



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:43 AM UTC

PDB ID : 9J97 / pdb_00009j97
EMDB ID : EMD-61254
Title : Closed structure of human XPR1
Authors : Wang, Y.; Wang, Y.; Yang, H.; Shen, H.
Deposited on : 2024-08-22
Resolution : 3.30 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

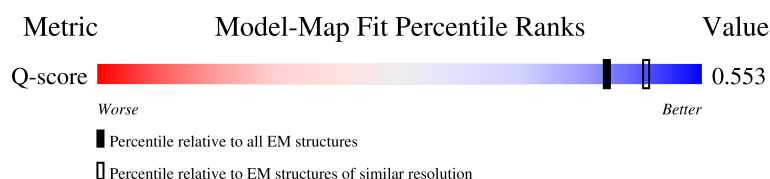
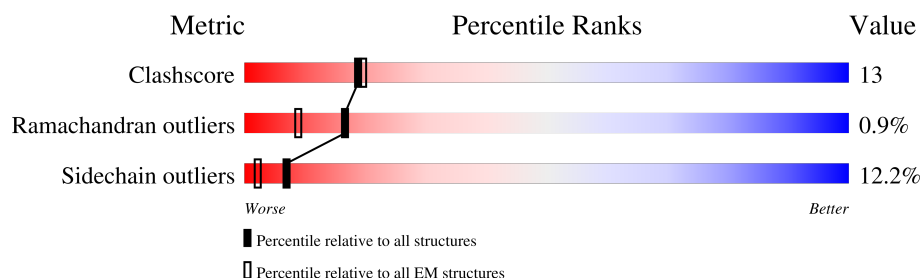
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	

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	PO4	A	1003	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6704 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	393	Total	C	N	O	S	0	0
			3272	2198	526	532	16		
1	B	393	Total	C	N	O	S	0	0
			3272	2198	526	532	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

Continued on next page...

Continued from previous page...

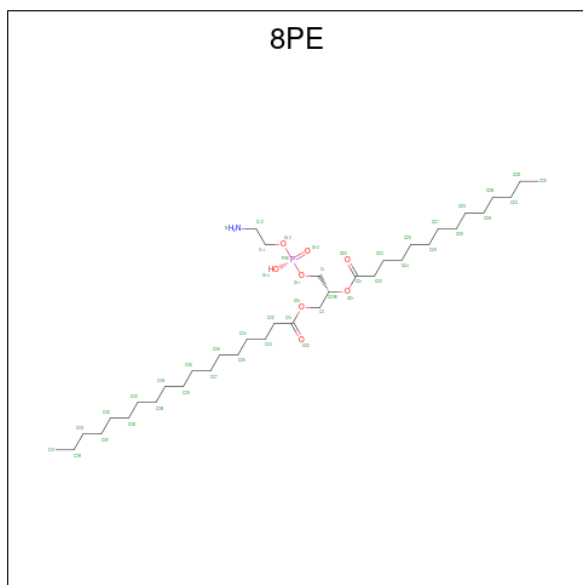
Chain	Residue	Modelled	Actual	Comment	Reference
A	955	ASP	-	expression tag	UNP P42212
A	956	TYR	-	expression tag	UNP P42212
A	957	LYS	-	expression tag	UNP P42212
A	958	ASP	-	expression tag	UNP P42212
A	959	HIS	-	expression tag	UNP P42212
A	960	ASP	-	expression tag	UNP P42212
A	961	ILE	-	expression tag	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

Continued on next page...

Continued from previous page...

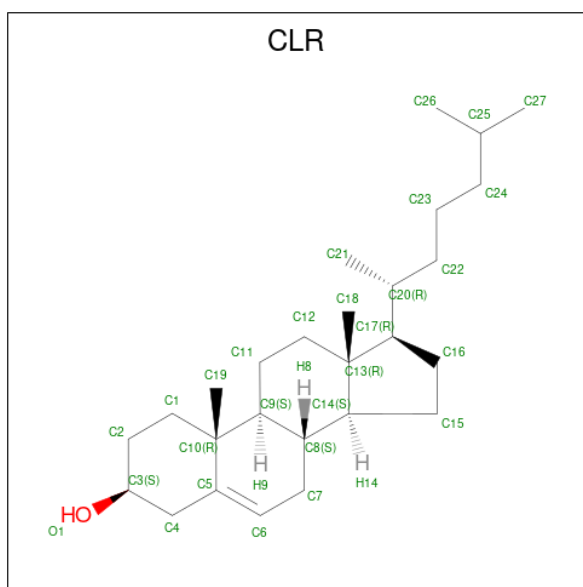
Chain	Residue	Modelled	Actual	Comment	Reference
B	956	TYR	-	expression tag	UNP P42212
B	957	LYS	-	expression tag	UNP P42212
B	958	ASP	-	expression tag	UNP P42212
B	959	HIS	-	expression tag	UNP P42212
B	960	ASP	-	expression tag	UNP P42212
B	961	ILE	-	expression tag	UNP P42212
B	962	ASP	-	expression tag	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).



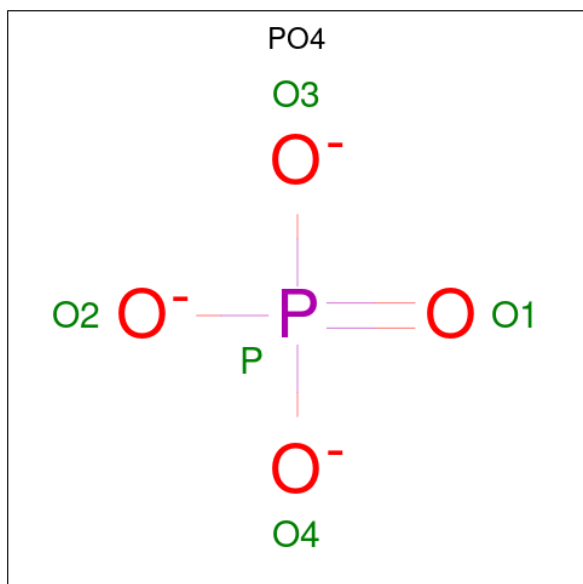
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
2	B	1	Total	C	N	O	P	0
			47	37	1	8	1	

- 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	

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	O	P	0
			5	4	1	

Continued on next page...

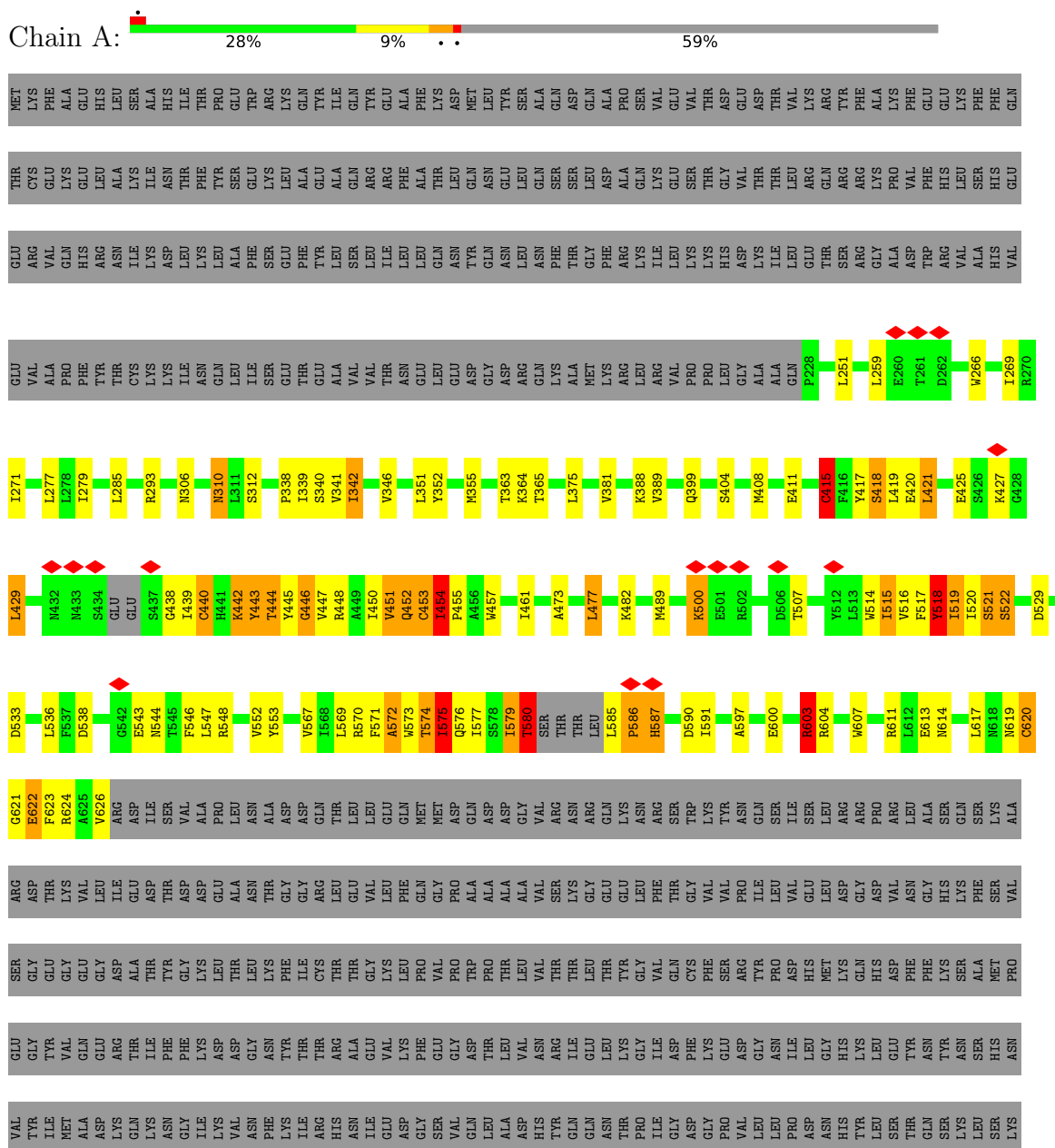
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
4	B	1	5	4	1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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



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

Frequency	Percentage
Often	29%
Sometimes	9%
Never	59%

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150104	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	7.760	Depositor
Minimum map value	-5.011	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.142	Depositor
Recommended contour level	0.738	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, PO4

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	0.83	16/3381 (0.5%)	1.04	40/4598 (0.9%)
1	B	0.81	15/3381 (0.4%)	1.02	34/4598 (0.7%)
All	All	0.82	31/6762 (0.5%)	1.03	74/9196 (0.8%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	454	ILE	C-N	14.27	1.50	1.34
1	A	454	ILE	C-N	14.13	1.49	1.34
1	B	454	ILE	C-O	-12.20	1.09	1.24
1	A	454	ILE	C-O	-12.13	1.09	1.24
1	A	621	GLY	C-O	-11.26	1.10	1.23
1	B	621	GLY	C-O	-11.24	1.10	1.23
1	B	620	CYS	C-O	-10.96	1.08	1.23
1	A	620	CYS	C-O	-10.96	1.08	1.23
1	A	603	ARG	C-O	-9.61	1.11	1.24
1	B	520	ILE	C-O	-8.37	1.14	1.24
1	A	520	ILE	C-O	-8.29	1.14	1.24
1	A	623	PHE	C-O	-7.88	1.13	1.24
1	B	623	PHE	C-O	-7.84	1.13	1.24
1	B	522	SER	CA-CB	-7.80	1.41	1.53
1	A	522	SER	CA-CB	-7.78	1.41	1.53
1	B	572	ALA	C-O	-7.58	1.14	1.24
1	A	572	ALA	C-O	-7.56	1.14	1.24
1	B	594	THR	C-N	7.12	1.43	1.33
1	A	451	VAL	C-O	-6.77	1.15	1.24
1	B	451	VAL	C-O	-6.73	1.15	1.24
1	A	516	VAL	C-O	-6.64	1.16	1.24
1	B	516	VAL	C-O	-6.59	1.16	1.24
1	A	570	ARG	C-O	-6.36	1.15	1.24
1	A	517	PHE	C-O	-6.18	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	517	PHE	C-O	-6.10	1.16	1.24
1	A	573	TRP	C-O	-5.81	1.17	1.24
1	B	573	TRP	C-O	-5.79	1.17	1.24
1	B	622	GLU	C-O	-5.77	1.16	1.24
1	A	622	GLU	C-O	-5.66	1.16	1.24
1	A	415	CYS	C-O	-5.36	1.17	1.24
1	B	415	CYS	C-O	-5.31	1.17	1.24

