



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:54 AM UTC

PDB ID : 7LG5 / pdb_00007lg5
EMDB ID : EMD-23311
Title : Synechocystis sp. UTEX2470 Cyanophycin synthetase 1 with ATP
Authors : Sharon, I.; Schmeing, T.M.
Deposited on : 2021-01-19
Resolution : 2.63 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

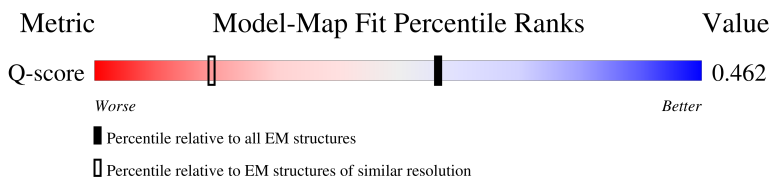
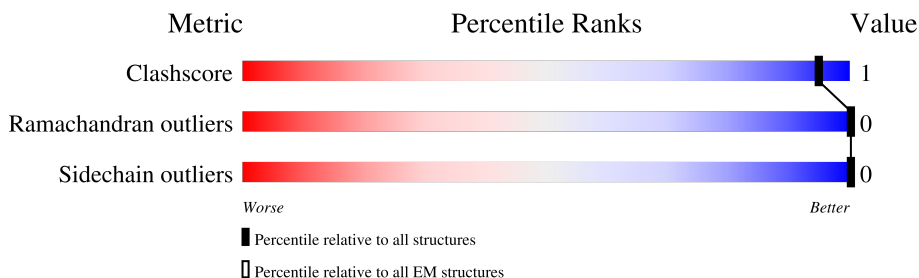
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.63 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	8888 (2.13 - 3.13)

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	879	 90% 8% .
1	B	879	 91% 8% .
1	C	879	 91% 8% ..
1	D	879	 91% 8% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26888 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 Cyanophycin synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	871	Total	C	N	O	S	0	0
			6657	4187	1164	1282	24		
1	B	871	Total	C	N	O	S	0	0
			6657	4187	1164	1282	24		
1	C	871	Total	C	N	O	S	0	0
			6657	4187	1164	1282	24		
1	D	871	Total	C	N	O	S	0	0
			6657	4187	1164	1282	24		

There are 24 discrepancies between the modelled and reference sequences:

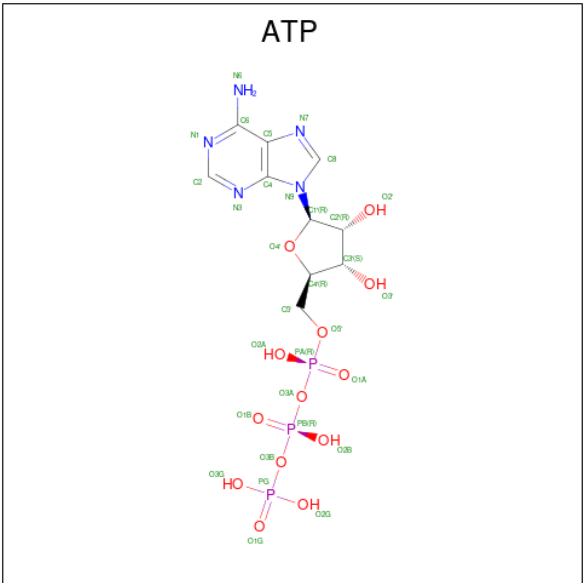
Chain	Residue	Modelled	Actual	Comment	Reference
A	874	GLU	-	expression tag	UNP A0A068N621
A	875	ASN	-	expression tag	UNP A0A068N621
A	876	LEU	-	expression tag	UNP A0A068N621
A	877	TYR	-	expression tag	UNP A0A068N621
A	878	PHE	-	expression tag	UNP A0A068N621
A	879	GLN	-	expression tag	UNP A0A068N621
B	874	GLU	-	expression tag	UNP A0A068N621
B	875	ASN	-	expression tag	UNP A0A068N621
B	876	LEU	-	expression tag	UNP A0A068N621
B	877	TYR	-	expression tag	UNP A0A068N621
B	878	PHE	-	expression tag	UNP A0A068N621
B	879	GLN	-	expression tag	UNP A0A068N621
C	874	GLU	-	expression tag	UNP A0A068N621
C	875	ASN	-	expression tag	UNP A0A068N621
C	876	LEU	-	expression tag	UNP A0A068N621
C	877	TYR	-	expression tag	UNP A0A068N621
C	878	PHE	-	expression tag	UNP A0A068N621
C	879	GLN	-	expression tag	UNP A0A068N621
D	874	GLU	-	expression tag	UNP A0A068N621
D	875	ASN	-	expression tag	UNP A0A068N621
D	876	LEU	-	expression tag	UNP A0A068N621
D	877	TYR	-	expression tag	UNP A0A068N621

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Chain	Residue	Modelled	Actual	Comment	Reference
D	878	PHE	-	expression tag	UNP A0A068N621
D	879	GLN	-	expression tag	UNP A0A068N621

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

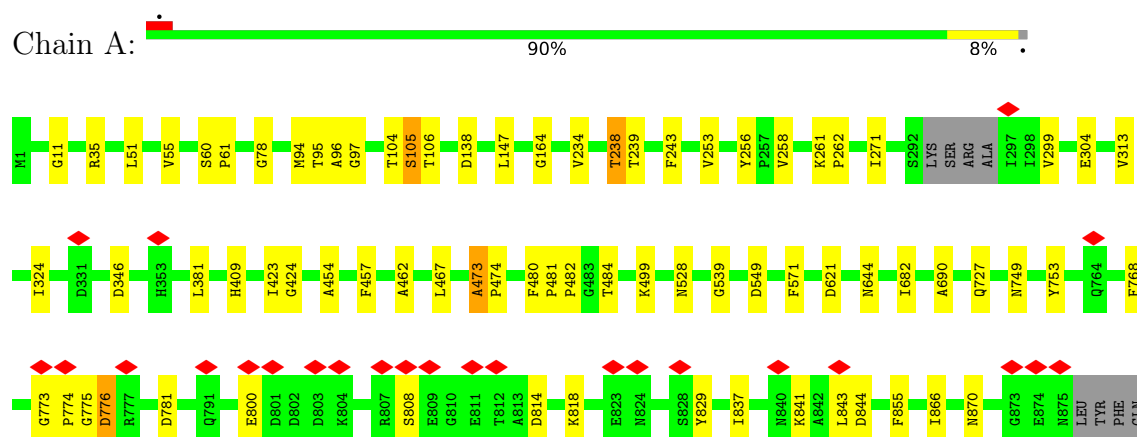
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	A	3	Total 3	Mg 3	0
3	B	3	Total 3	Mg 3	0
3	C	3	Total 3	Mg 3	0
3	D	3	Total 3	Mg 3	0

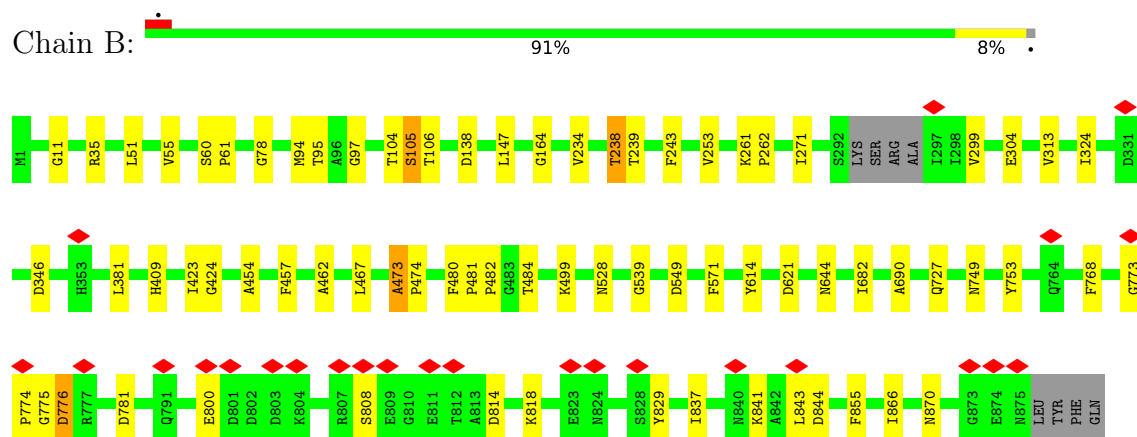
3 Residue-property plots

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.

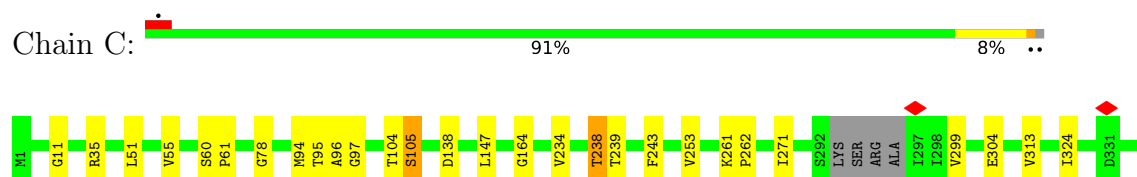
• Molecule 1: Cyanophycin synthase

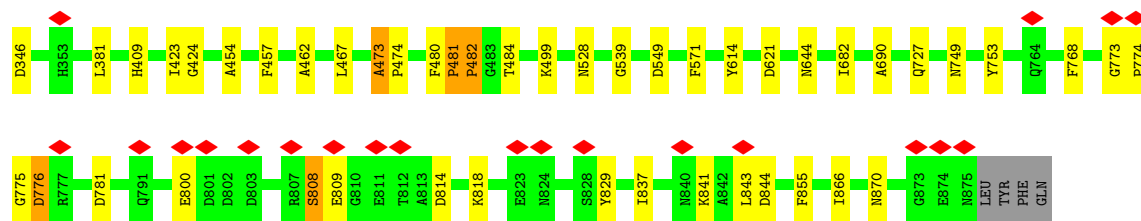


• Molecule 1: Cyanophycin synthase



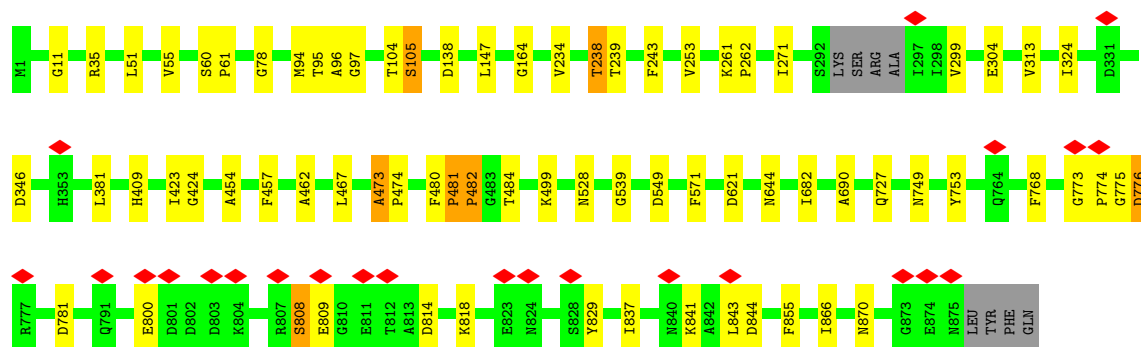
• Molecule 1: Cyanophycin synthase





• Molecule 1: Cyanophycin synthase

Chain D: 91% 8% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	311861	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 ($e^-/\text{\AA}^2$)	60.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.350	Depositor
Minimum map value	-0.408	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	342.0, 342.0, 342.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.99	4/6770 (0.1%)	1.32	82/9199 (0.9%)
1	B	0.99	4/6770 (0.1%)	1.32	82/9199 (0.9%)
1	C	0.99	4/6770 (0.1%)	1.32	83/9199 (0.9%)
1	D	0.99	4/6770 (0.1%)	1.32	82/9199 (0.9%)
All	All	0.99	16/27080 (0.1%)	1.32	329/36796 (0.9%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	481	PRO	C-O	-7.52	1.16	1.24
1	A	481	PRO	C-O	-7.51	1.16	1.24
1	B	481	PRO	C-O	-7.51	1.16	1.24
1	D	481	PRO	C-O	-7.48	1.16	1.24
1	A	35	ARG	NE-CZ	5.31	1.38	1.33
1	D	35	ARG	NE-CZ	5.29	1.38	1.33
1	B	35	ARG	NE-CZ	5.29	1.38	1.33
1	A	528	ASN	CB-CG	-5.24	1.39	1.52
1	C	35	ARG	NE-CZ	5.23	1.38	1.33
1	C	528	ASN	CB-CG	-5.23	1.39	1.52
1	D	528	ASN	CB-CG	-5.23	1.39	1.52
1	B	528	ASN	CB-CG	-5.20	1.39	1.52
1	C	768	PHE	CB-CG	-5.09	1.39	1.50
1	D	768	PHE	CB-CG	-5.07	1.39	1.50
1	B	768	PHE	CB-CG	-5.05	1.39	1.50
1	A	768	PHE	CB-CG	-5.05	1.39	1.50

