



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:50 PM UTC

PDB ID : 7UJN / pdb_00007ujn
EMDB ID : EMD-26567
Title : Structure of Human SAMHD1 with Non-Hydrolysable dGTP Analog
Authors : Huynh, K.W.; Ammirati, M.; Han, S.
Deposited on : 2022-03-31
Resolution : 2.89 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

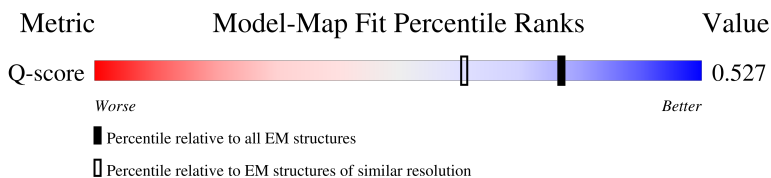
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.89 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	12148 (2.39 - 3.39)

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	626	18% 65% 13% 22%
1	B	626	19% 63% 15% 22%
1	C	626	19% 64% 14% 22%
1	D	626	19% 65% 13% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	T8T	A	702	-	-	X	-
2	T8T	A	703	-	-	X	-
2	T8T	B	701	-	-	X	-
2	T8T	B	703	-	-	X	-
2	T8T	C	701	-	-	X	-
2	T8T	C	702	-	-	X	-
2	T8T	D	701	-	-	X	-
2	T8T	D	702	-	-	X	-

2 Entry composition [i](#)

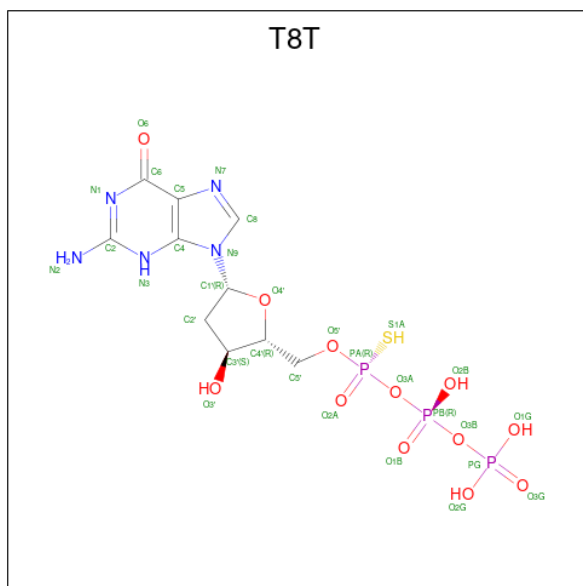
There are 2 unique types of molecules in this entry. The entry contains 16272 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	487	Total	C	N	O	S	0	0
			3975	2542	689	724	20		
1	B	487	Total	C	N	O	S	0	0
			3975	2542	689	724	20		
1	C	487	Total	C	N	O	S	0	0
			3975	2542	689	724	20		
1	D	487	Total	C	N	O	S	0	0
			3975	2542	689	724	20		

- Molecule 2 is 2'-deoxyguanosine-5'-O-(1-thiotriphosphate) (CCD ID: T8T) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
2	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

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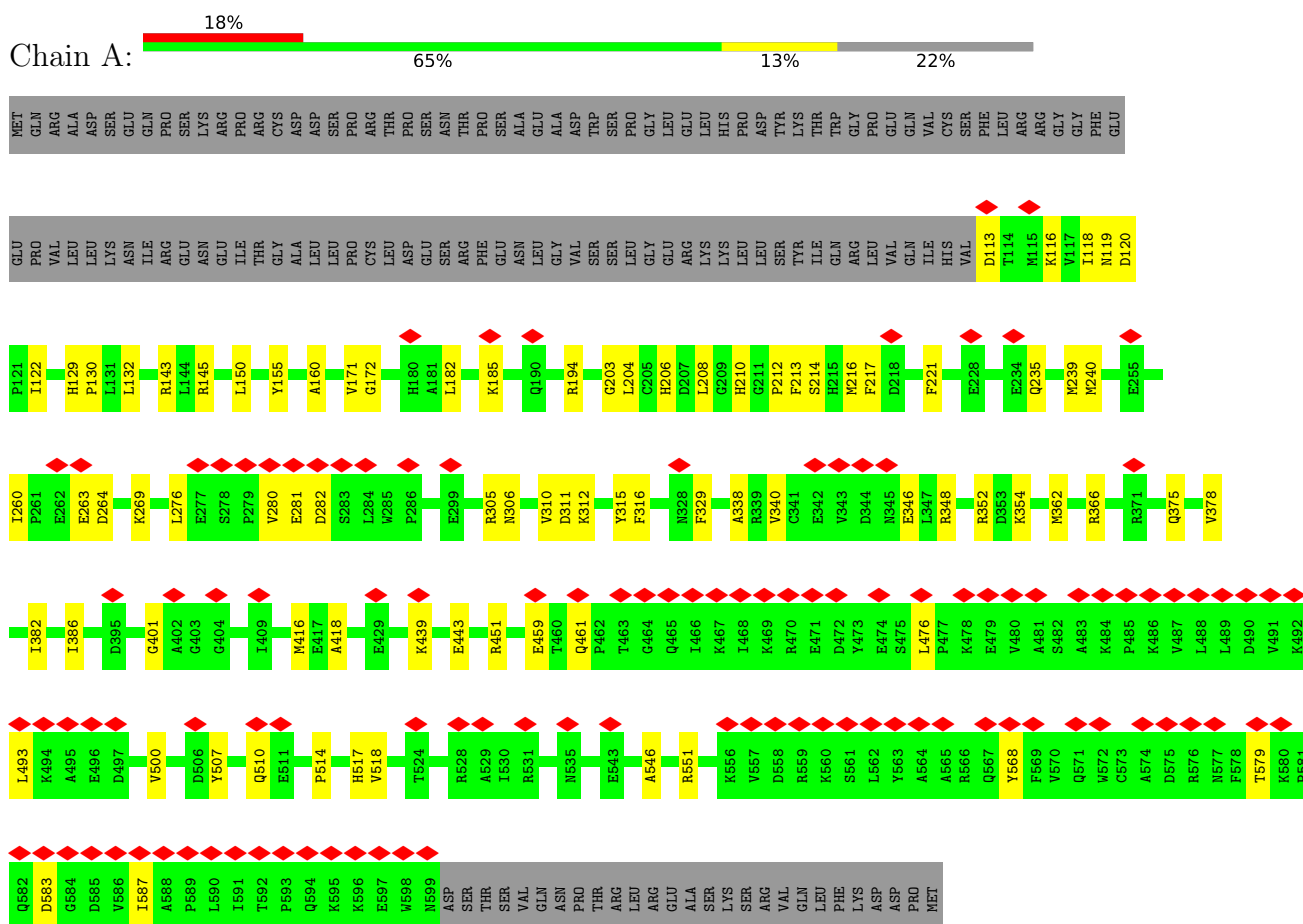
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Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
2	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
2	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
2	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
2	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
2	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
2	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
2	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
2	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
2	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

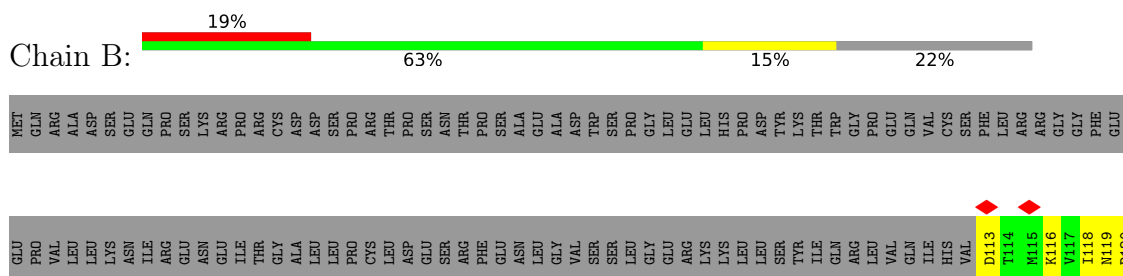
3 Residue-property plots

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

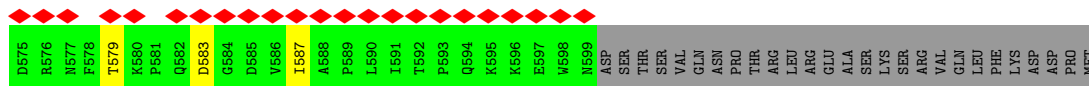
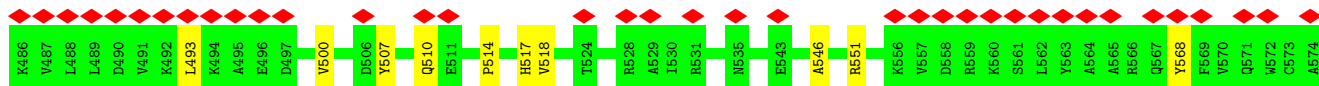
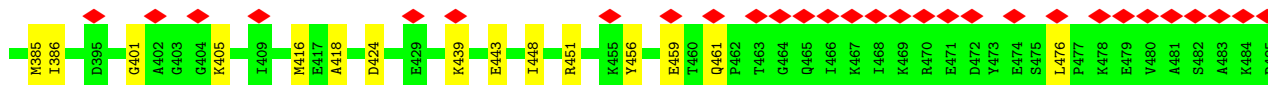
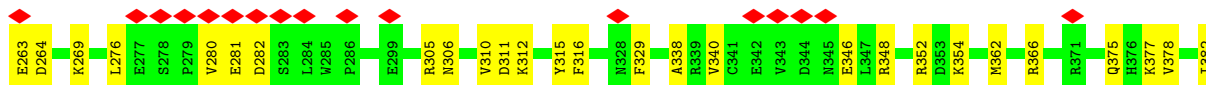
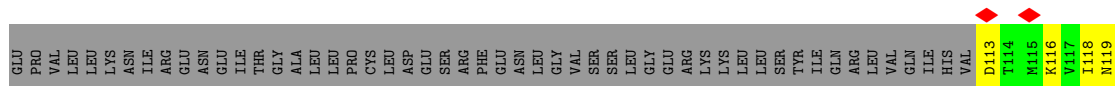
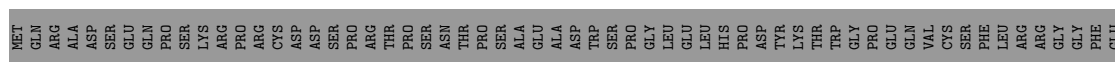
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



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MET	GLN	ARG	ALA	ASP	SER	GLU	GLN	PRO	ARG	PRO	THR	PRO	ASP	GLU	SER	ASN	SER	THR	PRO	SER	ALA	GLU	ALA	ALA	ASP	TRP	SER	SER	PRO	PRO	GLY	GLY	LEU	GLU	GLN	VAL	CYS	SER	SER	PHE	LEU	ARG	ARG	GLY	PHE	GLU									
GLU	PRO	VAL	LEU	ASP	SER	LYS	ASN	ILE	GLN	ALA	GLY	ASP	GLU	LEU	PRO	CYS	LEU	THR	ASP	GLU	ASN	ARG	PHE	GLU	ASN	LEU	GLY	VAL	SER	SER	LEU	LYS	LYS	THR	TRP	GLN	ARG	LEU	VAL	GLN	ILE	CYS	VAL	D113	T114	M115	K116	V117	I118	N119	D120				
P121	I122	H129	P130	L131	L132	R143	L144	R145	L150	Y155	A160	V171	G172	H180	A181	L182	K185	Q190	R194	G203	L204	C205	H206	D207	L208	G209	H210	G211	P212	F213	S214	H215	M216	F217	D218	F221	E228	E234	Q235	M239	M240	E255													
I260	P261	E262	E263	D264	K269	L276	E277	S278	P279	V280	E281	D282	S283	L284	W285	P286	E299	R305	N306	V310	D311	K312	Y315	F316	N328	F329	A338	R339	V340	C341	E342	V343	D344	N345	E346	L347	R348	R352	D353	K354	M362	R366	R371	Q375	H376	K377									
V378	T382	I386	D395	Q401	A402	G403	G404	I409	M416	E417	A418	D424	E429	K439	R451	K455	Y456	E459	T460	Q461	P462	T463	G464	Q465	I466	K467	I468	K469	R470	E471	D472	Y473	E474	S475	L476	P477	K478	E479	V480	A481	S482	A483	K484	P485	K486	V487	L488								
L489	D490	V491	K492	L493	K494	A495	E496	D497	D506	Y507	Q510	E511	P514	H517	V518	T524	R528	A529	I530	R531	N535	E543	A546	R551	K556	V557	D558	R559	K560	S561	L562	Y563	A564	A565	R566	Q567	Y568	F569	V570	Q571	W572	C573	A574	D575	R576	N577	F578	T579							
K580	F581	Q582	D583	G584	D585	V586	I587	A588	F589	L590	I591	T592	F593	Q594	K595	K596	E597	W598	N599	ASP	SER	THR	SER	VAL	GLN	ASN	PRO	PRO	THR	ARG	LEU	ARG	GLU	ALA	ALA	SER	LYS	SER	ARG	VAL	GLN	LEU	PHE	LYS	ASP	ASP	PRO	PRO	MET						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114078	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57.36	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.083	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	251.99998, 251.99998, 251.99998	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.84, 0.84, 0.84	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: T8T

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	0.12	0/4070	0.32	0/5498
1	B	0.12	0/4070	0.32	0/5498
1	C	0.12	0/4070	0.32	0/5498
1	D	0.12	0/4070	0.32	0/5498
All	All	0.12	0/16280	0.32	0/21992

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3975	0	3950	72	0
1	B	3975	0	3950	77	0
1	C	3975	0	3950	76	0
1	D	3975	0	3950	72	0
2	A	93	0	39	24	0
2	B	93	0	39	24	0
2	C	93	0	39	24	0
2	D	93	0	39	24	0
All	All	16272	0	15956	293	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 9.

