HD12	1.88	0.53
1:A:266:TRP:NE1	1:A:587:HIS:HD2	2.05	0.53
1:A:595:VAL:HG12	1:A:595:VAL:O	2.08	0.53
1:B:270:ARG:O	1:B:409:ASP:OD1	2.26	0.53
1:B:579:ILE:O	1:B:584:LEU:HD21	2.08	0.53
1:B:615:GLU:O	1:B:624:ARG:NH2	2.43	0.52
3:A:1002:CLR:H242	3:A:1002:CLR:C21	2.28	0.52
1:B:575:ILE:N	1:B:575:ILE:CD1	2.73	0.52
1:A:575:ILE:N	1:A:575:ILE:CD1	2.73	0.52
1:B:285:LEU:HD21	2:B:1001:8PE:H23A	1.91	0.52
1:A:285:LEU:HD21	2:A:1001:8PE:H23A	1.92	0.52
1:A:385:PRO:O	1:A:465:ARG:NE	2.28	0.51
1:B:361:ASN:ND2	1:B:363:THR:OG1	2.40	0.51
1:A:402:SER:HB3	1:A:604:ARG:HH21	1.76	0.51
1:B:402:SER:HB3	1:B:604:ARG:HH21	1.76	0.50
1:B:385:PRO:O	1:B:465:ARG:NE	2.28	0.50
1:B:399:GLN:HE22	1:B:608:ASN:ND2	2.09	0.50
1:B:273:ARG:NH2	1:B:594:THR:OG1	2.44	0.50
1:B:488:PHE:HB3	1:B:517:PHE:CD2	2.47	0.50
1:B:575:ILE:O	1:B:579:ILE:N	2.38	0.50
1:A:571:PHE:O	1:A:573:TRP:N	2.43	0.50
1:A:488:PHE:HB3	1:A:517:PHE:CD2	2.47	0.49
1:A:502:ARG:HD2	1:A:504:HIS:CD2	2.48	0.49
1:A:576:GLN:NE2	1:A:576:GLN:N	2.60	0.49
1:A:399:GLN:HE22	1:A:608:ASN:ND2	2.09	0.49
1:A:589:GLY:O	1:A:592:ILE:HG12	2.14	0.48
1:A:403:LEU:HG	1:A:406:ILE:HD12	1.96	0.48
1:B:266:TRP:HE1	1:B:587:HIS:CD2	2.31	0.48
1:B:576:GLN:NE2	1:B:596:PHE:CB	2.76	0.48
1:B:502:ARG:HD2	1:B:504:HIS:CD2	2.48	0.48
1:A:466:ARG:HE	1:A:476:HIS:HD2	1.62	0.47
1:B:403:LEU:HG	1:B:406:ILE:HD12	1.96	0.47
1:B:570:ARG:HD2	1:B:570:ARG:HA	1.67	0.47
1:A:273:ARG:NH1	1:A:594:THR:HG1	2.12	0.47
1:B:496:TYR:HB2	1:B:510:PHE:HB3	1.96	0.47
1:A:496:TYR:HB2	1:A:510:PHE:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LYS:HG3	1:A:368:TYR:CD2	2.50	0.47
1:A:620:CYS:SG	1:A:621:GLY:N	2.85	0.47
1:B:363:THR:OG1	1:B:365:THR:OG1	2.26	0.47
1:A:570:ARG:HD2	1:A:570:ARG:HA	1.67	0.46
1:B:611:ARG:NH1	1:B:620:CYS:SG	2.89	0.46
1:B:584:LEU:H	1:B:584:LEU:HG	1.26	0.46
1:A:538:ASP:OD1	1:A:539:LYS:N	2.49	0.46
1:B:538:ASP:OD1	1:B:539:LYS:N	2.49	0.46
1:A:251:LEU:HD13	1:A:332:LEU:HD13	1.98	0.46
1:B:620:CYS:SG	1:B:621:GLY:N	2.85	0.46
1:B:364:LYS:HG3	1:B:368:TYR:CD2	2.50	0.46
1:B:466:ARG:HE	1:B:476:HIS:HD2	1.62	0.46
1:B:594:THR:O	1:B:594:THR:HG23	2.17	0.45
1:A:584:LEU:H	1:A:584:LEU:HG	1.30	0.45
1:A:611:ARG:NH1	1:A:620:CYS:SG	2.89	0.45
1:B:422:LYS:H	1:B:422:LYS:HG2	1.50	0.45
1:A:271:ILE:O	1:A:352:TYR:OH	2.34	0.44
1:A:361:ASN:ND2	1:A:363:THR:OG1	2.40	0.44
1:B:384:ALA:HB1	1:B:385:PRO:HD2	1.99	0.44
1:B:571:PHE:O	1:B:573:TRP:N	2.43	0.44
1:A:576:GLN:HE21	1:A:576:GLN:N	2.14	0.44
1:B:251:LEU:HD13	1:B:332:LEU:HD13	1.98	0.44
1:A:332:LEU:HD12	1:A:332:LEU:HA	1.85	0.44
1:A:405:VAL:O	1:A:409:ASP:HB2	2.17	0.44
1:A:594:THR:O	1:A:594:THR:HG23	2.17	0.44
2:B:1001:8PE:H38	2:B:1001:8PE:H3BA	1.65	0.44
1:B:405:VAL:O	1:B:409:ASP:HB2	2.18	0.44
1:A:454:ILE:N	1:A:455:PRO:HD2	2.33	0.43
1:B:454:ILE:N	1:B:455:PRO:HD2	2.33	0.43
1:B:466:ARG:HE	1:B:476:HIS:CD2	2.37	0.43
1:A:384:ALA:HB1	1:A:385:PRO:HD2	1.99	0.43
1:B:406:ILE:HG23	2:B:1001:8PE:H3HA	2.00	0.43
1:A:548:ARG:NH1	1:A:613:GLU:OE1	2.51	0.43
1:B:548:ARG:NH1	1:B:613:GLU:OE1	2.51	0.43
1:A:252:VAL:O	1:A:256:VAL:HG23	2.19	0.43
1:A:495:LEU:HD23	1:A:495:LEU:HA	1.89	0.42
1:B:252:VAL:O	1:B:256:VAL:HG23	2.19	0.42
3:A:1002:CLR:H273	3:A:1002:CLR:H232	1.75	0.42
1:A:361:ASN:HB3	1:A:371:ARG:NH1	2.35	0.42
1:A:575:ILE:O	1:A:579:ILE:N	2.49	0.42
1:B:264:SER:HB3	1:B:431:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ARG:HE	1:A:476:HIS:CD2	2.36	0.42
1:A:573:TRP:O	1:A:577:ILE:HG22	2.19	0.42
1:B:278:LEU:HD21	2:B:1001:8PE:H3AB	2.00	0.42
1:B:463:CYS:SG	1:B:479:ASN:HB3	2.60	0.42
1:A:278:LEU:HD21	2:A:1001:8PE:H3AB	2.01	0.42
1:A:310:ASN:HA	2:A:1001:8PE:O14	2.20	0.42
1:B:516:VAL:O	1:B:519:ILE:HB	2.20	0.42
1:A:264:SER:HB3	1:A:431:PRO:HD2	2.02	0.42
1:A:463:CYS:SG	1:A:479:ASN:HB3	2.60	0.42
1:A:516:VAL:O	1:A:519:ILE:HB	2.20	0.42
1:A:573:TRP:HA	1:A:576:GLN:NE2	2.34	0.42
1:B:361:ASN:HB3	1:B:371:ARG:NH1	2.35	0.42
1:B:573:TRP:O	1:B:577:ILE:HG22	2.19	0.42
1:B:492:PHE:CE2	1:B:513:LEU:HB3	2.55	0.42
1:B:544:ASN:HB3	1:B:547:LEU:HB2	2.02	0.42
1:A:406:ILE:HG23	2:A:1001:8PE:H3HA	2.00	0.41
1:B:263:ARG:HG3	1:B:430:LEU:HB3	2.01	0.41
1:B:361:ASN:HB3	1:B:371:ARG:HH12	1.86	0.41
1:A:492:PHE:CE2	1:A:513:LEU:HB3	2.55	0.41
1:A:544:ASN:HB3	1:A:547:LEU:HB2	2.02	0.41
1:A:564:ILE:HD13	1:A:564:ILE:HA	1.96	0.41
1:A:263:ARG:HG3	1:A:430:LEU:HB3	2.01	0.41
1:A:442:LYS:HE3	1:A:442:LYS:HB2	1.84	0.41
1:B:306:ASN:HD21	1:B:308:ARG:HG3	1.86	0.41
1:A:594:THR:O	1:A:594:THR:CG2	2.69	0.41
1:B:271:ILE:O	1:B:352:TYR:OH	2.34	0.41
1:B:425:GLU:OE1	1:B:427:LYS:N	2.54	0.41
1:A:270:ARG:NH1	1:A:412:TYR:OH	2.54	0.41
1:A:441:HIS:CE1	1:A:442:LYS:HG3	2.55	0.41
1:A:595:VAL:O	1:A:595:VAL:CG1	2.67	0.41
1:B:270:ARG:NH1	1:B:412:TYR:OH	2.54	0.41
1:B:512:TYR:O	1:B:516:VAL:HG23	2.21	0.41
1:B:576:GLN:HG2	1:B:592:ILE:HB	2.03	0.41
1:A:329:LEU:HD23	1:A:329:LEU:HA	1.87	0.41
1:B:285:LEU:HD12	1:B:285:LEU:HA	1.91	0.41
1:B:441:HIS:CE1	1:B:442:LYS:HG3	2.55	0.41
1:A:361:ASN:HB3	1:A:371:ARG:HH12	1.86	0.40
1:A:386:PHE:C	1:A:465:ARG:HH21	2.29	0.40
1:B:310:ASN:HA	2:B:1001:8PE:O14	2.21	0.40
1:A:425:GLU:OE1	1:A:427:LYS:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	393/969 (41%)	351 (89%)	41 (10%)	1 (0%)	36	65
1	B	393/969 (41%)	352 (90%)	40 (10%)	1 (0%)	36	65
All	All	786/1938 (41%)	703 (89%)	81 (10%)	2 (0%)	37	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	PRO
1	B	230	PRO