All (329) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	843	LEU	N-CA-C	-13.09	97.40	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	843	LEU	N-CA-C	-13.09	97.40	113.50
1	C	843	LEU	N-CA-C	-13.08	97.41	113.50
1	D	843	LEU	N-CA-C	-13.07	97.43	113.50
1	D	78	GLY	N-CA-C	-10.98	97.67	112.82
1	C	78	GLY	N-CA-C	-10.98	97.67	112.82
1	A	78	GLY	N-CA-C	-10.97	97.68	112.82
1	B	78	GLY	N-CA-C	-10.96	97.69	112.82
1	B	454	ALA	CA-C-N	8.54	128.49	120.03
1	B	454	ALA	C-N-CA	8.54	128.49	120.03
1	A	454	ALA	CA-C-N	8.52	128.46	120.03
1	A	454	ALA	C-N-CA	8.52	128.46	120.03
1	D	454	ALA	CA-C-N	8.51	128.46	120.03
1	D	454	ALA	C-N-CA	8.51	128.46	120.03
1	C	454	ALA	CA-C-N	8.50	128.45	120.03
1	C	454	ALA	C-N-CA	8.50	128.45	120.03
1	B	94	MET	N-CA-C	-8.07	95.42	108.41
1	A	94	MET	N-CA-C	-8.06	95.43	108.41
1	C	94	MET	N-CA-C	-8.05	95.45	108.41
1	D	94	MET	N-CA-C	-8.05	95.46	108.41
1	D	55	VAL	N-CA-C	-7.94	105.75	113.53
1	A	55	VAL	N-CA-C	-7.92	105.77	113.53
1	C	55	VAL	N-CA-C	-7.92	105.77	113.53
1	B	55	VAL	N-CA-C	-7.91	105.78	113.53
1	B	773	GLY	CA-C-N	7.89	127.81	119.85
1	B	773	GLY	C-N-CA	7.89	127.81	119.85
1	D	773	GLY	CA-C-N	7.87	127.80	119.85
1	D	773	GLY	C-N-CA	7.87	127.80	119.85
1	A	773	GLY	CA-C-N	7.87	127.80	119.85
1	A	773	GLY	C-N-CA	7.87	127.80	119.85
1	C	773	GLY	CA-C-N	7.84	127.77	119.85
1	C	773	GLY	C-N-CA	7.84	127.77	119.85
1	A	549	ASP	CA-C-N	7.76	127.43	119.82
1	A	549	ASP	C-N-CA	7.76	127.43	119.82
1	C	549	ASP	CA-C-N	7.76	127.42	119.82
1	C	549	ASP	C-N-CA	7.76	127.42	119.82
1	D	549	ASP	CA-C-N	7.73	127.40	119.82
1	D	549	ASP	C-N-CA	7.73	127.40	119.82
1	B	549	ASP	CA-C-N	7.70	127.37	119.82
1	B	549	ASP	C-N-CA	7.70	127.37	119.82
1	D	51	LEU	CA-C-N	7.69	127.40	119.56
1	D	51	LEU	C-N-CA	7.69	127.40	119.56
1	A	51	LEU	CA-C-N	7.65	127.36	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	LEU	C-N-CA	7.65	127.36	119.56
1	B	51	LEU	CA-C-N	7.63	127.35	119.56
1	B	51	LEU	C-N-CA	7.63	127.35	119.56
1	C	51	LEU	CA-C-N	7.63	127.34	119.56
1	C	51	LEU	C-N-CA	7.63	127.34	119.56
1	B	313	VAL	N-CA-C	7.55	118.06	111.56
1	C	313	VAL	N-CA-C	7.55	118.06	111.56
1	D	313	VAL	N-CA-C	7.55	118.06	111.56
1	A	313	VAL	N-CA-C	7.54	118.05	111.56
1	B	539	GLY	CA-C-N	7.44	127.15	119.56
1	B	539	GLY	C-N-CA	7.44	127.15	119.56
1	C	539	GLY	CA-C-N	7.44	127.15	119.56
1	C	539	GLY	C-N-CA	7.44	127.15	119.56
1	A	539	GLY	CA-C-N	7.42	127.13	119.56
1	A	539	GLY	C-N-CA	7.42	127.13	119.56
1	D	539	GLY	CA-C-N	7.41	127.11	119.56
1	D	539	GLY	C-N-CA	7.41	127.11	119.56
1	C	467	LEU	CA-C-N	7.35	127.33	119.76
1	C	467	LEU	C-N-CA	7.35	127.33	119.76
1	B	467	LEU	CA-C-N	7.35	127.33	119.76
1	B	467	LEU	C-N-CA	7.35	127.33	119.76
1	D	467	LEU	CA-C-N	7.35	127.33	119.76
1	D	467	LEU	C-N-CA	7.35	127.33	119.76
1	A	467	LEU	CA-C-N	7.32	127.30	119.76
1	A	467	LEU	C-N-CA	7.32	127.30	119.76
1	D	346	ASP	CA-C-N	7.32	126.99	119.82
1	D	346	ASP	C-N-CA	7.32	126.99	119.82
1	C	346	ASP	CA-C-N	7.27	126.95	119.82
1	C	346	ASP	C-N-CA	7.27	126.95	119.82
1	A	346	ASP	CA-C-N	7.27	126.94	119.82
1	A	346	ASP	C-N-CA	7.27	126.94	119.82
1	B	346	ASP	CA-C-N	7.24	126.92	119.82
1	B	346	ASP	C-N-CA	7.24	126.92	119.82
1	D	855	PHE	CA-C-N	7.16	127.33	120.31
1	D	855	PHE	C-N-CA	7.16	127.33	120.31
1	C	855	PHE	CA-C-N	7.12	127.29	120.31
1	C	855	PHE	C-N-CA	7.12	127.29	120.31
1	A	855	PHE	CA-C-N	7.12	127.29	120.31
1	A	855	PHE	C-N-CA	7.12	127.29	120.31
1	B	855	PHE	CA-C-N	7.12	127.29	120.31
1	B	855	PHE	C-N-CA	7.12	127.29	120.31
1	B	164	GLY	CA-C-N	7.03	126.73	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	GLY	C-N-CA	7.03	126.73	119.56
1	C	682	ILE	CA-C-N	7.01	127.60	119.47
1	C	682	ILE	C-N-CA	7.01	127.60	119.47
1	C	164	GLY	CA-C-N	7.01	126.71	119.56
1	C	164	GLY	C-N-CA	7.01	126.71	119.56
1	A	164	GLY	CA-C-N	7.00	126.70	119.56
1	A	164	GLY	C-N-CA	7.00	126.70	119.56
1	D	424	GLY	N-CA-C	6.99	126.08	114.48
1	D	164	GLY	CA-C-N	6.98	126.68	119.56
1	D	164	GLY	C-N-CA	6.98	126.68	119.56
1	D	682	ILE	CA-C-N	6.98	127.57	119.47
1	D	682	ILE	C-N-CA	6.98	127.57	119.47
1	A	682	ILE	CA-C-N	6.97	127.56	119.47
1	A	682	ILE	C-N-CA	6.97	127.56	119.47
1	A	424	GLY	N-CA-C	6.97	126.05	114.48
1	B	682	ILE	CA-C-N	6.97	127.55	119.47
1	B	682	ILE	C-N-CA	6.97	127.55	119.47
1	B	424	GLY	N-CA-C	6.96	126.03	114.48
1	C	424	GLY	N-CA-C	6.95	126.02	114.48
1	B	105	SER	CB-CA-C	-6.84	108.67	116.54
1	C	105	SER	CB-CA-C	-6.81	108.70	116.54
1	A	105	SER	CB-CA-C	-6.80	108.72	116.54
1	D	105	SER	CB-CA-C	-6.80	108.72	116.54
1	C	690	ALA	CA-C-N	6.74	127.29	119.47
1	C	690	ALA	C-N-CA	6.74	127.29	119.47
1	A	690	ALA	CA-C-N	6.72	127.26	119.47
1	A	690	ALA	C-N-CA	6.72	127.26	119.47
1	D	690	ALA	CA-C-N	6.71	127.26	119.47
1	D	690	ALA	C-N-CA	6.71	127.26	119.47
1	B	690	ALA	CA-C-N	6.70	127.24	119.47
1	B	690	ALA	C-N-CA	6.70	127.24	119.47
1	D	462	ALA	CA-C-N	6.65	126.61	120.03
1	D	462	ALA	C-N-CA	6.65	126.61	120.03
1	A	462	ALA	CA-C-N	6.60	126.57	120.03
1	A	462	ALA	C-N-CA	6.60	126.57	120.03
1	B	462	ALA	CA-C-N	6.59	126.56	120.03
1	B	462	ALA	C-N-CA	6.59	126.56	120.03
1	C	866	ILE	N-CA-C	-6.59	106.14	111.81
1	D	866	ILE	N-CA-C	-6.59	106.14	111.81
1	B	866	ILE	N-CA-C	-6.59	106.14	111.81
1	A	866	ILE	N-CA-C	-6.59	106.14	111.81
1	C	462	ALA	CA-C-N	6.53	126.50	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	462	ALA	C-N-CA	6.53	126.50	120.03
1	D	409	HIS	CA-C-N	6.49	126.99	119.47
1	D	409	HIS	C-N-CA	6.49	126.99	119.47
1	B	409	HIS	CA-C-N	6.48	126.99	119.47
1	B	409	HIS	C-N-CA	6.48	126.99	119.47
1	C	409	HIS	CA-C-N	6.47	126.97	119.47
1	C	409	HIS	C-N-CA	6.47	126.97	119.47
1	C	727	GLN	N-CA-C	-6.45	105.42	113.55
1	A	409	HIS	CA-C-N	6.45	126.95	119.47
1	A	409	HIS	C-N-CA	6.45	126.95	119.47
1	D	727	GLN	N-CA-C	-6.45	105.43	113.55
1	A	727	GLN	N-CA-C	-6.43	105.45	113.55
1	B	727	GLN	N-CA-C	-6.39	105.50	113.55
1	D	482	PRO	CB-CA-C	6.38	119.67	111.56
1	B	482	PRO	CB-CA-C	6.37	119.64	111.56
1	A	482	PRO	CB-CA-C	6.36	119.64	111.56
1	C	482	PRO	CB-CA-C	6.36	119.64	111.56
1	C	238	THR	N-CA-C	6.36	116.67	108.34
1	D	238	THR	N-CA-C	6.36	116.67	108.34
1	A	238	THR	N-CA-C	6.36	116.67	108.34
1	B	238	THR	N-CA-C	6.35	116.66	108.34
1	A	11	GLY	CA-C-N	6.33	126.36	119.90
1	A	11	GLY	C-N-CA	6.33	126.36	119.90
1	C	11	GLY	CA-C-N	6.33	126.36	119.90
1	C	11	GLY	C-N-CA	6.33	126.36	119.90
1	B	808	SER	CB-CA-C	-6.31	109.28	116.54
1	B	11	GLY	CA-C-N	6.29	126.32	119.90
1	B	11	GLY	C-N-CA	6.29	126.32	119.90
1	C	808	SER	CB-CA-C	-6.29	109.31	116.54
1	C	775	GLY	CA-C-N	6.29	129.34	120.28
1	C	775	GLY	C-N-CA	6.29	129.34	120.28
1	D	11	GLY	CA-C-N	6.29	126.31	119.90
1	D	11	GLY	C-N-CA	6.29	126.31	119.90
1	A	775	GLY	CA-C-N	6.28	129.32	120.28
1	A	775	GLY	C-N-CA	6.28	129.32	120.28
1	A	808	SER	CB-CA-C	-6.27	109.33	116.54
1	B	775	GLY	CA-C-N	6.27	129.31	120.28
1	B	775	GLY	C-N-CA	6.27	129.31	120.28
1	D	775	GLY	CA-C-N	6.26	129.29	120.28
1	D	775	GLY	C-N-CA	6.26	129.29	120.28
1	D	808	SER	CB-CA-C	-6.25	109.35	116.54
1	D	481	PRO	CB-CA-C	6.22	118.51	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	481	PRO	CB-CA-C	6.20	118.49	110.92
1	C	481	PRO	CB-CA-C	6.20	118.48	110.92
1	A	481	PRO	CB-CA-C	6.20	118.48	110.92
1	A	324	ILE	CA-C-N	6.13	126.09	120.03
1	A	324	ILE	C-N-CA	6.13	126.09	120.03
1	C	324	ILE	CA-C-N	6.12	126.09	120.03
1	C	324	ILE	C-N-CA	6.12	126.09	120.03
1	C	473	ALA	CA-C-N	6.11	125.79	119.56
1	C	473	ALA	C-N-CA	6.11	125.79	119.56
1	B	324	ILE	CA-C-N	6.11	126.08	120.03
1	B	324	ILE	C-N-CA	6.11	126.08	120.03
1	D	870	ASN	CA-C-N	6.11	126.08	120.03
1	D	870	ASN	C-N-CA	6.11	126.08	120.03
1	B	381	LEU	CA-C-N	6.10	126.06	119.78
1	B	381	LEU	C-N-CA	6.10	126.06	119.78
1	B	473	ALA	CA-C-N	6.08	125.77	119.56
1	B	473	ALA	C-N-CA	6.08	125.77	119.56
1	D	324	ILE	CA-C-N	6.08	126.05	120.03
1	D	324	ILE	C-N-CA	6.08	126.05	120.03
1	D	381	LEU	CA-C-N	6.08	126.05	119.78
1	D	381	LEU	C-N-CA	6.08	126.05	119.78
1	A	473	ALA	CA-C-N	6.08	125.76	119.56
1	A	473	ALA	C-N-CA	6.08	125.76	119.56
1	D	473	ALA	CA-C-N	6.08	125.76	119.56
1	D	473	ALA	C-N-CA	6.08	125.76	119.56
1	A	381	LEU	CA-C-N	6.07	126.03	119.78
1	A	381	LEU	C-N-CA	6.07	126.03	119.78
1	A	870	ASN	CA-C-N	6.07	126.04	120.03
1	A	870	ASN	C-N-CA	6.07	126.04	120.03
1	B	870	ASN	CA-C-N	6.07	126.04	120.03
1	B	870	ASN	C-N-CA	6.07	126.04	120.03
1	C	870	ASN	CA-C-N	6.07	126.04	120.03
1	C	870	ASN	C-N-CA	6.07	126.04	120.03
1	C	381	LEU	CA-C-N	6.07	126.03	119.78
1	C	381	LEU	C-N-CA	6.07	126.03	119.78
1	C	837	ILE	N-CA-C	6.00	118.55	111.05
1	D	837	ILE	N-CA-C	5.99	118.54	111.05
1	A	837	ILE	N-CA-C	5.97	118.52	111.05
1	B	837	ILE	N-CA-C	5.97	118.51	111.05
1	A	271	ILE	N-CA-C	5.93	116.47	108.17
1	C	271	ILE	N-CA-C	5.92	116.46	108.17
1	B	271	ILE	N-CA-C	5.92	116.46	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	271	ILE	N-CA-C	5.90	116.44	108.17
1	B	749	ASN	CA-C-N	5.82	126.22	119.47
1	B	749	ASN	C-N-CA	5.82	126.22	119.47
1	A	749	ASN	CA-C-N	5.79	126.19	119.47
1	A	749	ASN	C-N-CA	5.79	126.19	119.47
1	B	571	PHE	N-CA-C	5.79	121.06	113.30
1	C	97	GLY	N-CA-C	5.79	126.89	113.18
1	C	749	ASN	CA-C-N	5.78	126.18	119.47
1	C	749	ASN	C-N-CA	5.78	126.18	119.47
1	D	749	ASN	CA-C-N	5.77	126.17	119.47
1	D	749	ASN	C-N-CA	5.77	126.17	119.47
1	A	97	GLY	N-CA-C	5.77	126.85	113.18
1	D	97	GLY	N-CA-C	5.76	126.84	113.18
1	D	571	PHE	N-CA-C	5.75	121.01	113.30
1	A	571	PHE	N-CA-C	5.75	121.01	113.30
1	C	571	PHE	N-CA-C	5.75	121.01	113.30
1	D	95	THR	CB-CA-C	-5.75	101.52	111.30
1	B	97	GLY	N-CA-C	5.75	126.81	113.18
1	A	95	THR	CB-CA-C	-5.75	101.53	111.30
1	C	95	THR	CB-CA-C	-5.74	101.55	111.30
1	B	95	THR	CB-CA-C	-5.72	101.58	111.30
1	A	480	PHE	O-C-N	5.71	126.51	121.37
1	B	480	PHE	O-C-N	5.71	126.51	121.37
1	C	781	ASP	CA-C-N	5.71	128.50	120.28
1	C	781	ASP	C-N-CA	5.71	128.50	120.28
1	D	480	PHE	O-C-N	5.70	126.50	121.37
1	A	781	ASP	CA-C-N	5.69	128.48	120.28
1	A	781	ASP	C-N-CA	5.69	128.48	120.28
1	C	480	PHE	O-C-N	5.67	126.48	121.37
1	D	781	ASP	CA-C-N	5.66	128.43	120.28
1	D	781	ASP	C-N-CA	5.66	128.43	120.28
1	B	781	ASP	CA-C-N	5.66	128.43	120.28
1	B	781	ASP	C-N-CA	5.66	128.43	120.28
1	B	243	PHE	N-CA-C	-5.65	101.34	110.32
1	C	243	PHE	N-CA-C	-5.64	101.35	110.32
1	A	243	PHE	N-CA-C	-5.63	101.37	110.32
1	D	147	LEU	N-CA-C	-5.63	106.46	113.55
1	B	147	LEU	N-CA-C	-5.63	106.46	113.55
1	D	243	PHE	N-CA-C	-5.62	101.38	110.32
1	C	621	ASP	CA-C-N	5.62	125.29	119.56
1	C	621	ASP	C-N-CA	5.62	125.29	119.56
1	A	147	LEU	N-CA-C	-5.60	106.50	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	147	LEU	N-CA-C	-5.59	106.51	113.55
1	C	262	PRO	N-CA-C	-5.55	102.39	111.21
1	D	484	THR	CB-CA-C	5.55	117.22	108.84
1	A	262	PRO	N-CA-C	-5.54	102.40	111.21
1	A	621	ASP	CA-C-N	5.54	125.21	119.56
1	A	621	ASP	C-N-CA	5.54	125.21	119.56
1	B	262	PRO	N-CA-C	-5.53	102.41	111.21
1	A	484	THR	CB-CA-C	5.53	117.19	108.84
1	D	262	PRO	N-CA-C	-5.53	102.42	111.21
1	C	484	THR	CB-CA-C	5.53	117.19	108.84
1	B	484	THR	CB-CA-C	5.53	117.19	108.84
1	B	621	ASP	CA-C-N	5.52	125.19	119.56
1	B	621	ASP	C-N-CA	5.52	125.19	119.56
1	D	621	ASP	CA-C-N	5.52	125.19	119.56
1	D	621	ASP	C-N-CA	5.52	125.19	119.56
1	B	481	PRO	N-CA-C	5.46	117.36	110.70
1	C	481	PRO	N-CA-C	5.43	117.33	110.70
1	A	481	PRO	N-CA-C	5.42	117.31	110.70
1	D	481	PRO	N-CA-C	5.42	117.31	110.70
1	A	644	ASN	CA-C-N	5.41	125.75	119.47
1	A	644	ASN	C-N-CA	5.41	125.75	119.47
1	B	644	ASN	CA-C-N	5.41	125.75	119.47
1	B	644	ASN	C-N-CA	5.41	125.75	119.47
1	C	644	ASN	CA-C-N	5.39	125.72	119.47
1	C	644	ASN	C-N-CA	5.39	125.72	119.47
1	D	644	ASN	CA-C-N	5.38	125.71	119.47
1	D	644	ASN	C-N-CA	5.38	125.71	119.47
1	D	261	LYS	CA-C-N	5.33	125.27	119.78
1	D	261	LYS	C-N-CA	5.33	125.27	119.78
1	B	261	LYS	CA-C-N	5.32	125.26	119.78
1	B	261	LYS	C-N-CA	5.32	125.26	119.78
1	A	261	LYS	CA-C-N	5.30	125.25	119.78
1	A	261	LYS	C-N-CA	5.30	125.25	119.78
1	D	499	LYS	N-CA-C	5.27	116.71	111.07
1	A	499	LYS	N-CA-C	5.27	116.71	111.07
1	C	261	LYS	CA-C-N	5.26	125.19	119.78
1	C	261	LYS	C-N-CA	5.26	125.19	119.78
1	B	499	LYS	N-CA-C	5.25	116.69	111.07
1	C	499	LYS	N-CA-C	5.25	116.68	111.07
1	C	776	ASP	N-CA-C	5.24	117.74	111.71
1	D	776	ASP	N-CA-C	5.23	117.73	111.71
1	A	776	ASP	N-CA-C	5.23	117.72	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	776	ASP	N-CA-C	5.20	117.68	111.71
1	D	96	ALA	N-CA-C	5.14	116.96	108.13
1	C	96	ALA	N-CA-C	5.13	116.96	108.13
1	A	96	ALA	N-CA-C	5.12	116.94	108.13
1	D	234	VAL	CA-C-N	5.12	125.03	119.76
1	D	234	VAL	C-N-CA	5.12	125.03	119.76
1	C	829	TYR	N-CA-C	5.11	118.44	111.39
1	A	234	VAL	CA-C-N	5.10	125.02	119.76
1	A	234	VAL	C-N-CA	5.10	125.02	119.76
1	C	753	TYR	N-CA-C	-5.10	105.42	111.69
1	A	753	TYR	N-CA-C	-5.09	105.42	111.69
1	B	138	ASP	N-CA-C	-5.09	106.16	112.93
1	B	234	VAL	CA-C-N	5.09	125.01	119.76
1	B	234	VAL	C-N-CA	5.09	125.01	119.76
1	A	829	TYR	N-CA-C	5.09	118.42	111.39
1	B	829	TYR	N-CA-C	5.09	118.41	111.39
1	D	829	TYR	N-CA-C	5.09	118.41	111.39
1	D	138	ASP	N-CA-C	-5.08	106.18	112.93
1	C	138	ASP	N-CA-C	-5.08	106.18	112.93
1	C	234	VAL	CA-C-N	5.08	124.99	119.76
1	C	234	VAL	C-N-CA	5.08	124.99	119.76
1	D	457	PHE	N-CA-C	5.08	121.17	114.12
1	C	457	PHE	N-CA-C	5.07	121.17	114.12
1	B	753	TYR	N-CA-C	-5.07	105.45	111.69
1	A	138	ASP	N-CA-C	-5.07	106.19	112.93
1	A	457	PHE	N-CA-C	5.07	121.16	114.12
1	B	457	PHE	N-CA-C	5.07	121.16	114.12
1	D	753	TYR	N-CA-C	-5.06	105.47	111.69
1	C	774	PRO	N-CA-C	5.04	119.39	111.38
1	A	774	PRO	N-CA-C	5.02	119.37	111.38
1	D	774	PRO	N-CA-C	5.02	119.36	111.38
1	B	614	TYR	N-CA-C	5.01	117.41	109.50
1	B	774	PRO	N-CA-C	5.01	119.34	111.38
1	C	614	TYR	N-CA-C	5.01	117.41	109.50