All (293) 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:D:451:ARG:NH1	2:D:702:T8T:C2	1.91	1.33
1:B:451:ARG:NH1	2:B:701:T8T:C2	1.90	1.33
1:C:451:ARG:NH1	2:C:702:T8T:C2	1.91	1.33
1:A:451:ARG:NH1	2:A:702:T8T:C2	1.92	1.32
1:D:451:ARG:HH12	2:D:702:T8T:C2	1.45	1.28
1:A:451:ARG:HH12	2:A:702:T8T:C2	1.47	1.26
1:C:451:ARG:HH12	2:C:702:T8T:C2	1.45	1.25
1:B:451:ARG:HH12	2:B:701:T8T:C2	1.46	1.25
2:A:703:T8T:O2A	1:C:354:LYS:NZ	1.87	1.07
1:B:354:LYS:NZ	2:D:701:T8T:O2A	1.88	1.07
2:B:703:T8T:O2A	1:D:354:LYS:NZ	1.88	1.06
1:A:354:LYS:NZ	2:C:701:T8T:O2A	1.88	1.05
1:A:451:ARG:NH1	2:A:702:T8T:N3	2.07	0.94
1:D:451:ARG:NH1	2:D:702:T8T:N3	2.07	0.93
1:B:451:ARG:NH1	2:B:701:T8T:N3	2.06	0.91
1:D:119:ASN:HD22	2:D:701:T8T:HN3	1.17	0.91
1:A:119:ASN:HD22	2:A:703:T8T:HN3	1.18	0.91
1:C:451:ARG:NH1	2:C:702:T8T:N3	2.07	0.90
1:B:119:ASN:HD22	2:B:703:T8T:HN3	1.17	0.88
1:C:119:ASN:HD22	2:C:701:T8T:HN3	1.18	0.87
2:B:703:T8T:S1A	1:D:354:LYS:NZ	2.52	0.83
1:C:451:ARG:NH1	2:C:702:T8T:N2	2.27	0.82
1:D:451:ARG:NH1	2:D:702:T8T:N2	2.27	0.82
2:A:703:T8T:S1A	1:C:354:LYS:NZ	2.51	0.81
1:B:451:ARG:NH1	2:B:701:T8T:N2	2.27	0.81
2:A:703:T8T:PA	1:C:354:LYS:NZ	2.53	0.81
1:B:354:LYS:NZ	2:D:701:T8T:S1A	2.51	0.81
1:B:354:LYS:NZ	2:D:701:T8T:PA	2.53	0.80
1:A:451:ARG:NH1	2:A:702:T8T:N2	2.29	0.80
1:B:119:ASN:ND2	2:B:703:T8T:HN3	1.79	0.80
1:A:354:LYS:NZ	2:C:701:T8T:PA	2.53	0.80
2:B:703:T8T:PA	1:D:354:LYS:NZ	2.53	0.79
1:D:119:ASN:ND2	2:D:701:T8T:HN3	1.79	0.79
1:C:119:ASN:ND2	2:C:701:T8T:HN3	1.80	0.79
1:A:354:LYS:NZ	2:C:701:T8T:S1A	2.52	0.78
1:B:451:ARG:HH12	2:B:701:T8T:C4	1.96	0.78
1:A:119:ASN:ND2	2:A:703:T8T:HN3	1.80	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ARG:HH12	2:A:702:T8T:C4	1.97	0.76
1:D:451:ARG:HH12	2:D:702:T8T:C4	1.98	0.75
1:C:451:ARG:HH12	2:C:702:T8T:C4	1.98	0.72
1:A:354:LYS:HZ3	2:C:701:T8T:PA	2.12	0.72
1:D:377:LYS:HD2	1:D:456:TYR:CG	2.25	0.71
1:C:377:LYS:HD2	1:C:456:TYR:CG	2.25	0.71
2:A:703:T8T:PA	1:C:354:LYS:HZ3	2.13	0.70
1:B:354:LYS:HZ3	2:D:701:T8T:PA	2.14	0.70
1:D:119:ASN:ND2	2:D:701:T8T:HN2A	1.94	0.66
1:A:172:GLY:HA3	1:A:204:LEU:HD12	1.78	0.66
1:D:172:GLY:HA3	1:D:204:LEU:HD12	1.78	0.66
1:B:119:ASN:ND2	2:B:703:T8T:HN2A	1.94	0.65
1:A:119:ASN:ND2	2:A:703:T8T:HN2A	1.94	0.65
1:D:378:VAL:HG21	2:D:702:T8T:H5'A	1.79	0.65
1:C:119:ASN:ND2	2:C:701:T8T:HN2A	1.94	0.65
1:C:378:VAL:HG21	2:C:702:T8T:H5'A	1.79	0.65
1:B:172:GLY:HA3	1:B:204:LEU:HD12	1.78	0.64
1:C:172:GLY:HA3	1:C:204:LEU:HD12	1.78	0.64
2:B:703:T8T:PA	1:D:354:LYS:HZ3	2.17	0.64
1:D:143:ARG:NH2	1:D:210:HIS:O	2.32	0.62
1:A:143:ARG:NH2	1:A:210:HIS:O	2.32	0.62
1:B:451:ARG:HH22	2:B:701:T8T:C5	2.11	0.62
1:A:451:ARG:HH22	2:A:702:T8T:C5	2.12	0.62
1:D:451:ARG:HH22	2:D:702:T8T:C5	2.12	0.62
1:C:451:ARG:HH22	2:C:702:T8T:C5	2.12	0.61
1:C:143:ARG:NH2	1:C:210:HIS:O	2.32	0.61
1:B:143:ARG:NH2	1:B:210:HIS:O	2.32	0.61
1:C:185:LYS:NZ	1:C:338:ALA:O	2.26	0.61
1:B:185:LYS:NZ	1:B:338:ALA:O	2.26	0.61
1:B:378:VAL:HG21	2:B:701:T8T:H5'A	1.84	0.60
1:C:451:ARG:HH22	2:C:702:T8T:C6	2.15	0.59
1:D:119:ASN:ND2	2:D:701:T8T:N3	2.44	0.59
1:B:451:ARG:HH22	2:B:701:T8T:C6	2.15	0.59
1:A:378:VAL:HG21	2:A:702:T8T:H5'A	1.85	0.59
1:B:119:ASN:HD21	2:B:703:T8T:HN2A	1.50	0.59
1:C:305:ARG:NH1	1:C:517:HIS:O	2.36	0.59
1:B:305:ARG:NH1	1:B:517:HIS:O	2.36	0.59
1:B:312:LYS:HA	1:B:315:TYR:CE2	2.38	0.58
1:A:269:LYS:HB3	1:A:276:LEU:HD21	1.85	0.58
1:A:312:LYS:HA	1:A:315:TYR:CE2	2.38	0.58
1:C:312:LYS:HA	1:C:315:TYR:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:LYS:HA	1:D:315:TYR:CE2	2.38	0.58
1:B:269:LYS:HB3	1:B:276:LEU:HD21	1.86	0.58
1:C:269:LYS:HB3	1:C:276:LEU:HD21	1.86	0.58
1:A:119:ASN:ND2	2:A:703:T8T:N3	2.45	0.58
1:D:269:LYS:HB3	1:D:276:LEU:HD21	1.86	0.58
1:D:451:ARG:HH22	2:D:702:T8T:C6	2.15	0.58
1:B:451:ARG:CZ	2:B:701:T8T:C2	2.78	0.58
1:D:119:ASN:HD21	2:D:701:T8T:HN2A	1.49	0.58
1:C:451:ARG:CZ	2:C:702:T8T:C2	2.79	0.58
1:C:119:ASN:HD21	2:C:701:T8T:HN2A	1.51	0.58
1:A:119:ASN:HD21	2:A:703:T8T:HN2A	1.50	0.57
1:D:305:ARG:NH1	1:D:517:HIS:O	2.36	0.57
1:A:185:LYS:NZ	1:A:338:ALA:O	2.26	0.57
1:A:305:ARG:NH1	1:A:517:HIS:O	2.36	0.57
1:C:378:VAL:HG21	2:C:702:T8T:C5'	2.34	0.57
1:D:451:ARG:CZ	2:D:702:T8T:C2	2.79	0.57
1:B:119:ASN:ND2	2:B:703:T8T:N3	2.44	0.57
1:A:451:ARG:HH22	2:A:702:T8T:C6	2.17	0.57
1:C:235:GLN:O	1:C:239:MET:HG3	2.05	0.56
1:D:378:VAL:HG21	2:D:702:T8T:C5'	2.34	0.56
1:B:235:GLN:O	1:B:239:MET:HG3	2.05	0.56
1:A:217:PHE:HA	1:A:221:PHE:HB3	1.87	0.56
1:A:451:ARG:CZ	2:A:702:T8T:C2	2.80	0.56
1:D:217:PHE:HA	1:D:221:PHE:HB3	1.87	0.56
1:A:203:GLY:O	1:A:206:HIS:ND1	2.38	0.55
1:C:217:PHE:HA	1:C:221:PHE:HB3	1.87	0.55
1:B:217:PHE:HA	1:B:221:PHE:HB3	1.87	0.55
1:C:119:ASN:ND2	2:C:701:T8T:N3	2.45	0.55
1:B:203:GLY:O	1:B:206:HIS:ND1	2.38	0.55
1:D:203:GLY:O	1:D:206:HIS:ND1	2.39	0.55
1:A:235:GLN:O	1:A:239:MET:HG3	2.05	0.55
1:C:203:GLY:O	1:C:206:HIS:ND1	2.39	0.55
1:D:235:GLN:O	1:D:239:MET:HG3	2.05	0.55
1:B:378:VAL:HG21	2:B:701:T8T:C5'	2.38	0.54
1:D:185:LYS:NZ	1:D:338:ALA:O	2.26	0.53
1:A:346:GLU:OE2	1:A:348:ARG:NH2	2.41	0.52
1:C:113:ASP:HB3	1:C:130:PRO:HB3	1.90	0.52
1:D:119:ASN:ND2	2:D:701:T8T:N2	2.57	0.52
1:B:113:ASP:HB3	1:B:130:PRO:HB3	1.90	0.52
1:D:346:GLU:OE2	1:D:348:ARG:NH2	2.41	0.52
1:D:113:ASP:HB3	1:D:130:PRO:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ASP:HB3	1:A:130:PRO:HB3	1.90	0.52
1:C:451:ARG:HD2	2:C:702:T8T:S1A	2.50	0.52
1:A:378:VAL:HG21	2:A:702:T8T:C5'	2.39	0.52
1:B:119:ASN:ND2	2:B:703:T8T:N2	2.57	0.52
1:C:280:VAL:O	1:C:281:GLU:HG3	2.10	0.52
1:A:119:ASN:ND2	2:A:703:T8T:N2	2.58	0.51
1:B:280:VAL:O	1:B:281:GLU:HG3	2.10	0.51
1:B:451:ARG:HD2	2:B:701:T8T:S1A	2.50	0.51
1:D:451:ARG:HD2	2:D:702:T8T:S1A	2.50	0.51
1:A:280:VAL:O	1:A:281:GLU:HG3	2.10	0.51
1:C:119:ASN:ND2	2:C:701:T8T:N2	2.58	0.50
1:D:280:VAL:O	1:D:281:GLU:HG3	2.10	0.50
1:B:451:ARG:NH2	2:B:701:T8T:C6	2.75	0.50
1:B:580:LYS:HD3	1:B:581:PRO:O	2.11	0.50
1:B:319:ASP:OD2	1:B:374:TYR:OH	2.18	0.50
1:C:451:ARG:NH2	2:C:702:T8T:C6	2.75	0.50
1:D:239:MET:HB2	1:D:416:MET:HE3	1.94	0.50
1:D:451:ARG:NH2	2:D:702:T8T:C6	2.75	0.50
1:A:239:MET:HB2	1:A:416:MET:HE3	1.94	0.49
1:B:375:GLN:O	1:B:551:ARG:NH2	2.40	0.49
1:A:507:TYR:HB3	1:A:514:PRO:HG3	1.95	0.49
1:D:507:TYR:HB3	1:D:514:PRO:HG3	1.95	0.49
1:A:451:ARG:HD2	2:A:702:T8T:S1A	2.52	0.49
1:A:451:ARG:NH2	2:A:702:T8T:C6	2.76	0.49
1:D:401:GLY:HA2	1:D:418:ALA:HB2	1.94	0.49
1:B:239:MET:HB2	1:B:416:MET:HE3	1.94	0.49
1:A:213:PHE:HB2	1:A:216:MET:HE2	1.94	0.49
1:C:239:MET:HB2	1:C:416:MET:HE3	1.94	0.49
1:A:401:GLY:HA2	1:A:418:ALA:HB2	1.94	0.48
1:B:507:TYR:HB3	1:B:514:PRO:HG3	1.95	0.48
1:C:459:GLU:HG2	1:C:551:ARG:HG3	1.95	0.48
1:C:507:TYR:HB3	1:C:514:PRO:HG3	1.95	0.48
1:B:346:GLU:OE2	1:B:348:ARG:NH2	2.41	0.48
1:B:401:GLY:HA2	1:B:418:ALA:HB2	1.95	0.48
1:C:401:GLY:HA2	1:C:418:ALA:HB2	1.94	0.48
1:D:459:GLU:HG2	1:D:551:ARG:HG3	1.94	0.48
1:C:346:GLU:OE2	1:C:348:ARG:NH2	2.41	0.48
1:A:375:GLN:O	1:A:551:ARG:NH2	2.40	0.48
1:A:171:VAL:HG13	1:A:310:VAL:HG23	1.96	0.47
1:B:260:ILE:N	1:B:264:ASP:OD2	2.46	0.47
1:D:171:VAL:HG13	1:D:310:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:PHE:HB2	1:B:216:MET:HE2	1.95	0.47
1:C:260:ILE:N	1:C:264:ASP:OD2	2.47	0.47
1:D:260:ILE:N	1:D:264:ASP:OD2	2.46	0.47
1:B:459:GLU:HG2	1:B:551:ARG:HG3	1.97	0.47
1:A:260:ILE:N	1:A:264:ASP:OD2	2.46	0.47
1:B:306:ASN:HD22	1:B:518:VAL:HG22	1.80	0.47
1:C:213:PHE:HB2	1:C:216:MET:HE2	1.96	0.47
1:C:306:ASN:HD22	1:C:518:VAL:HG22	1.80	0.47
1:A:306:ASN:HD22	1:A:518:VAL:HG22	1.80	0.46
1:D:306:ASN:HD22	1:D:518:VAL:HG22	1.80	0.46
1:B:150:LEU:HD12	1:B:160:ALA:HB1	1.98	0.46
1:B:171:VAL:HG13	1:B:310:VAL:HG23	1.96	0.46
1:B:212:PRO:HD2	1:B:217:PHE:CD2	2.51	0.46
1:C:171:VAL:HG13	1:C:310:VAL:HG23	1.96	0.46
1:A:150:LEU:HD12	1:A:160:ALA:HB1	1.98	0.46
1:A:194:ARG:NH2	1:A:263:GLU:OE2	2.49	0.46
1:A:493:LEU:HB2	1:A:568:TYR:HE2	1.80	0.46
1:B:194:ARG:NH2	1:B:263:GLU:OE2	2.49	0.46
1:C:212:PRO:HD2	1:C:217:PHE:CD2	2.50	0.46
1:C:150:LEU:HD12	1:C:160:ALA:HB1	1.98	0.46
1:D:213:PHE:HB2	1:D:216:MET:HE2	1.96	0.46
1:A:212:PRO:C	1:A:214:SER:H	2.24	0.46
1:C:194:ARG:NH2	1:C:263:GLU:OE2	2.49	0.46
1:A:352:ARG:HG3	1:A:354:LYS:HG2	1.98	0.46
1:D:150:LEU:HD12	1:D:160:ALA:HB1	1.98	0.46
1:D:212:PRO:C	1:D:214:SER:H	2.24	0.46
1:D:212:PRO:HD2	1:D:217:PHE:CD2	2.50	0.46
1:D:352:ARG:HG3	1:D:354:LYS:HG2	1.98	0.46
1:A:212:PRO:HD2	1:A:217:PHE:CD2	2.51	0.46
1:B:493:LEU:HB2	1:B:568:TYR:HE2	1.80	0.46
1:D:194:ARG:NH2	1:D:263:GLU:OE2	2.49	0.45
1:A:459:GLU:HG2	1:A:551:ARG:HG3	1.97	0.45
1:B:182:LEU:HD22	1:B:340:VAL:HG23	1.98	0.45
1:C:155:TYR:HA	1:D:145:ARG:NH2	2.32	0.45
1:C:182:LEU:HD22	1:C:340:VAL:HG23	1.98	0.45
1:A:182:LEU:HD22	1:A:340:VAL:HG23	1.98	0.45
1:A:208:LEU:HD23	1:A:208:LEU:HA	1.86	0.45
1:A:280:VAL:O	1:A:282:ASP:N	2.50	0.45
1:D:280:VAL:O	1:D:282:ASP:N	2.50	0.45
1:D:375:GLN:O	1:D:551:ARG:NH2	2.49	0.45
1:A:145:ARG:NH2	1:B:155:TYR:HA	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:VAL:O	1:C:282:ASP:N	2.50	0.45
1:D:182:LEU:HD22	1:D:340:VAL:HG23	1.98	0.45
1:B:280:VAL:O	1:B:282:ASP:N	2.50	0.45
1:C:145:ARG:NH2	1:D:155:TYR:HA	2.32	0.45
1:B:352:ARG:HG3	1:B:354:LYS:HG2	1.98	0.45
1:D:208:LEU:HD23	1:D:208:LEU:HA	1.86	0.44
1:D:493:LEU:HB2	1:D:568:TYR:HE2	1.82	0.44
1:C:352:ARG:HG3	1:C:354:LYS:HG2	1.99	0.44
1:A:155:TYR:HA	1:B:145:ARG:NH2	2.32	0.44
1:B:212:PRO:C	1:B:214:SER:H	2.24	0.44
1:B:240:MET:HE2	1:B:240:MET:HB2	1.86	0.44
1:D:213:PHE:N	1:D:424:ASP:OD1	2.45	0.44
1:C:212:PRO:C	1:C:214:SER:H	2.24	0.44
1:C:493:LEU:HB2	1:C:568:TYR:HE2	1.82	0.43
2:A:702:T8T:O2A	1:B:116:LYS:NZ	2.50	0.43
1:B:583:ASP:O	1:B:587:ILE:HG12	2.17	0.43
1:A:476:LEU:HB2	1:A:500:VAL:HG21	2.00	0.43
1:C:240:MET:HE2	1:C:240:MET:HB2	1.86	0.43
1:C:116:LYS:NZ	2:D:702:T8T:O2A	2.50	0.43
1:A:120:ASP:OD1	1:A:122:ILE:N	2.47	0.43
1:B:213:PHE:N	1:B:424:ASP:OD1	2.45	0.43
1:B:280:VAL:C	1:B:282:ASP:H	2.26	0.43
1:C:280:VAL:C	1:C:282:ASP:H	2.26	0.43
1:D:382:ILE:O	1:D:386:ILE:HG13	2.19	0.43
1:D:461:GLN:H	1:D:579:THR:HG22	1.84	0.43
1:A:461:GLN:H	1:A:579:THR:HG22	1.84	0.43
1:D:451:ARG:O	1:D:451:ARG:HG3	2.19	0.43
1:A:451:ARG:O	1:A:451:ARG:HG3	2.19	0.43
1:C:213:PHE:N	1:C:424:ASP:OD1	2.45	0.43
1:D:143:ARG:HH12	1:D:210:HIS:H	1.67	0.43
1:A:143:ARG:HH12	1:A:210:HIS:H	1.67	0.43
1:B:118:ILE:HA	2:B:703:T8T:H4'	2.01	0.43
1:B:129:HIS:H	1:B:132:LEU:HD12	1.84	0.43
1:C:118:ILE:HA	2:C:701:T8T:H4'	2.01	0.43
1:C:129:HIS:H	1:C:132:LEU:HD12	1.84	0.43
1:B:451:ARG:O	1:B:451:ARG:HG3	2.19	0.42
1:C:451:ARG:HG3	1:C:451:ARG:O	2.19	0.42
1:C:583:ASP:O	1:C:587:ILE:HG12	2.18	0.42
1:D:129:HIS:H	1:D:132:LEU:HD12	1.84	0.42
1:A:510:GLN:O	1:A:546:ALA:HB2	2.19	0.42
1:B:510:GLN:O	1:B:546:ALA:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ASP:OD1	1:D:122:ILE:N	2.47	0.42
1:D:510:GLN:O	1:D:546:ALA:HB2	2.19	0.42
1:A:382:ILE:O	1:A:386:ILE:HG13	2.19	0.42
1:C:382:ILE:O	1:C:386:ILE:HG13	2.19	0.42
1:A:129:HIS:H	1:A:132:LEU:HD12	1.85	0.42
1:B:382:ILE:O	1:B:386:ILE:HG13	2.19	0.42
1:C:510:GLN:O	1:C:546:ALA:HB2	2.19	0.42
1:B:120:ASP:OD1	1:B:122:ILE:N	2.47	0.42
1:B:143:ARG:HH12	1:B:210:HIS:H	1.67	0.42
1:D:118:ILE:HA	2:D:701:T8T:H4'	2.01	0.42
2:C:702:T8T:O2A	1:D:116:LYS:NZ	2.50	0.42
1:D:377:LYS:HD2	1:D:456:TYR:CD1	2.54	0.42
1:D:583:ASP:O	1:D:587:ILE:HG12	2.18	0.42
1:A:583:ASP:O	1:A:587:ILE:HG12	2.18	0.42
1:C:143:ARG:HH12	1:C:210:HIS:H	1.67	0.42
1:B:207:ASP:CG	1:B:210:HIS:HE2	2.28	0.42
1:C:207:ASP:CG	1:C:210:HIS:HE2	2.28	0.42
1:D:280:VAL:C	1:D:282:ASP:H	2.27	0.42
1:A:240:MET:HE2	1:A:240:MET:HB2	1.86	0.41
1:A:280:VAL:C	1:A:282:ASP:H	2.26	0.41
1:D:171:VAL:HG22	1:D:311:ASP:HA	2.02	0.41
1:A:171:VAL:HG22	1:A:311:ASP:HA	2.02	0.41
1:B:401:GLY:N	1:B:405:LYS:O	2.41	0.41
1:C:171:VAL:HG22	1:C:311:ASP:HA	2.02	0.41
1:B:171:VAL:HG22	1:B:311:ASP:HA	2.02	0.41
1:C:401:GLY:N	1:C:405:LYS:O	2.41	0.41
1:A:116:LYS:NZ	2:B:701:T8T:O2A	2.51	0.41
1:C:377:LYS:HD2	1:C:456:TYR:CD1	2.54	0.41
1:A:316:PHE:HZ	1:A:366:ARG:HB2	1.86	0.41
1:C:461:GLN:H	1:C:579:THR:HG22	1.84	0.41
1:D:240:MET:HE2	1:D:240:MET:HB2	1.86	0.41
1:D:316:PHE:HZ	1:D:366:ARG:HB2	1.86	0.41
1:A:329:PHE:CD1	1:A:362:MET:HB2	2.56	0.41
1:B:476:LEU:HD12	1:B:500:VAL:HG21	2.03	0.41
1:A:118:ILE:HA	2:A:703:T8T:H4'	2.02	0.41
1:C:329:PHE:CD1	1:C:362:MET:HB2	2.56	0.41
1:C:476:LEU:HD12	1:C:500:VAL:HG21	2.03	0.41
1:D:329:PHE:CD1	1:D:362:MET:HB2	2.56	0.41
1:B:329:PHE:CD1	1:B:362:MET:HB2	2.56	0.41
1:B:385:MET:HE2	1:B:448:ILE:HG12	2.02	0.41
1:C:208:LEU:HA	1:C:208:LEU:HD23	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:MET:HE2	1:C:448:ILE:HG12	2.02	0.41
1:B:316:PHE:HZ	1:B:366:ARG:HB2	1.85	0.40
1:C:375:GLN:O	1:C:551:ARG:NH2	2.49	0.40
1:C:316:PHE:HZ	1:C:366:ARG:HB2	1.86	0.40
1:B:439:LYS:O	1:B:443:GLU:HG2	2.22	0.40
1:C:439:LYS:O	1:C:443:GLU:HG2	2.22	0.40
1:A:439:LYS:O	1:A:443:GLU:HG2	2.21	0.40
1:B:208:LEU:HA	1:B:208:LEU:HD23	1.86	0.40
1:B:592:THR:OG1	1:B:593:PRO:HD3	2.22	0.40
1:A:306:ASN:ND2	1:A:518:VAL:HG22	2.37	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	485/626 (78%)	469 (97%)	16 (3%)	0	100	100
1	B	485/626 (78%)	469 (97%)	16 (3%)	0	100	100
1	C	485/626 (78%)	469 (97%)	16 (3%)	0	100	100
1	D	485/626 (78%)	469 (97%)	16 (3%)	0	100	100
All	All	1940/2504 (78%)	1876 (97%)	64 (3%)	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	433/560 (77%)	433 (100%)	0	100	100
1	B	433/560 (77%)	433 (100%)	0	100	100
1	C	433/560 (77%)	433 (100%)	0	100	100
1	D	433/560 (77%)	433 (100%)	0	100	100
All	All	1732/2240 (77%)	1732 (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 (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	235	GLN
1	A	447	GLN
1	A	517	HIS
1	B	119	ASN
1	B	235	GLN
1	B	447	GLN
1	B	517	HIS
1	C	119	ASN
1	C	235	GLN
1	C	376	HIS
1	C	447	GLN
1	C	517	HIS
1	D	119	ASN
1	D	235	GLN
1	D	376	HIS
1	D	447	GLN
1	D	517	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	T8T	C	701	-	29,33,33	1.06	1 (3%)	36,52,52	0.74	1 (2%)
2	T8T	C	702	-	29,33,33	1.05	1 (3%)	36,52,52	0.76	1 (2%)
2	T8T	B	702	-	29,33,33	1.08	1 (3%)	36,52,52	0.75	1 (2%)
2	T8T	A	701	-	29,33,33	1.08	1 (3%)	36,52,52	0.76	1 (2%)
2	T8T	B	703	-	29,33,33	1.06	1 (3%)	36,52,52	0.74	1 (2%)
2	T8T	D	701	-	29,33,33	1.06	1 (3%)	36,52,52	0.74	1 (2%)
2	T8T	D	703	-	29,33,33	1.08	1 (3%)	36,52,52	0.76	1 (2%)
2	T8T	A	702	-	29,33,33	1.05	1 (3%)	36,52,52	0.76	1 (2%)
2	T8T	D	702	-	29,33,33	1.05	1 (3%)	36,52,52	0.76	1 (2%)
2	T8T	C	703	-	29,33,33	1.08	1 (3%)	36,52,52	0.76	1 (2%)
2	T8T	A	703	-	29,33,33	1.06	1 (3%)	36,52,52	0.74	1 (2%)
2	T8T	B	701	-	29,33,33	1.05	1 (3%)	36,52,52	0.76	1 (2%)