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	352/857 (41%)	321 (91%)	31 (9%)	9	33
1	B	352/857 (41%)	322 (92%)	30 (8%)	10	34
All	All	704/1714 (41%)	643 (91%)	61 (9%)	12	33

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	LEU
1	A	280	GLU
1	A	314	GLN
1	A	342	ILE

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Mol	Chain	Res	Type
1	A	378	LEU
1	A	382	PHE
1	A	407	LEU
1	A	409	ASP
1	A	419	LEU
1	A	422	LYS
1	A	439	ILE
1	A	441	HIS
1	A	445	TYR
1	A	447	VAL
1	A	470	THR
1	A	477	LEU
1	A	498	THR
1	A	504	HIS
1	A	506	ASP
1	A	561	CYS
1	A	575	ILE
1	A	576	GLN
1	A	579	ILE
1	A	584	LEU
1	A	585	LEU
1	A	592	ILE
1	A	594	THR
1	A	613	GLU
1	A	618	ASN
1	A	622	GLU
1	A	626	VAL
1	B	259	LEU
1	B	280	GLU
1	B	314	GLN
1	B	342	ILE
1	B	378	LEU
1	B	382	PHE
1	B	407	LEU
1	B	409	ASP
1	B	419	LEU
1	B	422	LYS
1	B	439	ILE
1	B	441	HIS
1	B	445	TYR
1	B	447	VAL
1	B	470	THR

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Mol	Chain	Res	Type
1	B	477	LEU
1	B	498	THR
1	B	504	HIS
1	B	506	ASP
1	B	561	CYS
1	B	575	ILE
1	B	579	ILE
1	B	584	LEU
1	B	585	LEU
1	B	592	ILE
1	B	594	THR
1	B	598	PRO
1	B	613	GLU
1	B	618	ASN
1	B	626	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	ASN
1	A	294	GLN
1	A	298	ASN
1	A	315	HIS
1	A	399	GLN
1	A	499	HIS
1	A	576	GLN
1	A	587	HIS
1	A	614	ASN
1	A	618	ASN
1	B	288	ASN
1	B	294	GLN
1	B	298	ASN
1	B	315	HIS
1	B	399	GLN
1	B	499	HIS
1	B	576	GLN
1	B	587	HIS
1	B	614	ASN
1	B	618	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 ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	8PE	A	1001	-	46,46,46	0.99	1 (2%)	49,51,51	0.82	2 (4%)
3	CLR	B	1002	-	31,31,31	1.08	1 (3%)	48,48,48	1.83	11 (22%)
3	CLR	A	1002	-	31,31,31	1.08	1 (3%)	48,48,48	1.84	12 (25%)
2	8PE	B	1001	-	46,46,46	0.99	1 (2%)	49,51,51	0.83	2 (4%)

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
2	8PE	A	1001	-	-	28/50/50/50	-
3	CLR	B	1002	-	-	6/10/68/68	0/4/4/4
3	CLR	A	1002	-	-	6/10/68/68	0/4/4/4
2	8PE	B	1001	-	-	28/50/50/50	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	8PE	C32-C31	-2.24	1.44	1.50
3	B	1002	CLR	C20-C17	-2.22	1.50	1.54
3	A	1002	CLR	C20-C17	-2.22	1.50	1.54
2	B	1001	8PE	C32-C31	-2.21	1.44	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	CLR	C16-C17-C20	-5.11	104.44	112.18
3	A	1002	CLR	C16-C17-C20	-5.11	104.44	112.18
3	A	1002	CLR	C2-C3-C4	-4.34	104.18	110.29
3	B	1002	CLR	C2-C3-C4	-4.34	104.19	110.29
3	A	1002	CLR	C7-C8-C14	-3.99	105.28	110.93
3	B	1002	CLR	C7-C8-C14	-3.97	105.31	110.93
3	B	1002	CLR	C18-C13-C17	-3.54	105.25	111.68
3	A	1002	CLR	C18-C13-C17	-3.54	105.26	111.68
3	B	1002	CLR	C12-C13-C17	3.32	121.50	116.60
3	A	1002	CLR	C12-C13-C17	3.29	121.45	116.60
3	A	1002	CLR	C11-C9-C8	-2.97	107.63	111.78
3	B	1002	CLR	C11-C9-C8	-2.93	107.69	111.78
3	B	1002	CLR	C15-C14-C13	-2.70	100.67	103.84
3	A	1002	CLR	C15-C14-C13	-2.67	100.70	103.84
3	A	1002	CLR	C15-C14-C8	-2.34	115.36	119.10
3	A	1002	CLR	C1-C10-C9	2.27	111.74	108.74
3	B	1002	CLR	C15-C14-C8	-2.27	115.48	119.10
3	B	1002	CLR	C1-C10-C9	2.27	111.74	108.74
3	A	1002	CLR	C13-C17-C20	-2.11	116.23	119.50
3	A	1002	CLR	C19-C10-C1	-2.10	106.23	109.43
3	B	1002	CLR	C19-C10-C1	-2.09	106.26	109.43
3	B	1002	CLR	C13-C17-C20	-2.08	116.28	119.50
2	B	1001	8PE	C2-O21-C21	2.06	122.72	117.80
2	B	1001	8PE	O13-C11-C12	-2.04	101.71	109.17
2	A	1001	8PE	C2-O21-C21	2.03	122.66	117.80
2	A	1001	8PE	O13-C11-C12	-2.02	101.77	109.17
3	A	1002	CLR	C21-C20-C17	-2.00	109.88	112.88

