



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 01:54 AM UTC

PDB ID : 8J6M / pdb_00008j6m
EMDB ID : EMD-36008
Title : SIDT1 protein
Authors : Zhang, J.T.; Jiang, D.H.
Deposited on : 2023-04-26
Resolution : 2.77 Å(reported)

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

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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

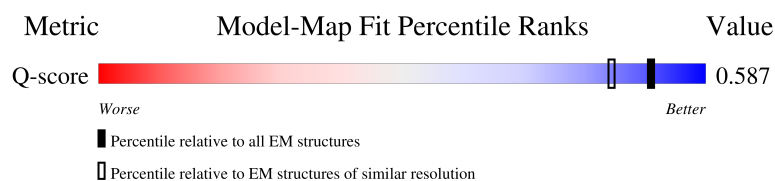
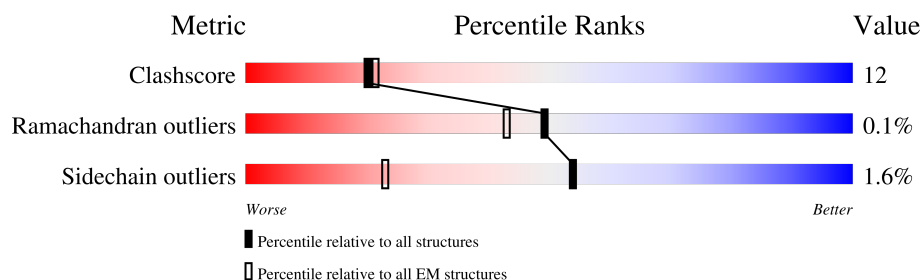
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.77 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	10695 (2.27 - 3.27)

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	1098	
1	B	1098	

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
2	CLR	A	905	-	-	X	-
2	CLR	B	904	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10599 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 Green fluorescent protein, SID1 transmembrane family member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	641	Total	C	N	O	S	1	0
			5165	3416	822	899	28		
1	A	641	Total	C	N	O	S	1	0
			5165	3416	822	899	28		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-270	MET	-	initiating methionine	UNP A0A059PIQ0
B	-269	TYR	-	expression tag	UNP A0A059PIQ0
B	-268	ARG	-	expression tag	UNP A0A059PIQ0
B	-267	MET	-	expression tag	UNP A0A059PIQ0
B	-266	GLN	-	expression tag	UNP A0A059PIQ0
B	-265	LEU	-	expression tag	UNP A0A059PIQ0
B	-264	LEU	-	expression tag	UNP A0A059PIQ0
B	-263	SER	-	expression tag	UNP A0A059PIQ0
B	-262	CYS	-	expression tag	UNP A0A059PIQ0
B	-261	ILE	-	expression tag	UNP A0A059PIQ0
B	-260	ALA	-	expression tag	UNP A0A059PIQ0
B	-259	LEU	-	expression tag	UNP A0A059PIQ0
B	-258	SER	-	expression tag	UNP A0A059PIQ0
B	-257	LEU	-	expression tag	UNP A0A059PIQ0
B	-256	ALA	-	expression tag	UNP A0A059PIQ0
B	-255	LEU	-	expression tag	UNP A0A059PIQ0
B	-254	VAL	-	expression tag	UNP A0A059PIQ0
B	-253	THR	-	expression tag	UNP A0A059PIQ0
B	-252	ASN	-	expression tag	UNP A0A059PIQ0
B	-251	SER	-	expression tag	UNP A0A059PIQ0
B	-250	TRP	-	expression tag	UNP A0A059PIQ0
B	-249	SER	-	expression tag	UNP A0A059PIQ0
B	-248	HIS	-	expression tag	UNP A0A059PIQ0
B	-247	PRO	-	expression tag	UNP A0A059PIQ0
B	-246	GLN	-	expression tag	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-245	PHE	-	expression tag	UNP A0A059PIQ0
B	-244	GLU	-	expression tag	UNP A0A059PIQ0
B	-243	LYS	-	expression tag	UNP A0A059PIQ0
B	-242	GLY	-	expression tag	UNP A0A059PIQ0
B	-241	GLY	-	expression tag	UNP A0A059PIQ0
B	-240	GLY	-	expression tag	UNP A0A059PIQ0
B	-239	SER	-	expression tag	UNP A0A059PIQ0
B	-238	GLY	-	expression tag	UNP A0A059PIQ0
B	-237	GLY	-	expression tag	UNP A0A059PIQ0
B	-236	GLY	-	expression tag	UNP A0A059PIQ0
B	-235	SER	-	expression tag	UNP A0A059PIQ0
B	-234	GLY	-	expression tag	UNP A0A059PIQ0
B	-233	GLY	-	expression tag	UNP A0A059PIQ0
B	-232	SER	-	expression tag	UNP A0A059PIQ0
B	-231	ALA	-	expression tag	UNP A0A059PIQ0
B	-230	TRP	-	expression tag	UNP A0A059PIQ0
B	-229	SER	-	expression tag	UNP A0A059PIQ0
B	-228	HIS	-	expression tag	UNP A0A059PIQ0
B	-227	PRO	-	expression tag	UNP A0A059PIQ0
B	-226	GLN	-	expression tag	UNP A0A059PIQ0
B	-225	PHE	-	expression tag	UNP A0A059PIQ0
B	-224	GLU	-	expression tag	UNP A0A059PIQ0
B	-223	LYS	-	expression tag	UNP A0A059PIQ0
B	-222	SER	-	expression tag	UNP A0A059PIQ0
B	-194	ARG	SER	conflict	UNP A0A059PIQ0
B	-152	SER	ALA	conflict	UNP A0A059PIQ0
B	-144	ARG	GLN	conflict	UNP A0A059PIQ0
B	-18	VAL	ALA	conflict	UNP A0A059PIQ0
B	13	GLU	-	linker	UNP A0A059PIQ0
B	14	VAL	-	linker	UNP A0A059PIQ0
B	15	LEU	-	linker	UNP A0A059PIQ0
B	16	PHE	-	linker	UNP A0A059PIQ0
B	17	GLN	-	linker	UNP A0A059PIQ0
B	18	GLY	-	linker	UNP A0A059PIQ0
B	19	PRO	-	linker	UNP A0A059PIQ0
A	-270	MET	-	initiating methionine	UNP A0A059PIQ0
A	-269	TYR	-	expression tag	UNP A0A059PIQ0
A	-268	ARG	-	expression tag	UNP A0A059PIQ0
A	-267	MET	-	expression tag	UNP A0A059PIQ0
A	-266	GLN	-	expression tag	UNP A0A059PIQ0
A	-265	LEU	-	expression tag	UNP A0A059PIQ0
A	-264	LEU	-	expression tag	UNP A0A059PIQ0

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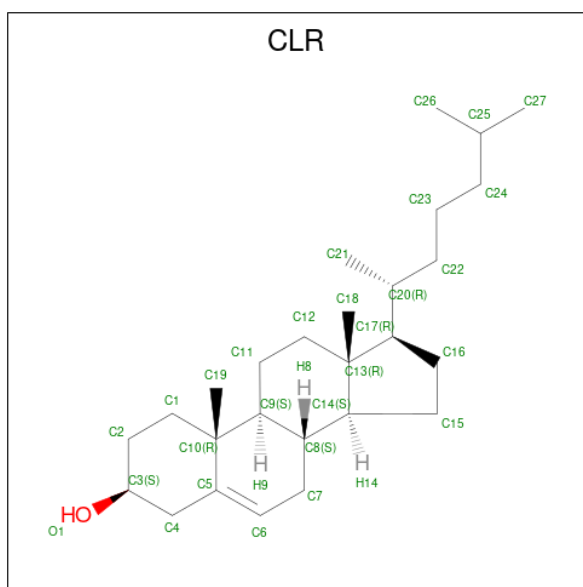
Chain	Residue	Modelled	Actual	Comment	Reference
A	-263	SER	-	expression tag	UNP A0A059PIQ0
A	-262	CYS	-	expression tag	UNP A0A059PIQ0
A	-261	ILE	-	expression tag	UNP A0A059PIQ0
A	-260	ALA	-	expression tag	UNP A0A059PIQ0
A	-259	LEU	-	expression tag	UNP A0A059PIQ0
A	-258	SER	-	expression tag	UNP A0A059PIQ0
A	-257	LEU	-	expression tag	UNP A0A059PIQ0
A	-256	ALA	-	expression tag	UNP A0A059PIQ0
A	-255	LEU	-	expression tag	UNP A0A059PIQ0
A	-254	VAL	-	expression tag	UNP A0A059PIQ0
A	-253	THR	-	expression tag	UNP A0A059PIQ0
A	-252	ASN	-	expression tag	UNP A0A059PIQ0
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A	-250	TRP	-	expression tag	UNP A0A059PIQ0
A	-249	SER	-	expression tag	UNP A0A059PIQ0
A	-248	HIS	-	expression tag	UNP A0A059PIQ0
A	-247	PRO	-	expression tag	UNP A0A059PIQ0
A	-246	GLN	-	expression tag	UNP A0A059PIQ0
A	-245	PHE	-	expression tag	UNP A0A059PIQ0
A	-244	GLU	-	expression tag	UNP A0A059PIQ0
A	-243	LYS	-	expression tag	UNP A0A059PIQ0
A	-242	GLY	-	expression tag	UNP A0A059PIQ0
A	-241	GLY	-	expression tag	UNP A0A059PIQ0
A	-240	GLY	-	expression tag	UNP A0A059PIQ0
A	-239	SER	-	expression tag	UNP A0A059PIQ0
A	-238	GLY	-	expression tag	UNP A0A059PIQ0
A	-237	GLY	-	expression tag	UNP A0A059PIQ0
A	-236	GLY	-	expression tag	UNP A0A059PIQ0
A	-235	SER	-	expression tag	UNP A0A059PIQ0
A	-234	GLY	-	expression tag	UNP A0A059PIQ0
A	-233	GLY	-	expression tag	UNP A0A059PIQ0
A	-232	SER	-	expression tag	UNP A0A059PIQ0
A	-231	ALA	-	expression tag	UNP A0A059PIQ0
A	-230	TRP	-	expression tag	UNP A0A059PIQ0
A	-229	SER	-	expression tag	UNP A0A059PIQ0
A	-228	HIS	-	expression tag	UNP A0A059PIQ0
A	-227	PRO	-	expression tag	UNP A0A059PIQ0
A	-226	GLN	-	expression tag	UNP A0A059PIQ0
A	-225	PHE	-	expression tag	UNP A0A059PIQ0
A	-224	GLU	-	expression tag	UNP A0A059PIQ0
A	-223	LYS	-	expression tag	UNP A0A059PIQ0
A	-222	SER	-	expression tag	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-194	ARG	SER	conflict	UNP A0A059PIQ0
A	-152	SER	ALA	conflict	UNP A0A059PIQ0
A	-144	ARG	GLN	conflict	UNP A0A059PIQ0
A	-18	VAL	ALA	conflict	UNP A0A059PIQ0
A	13	GLU	-	linker	UNP A0A059PIQ0
A	14	VAL	-	linker	UNP A0A059PIQ0
A	15	LEU	-	linker	UNP A0A059PIQ0
A	16	PHE	-	linker	UNP A0A059PIQ0
A	17	GLN	-	linker	UNP A0A059PIQ0
A	18	GLY	-	linker	UNP A0A059PIQ0
A	19	PRO	-	linker	UNP A0A059PIQ0

- Molecule 2 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



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

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

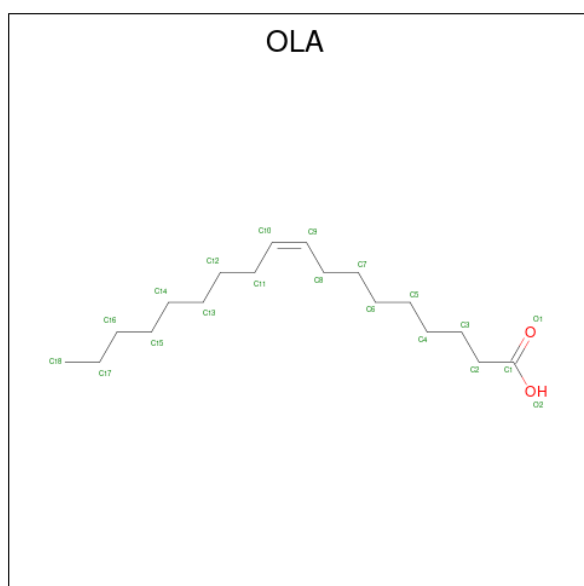
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	A	1	Total	Zn	0
			1	1	

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Na	0
			1	1	

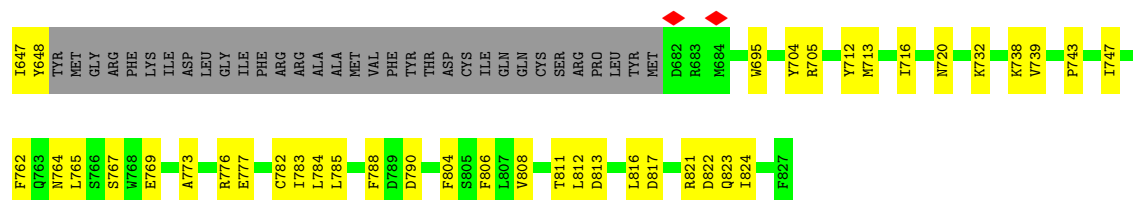
- Molecule 5 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂) (labeled as "Ligand of Interest" by depositor).