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	T8T	C	701	-	-	7/19/34/34	0/3/3/3
2	T8T	C	702	-	-	3/19/34/34	0/3/3/3
2	T8T	B	702	-	-	6/19/34/34	0/3/3/3
2	T8T	A	701	-	-	6/19/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	T8T	B	703	-	-	7/19/34/34	0/3/3/3
2	T8T	D	701	-	-	7/19/34/34	0/3/3/3
2	T8T	D	703	-	-	6/19/34/34	0/3/3/3
2	T8T	A	702	-	-	3/19/34/34	0/3/3/3
2	T8T	D	702	-	-	3/19/34/34	0/3/3/3
2	T8T	C	703	-	-	6/19/34/34	0/3/3/3
2	T8T	A	703	-	-	7/19/34/34	0/3/3/3
2	T8T	B	701	-	-	3/19/34/34	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	703	T8T	PA-O2A	4.44	1.56	1.46
2	A	701	T8T	PA-O2A	4.43	1.56	1.46
2	B	702	T8T	PA-O2A	4.43	1.56	1.46
2	C	703	T8T	PA-O2A	4.43	1.56	1.46
2	D	701	T8T	PA-O2A	4.40	1.56	1.46
2	A	703	T8T	PA-O2A	4.38	1.56	1.46
2	B	703	T8T	PA-O2A	4.38	1.56	1.46
2	C	701	T8T	PA-O2A	4.38	1.56	1.46
2	B	701	T8T	PA-O2A	4.30	1.56	1.46
2	A	702	T8T	PA-O2A	4.29	1.56	1.46
2	C	702	T8T	PA-O2A	4.29	1.56	1.46
2	D	702	T8T	PA-O2A	4.29	1.56	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	703	T8T	C6-N1-C2	2.04	125.22	119.24
2	B	702	T8T	C6-N1-C2	2.03	125.21	119.24
2	C	701	T8T	C6-N1-C2	2.03	125.21	119.24
2	C	702	T8T	C6-N1-C2	2.03	125.20	119.24
2	A	702	T8T	C6-N1-C2	2.03	125.20	119.24
2	B	701	T8T	C6-N1-C2	2.03	125.20	119.24
2	D	702	T8T	C6-N1-C2	2.03	125.20	119.24
2	A	701	T8T	C6-N1-C2	2.03	125.19	119.24
2	C	703	T8T	C6-N1-C2	2.03	125.19	119.24
2	D	703	T8T	C6-N1-C2	2.03	125.19	119.24
2	B	703	T8T	C6-N1-C2	2.03	125.19	119.24
2	D	701	T8T	C6-N1-C2	2.01	125.15	119.24