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	8PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
2	A	1001	8PE	C11-O13-P-O11
2	A	1001	8PE	C11-O13-P-O12
2	A	1001	8PE	C22-C21-O21-C2
2	B	1001	8PE	C1-O11-P-O13
2	B	1001	8PE	C11-O13-P-O11
2	B	1001	8PE	C11-O13-P-O12
2	B	1001	8PE	C22-C21-O21-C2
2	A	1001	8PE	O22-C21-O21-C2
2	B	1001	8PE	O22-C21-O21-C2
3	A	1002	CLR	C21-C20-C22-C23
3	B	1002	CLR	C21-C20-C22-C23
2	A	1001	8PE	C3A-C3B-C3C-C3D
2	B	1001	8PE	C3A-C3B-C3C-C3D
2	A	1001	8PE	C38-C39-C3A-C3B
2	B	1001	8PE	C38-C39-C3A-C3B
2	A	1001	8PE	C21-C22-C23-C24
2	B	1001	8PE	C21-C22-C23-C24
2	B	1001	8PE	C29-C2A-C2B-C2C
2	A	1001	8PE	C29-C2A-C2B-C2C
3	A	1002	CLR	C17-C20-C22-C23
2	A	1001	8PE	C3C-C3D-C3E-C3F
2	B	1001	8PE	C3C-C3D-C3E-C3F
3	B	1002	CLR	C17-C20-C22-C23
2	A	1001	8PE	C36-C37-C38-C39
2	B	1001	8PE	C36-C37-C38-C39
2	B	1001	8PE	C33-C34-C35-C36
2	A	1001	8PE	C33-C34-C35-C36
2	A	1001	8PE	C35-C36-C37-C38
2	B	1001	8PE	C35-C36-C37-C38
2	B	1001	8PE	C37-C38-C39-C3A
2	A	1001	8PE	C37-C38-C39-C3A
2	A	1001	8PE	C31-C32-C33-C34
2	B	1001	8PE	C31-C32-C33-C34
2	A	1001	8PE	C3F-C3G-C3H-C3I
2	B	1001	8PE	C3F-C3G-C3H-C3I
3	A	1002	CLR	C23-C24-C25-C26
3	A	1002	CLR	C23-C24-C25-C27
3	B	1002	CLR	C23-C24-C25-C26
3	B	1002	CLR	C23-C24-C25-C27
2	A	1001	8PE	O11-C1-C2-O21
2	B	1001	8PE	O11-C1-C2-O21
2	B	1001	8PE	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
2	A	1001	8PE	C2B-C2C-C2D-C2E
2	A	1001	8PE	C26-C27-C28-C29
2	B	1001	8PE	C26-C27-C28-C29
3	A	1002	CLR	C13-C17-C20-C21
3	B	1002	CLR	C13-C17-C20-C21
2	A	1001	8PE	O21-C2-C3-O31
2	B	1001	8PE	O21-C2-C3-O31
2	A	1001	8PE	O11-C1-C2-C3
2	B	1001	8PE	O11-C1-C2-C3
2	A	1001	8PE	C1-O11-P-O12
2	B	1001	8PE	C1-O11-P-O12
2	A	1001	8PE	C28-C29-C2A-C2B
2	B	1001	8PE	C28-C29-C2A-C2B
2	A	1001	8PE	C1-C2-C3-O31
2	B	1001	8PE	C1-C2-C3-O31
3	A	1002	CLR	C13-C17-C20-C22
3	B	1002	CLR	C13-C17-C20-C22
2	A	1001	8PE	C39-C3A-C3B-C3C
2	B	1001	8PE	C39-C3A-C3B-C3C
2	B	1001	8PE	C34-C35-C36-C37
2	A	1001	8PE	C34-C35-C36-C37
2	A	1001	8PE	O21-C21-C22-C23
2	B	1001	8PE	O21-C21-C22-C23
2	A	1001	8PE	O22-C21-C22-C23
2	B	1001	8PE	O22-C21-C22-C23

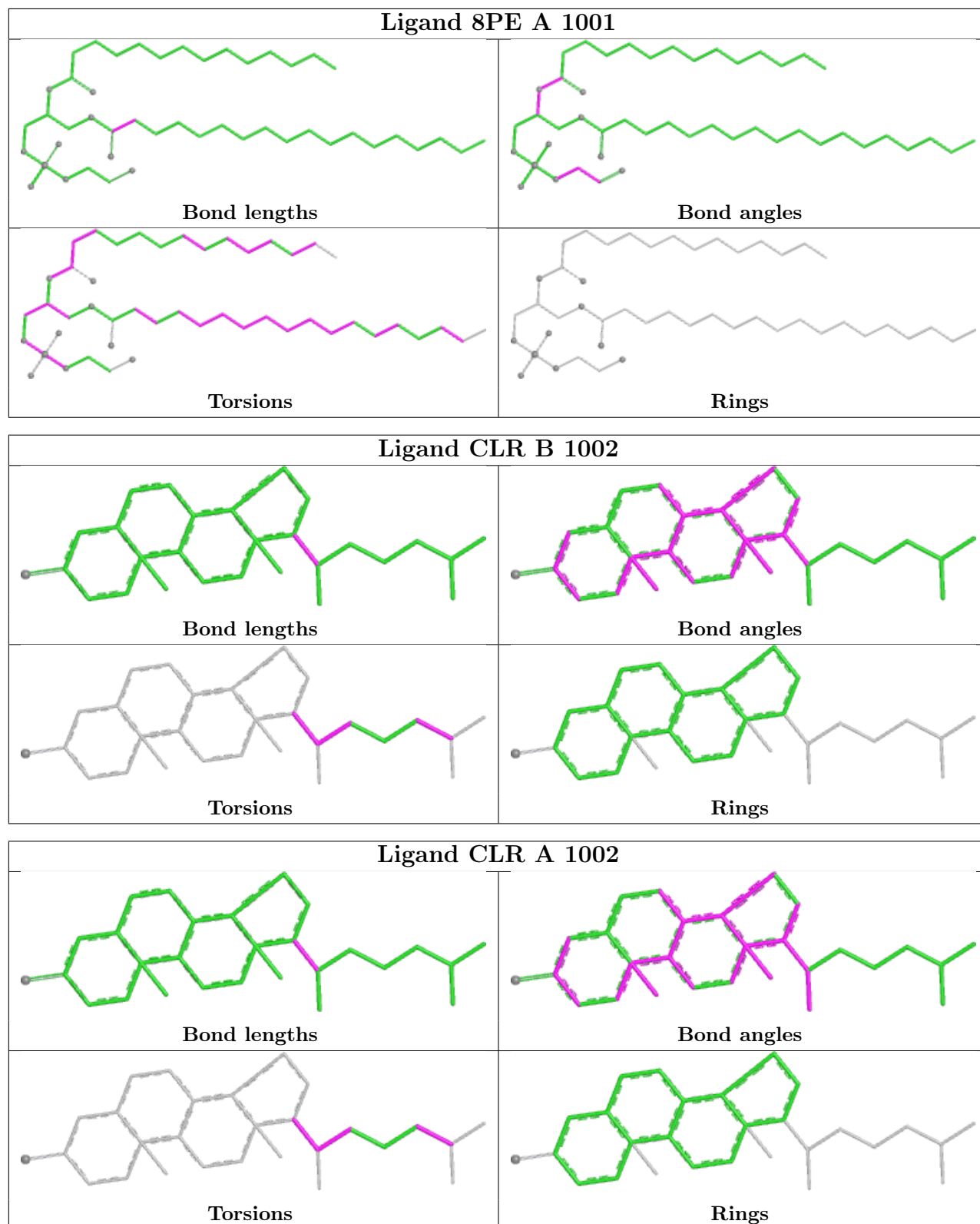
There are no ring outliers.