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	454	ILE	CA-C-N	16.43	136.95	119.87
1	B	454	ILE	C-N-CA	16.43	136.95	119.87
1	A	454	ILE	CA-C-N	16.31	136.83	119.87
1	A	454	ILE	C-N-CA	16.31	136.83	119.87
1	A	575	ILE	N-CA-C	-13.55	98.41	110.74
1	B	575	ILE	N-CA-C	-13.49	98.46	110.74
1	B	624	ARG	CB-CG-CD	-9.71	88.96	111.30
1	A	522	SER	N-CA-C	-9.37	101.97	113.50
1	B	522	SER	N-CA-C	-9.32	102.03	113.50
1	A	580	THR	CA-CB-OG1	-7.99	97.61	109.60
1	A	579	ILE	O-C-N	7.99	129.74	121.91
1	B	621	GLY	CA-C-N	7.89	136.61	121.54
1	B	621	GLY	C-N-CA	7.89	136.61	121.54
1	A	621	GLY	CA-C-N	7.86	136.55	121.54
1	A	621	GLY	C-N-CA	7.86	136.55	121.54
1	B	518	TYR	CB-CA-C	7.58	123.74	110.85
1	B	446	GLY	CA-C-N	-7.58	113.73	122.14
1	B	446	GLY	C-N-CA	-7.58	113.73	122.14
1	A	518	TYR	CB-CA-C	7.56	123.71	110.85
1	B	624	ARG	CB-CA-C	-7.32	96.85	109.65
1	A	624	ARG	CB-CG-CD	-7.21	94.71	111.30
1	B	517	PHE	CA-C-O	-7.07	112.93	120.42
1	A	517	PHE	CA-C-O	-7.01	112.99	120.42
1	A	579	ILE	CA-C-N	6.85	134.03	121.70
1	A	579	ILE	C-N-CA	6.85	134.03	121.70
1	A	624	ARG	CB-CA-C	-6.78	97.79	109.65
1	A	454	ILE	CA-C-O	-6.69	110.99	119.95
1	B	454	ILE	CA-C-O	-6.66	111.03	119.95
1	B	590	ASP	CA-CB-CG	-6.38	106.22	112.60
1	A	620	CYS	CB-CA-C	-6.38	99.44	110.09
1	A	590	ASP	CA-CB-CG	-6.33	106.27	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	445	TYR	CA-C-N	6.31	129.64	120.11
1	B	445	TYR	C-N-CA	6.31	129.64	120.11
1	B	620	CYS	CB-CA-C	-6.26	99.64	110.09
1	B	621	GLY	O-C-N	5.98	127.93	122.19
1	A	621	GLY	O-C-N	5.97	127.92	122.19
1	A	570	ARG	CB-CG-CD	-5.91	97.70	111.30
1	B	620	CYS	CA-CB-SG	-5.80	101.05	114.40
1	A	452	GLN	CB-CA-C	-5.80	101.78	110.88
1	B	452	GLN	CB-CA-C	-5.79	101.79	110.88
1	A	620	CYS	CA-CB-SG	-5.76	101.15	114.40
1	A	571	PHE	CA-CB-CG	-5.75	108.05	113.80
1	B	571	PHE	CA-CB-CG	-5.73	108.07	113.80
1	A	438	GLY	CA-C-O	-5.72	117.42	121.88
1	B	575	ILE	CA-C-N	5.69	129.71	120.60
1	B	575	ILE	C-N-CA	5.69	129.71	120.60
1	A	575	ILE	CA-C-N	5.67	129.68	120.60
1	A	575	ILE	C-N-CA	5.67	129.68	120.60
1	A	604	ARG	N-CA-C	-5.66	105.49	112.90
1	B	438	GLY	CA-C-O	-5.64	117.48	121.88
1	A	443	TYR	CA-C-N	5.59	131.02	121.29
1	A	443	TYR	C-N-CA	5.59	131.02	121.29
1	B	621	GLY	CA-C-O	-5.55	115.03	120.75
1	B	452	GLN	CA-C-O	-5.54	115.00	120.82
1	A	620	CYS	CA-C-O	-5.51	112.90	119.35
1	A	621	GLY	CA-C-O	-5.51	115.08	120.75
1	B	620	CYS	CA-C-O	-5.50	112.91	119.35
1	A	452	GLN	CA-C-O	-5.48	115.06	120.82
1	A	623	PHE	CB-CA-C	-5.47	101.31	110.56
1	B	580	THR	N-CA-C	5.46	126.30	111.00
1	B	453	CYS	CA-CB-SG	-5.39	102.01	114.40
1	A	453	CYS	CA-CB-SG	-5.38	102.02	114.40
1	B	623	PHE	CB-CA-C	-5.13	101.88	110.56
1	B	623	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	452	GLN	CA-C-N	-5.09	111.82	121.54
1	A	452	GLN	C-N-CA	-5.09	111.82	121.54
1	B	452	GLN	CA-C-N	-5.09	111.82	121.54
1	B	452	GLN	C-N-CA	-5.09	111.82	121.54
1	B	517	PHE	CA-CB-CG	-5.05	108.75	113.80
1	A	619	ASN	CA-C-N	-5.02	114.26	122.54
1	A	619	ASN	C-N-CA	-5.02	114.26	122.54
1	A	446	GLY	CA-C-N	-5.01	117.51	122.77
1	A	446	GLY	C-N-CA	-5.01	117.51	122.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	517	PHE	CA-CB-CG	-5.01	108.79	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3272	0	3258	76	0
1	B	3272	0	3258	78	0
2	A	47	0	73	8	0
2	B	47	0	73	8	0
3	A	28	0	46	5	0
3	B	28	0	46	4	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
All	All	6704	0	6754	173	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 13.