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	T8T	O4'-C1'-N9-C8
2	A	701	T8T	C5'-O5'-PA-O3A
2	A	701	T8T	O4'-C4'-C5'-O5'
2	A	703	T8T	PB-O3B-PG-O2G
2	B	702	T8T	O4'-C1'-N9-C8
2	B	702	T8T	C5'-O5'-PA-O3A
2	B	702	T8T	O4'-C4'-C5'-O5'
2	B	703	T8T	PB-O3B-PG-O2G
2	C	701	T8T	PB-O3B-PG-O2G
2	C	703	T8T	O4'-C1'-N9-C8
2	C	703	T8T	C5'-O5'-PA-O3A
2	C	703	T8T	O4'-C4'-C5'-O5'
2	D	701	T8T	PB-O3B-PG-O2G
2	D	703	T8T	O4'-C1'-N9-C8
2	D	703	T8T	C5'-O5'-PA-O3A
2	D	703	T8T	O4'-C4'-C5'-O5'
2	A	701	T8T	C3'-C4'-C5'-O5'
2	B	702	T8T	C3'-C4'-C5'-O5'
2	C	703	T8T	C3'-C4'-C5'-O5'
2	D	703	T8T	C3'-C4'-C5'-O5'
2	A	701	T8T	C4'-C5'-O5'-PA
2	B	702	T8T	C4'-C5'-O5'-PA
2	C	703	T8T	C4'-C5'-O5'-PA
2	D	703	T8T	C4'-C5'-O5'-PA
2	A	701	T8T	O4'-C1'-N9-C4
2	B	702	T8T	O4'-C1'-N9-C4
2	C	703	T8T	O4'-C1'-N9-C4
2	D	703	T8T	O4'-C1'-N9-C4
2	A	702	T8T	PA-O3A-PB-O3B
2	B	701	T8T	PA-O3A-PB-O3B
2	C	702	T8T	PA-O3A-PB-O3B
2	D	702	T8T	PA-O3A-PB-O3B
2	A	702	T8T	PA-O3A-PB-O2B
2	B	701	T8T	PA-O3A-PB-O2B
2	C	702	T8T	PA-O3A-PB-O2B
2	D	702	T8T	PA-O3A-PB-O2B
2	A	703	T8T	O4'-C4'-C5'-O5'
2	B	703	T8T	O4'-C4'-C5'-O5'
2	C	701	T8T	O4'-C4'-C5'-O5'
2	D	701	T8T	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	A	703	T8T	PG-O3B-PB-O2B
2	B	703	T8T	PG-O3B-PB-O2B
2	C	701	T8T	PG-O3B-PB-O2B
2	D	701	T8T	PG-O3B-PB-O2B
2	A	703	T8T	PB-O3B-PG-O3G
2	B	703	T8T	PB-O3B-PG-O3G
2	C	701	T8T	PB-O3B-PG-O3G
2	D	701	T8T	PB-O3B-PG-O3G
2	A	702	T8T	PB-O3B-PG-O2G
2	A	703	T8T	PB-O3B-PG-O1G
2	B	701	T8T	PB-O3B-PG-O2G
2	B	703	T8T	PB-O3B-PG-O1G
2	C	701	T8T	PB-O3B-PG-O1G
2	C	702	T8T	PB-O3B-PG-O2G
2	D	701	T8T	PB-O3B-PG-O1G
2	D	702	T8T	PB-O3B-PG-O2G
2	A	703	T8T	C5'-O5'-PA-O2A
2	B	703	T8T	C5'-O5'-PA-O2A
2	C	701	T8T	C5'-O5'-PA-O2A
2	D	701	T8T	C5'-O5'-PA-O2A
2	A	703	T8T	PG-O3B-PB-O1B
2	B	703	T8T	PG-O3B-PB-O1B
2	C	701	T8T	PG-O3B-PB-O1B
2	D	701	T8T	PG-O3B-PB-O1B

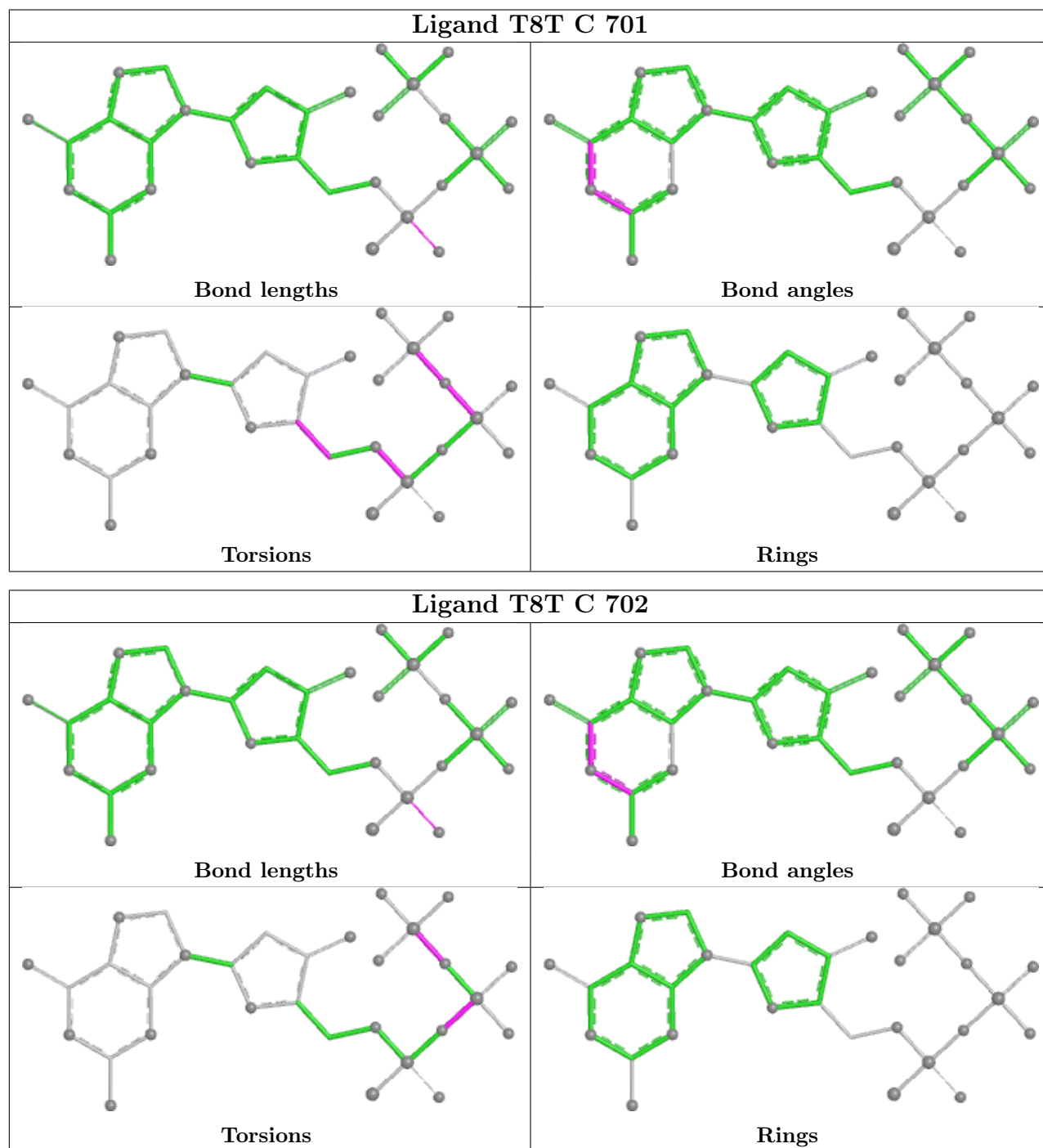
There are no ring outliers.

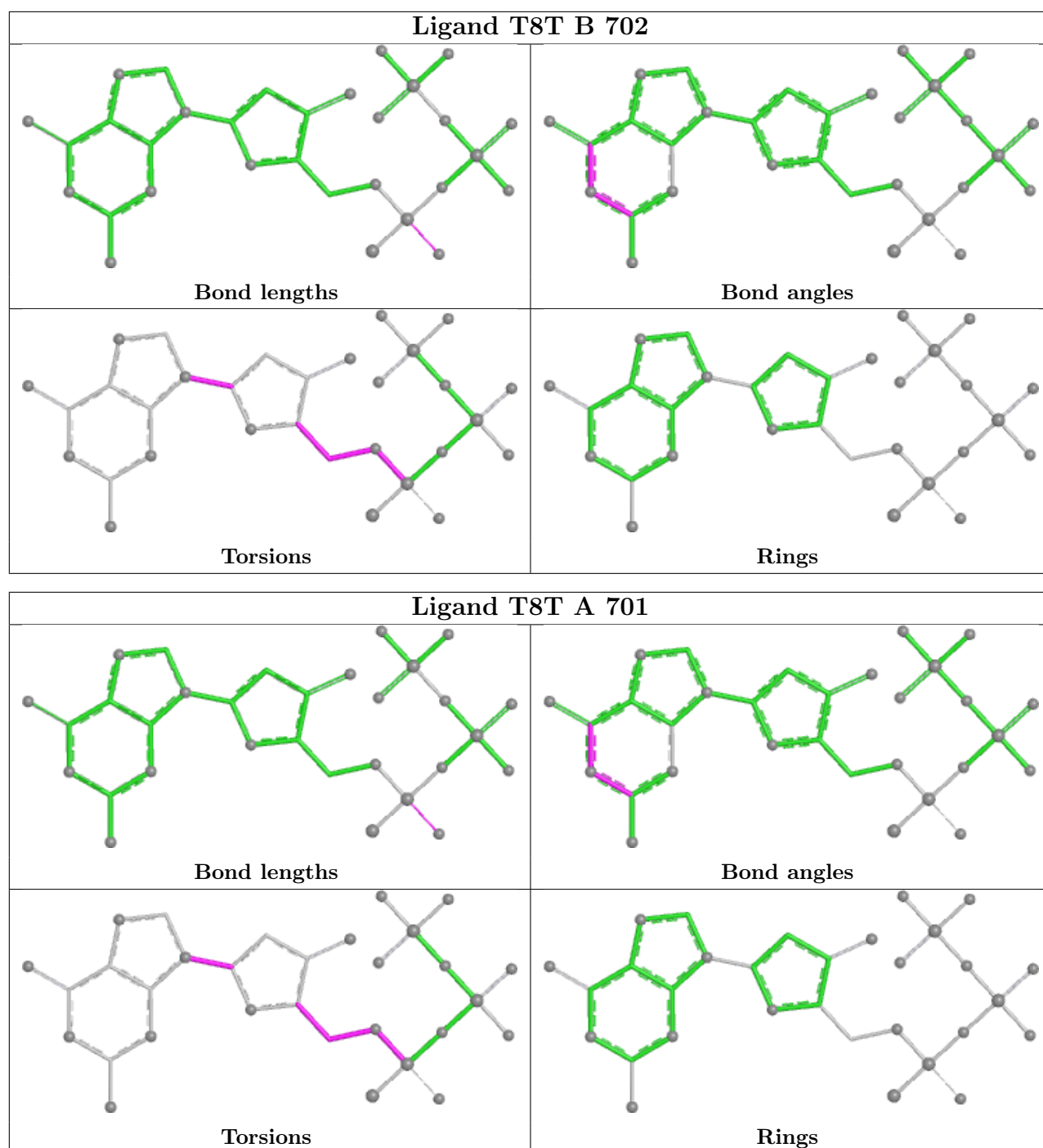
8 monomers are involved in 96 short contacts:

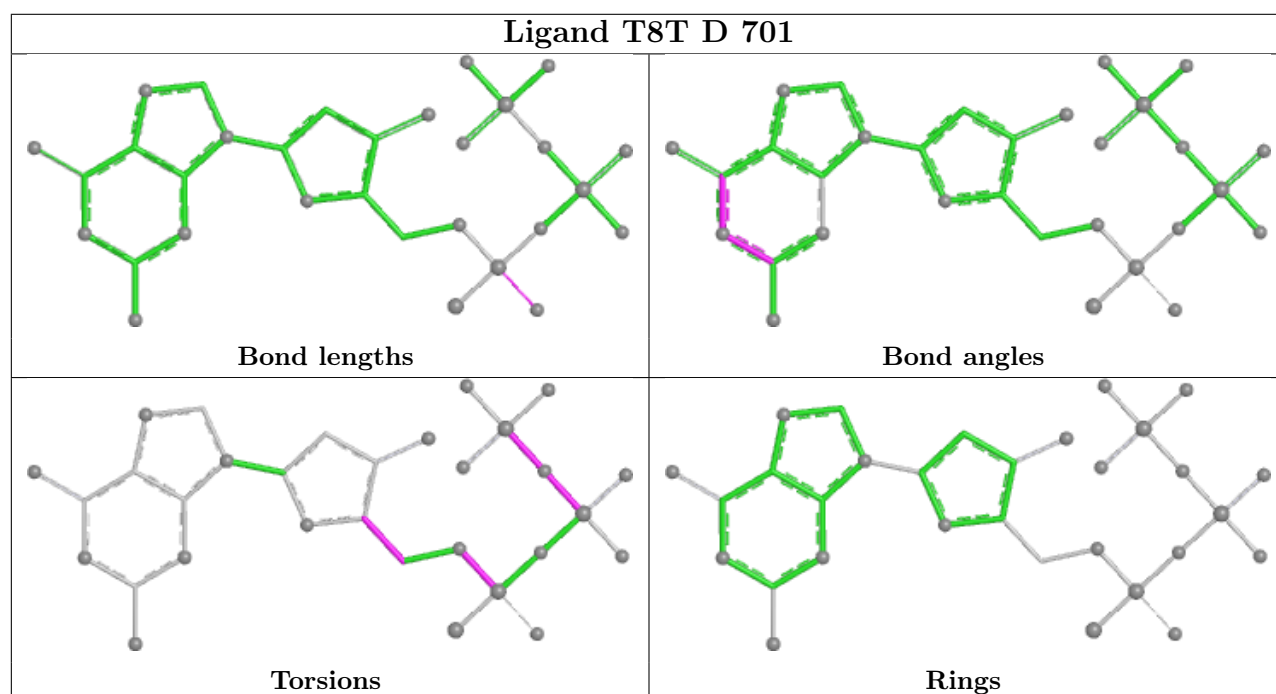
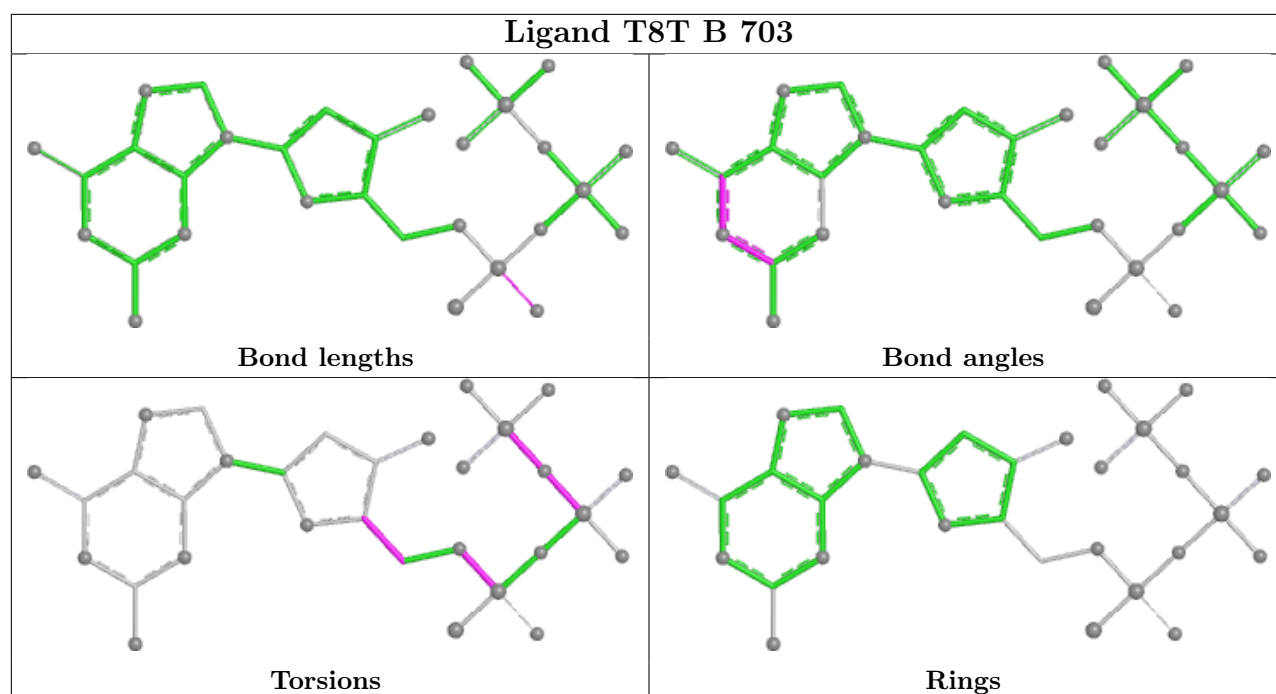
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	T8T	11	0
2	C	702	T8T	13	0
2	B	703	T8T	11	0
2	D	701	T8T	11	0
2	A	702	T8T	13	0
2	D	702	T8T	13	0
2	A	703	T8T	11	0
2	B	701	T8T	13	0

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

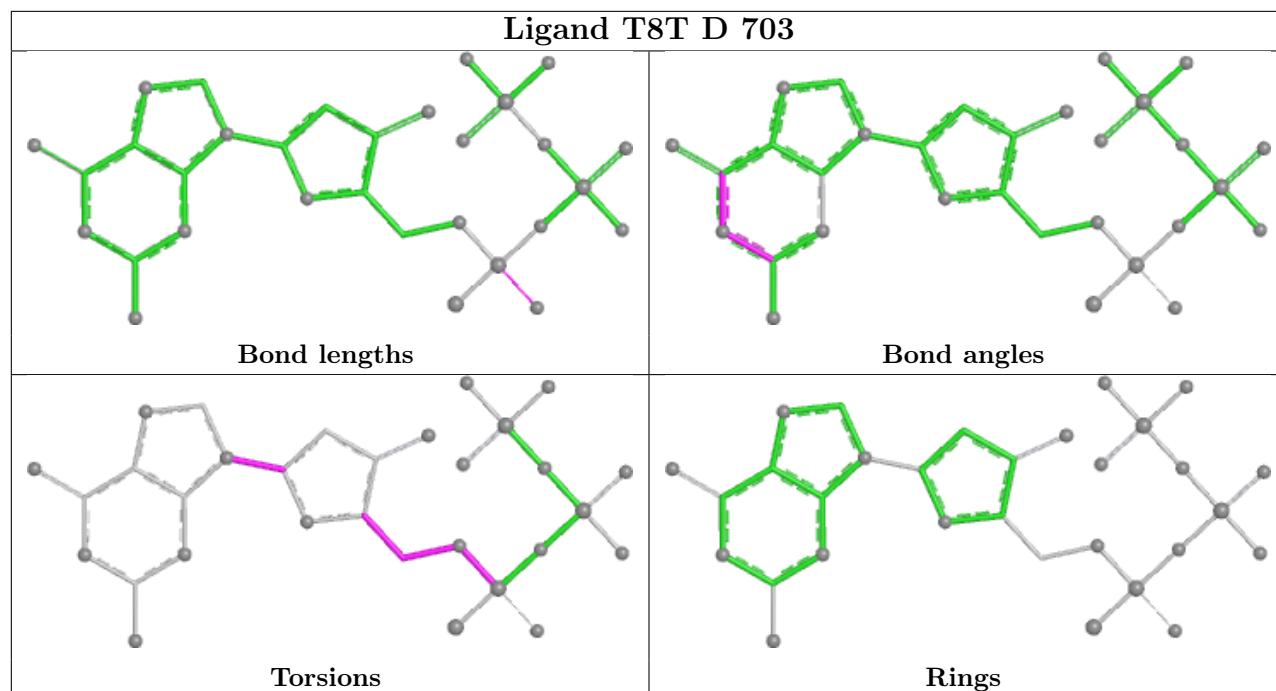
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