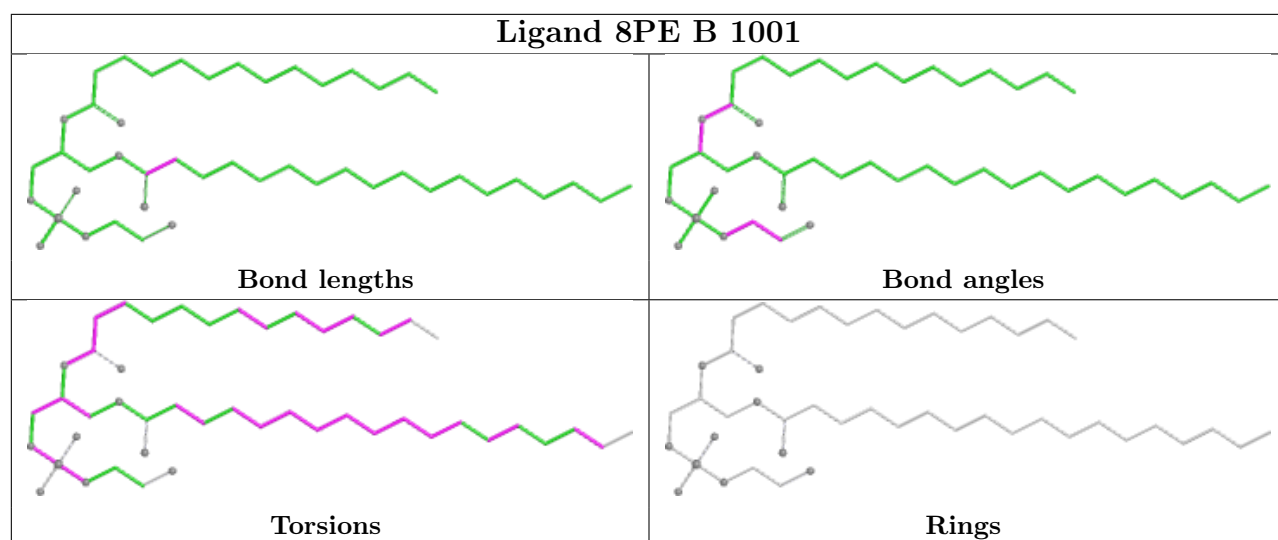
4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	8PE	5	0
3	B	1002	CLR	4	0
3	A	1002	CLR	7	0
2	B	1001	8PE	6	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.

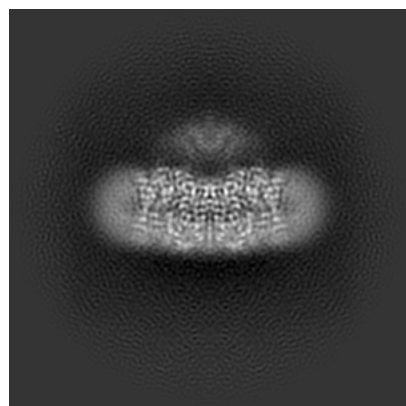
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61255. These allow visual inspection of the internal detail of the map and identification of artifacts.

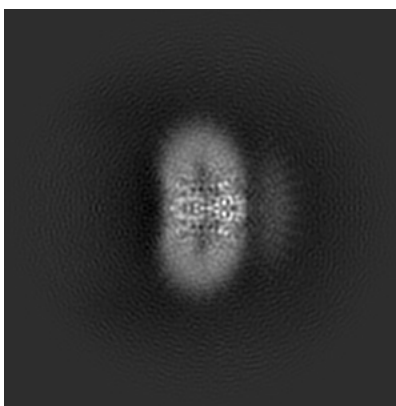
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

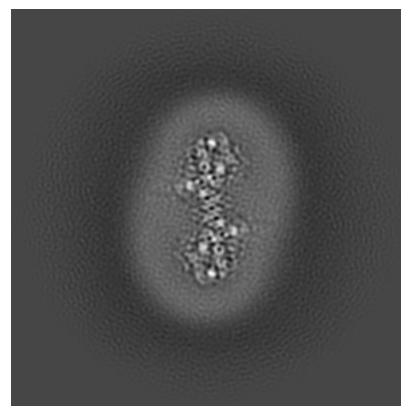
6.1.1 Primary map



X

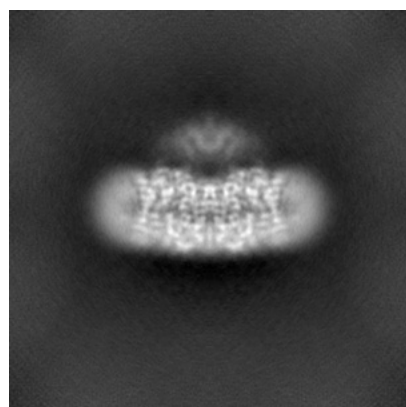


Y

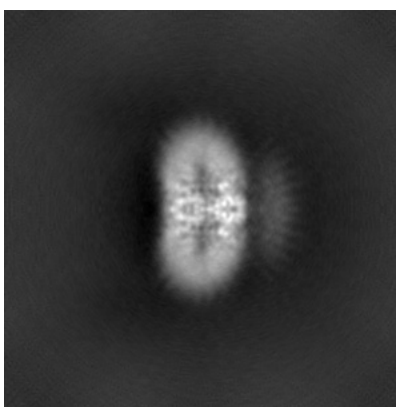


Z

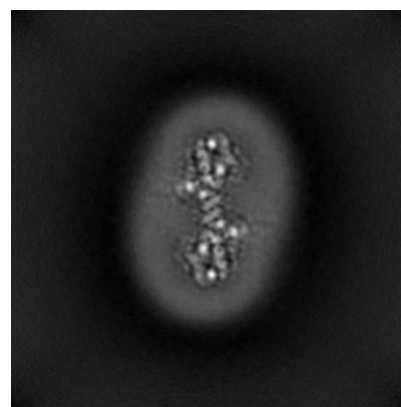
6.1.2 Raw map



X



Y

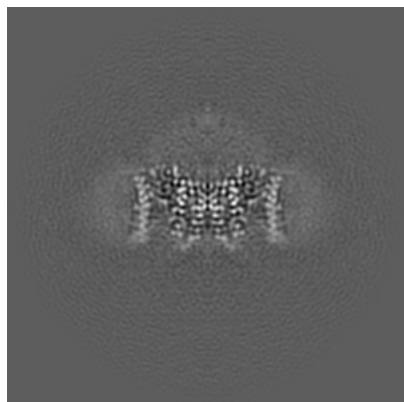


Z

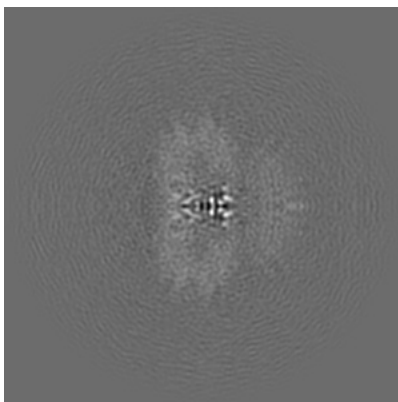
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