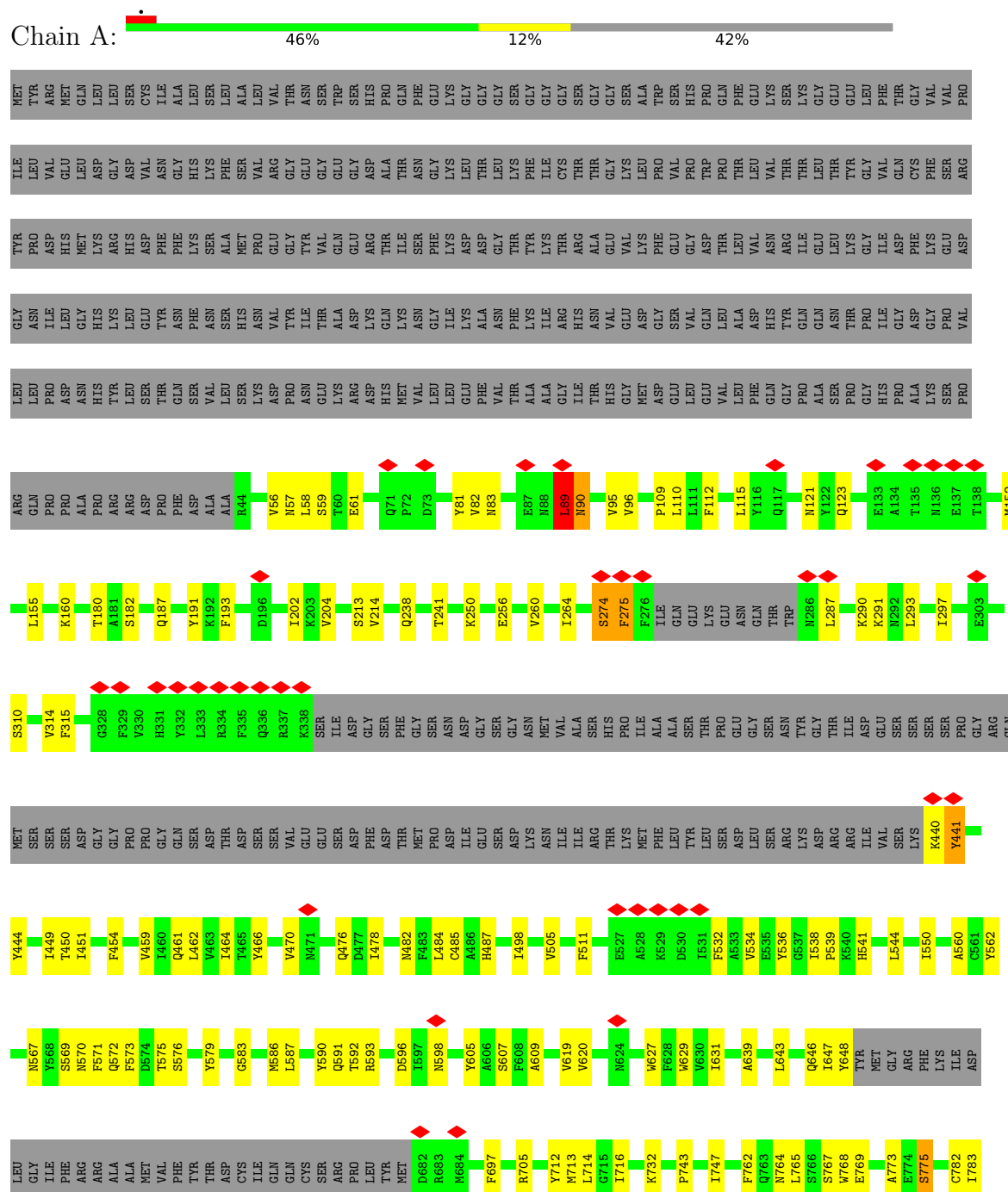
Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	C	O	0
			20	18	2	
5	A	1	Total	C	O	0
			20	18	2	

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	B	2	Total	O	0
			2	2	



- Molecule 1: Green fluorescent protein, SID1 transmembrane family member 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145765	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	7.900	Depositor
Minimum map value	-5.857	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.153	Depositor
Recommended contour level	0.962	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/5308	0.75	14/7222 (0.2%)
1	B	0.46	0/5308	0.66	16/7222 (0.2%)
All	All	0.53	0/10616	0.71	30/14444 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	534	VAL	N-CA-C	9.51	119.47	110.53
1	A	274	SER	N-CA-C	8.98	121.07	111.28
1	B	534	VAL	N-CA-C	8.92	118.91	110.53
1	B	275	PHE	N-CA-C	7.73	119.77	110.19
1	A	155	LEU	N-CA-C	-7.44	98.20	110.17
1	B	155	LEU	N-CA-C	-7.41	98.23	110.17
1	A	478	ILE	N-CA-C	7.02	117.78	110.62
1	B	315	PHE	N-CA-C	6.91	118.81	111.28
1	A	315	PHE	N-CA-C	6.87	118.77	111.28
1	B	598	ASN	N-CA-C	6.80	118.34	111.07
1	B	576	SER	N-CA-C	6.42	118.27	111.28
1	A	576	SER	N-CA-C	6.29	118.13	111.28
1	B	89	LEU	N-CA-C	-6.16	105.42	113.17
1	A	89	LEU	N-CA-C	-6.12	105.46	113.17
1	B	739	VAL	N-CA-C	-6.11	98.83	107.75
1	A	579	TYR	N-CA-C	-6.11	104.18	111.69
1	B	59	SER	N-CA-C	6.02	117.92	111.36
1	A	59	SER	N-CA-C	6.00	117.89	111.36
1	B	61	GLU	N-CA-C	-5.83	99.91	109.40
1	A	61	GLU	N-CA-C	-5.79	99.96	109.40
1	B	441	TYR	N-CA-C	5.74	116.66	108.74
1	A	441	TYR	N-CA-C	5.71	116.62	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	ASN	N-CA-C	-5.68	105.08	112.23
1	A	90	ASN	N-CA-C	-5.67	105.09	112.23
1	B	704	TYR	N-CA-C	5.62	117.49	111.36
1	A	123	GLN	N-CA-C	5.35	118.02	111.82
1	B	738	LYS	N-CA-C	5.22	116.83	110.41
1	B	599	ALA	N-CA-C	5.20	117.52	111.02
1	A	598	ASN	N-CA-C	5.07	116.81	111.28
1	B	573	PHE	N-CA-C	5.05	118.54	112.38

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	5165	0	5134	116	0
1	B	5165	0	5134	136	0
2	A	112	0	184	40	0
2	B	112	0	184	38	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	1	0	0	0	0
5	A	20	0	33	6	0
5	B	20	0	33	3	0
6	B	2	0	0	0	0
All	All	10599	0	10702	262	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 12.

