



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:51 PM UTC

PDB ID : 6N7V / pdb_00006n7v
EMDB ID : EMD-0364
Title : Structure of bacteriophage T7 gp4 (helicase-primase, E343Q mutant) in complex with ssDNA, dTTP, AC dinucleotide, and CTP (from multiple lead complexes)
Authors : Gao, Y.; Fox, T.; Val, N.; Yang, W.
Deposited on : 2018-11-28
Resolution : 3.80 Å (reported)
Based on initial model : 1E0J

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

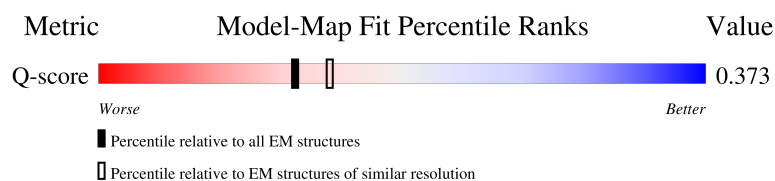
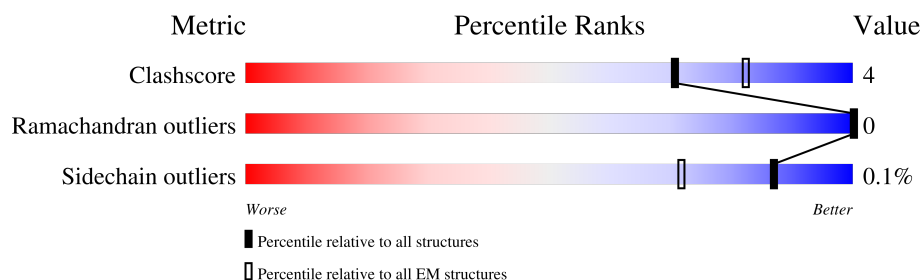
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	566	
1	B	566	
1	C	566	

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Mol	Chain	Length	Quality of chain
1	D	566	43% 52%
1	E	566	42% 54%
1	F	566	12% 42% 55%
2	T	76	9% 12% 79%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12861 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 DNA primase/helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	271	Total	C	N	O	S	0	0
			2093	1309	374	397	13		
1	B	274	Total	C	N	O	S	0	0
			2111	1318	377	403	13		
1	C	276	Total	C	N	O	S	0	0
			2127	1327	378	409	13		
1	D	271	Total	C	N	O	S	0	0
			2086	1304	373	396	13		
1	E	259	Total	C	N	O	S	0	0
			2003	1257	360	373	13		
1	F	255	Total	C	N	O	S	0	0
			1971	1238	354	366	13		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	343	GLN	GLU	engineered mutation	UNP P03692
B	343	GLN	GLU	engineered mutation	UNP P03692
C	343	GLN	GLU	engineered mutation	UNP P03692
D	343	GLN	GLU	engineered mutation	UNP P03692
E	343	GLN	GLU	engineered mutation	UNP P03692
F	343	GLN	GLU	engineered mutation	UNP P03692

- Molecule 2 is a DNA chain called DNA (93-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	16	Total	C	N	O	P	0	0
			320	160	32	112	16		

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).





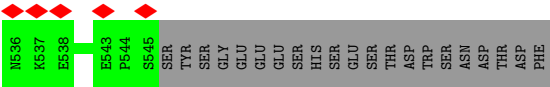
Chain E:



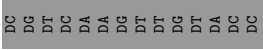
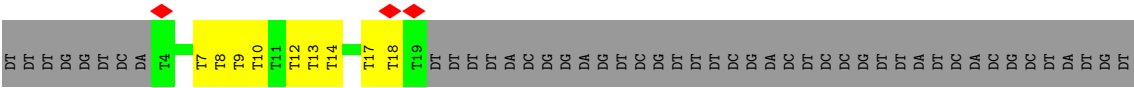
SER	D395	CYS	GLY	GLN	GLY
GLY	SER	HIS	ALA	LYS	LYS
GLU	PHE	LEU	SER	VAL	PRO
GLU	ALA	ASN	ALA	ARG	MET
GLU	GLU	GLY	ALA	ASP	THR
SER	ALA	HIS	LYS	LYS	TYR
HIS	GLU	ASP	LYS	ASP	ASN
SER	THR	ARG	THR	LYS	VAL
GLU	ASP	GLU	CYS	ASN	TRP
SER	R404	ILE	ALA	PHE	ASN
THR	L405	MET	ALA	LYS	VAL
ASP	L406	GLU	THR	THR	GLY
TRP		GLN	TYR	THR	GLY
SER	N412	VAL	GLY	SER	SER
ASN		TRP	TYR	GLY	ASN
ASP	D419	ASN	PHE	HIS	PRO
THR		ALA	ASP	LYS	ARG
ASP	H425	GLY	GLN	SER	ASP
PHE	T426	PRO	PHE	ASP	ASN
	S427	TRP	GLU	ALA	CYS
	T428	ILE	GLN	LEU	GLY
	V429	PRO	ILE	PHE	THR
			ILE	GLY	ALA
	VAL	D263	ILE	LYS	SER
SER	SER		LEU	HIS	ARG
ALA	ALA		MET	LYS	GLY
SER	SER		PHE	LEU	ILE
SER	SER		ASP	TRP	SER
GLU	GLY	L269	MET	ASN	LYS
SER	GLU		ASP	GLY	PHE
ASP	SER	S280	GLU	GLY	SER
GLU	GLU	SER	ALA	LYS	ASP
	R439	GLU	GLY	LYS	GLY
	L449	SER	VAL	VAL	HIS
	K454		VAL	THR	PHE
			VAL	THR	CYS
	L460	L288	GLU	GLU	TYR
			GLY	GLY	ILE
	D470	G294	ALA	GLU	VAL
		T295	ALA	ILE	LYS
	E476	N296	GLN	ASP	LYS
	B504	D297	VAL	MET	TRP
	Q507		LEU	LEU	THR
		M316	PRO	THR	ALA
	L515	G317	ALA	VAL	GLY
	Q525	K318	GLY	MET	ASN
	W529	S319	LYS	GLU	GLU
	Y535		VAL	LEU	ASP
	L542	V322	ARG	GLN	THR
	SS45	L339	VAL	ASP	ASP
		A340	ALA	ASP	LYS
		K341	VAL	CYS	GLU
			LEU	LYS	TYR
			PRO	TYR	ARG
			CYS	PRO	ALA
			LYS	VAL	SER
			ASP	VAL	GLN
			ALA	SER	ASP
			ASN	LEU	LYS
			CYS	ILE	PRO
			THR	GLY	VAL
			ASN	THR	SER
			GLY	ASN	GLY
			THR	THR	THR
			ASP	ASP	ASP
			ASN	ASN	ASN
			GLY	GLY	GLY
			THR	THR	THR
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			GLY	GLY	GLY
			THR	THR	THR
			ASP	ASP	ASP
			ASN	ASN	ASN

Chain F:

[illegible]



• Molecule 2: DNA (93-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	180907	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.324	Depositor
Minimum map value	-0.133	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	412.80002, 412.80002, 412.80002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.72, 1.72, 1.72	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: TTP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/2118	0.40	0/2841
1	B	0.21	0/2136	0.44	0/2865
1	C	0.24	0/2152	0.48	0/2887
1	D	0.23	0/2111	0.49	0/2833
1	E	0.22	0/2026	0.47	0/2716
1	F	0.22	0/1993	0.51	0/2671
2	T	0.29	0/351	0.62	0/540
All	All	0.22	0/12887	0.47	0/17353

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	2093	0	2122	15	0
1	B	2111	0	2136	10	0
1	C	2127	0	2148	16	0
1	D	2086	0	2110	15	0
1	E	2003	0	2041	15	0
1	F	1971	0	2014	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	320	0	193	11	0
3	B	29	0	13	2	0
3	C	29	0	13	1	0
3	D	29	0	13	0	0
3	E	29	0	13	4	0
3	F	29	0	13	3	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	12861	0	12829	91	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 4.