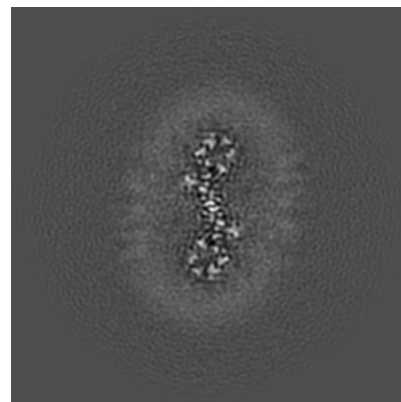
6.2.1 Primary map



X Index: 128

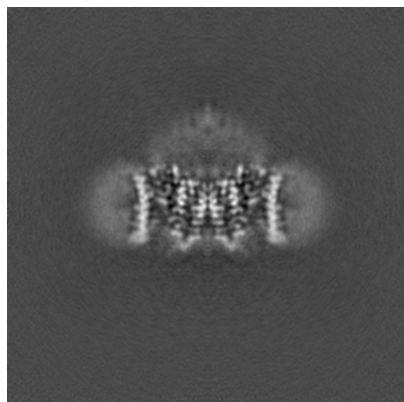


Y Index: 128

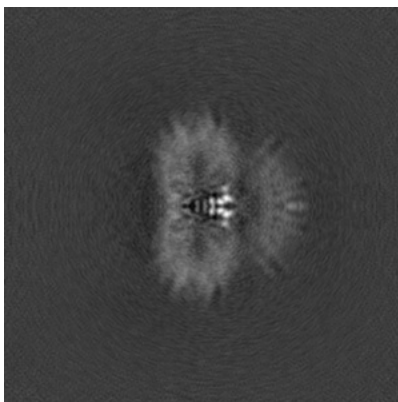


Z Index: 128

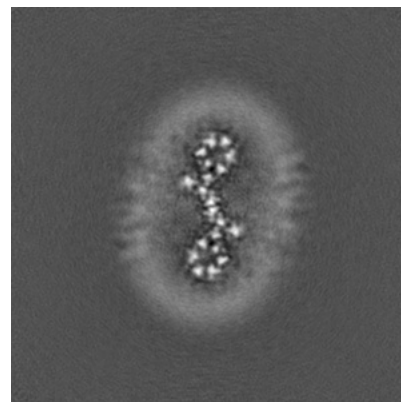
6.2.2 Raw map



X Index: 128



Y Index: 128

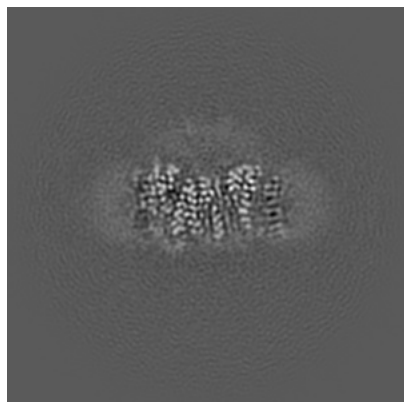


Z Index: 128

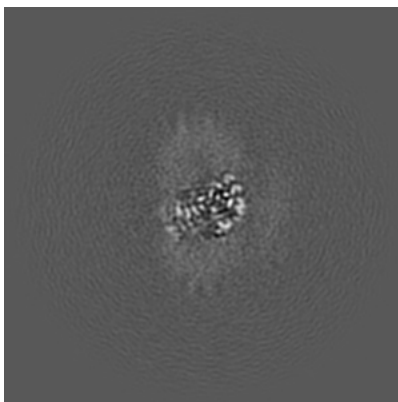
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

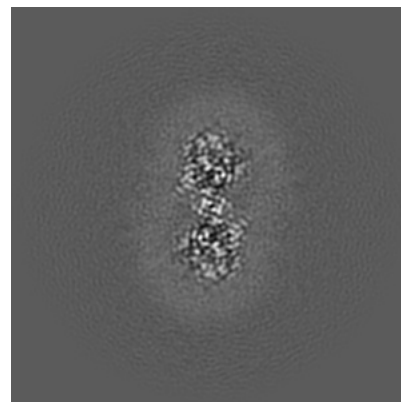
6.3.1 Primary map



X Index: 132

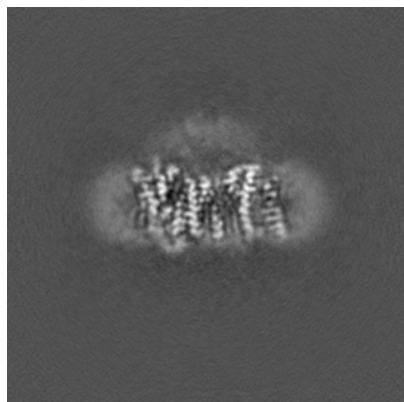


Y Index: 149

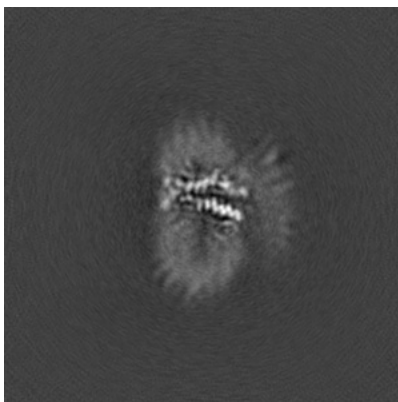


Z Index: 141

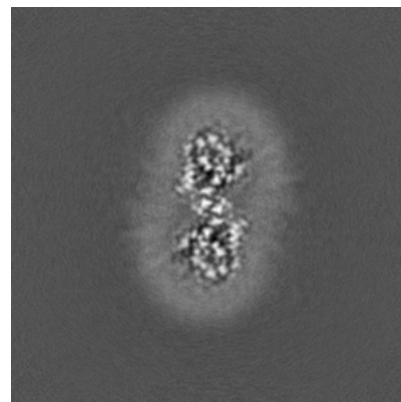
6.3.2 Raw map



X Index: 133



Y Index: 112

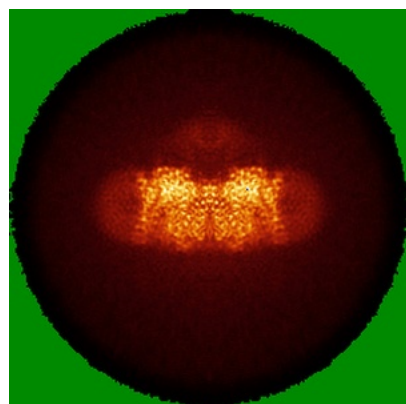


Z Index: 141

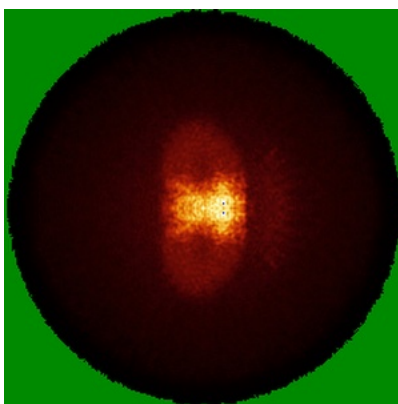
The images above show the largest variance slices of the map in three orthogonal directions.

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

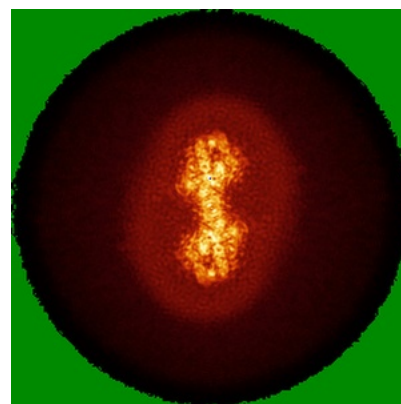
6.4.1 Primary map



X

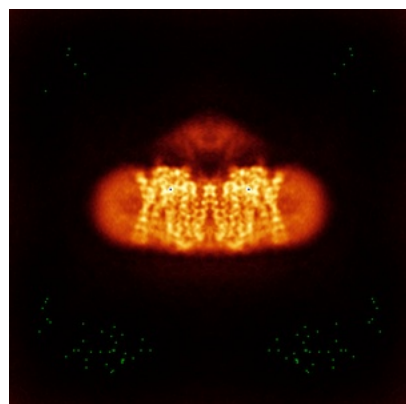


Y

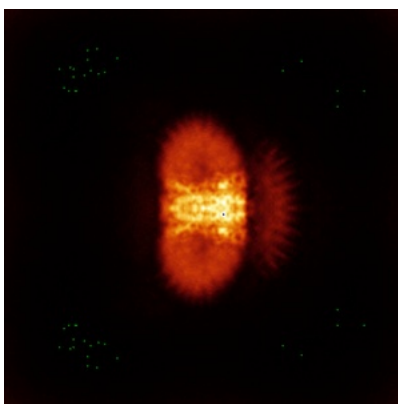


Z

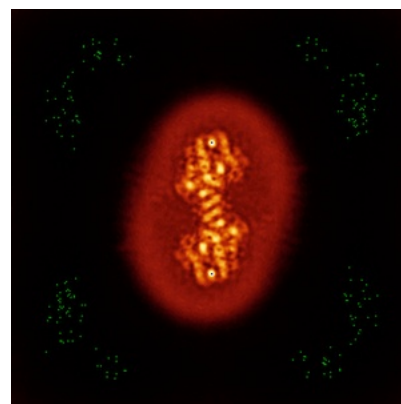
6.4.2 Raw map



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 0.641. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

