



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 02:07 PM EST

PDB ID : 7TXV
EMDB ID : EMD-26161
Title : Cyanophycin synthetase 1 from *Synechocystis* sp. UTEX2470 E82Q with ATP and 16x(Asp-Arg)
Authors : Sharon, I.; Grogg, M.; Hilvert, D.; Schmeing, T.M.
Deposited on : 2022-02-09
Resolution : 2.70 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

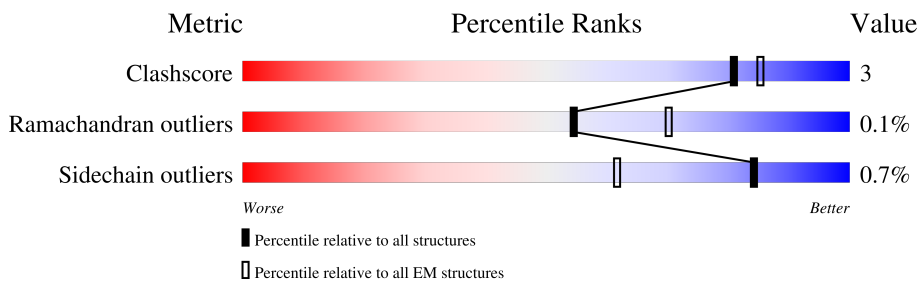
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
1	B	879	
1	C	879	
1	D	879	
2	E	16	
2	F	16	
2	G	16	
2	H	16	

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Mol	Chain	Length	Quality of chain
2	I	16	
2	J	16	
2	K	16	
2	L	16	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 27648 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
			Total	C	N	O	S		
1	A	870	6650	4185	1164	1277	24	0	0
1	B	870	6650	4185	1164	1277	24	0	0
1	C	870	6650	4185	1164	1277	24	0	0
1	D	870	6650	4185	1164	1277	24	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	GLN	GLU	engineered mutation	UNP A0A068N621
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	82	GLN	GLU	engineered mutation	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	82	GLN	GLU	engineered mutation	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	82	GLN	GLU	engineered mutation	UNP A0A068N621

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

- Molecule 2 is a protein called 16x(Asp-Arg).

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	4	Total	C	N	O	0	0
			61	33	16	12		
2	F	4	Total	C	N	O	0	0
			61	33	16	12		
2	G	4	Total	C	N	O	0	0
			61	33	16	12		
2	H	4	Total	C	N	O	0	0
			61	33	16	12		
2	I	8	Total	C	N	O	0	1
			134	70	36	28		
2	J	8	Total	C	N	O	0	1
			134	70	36	28		
2	K	8	Total	C	N	O	0	1
			134	70	36	28		
2	L	8	Total	C	N	O	0	1
			134	70	36	28		

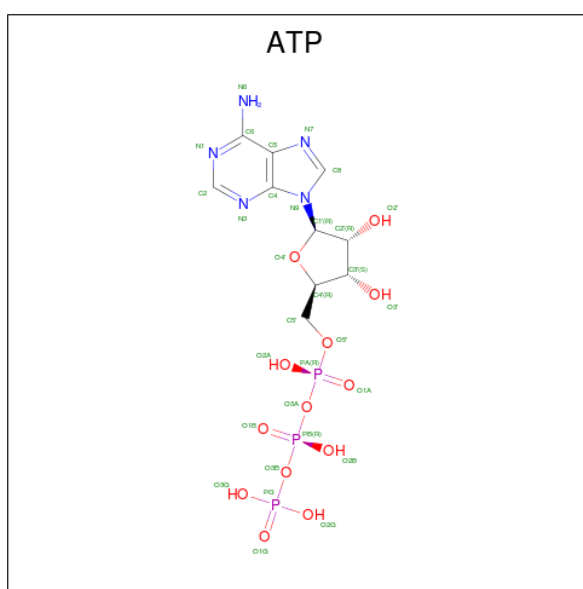
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	A	4	Total	Mg	0
			4	4	
3	B	4	Total	Mg	0
			4	4	
3	C	4	Total	Mg	0
			4	4	
3	D	4	Total	Mg	0
			4	4	

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	B	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	
4	D	1	Total	Zn	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms				AltConf	
5	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	D	1	Total	C	N	O	P	0
			62	20	10	26	6	

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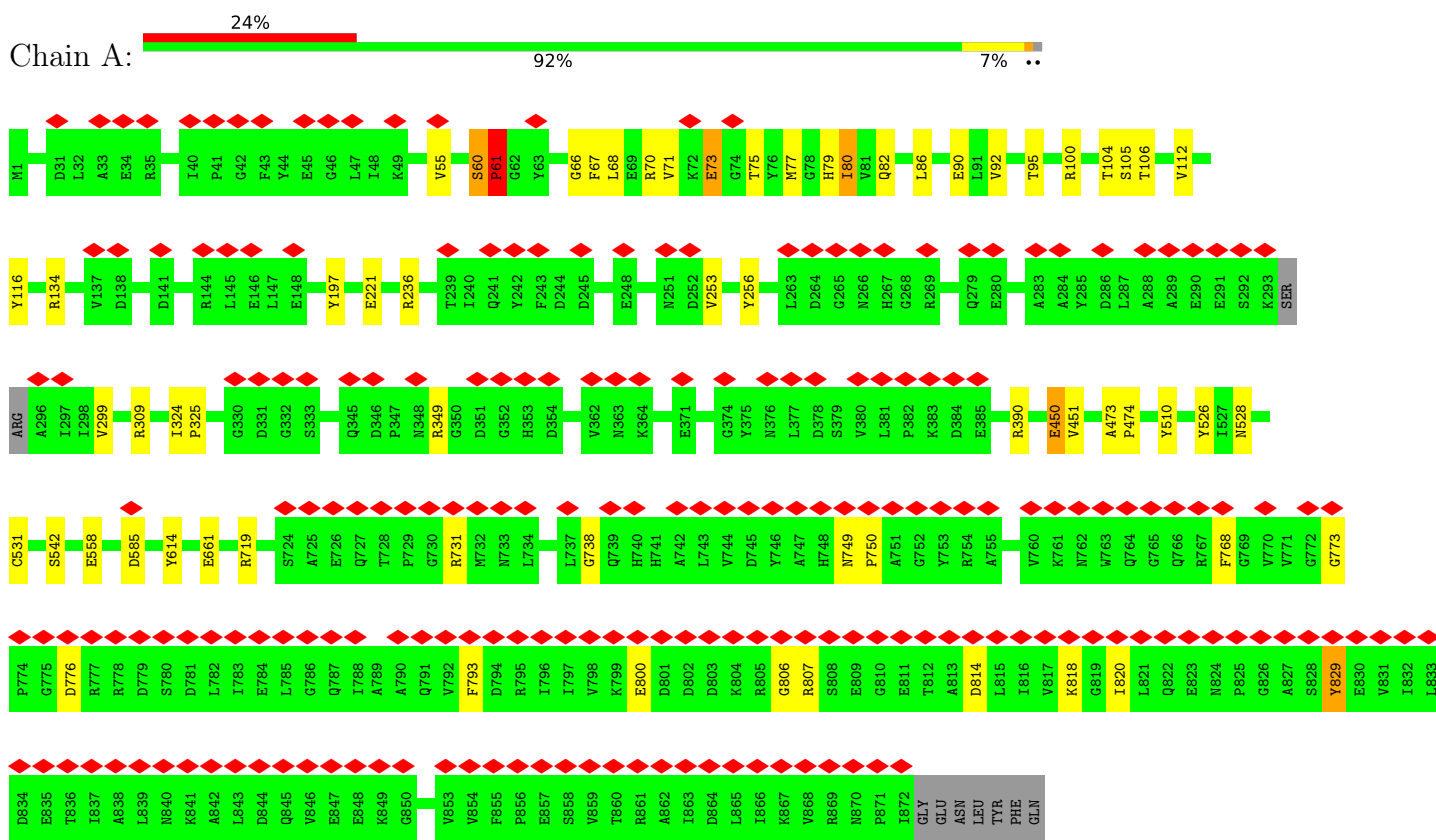
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	D	1	62	20	10	26	6	0

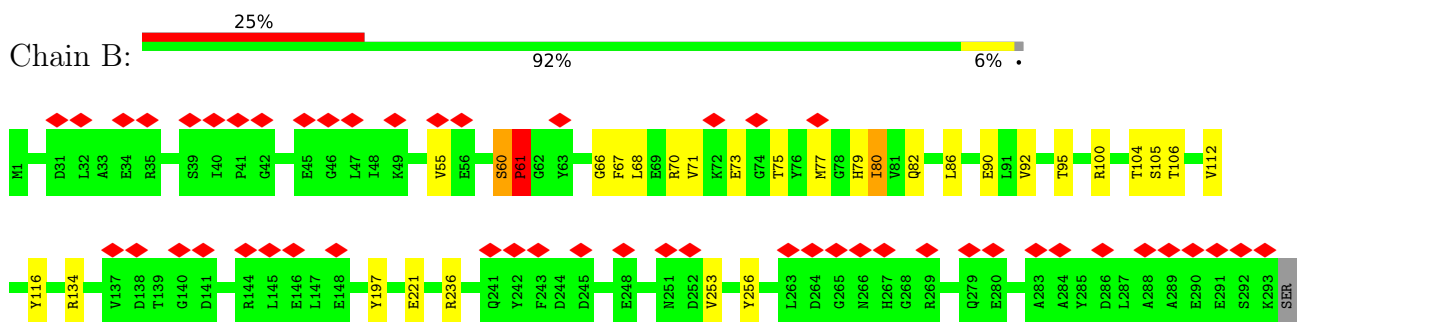
3 Residue-property plots

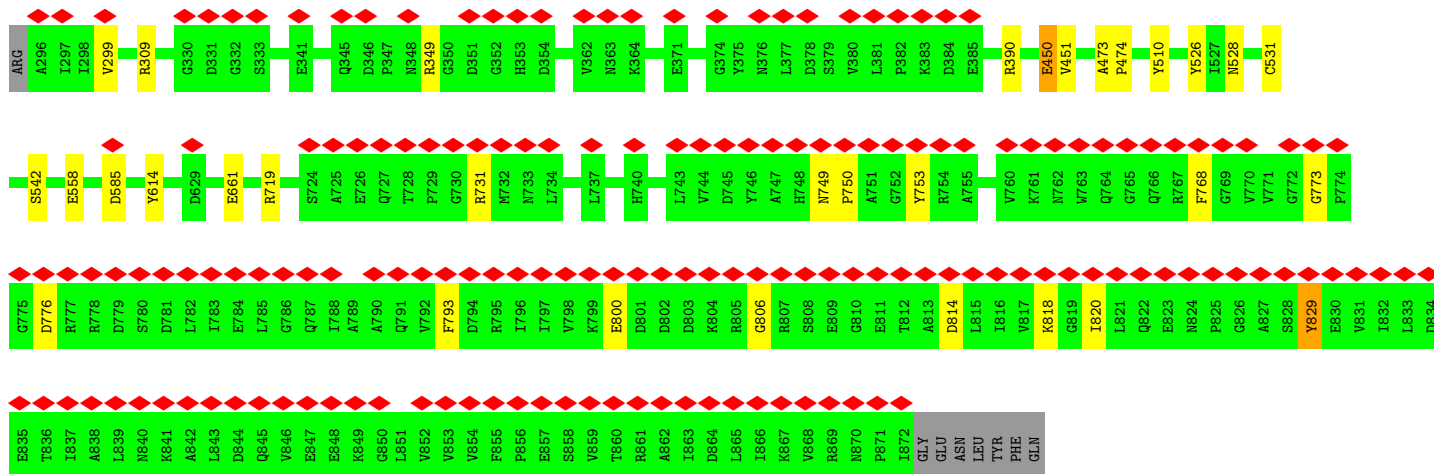
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

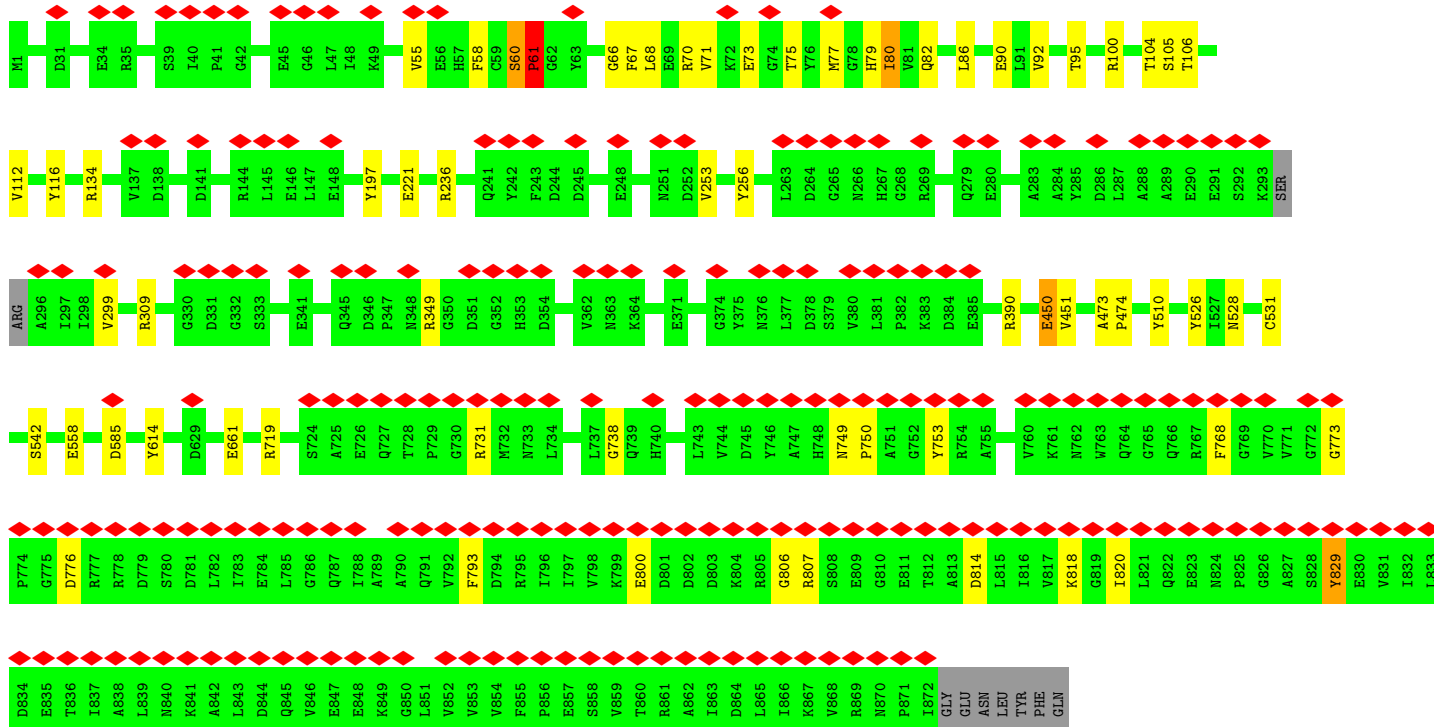
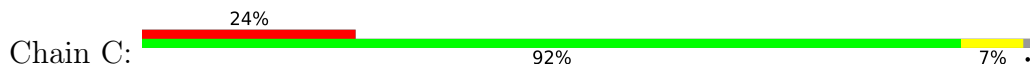


- Molecule 1: Cyanophycin synthase

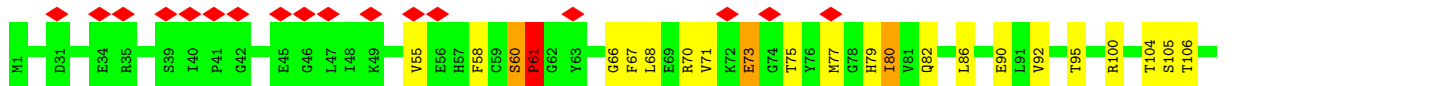
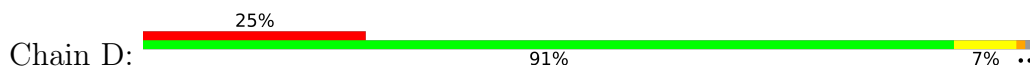


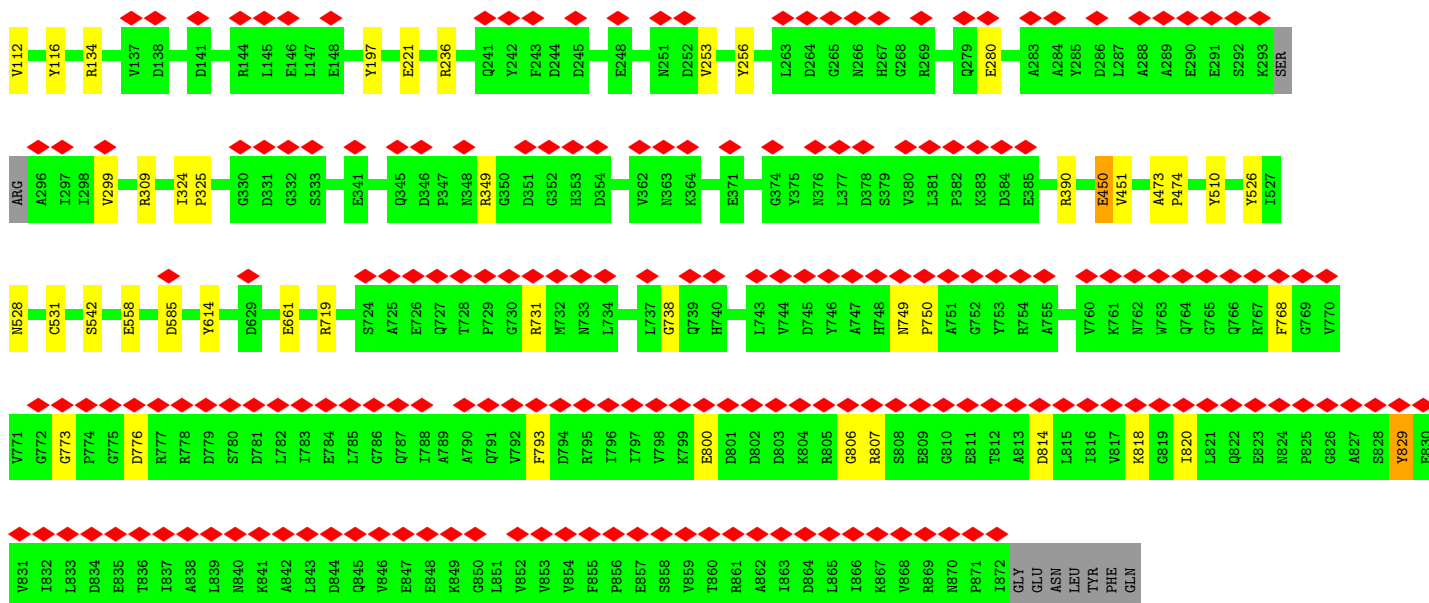


• Molecule 1: Cyanophycin synthase

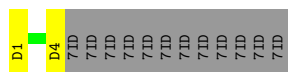


• Molecule 1: Cyanophycin synthase

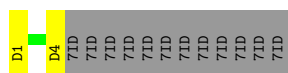




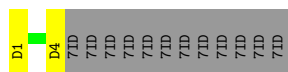
- Molecule 2: 16x(Asp-Arg)



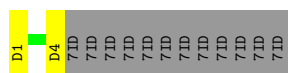
- Molecule 2: 16x(Asp-Arg)



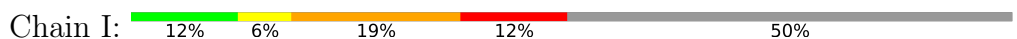
- Molecule 2: 16x(Asp-Arg)