All (173) 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:489:MET:HE1	1:B:574:THR:OG1	1.43	1.16
1:A:489:MET:HE1	1:A:574:THR:OG1	1.48	1.12
1:B:489:MET:HE2	1:B:518:TYR:HB2	1.35	1.05
1:A:489:MET:HE2	1:A:518:TYR:HB2	1.35	1.02
1:B:572:ALA:HA	1:B:575:ILE:HG13	1.49	0.95
1:A:453:CYS:O	1:A:453:CYS:SG	2.25	0.95
1:B:489:MET:CE	1:B:574:THR:OG1	2.15	0.94
1:A:572:ALA:HA	1:A:575:ILE:HG13	1.49	0.93
1:B:453:CYS:SG	1:B:453:CYS:O	2.25	0.92
1:B:415:CYS:SG	1:B:415:CYS:O	2.30	0.89
1:A:489:MET:CE	1:A:574:THR:OG1	2.20	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:CYS:SG	1:A:415:CYS:O	2.32	0.87
1:A:548:ARG:NH2	1:A:613:GLU:OE2	2.16	0.79
1:B:548:ARG:NH2	1:B:613:GLU:OE2	2.16	0.78
1:B:448:ARG:HG3	1:B:448:ARG:NH1	2.00	0.77
1:A:448:ARG:HG3	1:A:448:ARG:NH1	2.00	0.76
2:A:1001:8PE:H23	2:A:1001:8PE:H3	1.70	0.74
1:A:310:ASN:HA	2:A:1001:8PE:O14	1.88	0.74
1:B:576:GLN:NE2	1:B:600:GLU:OE1	2.19	0.73
1:A:489:MET:HE2	1:A:518:TYR:CB	2.17	0.73
1:B:285:LEU:HD21	2:B:1001:8PE:H23A	1.71	0.72
2:B:1001:8PE:H23	2:B:1001:8PE:H3	1.70	0.72
1:B:310:ASN:HA	2:B:1001:8PE:O14	1.89	0.71
1:A:285:LEU:HD21	2:A:1001:8PE:H23A	1.72	0.69
1:B:489:MET:HE2	1:B:518:TYR:CB	2.18	0.69
1:A:448:ARG:HG3	1:A:448:ARG:HH11	1.57	0.67
1:B:448:ARG:HG3	1:B:448:ARG:HH11	1.57	0.67
2:B:1001:8PE:H3	2:B:1001:8PE:C23	2.24	0.67
1:A:576:GLN:NE2	1:A:600:GLU:OE1	2.24	0.67
2:A:1001:8PE:H3	2:A:1001:8PE:C23	2.24	0.67
1:A:351:LEU:HD11	1:A:355:MET:HE3	1.78	0.65
1:A:266:TRP:CD1	1:A:587:HIS:HE2	2.15	0.65
1:B:351:LEU:HD11	1:B:355:MET:HE3	1.78	0.65
1:A:442:LYS:HE3	1:A:442:LYS:HA	1.80	0.63
1:B:500:LYS:HD3	1:B:507:THR:HG21	1.81	0.62
1:A:457:TRP:CE2	1:A:461:ILE:HD11	2.35	0.61
1:A:500:LYS:HD3	1:A:507:THR:HG21	1.81	0.61
1:B:411:GLU:OE1	1:B:448:ARG:NH1	2.31	0.61
1:B:457:TRP:CE2	1:B:461:ILE:HD11	2.35	0.61
1:A:444:THR:O	1:A:446:GLY:N	2.33	0.60
1:B:306:ASN:O	1:B:310:ASN:ND2	2.35	0.59
1:A:306:ASN:O	1:A:310:ASN:ND2	2.35	0.59
1:B:442:LYS:HA	1:B:442:LYS:HE3	1.84	0.59
1:A:442:LYS:HE3	1:A:442:LYS:CA	2.33	0.57
1:B:442:LYS:HE3	1:B:442:LYS:CA	2.35	0.57
1:B:447:VAL:HG13	1:B:447:VAL:O	2.04	0.57
1:B:572:ALA:CA	1:B:575:ILE:HG13	2.31	0.57
1:B:580:THR:HG23	1:B:580:THR:O	2.05	0.57
1:A:411:GLU:OE1	1:A:448:ARG:NH1	2.30	0.56
1:A:489:MET:HE2	1:A:518:TYR:HA	1.87	0.56
1:A:607:TRP:CZ2	1:A:611:ARG:HG3	2.41	0.56
1:B:489:MET:CE	1:B:574:THR:HG1	2.13	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:TRP:CZ2	1:B:611:ARG:HG3	2.41	0.55
1:B:489:MET:HE2	1:B:518:TYR:HA	1.87	0.55
1:A:489:MET:CE	1:A:574:THR:HG1	2.18	0.55
1:A:448:ARG:HH11	1:A:448:ARG:CG	2.20	0.55
1:A:574:THR:OG1	1:A:574:THR:O	2.23	0.55
1:A:572:ALA:CA	1:A:575:ILE:HG13	2.31	0.54
2:A:1001:8PE:C3	2:A:1001:8PE:C22	2.85	0.54
1:B:574:THR:OG1	1:B:574:THR:O	2.23	0.54
1:B:604:ARG:NH1	4:B:1003:PO4:O2	2.34	0.54
2:B:1001:8PE:C3	2:B:1001:8PE:C22	2.85	0.54
1:A:572:ALA:HA	1:A:575:ILE:CG1	2.30	0.54
1:B:293:ARG:HH22	1:B:312:SER:HA	1.72	0.54
1:A:293:ARG:HH22	1:A:312:SER:HA	1.72	0.53
1:A:529:ASP:HA	1:A:533:ASP:HB2	1.90	0.53
1:A:603:ARG:O	1:A:603:ARG:HG2	2.08	0.53
1:B:591:ILE:HG22	1:B:591:ILE:O	2.08	0.53
1:A:457:TRP:O	1:A:461:ILE:HG13	2.08	0.53
1:A:271:ILE:O	1:A:352:TYR:OH	2.23	0.53
1:A:451:VAL:O	1:A:451:VAL:HG12	2.08	0.53
1:A:489:MET:CE	1:A:518:TYR:HA	2.39	0.53
1:B:457:TRP:O	1:B:461:ILE:HG13	2.08	0.53
1:B:521:SER:O	1:B:521:SER:OG	2.22	0.53
1:A:591:ILE:HG22	1:A:591:ILE:O	2.08	0.53
1:B:451:VAL:HG12	1:B:451:VAL:O	2.08	0.53
1:A:266:TRP:CD1	1:A:587:HIS:NE2	2.76	0.52
1:B:585:LEU:N	1:B:585:LEU:CD2	2.73	0.52
1:B:489:MET:CE	1:B:518:TYR:HA	2.39	0.52
1:A:277:LEU:HD11	1:A:597:ALA:HB1	1.92	0.51
1:B:266:TRP:CD1	1:B:587:HIS:HE2	2.28	0.51
1:B:277:LEU:HD11	1:B:597:ALA:HB1	1.92	0.51
1:B:529:ASP:HA	1:B:533:ASP:HB2	1.90	0.51
1:B:572:ALA:HA	1:B:575:ILE:CG1	2.30	0.51
1:A:585:LEU:N	1:A:585:LEU:CD2	2.73	0.51
2:B:1001:8PE:H22A	2:B:1001:8PE:H3A	1.93	0.51
1:B:388:LYS:HD2	1:B:389:VAL:H	1.76	0.50
1:B:448:ARG:HH11	1:B:448:ARG:CG	2.20	0.50
1:A:388:LYS:HD2	1:A:389:VAL:H	1.75	0.50
1:A:603:ARG:CG	1:A:603:ARG:HH11	2.25	0.50
2:A:1001:8PE:H3A	2:A:1001:8PE:H22A	1.93	0.50
1:A:340:SER:O	1:A:342:ILE:N	2.46	0.49
1:A:580:THR:O	1:A:580:THR:HG23	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:SER:O	1:A:408:MET:HG2	2.13	0.48
1:A:473:ALA:O	1:A:477:LEU:HB2	2.13	0.48
1:B:340:SER:O	1:B:342:ILE:N	2.46	0.48
1:A:603:ARG:CG	1:A:603:ARG:NH1	2.72	0.48
1:B:404:SER:O	1:B:408:MET:HG2	2.13	0.48
1:A:603:ARG:HG2	1:A:603:ARG:NH1	2.29	0.48
1:B:515:ILE:HD12	1:B:515:ILE:HA	1.70	0.48
1:B:519:ILE:HD13	1:B:519:ILE:O	2.14	0.47
1:B:443:TYR:CE1	1:B:448:ARG:HD3	2.50	0.47
1:B:457:TRP:NE1	1:B:461:ILE:HD11	2.30	0.47
1:A:614:ASN:ND2	1:A:620:CYS:SG	2.88	0.47
1:B:473:ALA:O	1:B:477:LEU:HB2	2.13	0.47
1:A:457:TRP:NE1	1:A:461:ILE:HD11	2.30	0.47
2:B:1001:8PE:C3	2:B:1001:8PE:H22A	2.45	0.47
1:A:519:ILE:O	1:A:519:ILE:HD13	2.15	0.46
3:B:1002:CLR:H211	3:B:1002:CLR:H232	1.62	0.46
1:B:271:ILE:O	1:B:352:TYR:OH	2.23	0.46
1:A:544:ASN:HB3	1:A:547:LEU:HB2	1.98	0.46
1:B:445:TYR:CD2	1:B:445:TYR:O	2.69	0.46
2:A:1001:8PE:H3	2:A:1001:8PE:C22	2.45	0.46
1:B:614:ASN:ND2	1:B:620:CYS:SG	2.89	0.45
2:B:1001:8PE:H3	2:B:1001:8PE:C22	2.45	0.45
1:A:515:ILE:HD12	1:A:515:ILE:HA	1.70	0.45
2:A:1001:8PE:C3	2:A:1001:8PE:H22A	2.45	0.45
1:A:420:GLU:OE2	1:A:440:CYS:SG	2.75	0.45
1:B:418:SER:OG	1:B:419:LEU:N	2.50	0.45
1:B:445:TYR:O	1:B:445:TYR:CG	2.70	0.45
1:B:364:LYS:H	1:B:364:LYS:HG2	1.40	0.45
1:B:544:ASN:HB3	1:B:547:LEU:HB2	1.98	0.45
1:A:418:SER:OG	1:A:419:LEU:N	2.50	0.44
1:A:443:TYR:CE1	1:A:448:ARG:HD3	2.53	0.44
1:A:519:ILE:HD13	1:A:519:ILE:HA	1.71	0.44
1:B:420:GLU:OE2	1:B:440:CYS:SG	2.75	0.44
1:A:251:LEU:HD23	1:A:251:LEU:HA	1.85	0.44
1:B:553:TYR:CD1	3:B:1002:CLR:H41	2.53	0.44
3:A:1002:CLR:H192	3:A:1002:CLR:H22	1.46	0.44
1:B:477:LEU:HD22	1:B:477:LEU:HA	1.91	0.43
1:A:553:TYR:CD1	3:A:1002:CLR:H41	2.53	0.43
1:A:569:LEU:HD23	1:A:569:LEU:HA	1.87	0.43
1:B:464:LEU:HD23	1:B:464:LEU:HA	1.84	0.43
3:A:1002:CLR:H182	3:A:1002:CLR:H111	1.77	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:ILE:HD13	1:B:454:ILE:HG21	1.77	0.43
1:B:429:LEU:HD23	1:B:429:LEU:HA	1.78	0.43
3:A:1002:CLR:H212	3:A:1002:CLR:H183	2.01	0.42
1:B:266:TRP:CD1	1:B:587:HIS:NE2	2.87	0.42
1:B:519:ILE:HD13	1:B:519:ILE:HA	1.72	0.42
1:B:339:ILE:HG22	1:B:340:SER:N	2.35	0.42
1:A:546:PHE:O	1:A:547:LEU:HD23	2.20	0.42
3:A:1002:CLR:H231	3:A:1002:CLR:H262	1.82	0.42
1:B:546:PHE:O	1:B:547:LEU:HD23	2.20	0.42
1:A:586:PRO:HB2	1:A:587:HIS:H	1.76	0.42
1:B:444:THR:OG1	1:B:445:TYR:N	2.53	0.42
1:B:619:ASN:CG	1:B:619:ASN:O	2.61	0.42
1:A:521:SER:O	1:A:521:SER:OG	2.22	0.42
1:B:536:LEU:O	1:B:538:ASP:N	2.53	0.41
1:B:591:ILE:O	1:B:591:ILE:CG2	2.68	0.41
3:B:1002:CLR:H272	3:B:1002:CLR:H231	1.81	0.41
1:A:454:ILE:N	1:A:455:PRO:CD	2.83	0.41
1:B:259:LEU:HD22	1:B:259:LEU:HA	1.82	0.41
1:A:417:TYR:HD1	1:A:421:LEU:HD22	1.84	0.41
1:A:591:ILE:O	1:A:591:ILE:CG2	2.68	0.41
1:B:417:TYR:HD1	1:B:421:LEU:HD22	1.84	0.41
1:B:495:LEU:HD12	1:B:495:LEU:HA	1.91	0.41
1:A:338:PRO:O	1:A:339:ILE:HG13	2.21	0.41
1:A:585:LEU:HD13	1:A:586:PRO:HD3	2.02	0.41
3:B:1002:CLR:H22	3:B:1002:CLR:H192	1.46	0.41
1:A:339:ILE:HG22	1:A:340:SER:N	2.35	0.41
1:A:514:TRP:CD1	1:A:514:TRP:C	2.99	0.41
1:A:603:ARG:O	1:A:603:ARG:CG	2.69	0.41
1:B:332:LEU:HD12	1:B:332:LEU:HA	1.92	0.41
1:B:454:ILE:N	1:B:455:PRO:CD	2.84	0.41
1:A:536:LEU:O	1:A:538:ASP:N	2.53	0.41
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.78	0.40
1:B:585:LEU:HD13	1:B:586:PRO:HD3	2.03	0.40
1:A:425:GLU:HG3	1:A:427:LYS:H	1.87	0.40
1:A:580:THR:O	1:A:580:THR:CG2	2.68	0.40
1:B:338:PRO:O	1:B:339:ILE:HG13	2.21	0.40
1:A:375:LEU:HD23	1:A:375:LEU:HA	1.84	0.40
1:B:425:GLU:HG3	1:B:427:LYS:H	1.87	0.40
1:B:519:ILE:O	1:B:519:ILE:CD1	2.70	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	387/969 (40%)	356 (92%)	27 (7%)	4 (1%)	12	40
1	B	387/969 (40%)	358 (92%)	26 (7%)	3 (1%)	16	45
All	All	774/1938 (40%)	714 (92%)	53 (7%)	7 (1%)	16	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	586	PRO
1	A	622	GLU
1	B	586	PRO
1	B	622	GLU
1	A	445	TYR
1	A	341	VAL
1	B	341	VAL

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	347/857 (40%)	304 (88%)	43 (12%)	4	19
1	B	347/857 (40%)	305 (88%)	42 (12%)	5	20
All	All	694/1714 (40%)	609 (88%)	85 (12%)	7	19

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	LEU
1	A	269	ILE
1	A	279	ILE
1	A	310	ASN
1	A	342	ILE
1	A	346	VAL
1	A	363	THR
1	A	364	LYS
1	A	365	THR
1	A	381	VAL
1	A	399	GLN
1	A	415	CYS
1	A	418	SER
1	A	421	LEU
1	A	429	LEU
1	A	439	ILE
1	A	440	CYS
1	A	442	LYS
1	A	444	THR
1	A	447	VAL
1	A	450	ILE
1	A	452	GLN
1	A	454	ILE
1	A	477	LEU
1	A	482	LYS
1	A	500	LYS
1	A	515	ILE
1	A	518	TYR
1	A	519	ILE
1	A	521	SER
1	A	522	SER
1	A	543	GLU
1	A	552	VAL
1	A	567	VAL
1	A	574	THR
1	A	575	ILE
1	A	577	ILE
1	A	579	ILE
1	A	580	THR
1	A	587	HIS
1	A	603	ARG
1	A	617	LEU
1	A	626	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	259	LEU
1	B	269	ILE
1	B	279	ILE
1	B	310	ASN
1	B	342	ILE
1	B	346	VAL
1	B	363	THR
1	B	364	LYS
1	B	365	THR
1	B	381	VAL
1	B	399	GLN
1	B	415	CYS
1	B	421	LEU
1	B	429	LEU
1	B	439	ILE
1	B	440	CYS
1	B	442	LYS
1	B	444	THR
1	B	445	TYR
1	B	447	VAL
1	B	450	ILE
1	B	452	GLN
1	B	454	ILE
1	B	477	LEU
1	B	482	LYS
1	B	500	LYS
1	B	515	ILE
1	B	518	TYR
1	B	519	ILE
1	B	521	SER
1	B	522	SER
1	B	543	GLU
1	B	552	VAL
1	B	567	VAL
1	B	574	THR
1	B	575	ILE
1	B	577	ILE
1	B	579	ILE
1	B	580	THR
1	B	587	HIS
1	B	617	LEU
1	B	626	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	499	HIS
1	A	614	ASN
1	B	479	ASN
1	B	499	HIS
1	B	614	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	CLR	B	1002	-	31,31,31	1.00	0	48,48,48	1.91	15 (31%)
4	PO4	A	1003	-	4,4,4	3.06	4 (100%)	6,6,6	0.46	0
4	PO4	B	1003	-	4,4,4	1.54	1 (25%)	6,6,6	1.03	0
3	CLR	A	1002	-	31,31,31	0.99	0	48,48,48	1.92	15 (31%)
2	8PE	A	1001	-	46,46,46	1.09	3 (6%)	49,51,51	1.39	6 (12%)
2	8PE	B	1001	-	46,46,46	1.09	3 (6%)	49,51,51	1.39	6 (12%)