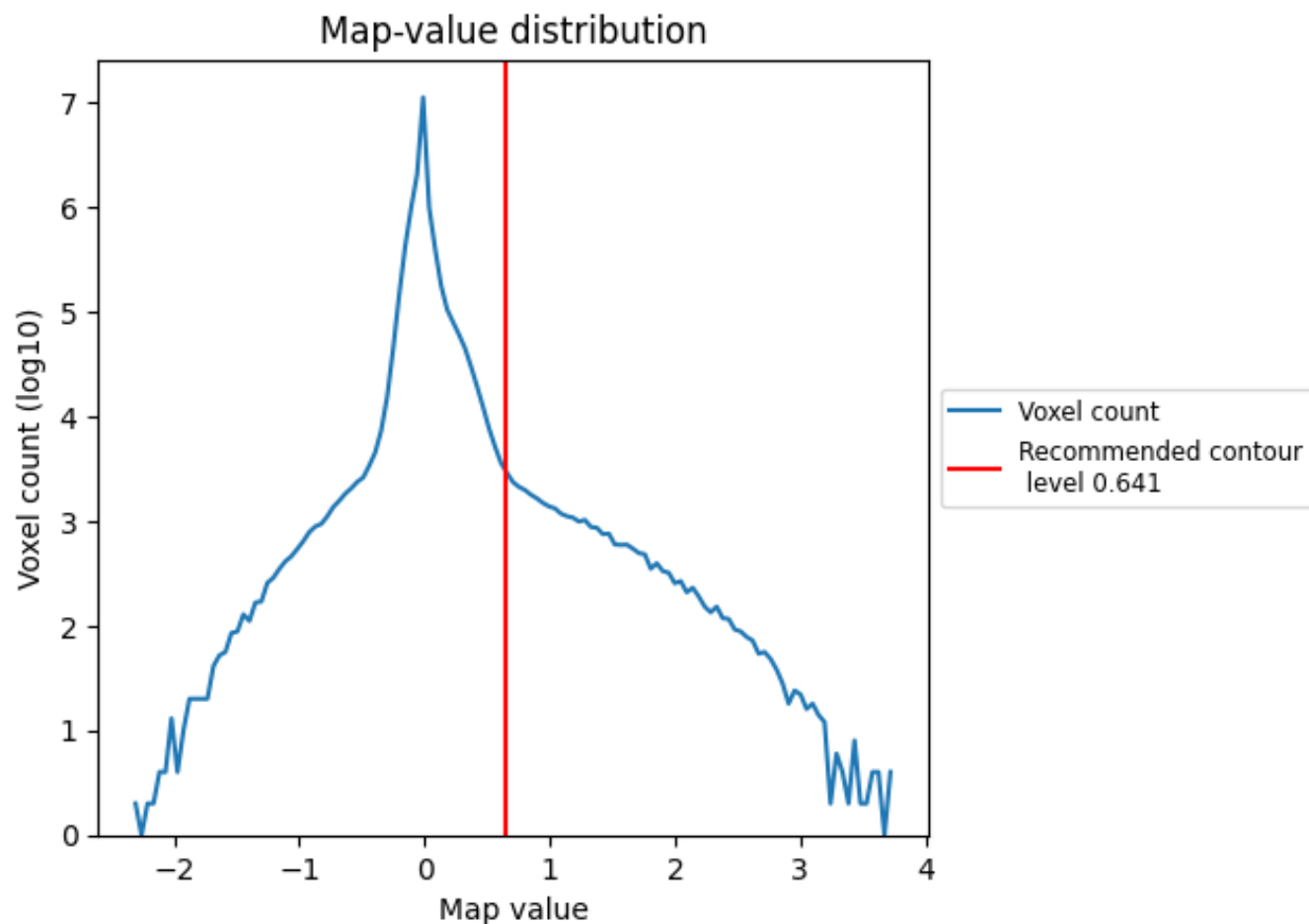
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

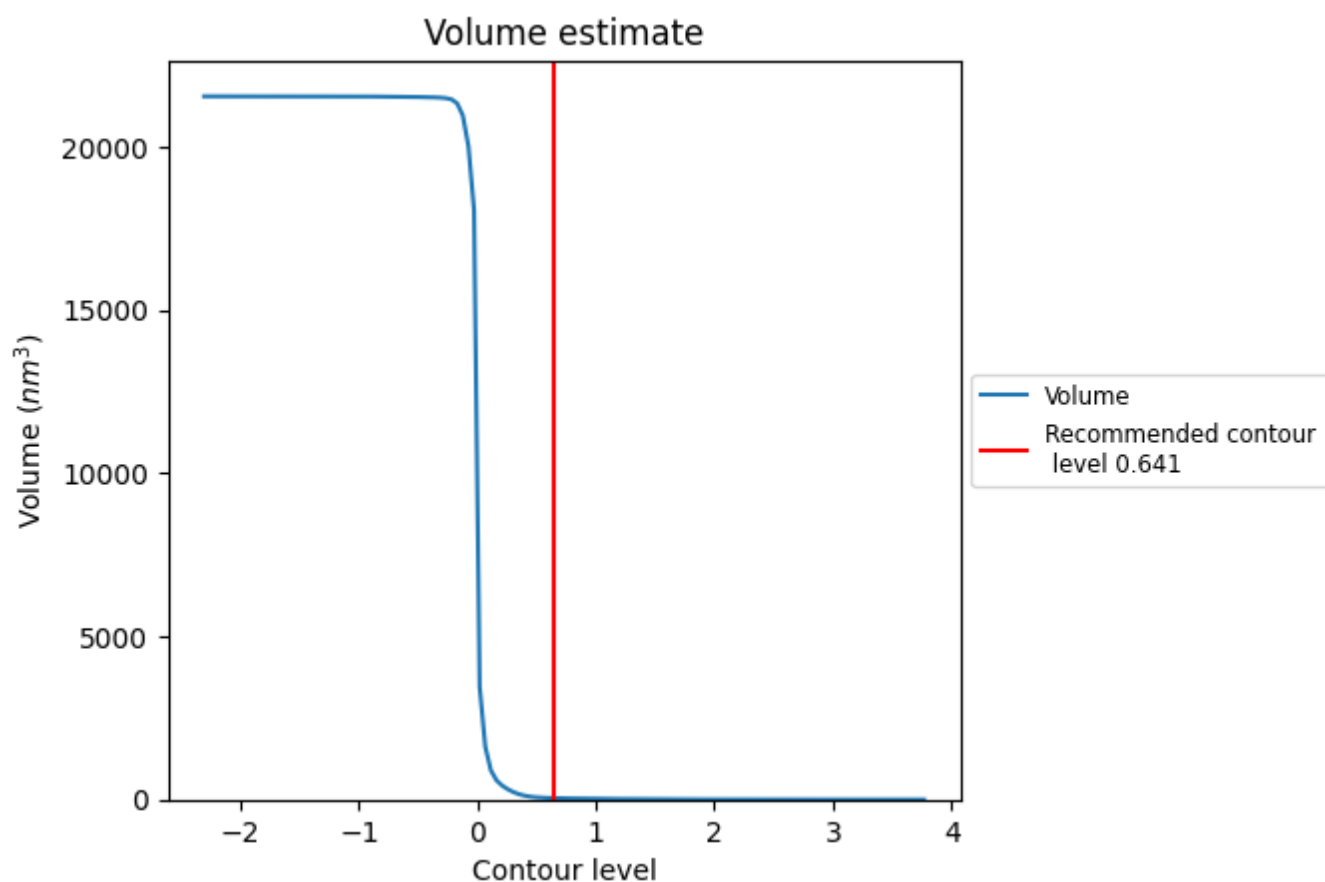
This section contains the results of statistical analysis of the map.

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.