- Molecule 2: 16x(Asp-Arg)

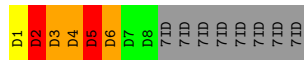
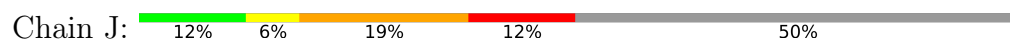


- Molecule 2: 16x(Asp-Arg)

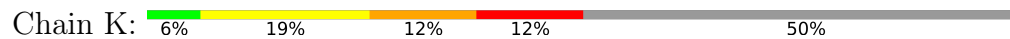




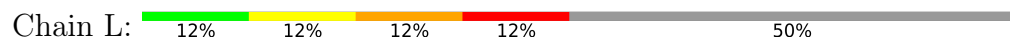
• Molecule 2: 16x(Asp-Arg)



• Molecule 2: 16x(Asp-Arg)



• Molecule 2: 16x(Asp-Arg)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	318594	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)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.385	Depositor
Minimum map value	-3.203	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.59	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: 7ID, ATP, ZN, 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	1.17	23/6763 (0.3%)	0.94	16/9189 (0.2%)
1	B	1.17	24/6763 (0.4%)	0.94	14/9189 (0.2%)
1	C	1.17	24/6763 (0.4%)	0.94	17/9189 (0.2%)
1	D	1.17	24/6763 (0.4%)	0.94	17/9189 (0.2%)
All	All	1.17	95/27052 (0.4%)	0.94	64/36756 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
2	F	0	1
2	G	0	1
2	H	0	1
2	I	0	4
2	J	0	4
2	K	0	4
2	L	0	4
All	All	0	20

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	450	GLU	CG-CD	-11.52	1.34	1.51
1	A	450	GLU	CG-CD	-11.47	1.34	1.51
1	C	450	GLU	CG-CD	-11.46	1.34	1.51
1	D	450	GLU	CG-CD	-11.45	1.34	1.51
1	D	526	TYR	CB-CG	-7.75	1.40	1.51
1	A	526	TYR	CB-CG	-7.74	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	526	TYR	CB-CG	-7.73	1.40	1.51
1	C	526	TYR	CB-CG	-7.73	1.40	1.51
1	D	558	GLU	CG-CD	7.41	1.63	1.51
1	A	558	GLU	CG-CD	7.40	1.63	1.51
1	C	558	GLU	CG-CD	7.40	1.63	1.51
1	B	558	GLU	CG-CD	7.40	1.63	1.51
1	C	116	TYR	CG-CD2	-6.83	1.30	1.39
1	B	116	TYR	CG-CD2	-6.81	1.30	1.39
1	D	116	TYR	CG-CD2	-6.79	1.30	1.39
1	A	116	TYR	CG-CD2	-6.78	1.30	1.39
1	B	531	CYS	CB-SG	-6.77	1.70	1.82
1	A	531	CYS	CB-SG	-6.75	1.70	1.82
1	C	531	CYS	CB-SG	-6.74	1.70	1.82
1	D	531	CYS	CB-SG	-6.72	1.70	1.82
1	D	528	ASN	CB-CG	-6.68	1.35	1.51
1	A	528	ASN	CB-CG	-6.67	1.35	1.51
1	B	528	ASN	CB-CG	-6.66	1.35	1.51
1	C	528	ASN	CB-CG	-6.66	1.35	1.51
1	B	197	TYR	CB-CG	-6.07	1.42	1.51
1	C	197	TYR	CB-CG	-6.04	1.42	1.51
1	A	197	TYR	CB-CG	-6.01	1.42	1.51
1	D	197	TYR	CB-CG	-5.99	1.42	1.51
1	A	661	GLU	CG-CD	-5.82	1.43	1.51
1	D	221	GLU	CD-OE2	-5.81	1.19	1.25
1	C	661	GLU	CG-CD	-5.80	1.43	1.51
1	B	661	GLU	CG-CD	-5.80	1.43	1.51
1	D	661	GLU	CG-CD	-5.77	1.43	1.51
1	A	221	GLU	CD-OE2	-5.76	1.19	1.25
1	C	221	GLU	CD-OE2	-5.76	1.19	1.25
1	B	221	GLU	CD-OE2	-5.73	1.19	1.25
1	C	92	VAL	CB-CG2	-5.69	1.41	1.52
1	B	92	VAL	CB-CG2	-5.68	1.41	1.52
1	C	542	SER	CB-OG	-5.68	1.34	1.42
1	D	92	VAL	CB-CG2	-5.66	1.41	1.52
1	A	92	VAL	CB-CG2	-5.66	1.41	1.52
1	A	542	SER	CB-OG	-5.65	1.34	1.42
1	B	542	SER	CB-OG	-5.63	1.34	1.42
1	D	542	SER	CB-OG	-5.63	1.34	1.42
1	A	829	TYR	CG-CD1	-5.60	1.31	1.39
1	B	829	TYR	CG-CD1	-5.59	1.31	1.39
1	C	829	TYR	CG-CD1	-5.58	1.31	1.39
1	D	526	TYR	CD1-CE1	-5.58	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	829	TYR	CG-CD1	-5.58	1.31	1.39
1	A	526	TYR	CD1-CE1	-5.57	1.30	1.39
1	A	829	TYR	CB-CG	-5.57	1.43	1.51
1	B	526	TYR	CD1-CE1	-5.57	1.30	1.39
1	C	526	TYR	CD1-CE1	-5.57	1.30	1.39
1	B	829	TYR	CB-CG	-5.56	1.43	1.51
1	D	829	TYR	CB-CG	-5.56	1.43	1.51
1	C	829	TYR	CB-CG	-5.54	1.43	1.51
1	C	829	TYR	CE1-CZ	-5.51	1.31	1.38
1	B	829	TYR	CE1-CZ	-5.44	1.31	1.38
1	A	829	TYR	CE1-CZ	-5.43	1.31	1.38
1	C	793	PHE	CB-CG	-5.42	1.42	1.51
1	B	793	PHE	CB-CG	-5.42	1.42	1.51
1	A	793	PHE	CB-CG	-5.41	1.42	1.51
1	D	829	TYR	CE1-CZ	-5.39	1.31	1.38
1	B	542	SER	CA-CB	-5.36	1.45	1.52
1	C	542	SER	CA-CB	-5.36	1.45	1.52
1	D	542	SER	CA-CB	-5.36	1.45	1.52
1	D	793	PHE	CB-CG	-5.35	1.42	1.51
1	A	542	SER	CA-CB	-5.32	1.45	1.52
1	C	558	GLU	CD-OE1	-5.22	1.20	1.25
1	A	558	GLU	CD-OE1	-5.21	1.20	1.25
1	C	197	TYR	CG-CD2	-5.21	1.32	1.39
1	D	197	TYR	CG-CD2	-5.20	1.32	1.39
1	D	510	TYR	CB-CG	-5.19	1.43	1.51
1	A	197	TYR	CG-CD2	-5.18	1.32	1.39
1	B	558	GLU	CD-OE1	-5.17	1.20	1.25
1	D	558	GLU	CD-OE1	-5.17	1.20	1.25
1	A	510	TYR	CB-CG	-5.16	1.44	1.51
1	B	197	TYR	CG-CD2	-5.16	1.32	1.39
1	B	510	TYR	CB-CG	-5.12	1.44	1.51
1	C	510	TYR	CB-CG	-5.10	1.44	1.51
1	D	116	TYR	CE2-CZ	-5.10	1.31	1.38
1	A	116	TYR	CE2-CZ	-5.06	1.31	1.38
1	C	60	SER	CA-CB	-5.06	1.45	1.52
1	A	526	TYR	CD2-CE2	-5.05	1.31	1.39
1	B	526	TYR	CD2-CE2	-5.05	1.31	1.39
1	C	526	TYR	CD2-CE2	-5.05	1.31	1.39
1	D	526	TYR	CD2-CE2	-5.05	1.31	1.39
1	D	60	SER	CA-CB	-5.04	1.45	1.52
1	D	280	GLU	CG-CD	-5.04	1.44	1.51
1	A	60	SER	CA-CB	-5.02	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	116	TYR	CE2-CZ	-5.02	1.32	1.38
1	C	753	TYR	CD2-CE2	-5.02	1.31	1.39
1	B	753	TYR	CD2-CE2	-5.01	1.31	1.39
1	B	60	SER	CA-CB	-5.00	1.45	1.52
1	B	116	TYR	CE2-CZ	-5.00	1.32	1.38

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	731	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	D	731	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	C	731	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	B	731	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	A	61	PRO	N-CA-CB	-6.99	94.91	102.60
1	D	61	PRO	N-CA-CB	-6.99	94.91	102.60
1	C	61	PRO	N-CA-CB	-6.98	94.92	102.60
1	B	61	PRO	N-CA-CB	-6.97	94.93	102.60
1	B	390	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	D	390	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	390	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	C	390	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	D	585	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	585	ASP	CB-CG-OD2	6.35	124.02	118.30
1	D	61	PRO	N-CA-C	-6.35	95.59	112.10
1	B	61	PRO	N-CA-C	-6.35	95.60	112.10
1	A	61	PRO	N-CA-C	-6.34	95.61	112.10
1	C	61	PRO	N-CA-C	-6.34	95.62	112.10
1	C	585	ASP	CB-CG-OD2	6.32	123.99	118.30
1	D	309	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	B	585	ASP	CB-CG-OD2	6.30	123.97	118.30
1	C	309	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	309	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	309	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	C	614	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	A	614	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	D	614	TYR	CB-CG-CD2	-5.86	117.48	121.00
1	B	614	TYR	CB-CG-CD2	-5.84	117.49	121.00
1	C	829	TYR	CB-CG-CD1	-5.54	117.68	121.00
1	B	829	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	D	236	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	829	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	C	256	TYR	CB-CG-CD1	-5.50	117.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	829	TYR	CB-CG-CD1	-5.49	117.71	121.00
1	B	236	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	256	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	A	256	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	D	349	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	C	349	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	236	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	349	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	256	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	B	349	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	C	236	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	768	PHE	CB-CG-CD2	5.30	124.51	120.80
1	B	719	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	719	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	719	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	768	PHE	CB-CG-CD2	5.26	124.48	120.80
1	A	768	PHE	CB-CG-CD2	5.26	124.48	120.80
1	B	134	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	C	768	PHE	CB-CG-CD2	5.24	124.47	120.80
1	C	134	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	D	134	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	134	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	D	719	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	807	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	D	58	PHE	CB-CG-CD1	5.03	124.32	120.80
1	D	738	GLY	N-CA-C	-5.02	100.55	113.10
1	A	807	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	C	738	GLY	N-CA-C	-5.01	100.56	113.10
1	C	58	PHE	CB-CG-CD1	5.01	124.31	120.80
1	A	738	GLY	N-CA-C	-5.01	100.58	113.10
1	D	807	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	1	7ID	Peptide
2	F	1	7ID	Peptide
2	G	1	7ID	Peptide
2	H	1	7ID	Peptide
2	I	1	7ID	Peptide
2	I	2	7ID	Peptide

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Mol	Chain	Res	Type	Group
2	I	3	7ID	Peptide
2	I	5	7ID	Peptide
2	J	1	7ID	Peptide
2	J	2	7ID	Peptide
2	J	3	7ID	Peptide
2	J	5	7ID	Peptide
2	K	1	7ID	Peptide
2	K	2	7ID	Peptide
2	K	3	7ID	Peptide
2	K	5	7ID	Peptide
2	L	1	7ID	Peptide
2	L	2	7ID	Peptide
2	L	3	7ID	Peptide
2	L	5	7ID	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6650	0	6688	33	0
1	B	6650	0	6688	31	0
1	C	6650	0	6688	31	0
1	D	6650	0	6688	33	0
2	E	61	0	0	0	0
2	F	61	0	0	0	0
2	G	61	0	0	0	0
2	H	61	0	0	0	0
2	I	134	0	0	6	0
2	J	134	0	0	6	0
2	K	134	0	0	6	0
2	L	134	0	0	6	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
5	A	62	0	24	1	0
5	B	62	0	24	1	0
5	C	62	0	24	1	0
5	D	62	0	24	1	0
All	All	27648	0	26848	140	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 3.

All (140) 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:C:90:GLU:HB2	2:K:4:7ID:NH2	1.90	0.86
1:B:90:GLU:HB2	2:J:4:7ID:NH1	1.90	0.86
1:A:90:GLU:HB2	2:I:4:7ID:NH1	1.90	0.85
1:D:90:GLU:HB2	2:L:4:7ID:NH2	1.90	0.84
1:A:68:LEU:H	1:A:71:VAL:HG23	1.45	0.82
1:D:68:LEU:H	1:D:71:VAL:HG23	1.45	0.82
1:B:68:LEU:H	1:B:71:VAL:HG23	1.45	0.81
1:C:68:LEU:H	1:C:71:VAL:HG23	1.44	0.81
1:B:95:THR:O	1:B:95:THR:HG23	1.81	0.79
1:C:95:THR:HG23	1:C:95:THR:O	1.81	0.79
1:D:95:THR:HG23	1:D:95:THR:O	1.81	0.79
1:A:95:THR:O	1:A:95:THR:HG23	1.81	0.78
1:D:75:THR:HG23	1:D:79:HIS:HD1	1.48	0.78
1:A:75:THR:HG23	1:A:79:HIS:HD1	1.48	0.78
1:C:75:THR:HG23	1:C:79:HIS:HD1	1.48	0.77
1:B:75:THR:HG23	1:B:79:HIS:HD1	1.48	0.77
1:D:77:MET:HA	1:D:80:ILE:HG13	1.69	0.74
1:A:77:MET:HA	1:A:80:ILE:HG13	1.69	0.73
1:C:77:MET:HA	1:C:80:ILE:HG13	1.69	0.73
1:B:77:MET:HA	1:B:80:ILE:HG13	1.69	0.73
1:B:299:VAL:HG12	1:B:299:VAL:O	1.87	0.73
1:C:299:VAL:HG12	1:C:299:VAL:O	1.87	0.73
1:A:299:VAL:HG12	1:A:299:VAL:O	1.87	0.73
1:D:299:VAL:O	1:D:299:VAL:HG12	1.87	0.73
1:C:86:LEU:HB3	2:K:4:7ID:NH1	2.06	0.70
1:B:86:LEU:HB3	2:J:4:7ID:NH2	2.06	0.70
1:A:86:LEU:HB3	2:I:4:7ID:NH2	2.06	0.70
1:D:86:LEU:HB3	2:L:4:7ID:NH1	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:PHE:O	1:A:68:LEU:HB2	1.96	0.66
1:D:67:PHE:O	1:D:68:LEU:HB2	1.96	0.66
1:B:67:PHE:O	1:B:68:LEU:HB2	1.96	0.64
1:C:67:PHE:O	1:C:68:LEU:HB2	1.96	0.64
1:B:95:THR:O	1:B:95:THR:CG2	2.48	0.60
1:B:82:GLN:HB2	1:B:112:VAL:HG13	1.84	0.60
1:C:95:THR:O	1:C:95:THR:CG2	2.48	0.60
1:A:95:THR:O	1:A:95:THR:CG2	2.48	0.60
1:C:82:GLN:HB2	1:C:112:VAL:HG13	1.84	0.60
1:D:95:THR:O	1:D:95:THR:CG2	2.48	0.60
1:A:82:GLN:HB2	1:A:112:VAL:HG13	1.84	0.60
1:D:82:GLN:HB2	1:D:112:VAL:HG13	1.84	0.60
1:B:253:VAL:HG21	1:B:299:VAL:O	2.04	0.57
1:C:253:VAL:HG21	1:C:299:VAL:O	2.04	0.57
1:D:253:VAL:HG21	1:D:299:VAL:O	2.04	0.57
1:A:253:VAL:HG21	1:A:299:VAL:O	2.04	0.57
1:C:75:THR:CG2	1:C:79:HIS:HD1	2.18	0.54
1:B:75:THR:CG2	1:B:79:HIS:HD1	2.18	0.54
1:D:75:THR:CG2	1:D:79:HIS:HD1	2.18	0.53
1:A:75:THR:CG2	1:A:79:HIS:HD1	2.18	0.53
2:I:6:7ID:C	2:I:6:7ID:OD1	2.57	0.53
2:K:6:7ID:OD1	2:K:6:7ID:C	2.57	0.53
2:L:6:7ID:OD1	2:L:6:7ID:C	2.57	0.53
2:J:6:7ID:OD1	2:J:6:7ID:C	2.57	0.53
1:B:55:VAL:HG12	1:B:68:LEU:HD12	1.92	0.52
1:C:55:VAL:HG12	1:C:68:LEU:HD12	1.92	0.52
1:D:55:VAL:HG12	1:D:68:LEU:HD12	1.92	0.52
1:A:55:VAL:HG12	1:A:68:LEU:HD12	1.92	0.51
1:D:100:ARG:NH1	2:L:3:7ID:O	2.44	0.51
1:A:100:ARG:NH1	2:I:3:7ID:O	2.44	0.51
2:L:4:7ID:O	2:L:5:7ID:C	2.59	0.51
1:C:100:ARG:NH1	2:K:3:7ID:O	2.44	0.50
2:I:4:7ID:O	2:I:5:7ID:C	2.59	0.50
1:B:100:ARG:NH1	2:J:3:7ID:O	2.44	0.50
2:J:4:7ID:O	2:J:5:7ID:C	2.59	0.50
2:K:4:7ID:O	2:K:5:7ID:C	2.59	0.50
1:A:68:LEU:H	1:A:71:VAL:CG2	2.21	0.48
1:C:68:LEU:H	1:C:71:VAL:CG2	2.21	0.48
1:D:68:LEU:H	1:D:71:VAL:CG2	2.21	0.48
1:B:68:LEU:H	1:B:71:VAL:CG2	2.21	0.48
1:D:814:ASP:OD2	1:D:818:LYS:NZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:ASP:OD2	1:A:818:LYS:NZ	2.47	0.48
1:C:814:ASP:OD2	1:C:818:LYS:NZ	2.46	0.48
1:B:814:ASP:OD2	1:B:818:LYS:NZ	2.47	0.48
1:A:299:VAL:O	1:A:299:VAL:CG1	2.59	0.48
1:A:104:THR:OG1	1:A:105:SER:N	2.47	0.47
1:D:104:THR:OG1	1:D:105:SER:N	2.47	0.47
1:D:299:VAL:O	1:D:299:VAL:CG1	2.59	0.47
1:B:75:THR:CG2	1:B:79:HIS:ND1	2.78	0.47
1:B:75:THR:HG23	1:B:79:HIS:ND1	2.25	0.47
1:C:75:THR:HG23	1:C:79:HIS:ND1	2.25	0.46
1:D:75:THR:CG2	1:D:79:HIS:ND1	2.78	0.46
1:A:75:THR:CG2	1:A:79:HIS:ND1	2.78	0.46
1:B:104:THR:OG1	1:B:105:SER:N	2.47	0.46
1:C:104:THR:OG1	1:C:105:SER:N	2.47	0.46
1:C:450:GLU:HG2	1:C:451:VAL:N	2.31	0.46
1:B:450:GLU:HG2	1:B:451:VAL:N	2.31	0.46
1:C:75:THR:CG2	1:C:79:HIS:ND1	2.78	0.46
1:A:82:GLN:HG2	1:A:82:GLN:O	2.15	0.45
1:B:82:GLN:O	1:B:82:GLN:HG2	2.15	0.45
1:C:82:GLN:O	1:C:82:GLN:HG2	2.15	0.45
1:B:100:ARG:NH2	2:J:2:7ID:O	2.50	0.45
1:C:100:ARG:NH2	2:K:2:7ID:O	2.50	0.45
1:D:82:GLN:O	1:D:82:GLN:HG2	2.15	0.45
1:A:473:ALA:HB3	1:A:474:PRO:HD3	1.98	0.45
1:D:473:ALA:HB3	1:D:474:PRO:HD3	1.99	0.45
1:C:473:ALA:HB3	1:C:474:PRO:HD3	1.99	0.44
1:B:473:ALA:HB3	1:B:474:PRO:HD3	1.98	0.44
1:A:450:GLU:HG2	1:A:451:VAL:N	2.31	0.44
1:D:450:GLU:HG2	1:D:451:VAL:N	2.31	0.44
1:A:749:ASN:HB2	1:A:750:PRO:HD2	2.00	0.44
1:D:749:ASN:HB2	1:D:750:PRO:HD2	2.00	0.44
1:D:67:PHE:HZ	1:D:80:ILE:HG23	1.83	0.44
1:A:105:SER:OG	1:A:106:THR:N	2.49	0.43
1:D:100:ARG:NH2	2:L:2:7ID:O	2.50	0.43
1:A:67:PHE:HZ	1:A:80:ILE:HG23	1.83	0.43
1:A:100:ARG:NH2	2:I:2:7ID:O	2.50	0.43
1:B:67:PHE:HZ	1:B:80:ILE:HG23	1.83	0.43
1:B:800:GLU:N	1:B:800:GLU:OE1	2.51	0.43
1:C:800:GLU:N	1:C:800:GLU:OE1	2.51	0.43
1:D:105:SER:OG	1:D:106:THR:N	2.49	0.43
1:C:67:PHE:HZ	1:C:80:ILE:HG23	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:GLU:OE1	1:A:800:GLU:N	2.51	0.43
1:C:61:PRO:HB2	1:C:66:GLY:HA3	2.01	0.43
1:D:800:GLU:N	1:D:800:GLU:OE1	2.51	0.43
1:B:61:PRO:HB2	1:B:66:GLY:HA3	2.01	0.43
1:B:105:SER:OG	1:B:106:THR:N	2.49	0.43
1:C:105:SER:OG	1:C:106:THR:N	2.49	0.43
1:A:61:PRO:HB2	1:A:66:GLY:HA3	2.01	0.42
1:B:749:ASN:HB2	1:B:750:PRO:HD2	2.00	0.42
1:D:61:PRO:HB2	1:D:66:GLY:HA3	2.01	0.42
1:C:749:ASN:HB2	1:C:750:PRO:HD2	2.01	0.42
5:A:907:ATP:O2B	5:A:907:ATP:O1G	2.38	0.42
5:D:907:ATP:O1G	5:D:907:ATP:O2B	2.38	0.42
1:D:324:ILE:HA	1:D:325:PRO:HD3	1.93	0.42
1:A:324:ILE:HA	1:A:325:PRO:HD3	1.93	0.42
5:B:907:ATP:O1G	5:B:907:ATP:O2B	2.38	0.42
1:C:450:GLU:CG	1:C:451:VAL:N	2.83	0.42
5:C:907:ATP:O1G	5:C:907:ATP:O2B	2.38	0.42
1:B:450:GLU:CG	1:B:451:VAL:N	2.83	0.41
1:A:776:ASP:OD2	1:A:806:GLY:N	2.53	0.41
1:C:820:ILE:HD12	1:C:829:TYR:CD1	2.56	0.41
1:B:776:ASP:OD2	1:B:806:GLY:N	2.53	0.41
1:B:820:ILE:HD12	1:B:829:TYR:CD1	2.56	0.41
1:C:776:ASP:OD2	1:C:806:GLY:N	2.53	0.41
1:D:776:ASP:OD2	1:D:806:GLY:N	2.53	0.41
1:A:450:GLU:CG	1:A:451:VAL:N	2.83	0.41
1:D:450:GLU:CG	1:D:451:VAL:N	2.83	0.41
1:A:73:GLU:H	1:A:73:GLU:HG3	1.62	0.41
1:D:73:GLU:H	1:D:73:GLU:HG3	1.62	0.41
1:D:820:ILE:HD12	1:D:829:TYR:CD1	2.56	0.41
1:A:820:ILE:HD12	1:A:829:TYR:CD1	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	866/879 (98%)	829 (96%)	36 (4%)	1 (0%)	51	78
1	B	866/879 (98%)	829 (96%)	36 (4%)	1 (0%)	51	78
1	C	866/879 (98%)	829 (96%)	36 (4%)	1 (0%)	51	78
1	D	866/879 (98%)	829 (96%)	36 (4%)	1 (0%)	51	78
All	All	3464/3516 (98%)	3316 (96%)	144 (4%)	4 (0%)	54	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	773	GLY
1	B	773	GLY
1	C	773	GLY
1	D	773	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	711/719 (99%)	706 (99%)	5 (1%)	84	94
1	B	711/719 (99%)	706 (99%)	5 (1%)	84	94
1	C	711/719 (99%)	706 (99%)	5 (1%)	84	94
1	D	711/719 (99%)	706 (99%)	5 (1%)	84	94
All	All	2844/2876 (99%)	2824 (99%)	20 (1%)	84	94