All (262) 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)
2:A:904:CLR:C19	2:A:905:CLR:H122	1.66	1.23
2:A:904:CLR:C18	2:A:905:CLR:H213	1.76	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:904:CLR:H191	2:A:905:CLR:C12	1.87	1.04
2:A:904:CLR:H183	2:A:905:CLR:H213	1.03	1.02
2:A:904:CLR:C19	2:A:905:CLR:C12	2.39	1.01
1:B:101:LYS:NZ	1:A:90:ASN:HA	1.76	1.00
1:A:646:GLN:HG3	2:A:905:CLR:H191	1.44	0.99
1:B:101:LYS:HZ3	1:A:90:ASN:HA	1.24	0.99
1:B:225:TYR:HE2	1:B:234:ASN:HD22	1.10	0.94
2:A:904:CLR:H191	2:A:905:CLR:H122	0.94	0.93
2:A:904:CLR:H183	2:A:905:CLR:C21	1.98	0.92
1:B:101:LYS:HZ3	1:A:90:ASN:CA	1.85	0.89
1:A:81[B]:TYR:HE2	1:A:83:ASN:HD22	1.19	0.86
1:A:646:GLN:HG3	2:A:905:CLR:C19	2.06	0.86
1:A:81[B]:TYR:CE2	1:A:83:ASN:ND2	2.42	0.85
1:B:607:SER:OG	2:B:903:CLR:H151	1.75	0.85
1:A:81[B]:TYR:HE2	1:A:83:ASN:ND2	1.75	0.83
1:B:225:TYR:HE2	1:B:234:ASN:ND2	1.79	0.81
1:B:454:PHE:CD2	1:A:454:PHE:CD2	2.69	0.81
1:A:586:MET:SD	2:A:905:CLR:H262	2.22	0.79
1:A:583:GLY:HA2	2:A:905:CLR:H273	1.64	0.79
1:B:225:TYR:CE2	1:B:234:ASN:ND2	2.52	0.78
1:A:646:GLN:CG	2:A:905:CLR:H191	2.13	0.78
1:B:242:LYS:HB2	1:B:777:GLU:HG2	1.67	0.77
1:B:485:CYS:SG	1:B:487:HIS:NE2	2.61	0.73
1:B:56:VAL:HG11	1:B:150:ALA:HA	1.72	0.72
1:B:454:PHE:CD2	1:A:454:PHE:HD2	2.07	0.71
1:A:607:SER:OG	2:A:903:CLR:C11	2.39	0.70
1:B:640:SER:HB3	2:B:904:CLR:H271	1.73	0.70
1:B:454:PHE:HD2	1:A:454:PHE:CD2	2.07	0.69
1:B:607:SER:CB	2:B:903:CLR:H151	2.22	0.69
1:B:541:HIS:HB2	1:B:591:GLN:HE22	1.58	0.69
1:B:238:GLN:HG2	1:B:476:GLN:HB2	1.76	0.68
1:A:583:GLY:HA2	2:A:905:CLR:C27	2.24	0.68
1:B:56:VAL:HG13	1:B:60:THR:O	1.93	0.68
1:A:590:TYR:CD2	2:A:905:CLR:H151	2.29	0.67
1:B:640:SER:HB3	2:B:904:CLR:C27	2.24	0.67
1:B:101:LYS:NZ	1:A:90:ASN:HD22	1.94	0.66
1:A:583:GLY:HA3	2:A:904:CLR:H242	1.78	0.66
1:B:605:TYR:CZ	1:A:450:THR:HG22	2.32	0.65
1:B:260:VAL:HG12	1:B:262:PHE:CZ	2.32	0.65
1:A:607:SER:OG	2:A:903:CLR:H112	1.95	0.65
1:A:593:ARG:HB3	1:A:826:VAL:HG13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:PHE:HD1	1:A:609:ALA:HB2	1.62	0.64
1:B:100:GLN:NE2	1:A:90:ASN:O	2.29	0.64
1:B:643:LEU:HD22	2:B:904:CLR:H242	1.79	0.64
1:A:83:ASN:OD1	1:A:160:LYS:HB2	1.98	0.64
1:A:238:GLN:HG2	1:A:476:GLN:HB2	1.79	0.64
1:B:603:SER:HB2	2:B:903:CLR:H6	1.80	0.64
1:B:155:LEU:N	1:B:155:LEU:HD12	2.13	0.63
1:B:607:SER:OG	2:B:903:CLR:C15	2.44	0.63
1:B:643:LEU:CD1	2:B:904:CLR:H161	2.29	0.63
1:A:590:TYR:CE2	2:A:905:CLR:H151	2.33	0.63
1:B:609:ALA:HB2	1:A:454:PHE:HD1	1.62	0.63
1:B:101:LYS:HZ2	1:A:90:ASN:HD22	1.44	0.62
1:A:646:GLN:OE1	2:A:905:CLR:C19	2.47	0.62
1:B:605:TYR:OH	1:A:451:ILE:HA	1.99	0.61
1:B:498:ILE:HG23	1:B:560:ALA:HB1	1.80	0.61
1:B:193:PHE:HB2	1:B:256:GLU:HB3	1.82	0.61
1:B:605:TYR:HE2	1:A:454:PHE:CD1	2.19	0.60
1:B:213:SER:HB2	1:B:264:ILE:HD13	1.83	0.60
1:A:627:TRP:O	1:A:631:ILE:HD12	2.02	0.59
1:A:202:ILE:HG12	1:A:297:ILE:HD13	1.85	0.59
1:A:732:LYS:NZ	1:A:813:ASP:OD1	2.30	0.59
1:B:627:TRP:O	1:B:631:ILE:HD12	2.02	0.59
1:B:202:ILE:HG12	1:B:297:ILE:HD13	1.85	0.59
2:B:903:CLR:H182	2:B:904:CLR:H112	1.85	0.59
1:A:193:PHE:HB2	1:A:256:GLU:HB3	1.85	0.59
2:A:902:CLR:H161	2:A:903:CLR:H17	1.85	0.58
1:B:101:LYS:NZ	1:A:90:ASN:CA	2.56	0.58
1:A:498:ILE:HG23	1:A:560:ALA:HB1	1.85	0.58
1:A:213:SER:HB2	1:A:264:ILE:HD13	1.83	0.58
1:B:239:SER:O	1:B:776:ARG:NH1	2.37	0.57
1:B:643:LEU:HB2	2:B:904:CLR:H162	1.86	0.57
1:A:590:TYR:CE2	2:A:905:CLR:H72	2.38	0.57
2:A:904:CLR:C19	2:A:905:CLR:C11	2.82	0.57
1:B:643:LEU:HD13	2:B:904:CLR:H161	1.85	0.57
1:B:101:LYS:NZ	1:A:90:ASN:ND2	2.53	0.57
2:A:902:CLR:H151	2:A:903:CLR:H14	1.87	0.57
1:A:784:LEU:HG	1:A:785:LEU:HD12	1.87	0.56
1:B:784:LEU:HG	1:B:785:LEU:HD12	1.87	0.56
1:A:590:TYR:CZ	2:A:905:CLR:H72	2.40	0.56
1:A:697:PHE:CZ	5:A:906:OLA:H10	2.40	0.56
1:B:464:ILE:CD1	1:A:620:VAL:HG11	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:TYR:HD1	1:B:570:ASN:HB3	1.71	0.55
1:A:646:GLN:OE1	2:A:905:CLR:H191	2.05	0.55
1:B:155:LEU:N	1:B:155:LEU:CD1	2.69	0.55
1:B:260:VAL:HG12	1:B:262:PHE:CE1	2.42	0.55
1:B:214:VAL:HG23	1:B:265:LYS:HE3	1.87	0.55
1:A:643:LEU:HG	1:A:647:ILE:HD13	1.88	0.55
1:B:712:TYR:HA	5:B:907:OLA:H9	1.89	0.55
1:B:541:HIS:O	1:B:588:LYS:NZ	2.40	0.54
2:B:903:CLR:C18	2:B:904:CLR:C11	2.84	0.54
1:B:260:VAL:CG1	1:B:262:PHE:CZ	2.90	0.54
1:B:454:PHE:HD2	1:A:454:PHE:HD2	1.48	0.54
1:A:646:GLN:CD	2:A:905:CLR:C19	2.81	0.54
1:A:646:GLN:CD	2:A:905:CLR:H191	2.33	0.54
1:A:712:TYR:HA	5:A:906:OLA:H9	1.89	0.54
1:B:101:LYS:HZ2	1:A:90:ASN:HA	1.66	0.53
1:B:607:SER:HA	2:B:903:CLR:H151	1.90	0.53
1:B:56:VAL:HG11	1:B:150:ALA:CA	2.38	0.53
1:A:646:GLN:CG	2:A:905:CLR:C19	2.78	0.53
1:B:182:SER:HB2	1:B:290:LYS:HD2	1.91	0.53
1:A:182:SER:HB2	1:A:290:LYS:HD2	1.91	0.53
1:B:607:SER:CA	2:B:903:CLR:H151	2.39	0.53
2:A:904:CLR:H192	2:A:905:CLR:H112	1.90	0.52
2:B:903:CLR:H242	2:B:904:CLR:H211	1.92	0.52
1:B:462:LEU:HD13	1:A:462:LEU:HD13	1.90	0.52
1:B:518:ARG:HH12	1:B:811:THR:HG22	1.73	0.52
1:B:536:TYR:HB3	1:B:817:ASP:O	2.09	0.52
1:A:562:TYR:HD1	1:A:570:ASN:HB3	1.75	0.52
1:A:646:GLN:OE1	2:A:905:CLR:H192	2.08	0.52
1:B:732:LYS:NZ	1:B:813:ASP:OD1	2.30	0.52
1:A:743:PRO:O	1:A:747:ILE:HG13	2.10	0.52
1:B:822:ASP:OD1	1:B:823:GLN:N	2.42	0.52
2:A:904:CLR:H192	2:A:905:CLR:C11	2.39	0.52
1:B:193:PHE:HB3	1:B:250:LYS:HE2	1.92	0.51
1:B:440:LYS:HA	1:B:544:LEU:HG	1.92	0.51
1:A:532:PHE:HA	1:A:536:TYR:HB2	1.93	0.51
1:B:743:PRO:O	1:B:747:ILE:HG13	2.10	0.51
1:B:180:THR:O	1:B:187:GLN:NE2	2.43	0.51
1:A:180:THR:O	1:A:187:GLN:NE2	2.44	0.51
1:B:821:ARG:HA	1:B:824:ILE:HD12	1.92	0.50
1:B:713:MET:HE3	1:B:716:ILE:HD12	1.93	0.50
1:A:538:ILE:HD13	1:A:592:THR:HG22	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LYS:HA	1:A:544:LEU:HG	1.93	0.50
1:A:713:MET:HE3	1:A:716:ILE:HD12	1.93	0.50
1:B:469:VAL:HG12	1:B:478:ILE:HD13	1.93	0.50
1:B:620:VAL:HG11	1:A:464:ILE:CD1	2.41	0.50
1:A:808:VAL:O	1:A:812:LEU:HB2	2.12	0.50
1:B:808:VAL:O	1:B:812:LEU:HB2	2.12	0.49
1:B:782:CYS:HB2	1:B:788:PHE:C	2.38	0.49
1:A:782:CYS:HB2	1:A:788:PHE:C	2.38	0.49
1:B:75:VAL:HG13	1:B:133:GLU:HG2	1.93	0.49
1:B:96:VAL:HG11	1:A:96:VAL:HG21	1.95	0.49
1:B:562:TYR:CD1	1:B:570:ASN:HB3	2.48	0.49
1:B:640:SER:HA	2:B:904:CLR:H272	1.93	0.49
1:B:605:TYR:CZ	1:A:605:TYR:CE2	3.01	0.49
2:B:902:CLR:H221	2:B:902:CLR:H162	1.58	0.48
1:B:572:GLN:HE22	1:A:461:GLN:HE22	1.59	0.48
1:B:455:TYR:OH	1:B:572:GLN:HG3	2.13	0.48
1:B:607:SER:OG	2:B:903:CLR:H72	2.14	0.48
1:B:640:SER:CB	2:B:904:CLR:C27	2.90	0.48
1:B:716:ILE:O	1:B:720:ASN:ND2	2.46	0.48
1:A:193:PHE:HB3	1:A:250:LYS:HE2	1.94	0.48
1:A:213:SER:OG	1:A:214:VAL:N	2.47	0.48
1:A:449:ILE:HD11	1:A:550:ILE:HG12	1.95	0.48
1:B:640:SER:CA	2:B:904:CLR:C27	2.91	0.48
2:A:902:CLR:H221	2:A:902:CLR:H162	1.58	0.47
1:B:56:VAL:HG11	1:B:151:SER:N	2.29	0.47
1:B:241:THR:HG23	1:B:773:ALA:HB1	1.97	0.47
1:B:98:ARG:HG2	1:B:146:PHE:HB2	1.96	0.47
1:B:310:SER:HA	1:B:499:LEU:HD21	1.96	0.47
1:A:647:ILE:HG13	1:A:648:TYR:CE1	2.50	0.47
1:B:637:VAL:HG22	1:B:695:TRP:CD1	2.49	0.47
2:B:901:CLR:H6	2:B:903:CLR:H191	1.97	0.47
1:B:57:ASN:OD1	1:B:57:ASN:N	2.47	0.47
1:A:57:ASN:OD1	1:A:57:ASN:N	2.47	0.47
1:B:643:LEU:HB2	2:B:904:CLR:C16	2.44	0.47
2:A:904:CLR:C19	2:A:905:CLR:H112	2.45	0.47
1:B:544:LEU:HD11	1:B:587:LEU:HD22	1.97	0.47
1:B:647:ILE:HG13	1:B:648:TYR:CD2	2.50	0.46
1:B:640:SER:HA	2:B:904:CLR:C27	2.45	0.46
2:B:903:CLR:C18	2:B:904:CLR:H112	2.42	0.46
1:B:275:PHE:O	1:B:276:PHE:HB3	2.15	0.46
1:A:241:THR:HG23	1:A:773:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:TYR:CD1	1:A:570:ASN:HB3	2.51	0.46
1:A:482:ASN:O	1:A:484:LEU:N	2.44	0.46
1:B:101:LYS:HZ3	1:A:90:ASN:CB	2.28	0.46
5:A:906:OLA:H71	5:A:906:OLA:H42	1.55	0.46
1:B:196:ASP:OD1	1:B:197:VAL:N	2.49	0.45
1:B:762:PHE:HD1	5:B:907:OLA:H41	1.82	0.45
5:B:907:OLA:H42	5:B:907:OLA:H71	1.55	0.45
1:B:532:PHE:HA	1:B:536:TYR:HD1	1.81	0.45
1:B:213:SER:OG	1:B:214:VAL:N	2.47	0.45
1:A:762:PHE:HD1	5:A:906:OLA:H41	1.81	0.45
2:A:904:CLR:H221	2:A:904:CLR:H162	1.45	0.45
2:B:901:CLR:H9	2:B:902:CLR:H152	1.99	0.45
2:B:903:CLR:H183	2:B:903:CLR:H20	1.80	0.45
1:A:539:PRO:HG3	1:A:821:ARG:HD3	1.98	0.45
1:B:441:TYR:O	1:B:444:TYR:HB2	2.17	0.45
1:B:720:ASN:ND2	2:B:904:CLR:H25	2.32	0.44
1:B:767:SER:HB2	1:B:769:GLU:OE2	2.17	0.44
1:A:767:SER:HB2	1:A:769:GLU:OE2	2.17	0.44
1:B:196:ASP:OD1	1:B:197:VAL:HG23	2.17	0.44
1:A:310:SER:O	1:A:314:VAL:HG23	2.16	0.44
1:B:58:LEU:HD13	1:B:152:MET:HG2	1.98	0.44
1:B:310:SER:O	1:B:314:VAL:HG23	2.16	0.44
1:A:82:VAL:HG21	1:A:95:VAL:HG11	2.00	0.44
1:A:541:HIS:HB2	1:A:591:GLN:HE22	1.81	0.44
1:A:639:ALA:HB1	2:A:902:CLR:H25	1.99	0.44
2:A:905:CLR:H232	2:A:905:CLR:H211	1.68	0.44
1:A:58:LEU:HD13	1:A:152:MET:HG2	1.98	0.44
1:A:767:SER:H	1:A:775:SER:HB3	1.82	0.44
1:A:783:ILE:HD13	1:A:783:ILE:HA	1.83	0.44
1:B:89:LEU:HD12	1:B:109:PRO:HG2	1.99	0.44
2:B:901:CLR:H162	2:B:901:CLR:H222	1.36	0.44
1:B:121:ASN:H	1:B:286:ASN:HA	1.83	0.44
1:B:643:LEU:HB2	2:B:904:CLR:H222	1.99	0.44
2:B:901:CLR:H41	2:B:902:CLR:C6	2.48	0.44
1:A:441:TYR:O	1:A:444:TYR:HB2	2.17	0.44
1:B:492:LEU:HD13	1:B:498:ILE:HD12	1.99	0.44
1:A:629:TRP:CD1	1:A:705:ARG:HG2	2.53	0.44
1:B:102:GLU:HG2	1:B:103:VAL:N	2.32	0.43
1:B:537:GLY:HA2	1:B:816:LEU:O	2.18	0.43
1:A:485:CYS:SG	1:A:487:HIS:NE2	2.91	0.43
1:B:765:LEU:HD11	1:B:790:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HD12	1:A:109:PRO:HG2	1.99	0.43
1:B:562:TYR:HB2	1:B:573:PHE:HB2	1.99	0.43
1:A:697:PHE:HZ	5:A:906:OLA:H10	1.83	0.43
1:A:571:PHE:CE2	1:A:619:VAL:HG21	2.54	0.43
1:B:629:TRP:CD1	1:B:705:ARG:HG2	2.53	0.43
1:A:567:ASN:OD1	1:A:569:SER:N	2.48	0.43
1:B:464:ILE:HD13	1:A:620:VAL:HG11	2.00	0.43
1:B:609:ALA:HB2	1:A:454:PHE:CD1	2.50	0.43
1:B:822:ASP:OD1	1:B:823:GLN:HG3	2.19	0.43
1:A:544:LEU:HD11	1:A:587:LEU:HD22	2.00	0.43
1:B:571:PHE:HZ	1:B:616:VAL:HA	1.84	0.42
1:B:56:VAL:HG11	1:B:150:ALA:C	2.44	0.42
1:B:56:VAL:CG1	1:B:151:SER:N	2.83	0.42
1:A:511:PHE:CZ	1:A:806:PHE:HB3	2.54	0.42
1:B:115:LEU:HD23	1:B:115:LEU:HA	1.82	0.42
2:B:902:CLR:H183	2:B:902:CLR:H20	1.72	0.42
2:B:904:CLR:H162	2:B:904:CLR:H222	1.62	0.42
1:A:575:THR:HB	1:A:714:LEU:HD22	2.02	0.42
2:A:904:CLR:H183	2:A:904:CLR:H20	1.77	0.42
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.83	0.42
1:A:769:GLU:H	1:A:769:GLU:CD	2.28	0.42
1:B:81[B]:TYR:OH	1:B:124:GLU:HG2	2.19	0.42
2:A:902:CLR:H193	2:A:902:CLR:H111	1.77	0.42
1:B:55:VAL:HG22	1:B:158:GLN:HG2	2.02	0.42
1:A:765:LEU:HD11	1:A:790:ASP:HB2	2.00	0.42
2:B:903:CLR:H191	2:B:904:CLR:H11	2.01	0.42
1:B:588:LYS:O	1:B:592:THR:OG1	2.36	0.42
1:B:191:TYR:CZ	1:B:297:ILE:HG21	2.55	0.41
1:A:532:PHE:HA	1:A:536:TYR:HD1	1.85	0.41
1:B:783:ILE:HD13	1:B:783:ILE:HA	1.83	0.41
1:B:96:VAL:HG21	1:A:96:VAL:HG11	2.03	0.41
1:B:646:GLN:HG3	2:B:902:CLR:H9	2.02	0.41
1:A:274:SER:O	1:A:275:PHE:HB3	2.21	0.41
1:B:769:GLU:CD	1:B:769:GLU:H	2.28	0.41
2:B:902:CLR:H272	2:B:902:CLR:H232	1.75	0.41
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.93	0.41
1:A:572:GLN:HG2	1:A:573:PHE:CD2	2.55	0.41
1:A:590:TYR:OH	2:A:905:CLR:H72	2.21	0.41
1:A:191:TYR:CZ	1:A:297:ILE:HG21	2.55	0.41
2:A:903:CLR:H222	2:A:903:CLR:H162	1.78	0.41
1:B:71:GLN:OE1	1:B:71:GLN:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LYS:HD3	1:B:293:LEU:HD21	2.03	0.41
1:B:466:TYR:O	1:B:470:VAL:HG23	2.21	0.41
1:B:804:PHE:O	1:B:808:VAL:HG23	2.21	0.41
2:B:902:CLR:H193	2:B:902:CLR:H111	1.86	0.41
1:A:466:TYR:O	1:A:470:VAL:HG23	2.21	0.41
1:A:571:PHE:HB2	1:A:768:TRP:CE2	2.55	0.41
1:A:804:PHE:O	1:A:808:VAL:HG23	2.21	0.41
1:A:291:LYS:HD3	1:A:293:LEU:HD21	2.03	0.41
2:B:903:CLR:H181	2:B:904:CLR:H121	2.02	0.40
1:B:511:PHE:CZ	1:B:806:PHE:HB3	2.57	0.40
1:A:697:PHE:CE2	5:A:906:OLA:H10	2.56	0.40
1:B:110:LEU:HD23	1:B:112:PHE:CE1	2.57	0.40
2:B:903:CLR:C19	2:B:904:CLR:H11	2.52	0.40
1:A:110:LEU:HD23	1:A:112:PHE:CE1	2.56	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	634/1098 (58%)	618 (98%)	15 (2%)	1 (0%)	43	70
1	B	634/1098 (58%)	620 (98%)	14 (2%)	0	100	100
All	All	1268/2196 (58%)	1238 (98%)	29 (2%)	1 (0%)	49	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	PHE

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	566/965 (59%)	556 (98%)	10 (2%)	51	79
1	B	566/965 (59%)	558 (99%)	8 (1%)	59	82
All	All	1132/1930 (59%)	1114 (98%)	18 (2%)	54	81