All (91) 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:E:525:GLY:HA3	3:F:700:TTP:H1'	1.63	0.81
2:T:17:DT:H2''	2:T:18:DT:H5''	1.65	0.78
2:T:17:DT:C2'	2:T:18:DT:H5''	2.18	0.74
1:A:491:ALA:HA	1:A:494:GLN:HG2	1.74	0.69
1:D:339:LEU:HD12	1:D:341:MET:HE3	1.83	0.60
1:A:276:ARG:HG3	1:B:373:ILE:HD11	1.84	0.58
1:B:413:ARG:HE	1:B:458:VAL:HB	1.69	0.58
1:D:486:LEU:HB3	1:D:492:LEU:HD12	1.85	0.58
1:A:515:LEU:HD21	1:A:529:ILE:HG12	1.86	0.57
1:F:317:GLY:HA3	3:F:700:TTP:HM51	1.86	0.57
1:D:425:HIS:HD2	1:D:428:ILE:HG12	1.70	0.57
1:F:310:VAL:HB	1:F:463:ILE:HG12	1.86	0.57
1:C:361:ARG:HG2	1:C:361:ARG:NH1	2.19	0.56
1:D:489:SER:HA	2:T:10:DT:H5''	1.87	0.56
1:A:360:VAL:HB	1:A:368:LEU:HD21	1.89	0.54
1:C:361:ARG:HG2	1:C:361:ARG:HH11	1.72	0.53
1:B:425:HIS:HD2	1:B:428:ILE:HG13	1.74	0.53
1:C:439:ARG:HG3	2:T:12:DT:H5''	1.91	0.53
1:E:515:LEU:HD21	1:E:529:ILE:HG12	1.92	0.52
1:C:435:GLU:HG3	1:C:441:MET:HG3	1.92	0.51
1:E:317:GLY:HA3	3:E:700:TTP:C5M	2.40	0.51
1:F:336:LYS:HB2	1:F:418:CYS:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:13:DT:H2''	2:T:14:DT:H5''	1.92	0.51
1:D:449:LEU:HD12	1:D:460:LEU:HD21	1.92	0.51
1:E:394:TYR:HB2	1:E:412:MET:HE1	1.92	0.50
1:D:486:LEU:HD13	1:D:492:LEU:HB2	1.94	0.50
1:F:317:GLY:HA2	3:F:700:TTP:O1A	2.11	0.50
1:D:413:ARG:HE	1:D:456:THR:HB	1.77	0.50
1:E:288:LEU:HD22	1:E:296:ASN:HD22	1.76	0.50
1:A:491:ALA:HA	1:A:494:GLN:CG	2.40	0.50
1:A:425:HIS:HD2	1:A:428:ILE:HG13	1.77	0.49
1:B:535:TYR:HD1	1:B:542:LEU:HB3	1.78	0.48
1:C:325:GLN:NE2	1:C:325:GLN:HA	2.28	0.48
1:F:521:CYS:HG	1:F:524:THR:HG1	1.60	0.48
1:A:491:ALA:HA	1:A:494:GLN:CD	2.38	0.48
2:T:17:DT:H6	2:T:17:DT:H3'	1.78	0.48
1:D:361:ARG:HH22	1:D:535:TYR:HE2	1.62	0.48
1:F:469:PRO:HG3	1:F:474:ALA:HA	1.96	0.48
1:C:413:ARG:HG2	1:C:456:THR:HB	1.96	0.48
1:D:290:SER:H	1:D:325:GLN:HE22	1.61	0.47
1:C:361:ARG:HH11	1:C:361:ARG:CG	2.27	0.47
1:E:316:MET:HE3	1:E:476:GLU:HG3	1.96	0.47
1:A:512:ASN:HD22	1:A:535:TYR:HD2	1.62	0.47
1:E:294:GLY:HA2	1:E:297:ASP:HB3	1.96	0.47
1:F:340:ALA:HB3	1:F:423:LEU:HA	1.96	0.46
1:A:491:ALA:CA	1:A:494:GLN:HG2	2.45	0.46
1:B:361:ARG:HG3	1:B:364:GLN:HB2	1.98	0.46
1:A:322:VAL:HG11	1:A:463:ILE:HD11	1.97	0.45
1:E:316:MET:SD	1:E:504:ARG:HG2	2.55	0.45
1:E:339:LEU:HD12	1:E:341:MET:HE2	1.97	0.45
2:T:7:DT:H2'	2:T:8:DT:H71	1.97	0.45
1:C:534:GLU:HG3	1:C:545:SER:HB2	1.97	0.45
2:T:8:DT:H2''	2:T:9:DT:H5'	1.99	0.45
1:C:475:HIS:HA	1:C:479:ARG:HB3	1.99	0.45
1:C:312:SER:HB3	1:C:316:MET:HB2	1.98	0.45
1:C:325:GLN:HA	1:C:325:GLN:HE21	1.82	0.45
1:D:504:ARG:HB3	1:D:514:VAL:HG12	1.99	0.45
1:A:483:ILE:HG12	1:A:493:ARG:HD2	1.98	0.45
1:D:525:GLY:HA3	3:E:700:TTP:H1'	1.99	0.44
3:B:700:TTP:H3'	3:B:700:TTP:H6	1.81	0.44
1:E:535:TYR:HA	1:E:542:LEU:HD13	1.99	0.44
1:B:340:ALA:HA	1:B:394:TYR:HB3	1.98	0.44
1:E:316:MET:O	3:E:700:TTP:HM52	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:TYR:HE1	1:D:408:LYS:HG2	1.82	0.44
1:B:504:ARG:HH11	1:B:506:GLN:HB3	1.83	0.43
1:D:504:ARG:NH1	1:D:511:PRO:HB2	2.34	0.43
1:C:325:GLN:HE21	1:C:325:GLN:CA	2.30	0.43
1:F:412:MET:HA	1:F:416:LEU:HD12	2.00	0.43
2:T:17:DT:C2'	2:T:18:DT:C5'	2.94	0.43
1:B:467:LYS:HB3	1:B:487:ARG:HB3	2.00	0.43
1:D:319:SER:HA	1:D:322:VAL:HG12	2.01	0.43
1:E:425:HIS:CE1	1:E:427:SER:HB2	2.54	0.43
1:D:488:GLY:O	2:T:10:DT:H4'	2.19	0.42
1:C:406:LEU:HD23	1:C:409:LEU:HD12	2.01	0.42
1:A:413:ARG:HE	1:A:458:VAL:HB	1.84	0.42
1:E:317:GLY:HA3	3:E:700:TTP:HM52	2.02	0.42
1:F:320:THR:HG21	1:F:535:TYR:HE1	1.84	0.42
1:F:504:ARG:HB3	1:F:514:VAL:HG12	2.02	0.42
1:B:311:THR:O	1:B:501:ALA:HA	2.20	0.42
1:B:316:MET:SD	1:B:504:ARG:HG2	2.60	0.42
1:C:425:HIS:CD2	1:C:465:HIS:HE1	2.37	0.42
1:E:449:LEU:HD12	1:E:460:LEU:HD21	2.00	0.42
1:A:357:HIS:CG	1:A:385:LEU:HD21	2.55	0.42
1:E:319:SER:HA	1:E:322:VAL:HG12	2.02	0.42
1:F:486:LEU:HD13	1:F:492:LEU:HB2	2.02	0.41
1:C:322:VAL:HG11	1:C:463:ILE:HD11	2.02	0.41
3:B:700:TTP:C6	3:B:700:TTP:C3'	3.03	0.41
1:A:312:SER:HB3	1:A:502:LEU:HB2	2.01	0.41
2:T:18:DT:H6	2:T:18:DT:H2'	1.70	0.40
1:C:512:ASN:OD1	3:C:700:TTP:N3	2.49	0.40
1:A:339:LEU:HB2	1:A:393:LEU:HD23	2.03	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	263/566 (46%)	257 (98%)	6 (2%)	0	100	100
1	B	266/566 (47%)	256 (96%)	10 (4%)	0	100	100
1	C	268/566 (47%)	256 (96%)	12 (4%)	0	100	100
1	D	263/566 (46%)	250 (95%)	13 (5%)	0	100	100
1	E	249/566 (44%)	241 (97%)	8 (3%)	0	100	100
1	F	245/566 (43%)	235 (96%)	10 (4%)	0	100	100
All	All	1554/3396 (46%)	1495 (96%)	59 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	228/475 (48%)	228 (100%)	0	100	100
1	B	231/475 (49%)	230 (100%)	1 (0%)	84	83
1	C	233/475 (49%)	233 (100%)	0	100	100
1	D	227/475 (48%)	226 (100%)	1 (0%)	84	83
1	E	217/475 (46%)	217 (100%)	0	100	100
1	F	213/475 (45%)	213 (100%)	0	100	100
All	All	1349/2850 (47%)	1347 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	504	ARG
1	D	468	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	GLN
1	A	357	HIS
1	A	392	HIS
1	A	507	GLN
1	A	512	ASN
1	B	505	ASN
1	B	536	ASN
1	C	328	GLN
1	C	465	HIS
1	D	278	HIS
1	D	325	GLN
1	D	392	HIS
1	D	425	HIS
1	D	475	HIS
1	D	506	GLN
1	D	507	GLN
1	E	278	HIS
1	E	328	GLN
1	E	425	HIS
1	E	465	HIS
1	E	507	GLN
1	F	328	GLN
1	F	392	HIS
1	F	425	HIS
1	F	465	HIS
1	F	507	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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
3	TTP	B	700	4	29,30,30	2.47	8 (27%)	43,47,47	3.24	10 (23%)
3	TTP	F	700	4	29,30,30	2.49	8 (27%)	43,47,47	3.23	10 (23%)
3	TTP	D	700	4	29,30,30	2.20	9 (31%)	43,47,47	3.28	10 (23%)
3	TTP	C	700	4	29,30,30	2.28	9 (31%)	43,47,47	3.25	10 (23%)
3	TTP	E	700	4	29,30,30	2.48	8 (27%)	43,47,47	3.23	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TTP	B	700	4	-	8/22/34/34	0/2/2/2
3	TTP	F	700	4	-	4/22/34/34	0/2/2/2
3	TTP	D	700	4	-	10/22/34/34	0/2/2/2
3	TTP	C	700	4	-	3/22/34/34	0/2/2/2
3	TTP	E	700	4	-	8/22/34/34	0/2/2/2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	700	TTP	C2-N1	6.88	1.49	1.38
3	E	700	TTP	C2-N1	6.86	1.49	1.38
3	B	700	TTP	C2-N1	6.85	1.49	1.38
3	D	700	TTP	C2-N1	6.77	1.49	1.38
3	C	700	TTP	C2-N1	6.56	1.48	1.38
3	F	700	TTP	PB-O3A	5.39	1.65	1.59
3	B	700	TTP	PA-O3A	5.35	1.65	1.59
3	B	700	TTP	PB-O3A	5.34	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	700	TTP	PB-O3B	5.33	1.65	1.59
3	F	700	TTP	PB-O3B	5.33	1.65	1.59
3	F	700	TTP	PA-O3A	5.32	1.65	1.59
3	E	700	TTP	PA-O3A	5.32	1.65	1.59
3	E	700	TTP	PB-O3A	5.30	1.65	1.59
3	B	700	TTP	PB-O3B	5.24	1.65	1.59
3	C	700	TTP	PB-O3B	4.76	1.64	1.59
3	C	700	TTP	PA-O3A	4.63	1.64	1.59
3	C	700	TTP	PB-O3A	4.50	1.64	1.59
3	D	700	TTP	PB-O3A	4.29	1.64	1.59
3	D	700	TTP	PA-O3A	4.20	1.64	1.59
3	D	700	TTP	PB-O3B	4.12	1.63	1.59
3	E	700	TTP	C6-N1	3.02	1.43	1.38
3	F	700	TTP	C6-N1	3.02	1.43	1.38
3	E	700	TTP	C4-C5	3.01	1.49	1.44
3	F	700	TTP	C4-C5	3.00	1.49	1.44
3	B	700	TTP	C6-N1	2.99	1.43	1.38
3	B	700	TTP	C4-C5	2.96	1.49	1.44
3	C	700	TTP	C4-C5	2.83	1.49	1.44
3	D	700	TTP	C4-C5	2.78	1.49	1.44
3	D	700	TTP	C6-N1	2.78	1.42	1.38
3	C	700	TTP	C6-N1	2.72	1.42	1.38
3	C	700	TTP	O2-C2	-2.49	1.18	1.23
3	F	700	TTP	C6-C5	2.48	1.38	1.34
3	B	700	TTP	C6-C5	2.45	1.38	1.34
3	E	700	TTP	C6-C5	2.44	1.38	1.34
3	D	700	TTP	O2-C2	-2.41	1.18	1.23
3	B	700	TTP	O2-C2	-2.33	1.18	1.23
3	E	700	TTP	O2-C2	-2.33	1.18	1.23
3	F	700	TTP	O2-C2	-2.32	1.18	1.23
3	C	700	TTP	C6-C5	2.27	1.38	1.34
3	D	700	TTP	C6-C5	2.16	1.38	1.34
3	C	700	TTP	C4-N3	-2.03	1.35	1.38
3	D	700	TTP	C4-N3	-2.00	1.35	1.38