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	SER
1	A	61	PRO
1	A	70	ARG
1	A	73	GLU

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Mol	Chain	Res	Type
1	A	80	ILE
1	B	60	SER
1	B	61	PRO
1	B	70	ARG
1	B	73	GLU
1	B	80	ILE
1	C	60	SER
1	C	61	PRO
1	C	70	ARG
1	C	73	GLU
1	C	80	ILE
1	D	60	SER
1	D	61	PRO
1	D	70	ARG
1	D	73	GLU
1	D	80	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

Of 48 non-standard protein/DNA/RNA residues modelled in this entry, 4 are modelled with single atom - leaving 44 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	7ID	G	1	2	3,4,19	0.58	0	2,4,24	0.85	0
2	7ID	G	4	2	16,17,19	1.69	1 (6%)	11,20,24	1.45	1 (9%)
2	7ID	I	4	2	17,18,19	0.67	1 (5%)	18,22,24	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	7ID	K	7	2	17,18,19	0.61	0	18,22,24	0.76	1 (5%)
2	7ID	I	3	2	17,18,19	0.63	0	18,22,24	0.67	0
2	7ID	E	2	2	17,18,19	0.61	0	18,22,24	0.93	0
2	7ID	H	4	2	16,17,19	1.69	1 (6%)	11,20,24	1.46	1 (9%)
2	7ID	E	1	2	3,4,19	0.59	0	2,4,24	0.84	0
2	7ID	E	4	2	16,17,19	1.68	1 (6%)	11,20,24	1.46	1 (9%)
2	7ID	I	5	2	17,18,19	0.56	0	18,22,24	1.07	1 (5%)
2	7ID	K	2	2	17,18,19	0.61	0	18,22,24	0.94	1 (5%)
2	7ID	K	6	2	17,18,19	0.66	1 (5%)	18,22,24	1.04	1 (5%)
2	7ID	L	2	2	17,18,19	0.61	0	18,22,24	0.94	1 (5%)
2	7ID	J	6	2	17,18,19	0.57	0	18,22,24	1.11	1 (5%)
2	7ID	J	7	2	17,18,19	0.61	0	18,22,24	0.78	0
2	7ID	I	2	2	17,18,19	0.60	0	18,22,24	0.90	1 (5%)
2	7ID	K	3	2	17,18,19	0.61	0	18,22,24	0.62	0
2	7ID	E	3	2	17,18,19	0.63	0	18,22,24	0.63	0
2	7ID	J	4	2	17,18,19	0.67	1 (5%)	18,22,24	0.55	0
2	7ID	H	2	2	17,18,19	0.60	0	18,22,24	0.88	0
2	7ID	K	1	2	17,18,19	0.59	0	18,22,24	0.92	0
2	7ID	L	7	2	17,18,19	0.61	0	18,22,24	0.76	0
2	7ID	F	3	2	17,18,19	0.63	0	18,22,24	0.63	0
2	7ID	J	2	2	17,18,19	0.60	0	18,22,24	0.90	1 (5%)
2	7ID	L	6	2	17,18,19	0.66	1 (5%)	18,22,24	1.04	1 (5%)
2	7ID	K	5	2	17,18,19	0.58	0	18,22,24	1.05	1 (5%)
2	7ID	F	1	2	3,4,19	0.59	0	2,4,24	0.84	0
2	7ID	I	7	2	17,18,19	0.61	0	18,22,24	0.78	0
2	7ID	J	3	2	17,18,19	0.62	0	18,22,24	0.66	0
2	7ID	G	3	2	17,18,19	0.57	0	18,22,24	0.69	0
2	7ID	L	1	2	17,18,19	0.59	0	18,22,24	0.91	0
2	7ID	H	3	2	17,18,19	0.57	0	18,22,24	0.69	0
2	7ID	J	5	2	17,18,19	0.57	0	18,22,24	1.07	1 (5%)
2	7ID	I	6	2	17,18,19	0.58	0	18,22,24	1.11	1 (5%)
2	7ID	L	3	2	17,18,19	0.62	0	18,22,24	0.62	0
2	7ID	K	4	2	17,18,19	0.62	0	18,22,24	0.66	0
2	7ID	I	1	2	17,18,19	0.61	0	18,22,24	0.92	0
2	7ID	G	2	2	17,18,19	0.60	0	18,22,24	0.89	0
2	7ID	L	5	2	17,18,19	0.58	0	18,22,24	1.06	1 (5%)
2	7ID	L	4	2	17,18,19	0.63	0	18,22,24	0.66	0
2	7ID	F	2	2	17,18,19	0.61	0	18,22,24	0.93	0
2	7ID	F	4	2	16,17,19	1.68	1 (6%)	11,20,24	1.46	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	7ID	H	1	2	3,4,19	0.57	0	2,4,24	0.84	0
2	7ID	J	1	2	17,18,19	0.61	0	18,22,24	0.92	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	7ID	G	1	2	-	0/0/2/23	-
2	7ID	G	4	2	-	11/18/19/23	-
2	7ID	I	4	2	-	10/20/21/23	-
2	7ID	K	7	2	-	8/20/21/23	-
2	7ID	I	3	2	-	10/20/21/23	-
2	7ID	E	2	2	-	12/20/21/23	-
2	7ID	H	4	2	-	11/18/19/23	-
2	7ID	E	1	2	-	0/0/2/23	-
2	7ID	E	4	2	-	11/18/19/23	-
2	7ID	I	5	2	-	12/20/21/23	-
2	7ID	K	2	2	-	11/20/21/23	-
2	7ID	K	6	2	-	7/20/21/23	-
2	7ID	L	2	2	-	11/20/21/23	-
2	7ID	J	6	2	-	7/20/21/23	-
2	7ID	J	7	2	-	9/20/21/23	-
2	7ID	I	2	2	-	11/20/21/23	-
2	7ID	K	3	2	-	8/20/21/23	-
2	7ID	E	3	2	-	5/20/21/23	-
2	7ID	J	4	2	-	10/20/21/23	-
2	7ID	H	2	2	-	12/20/21/23	-
2	7ID	K	1	2	-	11/20/21/23	-
2	7ID	L	7	2	-	8/20/21/23	-
2	7ID	F	3	2	-	5/20/21/23	-
2	7ID	J	2	2	-	11/20/21/23	-
2	7ID	L	6	2	-	7/20/21/23	-
2	7ID	K	5	2	-	14/20/21/23	-
2	7ID	F	1	2	-	0/0/2/23	-
2	7ID	I	7	2	-	9/20/21/23	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	7ID	J	3	2	-	10/20/21/23	-
2	7ID	G	3	2	-	5/20/21/23	-
2	7ID	L	1	2	-	11/20/21/23	-
2	7ID	H	3	2	-	5/20/21/23	-
2	7ID	J	5	2	-	12/20/21/23	-
2	7ID	I	6	2	-	7/20/21/23	-
2	7ID	L	3	2	-	8/20/21/23	-
2	7ID	K	4	2	-	10/20/21/23	-
2	7ID	I	1	2	-	9/20/21/23	-
2	7ID	G	2	2	-	12/20/21/23	-
2	7ID	L	5	2	-	14/20/21/23	-
2	7ID	L	4	2	-	10/20/21/23	-
2	7ID	F	2	2	-	12/20/21/23	-
2	7ID	F	4	2	-	11/18/19/23	-
2	7ID	H	1	2	-	0/0/2/23	-
2	7ID	J	1	2	-	9/20/21/23	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	7ID	CG-N2	-6.20	1.33	1.47
2	E	4	7ID	CG-N2	-6.19	1.33	1.47
2	G	4	7ID	CG-N2	-6.18	1.33	1.47
2	H	4	7ID	CG-N2	-6.18	1.33	1.47
2	I	4	7ID	OX2-CO2	-2.17	1.23	1.30
2	J	4	7ID	OX2-CO2	-2.15	1.23	1.30
2	L	6	7ID	OX2-CO2	-2.07	1.23	1.30
2	K	6	7ID	OX2-CO2	-2.05	1.23	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	4	7ID	CG-N2-CA2	4.35	121.68	114.04
2	E	4	7ID	CG-N2-CA2	4.35	121.67	114.04
2	F	4	7ID	CG-N2-CA2	4.34	121.65	114.04
2	G	4	7ID	CG-N2-CA2	4.33	121.64	114.04
2	K	5	7ID	CB-CA-C	-3.61	104.69	111.47
2	L	5	7ID	CB-CA-C	-3.61	104.69	111.47
2	J	5	7ID	CB-CA-C	-3.61	104.70	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	5	7ID	CB-CA-C	-3.61	104.70	111.47
2	L	2	7ID	CB-CA-C	-2.88	106.07	111.47
2	I	2	7ID	CB-CA-C	-2.87	106.08	111.47
2	J	2	7ID	CB-CA-C	-2.86	106.10	111.47
2	K	2	7ID	CB-CA-C	-2.85	106.12	111.47
2	I	6	7ID	CB2-CA2-N2	2.08	115.07	110.88
2	J	6	7ID	CB2-CA2-N2	2.08	115.07	110.88
2	L	6	7ID	CB2-CA2-N2	2.07	115.06	110.88
2	K	6	7ID	CB2-CA2-N2	2.07	115.06	110.88
2	K	7	7ID	CB-CA-C	-2.01	107.70	111.47

There are no chirality outliers.

All (386) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1	7ID	CB-CG-N2-CA2
2	I	1	7ID	OD1-CG-N2-CA2
2	J	1	7ID	CB-CG-N2-CA2
2	J	1	7ID	OD1-CG-N2-CA2
2	K	1	7ID	CB-CG-N2-CA2
2	K	1	7ID	OD1-CG-N2-CA2
2	L	1	7ID	CB-CG-N2-CA2
2	L	1	7ID	OD1-CG-N2-CA2
2	E	2	7ID	C-CA-CB-CG
2	E	2	7ID	CB-CG-N2-CA2
2	E	2	7ID	OD1-CG-N2-CA2
2	F	2	7ID	C-CA-CB-CG
2	F	2	7ID	CB-CG-N2-CA2
2	F	2	7ID	OD1-CG-N2-CA2
2	G	2	7ID	C-CA-CB-CG
2	G	2	7ID	CB-CG-N2-CA2
2	G	2	7ID	OD1-CG-N2-CA2
2	H	2	7ID	C-CA-CB-CG
2	H	2	7ID	CB-CG-N2-CA2
2	H	2	7ID	OD1-CG-N2-CA2
2	I	2	7ID	CB-CG-N2-CA2
2	I	2	7ID	OD1-CG-N2-CA2
2	J	2	7ID	CB-CG-N2-CA2
2	J	2	7ID	OD1-CG-N2-CA2
2	K	2	7ID	CB-CG-N2-CA2
2	K	2	7ID	OD1-CG-N2-CA2
2	K	2	7ID	NH2-CZ2-NE2-CD2

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Mol	Chain	Res	Type	Atoms
2	L	2	7ID	CB-CG-N2-CA2
2	L	2	7ID	OD1-CG-N2-CA2
2	L	2	7ID	NH2-CZ2-NE2-CD2
2	E	3	7ID	CB-CG-N2-CA2
2	E	3	7ID	OD1-CG-N2-CA2
2	E	3	7ID	NH1-CZ2-NE2-CD2
2	E	3	7ID	NH2-CZ2-NE2-CD2
2	F	3	7ID	CB-CG-N2-CA2
2	F	3	7ID	OD1-CG-N2-CA2
2	F	3	7ID	NH1-CZ2-NE2-CD2
2	F	3	7ID	NH2-CZ2-NE2-CD2
2	G	3	7ID	CB-CG-N2-CA2
2	G	3	7ID	OD1-CG-N2-CA2
2	G	3	7ID	NH1-CZ2-NE2-CD2
2	G	3	7ID	NH2-CZ2-NE2-CD2
2	H	3	7ID	CB-CG-N2-CA2
2	H	3	7ID	OD1-CG-N2-CA2
2	H	3	7ID	NH1-CZ2-NE2-CD2
2	H	3	7ID	NH2-CZ2-NE2-CD2
2	I	3	7ID	O-C-CA-CB
2	I	3	7ID	CB-CG-N2-CA2
2	I	3	7ID	OD1-CG-N2-CA2
2	I	3	7ID	CG2-CD2-NE2-CZ2
2	I	3	7ID	NH2-CZ2-NE2-CD2
2	J	3	7ID	O-C-CA-CB
2	J	3	7ID	CB-CG-N2-CA2
2	J	3	7ID	OD1-CG-N2-CA2
2	J	3	7ID	CG2-CD2-NE2-CZ2
2	J	3	7ID	NH2-CZ2-NE2-CD2
2	K	3	7ID	O-C-CA-CB
2	K	3	7ID	CB-CG-N2-CA2
2	K	3	7ID	OD1-CG-N2-CA2
2	K	3	7ID	CG2-CD2-NE2-CZ2
2	L	3	7ID	O-C-CA-CB
2	L	3	7ID	CB-CG-N2-CA2
2	L	3	7ID	OD1-CG-N2-CA2
2	L	3	7ID	CG2-CD2-NE2-CZ2
2	E	4	7ID	CA-CB-CG-N2
2	E	4	7ID	CO2-CA2-N2-CG
2	E	4	7ID	NH1-CZ2-NE2-CD2
2	E	4	7ID	NH2-CZ2-NE2-CD2
2	F	4	7ID	CA-CB-CG-N2