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

Mol	Chain	Res	Type
1	B	75	VAL
1	B	89	LEU
1	B	124	GLU
1	B	204	VAL
1	B	459	VAL
1	B	596	ASP
1	B	638	LEU
1	B	764	ASN
1	A	56	VAL
1	A	89	LEU
1	A	121	ASN
1	A	204	VAL
1	A	260	VAL
1	A	459	VAL
1	A	505	VAL
1	A	596	ASP
1	A	764	ASN
1	A	775	SER

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

Mol	Chain	Res	Type
1	B	90	ASN
1	B	117	GLN
1	B	447	ASN
1	B	461	GLN

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Mol	Chain	Res	Type
1	B	501	ASN
1	B	720	ASN
1	B	764	ASN
1	B	779	ASN
1	A	90	ASN
1	A	117	GLN
1	A	121	ASN
1	A	123	GLN
1	A	447	ASN
1	A	461	GLN
1	A	476	GLN
1	A	501	ASN
1	A	522	HIS
1	A	764	ASN
1	A	779	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CLR	B	904	-	31,31,31	0.80	1 (3%)	48,48,48	1.55	9 (18%)
2	CLR	B	903	-	31,31,31	0.79	1 (3%)	48,48,48	1.41	7 (14%)
2	CLR	A	903	-	31,31,31	0.80	1 (3%)	48,48,48	1.00	2 (4%)
2	CLR	A	902	-	31,31,31	0.83	1 (3%)	48,48,48	1.29	8 (16%)
5	OLA	B	907	-	19,19,19	0.81	1 (5%)	19,19,19	0.90	1 (5%)
2	CLR	B	901	-	31,31,31	0.85	1 (3%)	48,48,48	1.63	12 (25%)
2	CLR	B	902	-	31,31,31	0.76	1 (3%)	48,48,48	1.28	6 (12%)
2	CLR	A	905	-	31,31,31	0.78	1 (3%)	48,48,48	1.18	5 (10%)
5	OLA	A	906	-	19,19,19	0.80	1 (5%)	19,19,19	0.90	1 (5%)
2	CLR	A	904	-	31,31,31	0.80	2 (6%)	48,48,48	1.53	8 (16%)

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	CLR	B	904	-	-	1/10/68/68	0/4/4/4
2	CLR	B	903	-	-	5/10/68/68	0/4/4/4
2	CLR	A	903	-	-	1/10/68/68	0/4/4/4
2	CLR	A	902	-	-	7/10/68/68	0/4/4/4
5	OLA	B	907	-	-	8/17/17/17	-
2	CLR	B	901	-	-	6/10/68/68	0/4/4/4
2	CLR	B	902	-	-	6/10/68/68	0/4/4/4
2	CLR	A	905	-	-	5/10/68/68	0/4/4/4
5	OLA	A	906	-	-	8/17/17/17	-
2	CLR	A	904	-	-	6/10/68/68	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	906	OLA	C10-C9	2.76	1.47	1.31
5	B	907	OLA	C10-C9	2.76	1.47	1.31
2	A	902	CLR	C10-C9	-2.39	1.52	1.56
2	B	904	CLR	C10-C9	-2.25	1.52	1.56
2	A	903	CLR	C10-C9	-2.21	1.52	1.56
2	B	901	CLR	C10-C9	-2.20	1.52	1.56
2	A	905	CLR	C10-C9	-2.18	1.52	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	CLR	C10-C9	-2.16	1.52	1.56
2	A	904	CLR	C13-C14	-2.14	1.51	1.55
2	A	904	CLR	C10-C9	-2.04	1.52	1.56
2	B	903	CLR	C10-C9	-2.01	1.52	1.56

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	904	CLR	C7-C6-C5	-4.63	117.19	125.02
2	A	904	CLR	C8-C7-C6	-4.33	106.77	112.76
2	A	904	CLR	C13-C17-C20	-4.20	113.01	119.50
2	B	903	CLR	C8-C7-C6	-4.19	106.95	112.76
2	B	902	CLR	C13-C17-C20	-3.95	113.40	119.50
2	B	901	CLR	C4-C5-C10	3.63	121.06	116.42
2	B	901	CLR	C8-C7-C6	-3.61	107.75	112.76
2	B	901	CLR	C7-C6-C5	-3.59	118.95	125.02
2	A	902	CLR	C13-C17-C20	-3.22	114.53	119.50
2	B	904	CLR	C7-C8-C9	3.21	113.43	109.72
2	A	904	CLR	C13-C14-C8	-3.21	109.86	114.41
2	B	904	CLR	C8-C7-C6	-2.96	108.67	112.76
2	A	904	CLR	C17-C13-C14	2.94	103.47	100.10
2	B	903	CLR	C13-C17-C20	-2.86	115.09	119.50
2	B	903	CLR	C19-C10-C9	-2.72	108.60	111.66
2	A	904	CLR	C19-C10-C9	-2.67	108.66	111.66
2	B	903	CLR	C3-C4-C5	-2.60	107.91	112.05
2	B	902	CLR	C11-C12-C13	-2.57	108.40	112.74
2	A	902	CLR	C11-C9-C10	-2.55	109.94	113.08
2	B	901	CLR	C14-C8-C9	-2.55	105.76	109.09
2	A	902	CLR	C19-C10-C9	-2.54	108.81	111.66
2	B	904	CLR	C13-C14-C8	-2.53	110.82	114.41
2	A	905	CLR	C11-C9-C10	-2.51	109.98	113.08
2	B	904	CLR	C1-C10-C9	2.51	112.06	108.74
2	A	903	CLR	C8-C7-C6	-2.46	109.35	112.76
2	B	903	CLR	C13-C14-C8	-2.44	110.94	114.41
2	B	904	CLR	C1-C2-C3	2.43	113.71	110.48
2	B	901	CLR	C22-C20-C17	-2.43	105.28	110.33
2	A	904	CLR	C11-C9-C10	-2.40	110.12	113.08
2	A	905	CLR	C8-C7-C6	-2.37	109.47	112.76
2	A	902	CLR	C11-C12-C13	-2.35	108.77	112.74
2	A	905	CLR	C19-C10-C9	-2.35	109.03	111.66
2	B	904	CLR	C4-C5-C10	2.35	119.43	116.42
2	B	904	CLR	C10-C5-C6	-2.33	119.52	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	CLR	C10-C5-C6	-2.32	119.55	122.93
2	A	904	CLR	C3-C4-C5	-2.31	108.37	112.05
2	A	904	CLR	C9-C10-C5	2.30	113.02	109.65
2	A	902	CLR	C18-C13-C17	-2.30	107.51	111.68
2	B	901	CLR	C16-C17-C20	-2.28	108.73	112.18
2	A	905	CLR	C13-C17-C20	-2.27	116.00	119.50
2	B	902	CLR	C17-C13-C14	2.24	102.67	100.10
2	A	902	CLR	C8-C7-C6	-2.21	109.70	112.76
2	A	905	CLR	C23-C22-C20	-2.20	108.91	115.08
2	B	901	CLR	C1-C2-C3	2.20	113.40	110.48
2	B	902	CLR	C8-C7-C6	-2.19	109.73	112.76
2	B	901	CLR	C7-C8-C9	2.19	112.25	109.72
2	A	902	CLR	C21-C20-C17	-2.16	109.64	112.88
2	B	901	CLR	C16-C17-C13	2.15	106.36	103.84
2	B	901	CLR	C19-C10-C9	-2.11	109.29	111.66
2	B	902	CLR	C18-C13-C17	-2.09	107.88	111.68
2	A	902	CLR	C10-C9-C8	-2.08	109.67	112.71
2	B	903	CLR	C9-C10-C5	2.08	112.70	109.65
2	A	903	CLR	C11-C12-C13	-2.08	109.23	112.74
5	A	906	OLA	O2-C1-C2	2.06	120.52	114.00
5	B	907	OLA	O2-C1-C2	2.06	120.50	114.00
2	B	903	CLR	C4-C5-C6	-2.05	117.79	120.57
2	B	902	CLR	C4-C5-C10	2.03	119.02	116.42
2	B	904	CLR	C14-C8-C9	-2.01	106.46	109.09
2	B	901	CLR	C1-C10-C9	2.00	111.39	108.74

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	903	CLR	C16-C17-C20-C21
2	B	902	CLR	C13-C17-C20-C21
2	B	903	CLR	C13-C17-C20-C21
2	B	902	CLR	C16-C17-C20-C21
2	B	902	CLR	C13-C17-C20-C22
2	B	903	CLR	C13-C17-C20-C22
5	B	907	OLA	C11-C10-C9-C8
5	A	906	OLA	C11-C10-C9-C8
2	B	903	CLR	C16-C17-C20-C22
2	A	904	CLR	C17-C20-C22-C23
2	A	902	CLR	C21-C20-C22-C23
2	A	902	CLR	C17-C20-C22-C23

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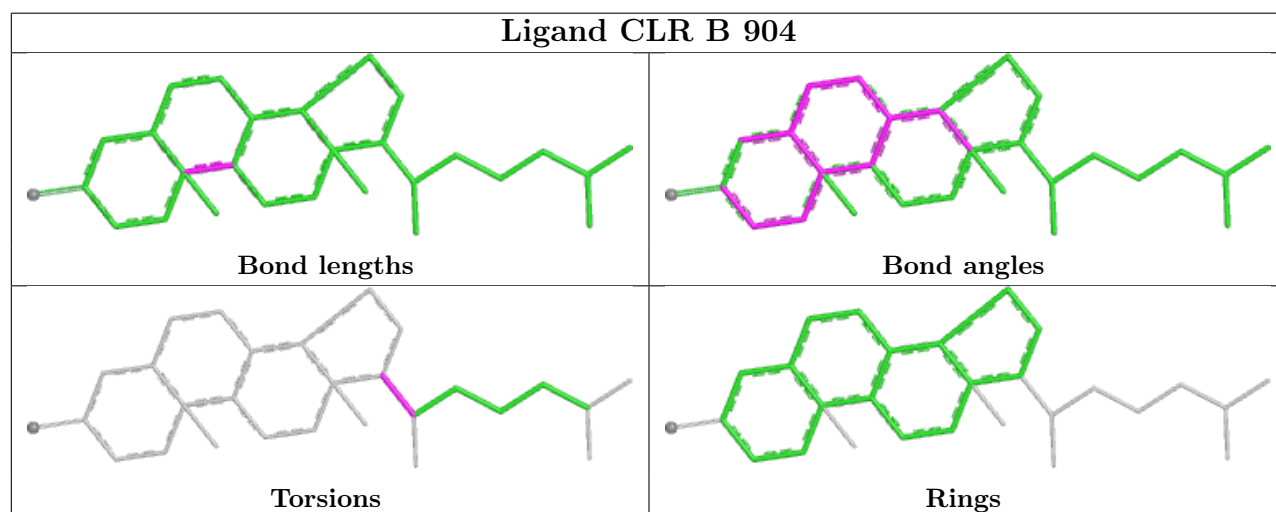
Mol	Chain	Res	Type	Atoms
2	A	904	CLR	C13-C17-C20-C22
5	B	907	OLA	C4-C5-C6-C7
5	A	906	OLA	C4-C5-C6-C7
2	A	904	CLR	C21-C20-C22-C23
2	B	902	CLR	C16-C17-C20-C22
2	A	902	CLR	C13-C17-C20-C22
2	B	902	CLR	C17-C20-C22-C23
5	B	907	OLA	C1-C2-C3-C4
5	A	906	OLA	C1-C2-C3-C4
2	A	902	CLR	C20-C22-C23-C24
2	A	904	CLR	C13-C17-C20-C21
2	B	901	CLR	C13-C17-C20-C21
2	A	902	CLR	C13-C17-C20-C21
5	B	907	OLA	C3-C4-C5-C6
5	A	906	OLA	C3-C4-C5-C6
2	B	901	CLR	C13-C17-C20-C22
2	A	905	CLR	C20-C22-C23-C24
2	B	901	CLR	C16-C17-C20-C21
2	A	904	CLR	C16-C17-C20-C21
2	A	902	CLR	C16-C17-C20-C21
2	A	904	CLR	C16-C17-C20-C22
2	A	902	CLR	C16-C17-C20-C22
2	B	901	CLR	C16-C17-C20-C22
2	B	903	CLR	C21-C20-C22-C23
2	B	901	CLR	C23-C24-C25-C26
2	B	901	CLR	C23-C24-C25-C27
2	A	905	CLR	C13-C17-C20-C21
5	B	907	OLA	C5-C6-C7-C8
5	A	906	OLA	C5-C6-C7-C8
2	A	905	CLR	C13-C17-C20-C22
2	B	902	CLR	C21-C20-C22-C23
2	A	903	CLR	C13-C17-C20-C21
2	A	905	CLR	C16-C17-C20-C22
2	B	904	CLR	C13-C17-C20-C21
5	A	906	OLA	C11-C12-C13-C14
5	B	907	OLA	C11-C12-C13-C14
5	A	906	OLA	C7-C8-C9-C10
5	B	907	OLA	C7-C8-C9-C10
5	B	907	OLA	C9-C10-C11-C12
5	A	906	OLA	C9-C10-C11-C12
2	A	905	CLR	C16-C17-C20-C21