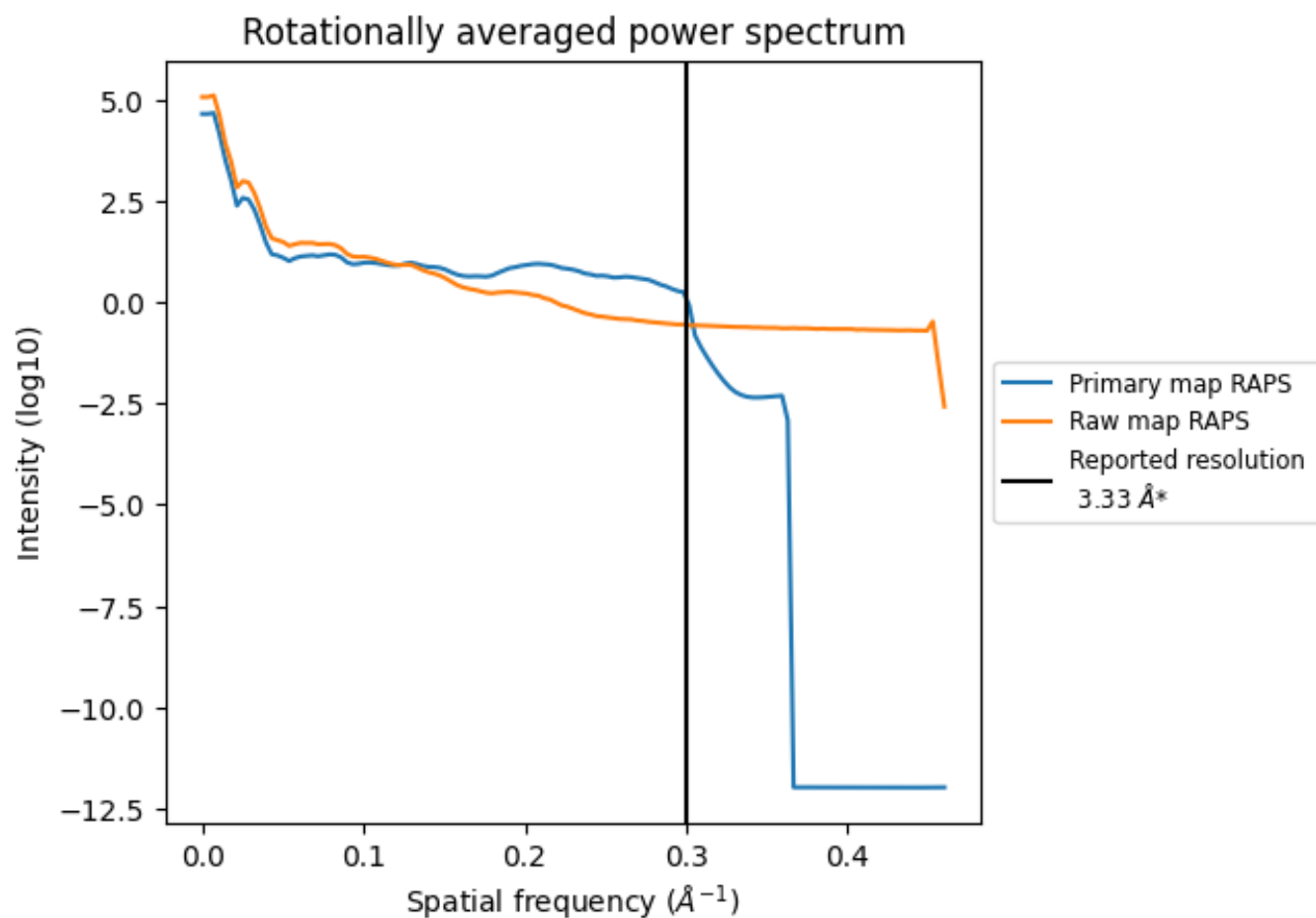
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 44 nm³; this corresponds to an approximate mass of 39 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 ⓘ

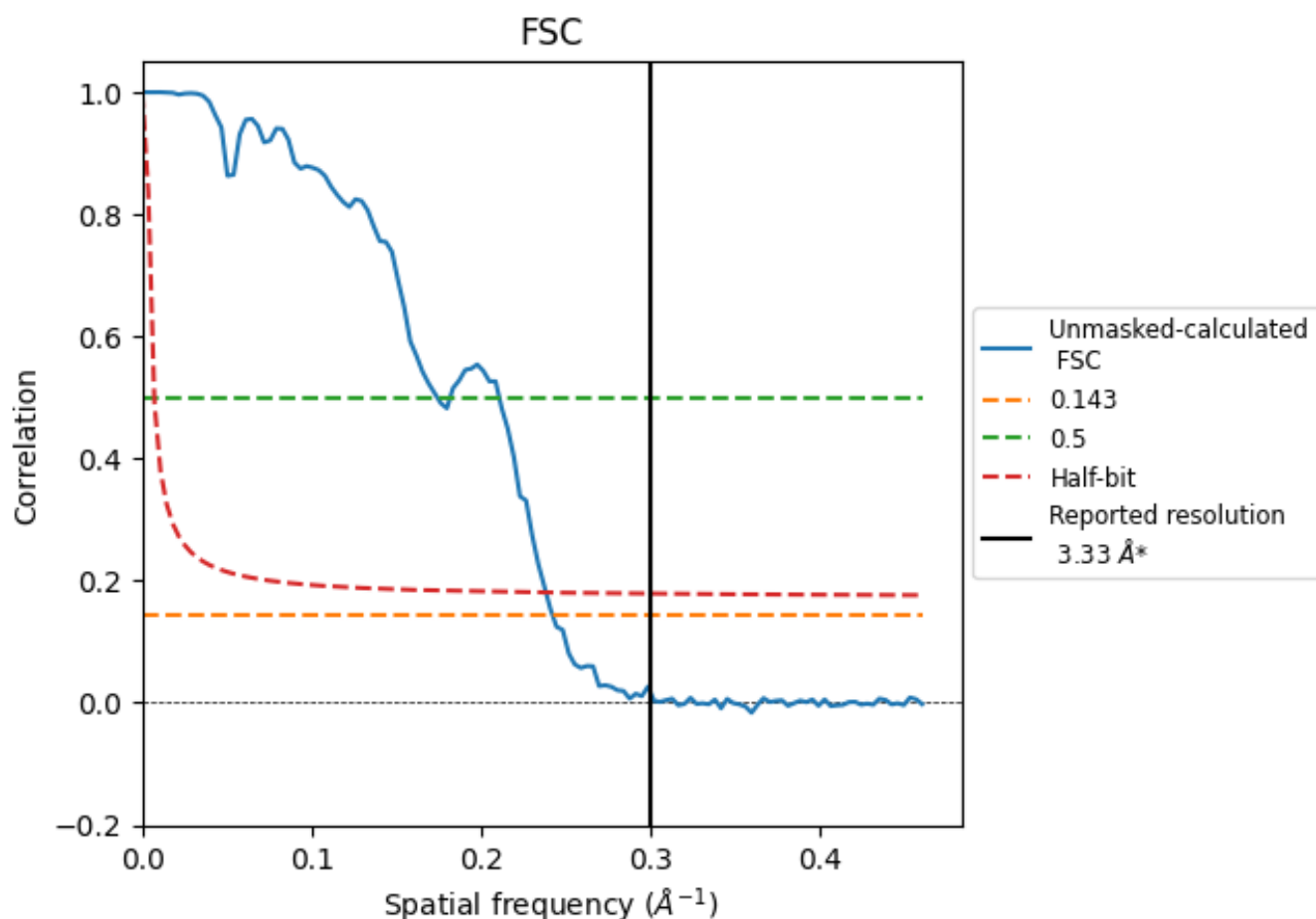


*Reported resolution corresponds to spatial frequency of 0.300 Å⁻¹

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 $0.300 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

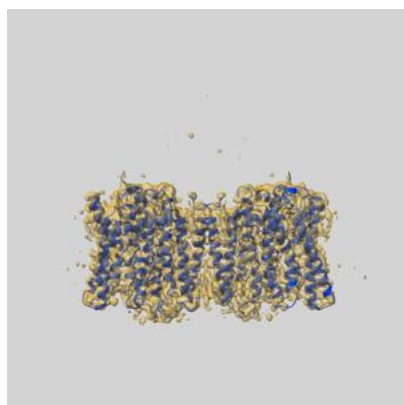
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.13	5.75	4.20

*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 4.13 differs from the reported value 3.33 by more than 10 %

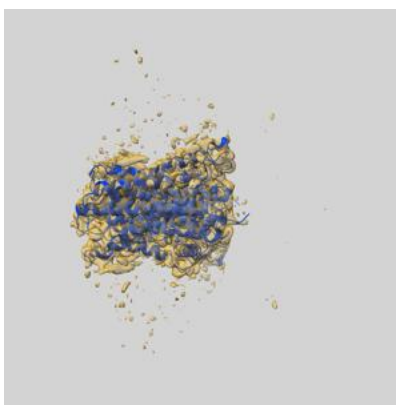
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61255 and PDB model 9J98. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