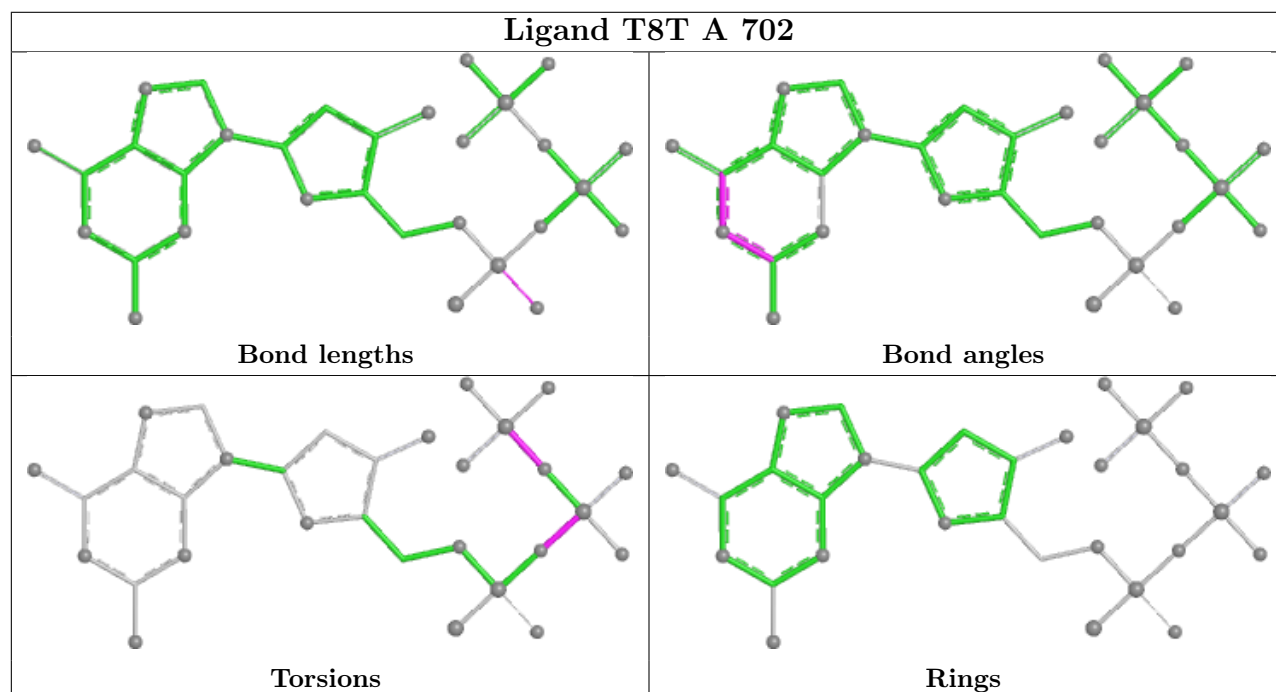


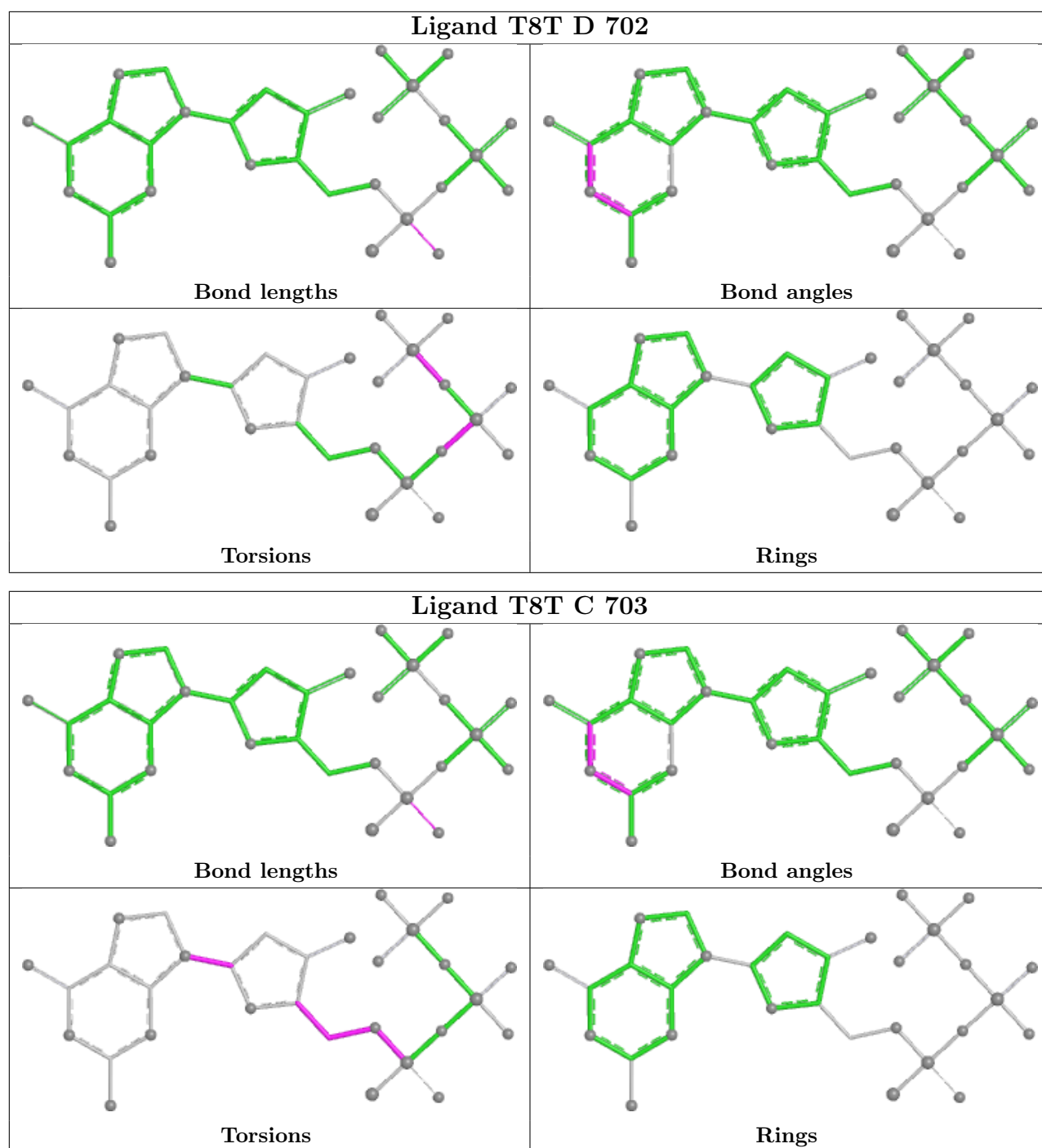


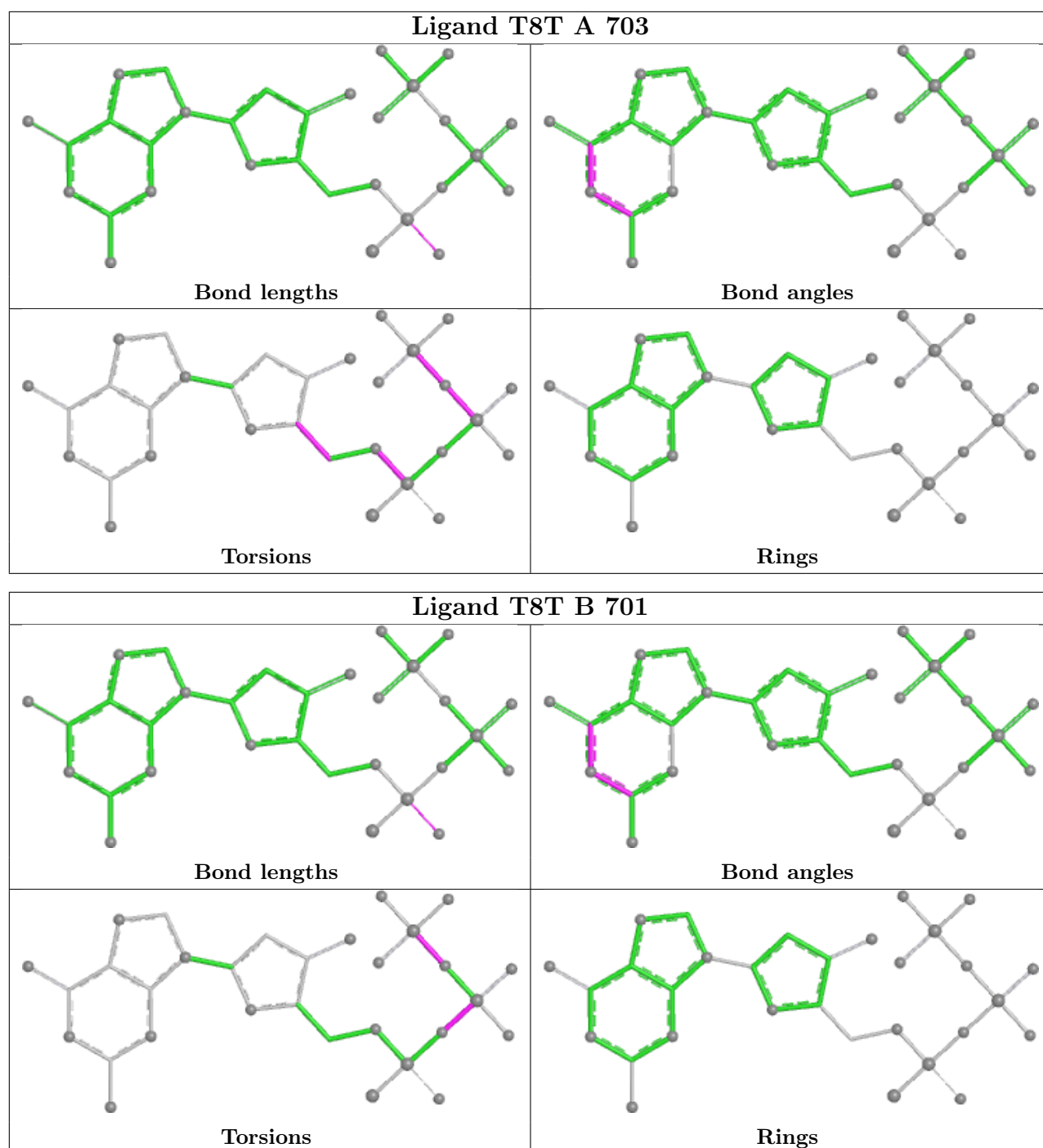
Ligand T8T D 703



Ligand T8T A 702







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.

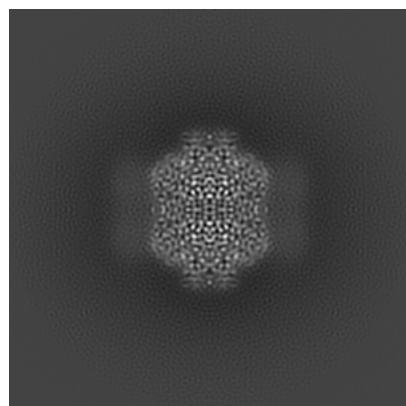
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26567. These allow visual inspection of the internal detail of the map and identification of artifacts.

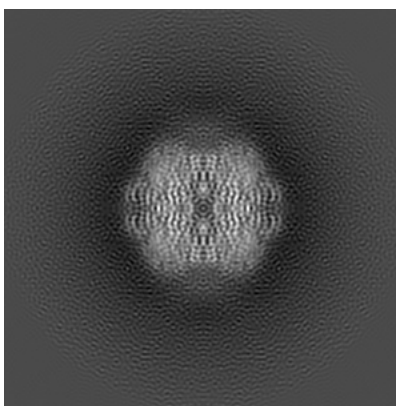
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

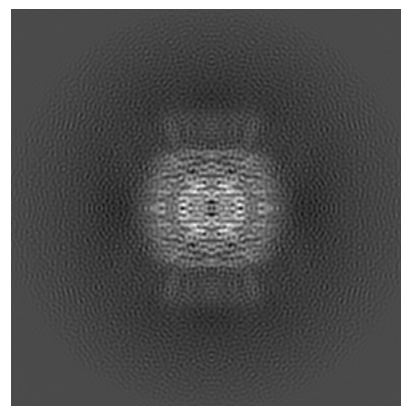
6.1.1 Primary map



X

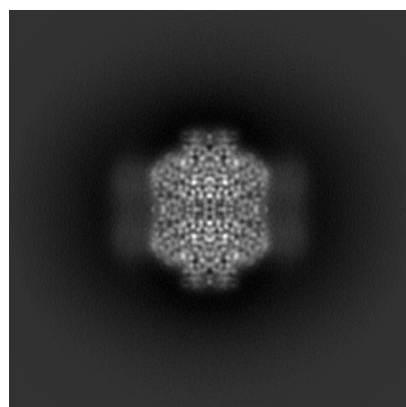


Y

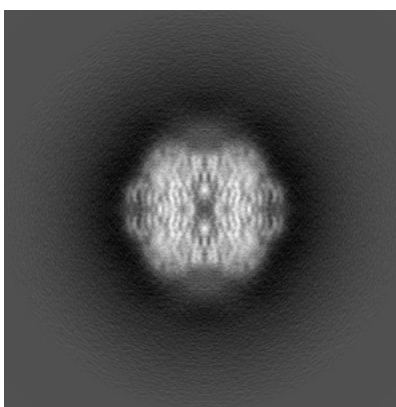


Z

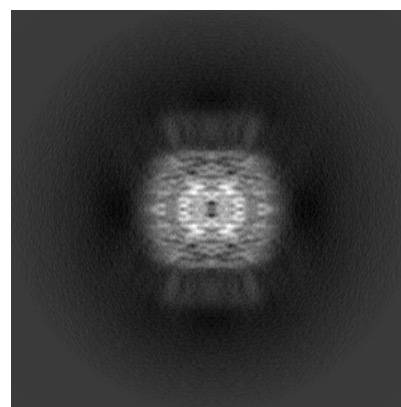
6.1.2 Raw map



X



Y

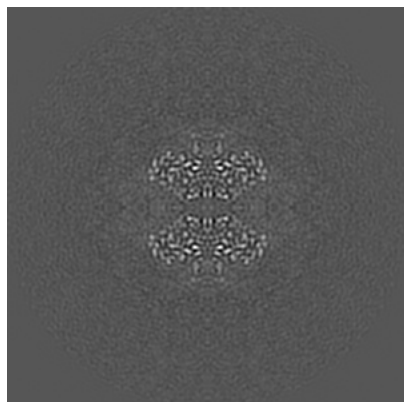


Z

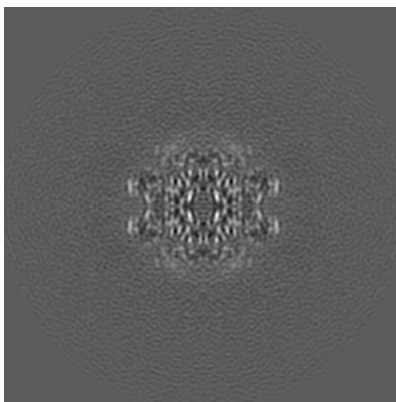
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

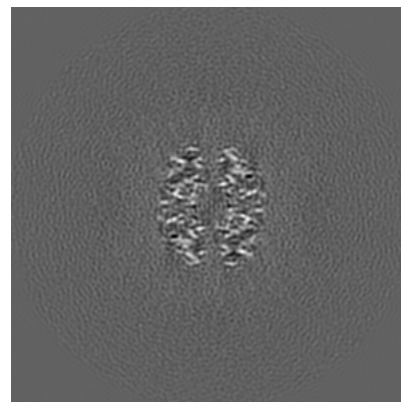
6.2.1 Primary map



X Index: 150

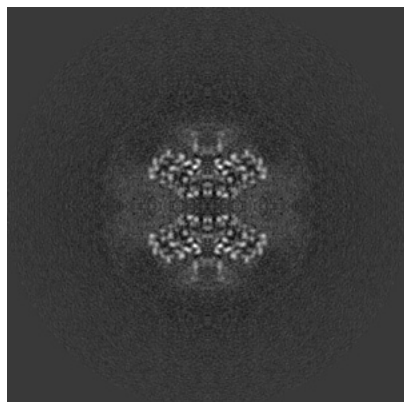


Y Index: 150

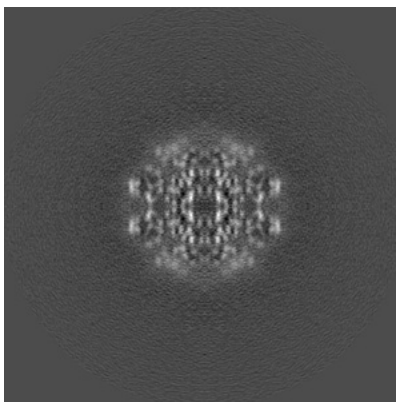


Z Index: 150

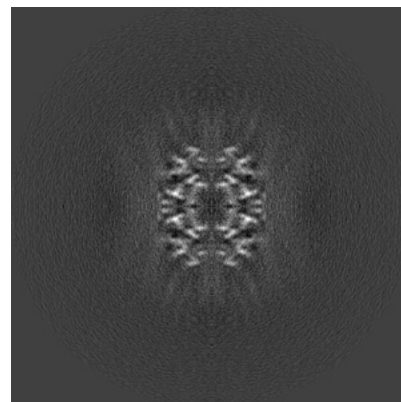
6.2.2 Raw map



X Index: 150



Y Index: 150

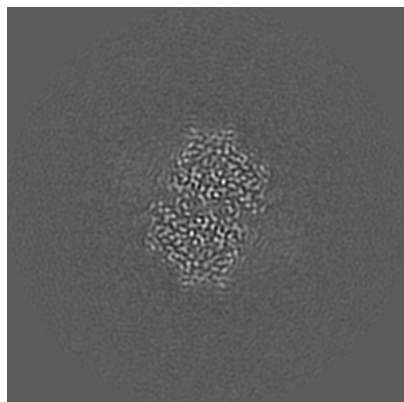


Z Index: 150

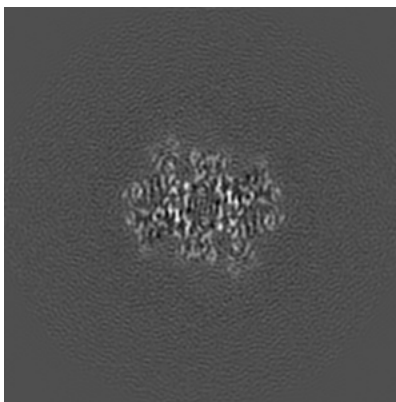
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