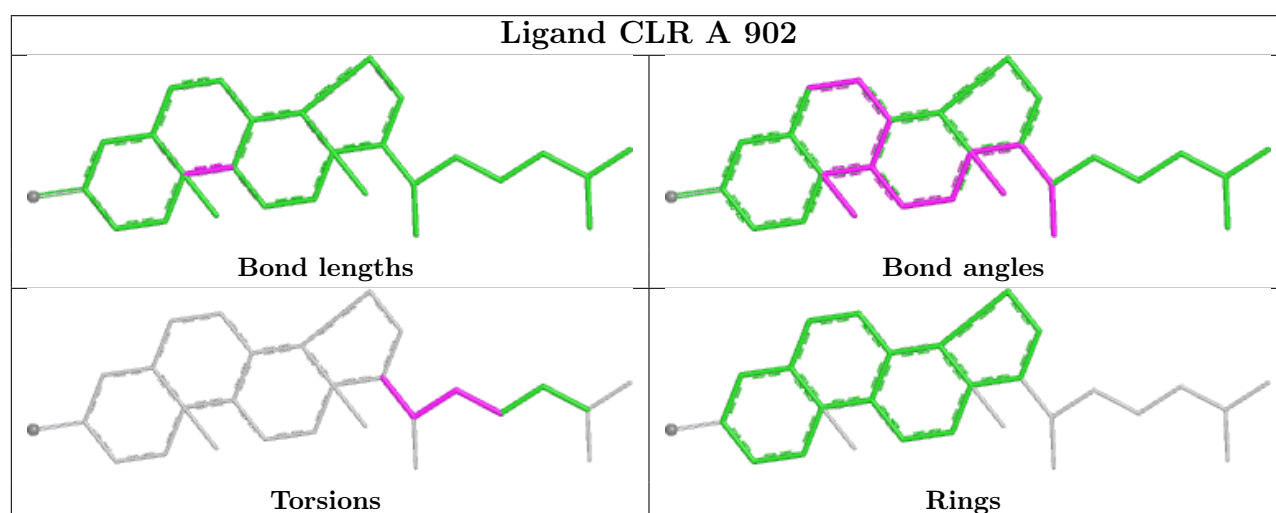
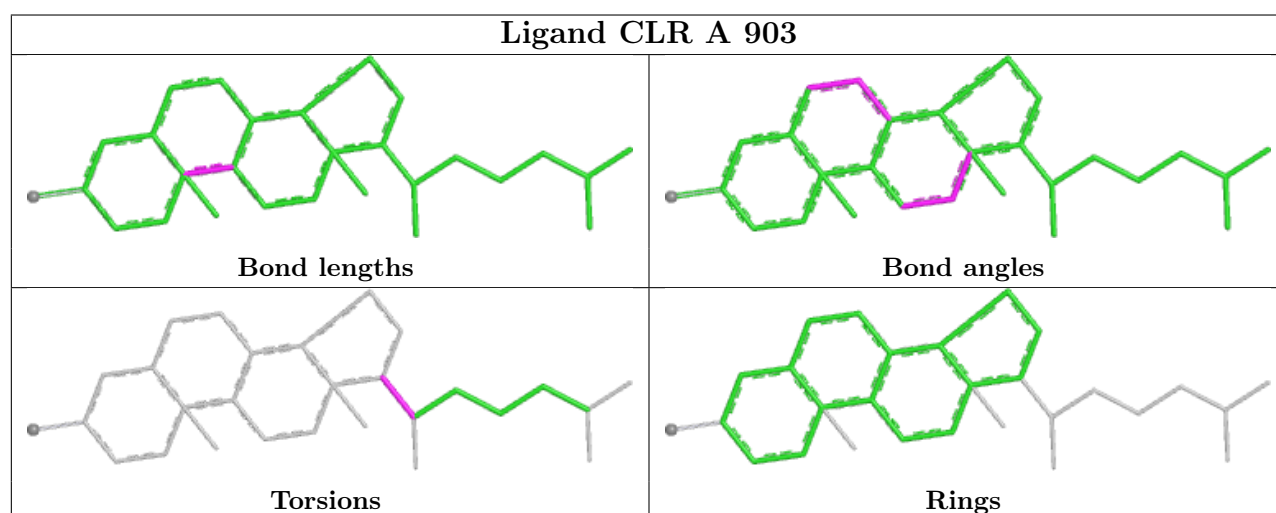
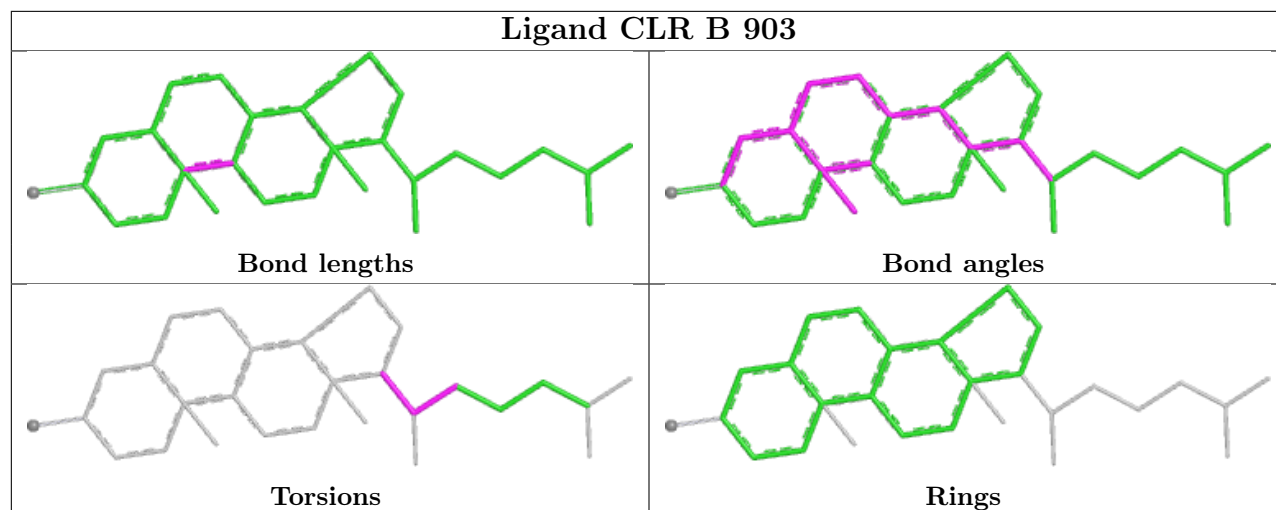
There are no ring outliers.

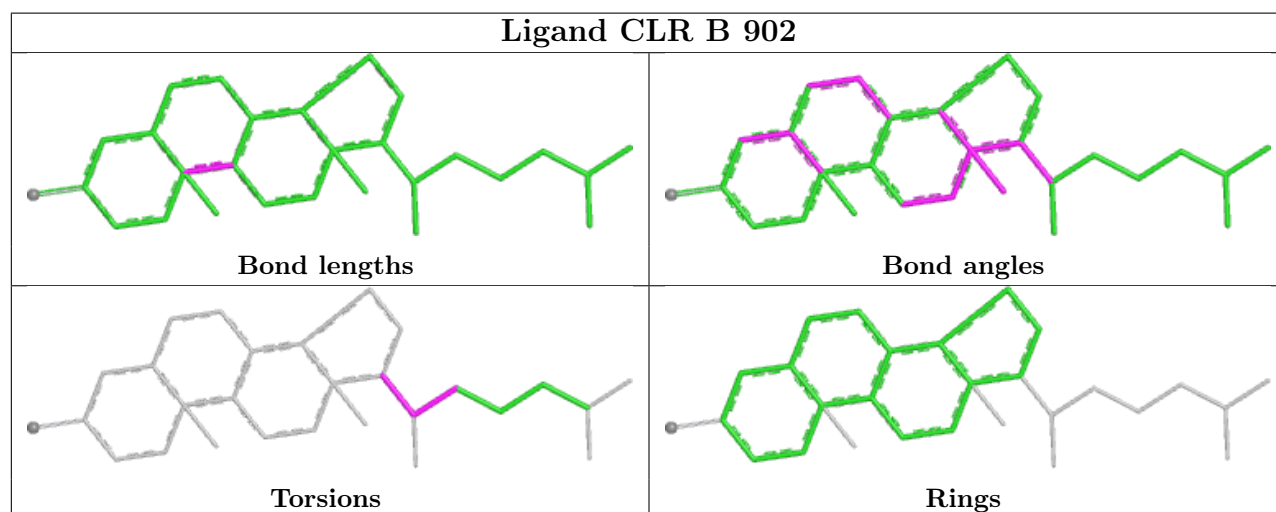
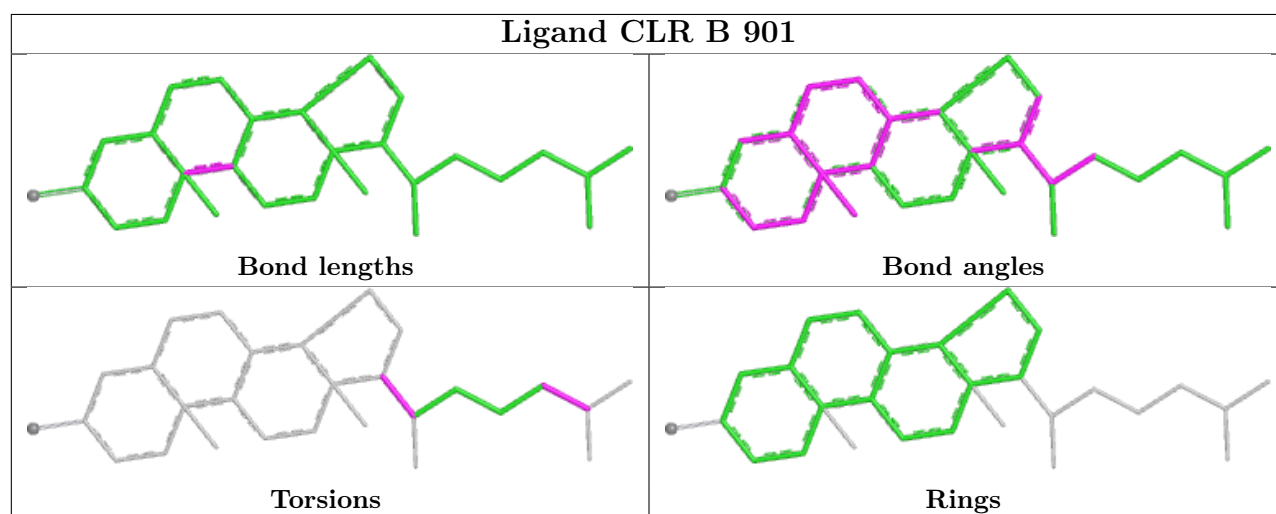
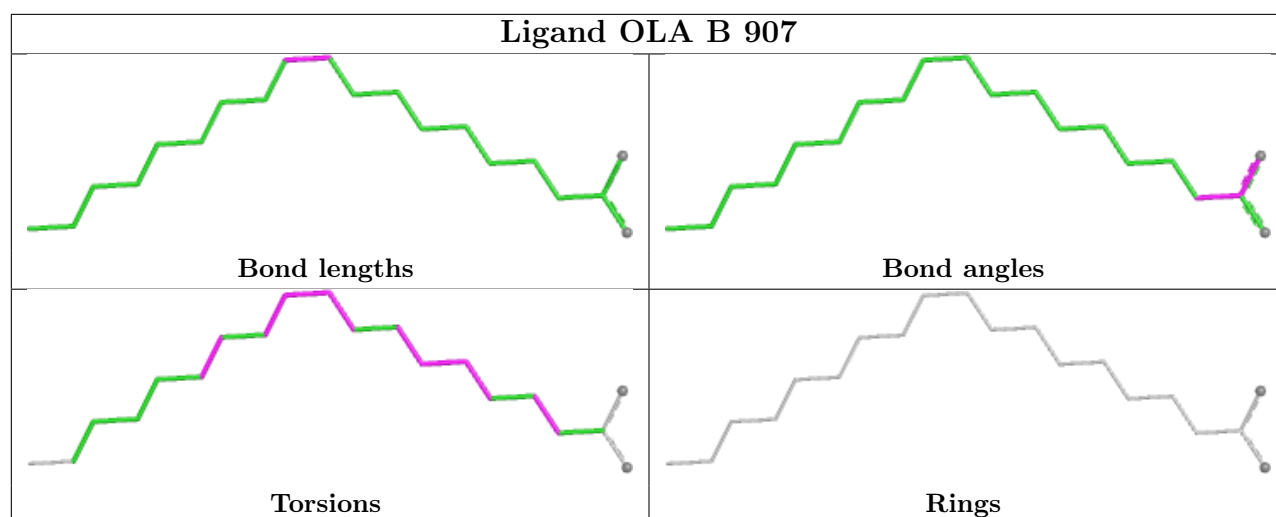
10 monomers are involved in 87 short contacts:

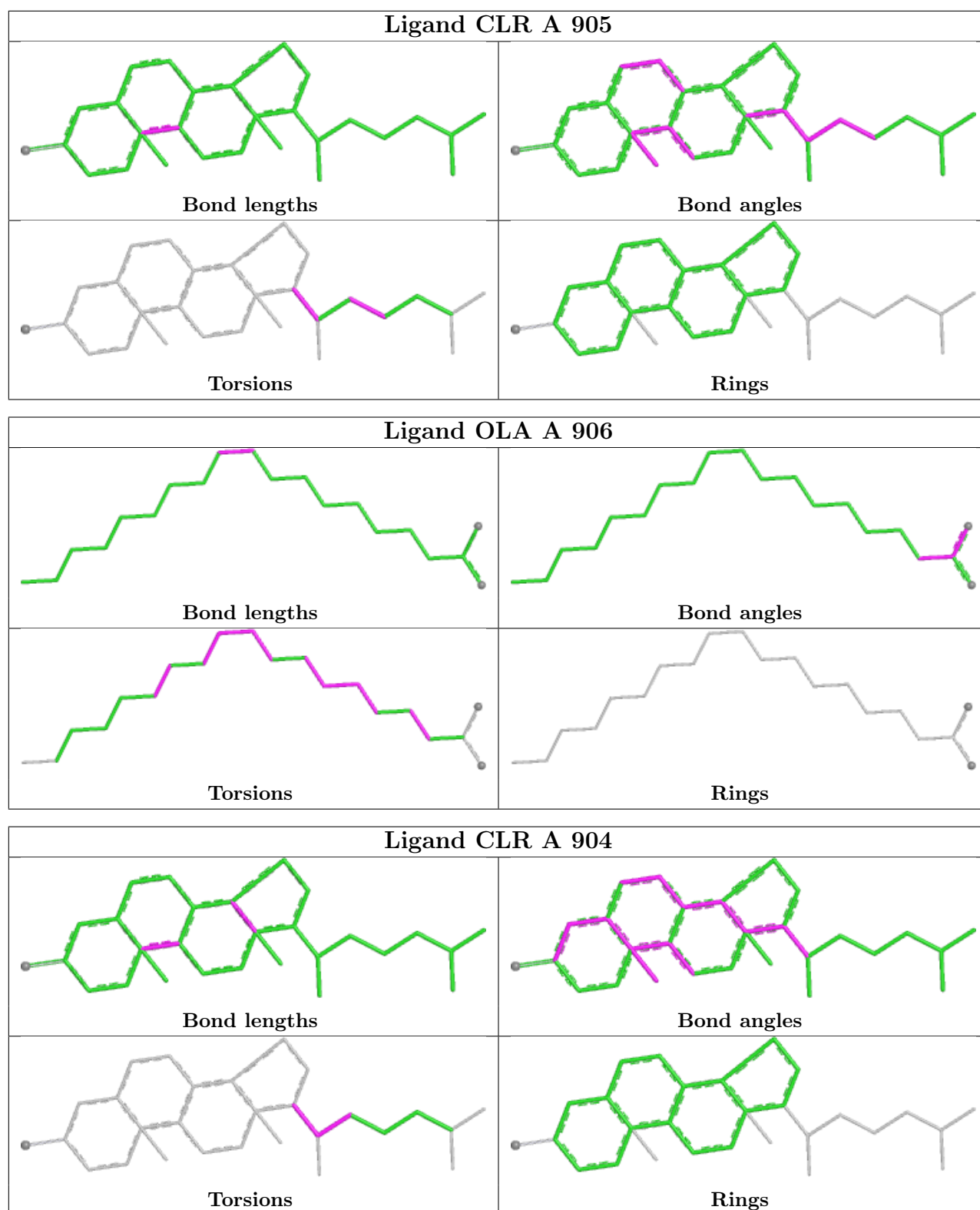
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	904	CLR	21	0
2	B	903	CLR	16	0
2	A	903	CLR	5	0
2	A	902	CLR	5	0
5	B	907	OLA	3	0
2	B	901	CLR	4	0
2	B	902	CLR	7	0
2	A	905	CLR	29	0
5	A	906	OLA	6	0
2	A	904	CLR	14	0

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.