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Mol	Chain	Res	Type	Atoms
2	F	4	7ID	CO2-CA2-N2-CG
2	F	4	7ID	NH1-CZ2-NE2-CD2
2	F	4	7ID	NH2-CZ2-NE2-CD2
2	G	4	7ID	CA-CB-CG-N2
2	G	4	7ID	CO2-CA2-N2-CG
2	G	4	7ID	NH1-CZ2-NE2-CD2
2	G	4	7ID	NH2-CZ2-NE2-CD2
2	H	4	7ID	CA-CB-CG-N2
2	H	4	7ID	CO2-CA2-N2-CG
2	H	4	7ID	NH1-CZ2-NE2-CD2
2	H	4	7ID	NH2-CZ2-NE2-CD2
2	I	4	7ID	N-CA-CB-CG
2	I	4	7ID	O-C-CA-CB
2	I	4	7ID	NH1-CZ2-NE2-CD2
2	I	4	7ID	NH2-CZ2-NE2-CD2
2	J	4	7ID	N-CA-CB-CG
2	J	4	7ID	O-C-CA-CB
2	J	4	7ID	NH1-CZ2-NE2-CD2
2	J	4	7ID	NH2-CZ2-NE2-CD2
2	K	4	7ID	N-CA-CB-CG
2	K	4	7ID	O-C-CA-CB
2	K	4	7ID	NH1-CZ2-NE2-CD2
2	K	4	7ID	NH2-CZ2-NE2-CD2
2	L	4	7ID	N-CA-CB-CG
2	L	4	7ID	O-C-CA-CB
2	L	4	7ID	NH1-CZ2-NE2-CD2
2	L	4	7ID	NH2-CZ2-NE2-CD2
2	I	5	7ID	CB-CG-N2-CA2
2	I	5	7ID	OD1-CG-N2-CA2
2	I	5	7ID	CB2-CA2-N2-CG
2	I	5	7ID	CG2-CD2-NE2-CZ2
2	I	5	7ID	NH1-CZ2-NE2-CD2
2	I	5	7ID	NH2-CZ2-NE2-CD2
2	J	5	7ID	CB-CG-N2-CA2
2	J	5	7ID	OD1-CG-N2-CA2
2	J	5	7ID	CB2-CA2-N2-CG
2	J	5	7ID	CG2-CD2-NE2-CZ2
2	J	5	7ID	NH1-CZ2-NE2-CD2
2	J	5	7ID	NH2-CZ2-NE2-CD2
2	K	5	7ID	CB-CG-N2-CA2
2	K	5	7ID	OD1-CG-N2-CA2
2	K	5	7ID	CB2-CA2-N2-CG

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Mol	Chain	Res	Type	Atoms
2	K	5	7ID	CG2-CD2-NE2-CZ2
2	K	5	7ID	NH1-CZ2-NE2-CD2
2	K	5	7ID	NH2-CZ2-NE2-CD2
2	L	5	7ID	CB-CG-N2-CA2
2	L	5	7ID	OD1-CG-N2-CA2
2	L	5	7ID	CB2-CA2-N2-CG
2	L	5	7ID	CG2-CD2-NE2-CZ2
2	L	5	7ID	NH1-CZ2-NE2-CD2
2	L	5	7ID	NH2-CZ2-NE2-CD2
2	I	6	7ID	O-C-CA-CB
2	I	6	7ID	NH1-CZ2-NE2-CD2
2	I	6	7ID	NH2-CZ2-NE2-CD2
2	J	6	7ID	O-C-CA-CB
2	J	6	7ID	NH1-CZ2-NE2-CD2
2	J	6	7ID	NH2-CZ2-NE2-CD2
2	K	6	7ID	O-C-CA-CB
2	K	6	7ID	NH1-CZ2-NE2-CD2
2	K	6	7ID	NH2-CZ2-NE2-CD2
2	L	6	7ID	O-C-CA-CB
2	L	6	7ID	NH1-CZ2-NE2-CD2
2	L	6	7ID	NH2-CZ2-NE2-CD2
2	I	7	7ID	N-CA-CB-CG
2	I	7	7ID	C-CA-CB-CG
2	J	7	7ID	N-CA-CB-CG
2	J	7	7ID	C-CA-CB-CG
2	K	7	7ID	N-CA-CB-CG
2	K	7	7ID	C-CA-CB-CG
2	K	7	7ID	NH2-CZ2-NE2-CD2
2	L	7	7ID	N-CA-CB-CG
2	L	7	7ID	C-CA-CB-CG
2	L	7	7ID	NH2-CZ2-NE2-CD2
2	I	1	7ID	N2-CA2-CB2-CG2
2	J	1	7ID	N2-CA2-CB2-CG2
2	K	1	7ID	N2-CA2-CB2-CG2
2	L	1	7ID	N2-CA2-CB2-CG2
2	E	4	7ID	N2-CA2-CB2-CG2
2	F	4	7ID	N2-CA2-CB2-CG2
2	G	4	7ID	N2-CA2-CB2-CG2
2	H	4	7ID	N2-CA2-CB2-CG2
2	E	2	7ID	NE2-CD2-CG2-CB2
2	F	2	7ID	NE2-CD2-CG2-CB2
2	G	2	7ID	NE2-CD2-CG2-CB2

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Mol	Chain	Res	Type	Atoms
2	H	2	7ID	NE2-CD2-CG2-CB2
2	K	2	7ID	NH1-CZ2-NE2-CD2
2	L	2	7ID	NH1-CZ2-NE2-CD2
2	E	4	7ID	NE2-CD2-CG2-CB2
2	F	4	7ID	NE2-CD2-CG2-CB2
2	G	4	7ID	NE2-CD2-CG2-CB2
2	H	4	7ID	NE2-CD2-CG2-CB2
2	I	4	7ID	NE2-CD2-CG2-CB2
2	J	4	7ID	NE2-CD2-CG2-CB2
2	K	4	7ID	NE2-CD2-CG2-CB2
2	L	4	7ID	NE2-CD2-CG2-CB2
2	E	2	7ID	N2-CA2-CB2-CG2
2	F	2	7ID	N2-CA2-CB2-CG2
2	G	2	7ID	N2-CA2-CB2-CG2
2	H	2	7ID	N2-CA2-CB2-CG2
2	I	3	7ID	NE2-CD2-CG2-CB2
2	J	3	7ID	NE2-CD2-CG2-CB2
2	K	3	7ID	NE2-CD2-CG2-CB2
2	L	3	7ID	NE2-CD2-CG2-CB2
2	I	1	7ID	CO2-CA2-CB2-CG2
2	J	1	7ID	CO2-CA2-CB2-CG2
2	K	1	7ID	CO2-CA2-CB2-CG2
2	L	1	7ID	CO2-CA2-CB2-CG2
2	E	2	7ID	CO2-CA2-CB2-CG2
2	F	2	7ID	CO2-CA2-CB2-CG2
2	G	2	7ID	CO2-CA2-CB2-CG2
2	H	2	7ID	CO2-CA2-CB2-CG2
2	E	4	7ID	CO2-CA2-CB2-CG2
2	F	4	7ID	CO2-CA2-CB2-CG2
2	G	4	7ID	CO2-CA2-CB2-CG2
2	H	4	7ID	CO2-CA2-CB2-CG2
2	E	2	7ID	CB2-CA2-N2-CG
2	F	2	7ID	CB2-CA2-N2-CG
2	G	2	7ID	CB2-CA2-N2-CG
2	H	2	7ID	CB2-CA2-N2-CG
2	I	7	7ID	N2-CA2-CB2-CG2
2	J	7	7ID	N2-CA2-CB2-CG2
2	K	7	7ID	N2-CA2-CB2-CG2
2	L	7	7ID	N2-CA2-CB2-CG2
2	I	5	7ID	CA2-CB2-CG2-CD2
2	J	5	7ID	CA2-CB2-CG2-CD2
2	K	5	7ID	CA2-CB2-CG2-CD2

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Mol	Chain	Res	Type	Atoms
2	L	5	7ID	CA2-CB2-CG2-CD2
2	K	2	7ID	CB2-CA2-CO2-O2
2	K	2	7ID	CB2-CA2-CO2-OX2
2	L	2	7ID	CB2-CA2-CO2-O2
2	L	2	7ID	CB2-CA2-CO2-OX2
2	I	2	7ID	NH1-CZ2-NE2-CD2
2	J	2	7ID	NH1-CZ2-NE2-CD2
2	I	6	7ID	CO2-CA2-CB2-CG2
2	J	6	7ID	CO2-CA2-CB2-CG2
2	K	6	7ID	CO2-CA2-CB2-CG2
2	L	6	7ID	CO2-CA2-CB2-CG2
2	I	3	7ID	CA2-CB2-CG2-CD2
2	J	3	7ID	CA2-CB2-CG2-CD2
2	K	3	7ID	CA2-CB2-CG2-CD2
2	L	3	7ID	CA2-CB2-CG2-CD2
2	I	5	7ID	N-CA-CB-CG
2	J	5	7ID	N-CA-CB-CG
2	K	5	7ID	N-CA-CB-CG
2	L	5	7ID	N-CA-CB-CG
2	I	1	7ID	N2-CA2-CO2-OX2
2	J	1	7ID	N2-CA2-CO2-OX2
2	I	2	7ID	CA2-CB2-CG2-CD2
2	J	2	7ID	CA2-CB2-CG2-CD2
2	K	2	7ID	CA2-CB2-CG2-CD2
2	L	2	7ID	CA2-CB2-CG2-CD2
2	I	1	7ID	N2-CA2-CO2-O2
2	J	1	7ID	N2-CA2-CO2-O2
2	K	1	7ID	N2-CA2-CO2-O2
2	K	1	7ID	N2-CA2-CO2-OX2
2	L	1	7ID	N2-CA2-CO2-O2
2	L	1	7ID	N2-CA2-CO2-OX2
2	H	4	7ID	N2-CA2-CO2-O2
2	K	6	7ID	N2-CA2-CO2-OX2
2	L	6	7ID	N2-CA2-CO2-OX2
2	K	4	7ID	CB2-CA2-CO2-OX2
2	L	4	7ID	CB2-CA2-CO2-OX2
2	I	7	7ID	NH1-CZ2-NE2-CD2
2	J	7	7ID	NH1-CZ2-NE2-CD2
2	K	7	7ID	NH1-CZ2-NE2-CD2
2	L	7	7ID	NH1-CZ2-NE2-CD2
2	E	2	7ID	CA-CB-CG-OD1
2	F	2	7ID	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
2	G	2	7ID	CA-CB-CG-OD1
2	H	2	7ID	CA-CB-CG-OD1
2	I	7	7ID	CA-CB-CG-OD1
2	J	7	7ID	CA-CB-CG-OD1
2	K	7	7ID	CA-CB-CG-OD1
2	L	7	7ID	CA-CB-CG-OD1
2	I	1	7ID	CA-CB-CG-N2
2	J	1	7ID	CA-CB-CG-N2
2	K	1	7ID	CA-CB-CG-N2
2	L	1	7ID	CA-CB-CG-N2
2	I	7	7ID	CA-CB-CG-N2
2	J	7	7ID	CA-CB-CG-N2
2	K	7	7ID	CA-CB-CG-N2
2	L	7	7ID	CA-CB-CG-N2
2	G	4	7ID	N2-CA2-CO2-O2
2	G	4	7ID	N2-CA2-CO2-OX2
2	H	4	7ID	N2-CA2-CO2-OX2
2	K	4	7ID	CB2-CA2-CO2-O2
2	L	4	7ID	CB2-CA2-CO2-O2
2	J	1	7ID	NE2-CD2-CG2-CB2
2	L	1	7ID	NE2-CD2-CG2-CB2
2	K	3	7ID	NH1-CZ2-NE2-CD2
2	L	3	7ID	NH1-CZ2-NE2-CD2
2	I	1	7ID	NE2-CD2-CG2-CB2
2	K	1	7ID	NE2-CD2-CG2-CB2
2	E	4	7ID	N2-CA2-CO2-O2
2	E	4	7ID	N2-CA2-CO2-OX2
2	F	4	7ID	N2-CA2-CO2-O2
2	F	4	7ID	N2-CA2-CO2-OX2
2	I	2	7ID	CO2-CA2-N2-CG
2	K	2	7ID	CO2-CA2-N2-CG
2	L	2	7ID	CO2-CA2-N2-CG
2	I	4	7ID	N2-CA2-CB2-CG2
2	J	4	7ID	N2-CA2-CB2-CG2
2	K	4	7ID	N2-CA2-CB2-CG2
2	L	4	7ID	N2-CA2-CB2-CG2
2	J	2	7ID	CO2-CA2-N2-CG
2	H	2	7ID	N-CA-CB-CG
2	I	2	7ID	N-CA-CB-CG
2	J	2	7ID	N-CA-CB-CG
2	K	2	7ID	N-CA-CB-CG
2	L	2	7ID	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	I	3	7ID	NH1-CZ2-NE2-CD2
2	J	3	7ID	NH1-CZ2-NE2-CD2
2	I	1	7ID	CA-CB-CG-OD1
2	J	1	7ID	CA-CB-CG-OD1
2	K	1	7ID	CA-CB-CG-OD1
2	L	1	7ID	CA-CB-CG-OD1
2	I	6	7ID	N2-CA2-CO2-O2
2	I	6	7ID	N2-CA2-CO2-OX2
2	J	6	7ID	N2-CA2-CO2-O2
2	J	6	7ID	N2-CA2-CO2-OX2
2	K	6	7ID	N2-CA2-CO2-O2
2	L	6	7ID	N2-CA2-CO2-O2
2	E	4	7ID	CB2-CA2-CO2-O2
2	E	4	7ID	CB2-CA2-CO2-OX2
2	F	4	7ID	CB2-CA2-CO2-O2
2	F	4	7ID	CB2-CA2-CO2-OX2
2	I	4	7ID	CO2-CA2-CB2-CG2
2	J	4	7ID	CO2-CA2-CB2-CG2
2	K	4	7ID	CO2-CA2-CB2-CG2
2	L	4	7ID	CO2-CA2-CB2-CG2
2	I	7	7ID	N2-CA2-CO2-OX2
2	J	7	7ID	N2-CA2-CO2-OX2
2	E	2	7ID	CB2-CA2-CO2-OX2
2	F	2	7ID	CB2-CA2-CO2-OX2
2	I	4	7ID	C-CA-CB-CG
2	J	4	7ID	C-CA-CB-CG
2	K	4	7ID	C-CA-CB-CG
2	L	4	7ID	C-CA-CB-CG
2	I	6	7ID	C-CA-CB-CG
2	J	6	7ID	C-CA-CB-CG
2	K	6	7ID	C-CA-CB-CG
2	L	6	7ID	C-CA-CB-CG
2	E	2	7ID	CA-CB-CG-N2
2	F	2	7ID	CA-CB-CG-N2
2	G	2	7ID	CA-CB-CG-N2
2	H	2	7ID	CA-CB-CG-N2
2	I	5	7ID	CA-CB-CG-N2
2	J	5	7ID	CA-CB-CG-N2
2	K	5	7ID	CA-CB-CG-N2
2	L	5	7ID	CA-CB-CG-N2
2	I	2	7ID	NH2-CZ2-NE2-CD2
2	J	2	7ID	NH2-CZ2-NE2-CD2

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Mol	Chain	Res	Type	Atoms
2	I	7	7ID	NH2-CZ2-NE2-CD2
2	J	7	7ID	NH2-CZ2-NE2-CD2
2	E	3	7ID	CA2-CB2-CG2-CD2
2	F	3	7ID	CA2-CB2-CG2-CD2
2	G	3	7ID	CA2-CB2-CG2-CD2
2	H	3	7ID	CA2-CB2-CG2-CD2
2	I	7	7ID	N2-CA2-CO2-O2
2	J	7	7ID	N2-CA2-CO2-O2
2	K	1	7ID	CB2-CA2-CO2-OX2
2	L	1	7ID	CB2-CA2-CO2-OX2
2	E	2	7ID	CB2-CA2-CO2-O2
2	F	2	7ID	CB2-CA2-CO2-O2
2	K	5	7ID	CB2-CA2-CO2-OX2
2	L	5	7ID	CB2-CA2-CO2-OX2
2	I	2	7ID	NE2-CD2-CG2-CB2
2	J	2	7ID	NE2-CD2-CG2-CB2
2	K	2	7ID	NE2-CD2-CG2-CB2
2	L	2	7ID	NE2-CD2-CG2-CB2
2	E	2	7ID	N-CA-CB-CG
2	F	2	7ID	N-CA-CB-CG
2	G	2	7ID	N-CA-CB-CG
2	I	5	7ID	CA-CB-CG-OD1
2	J	5	7ID	CA-CB-CG-OD1
2	K	5	7ID	CA-CB-CG-OD1
2	L	5	7ID	CA-CB-CG-OD1
2	G	2	7ID	CB2-CA2-CO2-OX2
2	H	2	7ID	CB2-CA2-CO2-OX2
2	I	3	7ID	CB2-CA2-CO2-OX2
2	J	3	7ID	CB2-CA2-CO2-OX2
2	K	1	7ID	CB2-CA2-CO2-O2
2	L	1	7ID	CB2-CA2-CO2-O2
2	I	3	7ID	CB2-CA2-CO2-O2
2	J	3	7ID	CB2-CA2-CO2-O2
2	K	7	7ID	N2-CA2-CO2-O2
2	L	7	7ID	N2-CA2-CO2-O2
2	I	2	7ID	CB2-CA2-CO2-O2
2	J	2	7ID	CB2-CA2-CO2-O2
2	G	4	7ID	CB2-CA2-CO2-O2
2	G	4	7ID	CB2-CA2-CO2-OX2
2	H	4	7ID	CB2-CA2-CO2-O2
2	H	4	7ID	CB2-CA2-CO2-OX2
2	I	4	7ID	CB2-CA2-CO2-O2

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Mol	Chain	Res	Type	Atoms
2	J	4	7ID	CB2-CA2-CO2-O2
2	G	2	7ID	CB2-CA2-CO2-O2
2	H	2	7ID	CB2-CA2-CO2-O2
2	I	2	7ID	CB2-CA2-CO2-OX2
2	J	2	7ID	CB2-CA2-CO2-OX2
2	I	4	7ID	CB2-CA2-CO2-OX2
2	J	4	7ID	CB2-CA2-CO2-OX2
2	K	5	7ID	CB2-CA2-CO2-O2
2	L	5	7ID	CB2-CA2-CO2-O2
2	I	2	7ID	C-CA-CB-CG
2	J	2	7ID	C-CA-CB-CG
2	K	2	7ID	C-CA-CB-CG
2	L	2	7ID	C-CA-CB-CG
2	I	5	7ID	C-CA-CB-CG
2	J	5	7ID	C-CA-CB-CG
2	K	5	7ID	C-CA-CB-CG
2	L	5	7ID	C-CA-CB-CG
2	J	5	7ID	NE2-CD2-CG2-CB2
2	I	5	7ID	NE2-CD2-CG2-CB2
2	K	5	7ID	NE2-CD2-CG2-CB2
2	K	3	7ID	NH2-CZ2-NE2-CD2
2	L	3	7ID	NH2-CZ2-NE2-CD2
2	L	5	7ID	NE2-CD2-CG2-CB2

There are no ring outliers.