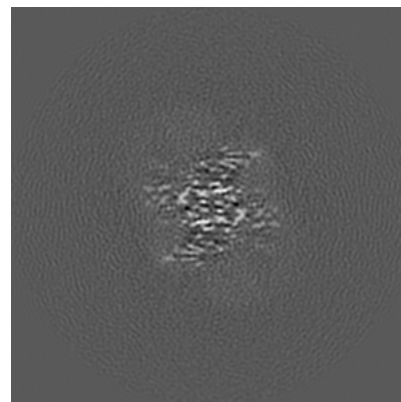
6.3.1 Primary map



X Index: 140

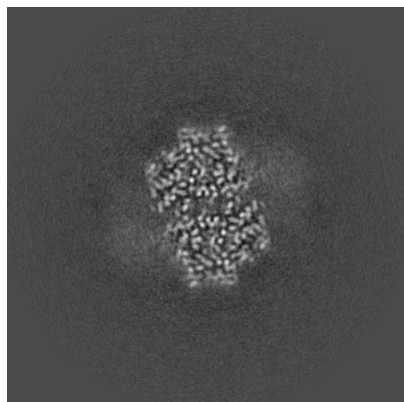


Y Index: 138

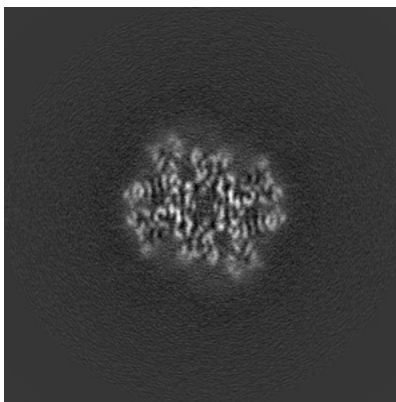


Z Index: 129

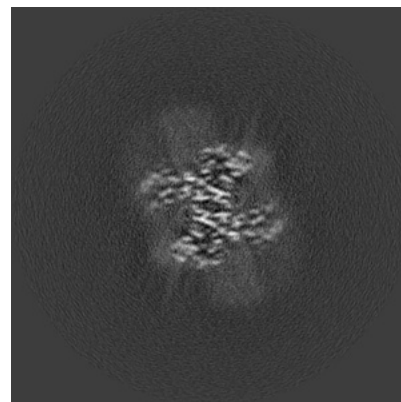
6.3.2 Raw map



X Index: 141



Y Index: 162

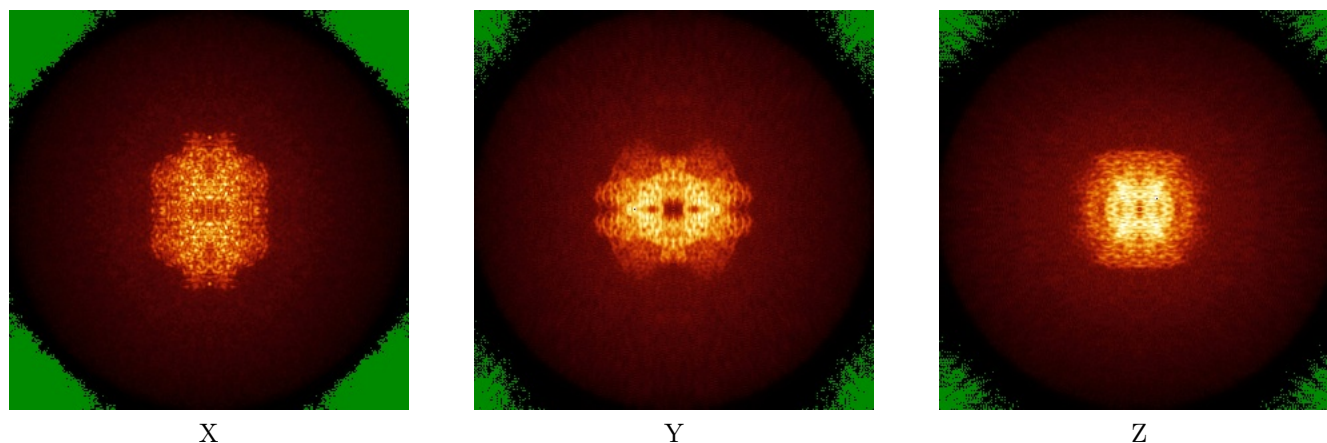


Z Index: 175

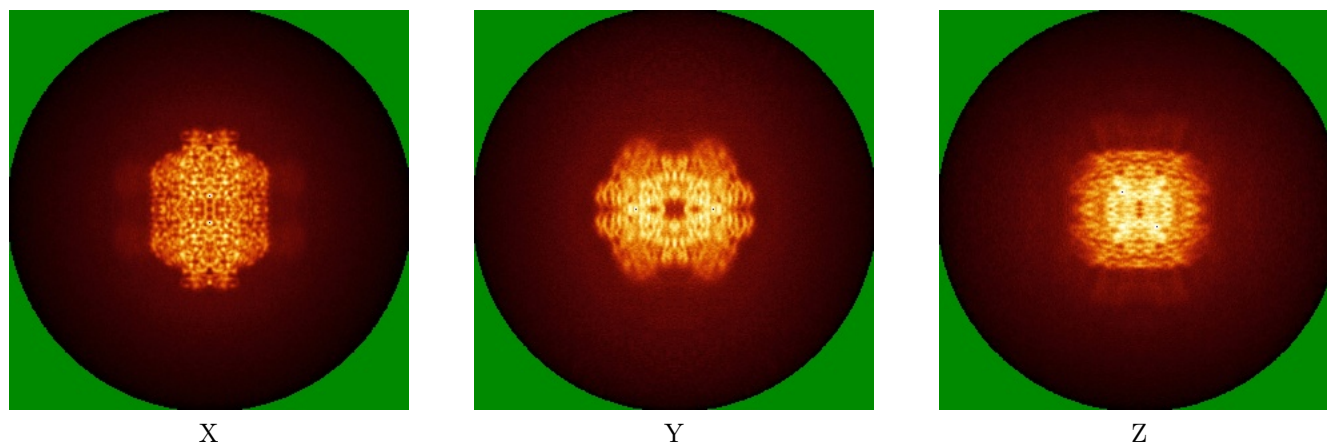
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

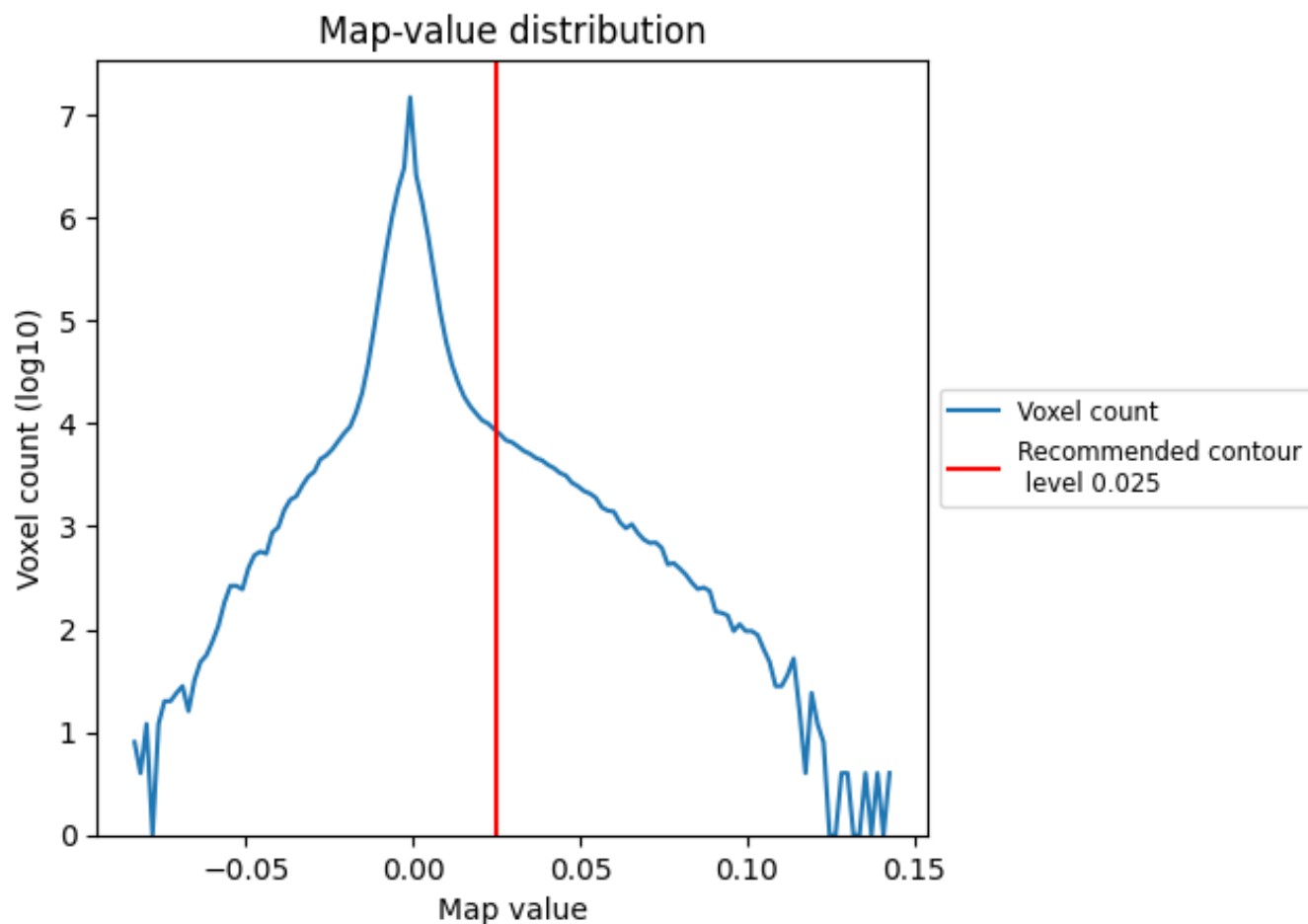
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

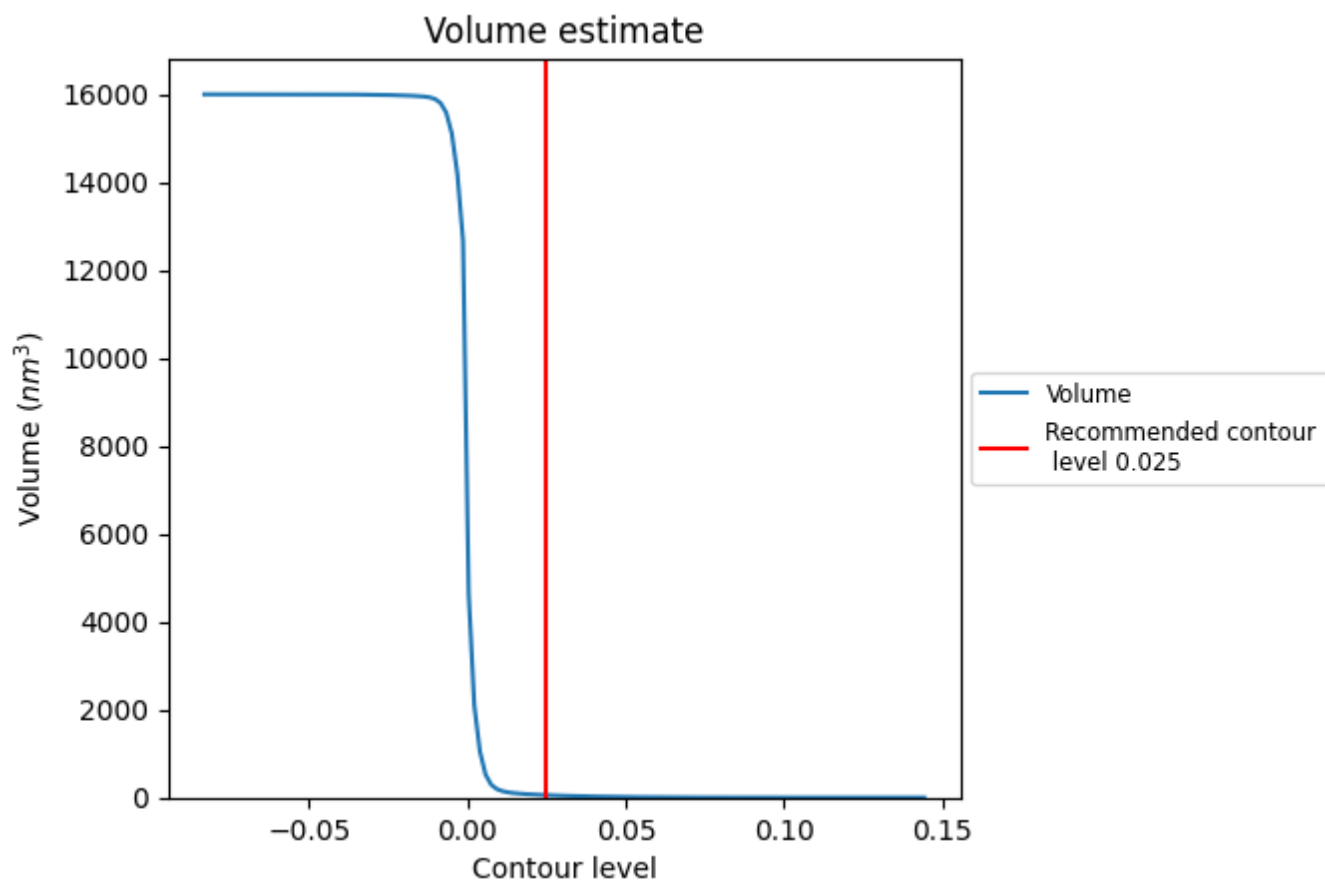
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

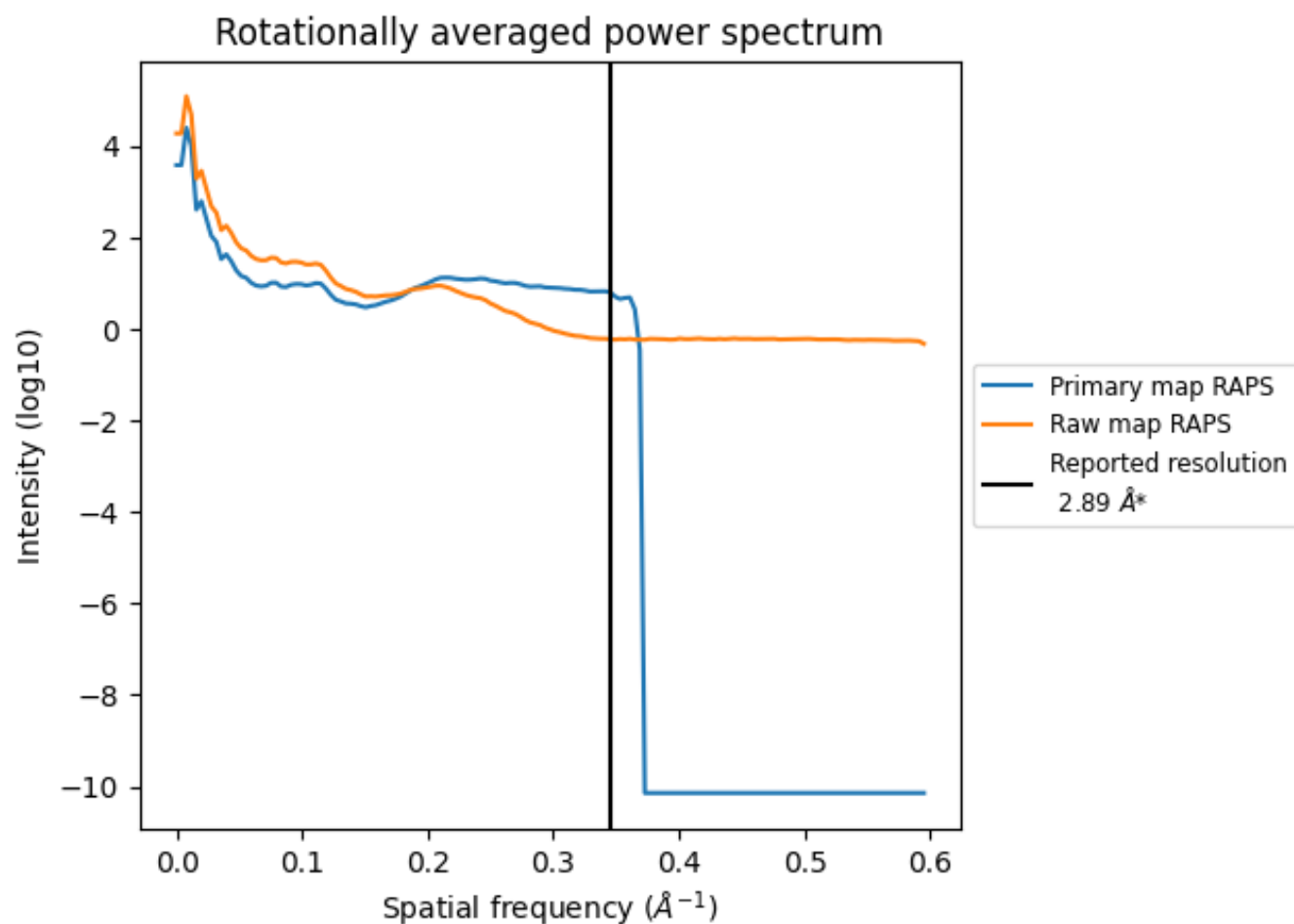
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 55 nm³; this corresponds to an approximate mass of 49 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 ⓘ