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	6657	0	6685	15	0
1	B	6657	0	6685	14	0
1	C	6657	0	6685	15	0
1	D	6657	0	6685	15	0
2	A	62	0	24	0	0
2	B	62	0	24	0	0
2	C	62	0	24	0	0
2	D	62	0	24	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
All	All	26888	0	26836	59	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 1.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ILE:HG22	1:A:423:ILE:O	1.74	0.88
1:B:423:ILE:O	1:B:423:ILE:HG22	1.74	0.87
1:D:423:ILE:HG22	1:D:423:ILE:O	1.73	0.85
1:C:423:ILE:HG22	1:C:423:ILE:O	1.73	0.85
1:A:423:ILE:O	1:A:423:ILE:CG2	2.39	0.70
1:D:423:ILE:O	1:D:423:ILE:CG2	2.39	0.70
1:B:423:ILE:O	1:B:423:ILE:CG2	2.39	0.70
1:C:423:ILE:O	1:C:423:ILE:CG2	2.39	0.70
1:C:814:ASP:OD2	1:C:818:LYS:NZ	2.41	0.54
1:D:814:ASP:OD2	1:D:818:LYS:NZ	2.41	0.54
1:A:814:ASP:OD2	1:A:818:LYS:NZ	2.41	0.53
1:B:814:ASP:OD2	1:B:818:LYS:NZ	2.41	0.53
1:A:776:ASP:N	1:A:776:ASP:OD1	2.42	0.52
1:C:776:ASP:OD1	1:C:776:ASP:N	2.42	0.52
1:D:776:ASP:N	1:D:776:ASP:OD1	2.42	0.52
1:A:841:LYS:NZ	1:A:844:ASP:OD2	2.46	0.48
1:B:776:ASP:N	1:B:776:ASP:OD1	2.42	0.48
1:B:841:LYS:NZ	1:B:844:ASP:OD2	2.46	0.48
1:D:841:LYS:NZ	1:D:844:ASP:OD2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:841:LYS:NZ	1:C:844:ASP:OD2	2.46	0.47
1:A:104:THR:OG1	1:A:105:SER:N	2.48	0.47
1:B:104:THR:OG1	1:B:105:SER:N	2.48	0.46
1:A:253:VAL:HG21	1:A:299:VAL:O	2.15	0.46
1:B:253:VAL:HG21	1:B:299:VAL:O	2.15	0.46
1:C:299:VAL:HG12	1:C:299:VAL:O	2.15	0.46
1:D:299:VAL:O	1:D:299:VAL:HG12	2.15	0.46
1:B:299:VAL:O	1:B:299:VAL:HG12	2.15	0.46
1:C:104:THR:OG1	1:C:105:SER:N	2.48	0.46
1:D:104:THR:OG1	1:D:105:SER:N	2.48	0.46
1:D:253:VAL:HG21	1:D:299:VAL:O	2.15	0.46
1:C:253:VAL:HG21	1:C:299:VAL:O	2.15	0.46
1:D:800:GLU:OE1	1:D:800:GLU:N	2.48	0.46
1:A:299:VAL:O	1:A:299:VAL:HG12	2.15	0.46
1:C:800:GLU:OE1	1:C:800:GLU:N	2.48	0.45
1:C:481:PRO:HA	1:C:482:PRO:HD3	1.93	0.45
1:D:481:PRO:HA	1:D:482:PRO:HD3	1.93	0.45
1:A:800:GLU:OE1	1:A:800:GLU:N	2.48	0.44
1:B:800:GLU:OE1	1:B:800:GLU:N	2.48	0.44
1:C:238:THR:OG1	1:C:239:THR:N	2.51	0.43
1:D:238:THR:OG1	1:D:239:THR:N	2.51	0.43
1:B:473:ALA:HB3	1:B:474:PRO:HD3	2.00	0.43
1:A:473:ALA:HB3	1:A:474:PRO:HD3	2.00	0.43
1:A:304:GLU:OE1	1:A:304:GLU:N	2.52	0.43
1:B:304:GLU:OE1	1:B:304:GLU:N	2.52	0.43
1:C:473:ALA:HB3	1:C:474:PRO:HD3	2.00	0.42
1:D:473:ALA:HB3	1:D:474:PRO:HD3	2.00	0.42
1:A:238:THR:OG1	1:A:239:THR:N	2.51	0.42
1:D:304:GLU:OE1	1:D:304:GLU:N	2.52	0.42
1:C:304:GLU:OE1	1:C:304:GLU:N	2.52	0.42
1:B:238:THR:OG1	1:B:239:THR:N	2.52	0.42
1:B:105:SER:OG	1:B:106:THR:N	2.53	0.41
1:A:105:SER:OG	1:A:106:THR:N	2.53	0.41
1:B:60:SER:N	1:B:61:PRO:CD	2.84	0.41
1:A:60:SER:N	1:A:61:PRO:CD	2.84	0.41
1:C:60:SER:N	1:C:61:PRO:CD	2.84	0.41
1:D:60:SER:N	1:D:61:PRO:CD	2.84	0.41
1:A:256:TYR:O	1:A:258:VAL:N	2.55	0.40
1:C:808:SER:OG	1:C:809:GLU:N	2.54	0.40
1:D:808:SER:OG	1:D:809:GLU:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	867/879 (99%)	833 (96%)	34 (4%)	0	100	100
1	B	867/879 (99%)	833 (96%)	34 (4%)	0	100	100
1	C	867/879 (99%)	833 (96%)	34 (4%)	0	100	100
1	D	867/879 (99%)	833 (96%)	34 (4%)	0	100	100
All	All	3468/3516 (99%)	3332 (96%)	136 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	712/719 (99%)	712 (100%)	0	100	100
1	B	712/719 (99%)	712 (100%)	0	100	100
1	C	712/719 (99%)	712 (100%)	0	100	100
1	D	712/719 (99%)	712 (100%)	0	100	100
All	All	2848/2876 (99%)	2848 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	460	HIS
1	A	586	HIS
1	A	650	HIS
1	B	460	HIS
1	B	586	HIS
1	B	650	HIS
1	C	460	HIS
1	C	586	HIS
1	C	650	HIS
1	D	460	HIS
1	D	586	HIS
1	D	650	HIS

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 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 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	ATP	B	902	3	32,33,33	0.55	0	48,52,52	0.60	0
2	ATP	D	902	3	32,33,33	0.53	0	48,52,52	0.60	0
2	ATP	B	901	3	32,33,33	0.90	3 (9%)	48,52,52	0.82	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	A	901	3	32,33,33	0.90	2 (6%)	48,52,52	0.82	1 (2%)
2	ATP	C	902	3	32,33,33	0.54	0	48,52,52	0.60	0
2	ATP	D	901	3	32,33,33	0.90	2 (6%)	48,52,52	0.82	1 (2%)
2	ATP	C	901	3	32,33,33	0.89	3 (9%)	48,52,52	0.82	1 (2%)
2	ATP	A	902	3	32,33,33	0.54	0	48,52,52	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	B	902	3	-	5/22/38/38	0/3/3/3
2	ATP	D	902	3	-	5/22/38/38	0/3/3/3
2	ATP	B	901	3	-	8/22/38/38	0/3/3/3
2	ATP	A	901	3	-	8/22/38/38	0/3/3/3
2	ATP	C	902	3	-	5/22/38/38	0/3/3/3
2	ATP	D	901	3	-	8/22/38/38	0/3/3/3
2	ATP	C	901	3	-	8/22/38/38	0/3/3/3
2	ATP	A	902	3	-	5/22/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ATP	PG-O2G	-2.25	1.46	1.54
2	A	901	ATP	PG-O2G	-2.24	1.46	1.54
2	C	901	ATP	PG-O2G	-2.24	1.46	1.54
2	D	901	ATP	PG-O2G	-2.22	1.46	1.54
2	C	901	ATP	PB-O2B	-2.06	1.45	1.55
2	A	901	ATP	PB-O2B	-2.06	1.45	1.55
2	D	901	ATP	PB-O2B	-2.05	1.45	1.55
2	B	901	ATP	PB-O2B	-2.04	1.45	1.55
2	C	901	ATP	PG-O3G	-2.02	1.47	1.54
2	B	901	ATP	PG-O3G	-2.01	1.47	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901	ATP	O2A-PA-O3A	2.65	114.43	107.27

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	ATP	O2A-PA-O3A	2.64	114.41	107.27
2	D	901	ATP	O2A-PA-O3A	2.64	114.41	107.27
2	B	901	ATP	O2A-PA-O3A	2.63	114.39	107.27

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	ATP	PB-O3B-PG-O2G
2	A	901	ATP	C5'-O5'-PA-O1A
2	A	901	ATP	C5'-O5'-PA-O3A
2	A	902	ATP	C5'-O5'-PA-O1A
2	A	902	ATP	C5'-O5'-PA-O2A
2	A	902	ATP	C5'-O5'-PA-O3A
2	B	901	ATP	PB-O3B-PG-O2G
2	B	901	ATP	C5'-O5'-PA-O1A
2	B	901	ATP	C5'-O5'-PA-O3A
2	B	902	ATP	C5'-O5'-PA-O1A
2	B	902	ATP	C5'-O5'-PA-O2A
2	B	902	ATP	C5'-O5'-PA-O3A
2	C	901	ATP	PB-O3B-PG-O2G
2	C	901	ATP	C5'-O5'-PA-O1A
2	C	901	ATP	C5'-O5'-PA-O3A
2	C	902	ATP	C5'-O5'-PA-O1A
2	C	902	ATP	C5'-O5'-PA-O2A
2	C	902	ATP	C5'-O5'-PA-O3A
2	D	901	ATP	PB-O3B-PG-O2G
2	D	901	ATP	C5'-O5'-PA-O1A
2	D	901	ATP	C5'-O5'-PA-O3A
2	D	902	ATP	C5'-O5'-PA-O1A
2	D	902	ATP	C5'-O5'-PA-O2A
2	D	902	ATP	C5'-O5'-PA-O3A
2	A	901	ATP	O4'-C4'-C5'-O5'
2	A	901	ATP	C3'-C4'-C5'-O5'
2	A	902	ATP	O4'-C4'-C5'-O5'
2	A	902	ATP	C3'-C4'-C5'-O5'
2	B	901	ATP	O4'-C4'-C5'-O5'
2	B	901	ATP	C3'-C4'-C5'-O5'
2	B	902	ATP	O4'-C4'-C5'-O5'
2	B	902	ATP	C3'-C4'-C5'-O5'
2	C	901	ATP	O4'-C4'-C5'-O5'
2	C	901	ATP	C3'-C4'-C5'-O5'

Continued on next page...