20 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	4	7ID	3	0
2	I	3	7ID	1	0
2	I	5	7ID	1	0
2	K	2	7ID	1	0
2	K	6	7ID	1	0
2	L	2	7ID	1	0
2	J	6	7ID	1	0
2	I	2	7ID	1	0
2	K	3	7ID	1	0
2	J	4	7ID	3	0
2	J	2	7ID	1	0
2	L	6	7ID	1	0
2	K	5	7ID	1	0
2	J	3	7ID	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	5	7ID	1	0
2	I	6	7ID	1	0
2	L	3	7ID	1	0
2	K	4	7ID	3	0
2	L	5	7ID	1	0
2	L	4	7ID	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 20 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
5	ATP	B	906	3	26,33,33	1.45	3 (11%)	31,52,52	2.20	8 (25%)
5	ATP	A	906	3	26,33,33	1.45	3 (11%)	31,52,52	2.21	8 (25%)
5	ATP	B	907	3	26,33,33	1.32	4 (15%)	31,52,52	2.00	5 (16%)
5	ATP	C	907	3	26,33,33	1.33	3 (11%)	31,52,52	2.00	5 (16%)
5	ATP	A	907	3	26,33,33	1.33	3 (11%)	31,52,52	2.00	5 (16%)
5	ATP	D	906	3	26,33,33	1.45	3 (11%)	31,52,52	2.20	8 (25%)
5	ATP	D	907	3	26,33,33	1.32	3 (11%)	31,52,52	2.00	5 (16%)
5	ATP	C	906	3	26,33,33	1.44	3 (11%)	31,52,52	2.21	8 (25%)

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
5	ATP	B	906	3	-	5/18/38/38	0/3/3/3
5	ATP	A	906	3	-	5/18/38/38	0/3/3/3
5	ATP	B	907	3	-	6/18/38/38	0/3/3/3
5	ATP	C	907	3	-	6/18/38/38	0/3/3/3
5	ATP	A	907	3	-	6/18/38/38	0/3/3/3
5	ATP	D	906	3	-	5/18/38/38	0/3/3/3
5	ATP	D	907	3	-	6/18/38/38	0/3/3/3
5	ATP	C	906	3	-	5/18/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	906	ATP	O4'-C1'	3.41	1.45	1.41
5	C	906	ATP	O4'-C1'	3.39	1.45	1.41
5	A	906	ATP	O4'-C1'	3.39	1.45	1.41
5	B	906	ATP	O4'-C1'	3.37	1.45	1.41
5	A	907	ATP	O4'-C1'	3.16	1.45	1.41
5	B	907	ATP	O4'-C1'	3.15	1.45	1.41
5	C	907	ATP	O4'-C1'	3.13	1.45	1.41
5	D	907	ATP	O4'-C1'	3.11	1.45	1.41
5	D	906	ATP	C2-N3	2.53	1.36	1.32
5	A	906	ATP	C2-N3	2.48	1.36	1.32
5	B	906	ATP	C2-N3	2.45	1.36	1.32
5	C	906	ATP	C2-N3	2.44	1.36	1.32
5	C	906	ATP	C8-N7	-2.29	1.30	1.34
5	B	906	ATP	C8-N7	-2.28	1.30	1.34
5	A	906	ATP	C8-N7	-2.26	1.30	1.34
5	D	906	ATP	C8-N7	-2.21	1.30	1.34
5	C	907	ATP	C4-N3	2.16	1.38	1.35
5	D	907	ATP	C4-N3	2.16	1.38	1.35
5	A	907	ATP	C4-N3	2.13	1.38	1.35
5	B	907	ATP	C4-N3	2.09	1.38	1.35
5	C	907	ATP	C2-N1	2.09	1.37	1.33
5	D	907	ATP	C2-N1	2.06	1.37	1.33
5	A	907	ATP	C2-N1	2.05	1.37	1.33
5	B	907	ATP	C2-N1	2.02	1.37	1.33
5	B	907	ATP	C8-N7	-2.01	1.31	1.34

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	907	ATP	PB-O3B-PG	-6.21	111.52	132.83
5	D	907	ATP	PB-O3B-PG	-6.20	111.55	132.83
5	A	907	ATP	PB-O3B-PG	-6.20	111.56	132.83
5	B	907	ATP	PB-O3B-PG	-6.19	111.58	132.83
5	A	906	ATP	PA-O3A-PB	-6.02	112.16	132.83
5	B	906	ATP	PA-O3A-PB	-6.02	112.16	132.83
5	C	906	ATP	PA-O3A-PB	-6.02	112.16	132.83
5	D	906	ATP	PA-O3A-PB	-6.02	112.18	132.83
5	C	906	ATP	PB-O3B-PG	-5.91	112.55	132.83
5	A	906	ATP	PB-O3B-PG	-5.91	112.56	132.83
5	B	906	ATP	PB-O3B-PG	-5.90	112.57	132.83
5	D	906	ATP	PB-O3B-PG	-5.90	112.58	132.83
5	D	907	ATP	PA-O3A-PB	-5.15	115.14	132.83
5	A	907	ATP	PA-O3A-PB	-5.14	115.20	132.83
5	C	907	ATP	PA-O3A-PB	-5.14	115.20	132.83
5	B	907	ATP	PA-O3A-PB	-5.13	115.22	132.83
5	C	907	ATP	N3-C2-N1	-4.34	121.90	128.68
5	D	907	ATP	N3-C2-N1	-4.33	121.90	128.68
5	A	907	ATP	N3-C2-N1	-4.33	121.91	128.68
5	B	907	ATP	N3-C2-N1	-4.32	121.93	128.68
5	C	906	ATP	N3-C2-N1	-4.29	121.97	128.68
5	D	906	ATP	N3-C2-N1	-4.29	121.97	128.68
5	B	906	ATP	N3-C2-N1	-4.29	121.97	128.68
5	A	906	ATP	N3-C2-N1	-4.29	121.97	128.68
5	D	906	ATP	O2G-PG-O3B	3.65	116.88	104.64
5	C	906	ATP	O2G-PG-O3B	3.65	116.88	104.64
5	A	906	ATP	O2G-PG-O3B	3.65	116.87	104.64
5	B	906	ATP	O2G-PG-O3B	3.64	116.83	104.64
5	B	907	ATP	C3'-C2'-C1'	3.44	106.16	100.98
5	C	907	ATP	C3'-C2'-C1'	3.44	106.15	100.98
5	D	907	ATP	C3'-C2'-C1'	3.43	106.14	100.98
5	A	907	ATP	C3'-C2'-C1'	3.43	106.14	100.98
5	A	906	ATP	C4-C5-N7	-3.02	106.25	109.40
5	B	906	ATP	C4-C5-N7	-3.02	106.25	109.40
5	C	906	ATP	C4-C5-N7	-3.02	106.25	109.40
5	D	906	ATP	C4-C5-N7	-2.97	106.30	109.40
5	D	906	ATP	O2A-PA-O1A	-2.94	97.69	112.24
5	B	906	ATP	O2A-PA-O1A	-2.94	97.70	112.24
5	C	906	ATP	O2A-PA-O1A	-2.94	97.71	112.24
5	A	906	ATP	O2A-PA-O1A	-2.94	97.71	112.24
5	D	906	ATP	C3'-C2'-C1'	2.62	104.92	100.98
5	A	906	ATP	C3'-C2'-C1'	2.60	104.89	100.98
5	B	906	ATP	C3'-C2'-C1'	2.59	104.88	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	906	ATP	C3'-C2'-C1'	2.58	104.86	100.98
5	D	907	ATP	O3G-PG-O3B	2.41	112.72	104.64
5	C	907	ATP	O3G-PG-O3B	2.40	112.69	104.64
5	A	907	ATP	O3G-PG-O3B	2.40	112.68	104.64
5	B	907	ATP	O3G-PG-O3B	2.39	112.66	104.64
5	C	906	ATP	O3G-PG-O1G	-2.07	102.58	110.68
5	B	906	ATP	O3G-PG-O1G	-2.07	102.59	110.68
5	A	906	ATP	O3G-PG-O1G	-2.06	102.60	110.68
5	D	906	ATP	O3G-PG-O1G	-2.06	102.60	110.68

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	906	ATP	C5'-O5'-PA-O2A
5	A	906	ATP	C5'-O5'-PA-O3A
5	A	907	ATP	C5'-O5'-PA-O2A
5	A	907	ATP	C5'-O5'-PA-O3A
5	B	906	ATP	C5'-O5'-PA-O2A
5	B	906	ATP	C5'-O5'-PA-O3A
5	B	907	ATP	C5'-O5'-PA-O2A
5	B	907	ATP	C5'-O5'-PA-O3A
5	C	906	ATP	C5'-O5'-PA-O2A
5	C	906	ATP	C5'-O5'-PA-O3A
5	C	907	ATP	C5'-O5'-PA-O2A
5	C	907	ATP	C5'-O5'-PA-O3A
5	D	906	ATP	C5'-O5'-PA-O2A
5	D	906	ATP	C5'-O5'-PA-O3A
5	D	907	ATP	C5'-O5'-PA-O2A
5	D	907	ATP	C5'-O5'-PA-O3A
5	A	906	ATP	O4'-C4'-C5'-O5'
5	A	906	ATP	C3'-C4'-C5'-O5'
5	B	906	ATP	O4'-C4'-C5'-O5'
5	B	906	ATP	C3'-C4'-C5'-O5'
5	C	906	ATP	O4'-C4'-C5'-O5'
5	C	906	ATP	C3'-C4'-C5'-O5'
5	D	906	ATP	O4'-C4'-C5'-O5'
5	D	906	ATP	C3'-C4'-C5'-O5'
5	A	907	ATP	PB-O3A-PA-O1A
5	B	907	ATP	PB-O3A-PA-O1A
5	C	907	ATP	PB-O3A-PA-O1A
5	D	907	ATP	PB-O3A-PA-O1A

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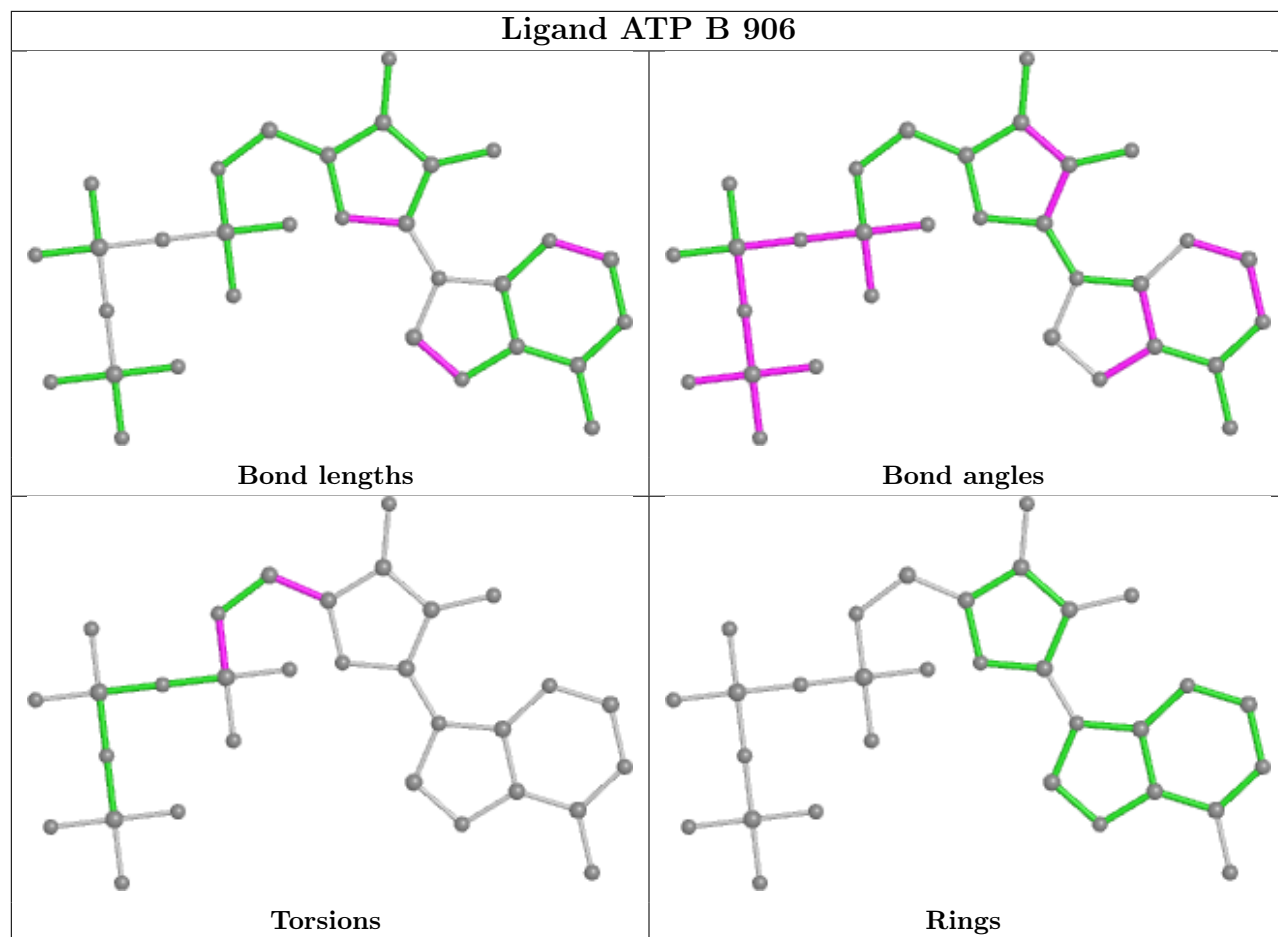
Mol	Chain	Res	Type	Atoms
5	A	906	ATP	C5'-O5'-PA-O1A
5	A	907	ATP	C5'-O5'-PA-O1A
5	B	906	ATP	C5'-O5'-PA-O1A
5	B	907	ATP	C5'-O5'-PA-O1A
5	C	906	ATP	C5'-O5'-PA-O1A
5	C	907	ATP	C5'-O5'-PA-O1A
5	D	906	ATP	C5'-O5'-PA-O1A
5	D	907	ATP	C5'-O5'-PA-O1A
5	A	907	ATP	O4'-C4'-C5'-O5'
5	B	907	ATP	O4'-C4'-C5'-O5'
5	C	907	ATP	O4'-C4'-C5'-O5'
5	D	907	ATP	O4'-C4'-C5'-O5'
5	A	907	ATP	PB-O3A-PA-O2A
5	B	907	ATP	PB-O3A-PA-O2A
5	C	907	ATP	PB-O3A-PA-O2A
5	D	907	ATP	PB-O3A-PA-O2A

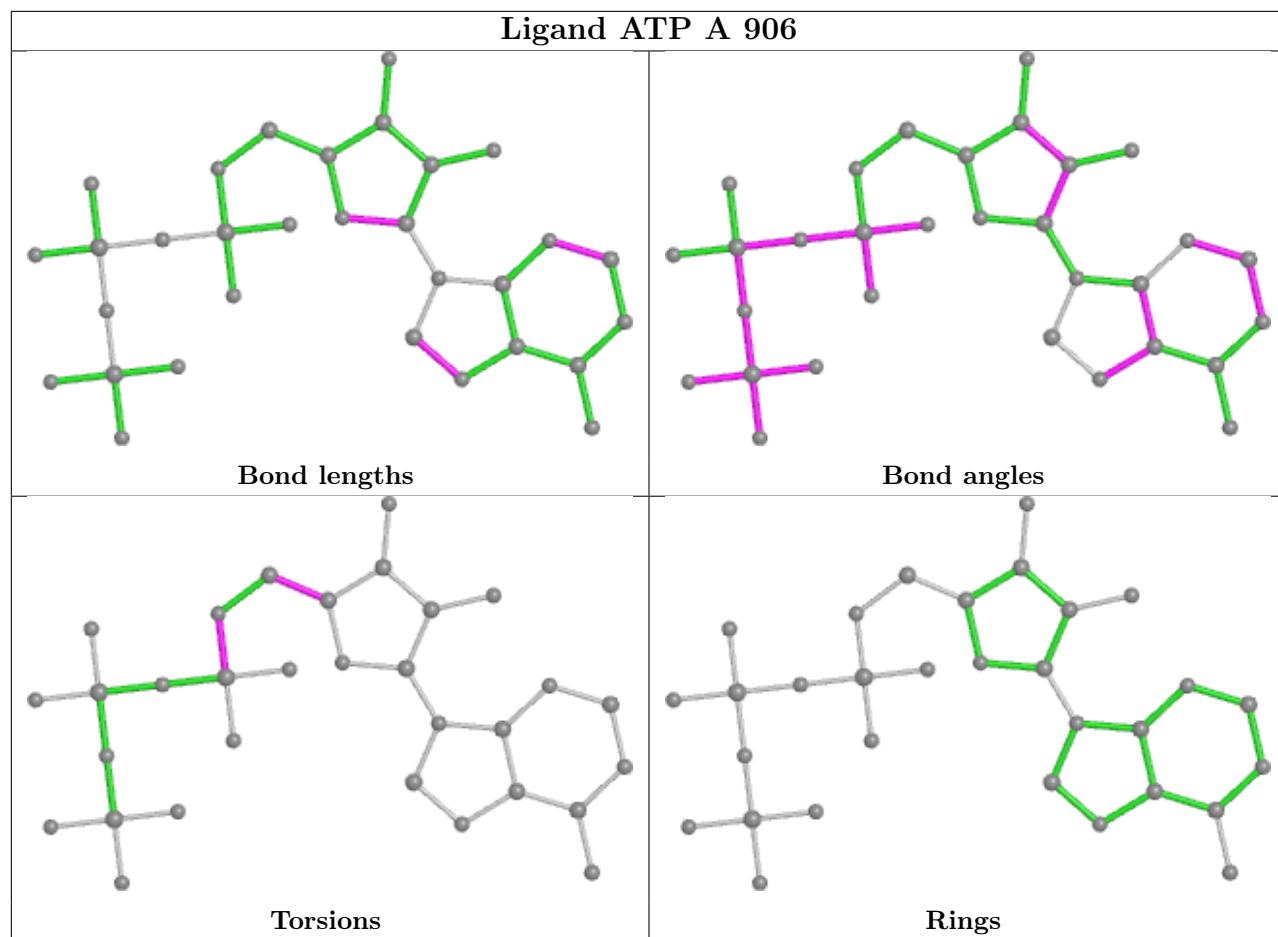
There are no ring outliers.