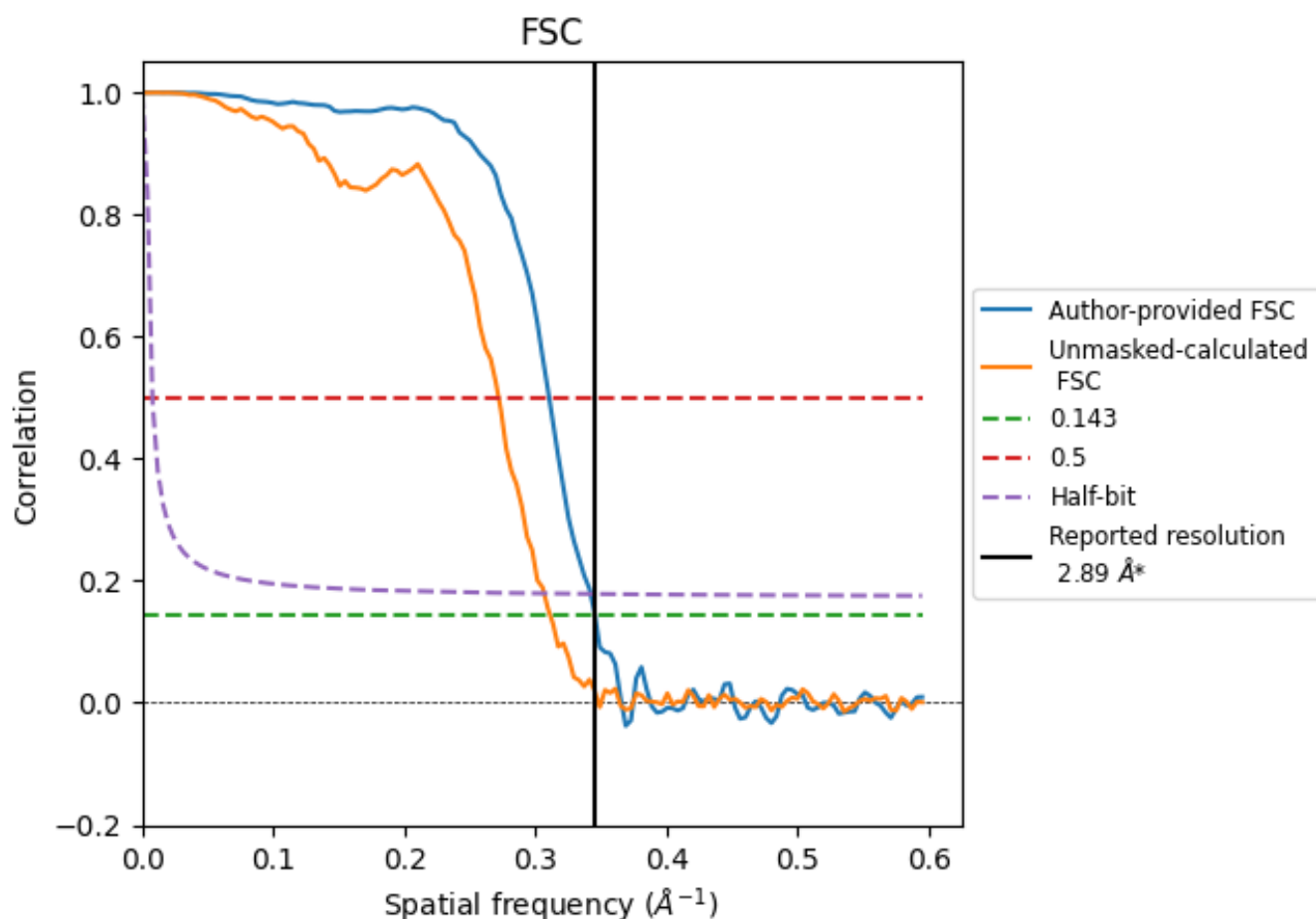


*Reported resolution corresponds to spatial frequency of 0.346 Å⁻¹

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 0.346 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

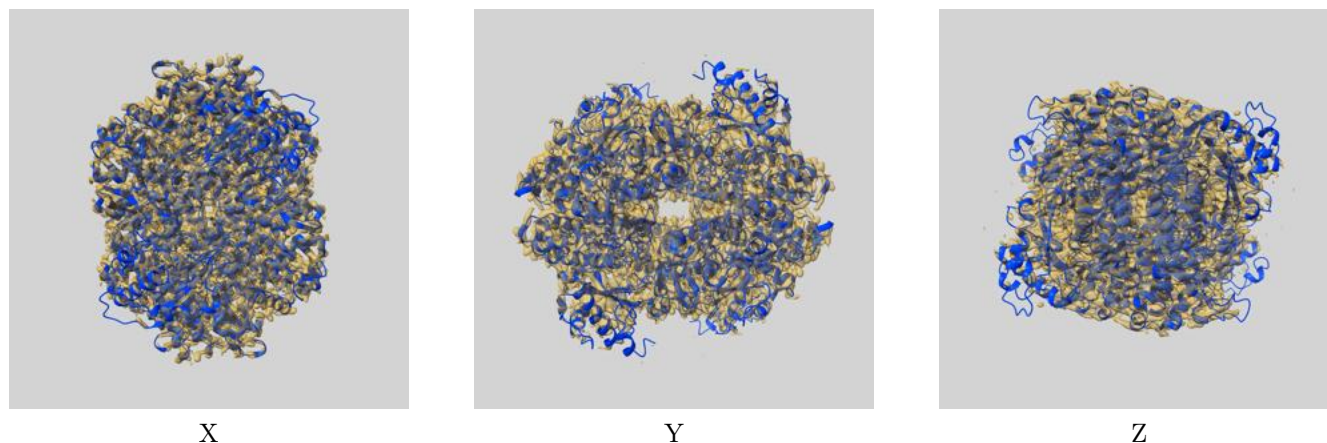
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	2.89	3.22	2.92
Unmasked-calculated*	3.21	3.68	3.26

*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 3.21 differs from the reported value 2.89 by more than 10 %

9 Map-model fit [i](#)

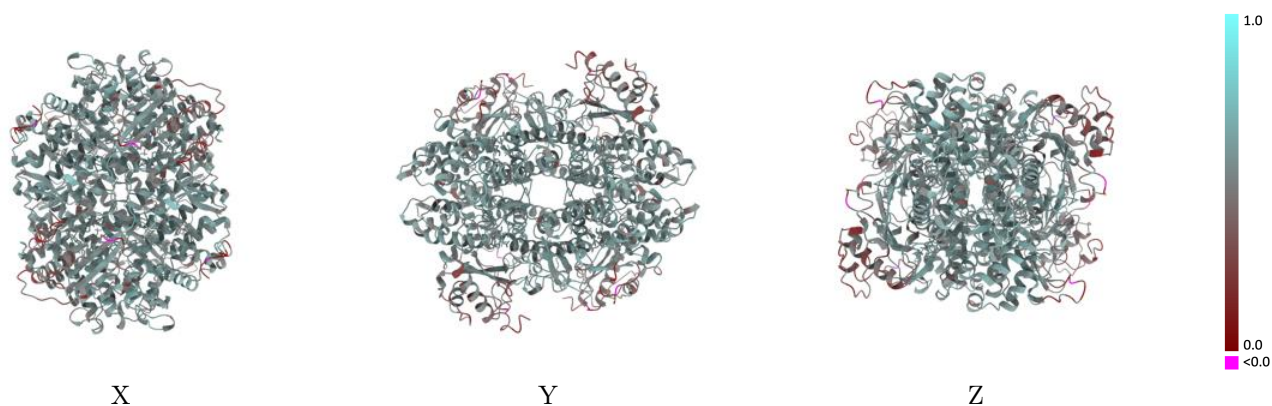
This section contains information regarding the fit between EMDB map EMD-26567 and PDB model 7UJN. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



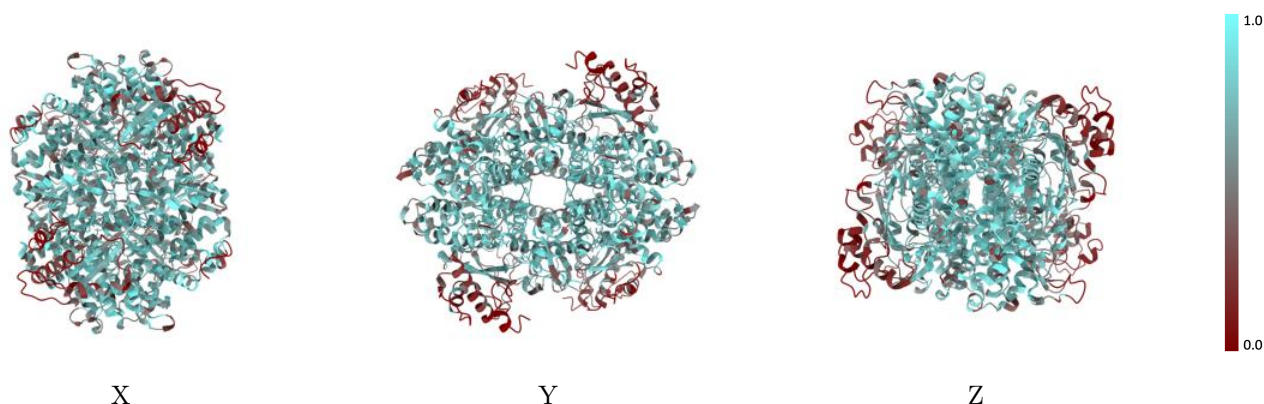
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



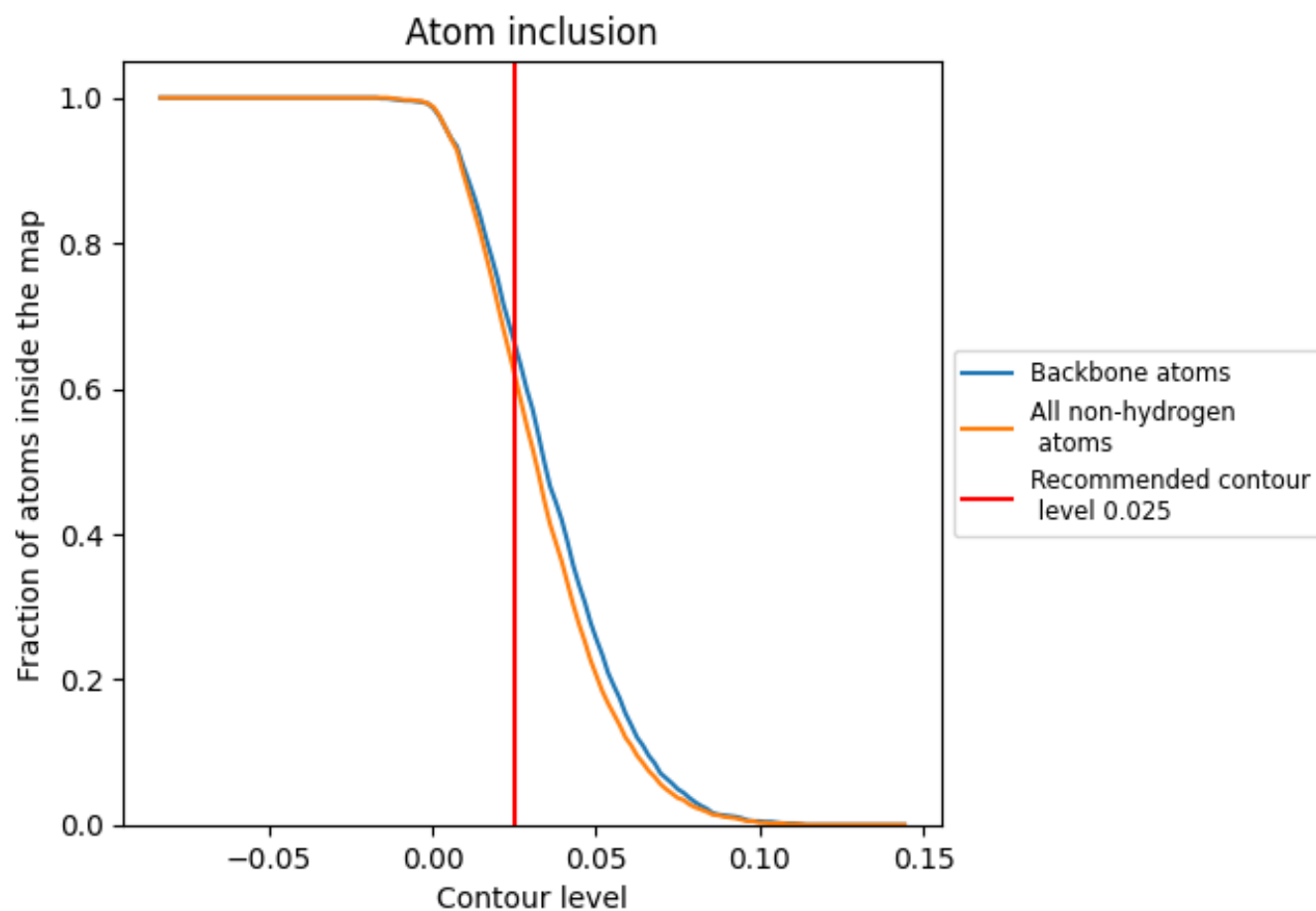
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 62% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6220	0.5270
A	0.6230	0.5280
B	0.6220	0.5260
C	0.6220	0.5270
D	0.6210	0.5270