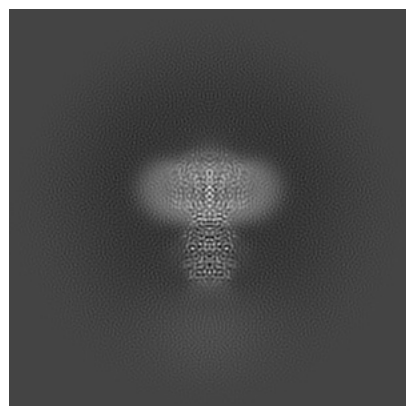
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36008. These allow visual inspection of the internal detail of the map and identification of artifacts.

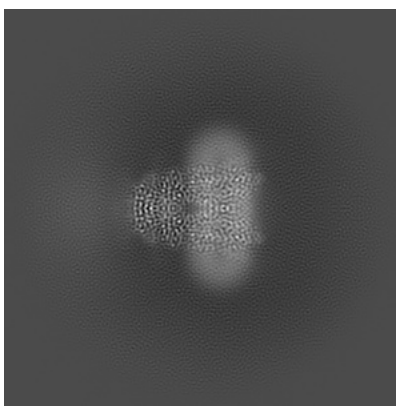
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

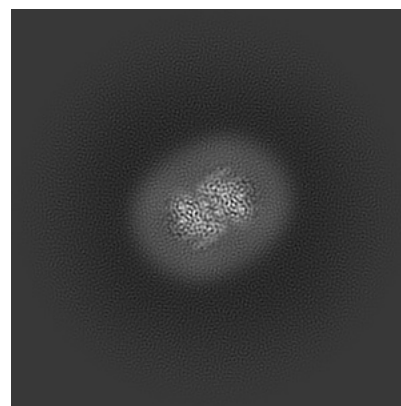
6.1.1 Primary map



X

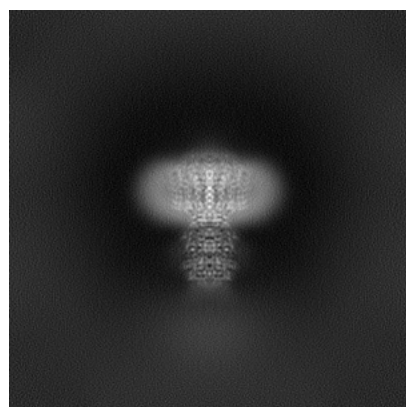


Y

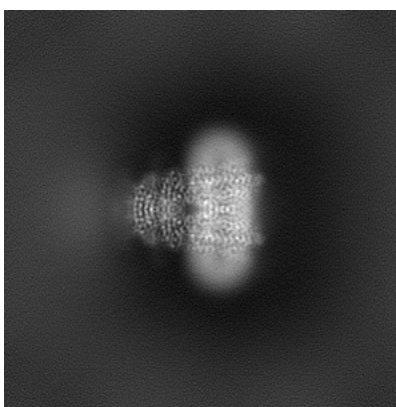


Z

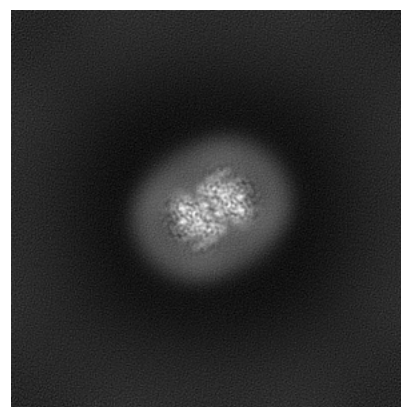
6.1.2 Raw map



X



Y

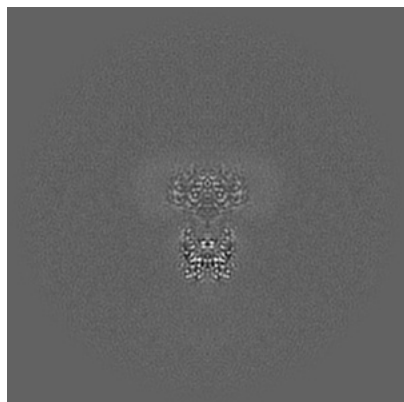


Z

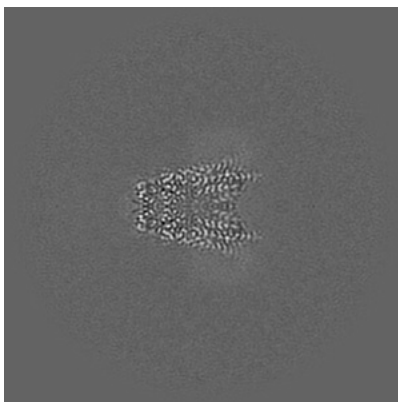
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

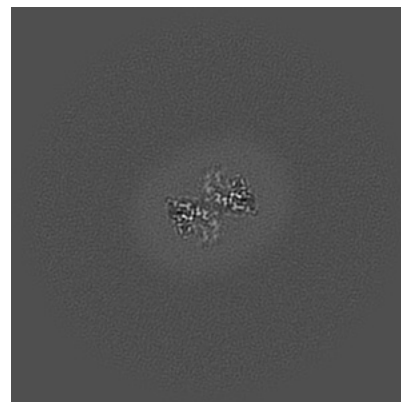
6.2.1 Primary map



X Index: 160

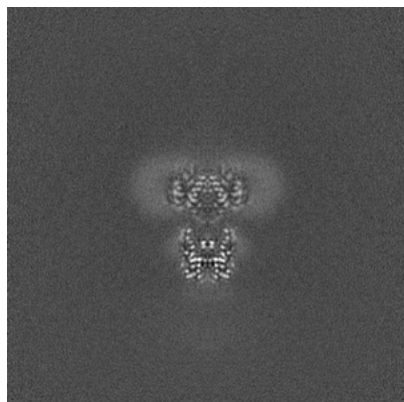


Y Index: 160

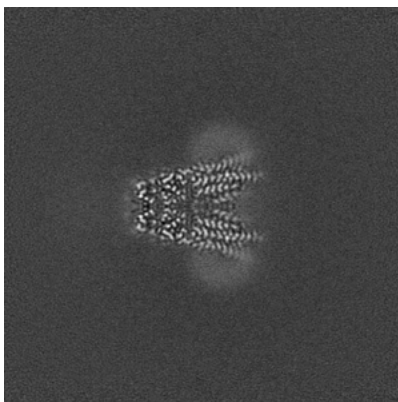


Z Index: 160

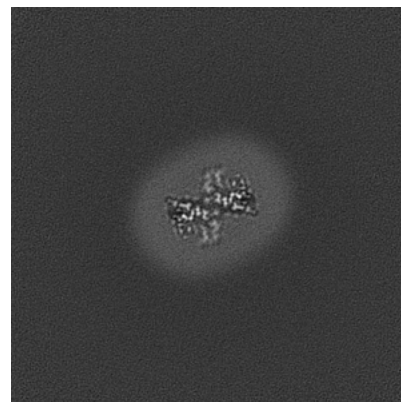
6.2.2 Raw map



X Index: 160



Y Index: 160

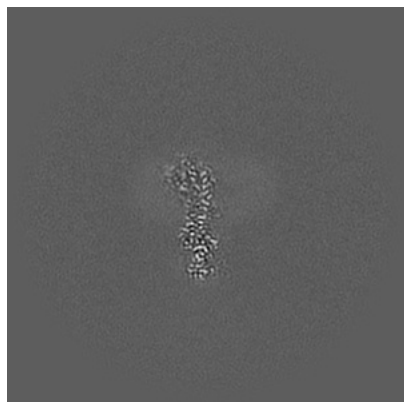


Z Index: 160

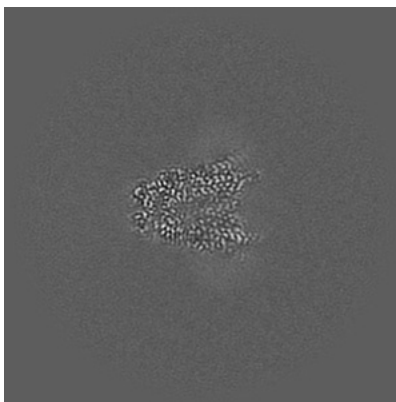
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

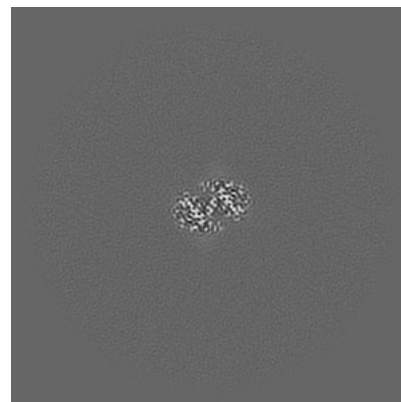
6.3.1 Primary map



X Index: 146

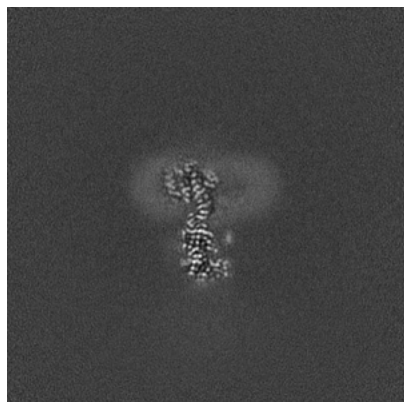


Y Index: 162

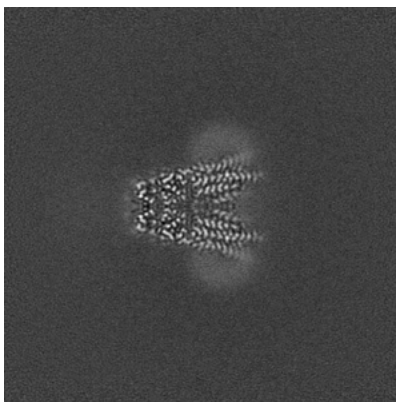


Z Index: 131

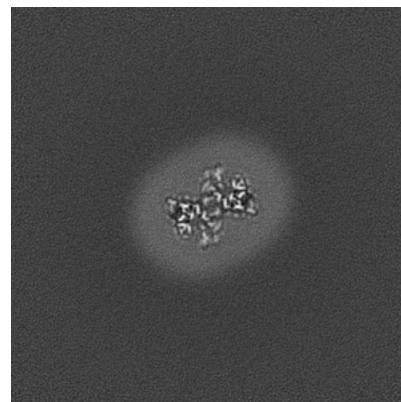
6.3.2 Raw map



X Index: 150



Y Index: 160

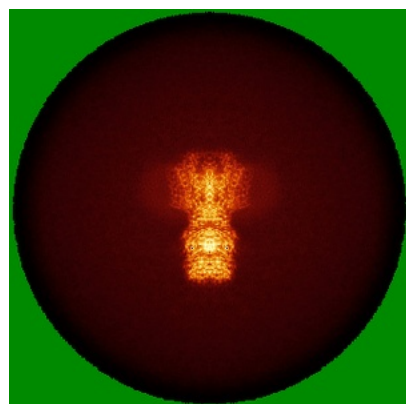


Z Index: 161

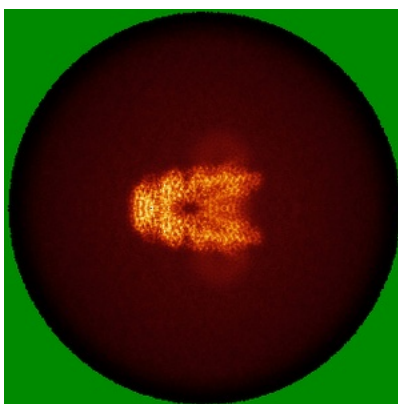
The images above show the largest variance slices of the map in three orthogonal directions.