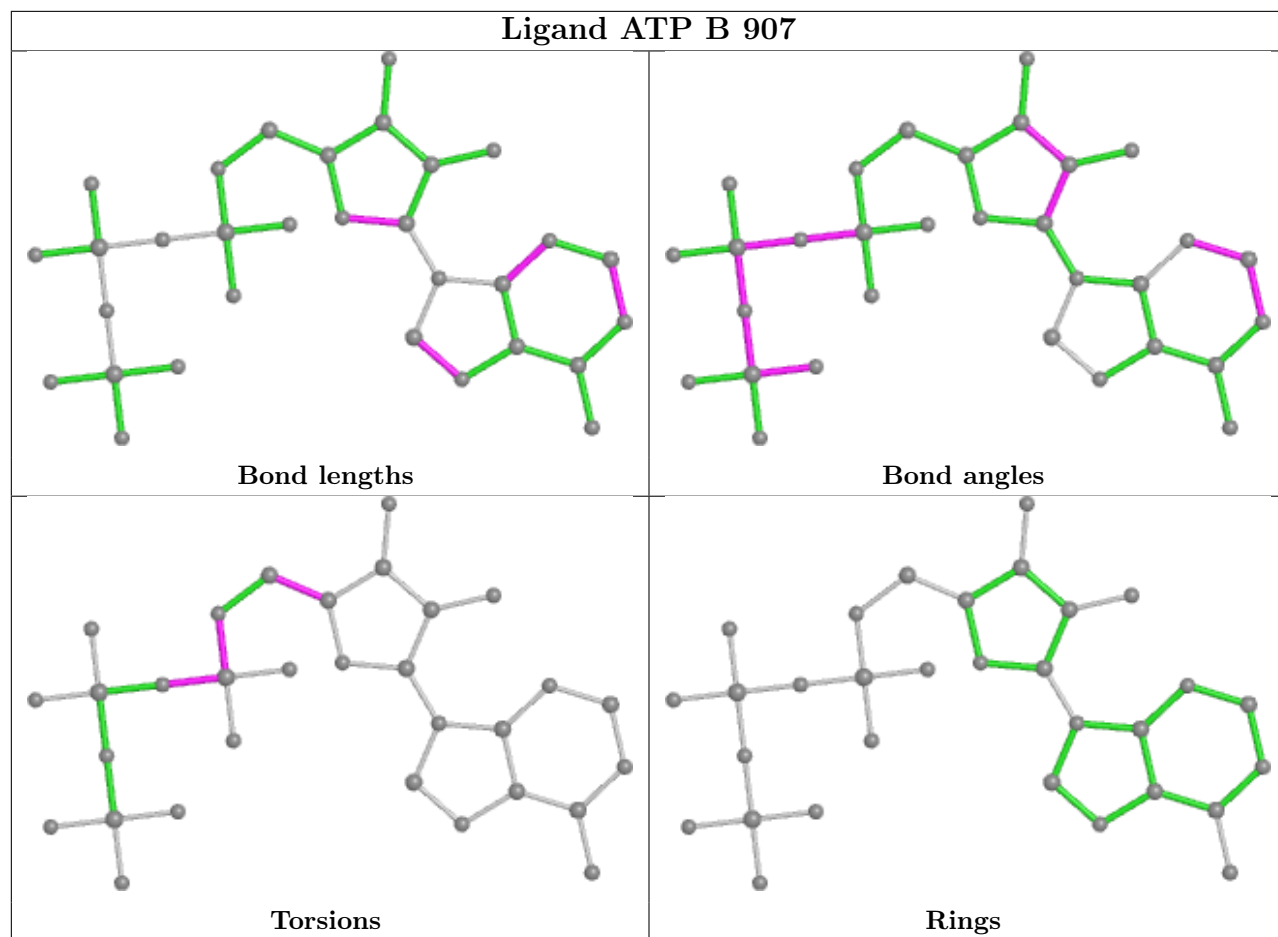
4 monomers are involved in 4 short contacts:

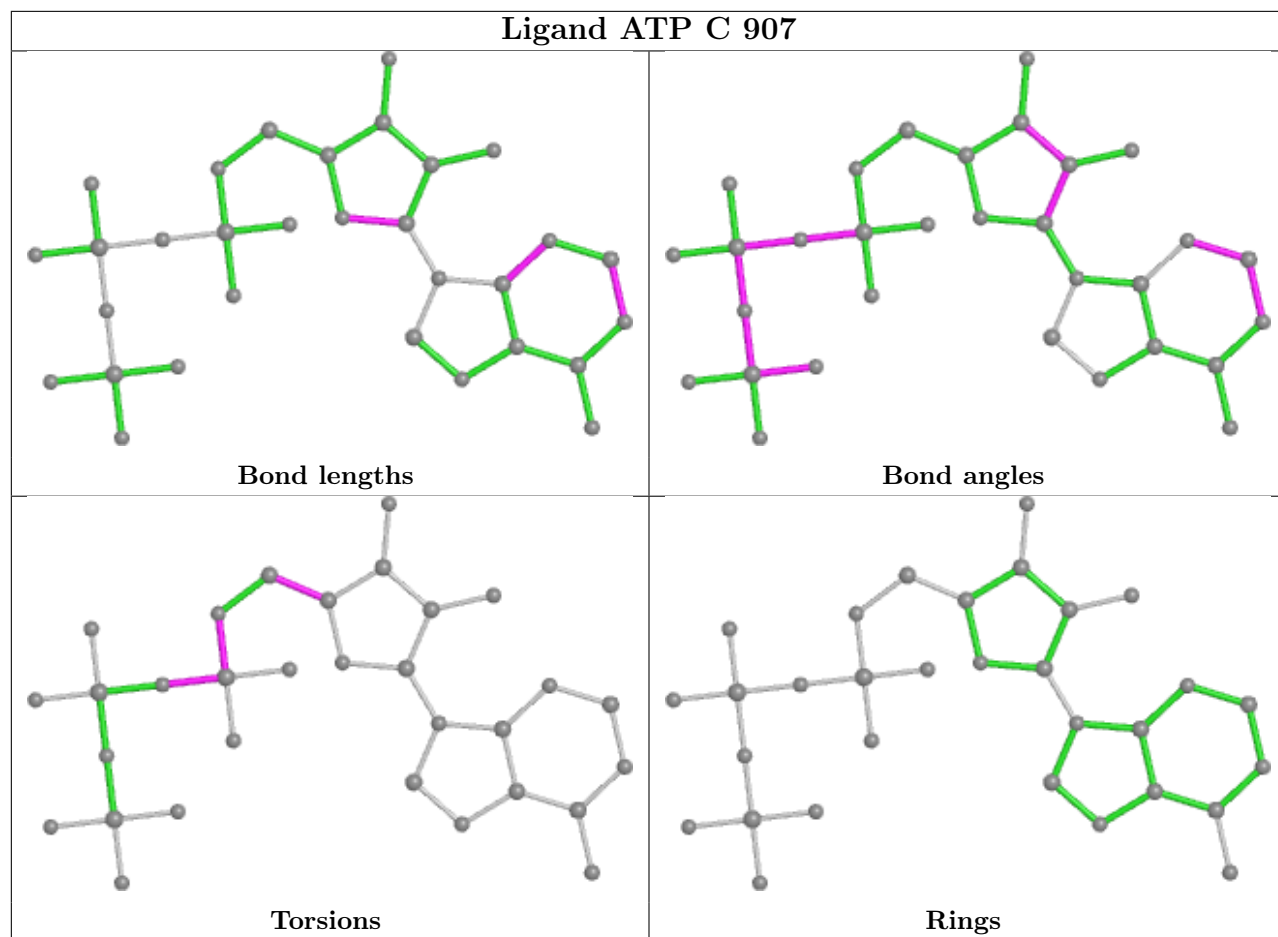
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	907	ATP	1	0
5	C	907	ATP	1	0
5	A	907	ATP	1	0
5	D	907	ATP	1	0

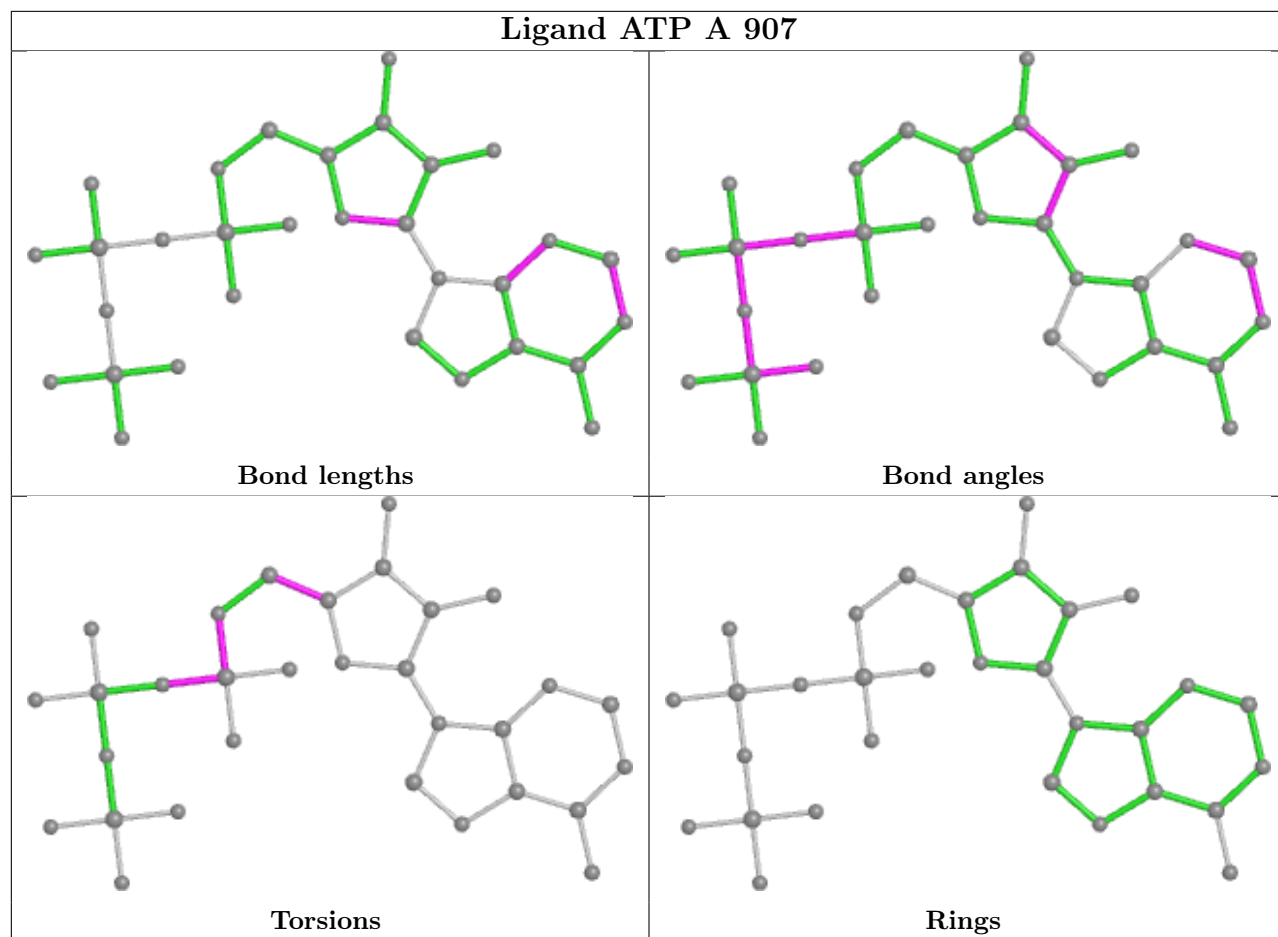
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

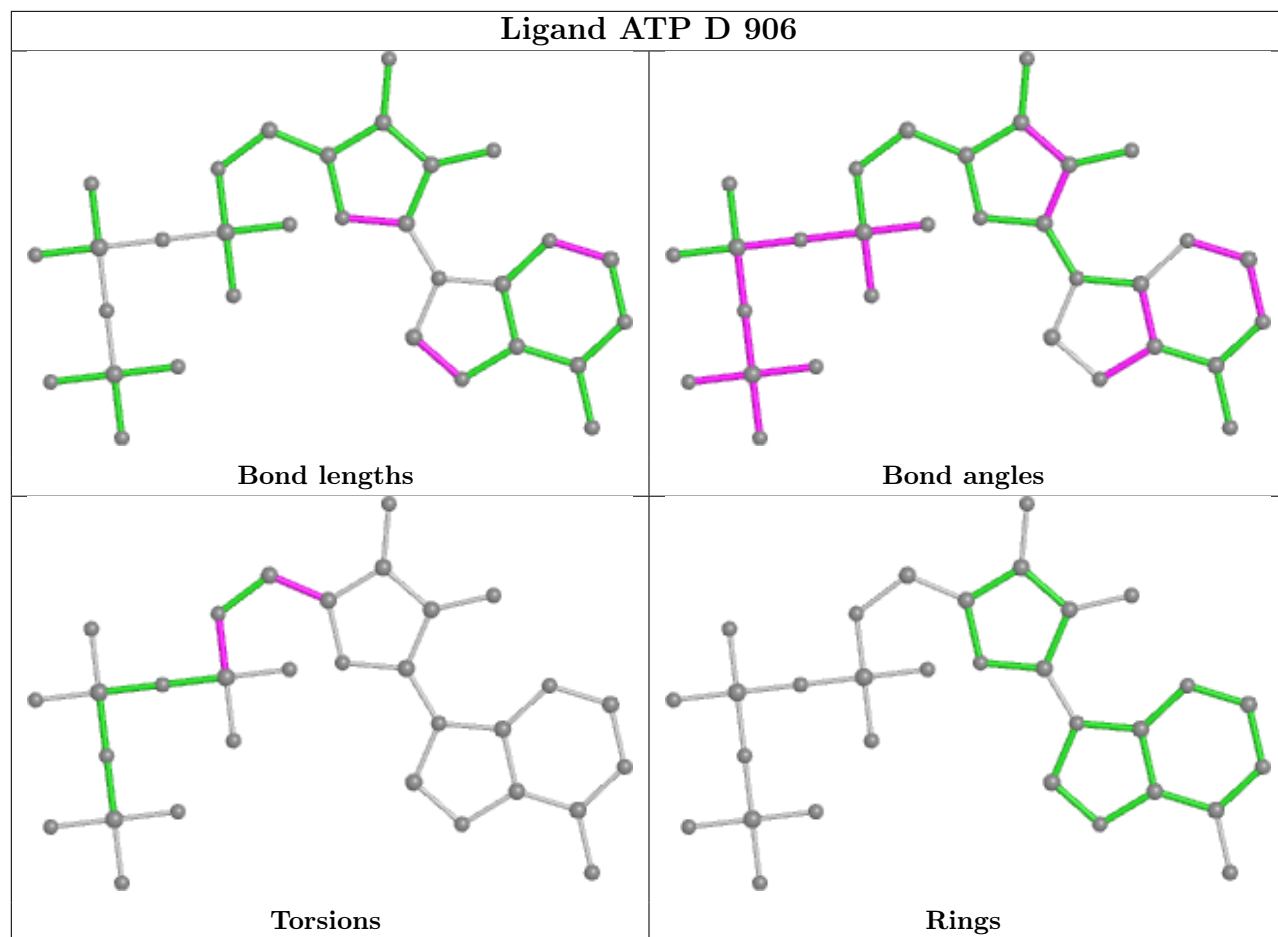


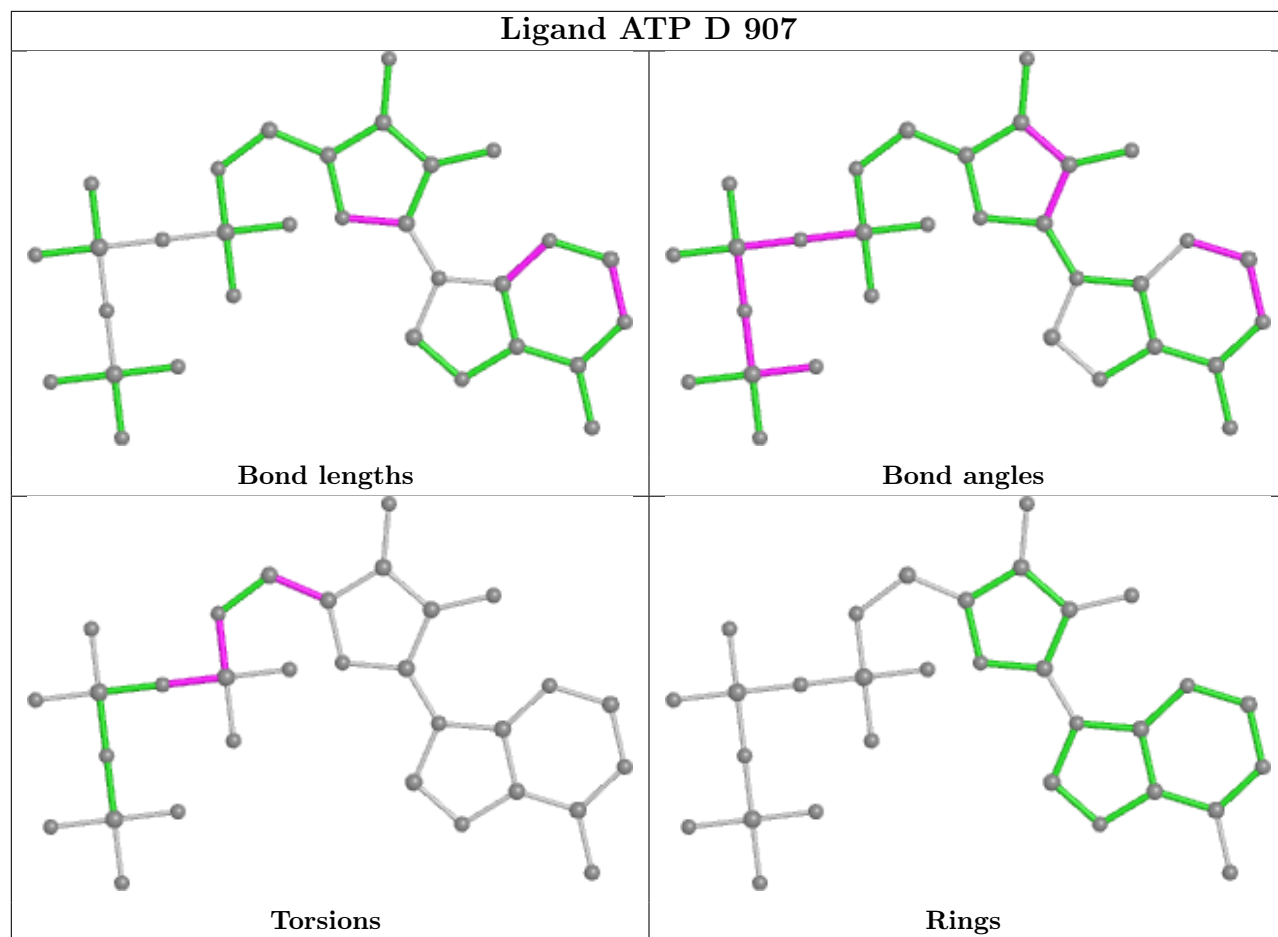


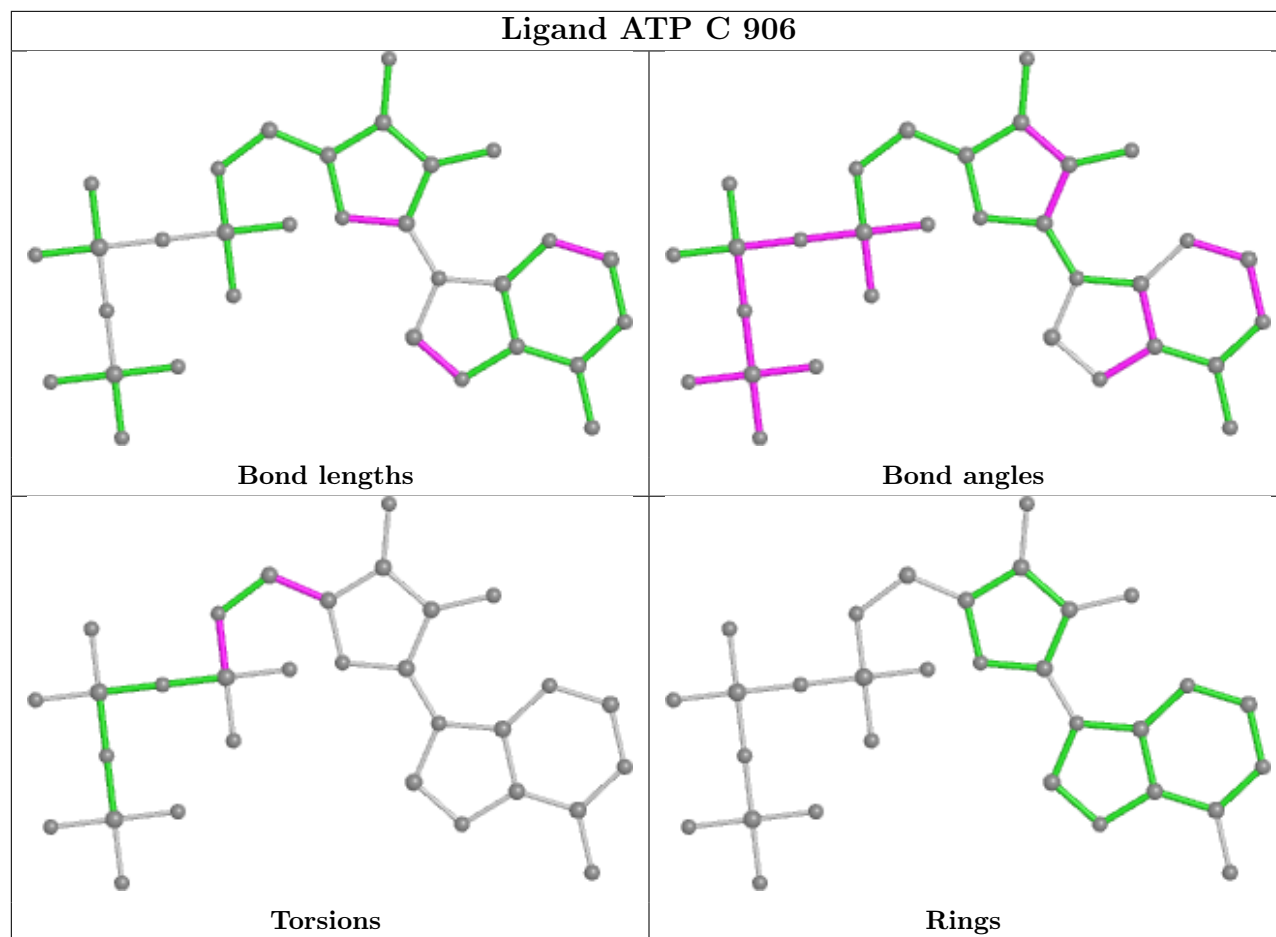












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

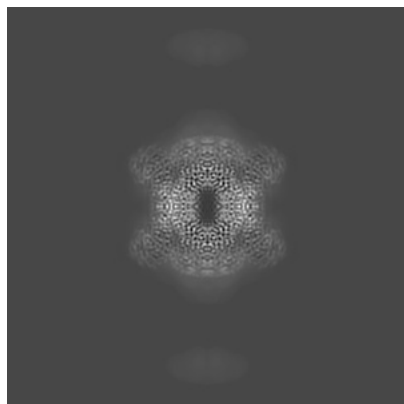
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26161. These allow visual inspection of the internal detail of the map and identification of artifacts.