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	CLR	A	1002	-	-	4/10/68/68	0/4/4/4
2	8PE	A	1001	-	-	21/50/50/50	-
3	CLR	B	1002	-	-	4/10/68/68	0/4/4/4
2	8PE	B	1001	-	-	21/50/50/50	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	PO4	P-O1	4.68	1.61	1.50
2	B	1001	8PE	O32-C31	-3.18	1.13	1.22
2	A	1001	8PE	O32-C31	-3.14	1.13	1.22
4	B	1003	PO4	P-O3	-2.41	1.47	1.54
4	A	1003	PO4	P-O3	2.36	1.61	1.54
4	A	1003	PO4	P-O2	2.34	1.61	1.54
2	A	1001	8PE	C22-C21	-2.29	1.44	1.50
2	B	1001	8PE	C22-C21	-2.26	1.44	1.50
2	B	1001	8PE	O22-C21	-2.22	1.15	1.22
2	A	1001	8PE	O22-C21	-2.21	1.15	1.22
4	A	1003	PO4	P-O4	-2.15	1.48	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	CLR	C19-C10-C1	-6.56	99.45	109.43
3	B	1002	CLR	C19-C10-C1	-6.52	99.51	109.43
2	A	1001	8PE	O21-C21-C22	5.69	123.79	111.48
2	B	1001	8PE	O21-C21-C22	5.68	123.76	111.48
2	B	1001	8PE	O13-P-O12	-4.29	91.92	108.94
2	A	1001	8PE	O13-P-O12	-4.28	91.95	108.94
3	B	1002	CLR	C19-C10-C5	4.26	114.89	108.38
3	A	1002	CLR	C19-C10-C5	4.24	114.85	108.38
3	A	1002	CLR	C1-C10-C9	4.13	114.21	108.74
3	B	1002	CLR	C1-C10-C9	4.13	114.20	108.74
2	B	1001	8PE	O22-C21-C22	-2.93	112.31	123.78
2	A	1001	8PE	O22-C21-C22	-2.92	112.35	123.78
3	B	1002	CLR	O1-C3-C4	2.80	116.02	109.71
3	A	1002	CLR	O1-C3-C4	2.78	115.96	109.71
2	B	1001	8PE	C2-O21-C21	2.76	124.40	117.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	8PE	C2-O21-C21	2.75	124.38	117.80
3	A	1002	CLR	C11-C12-C13	-2.62	108.31	112.74
3	B	1002	CLR	C11-C12-C13	-2.62	108.32	112.74
3	A	1002	CLR	C18-C13-C12	-2.56	106.83	110.61
3	B	1002	CLR	C10-C9-C8	2.53	116.42	112.71
3	B	1002	CLR	C18-C13-C12	-2.51	106.90	110.61
3	A	1002	CLR	C10-C9-C8	2.49	116.36	112.71
3	A	1002	CLR	C2-C1-C10	-2.48	107.50	112.78
3	B	1002	CLR	C2-C1-C10	-2.48	107.51	112.78
3	A	1002	CLR	C19-C10-C9	2.34	114.29	111.66
3	B	1002	CLR	C12-C11-C9	-2.30	109.23	113.14
3	A	1002	CLR	C12-C11-C9	-2.30	109.23	113.14
3	B	1002	CLR	C19-C10-C9	2.25	114.18	111.66
3	A	1002	CLR	C16-C17-C20	-2.22	108.82	112.18
3	B	1002	CLR	C16-C17-C20	-2.15	108.93	112.18
2	B	1001	8PE	C3-O31-C31	-2.14	109.30	117.12
2	A	1001	8PE	C3-O31-C31	-2.13	109.34	117.12
3	A	1002	CLR	C1-C10-C5	-2.10	105.13	108.74
3	B	1002	CLR	C1-C10-C5	-2.09	105.14	108.74
3	B	1002	CLR	C2-C3-C4	-2.03	107.43	110.29
3	B	1002	CLR	C11-C9-C8	-2.02	108.96	111.78
3	B	1002	CLR	C17-C13-C14	2.02	102.42	100.10
3	A	1002	CLR	C2-C3-C4	-2.01	107.46	110.29
2	B	1001	8PE	O14-P-O11	2.01	116.67	107.57
2	A	1001	8PE	O14-P-O11	2.00	116.65	107.57
3	A	1002	CLR	C17-C13-C14	2.00	102.40	100.10
3	A	1002	CLR	C11-C9-C8	-2.00	108.99	111.78

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	8PE	O22-C21-O21-C2
2	A	1001	8PE	C22-C21-O21-C2
2	B	1001	8PE	O22-C21-O21-C2
2	B	1001	8PE	C22-C21-O21-C2
3	A	1002	CLR	C21-C20-C22-C23
3	B	1002	CLR	C21-C20-C22-C23
2	A	1001	8PE	C32-C31-O31-C3
2	B	1001	8PE	C32-C31-O31-C3
2	A	1001	8PE	O32-C31-O31-C3
2	B	1001	8PE	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

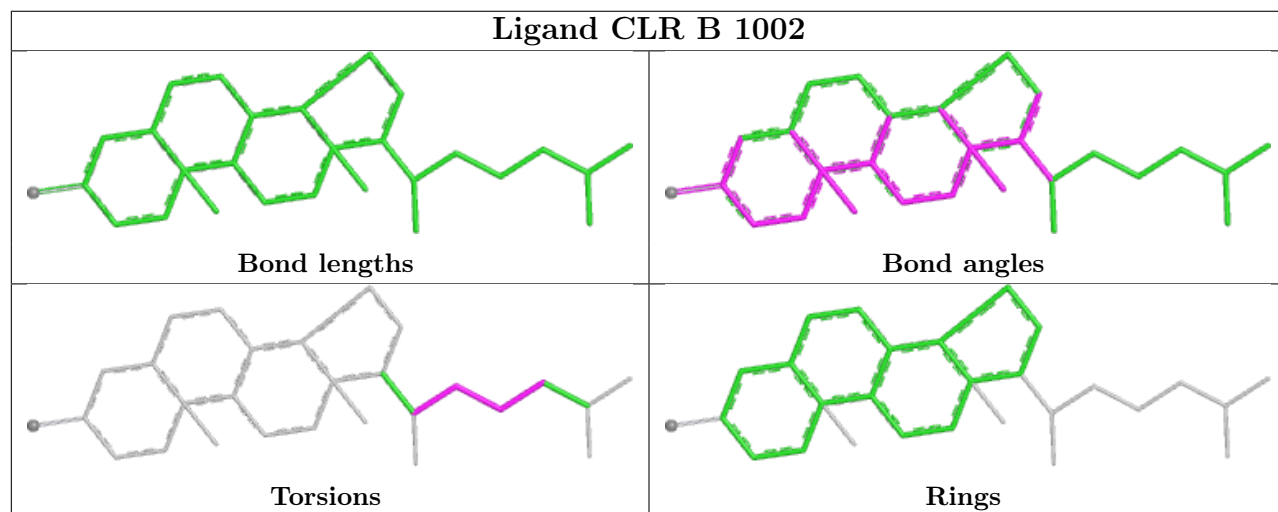
Mol	Chain	Res	Type	Atoms
3	A	1002	CLR	C22-C23-C24-C25
3	B	1002	CLR	C22-C23-C24-C25
2	A	1001	8PE	C3-C2-O21-C21
2	B	1001	8PE	C3-C2-O21-C21
2	A	1001	8PE	C28-C29-C2A-C2B
2	B	1001	8PE	C28-C29-C2A-C2B
2	A	1001	8PE	C29-C2A-C2B-C2C
2	B	1001	8PE	C29-C2A-C2B-C2C
3	B	1002	CLR	C20-C22-C23-C24
3	A	1002	CLR	C20-C22-C23-C24
2	B	1001	8PE	C23-C24-C25-C26
2	A	1001	8PE	C23-C24-C25-C26
2	A	1001	8PE	C38-C39-C3A-C3B
2	B	1001	8PE	C38-C39-C3A-C3B
2	A	1001	8PE	C2B-C2C-C2D-C2E
2	B	1001	8PE	C2B-C2C-C2D-C2E
2	A	1001	8PE	C21-C22-C23-C24
2	B	1001	8PE	C21-C22-C23-C24
2	B	1001	8PE	C27-C28-C29-C2A
2	A	1001	8PE	C27-C28-C29-C2A
2	A	1001	8PE	C37-C38-C39-C3A
2	B	1001	8PE	C37-C38-C39-C3A
3	A	1002	CLR	C17-C20-C22-C23
3	B	1002	CLR	C17-C20-C22-C23
2	A	1001	8PE	C3F-C3G-C3H-C3I
2	B	1001	8PE	C3F-C3G-C3H-C3I
2	B	1001	8PE	C31-C32-C33-C34
2	A	1001	8PE	C31-C32-C33-C34
2	A	1001	8PE	C3A-C3B-C3C-C3D
2	B	1001	8PE	C3A-C3B-C3C-C3D
2	A	1001	8PE	C35-C36-C37-C38
2	B	1001	8PE	C35-C36-C37-C38
2	A	1001	8PE	C3B-C3C-C3D-C3E
2	B	1001	8PE	C3B-C3C-C3D-C3E
2	A	1001	8PE	C3C-C3D-C3E-C3F
2	B	1001	8PE	C3C-C3D-C3E-C3F
2	B	1001	8PE	O21-C21-C22-C23
2	A	1001	8PE	O21-C21-C22-C23
2	B	1001	8PE	O22-C21-C22-C23
2	A	1001	8PE	O22-C21-C22-C23

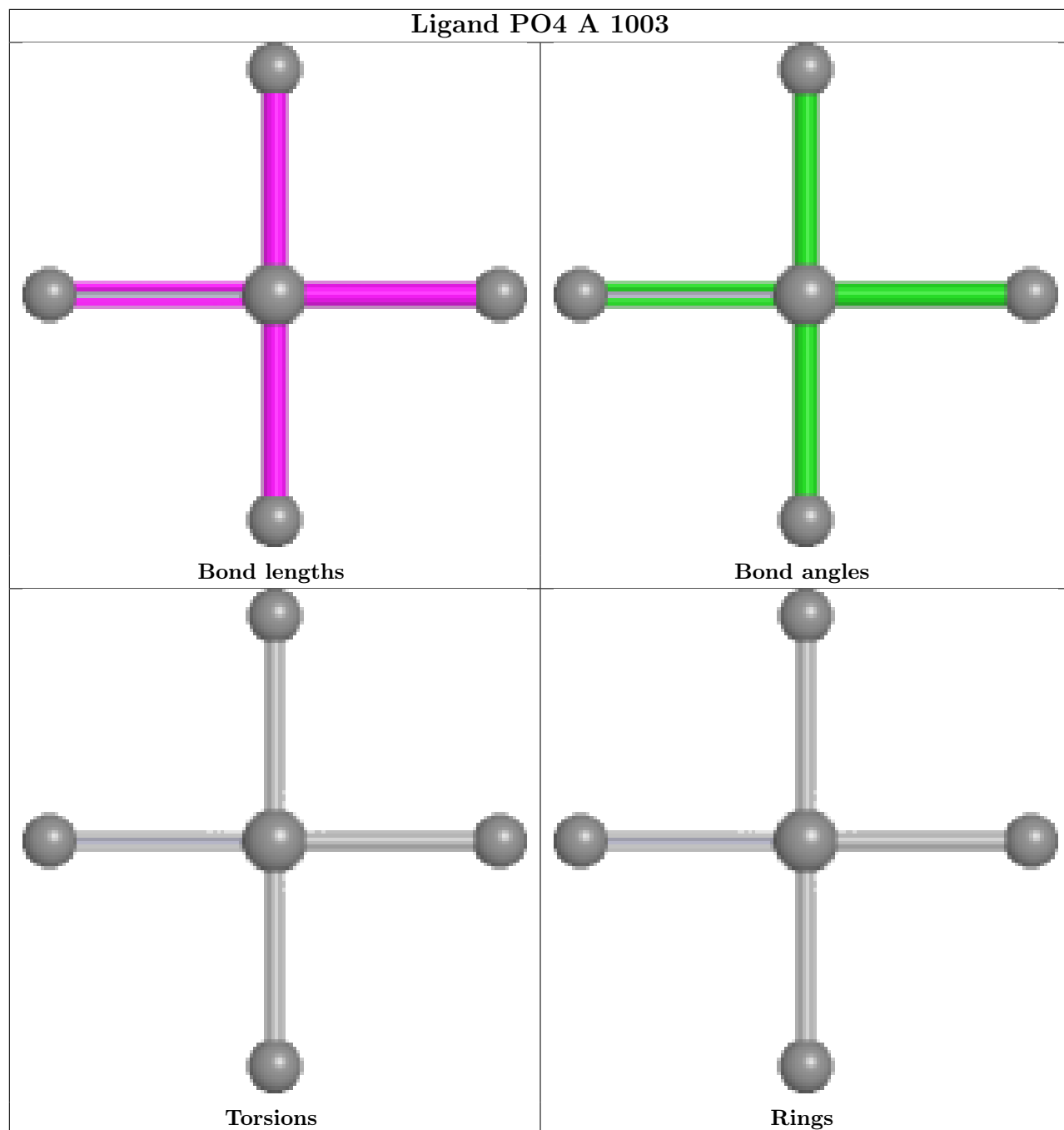
There are no ring outliers.