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

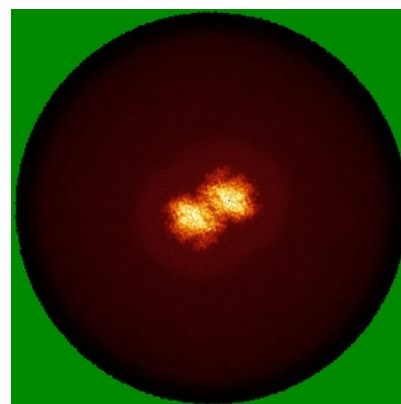
6.4.1 Primary map



X

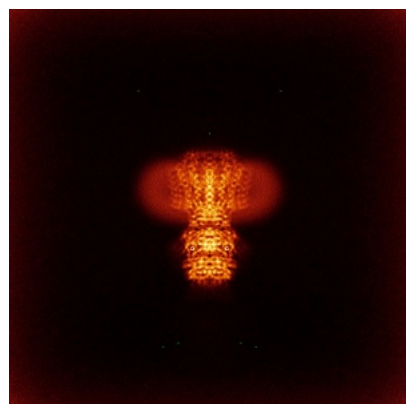


Y

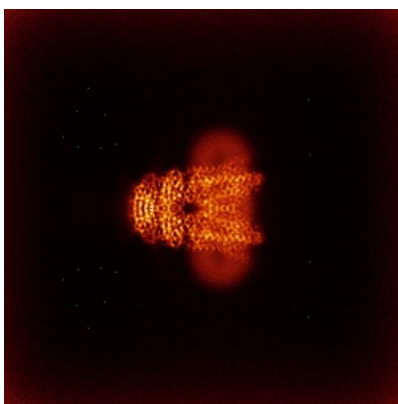


Z

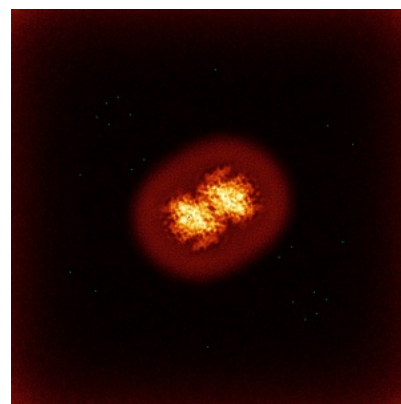
6.4.2 Raw map



X



Y

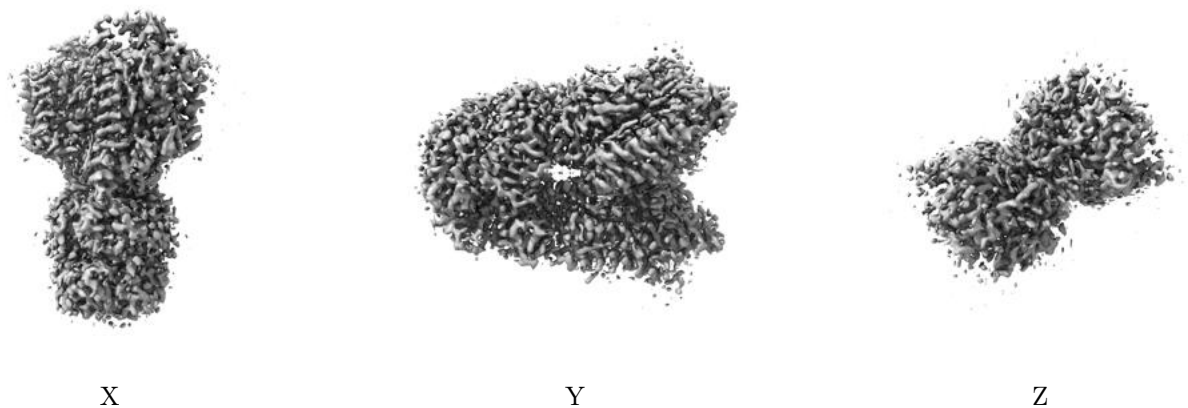


Z

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.

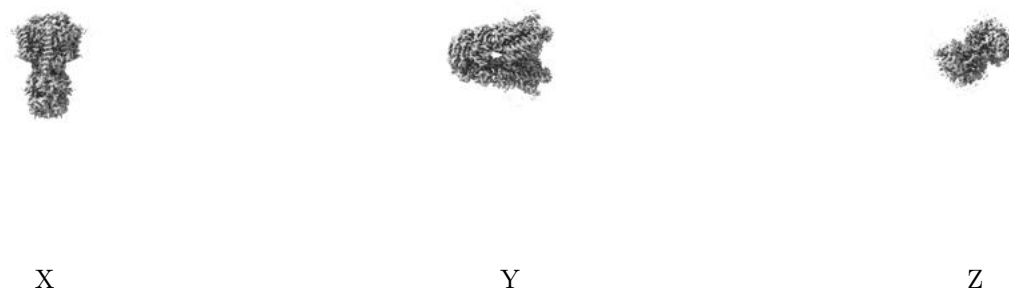
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.962. 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.

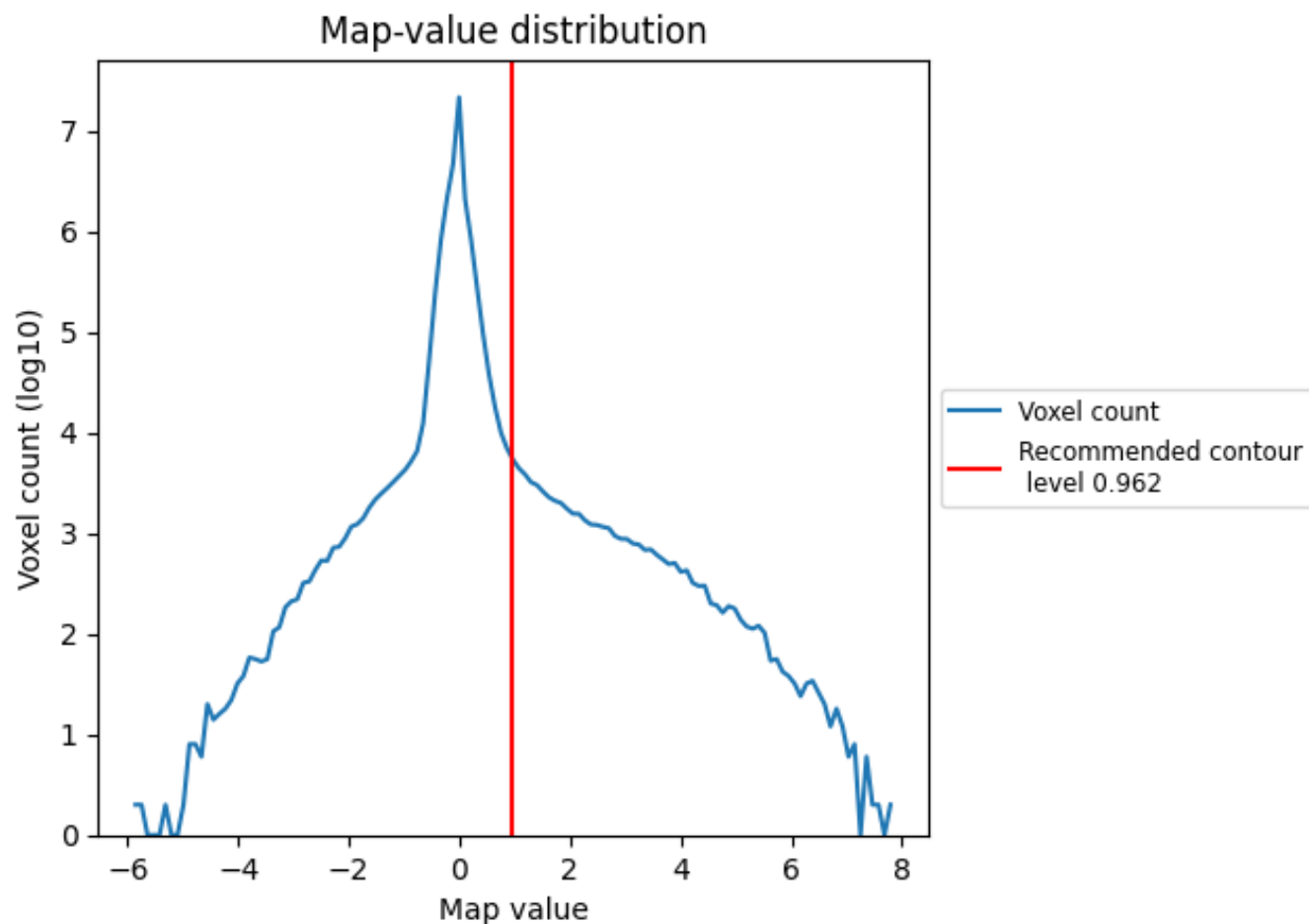
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

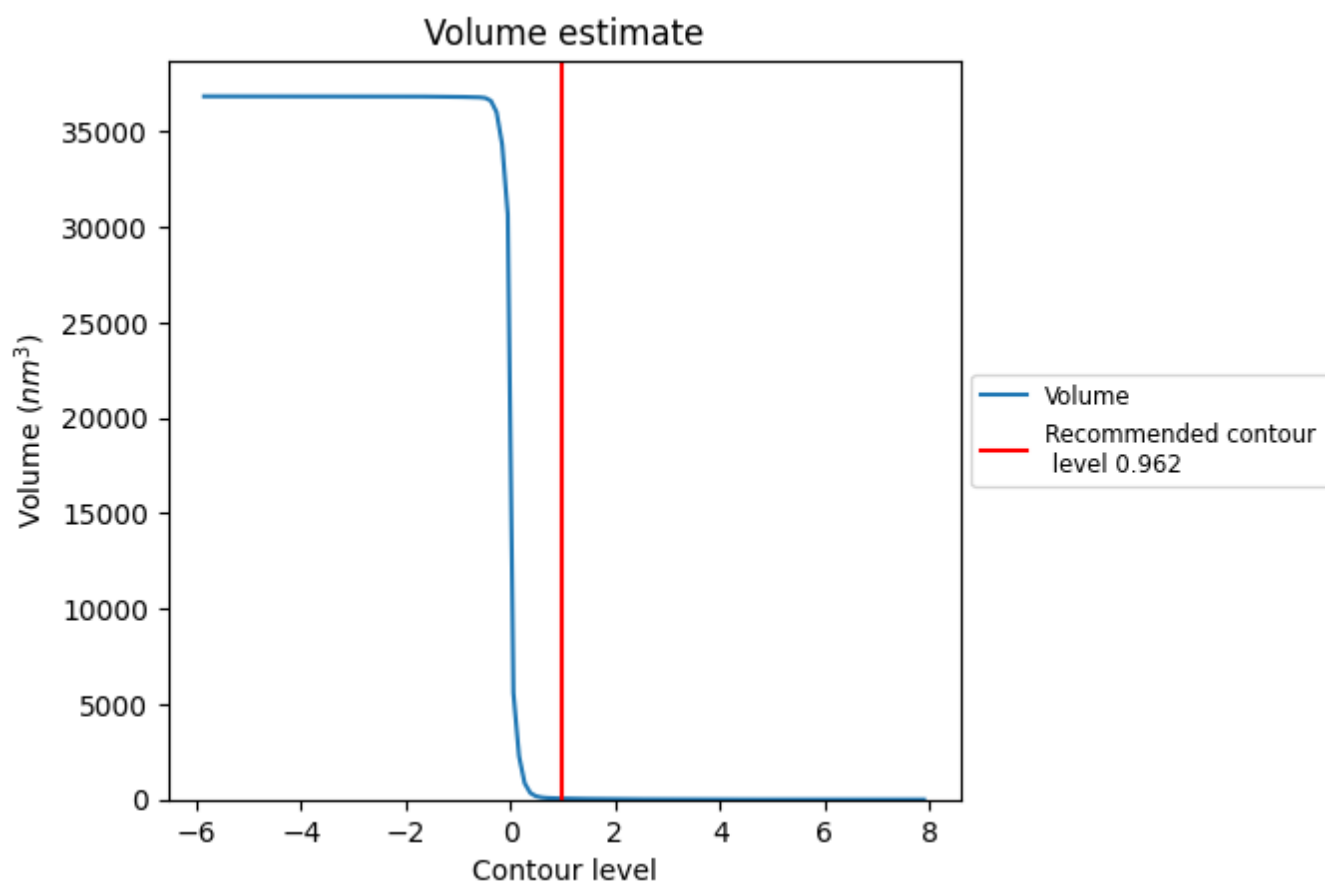
This section contains the results of statistical analysis of the map.

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.

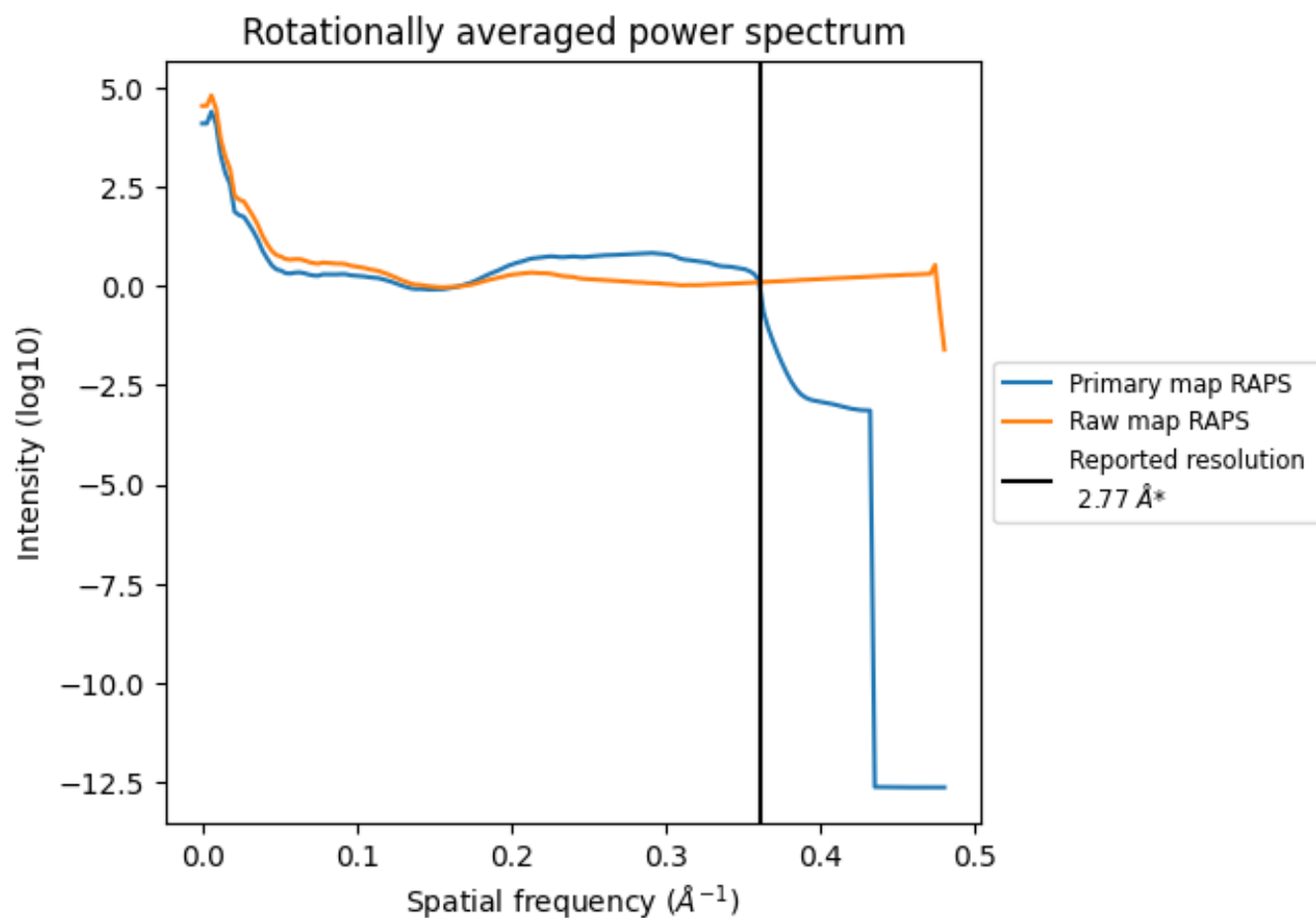
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 58 nm³; this corresponds to an approximate mass of 52 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 ⓘ