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	700	TTP	C5-C4-N3	12.72	126.38	115.32
3	B	700	TTP	C5-C4-N3	12.48	126.17	115.32
3	C	700	TTP	C5-C4-N3	12.47	126.16	115.32
3	F	700	TTP	C5-C4-N3	12.45	126.14	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	700	TTP	C5-C4-N3	12.45	126.14	115.32
3	D	700	TTP	C4-N3-C2	-10.33	113.79	127.34
3	C	700	TTP	C4-N3-C2	-10.33	113.79	127.34
3	B	700	TTP	C4-N3-C2	-10.30	113.84	127.34
3	E	700	TTP	C4-N3-C2	-10.25	113.90	127.34
3	F	700	TTP	C4-N3-C2	-10.24	113.91	127.34
3	C	700	TTP	N3-C2-N1	7.96	125.25	114.89
3	B	700	TTP	N3-C2-N1	7.94	125.22	114.89
3	F	700	TTP	N3-C2-N1	7.94	125.22	114.89
3	E	700	TTP	N3-C2-N1	7.92	125.20	114.89
3	D	700	TTP	N3-C2-N1	7.84	125.09	114.89
3	D	700	TTP	O4-C4-C5	-7.17	116.72	124.92
3	E	700	TTP	O4-C4-C5	-6.99	116.92	124.92
3	F	700	TTP	O4-C4-C5	-6.98	116.93	124.92
3	B	700	TTP	O4-C4-C5	-6.97	116.95	124.92
3	C	700	TTP	O4-C4-C5	-6.95	116.96	124.92
3	F	700	TTP	C6-N1-C2	-4.86	116.47	121.30
3	B	700	TTP	C6-N1-C2	-4.85	116.48	121.30
3	E	700	TTP	C6-N1-C2	-4.82	116.50	121.30
3	C	700	TTP	C6-N1-C2	-4.71	116.62	121.30
3	D	700	TTP	C6-N1-C2	-4.66	116.66	121.30
3	C	700	TTP	O2-C2-N1	-4.25	117.27	122.80
3	F	700	TTP	O2-C2-N1	-4.15	117.39	122.80
3	E	700	TTP	O2-C2-N1	-4.15	117.39	122.80
3	B	700	TTP	O2-C2-N1	-4.10	117.46	122.80
3	D	700	TTP	O2-C2-N1	-3.76	117.90	122.80
3	C	700	TTP	C5-C6-N1	-2.61	120.48	123.31
3	D	700	TTP	C5-C6-N1	-2.58	120.51	123.31
3	E	700	TTP	C5-C6-N1	-2.53	120.56	123.31
3	F	700	TTP	C5-C6-N1	-2.52	120.57	123.31
3	B	700	TTP	C5-C6-N1	-2.47	120.64	123.31
3	D	700	TTP	C1'-N1-C2	2.43	122.41	117.66
3	D	700	TTP	O2-C2-N3	-2.43	117.01	121.49
3	C	700	TTP	C5M-C5-C4	2.27	121.21	118.78
3	B	700	TTP	O2-C2-N3	-2.26	117.31	121.49
3	B	700	TTP	C5M-C5-C4	2.26	121.19	118.78
3	E	700	TTP	C5M-C5-C4	2.23	121.17	118.78
3	D	700	TTP	C5M-C5-C4	2.23	121.16	118.78
3	F	700	TTP	C5M-C5-C4	2.23	121.16	118.78
3	F	700	TTP	O2-C2-N3	-2.22	117.39	121.49
3	E	700	TTP	O2-C2-N3	-2.22	117.40	121.49
3	C	700	TTP	O2-C2-N3	-2.17	117.48	121.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	700	TTP	C1'-N1-C2	2.13	121.83	117.66
3	B	700	TTP	C1'-N1-C2	2.12	121.81	117.66
3	E	700	TTP	C1'-N1-C2	2.04	121.64	117.66
3	F	700	TTP	C1'-N1-C2	2.01	121.59	117.66

There are no chirality outliers.

All (33) torsion outliers are listed below:

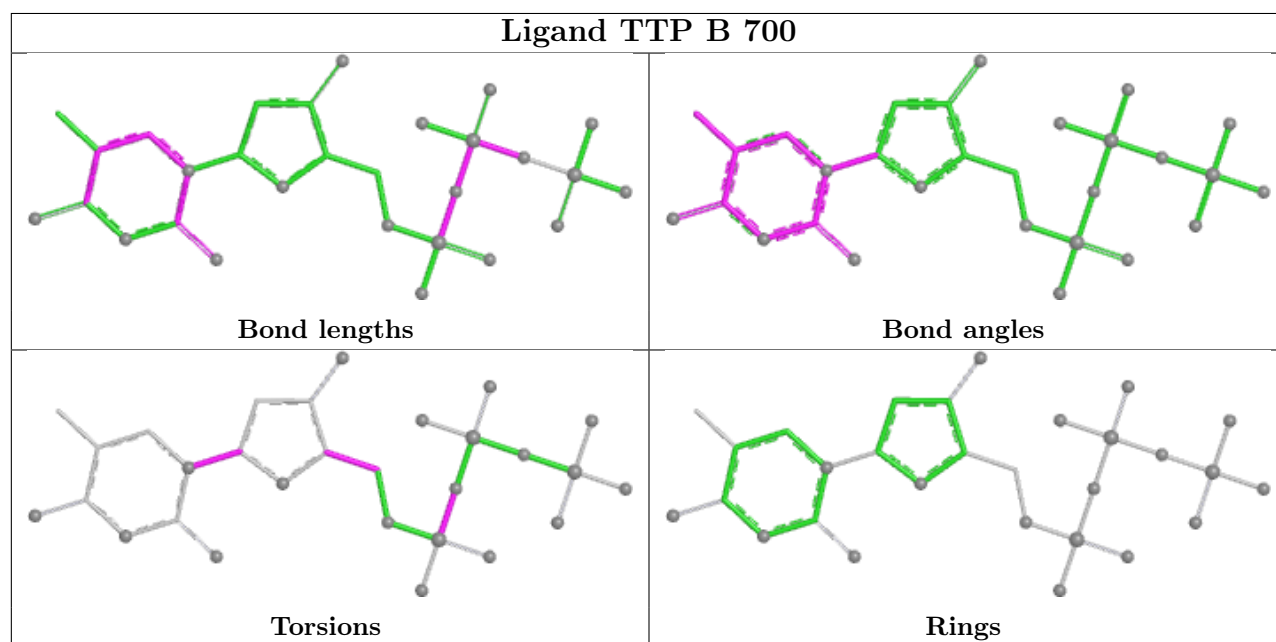
Mol	Chain	Res	Type	Atoms
3	C	700	TTP	PB-O3B-PG-O3G
3	D	700	TTP	C5'-O5'-PA-O1A
3	D	700	TTP	C5'-O5'-PA-O3A
3	D	700	TTP	PB-O3B-PG-O2G
3	D	700	TTP	O4'-C4'-C5'-O5'
3	D	700	TTP	C3'-C4'-C5'-O5'
3	E	700	TTP	PB-O3B-PG-O2G
3	F	700	TTP	PB-O3B-PG-O2G
3	F	700	TTP	C3'-C4'-C5'-O5'
3	F	700	TTP	O4'-C4'-C5'-O5'
3	E	700	TTP	O4'-C4'-C5'-O5'
3	E	700	TTP	C3'-C4'-C5'-O5'
3	C	700	TTP	O4'-C4'-C5'-O5'
3	C	700	TTP	C3'-C4'-C5'-O5'
3	B	700	TTP	C2'-C1'-N1-C6
3	D	700	TTP	PB-O3B-PG-O3G
3	D	700	TTP	PA-O3A-PB-O2B
3	B	700	TTP	C2'-C1'-N1-C2
3	B	700	TTP	O4'-C1'-N1-C6
3	F	700	TTP	PB-O3B-PG-O1G
3	D	700	TTP	PG-O3B-PB-O2B
3	E	700	TTP	PG-O3B-PB-O2B
3	B	700	TTP	O4'-C4'-C5'-O5'
3	E	700	TTP	PA-O3A-PB-O2B
3	B	700	TTP	O4'-C1'-N1-C2
3	E	700	TTP	PB-O3B-PG-O1G
3	E	700	TTP	PB-O3B-PG-O3G
3	B	700	TTP	PB-O3A-PA-O2A
3	D	700	TTP	PA-O3A-PB-O1B
3	E	700	TTP	PG-O3B-PB-O1B
3	B	700	TTP	C3'-C4'-C5'-O5'
3	B	700	TTP	PB-O3A-PA-O1A
3	D	700	TTP	PG-O3B-PB-O1B

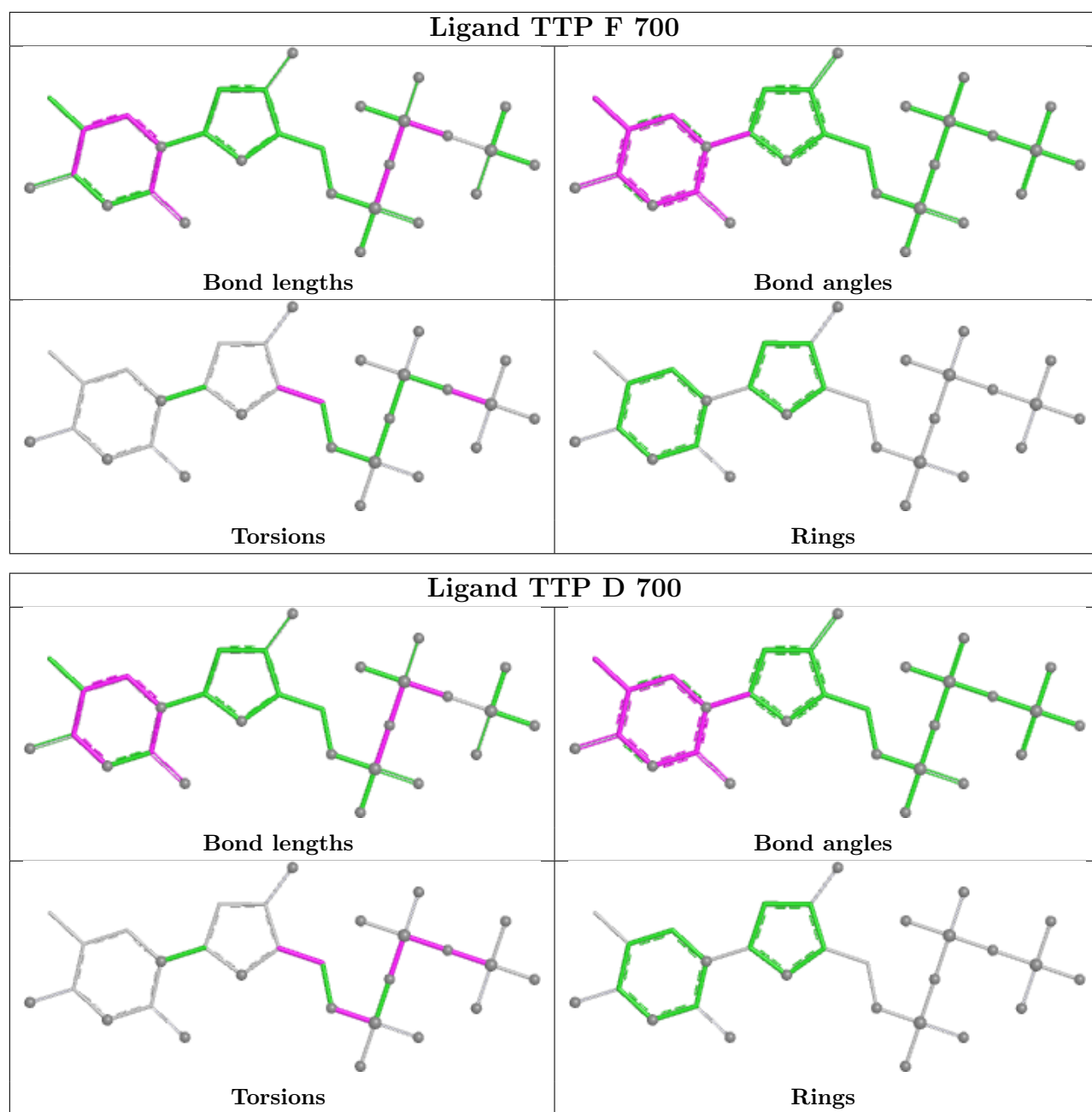
There are no ring outliers.