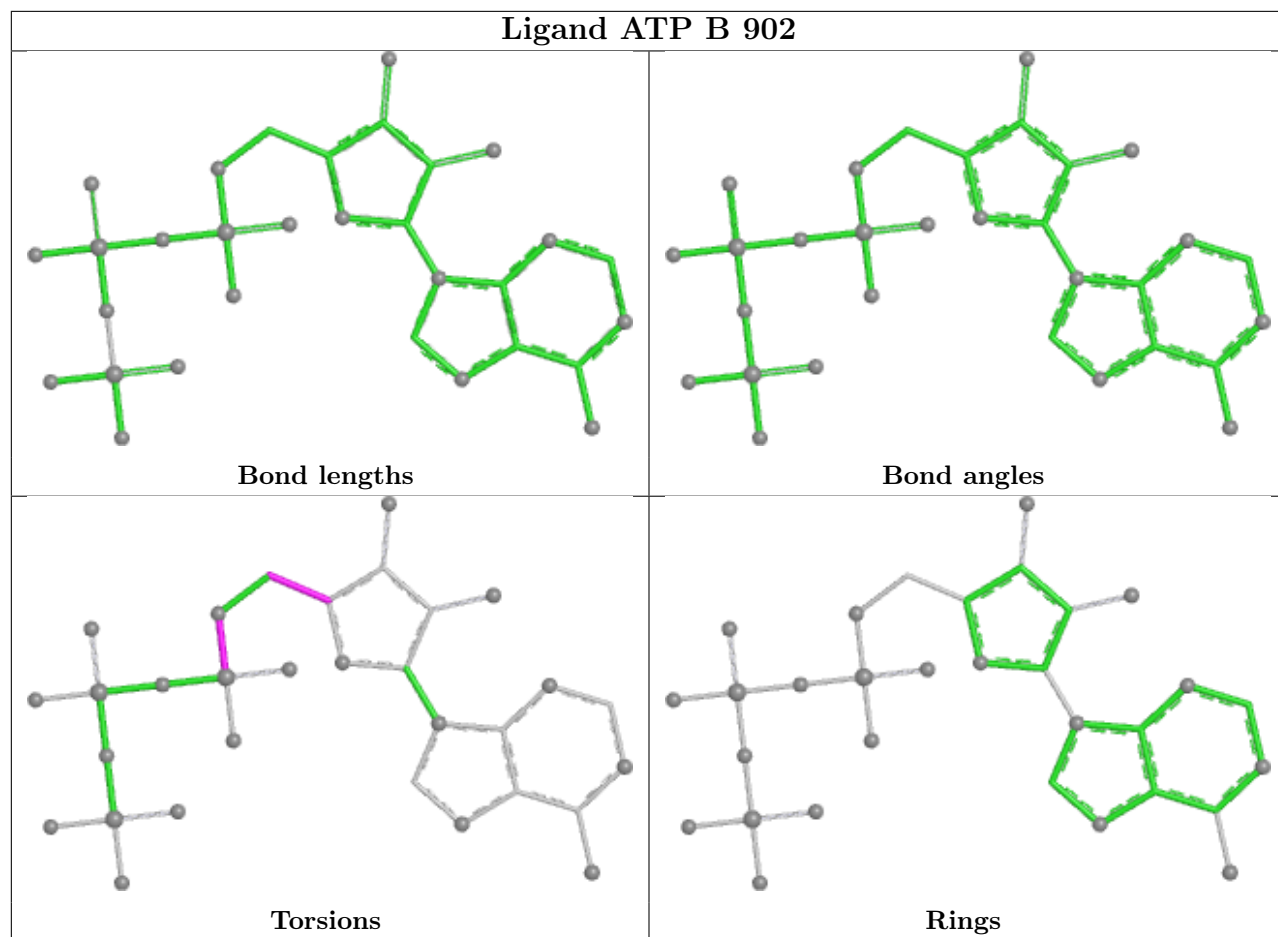
Continued from previous page...

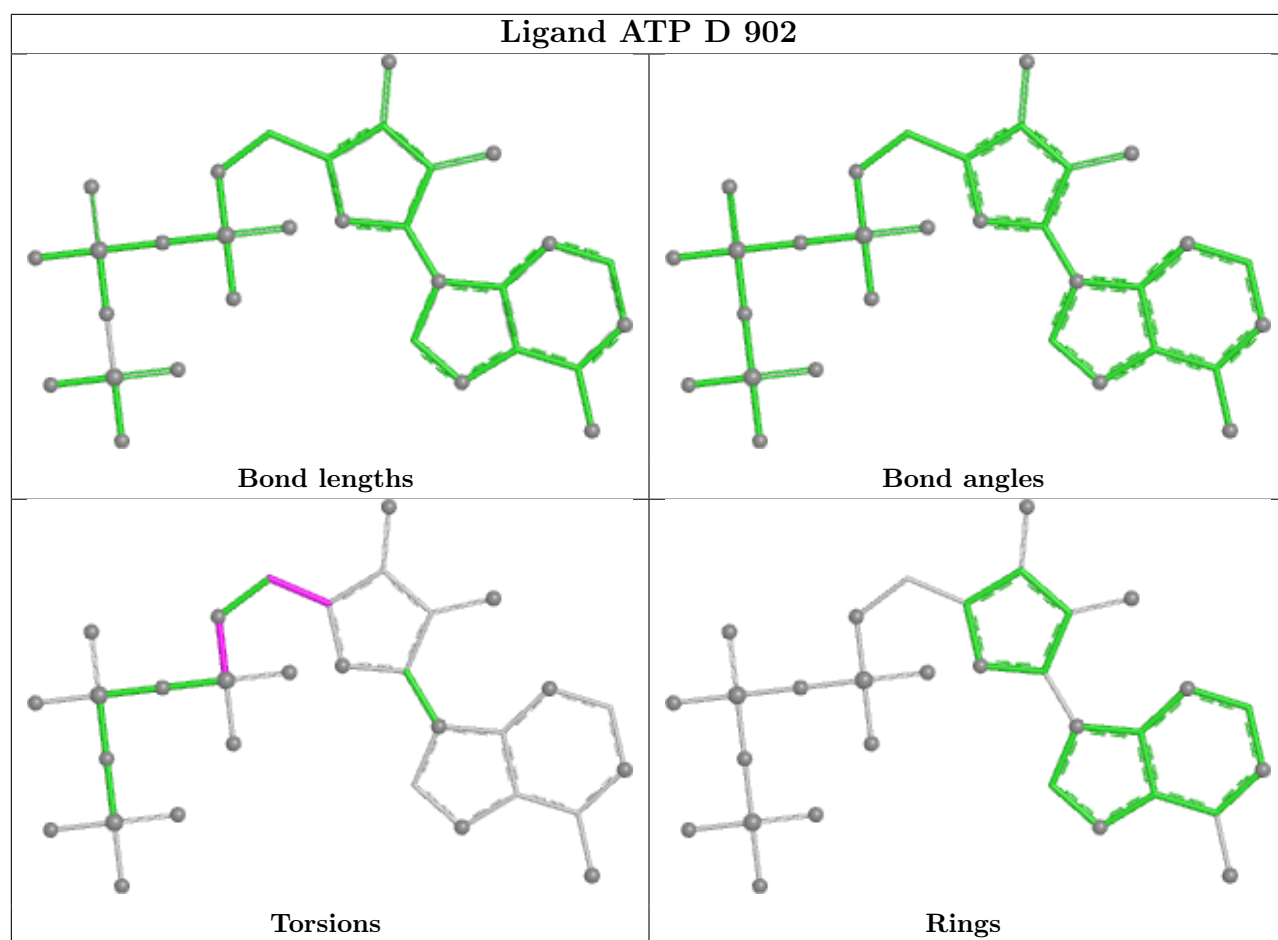
Mol	Chain	Res	Type	Atoms
2	C	902	ATP	O4'-C4'-C5'-O5'
2	C	902	ATP	C3'-C4'-C5'-O5'
2	D	901	ATP	O4'-C4'-C5'-O5'
2	D	901	ATP	C3'-C4'-C5'-O5'
2	D	902	ATP	O4'-C4'-C5'-O5'
2	D	902	ATP	C3'-C4'-C5'-O5'
2	A	901	ATP	PA-O3A-PB-O1B
2	B	901	ATP	PA-O3A-PB-O1B
2	C	901	ATP	PA-O3A-PB-O1B
2	D	901	ATP	PA-O3A-PB-O1B
2	A	901	ATP	PA-O3A-PB-O2B
2	B	901	ATP	PA-O3A-PB-O2B
2	C	901	ATP	PA-O3A-PB-O2B
2	D	901	ATP	PA-O3A-PB-O2B
2	A	901	ATP	C2'-C1'-N9-C8
2	B	901	ATP	C2'-C1'-N9-C8
2	C	901	ATP	C2'-C1'-N9-C8
2	D	901	ATP	C2'-C1'-N9-C8

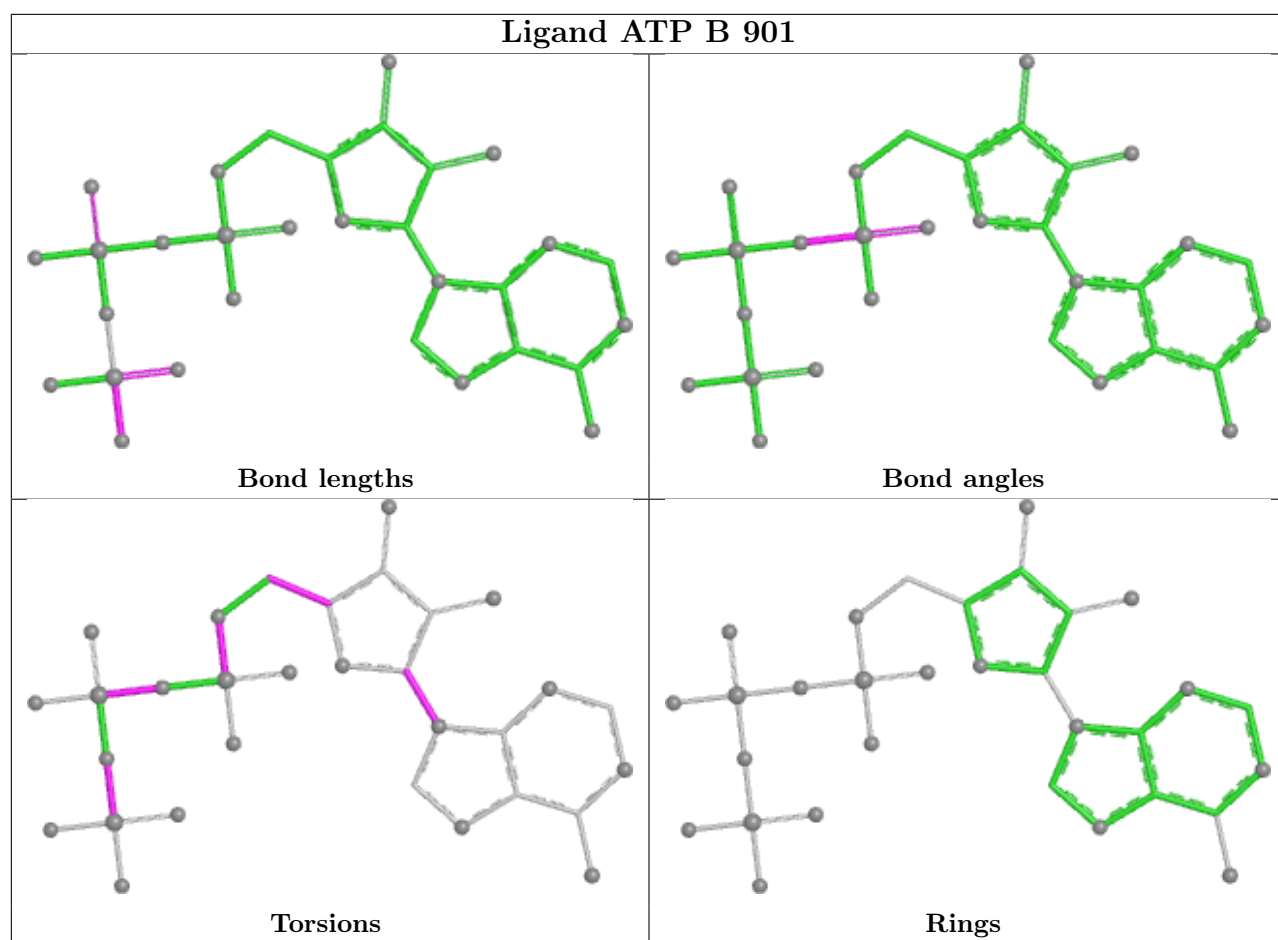
There are no ring outliers.