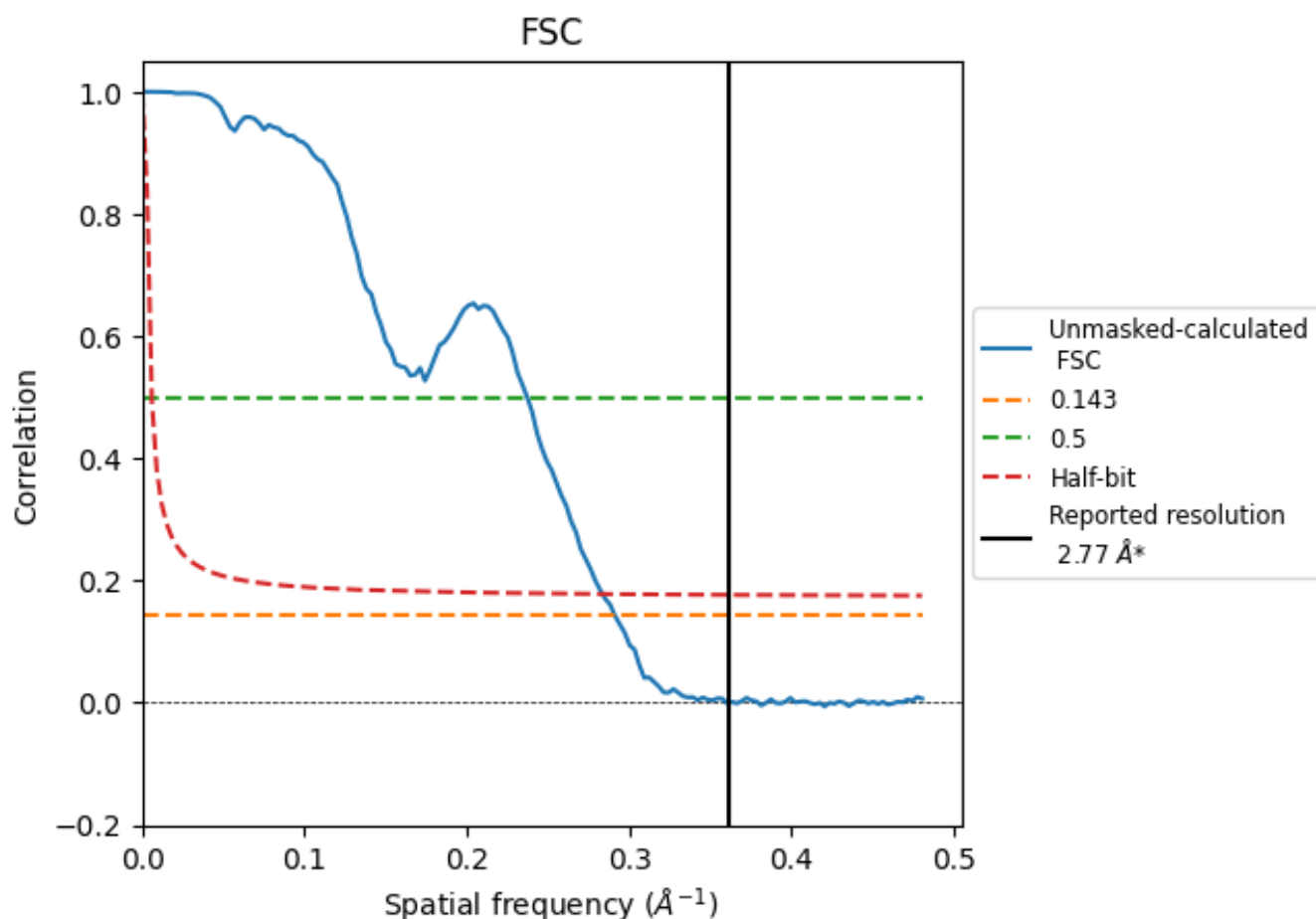


*Reported resolution corresponds to spatial frequency of 0.361 $\text{\AA}^{-1}$

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 0.361 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

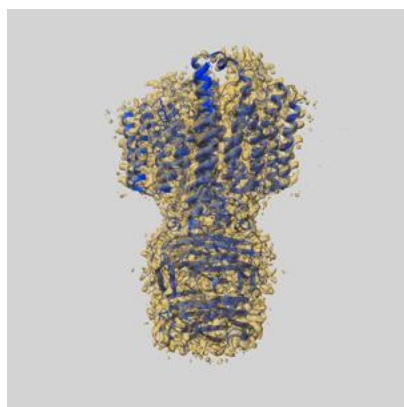
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.43	4.21	3.52

*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 3.43 differs from the reported value 2.77 by more than 10 %

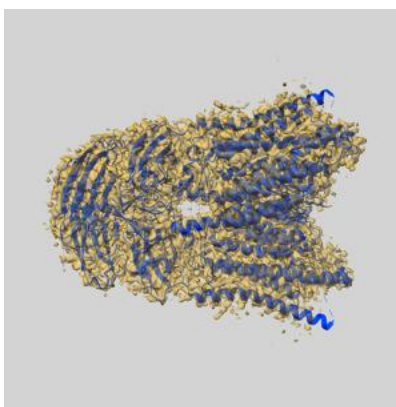
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36008 and PDB model 8J6M. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

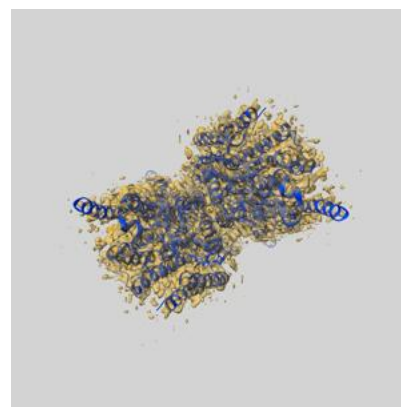
9.1 Map-model overlay [i](#)



X



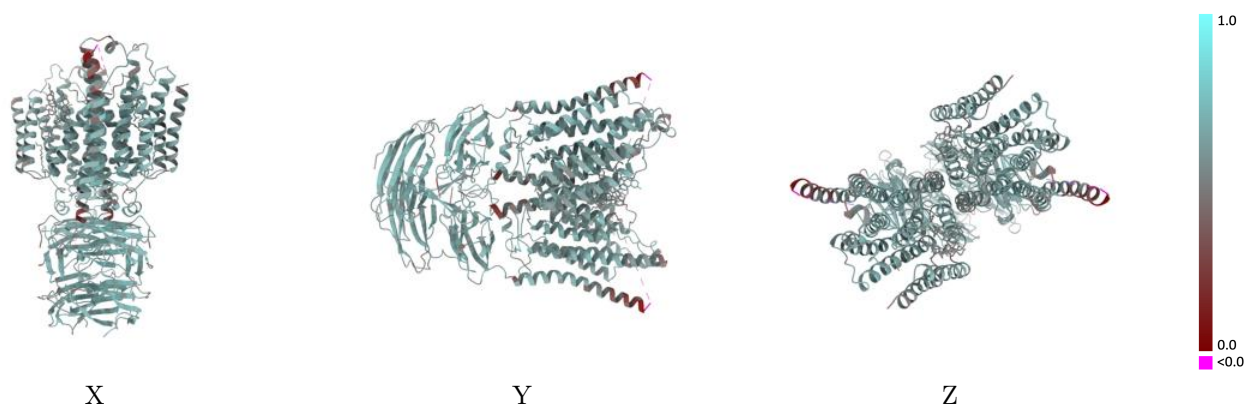
Y



Z

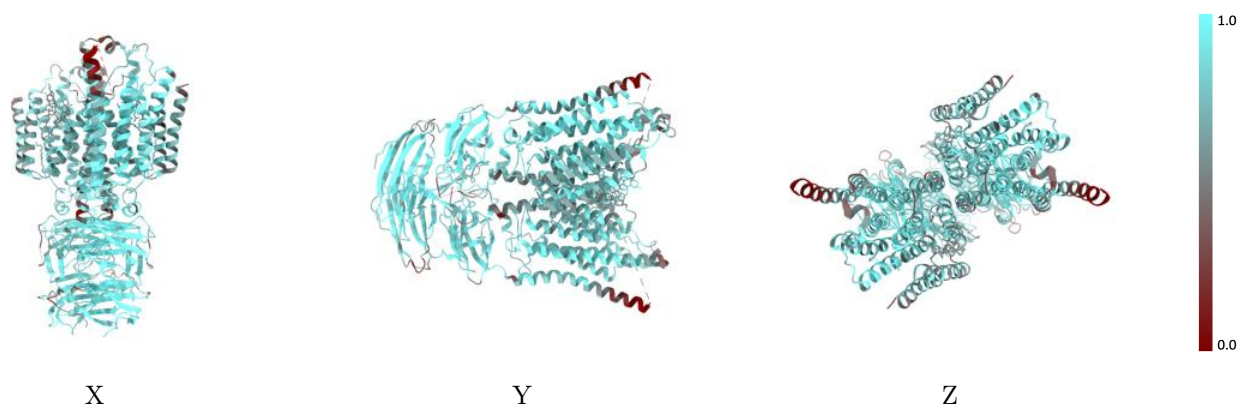
The images above show the 3D surface view of the map at the recommended contour level 0.962 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



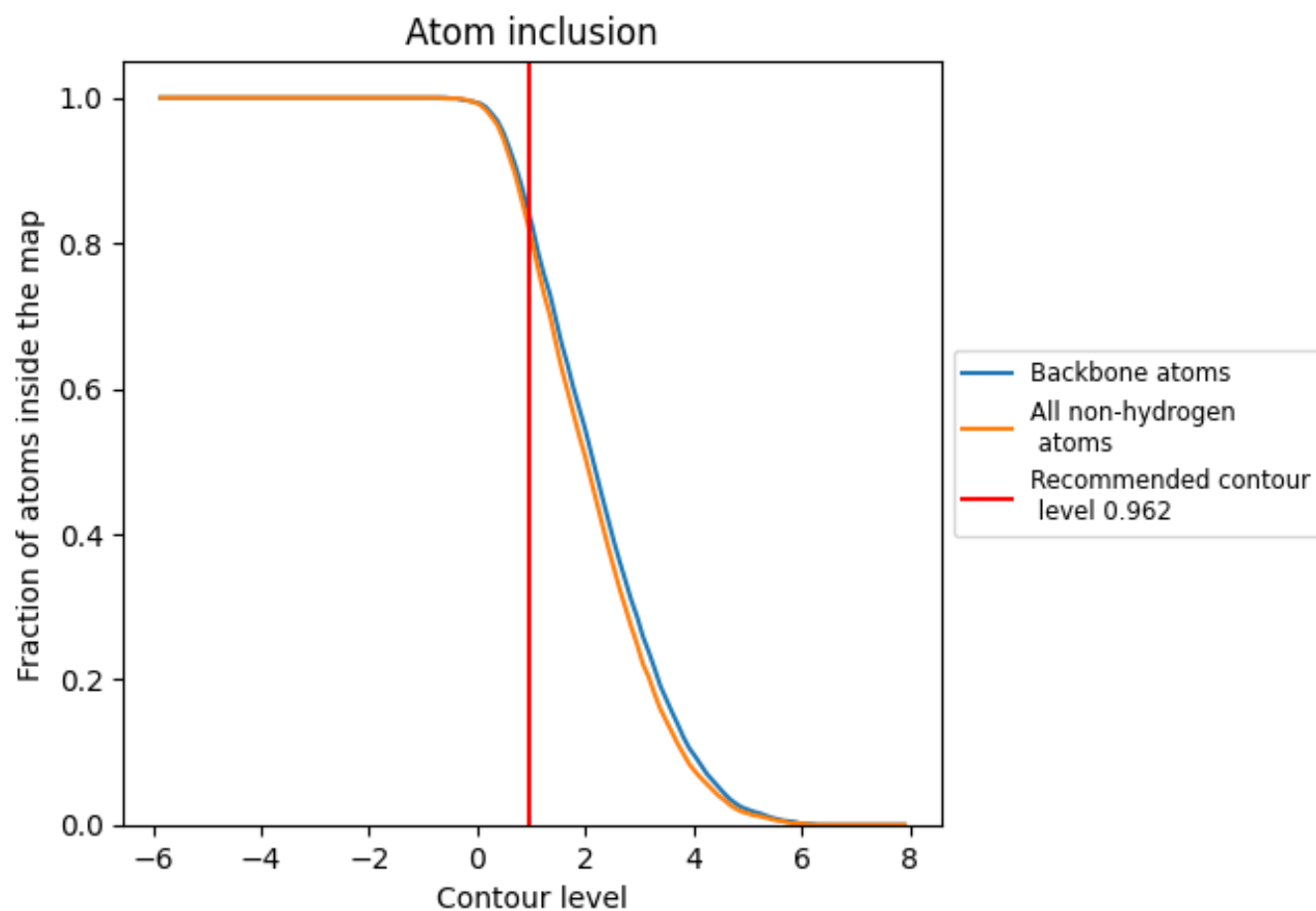
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.962).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 82% 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 (0.962) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8180	0.5870
A	0.8180	0.5880
B	0.8250	0.5860