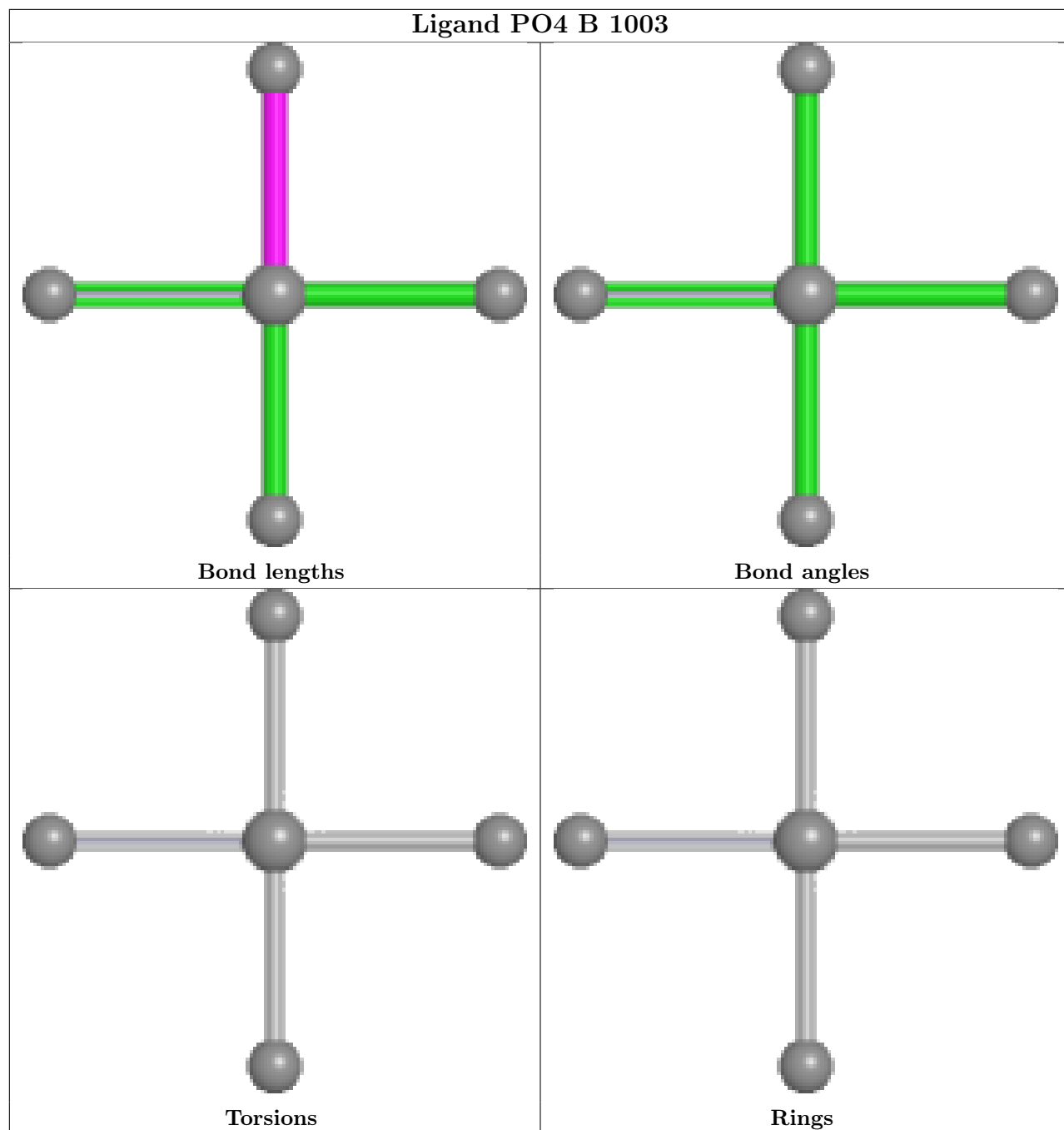
5 monomers are involved in 26 short contacts:

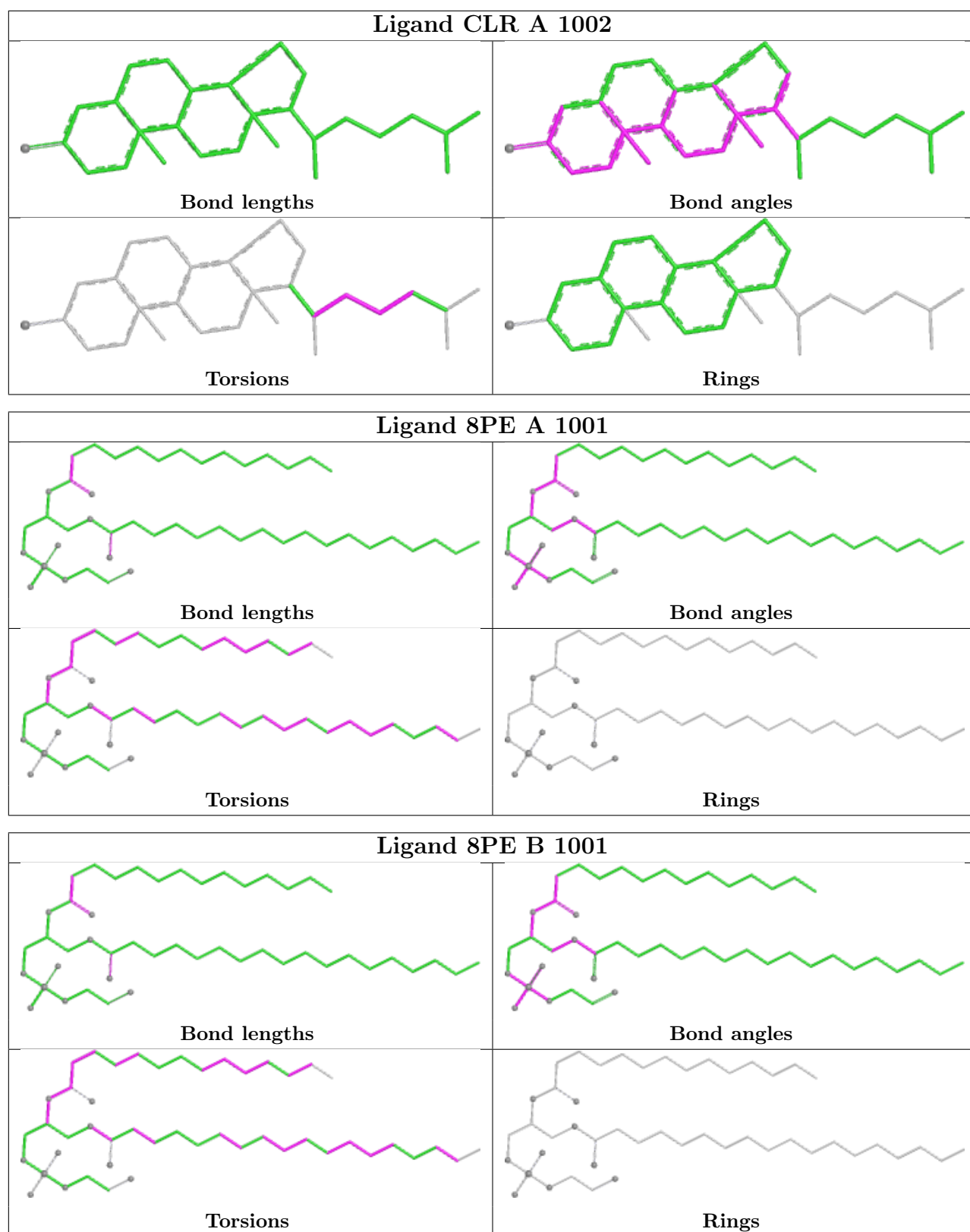
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	CLR	4	0
4	B	1003	PO4	1	0
3	A	1002	CLR	5	0
2	A	1001	8PE	8	0
2	B	1001	8PE	8	0

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 ⓘ

There are no chain breaks in this entry.

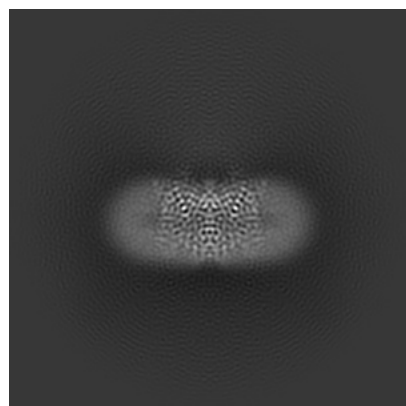
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61254. These allow visual inspection of the internal detail of the map and identification of artifacts.

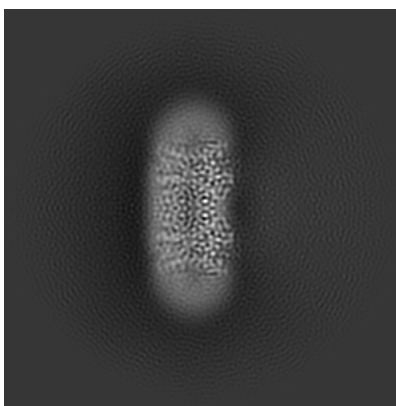
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