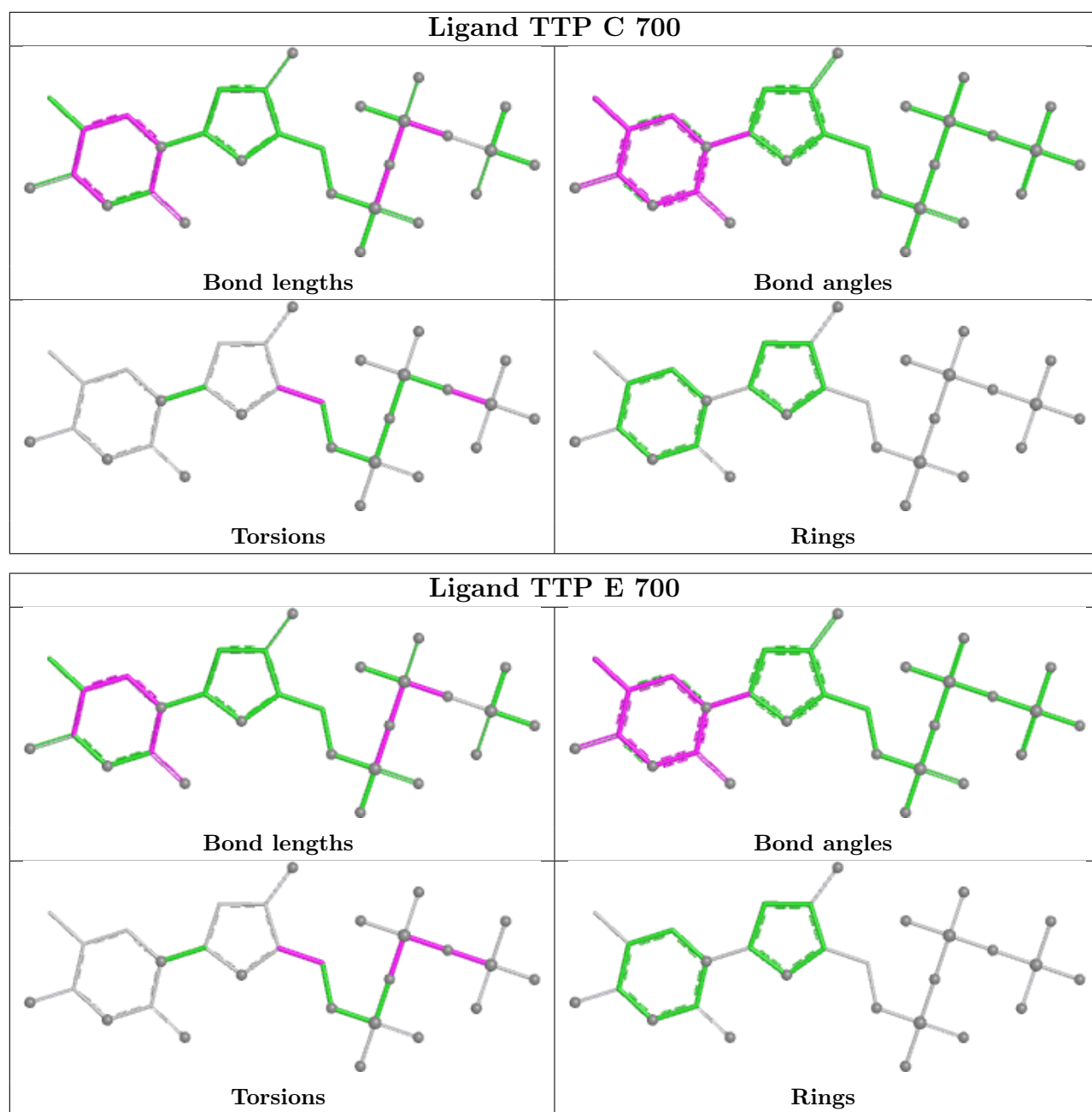
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	700	TTP	2	0
3	F	700	TTP	3	0
3	C	700	TTP	1	0
3	E	700	TTP	4	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.

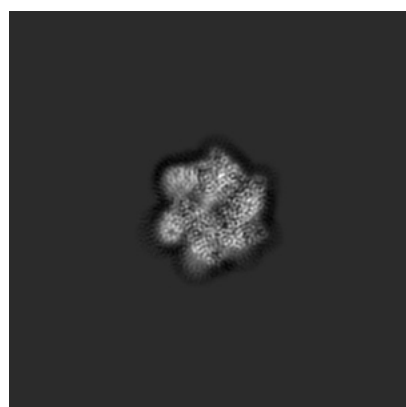
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0364. These allow visual inspection of the internal detail of the map and identification of artifacts.

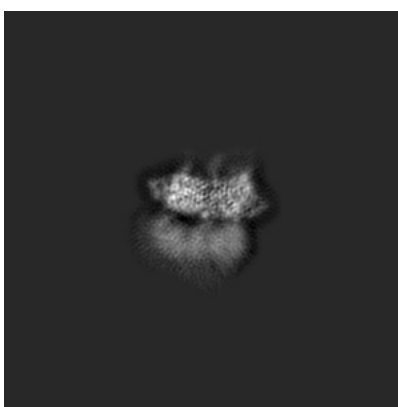
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

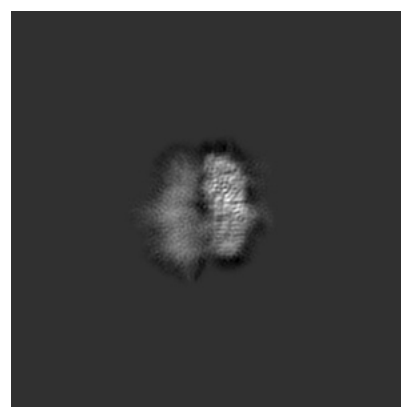
6.1.1 Primary map



X



Y

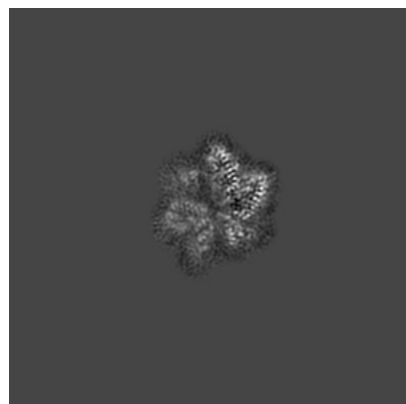


Z

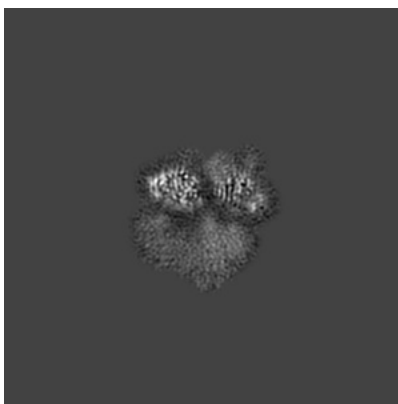
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

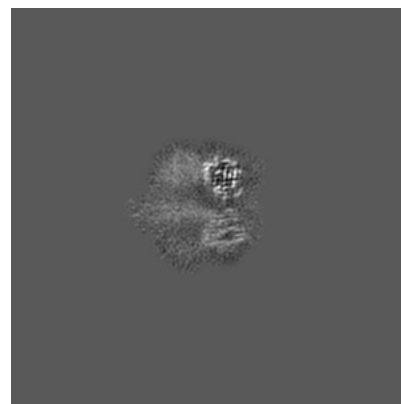
6.2.1 Primary map



X Index: 120



Y Index: 120

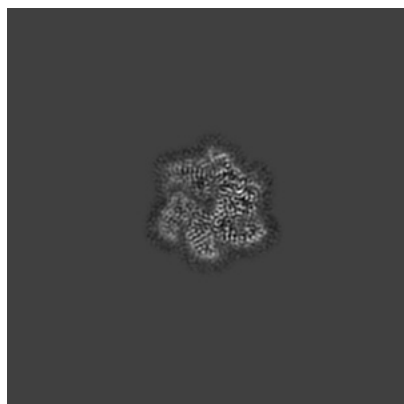


Z Index: 120

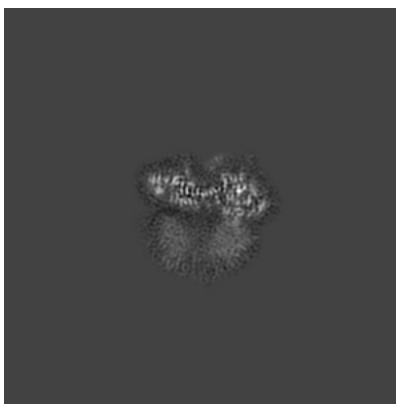
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 128



Y Index: 126

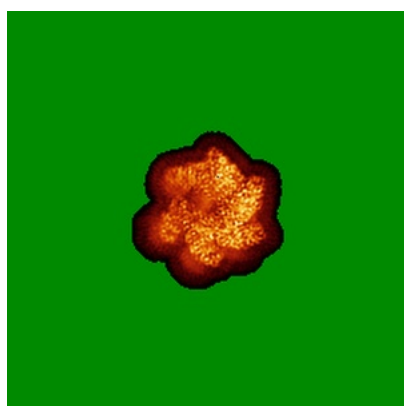


Z Index: 108

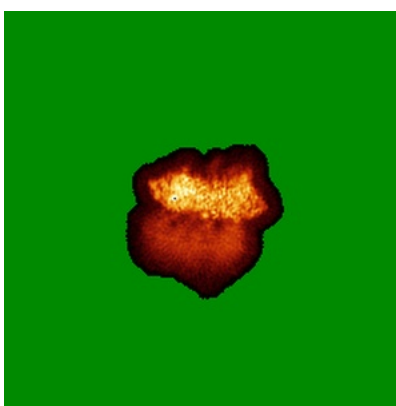
The images above show the largest variance slices of the map in three orthogonal directions.