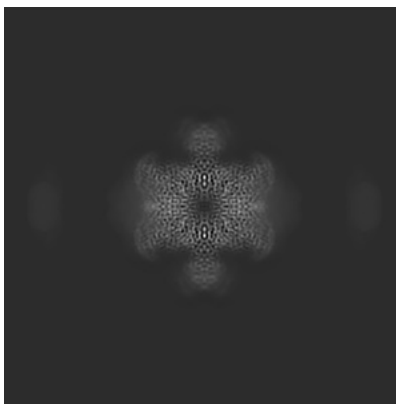
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

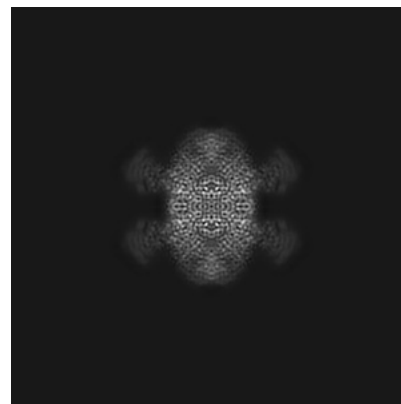
6.1.1 Primary map



X

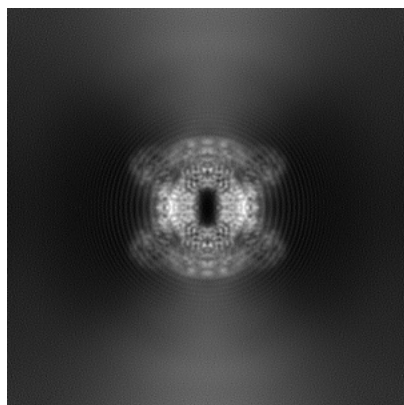


Y

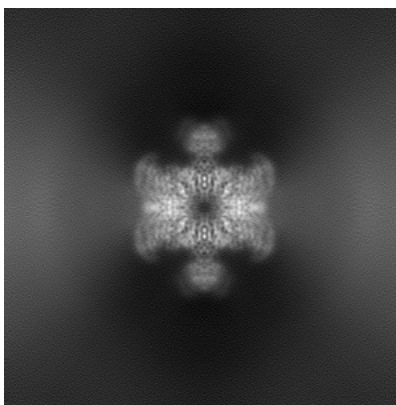


Z

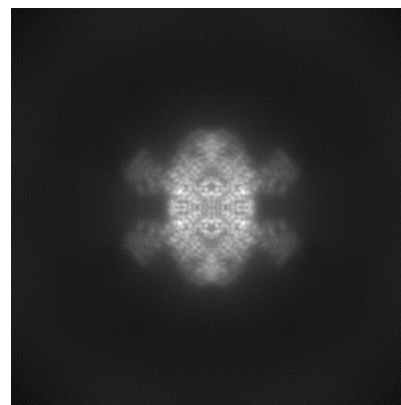
6.1.2 Raw map



X



Y

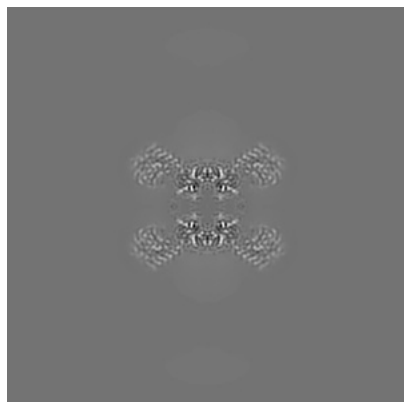


Z

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

6.2 Central slices [i](#)

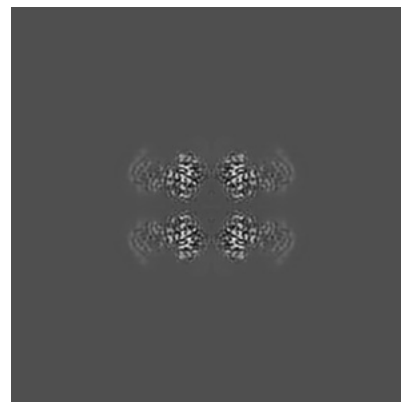
6.2.1 Primary map



X Index: 200

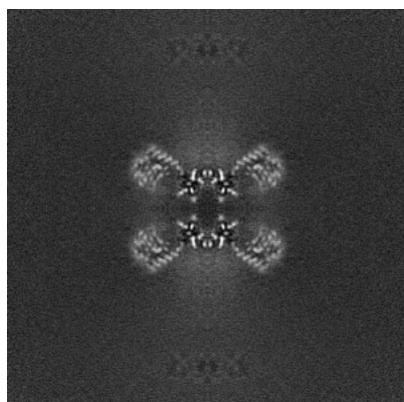


Y Index: 200

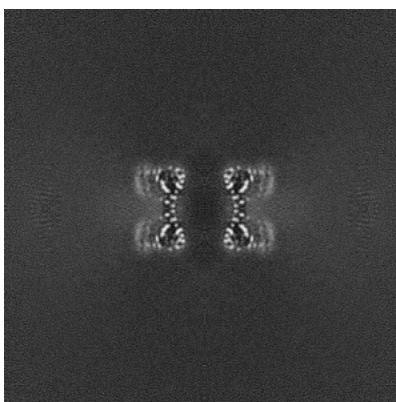


Z Index: 200

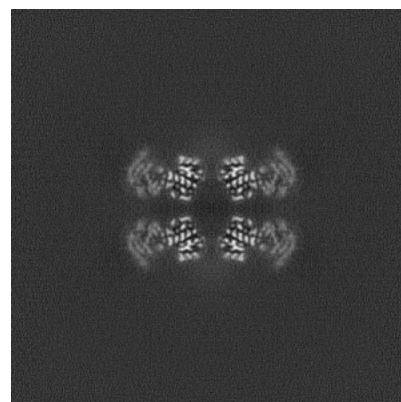
6.2.2 Raw map



X Index: 200



Y Index: 200

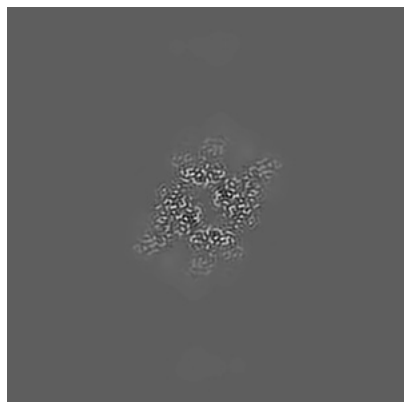


Z Index: 200

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: 178

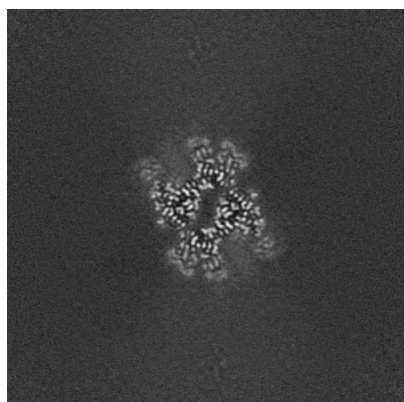


Y Index: 186

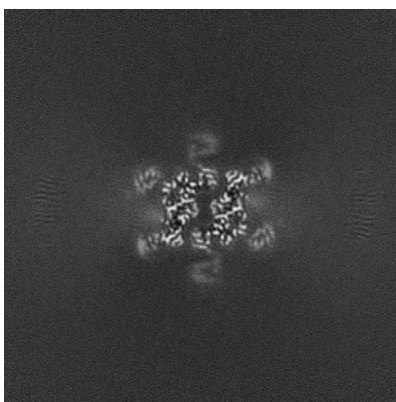


Z Index: 195

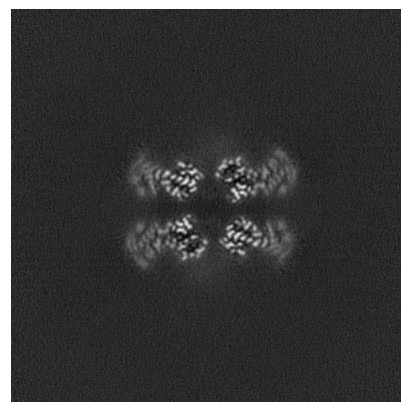
6.3.2 Raw map



X Index: 228



Y Index: 214

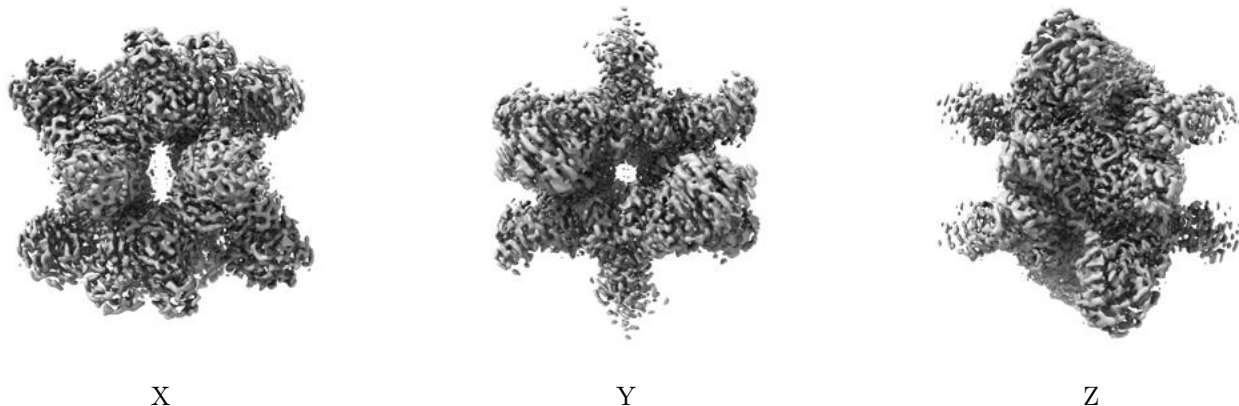


Z Index: 196

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

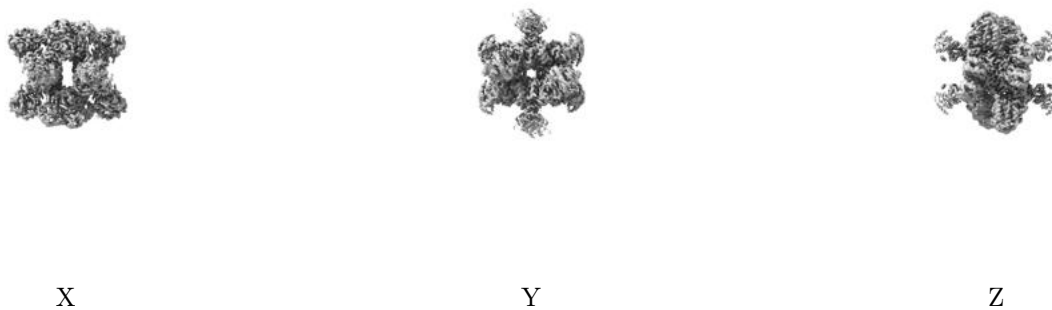
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.59. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

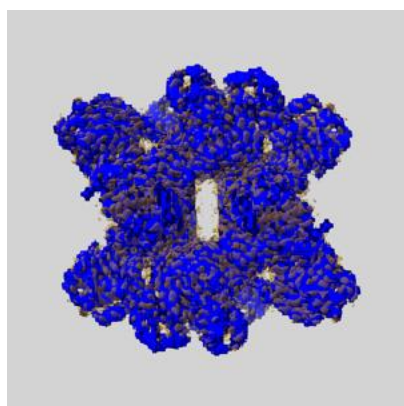
6.5 Mask visualisation [i](#)

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

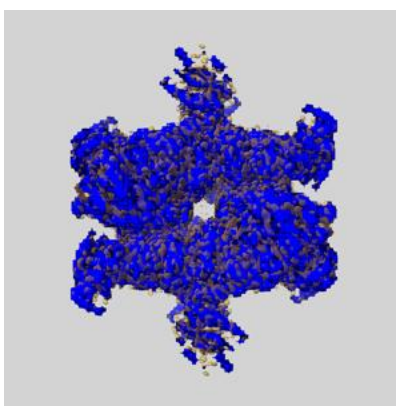
A mask typically either:

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

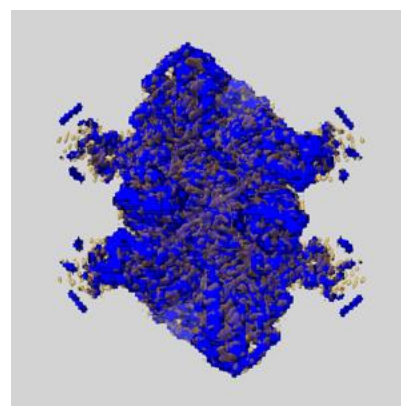
6.5.1 emd_26161_msk_1.map [i](#)



X



Y

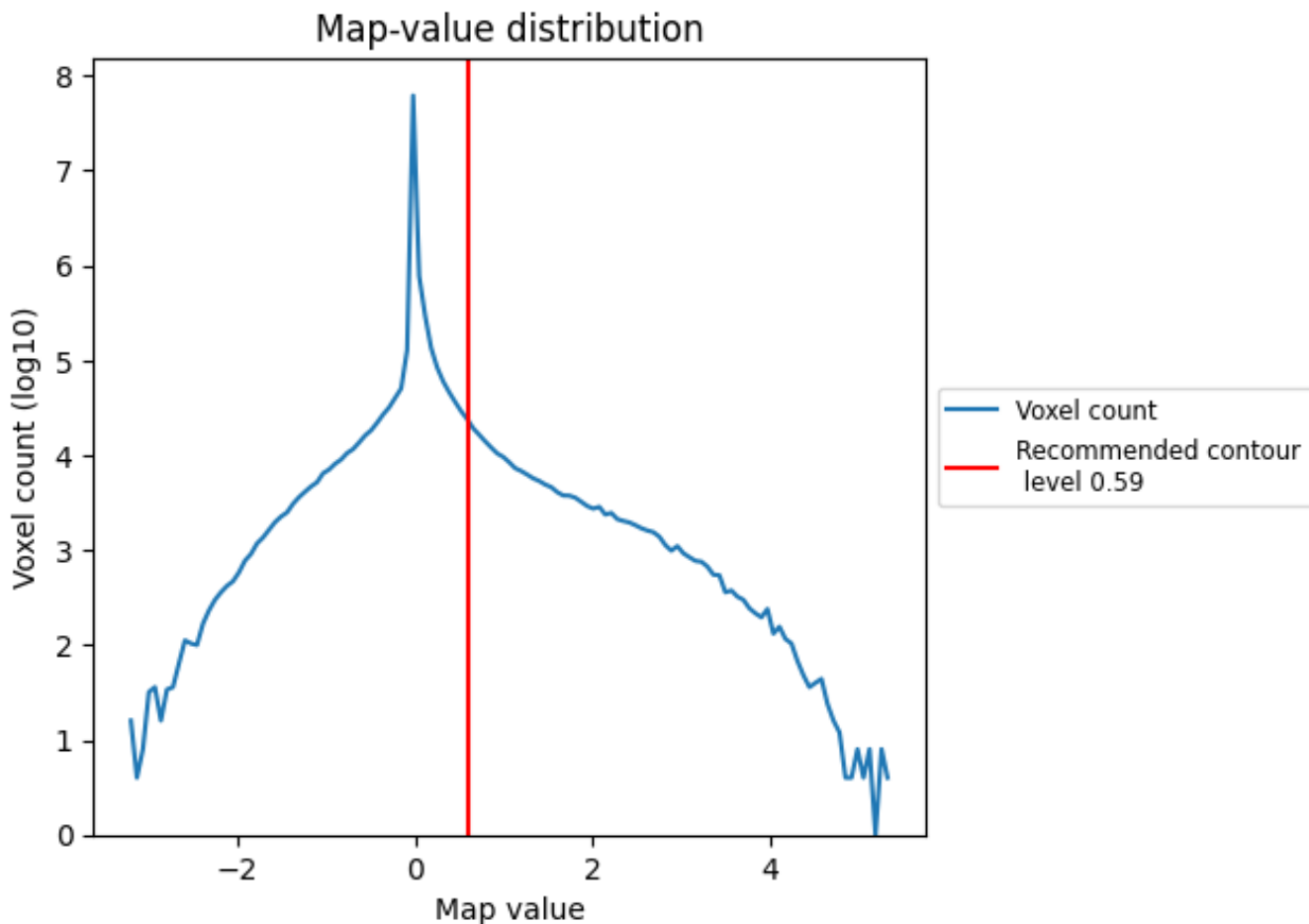


Z

7 Map analysis [i](#)

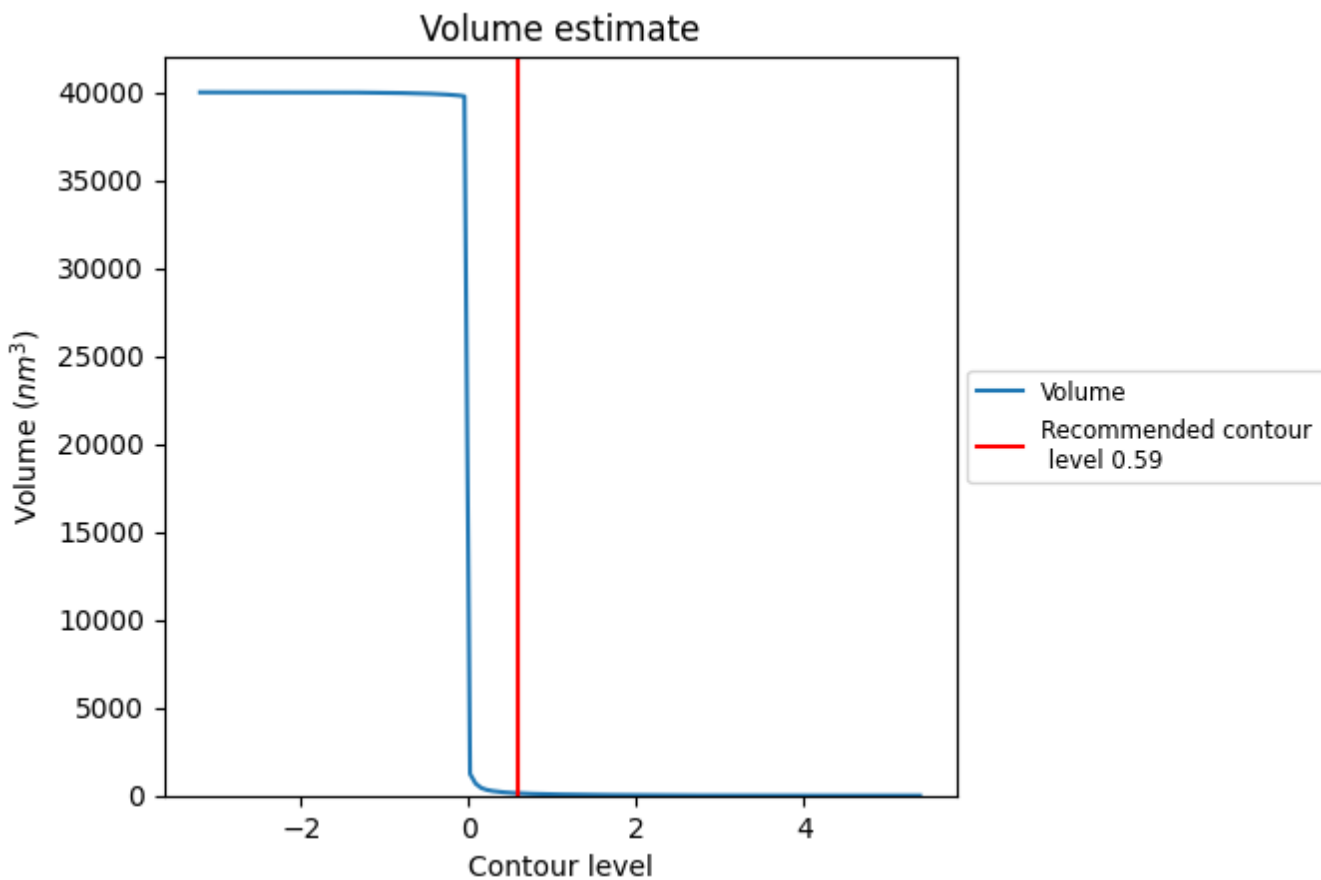
This section contains the results of statistical analysis of the map.