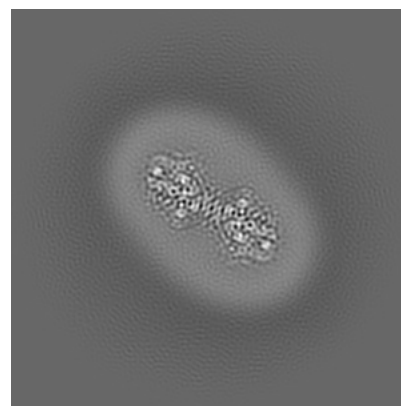
6.1.1 Primary map



X

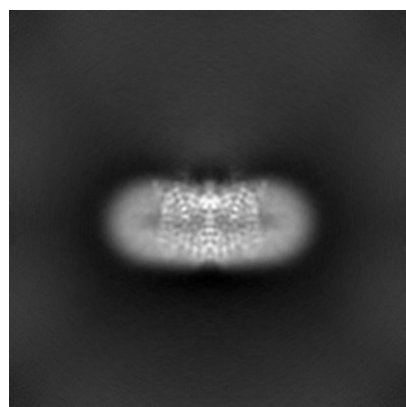


Y

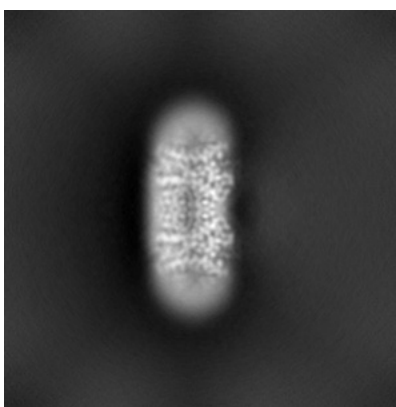


Z

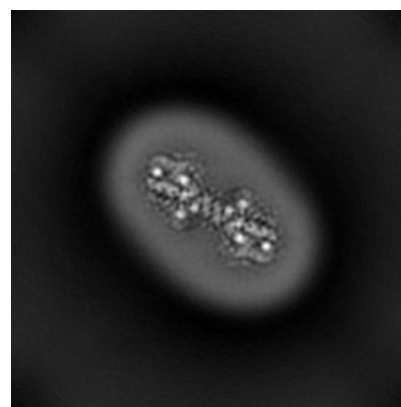
6.1.2 Raw map



X



Y

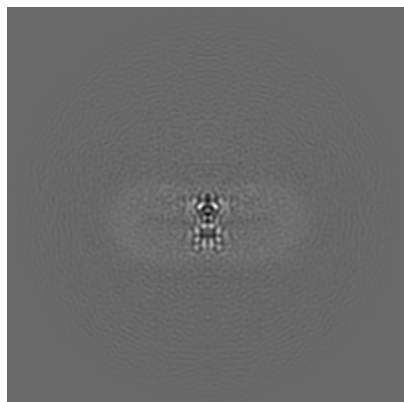


Z

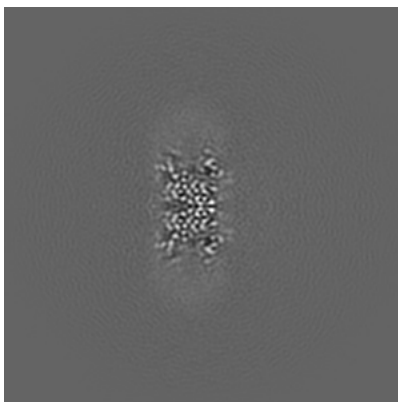
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

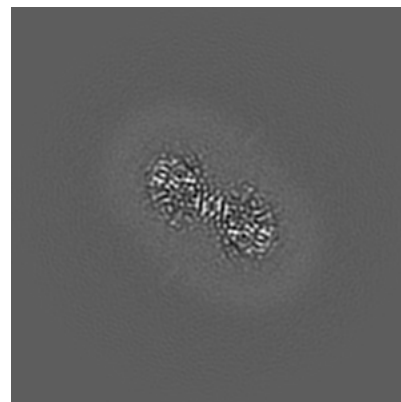
6.2.1 Primary map



X Index: 128

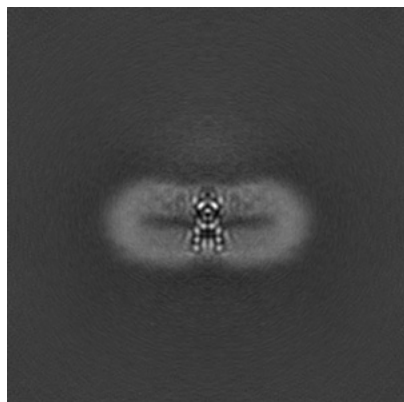


Y Index: 128

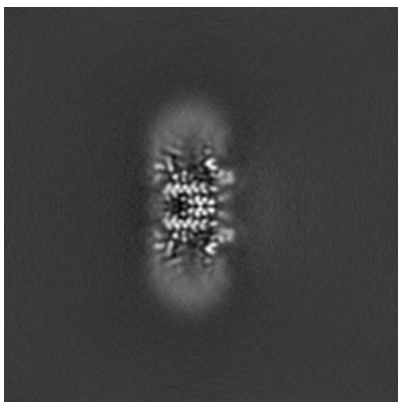


Z Index: 128

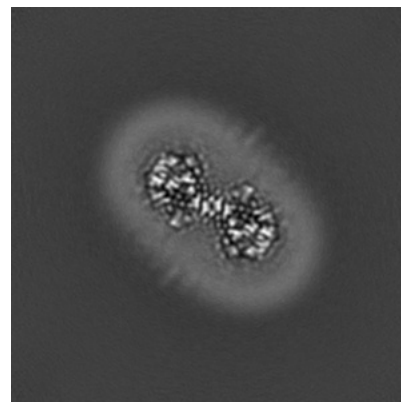
6.2.2 Raw map



X Index: 128



Y Index: 128

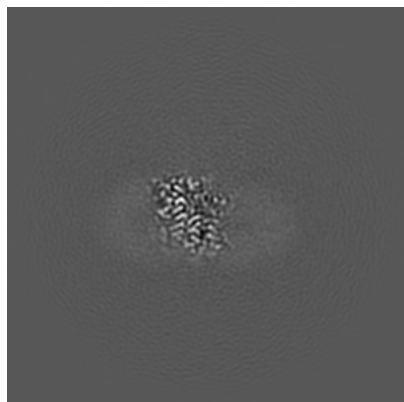


Z Index: 128

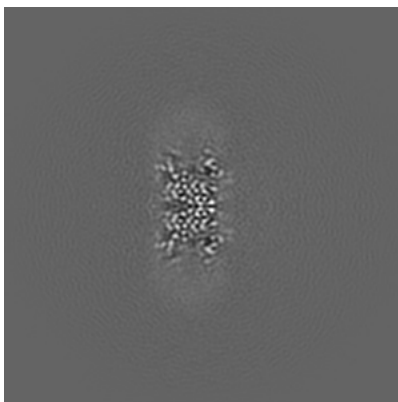
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

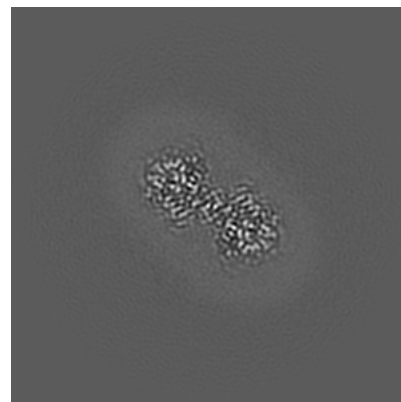
6.3.1 Primary map



X Index: 146

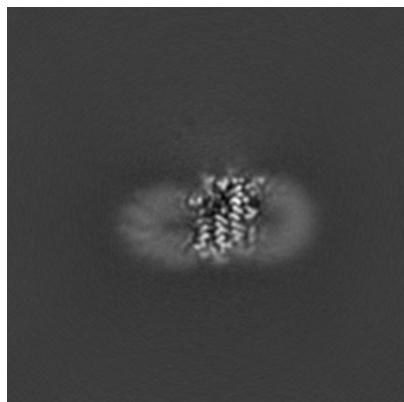


Y Index: 128

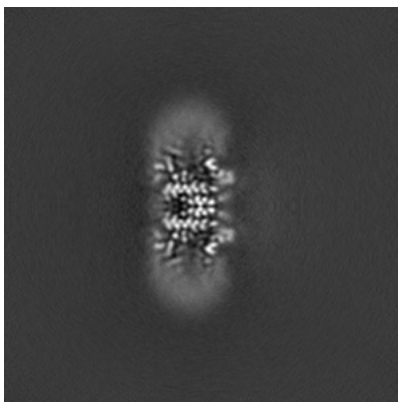


Z Index: 132

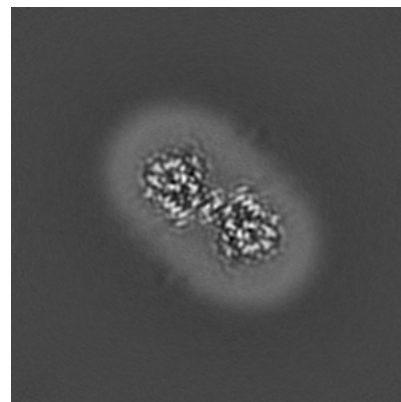
6.3.2 Raw map



X Index: 110



Y Index: 128

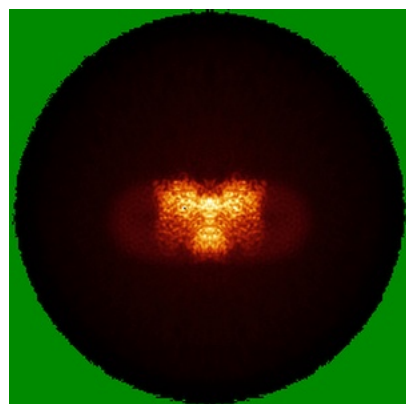


Z Index: 132

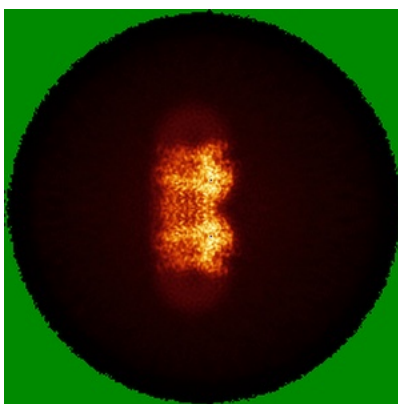
The images above show the largest variance slices of the map in three orthogonal directions.