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

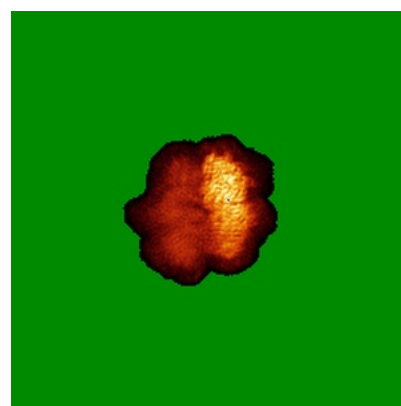
6.4.1 Primary map



X



Y

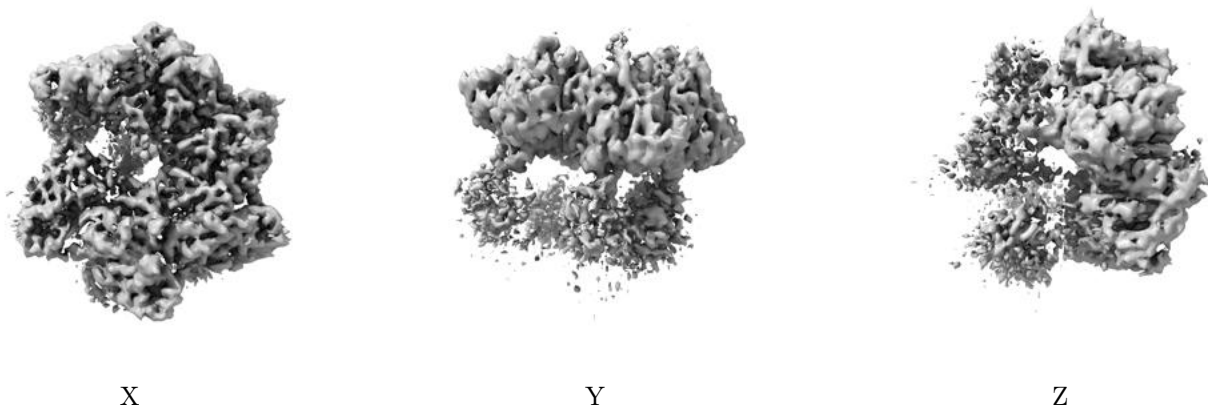


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

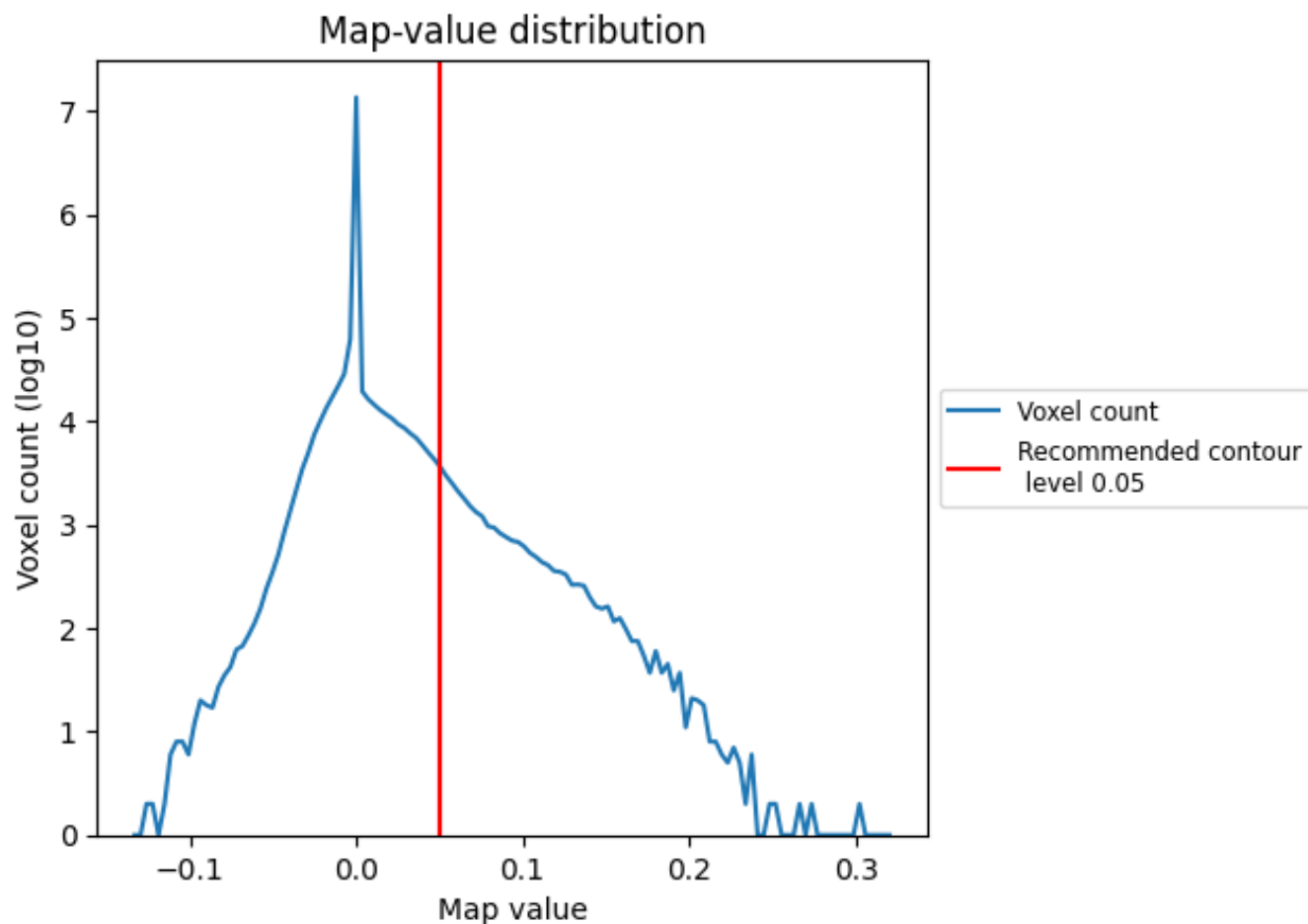
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

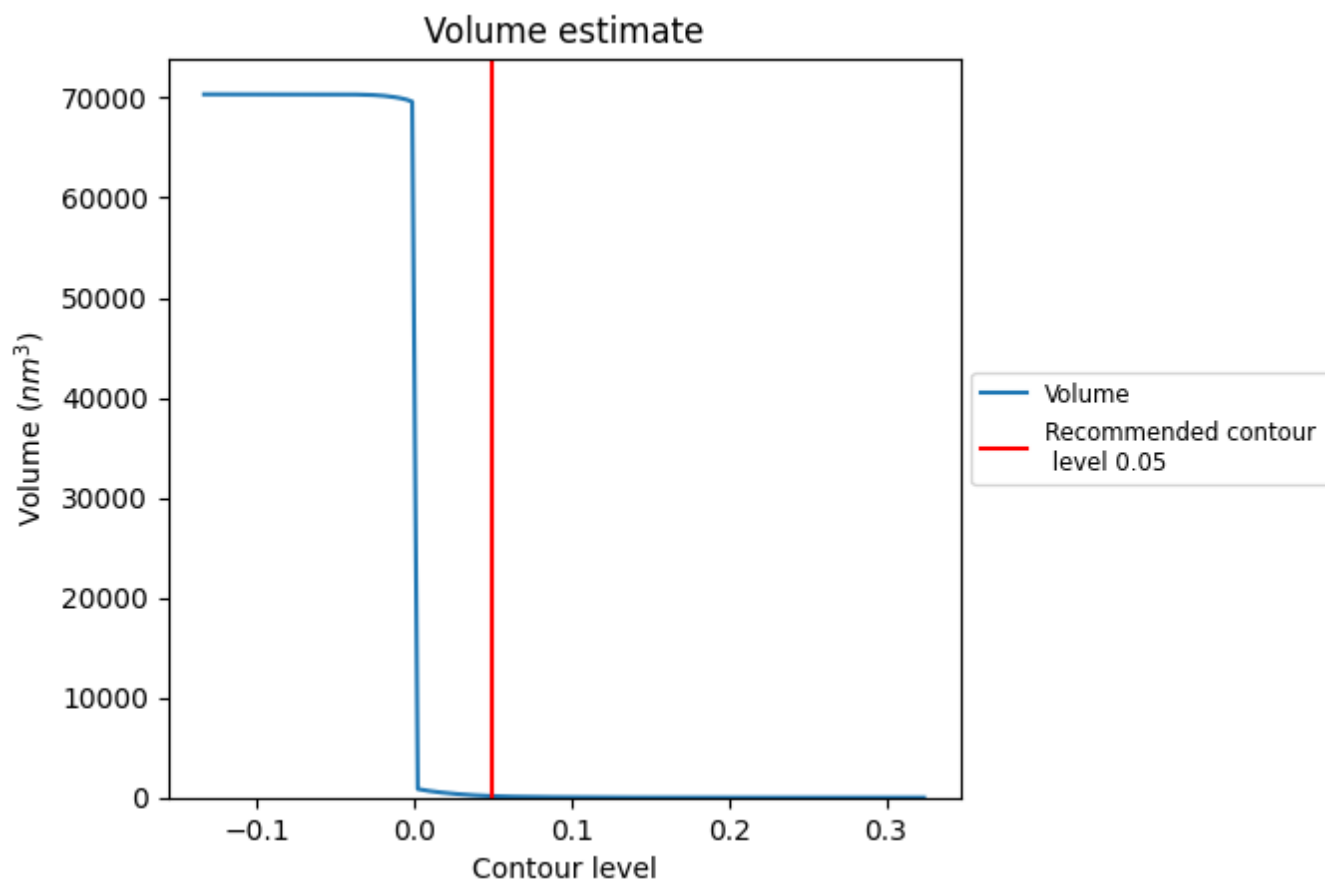
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