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.

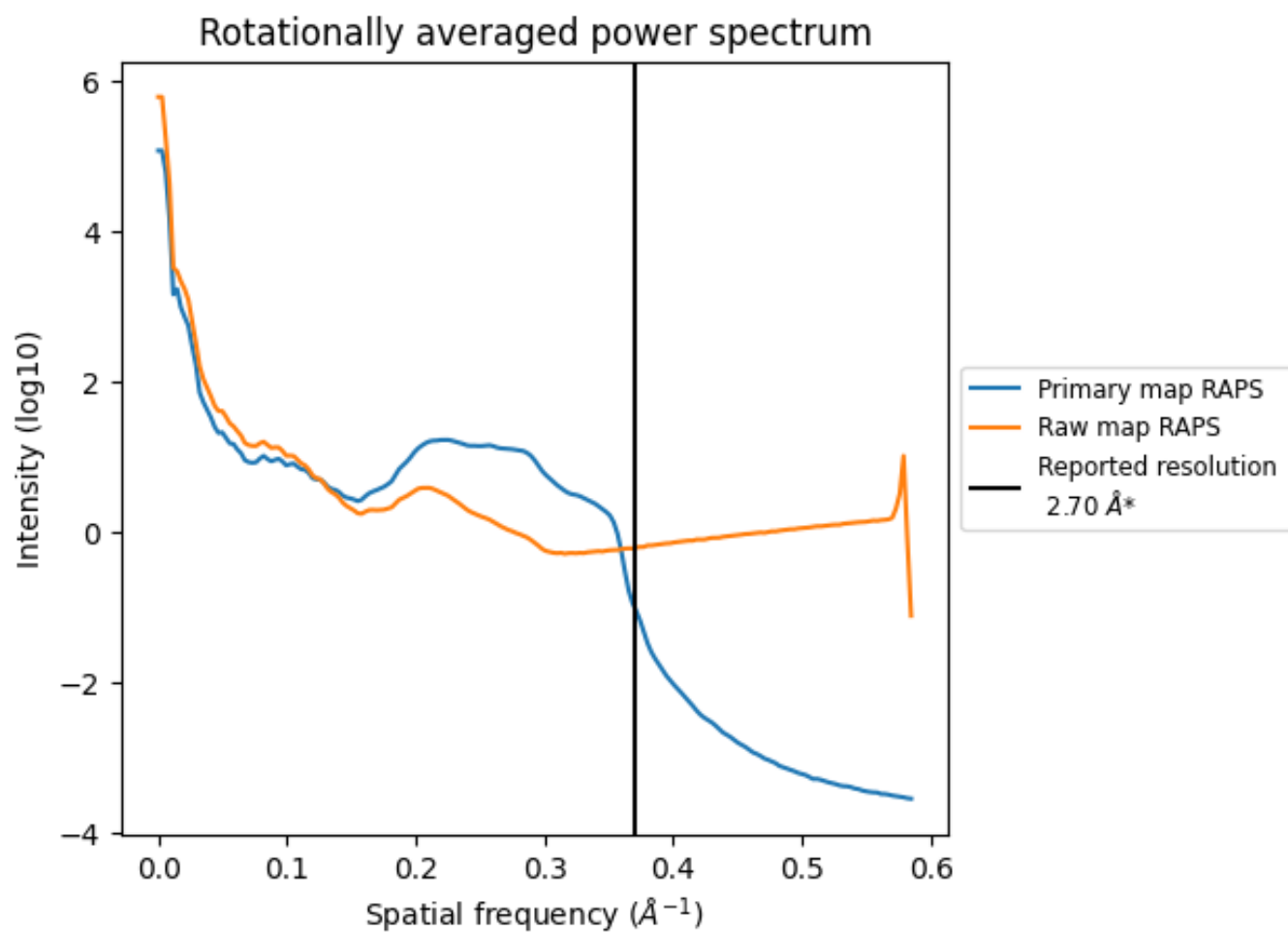
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132 nm³; this corresponds to an approximate mass of 119 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 i

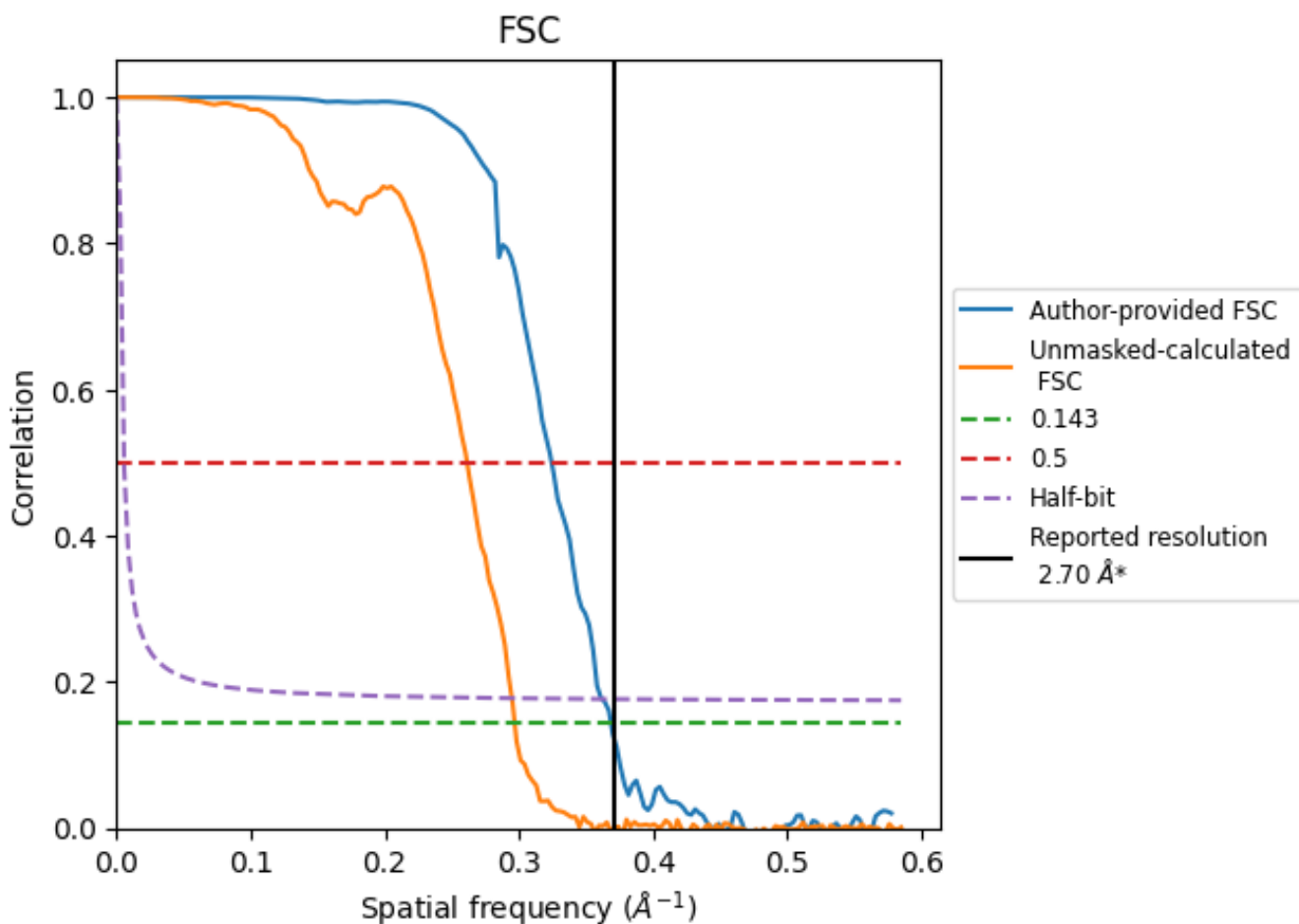


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

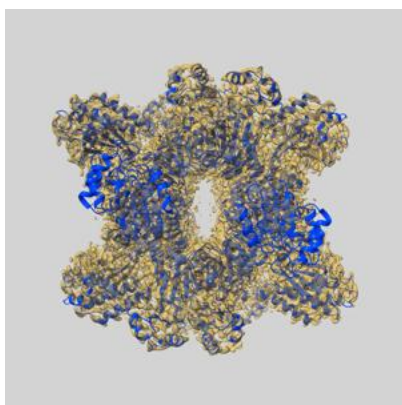
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.71	3.08	2.76
Unmasked-calculated*	3.37	3.83	3.39

*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 3.37 differs from the reported value 2.7 by more than 10 %

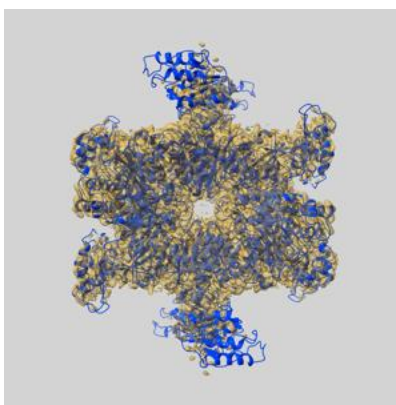
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26161 and PDB model 7TXV. Per-residue inclusion information can be found in section 3 on page 8.

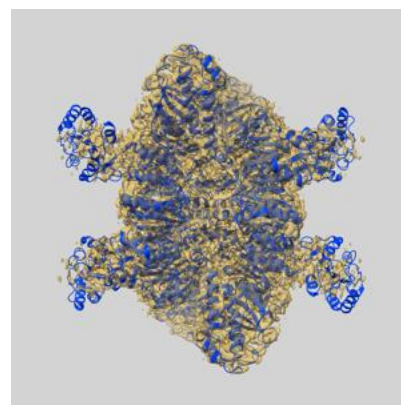
9.1 Map-model overlay [i](#)



X



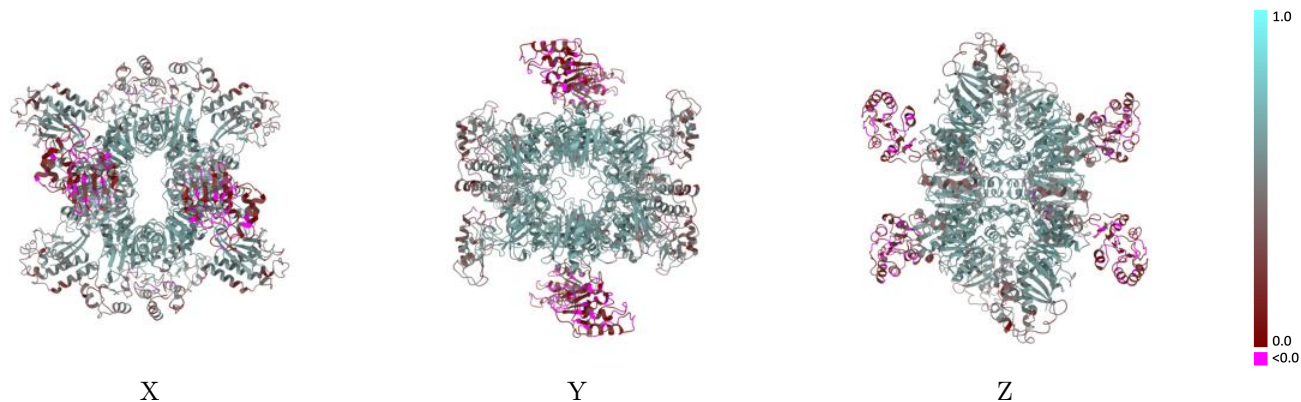
Y



Z

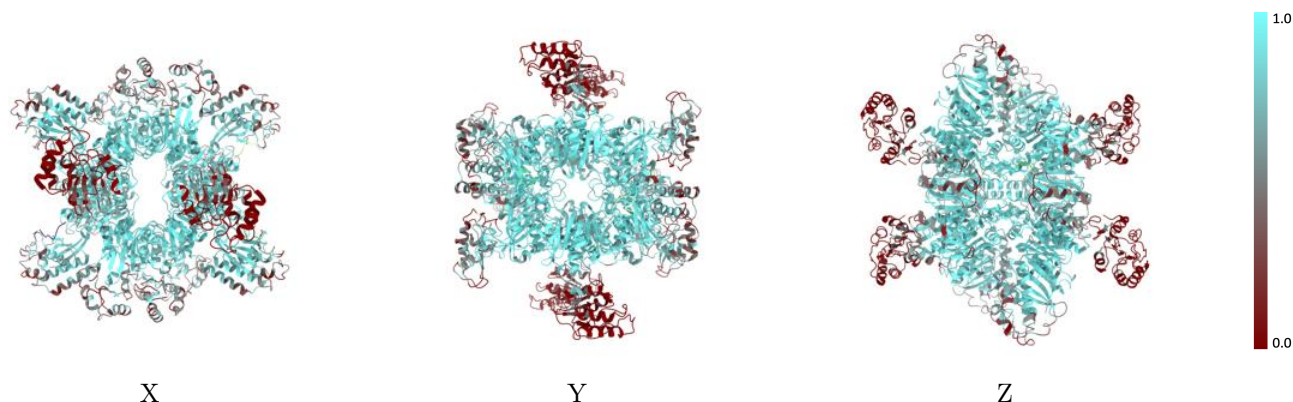
The images above show the 3D surface view of the map at the recommended contour level 0.59 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



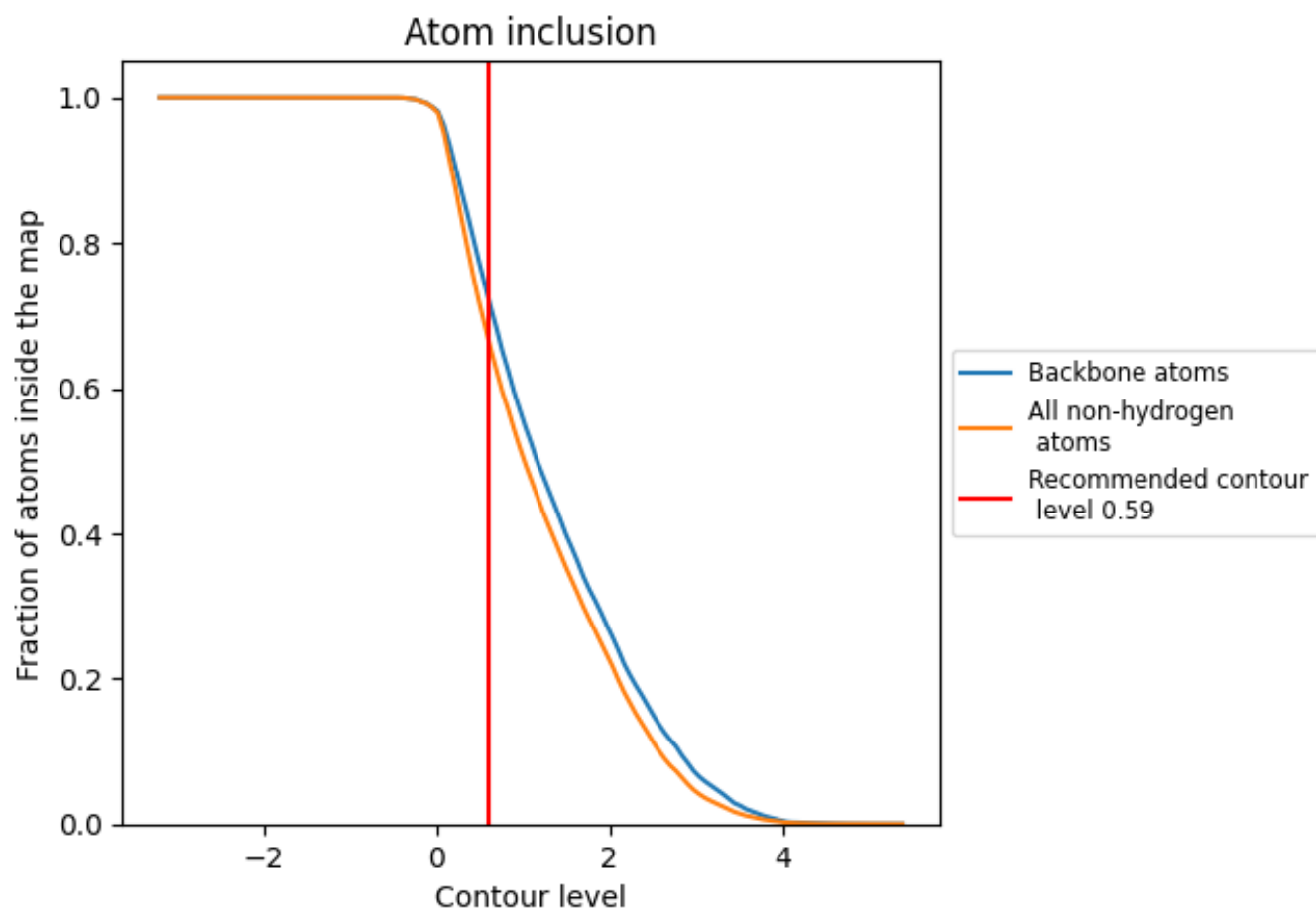
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.59).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.59) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6695	 0.4720
A	 0.6777	 0.4800
B	 0.6680	 0.4650
C	 0.6695	 0.4680
D	 0.6687	 0.4690
E	 0.5636	 0.5600
F	 0.5636	 0.5460
G	 0.5636	 0.5480
H	 0.5636	 0.5550
I	 0.6750	 0.5200
J	 0.6250	 0.4910
K	 0.6250	 0.4920
L	 0.6250	 0.4930