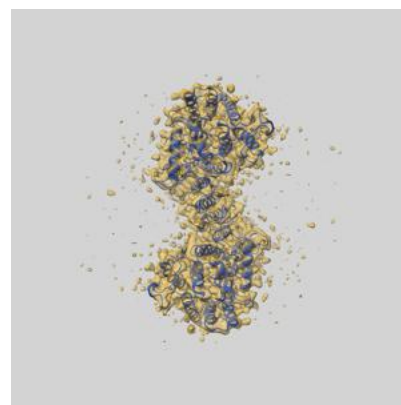
9.1 Map-model overlay [i](#)



X



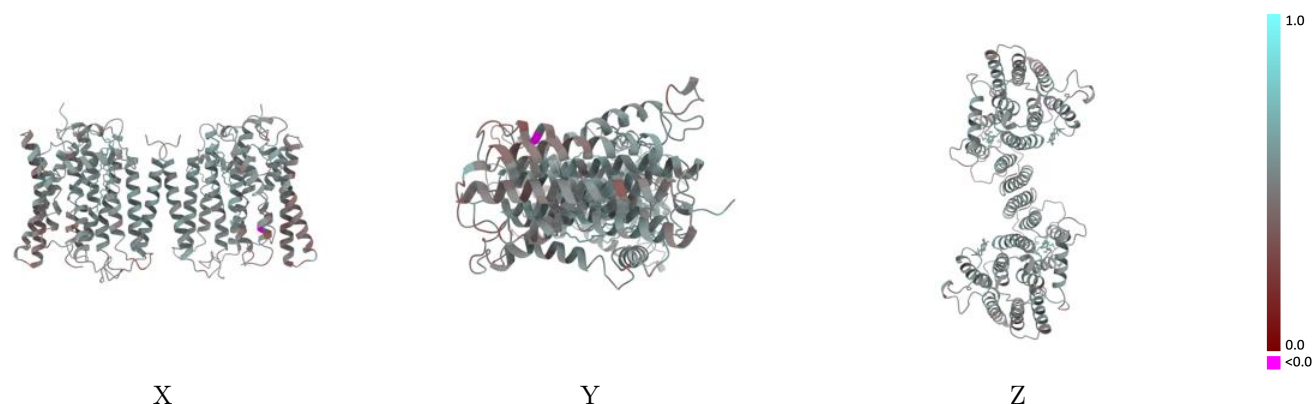
Y



Z

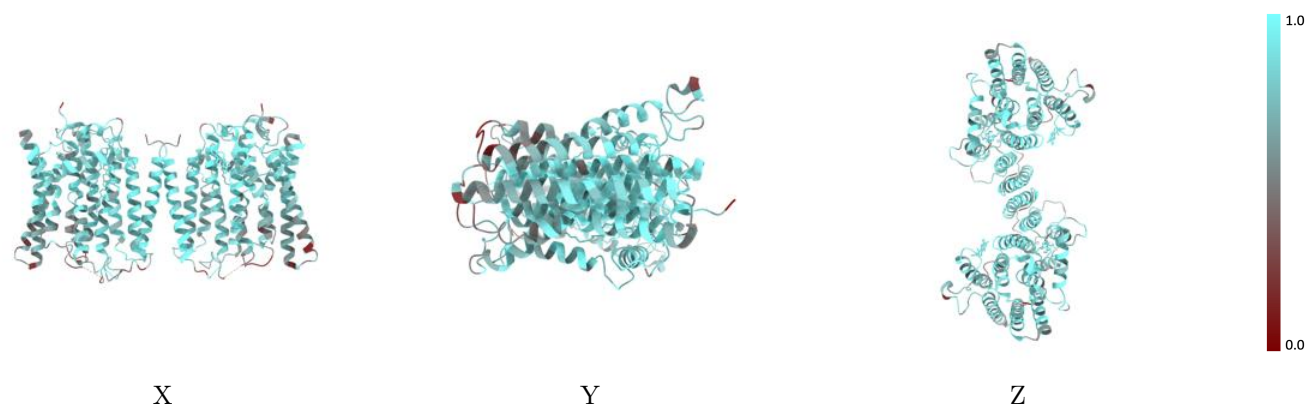
The images above show the 3D surface view of the map at the recommended contour level 0.641 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



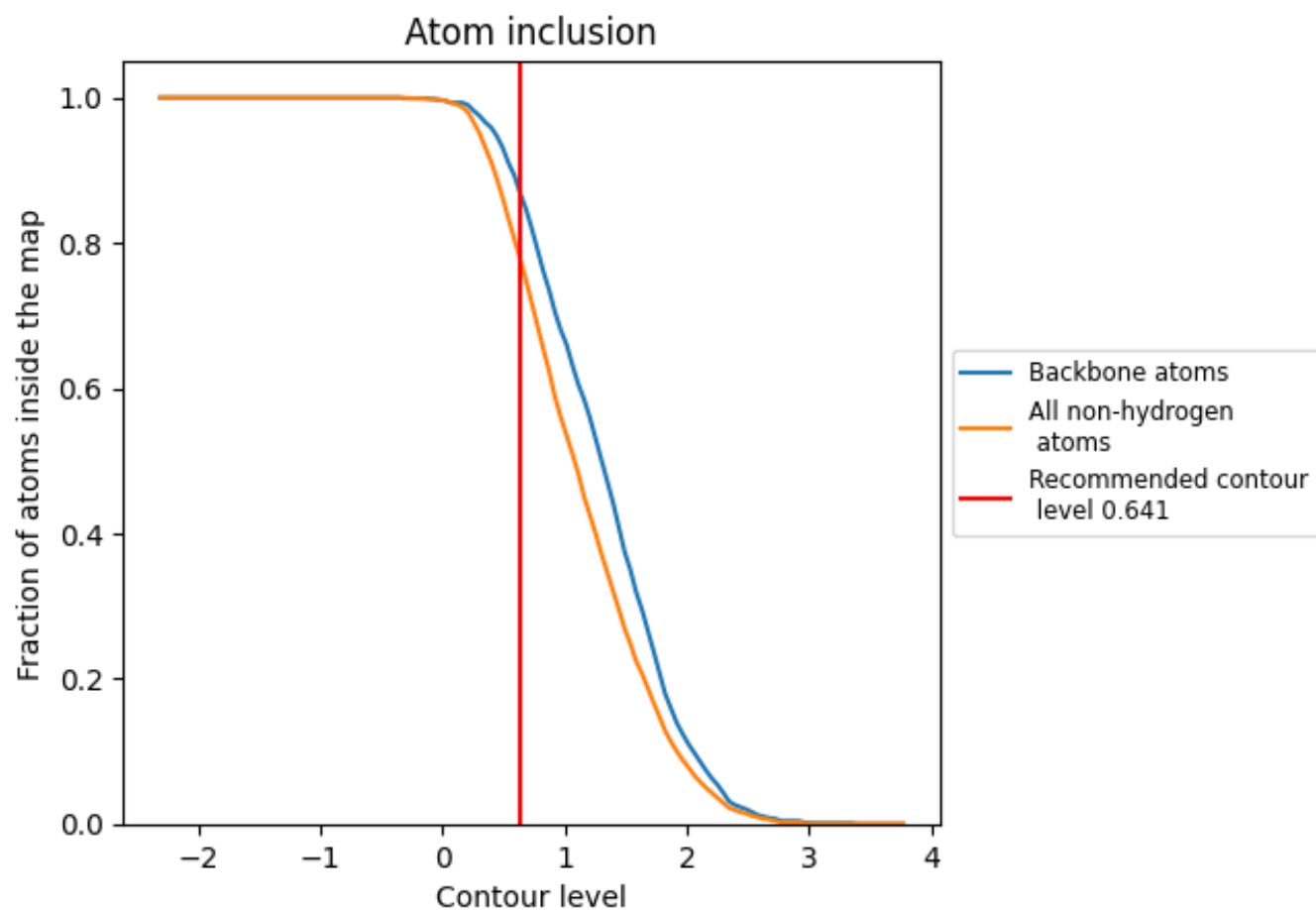
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.641).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 78% 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 (0.641) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7750	0.5060
A	0.7750	0.5050
B	0.7750	0.5060