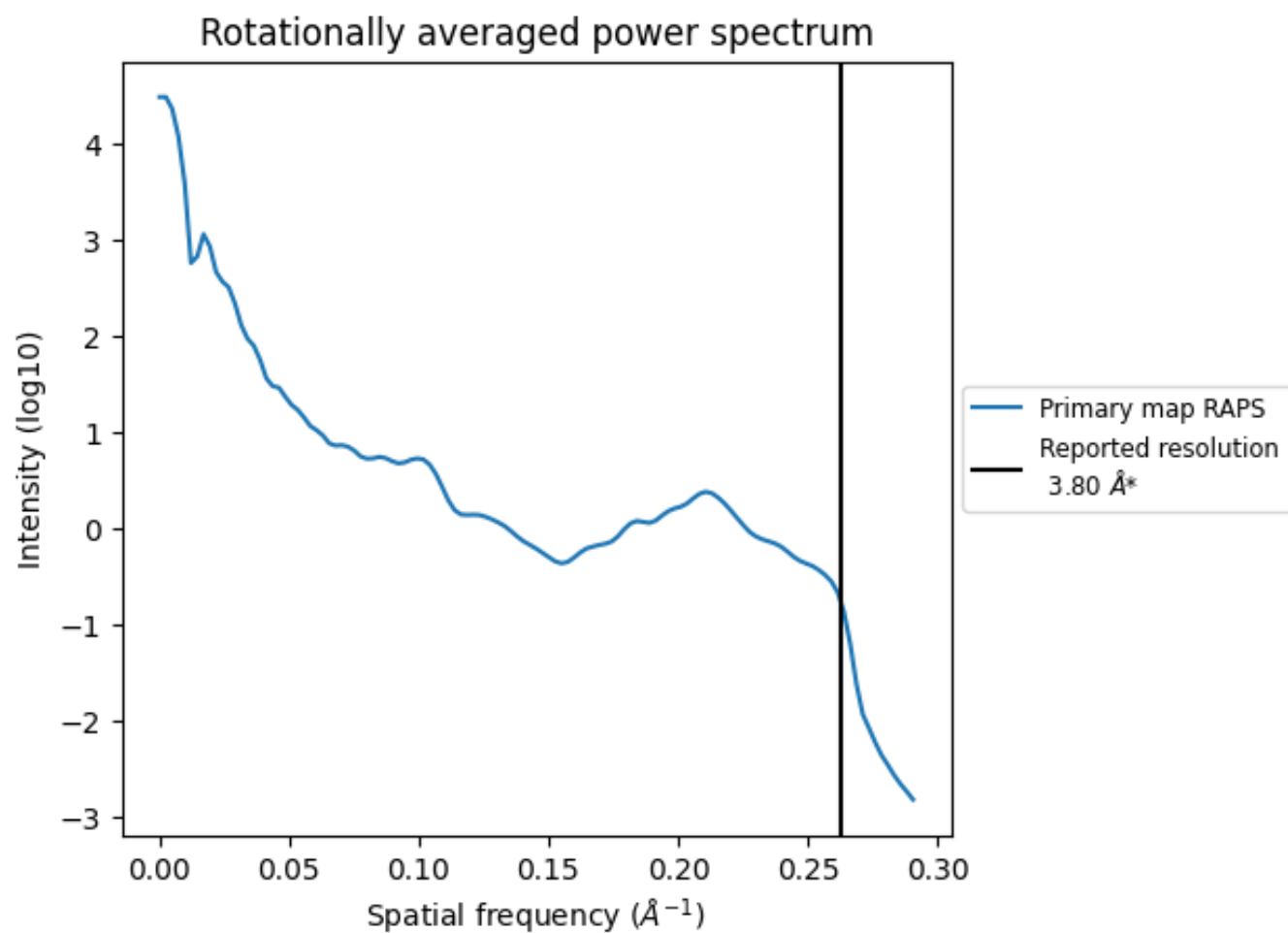
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 144 nm³; this corresponds to an approximate mass of 130 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 ⓘ

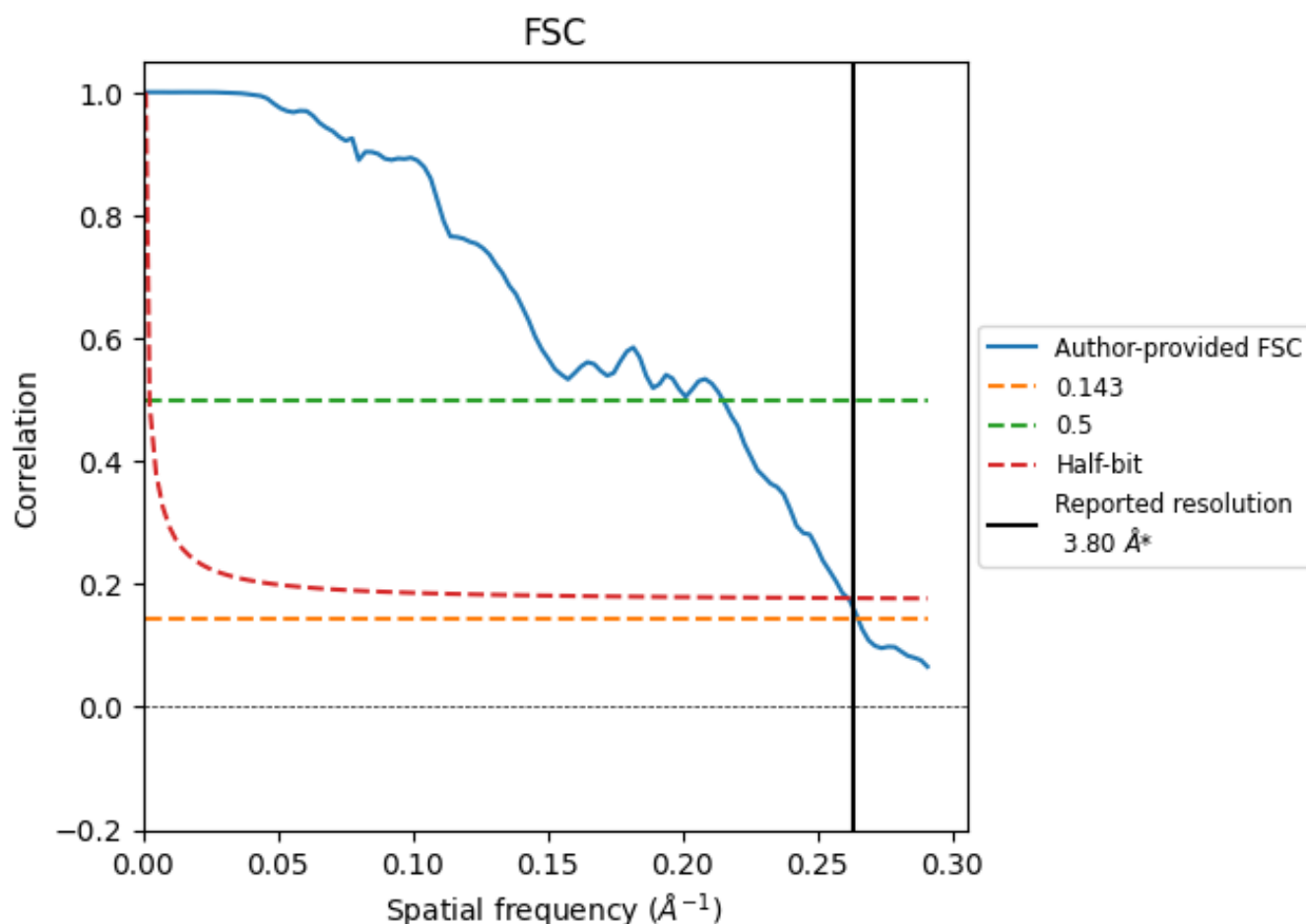


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

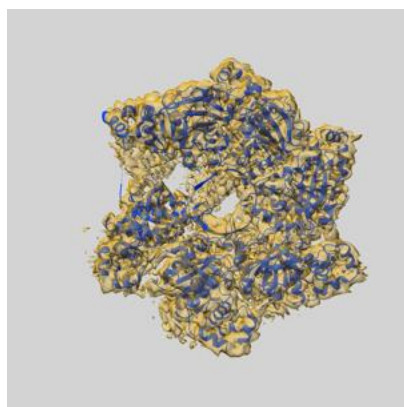
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.77	4.66	3.83
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

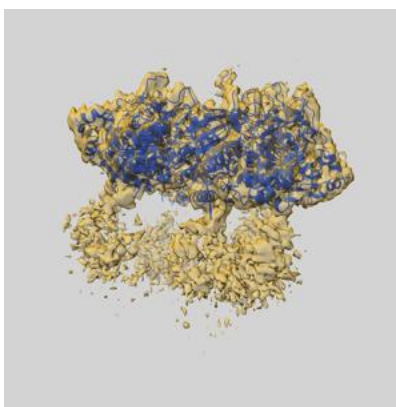
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0364 and PDB model 6N7V. Per-residue inclusion information can be found in section [3](#) on page [6](#).