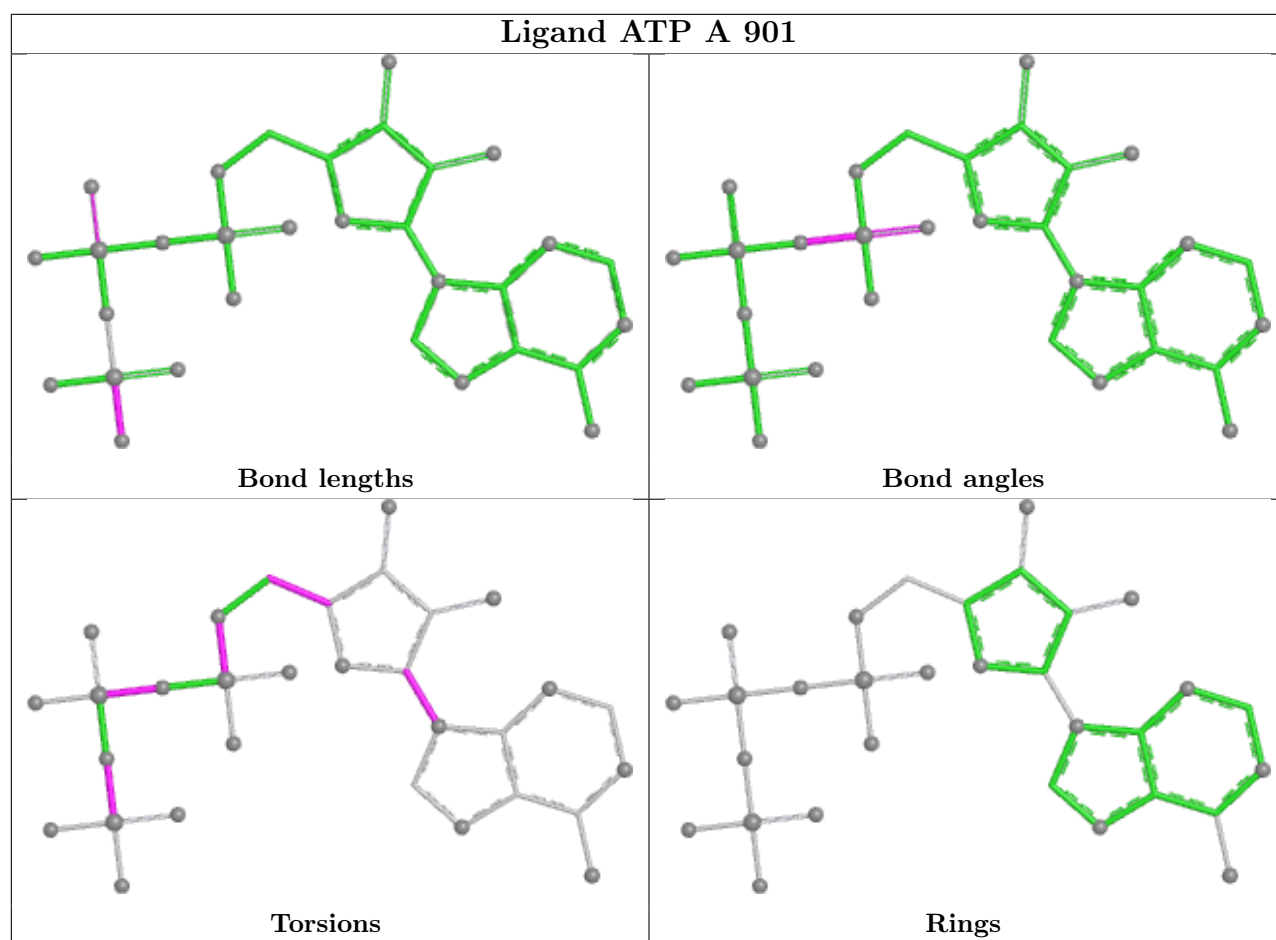
No monomer is involved in short contacts.

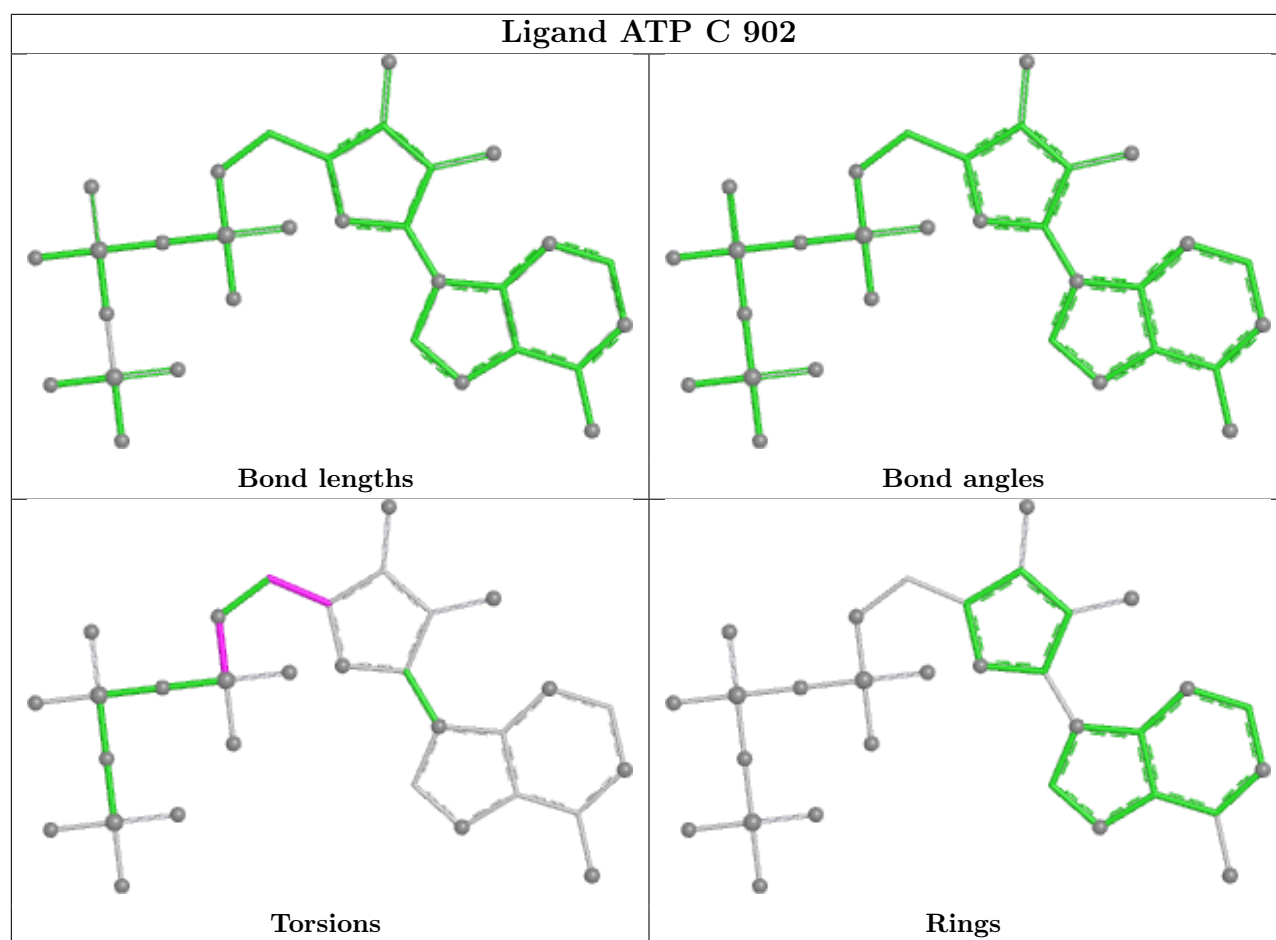
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