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

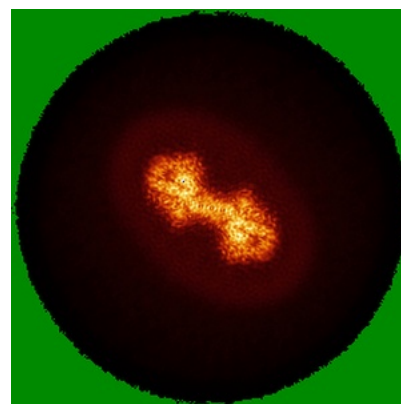
6.4.1 Primary map



X

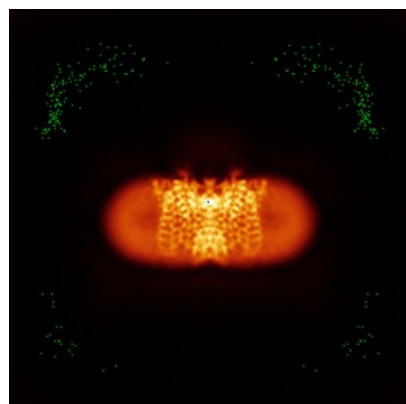


Y

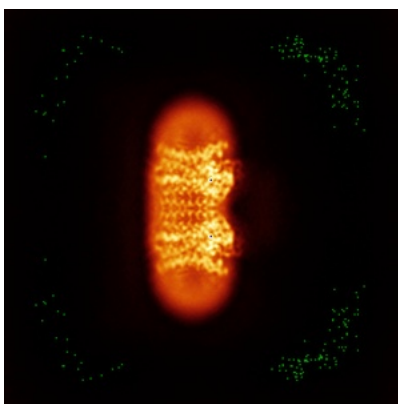


Z

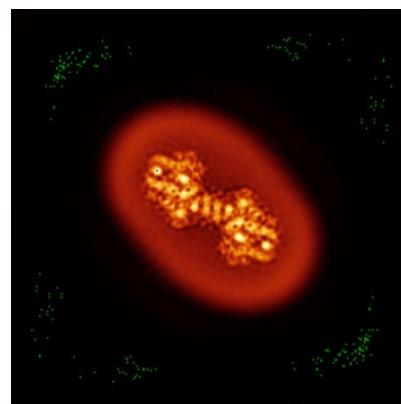
6.4.2 Raw map



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

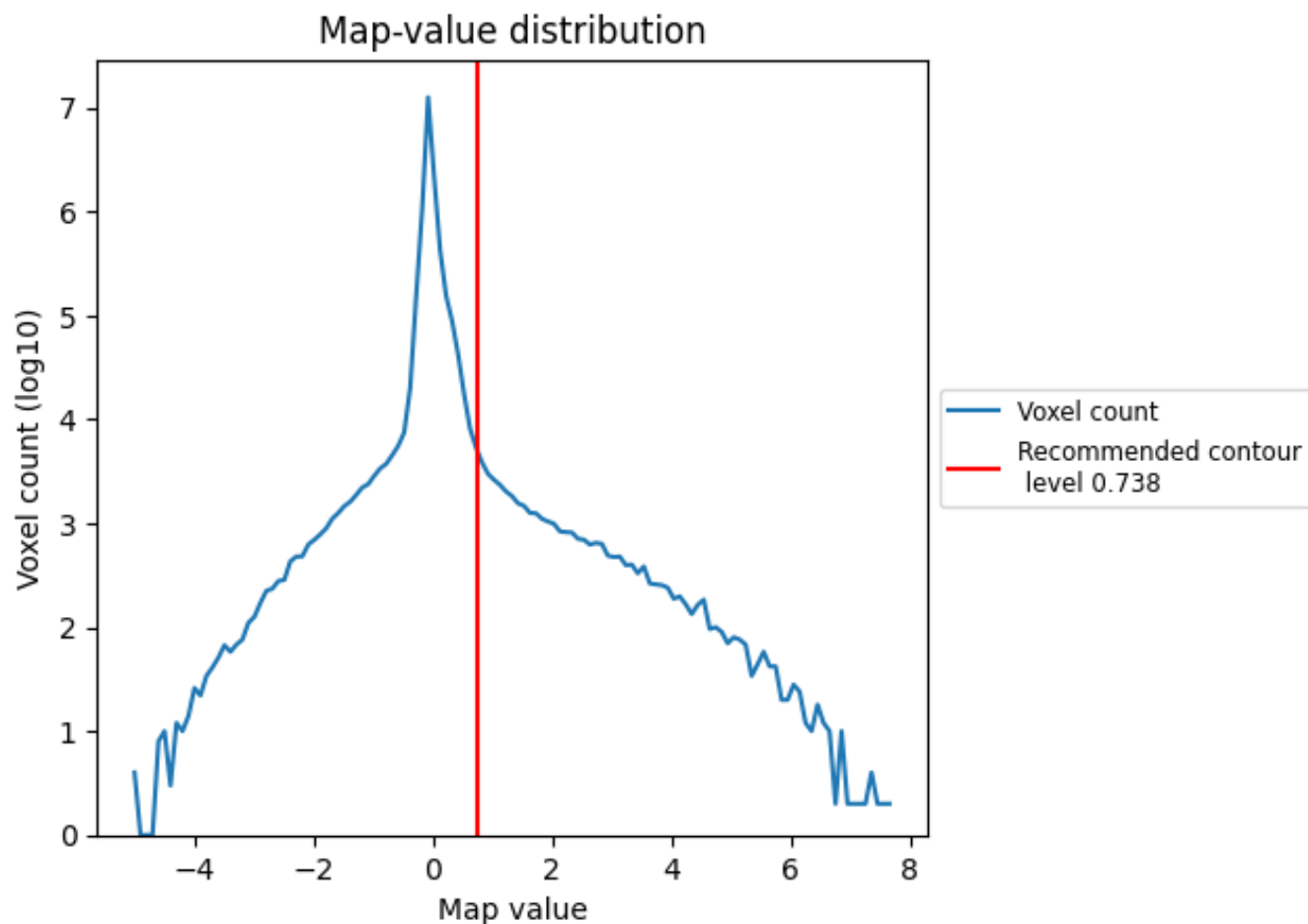
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

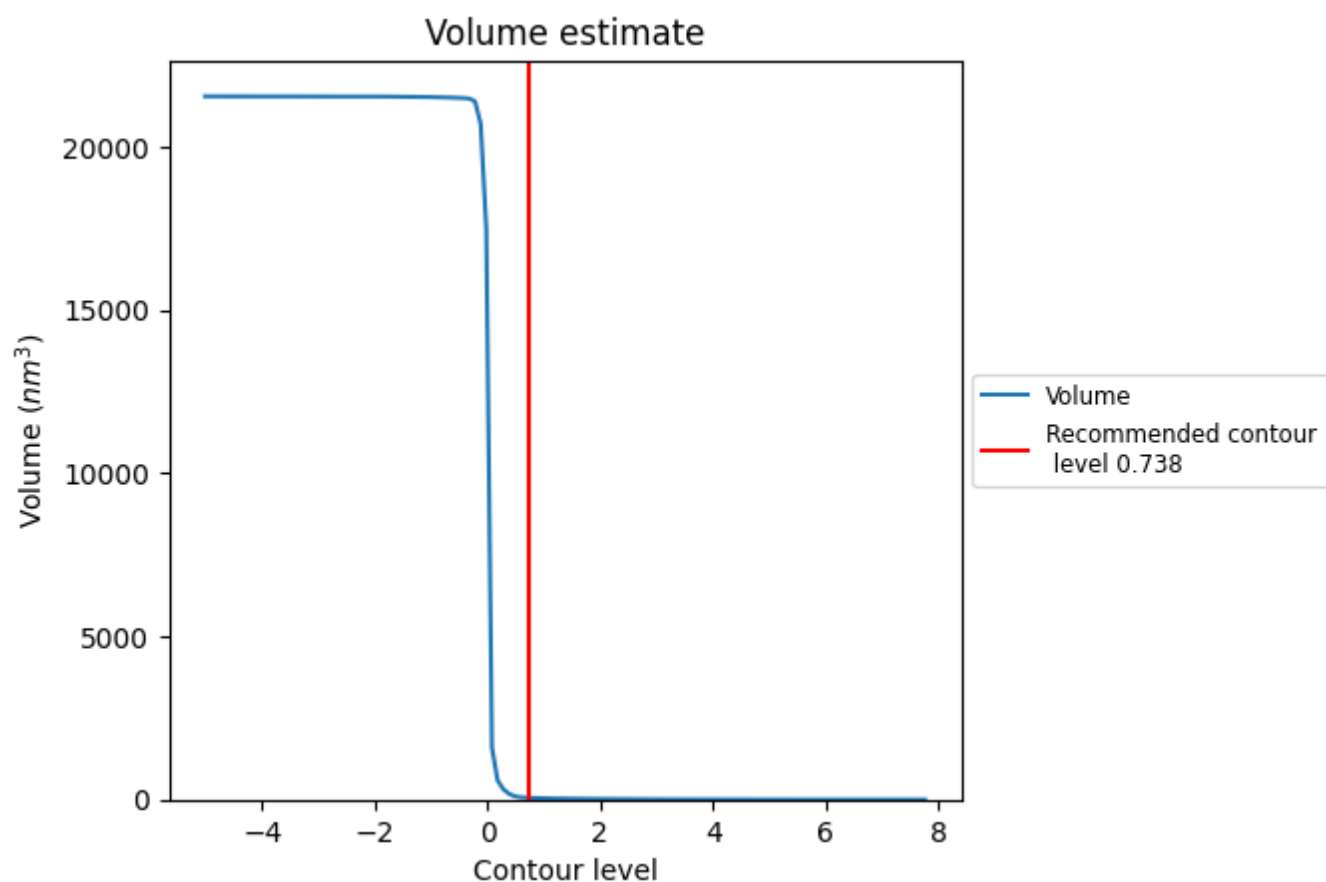
This section contains the results of statistical analysis of the map.

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.

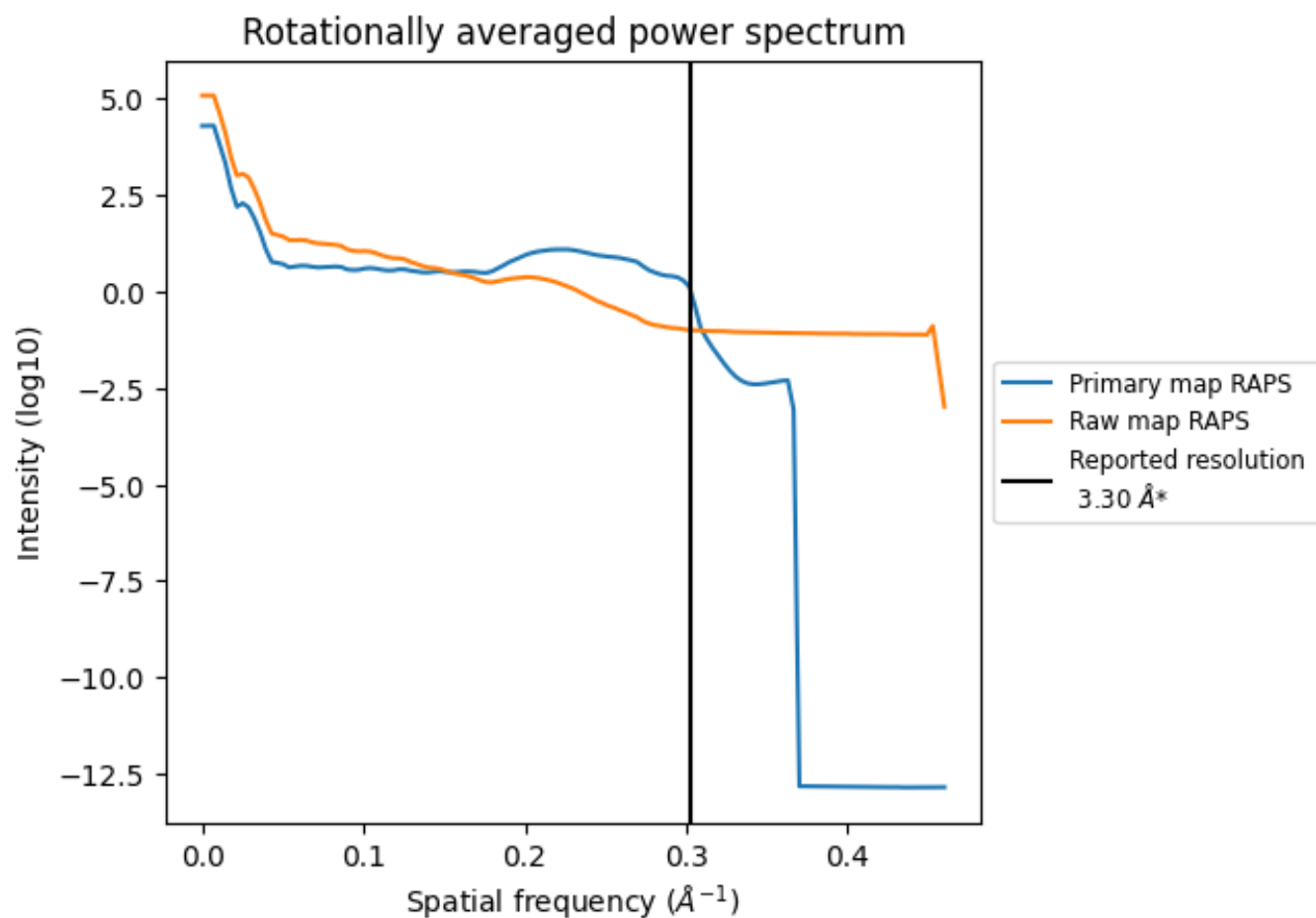
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 52 nm^3 ; this corresponds to an approximate mass of 47 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 ⓘ