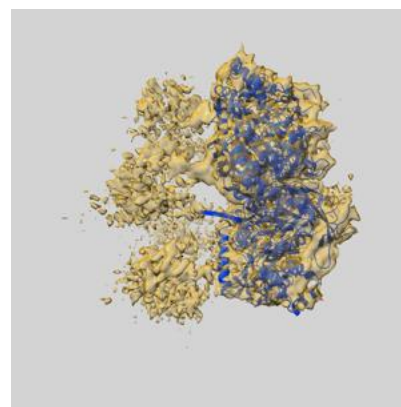
9.1 Map-model overlay [i](#)



X



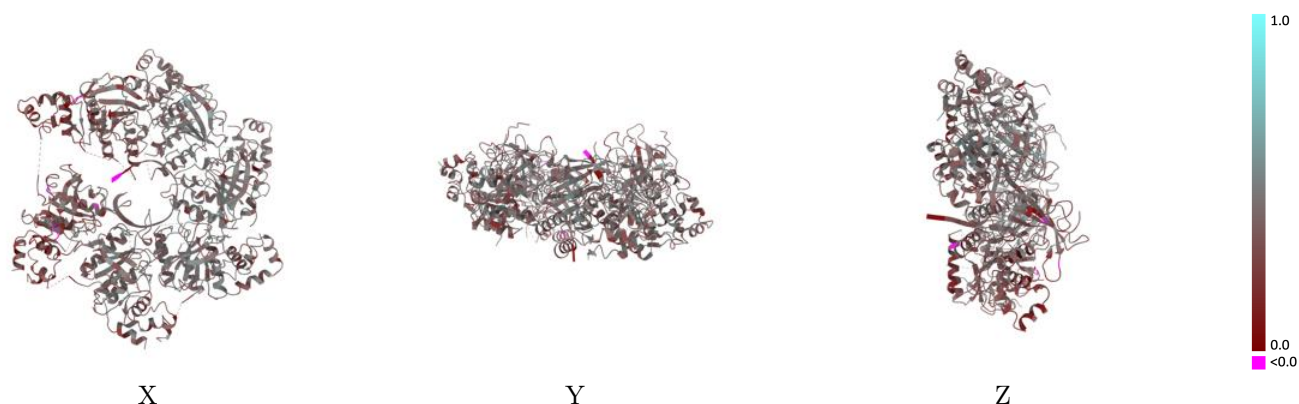
Y



Z

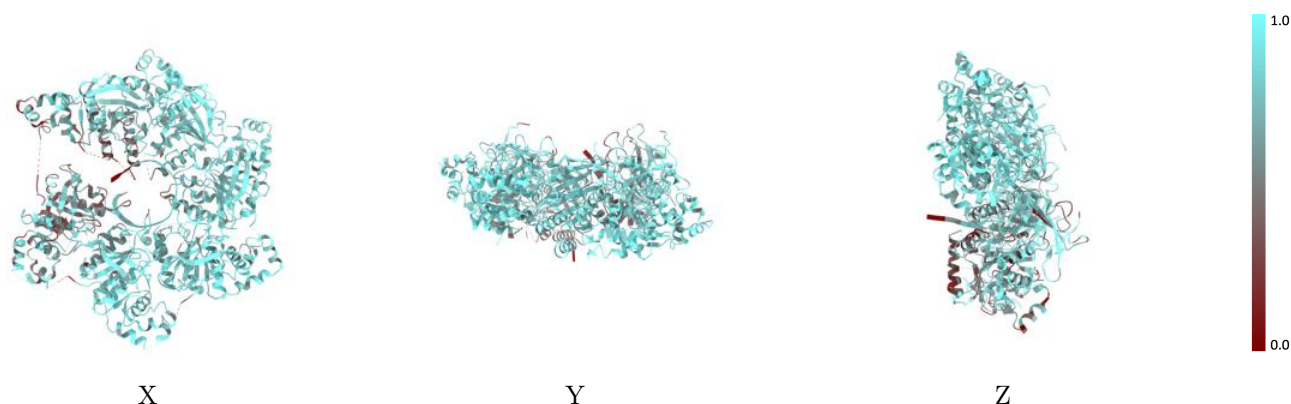
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



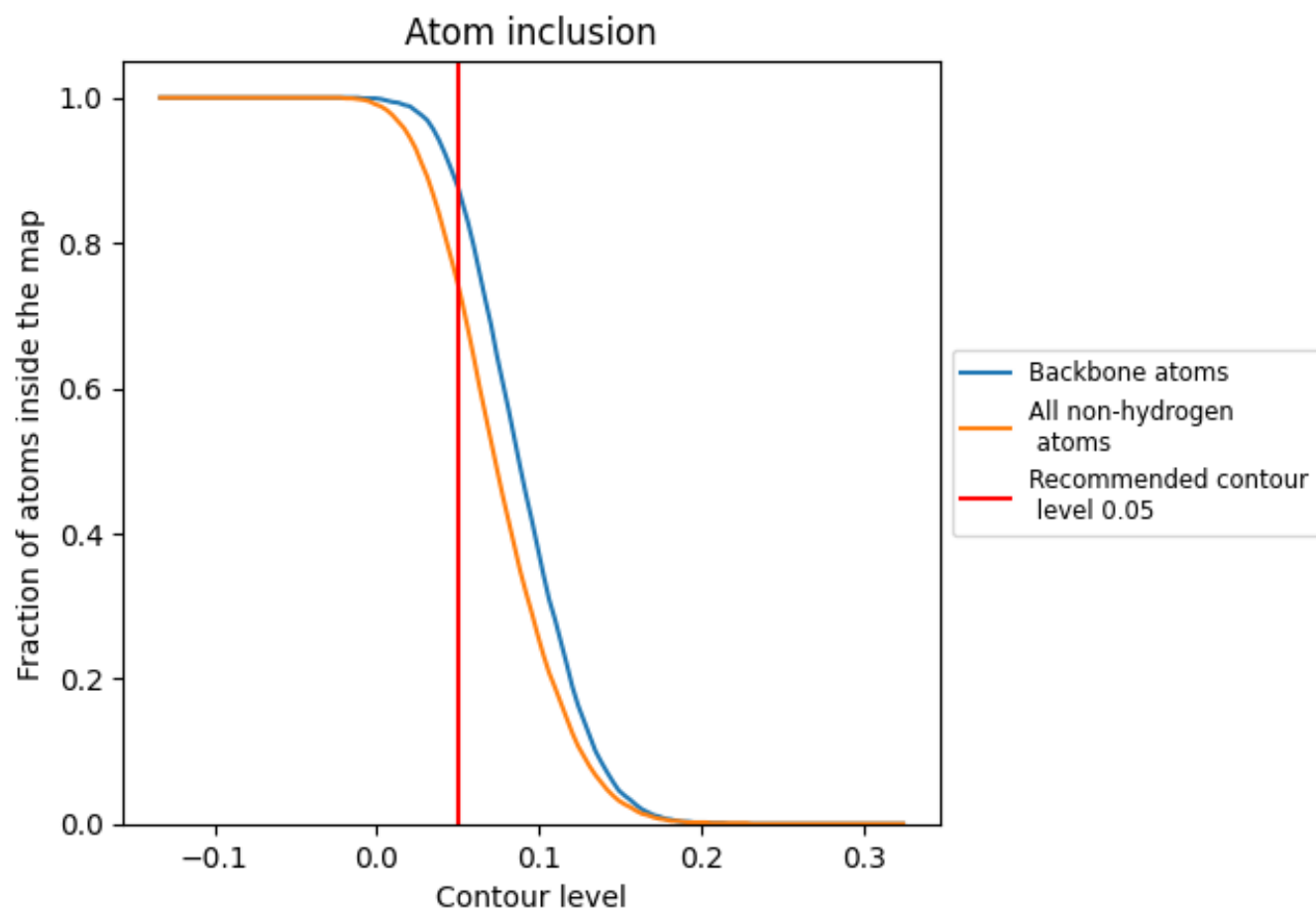
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 74% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7430	0.3730
A	0.6530	0.3260
B	0.8280	0.4110
C	0.8040	0.4100
D	0.8190	0.4120
E	0.7820	0.3840
F	0.5740	0.3000
T	0.6530	0.3080

1.0

0.0

<0.0