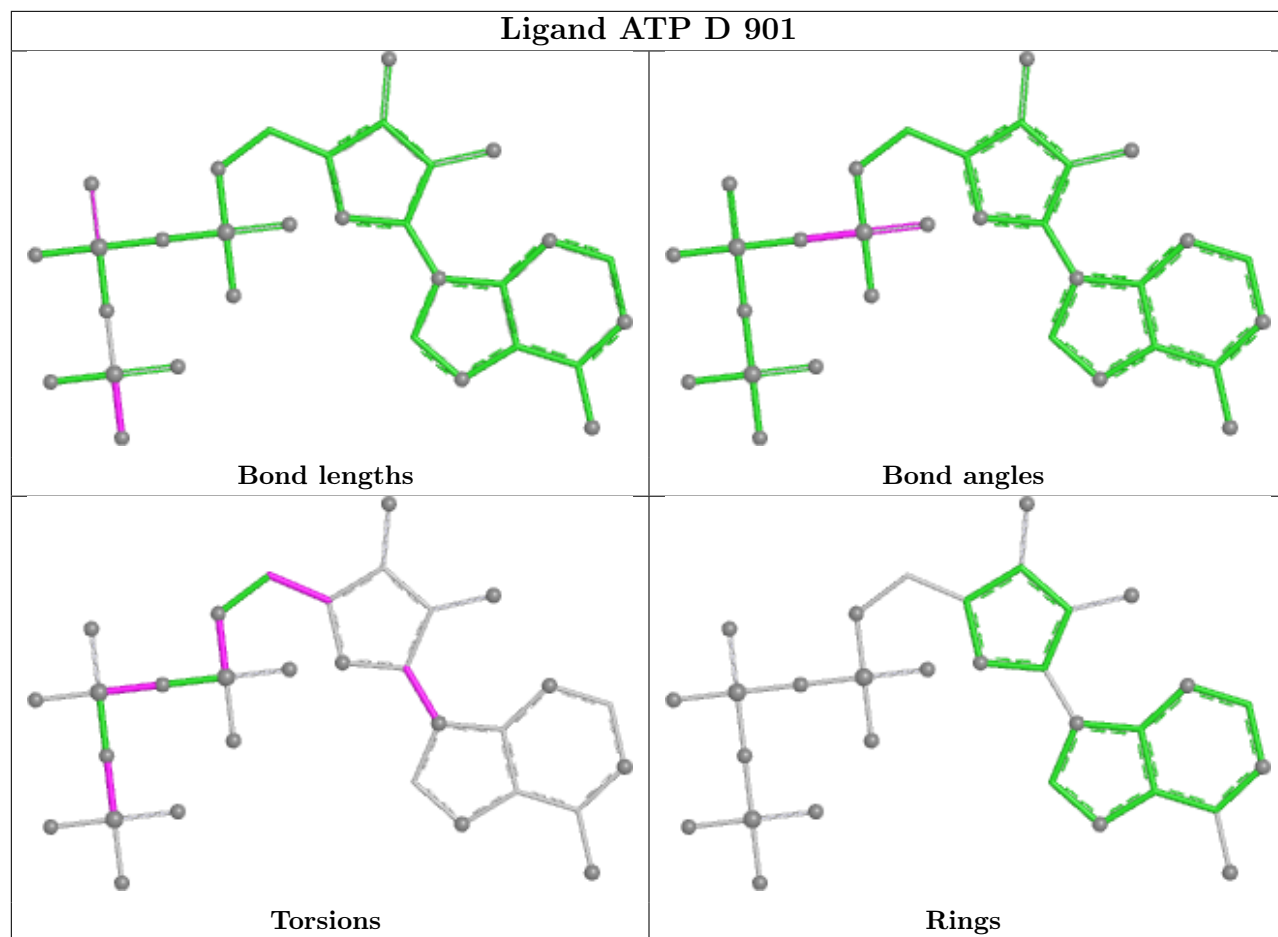


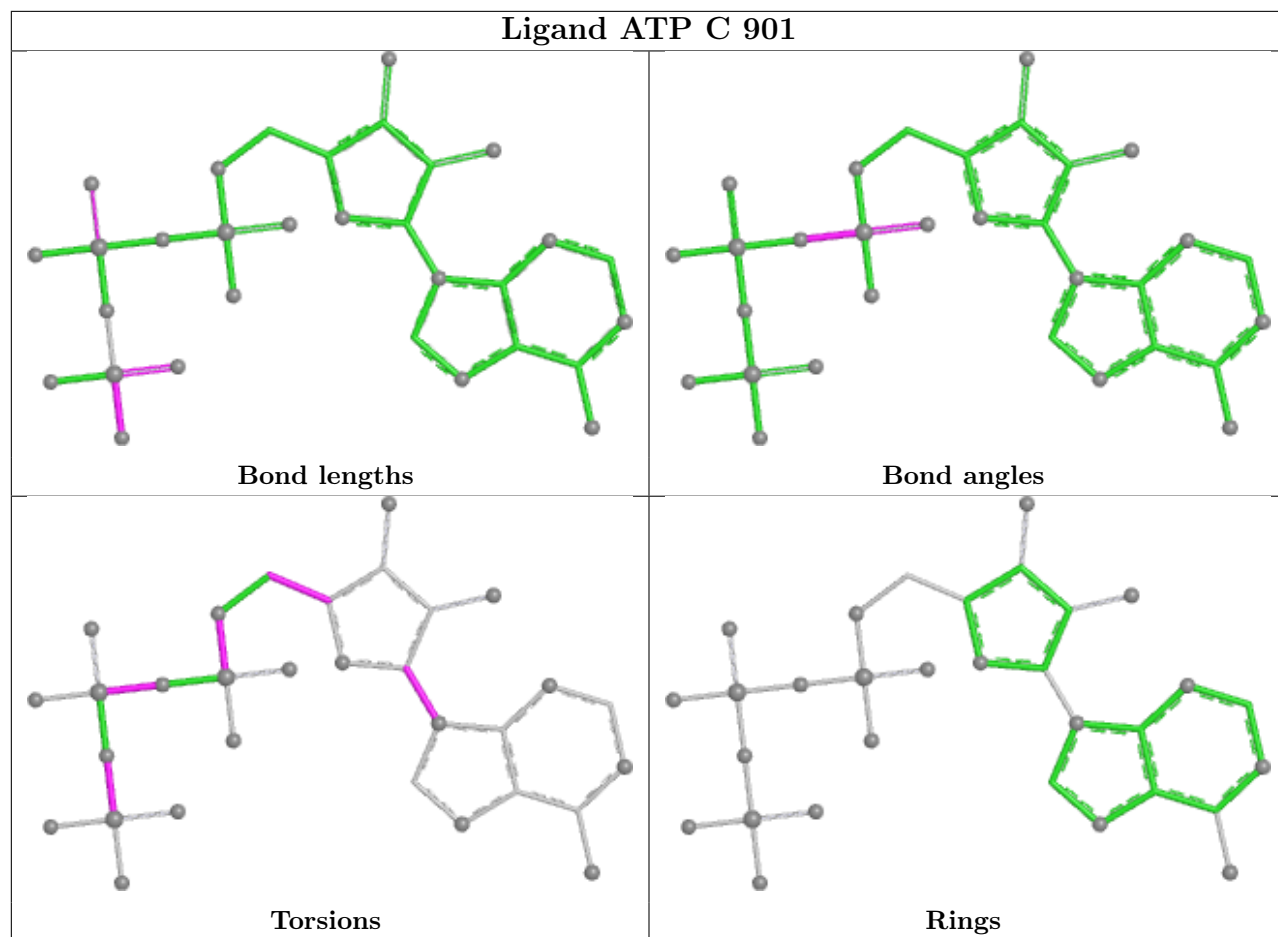


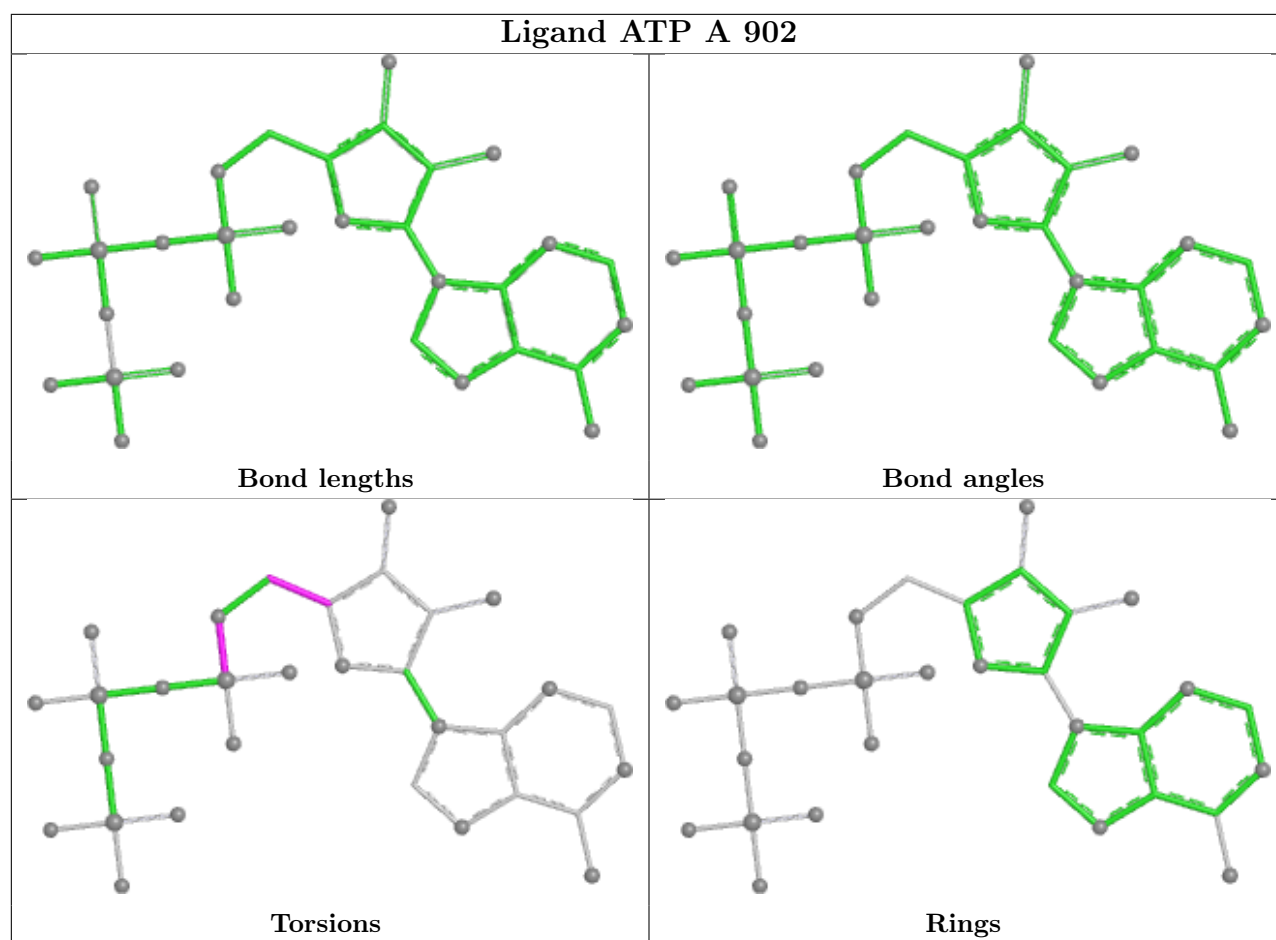












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

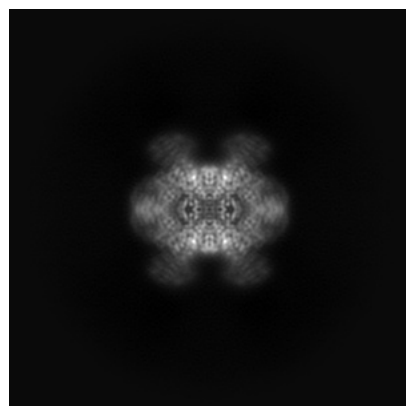
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23311. These allow visual inspection of the internal detail of the map and identification of artifacts.

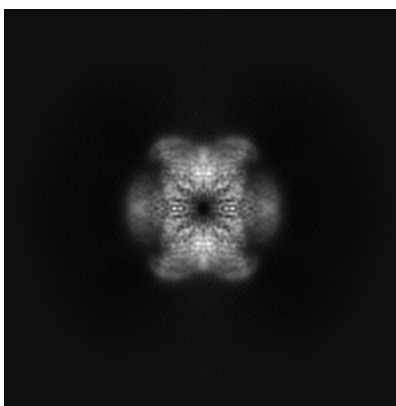
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

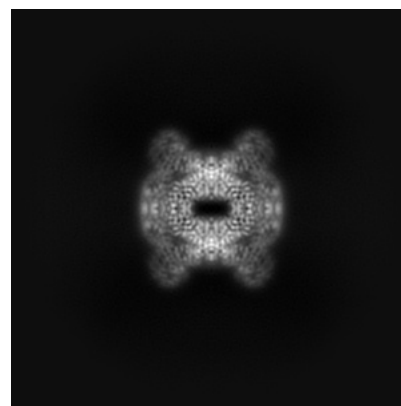
6.1.1 Primary map



X

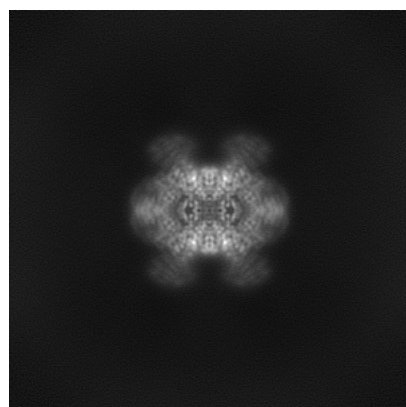


Y

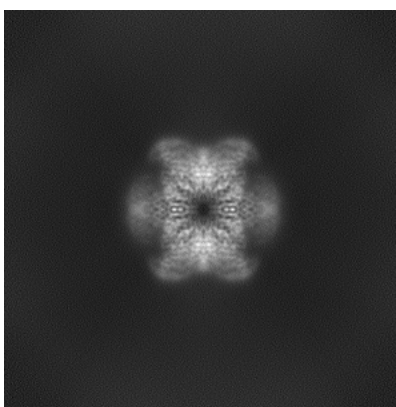


Z

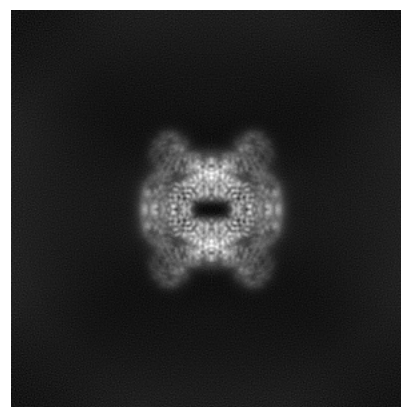
6.1.2 Raw map



X



Y

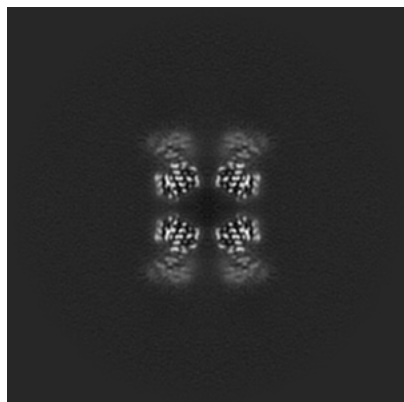


Z

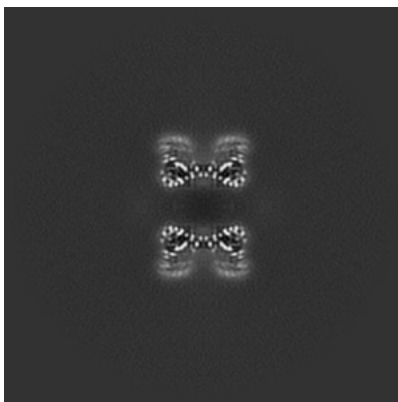
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

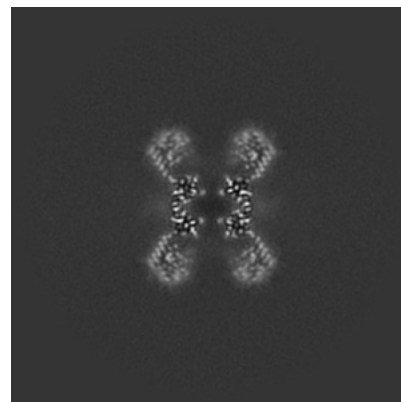
6.2.1 Primary map



X Index: 200

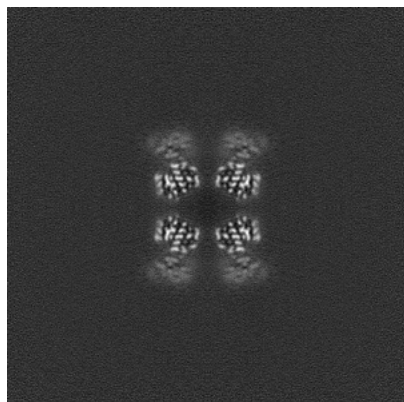


Y Index: 200

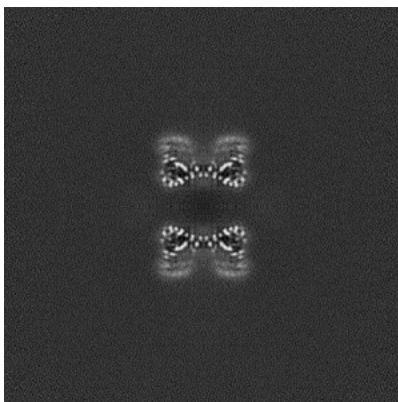


Z Index: 200

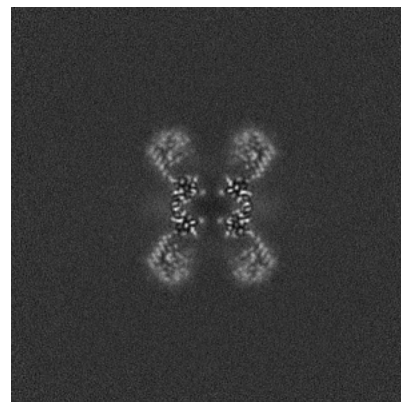
6.2.2 Raw map



X Index: 200



Y Index: 200

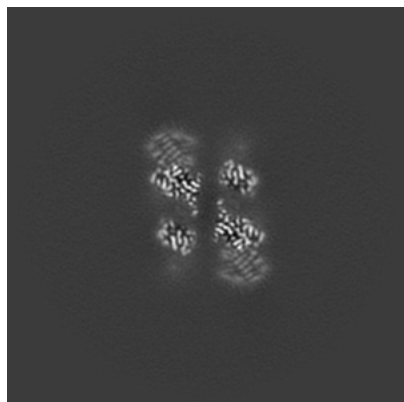


Z Index: 200

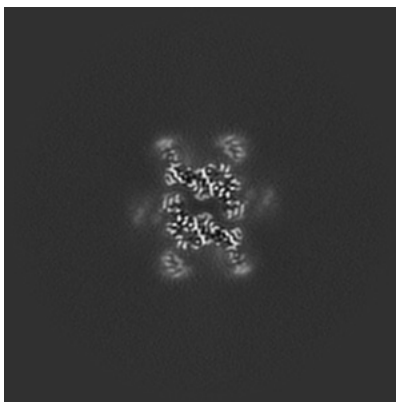
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

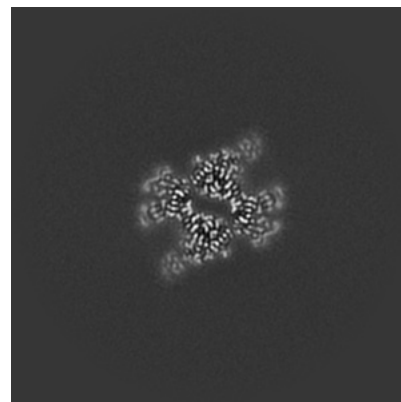
6.3.1 Primary map



X Index: 188

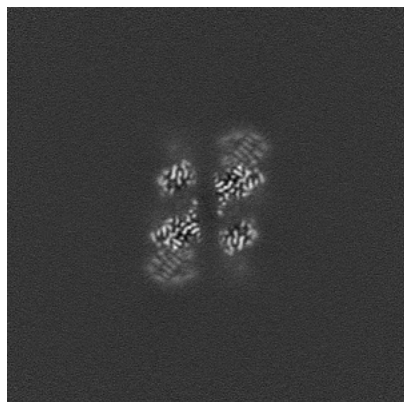


Y Index: 214

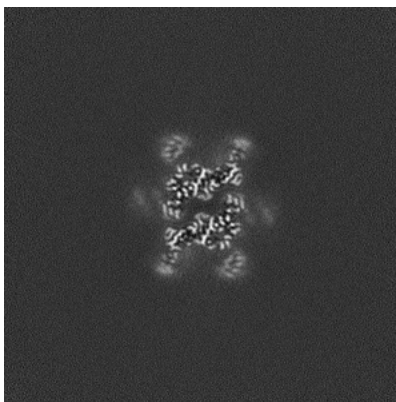


Z Index: 227

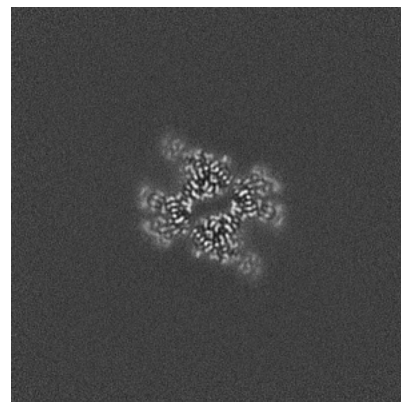
6.3.2 Raw map



X Index: 212



Y Index: 186

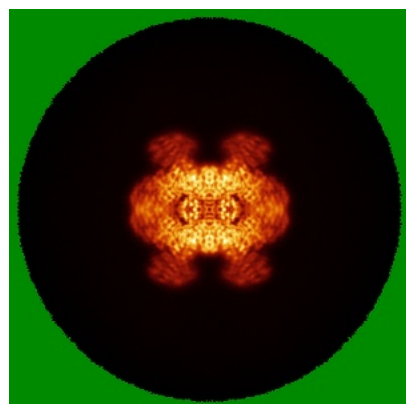


Z Index: 171

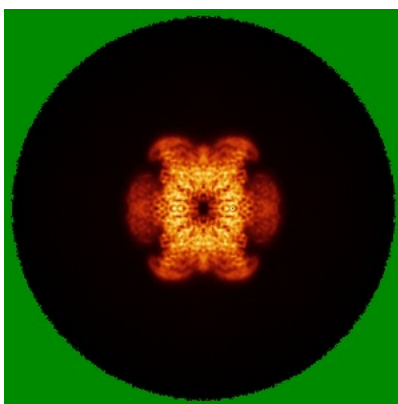
The images above show the largest variance slices of the map in three orthogonal directions.