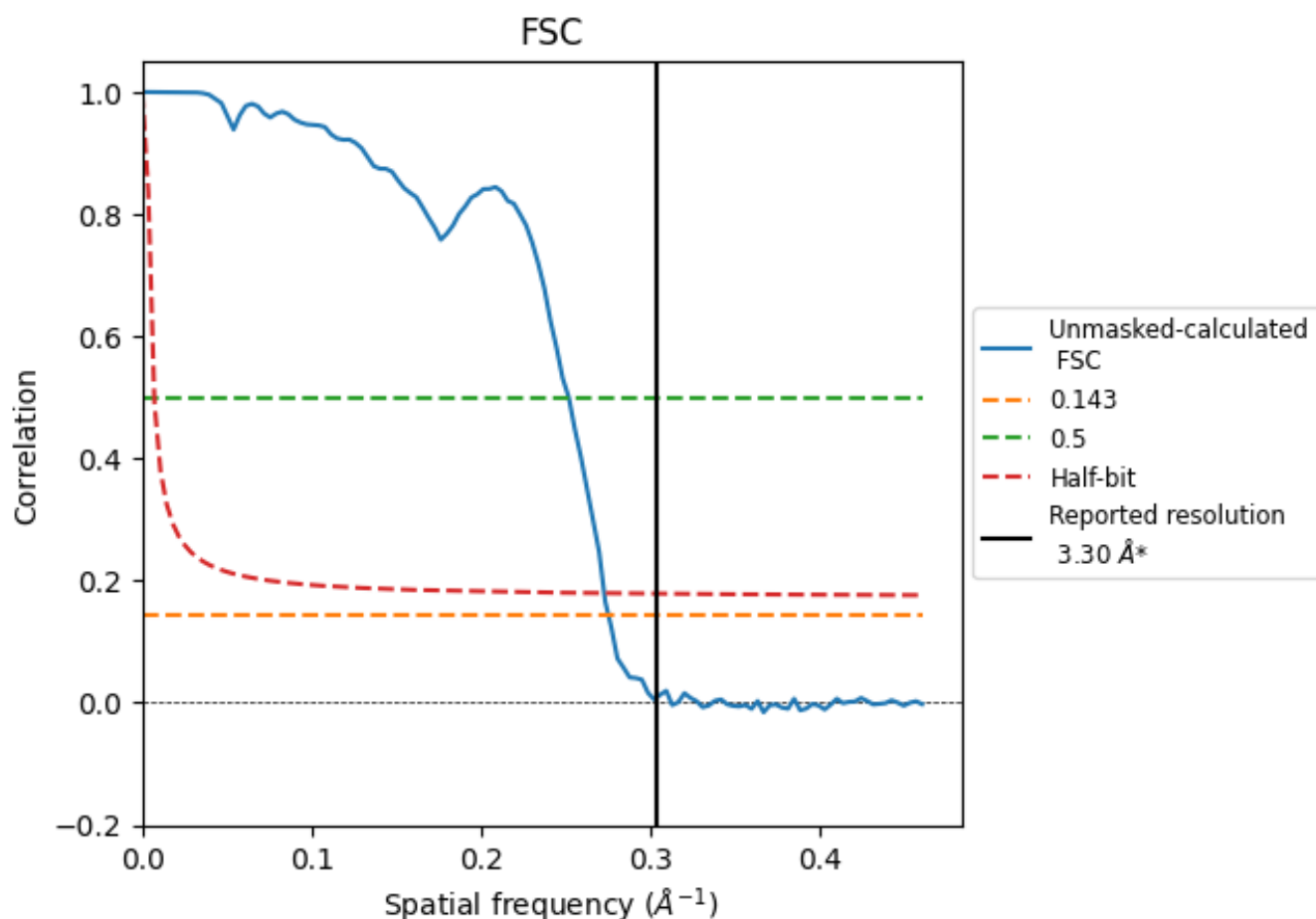


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

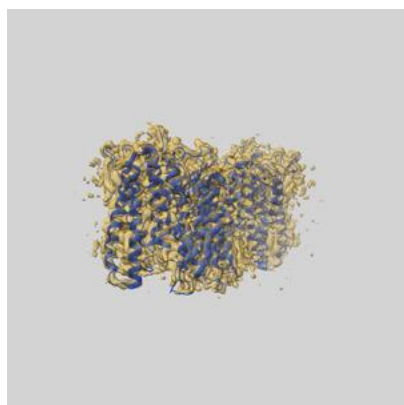
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.64	3.98	3.67

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.64 differs from the reported value 3.3 by more than 10 %

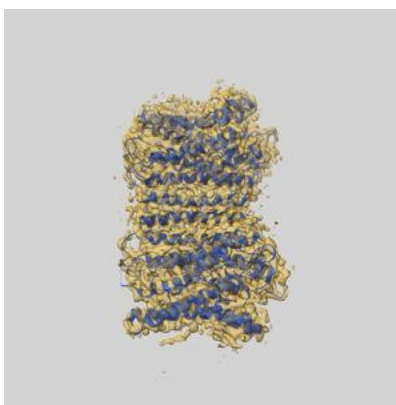
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61254 and PDB model 9J97. Per-residue inclusion information can be found in section [3](#) on page [9](#).

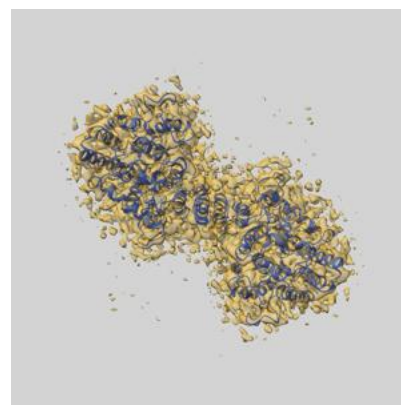
9.1 Map-model overlay [i](#)



X



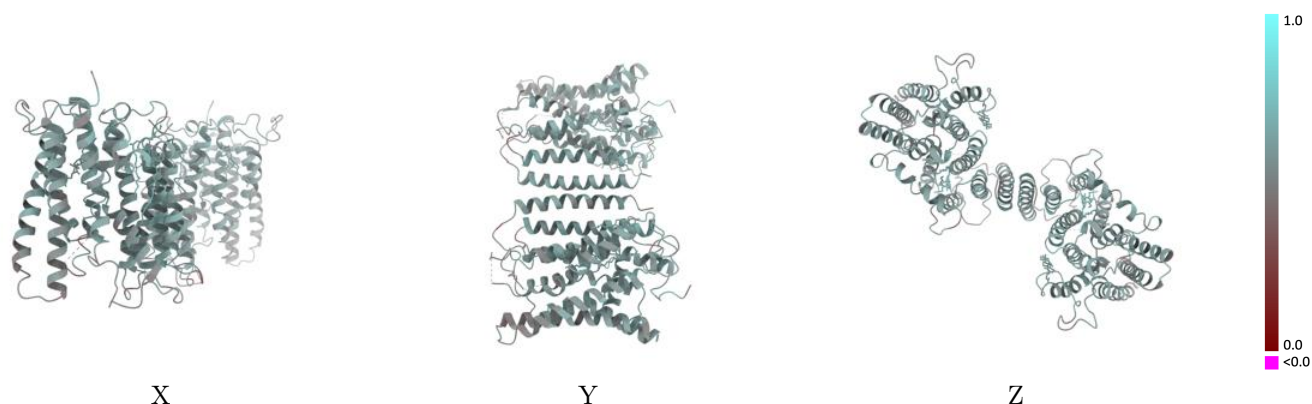
Y



Z

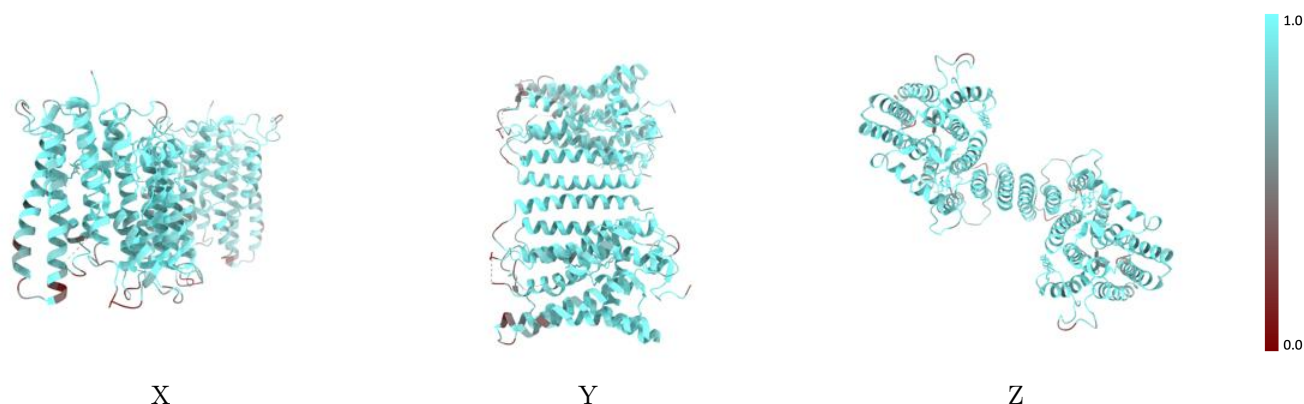
The images above show the 3D surface view of the map at the recommended contour level 0.738 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



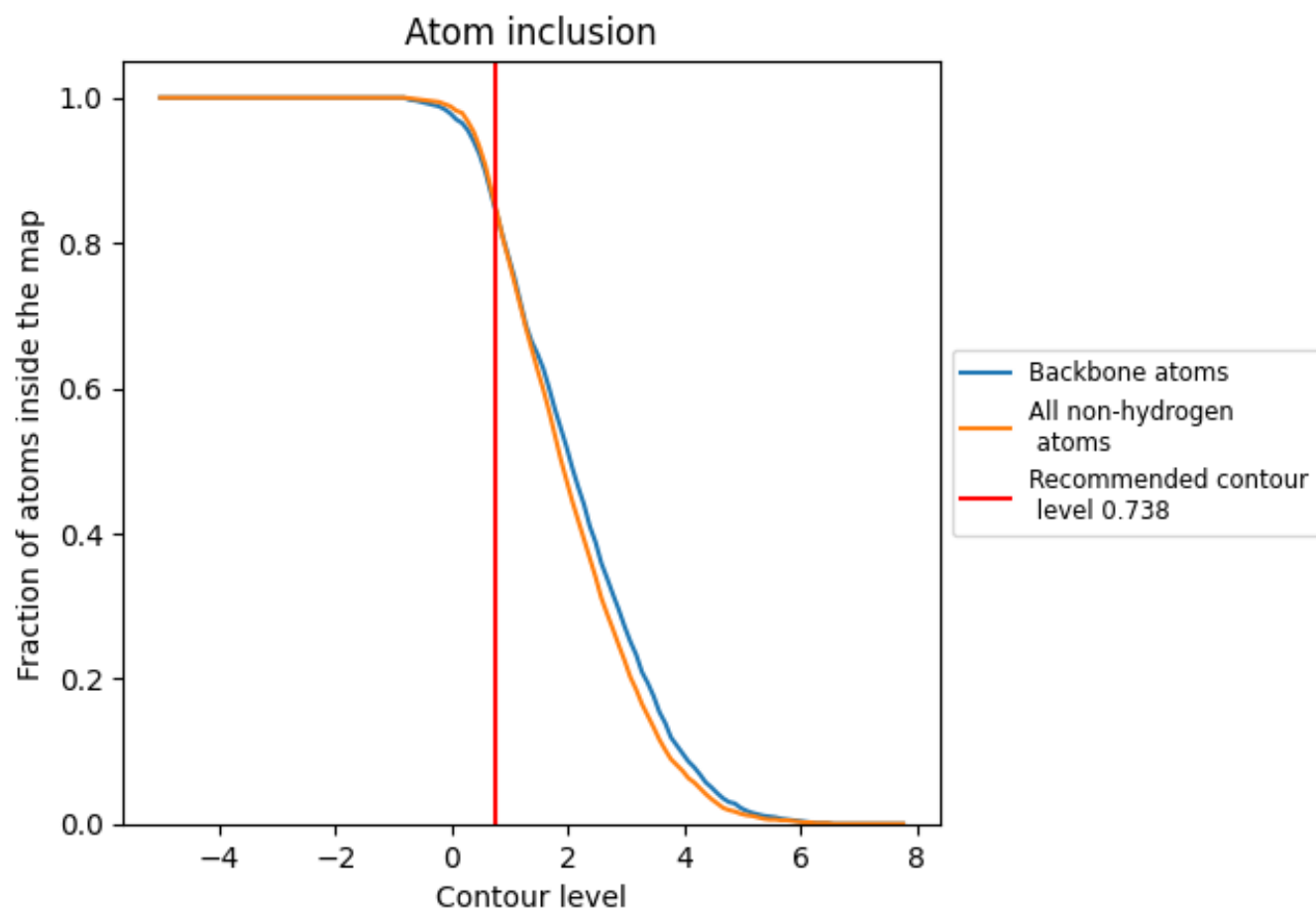
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.738).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.738) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8530	0.5530
A	0.8530	0.5530
B	0.8540	0.5540