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

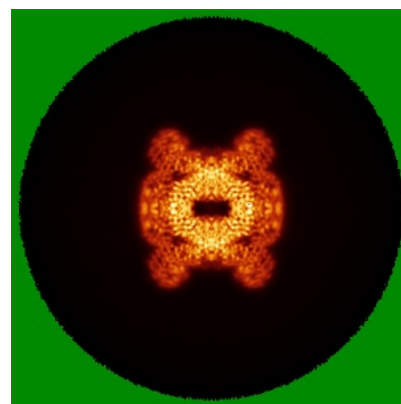
6.4.1 Primary map



X

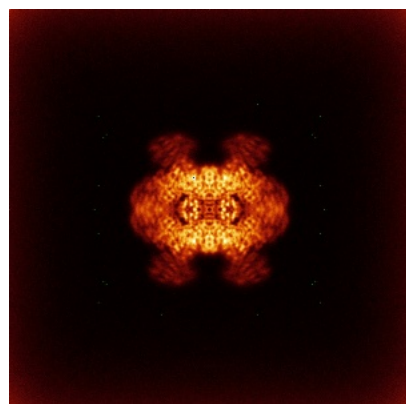


Y

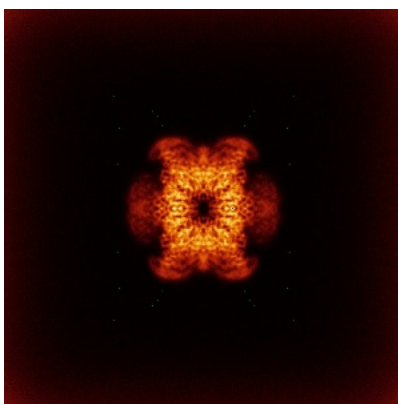


Z

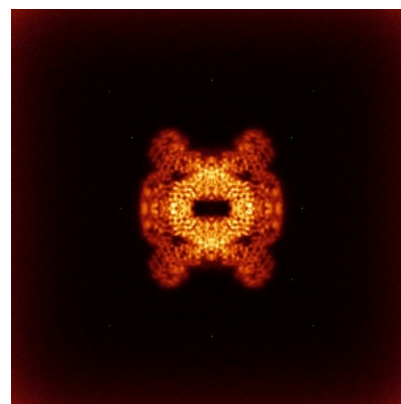
6.4.2 Raw map



X



Y

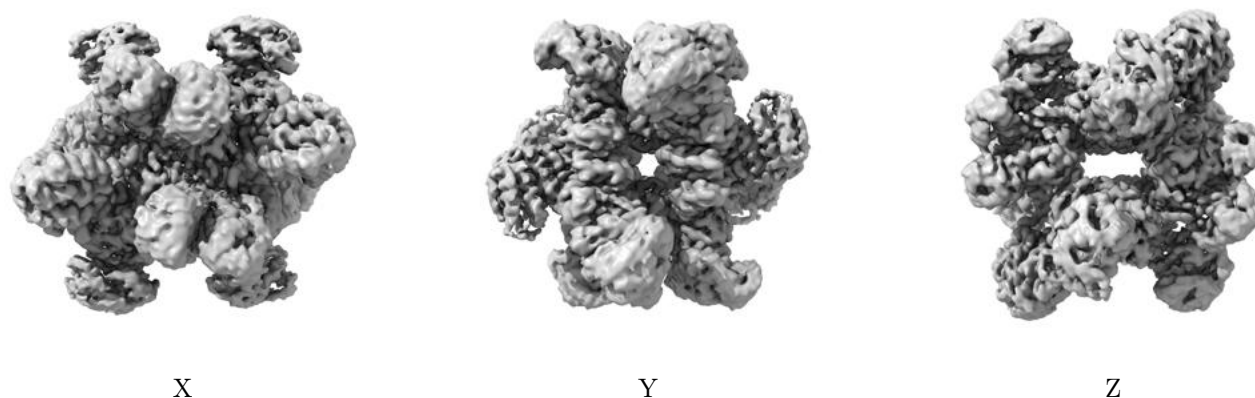


Z

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.

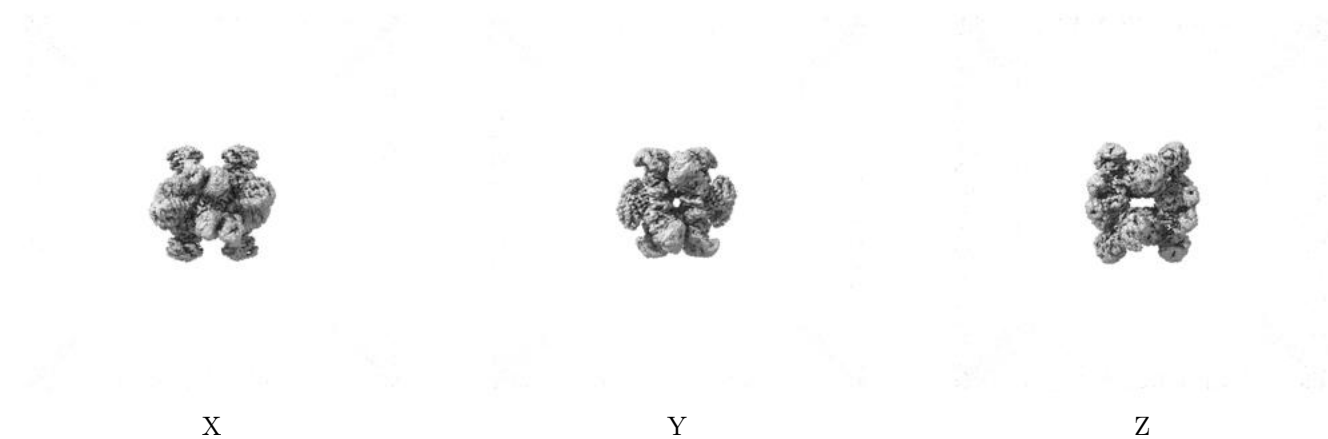
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.22. 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.

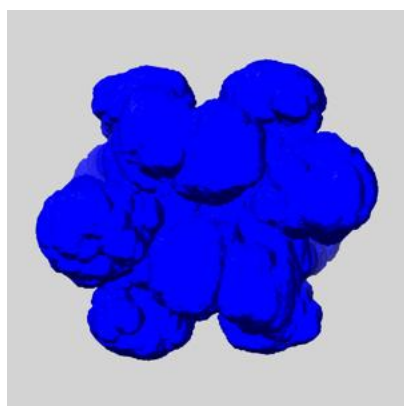
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

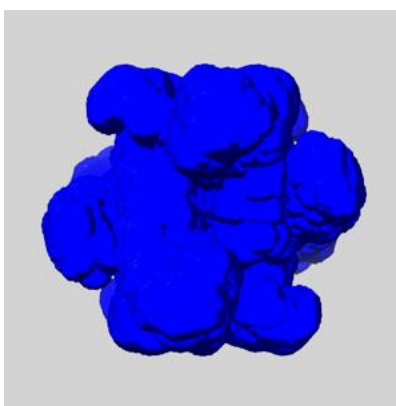
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

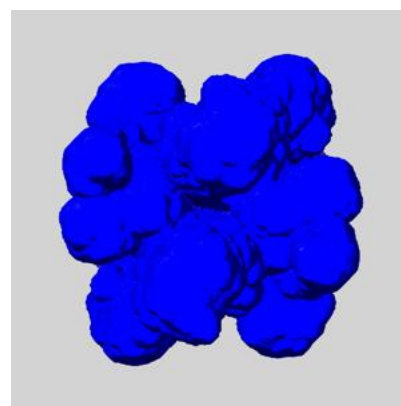
6.6.1 emd_23311_msk_1.map [i](#)



X



Y

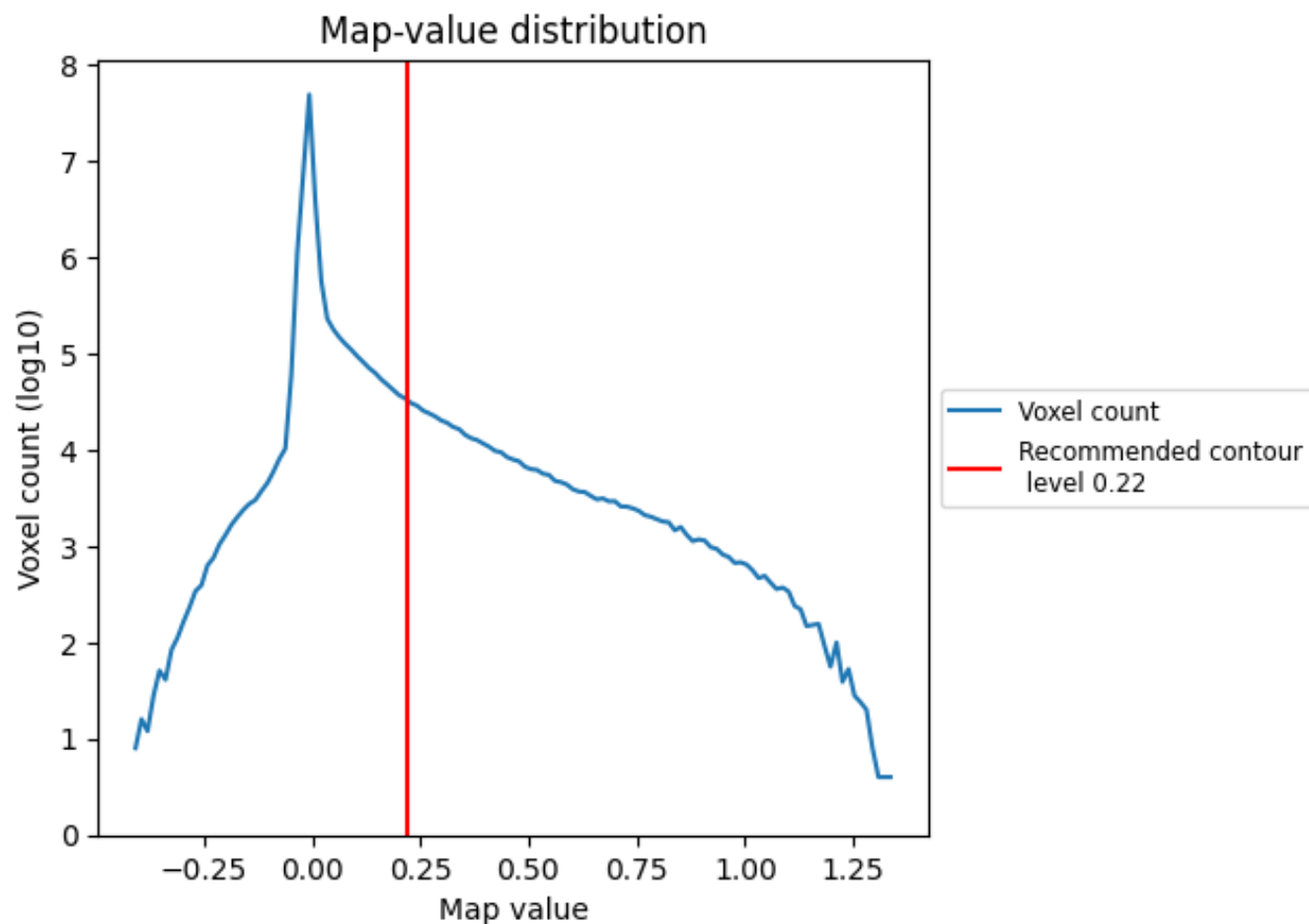


Z

7 Map analysis [i](#)

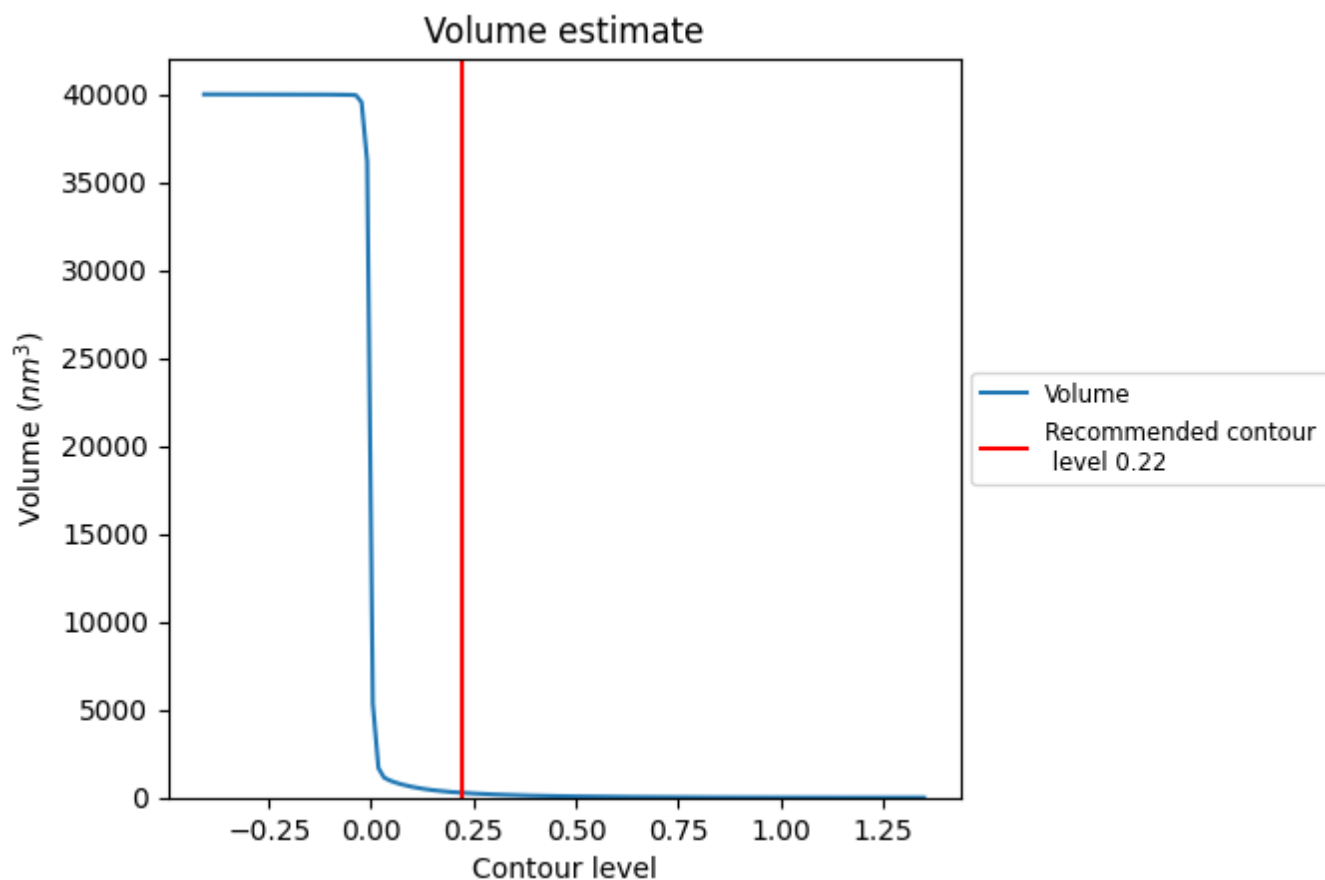
This section contains the results of statistical analysis of the map.

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.

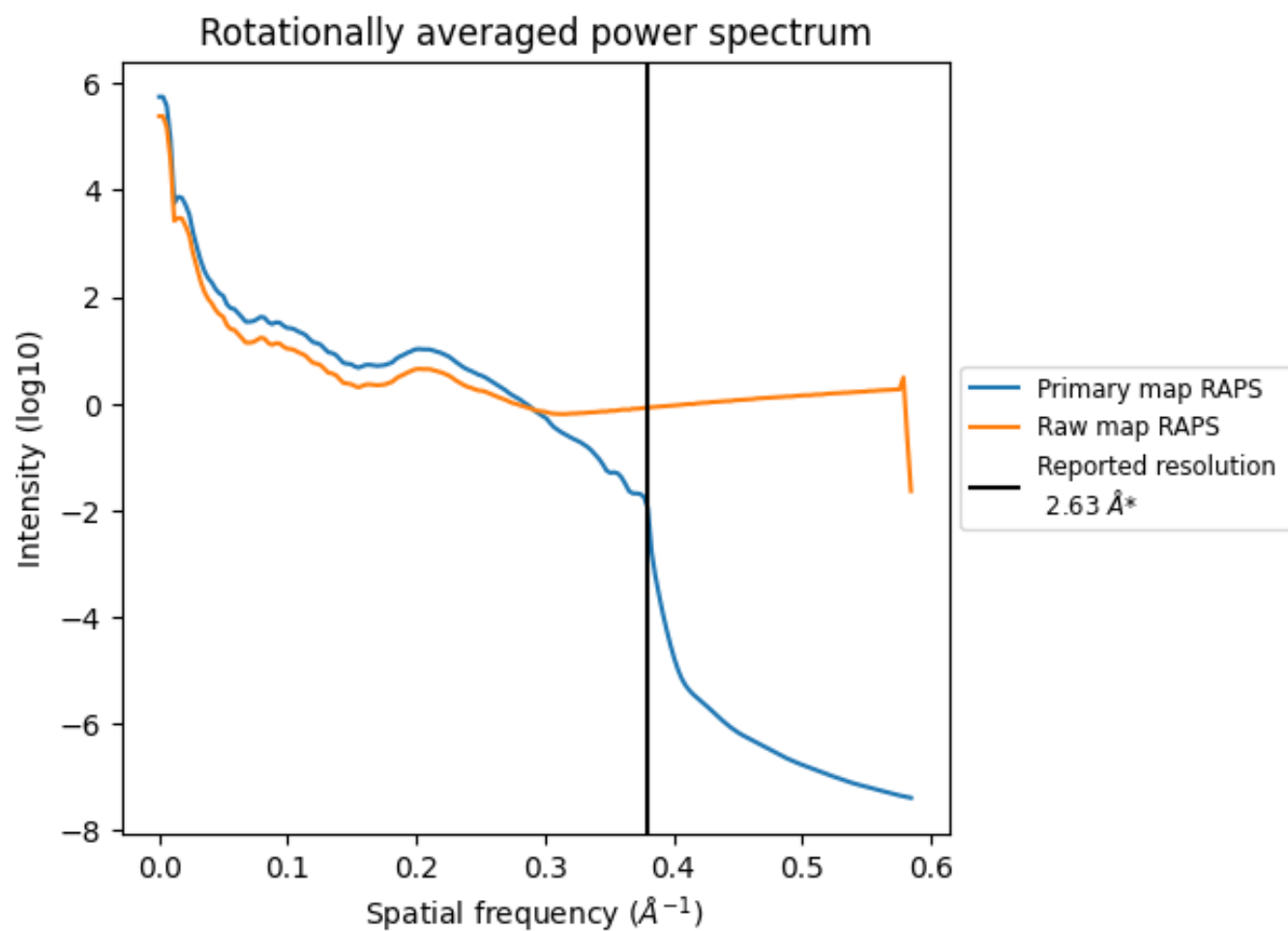
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 275 nm^3 ; this corresponds to an approximate mass of 249 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 ⓘ

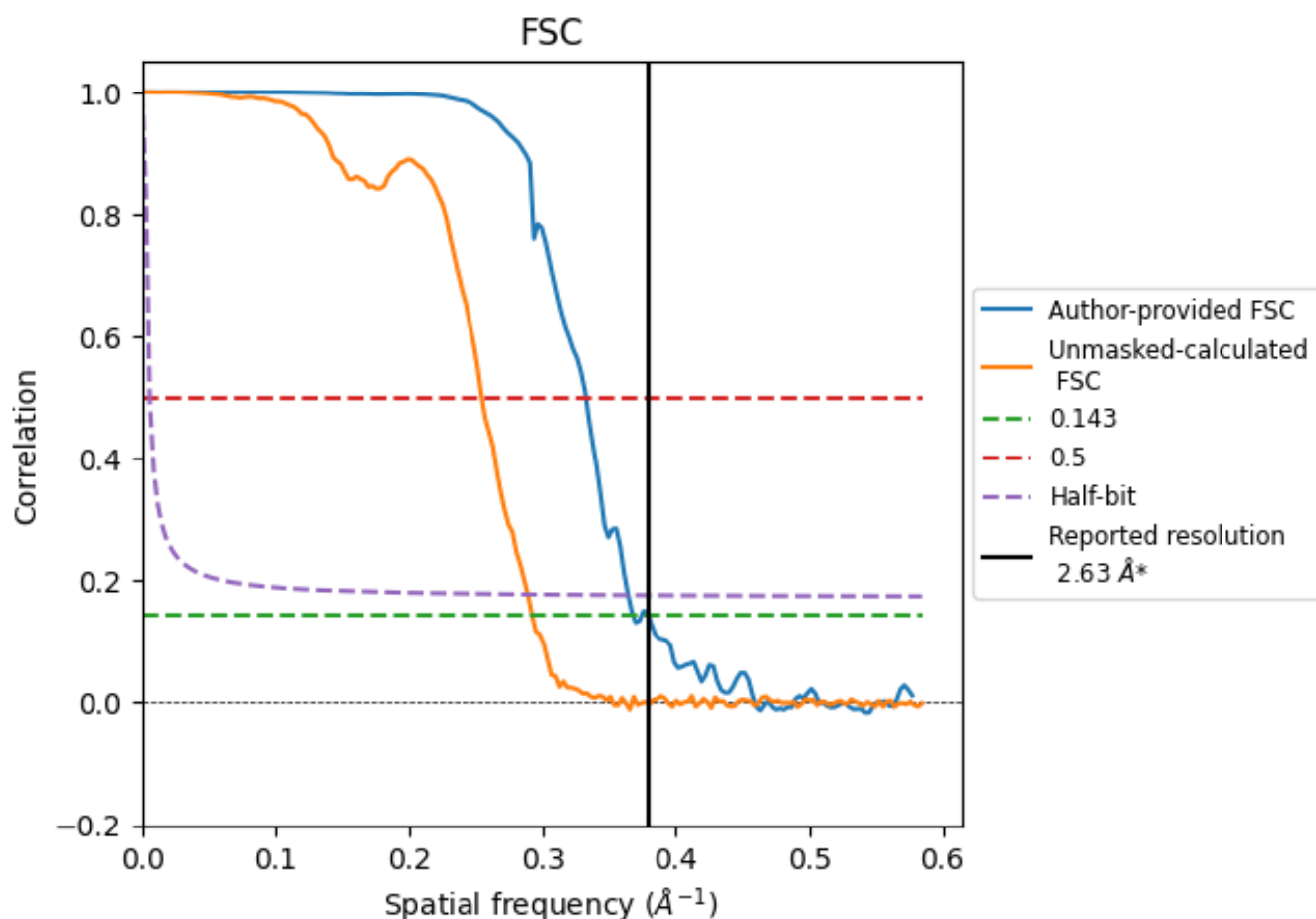


*Reported resolution corresponds to spatial frequency of 0.380 Å⁻¹

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 0.380 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

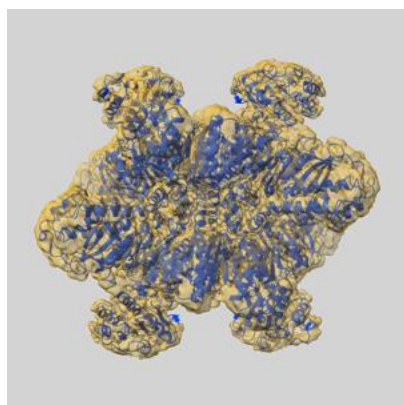
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	2.72	3.01	2.74
Unmasked-calculated*	3.42	3.93	3.46

*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 3.42 differs from the reported value 2.63 by more than 10 %

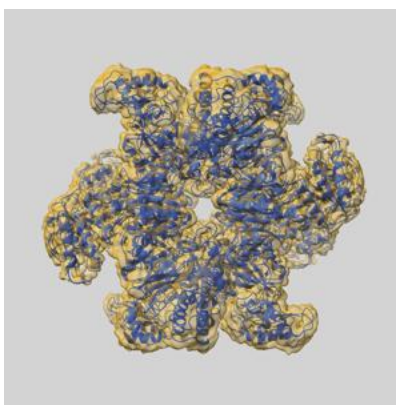
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23311 and PDB model 7LG5. Per-residue inclusion information can be found in section [3](#) on page [6](#).

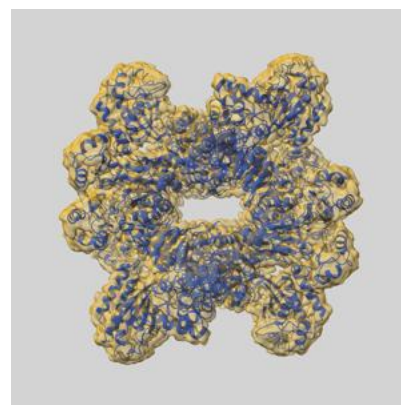
9.1 Map-model overlay [i](#)



X



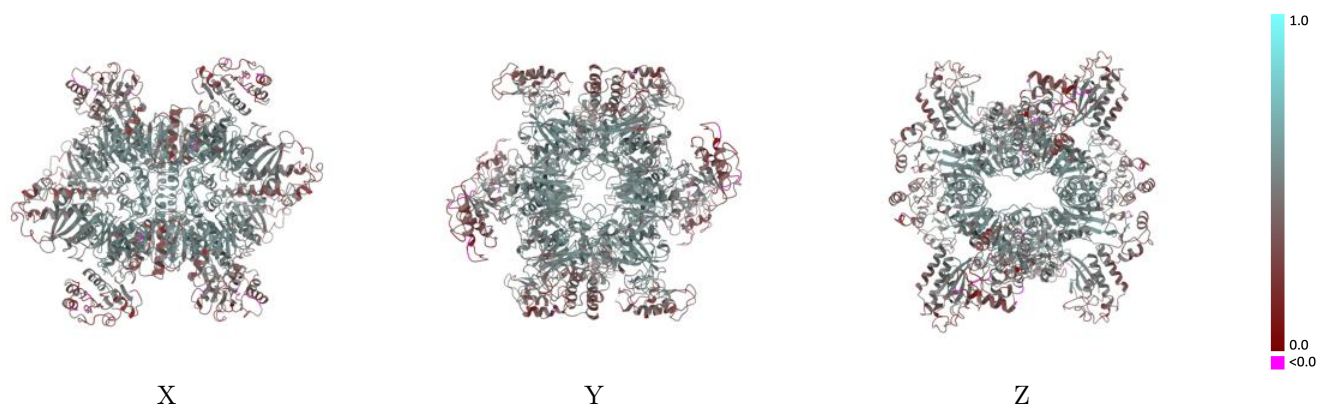
Y



Z

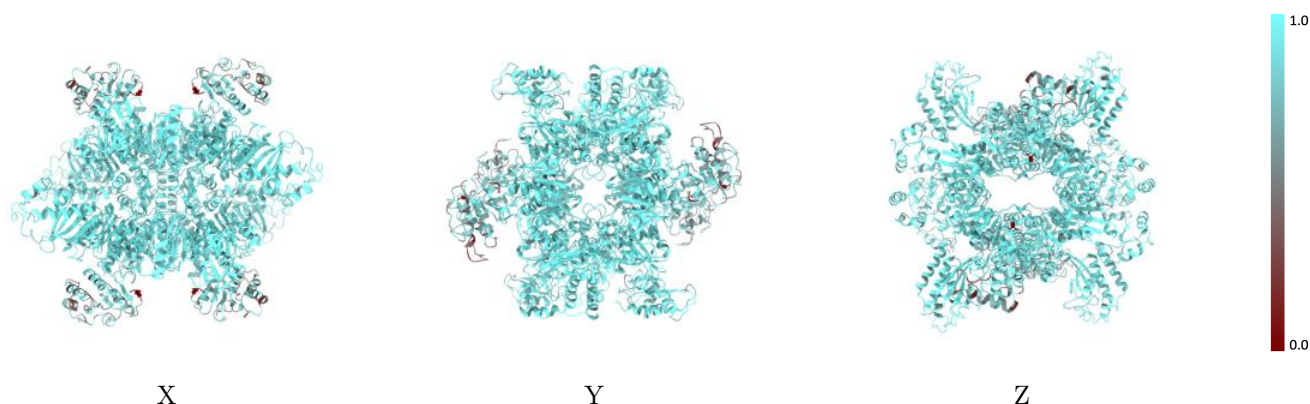
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



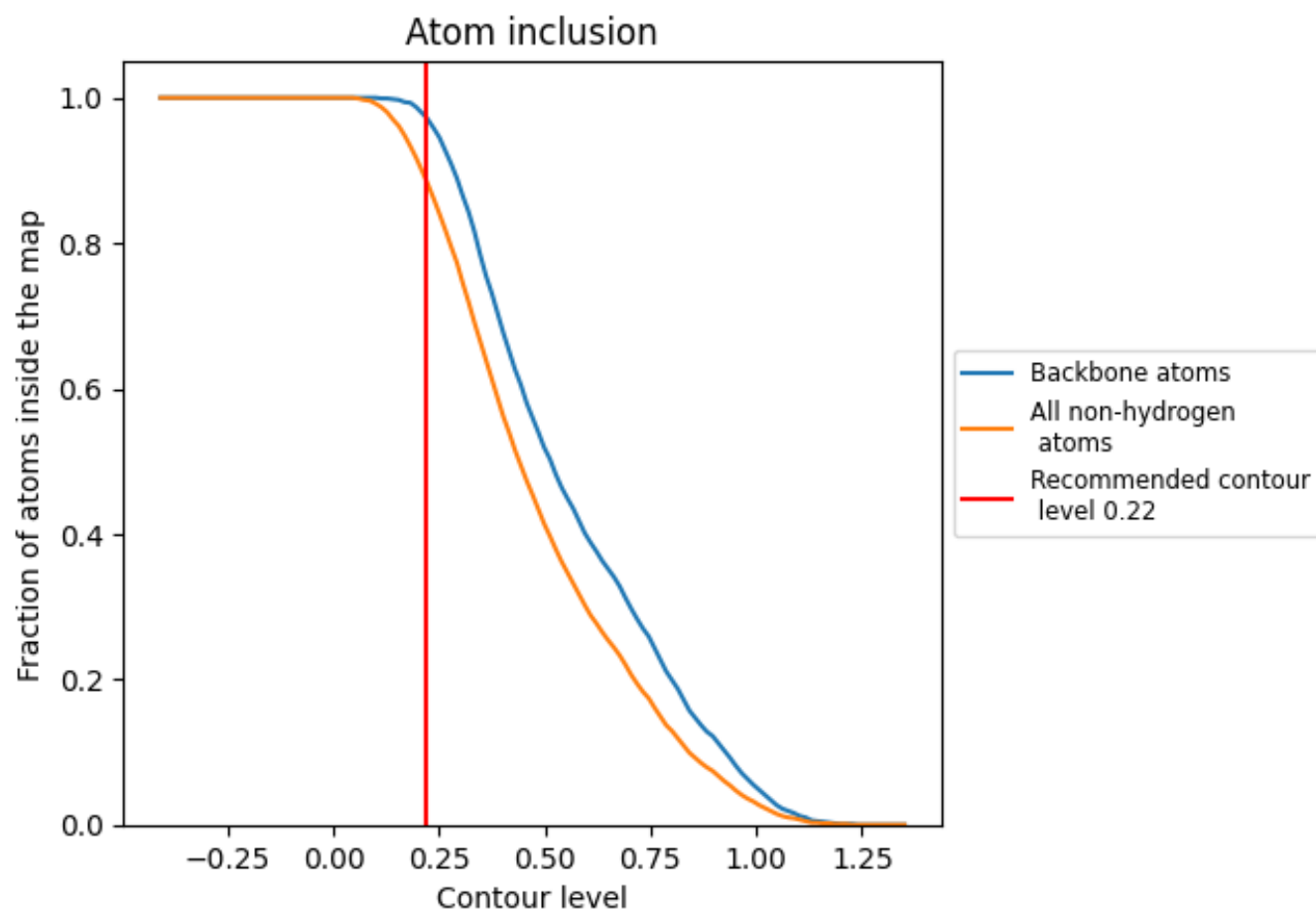
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 89% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8860	0.4620
A	0.8860	0.4620
B	0.8860	0.4610
C	0.8870	0.4630
D	0.8870	0.4610

