



Full wwPDB EM Validation Report ⓘ

Jun 7, 2023 – 04:17 PM EDT

PDB ID : 8D4G
EMDB ID : EMD-27185
Title : gamma-Arf1 mediated dimeric assembly of AP-1, Arf1, Nef complex within lattice on MHC-I lipopeptide incorporated wide(r) membrane tubes
Authors : Hooy, R.M.; Hurley, J.H.
Deposited on : 2022-06-01
Resolution : 11.60 Å (reported)
Based on initial models : 6CM9, 4EN2

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:

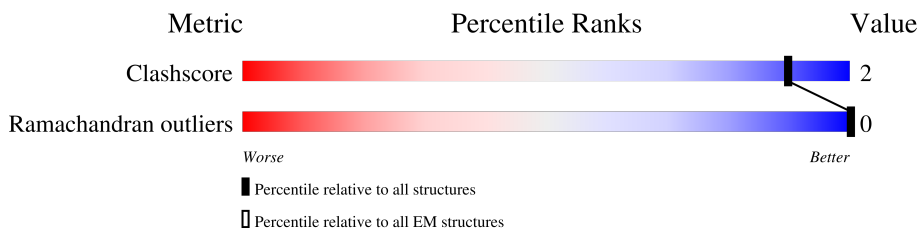
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.33

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 11.60 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.



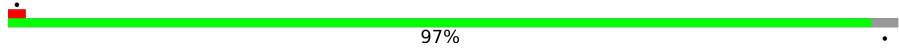
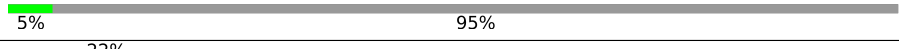

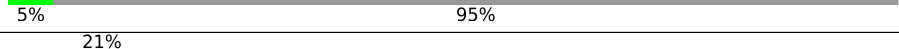

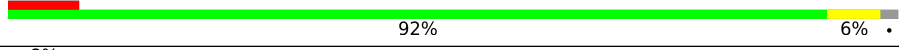
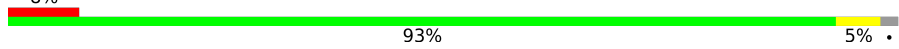

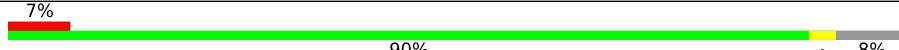

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	949	60% 40%
1	B	949	60% 40%
2	C	181	15% 98% ..
2	D	181	16% 99% .
2	F	181	13% 98% ..
2	H	181	13% 98% ..
2	Q	181	31% 98% ..
2	Z	181	30% 98% ..
3	E	601	97% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	601	 97%
4	I	213	 5% 95%
4	K	213	 22% 62% 36%
4	L	213	 5% 95%
4	N	213	 21% 62% 36%
5	J	423	 8% 92% 6%
5	M	423	 8% 93% 5%
6	O	154	 8% 88% 8%
6	S	154	 7% 90% 8%
7	P	39	 10% 46% 54%
7	Y	39	 15% 46% 54%

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 19534 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 AP-1 complex subunit beta-1.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
1	B	570	2280	1140	570	570	0	0
1	A	570	2280	1140	570	570	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	359	ARG	LYS	engineered mutation	UNP Q10567
B	476	LYS	GLU	engineered mutation	UNP Q10567
A	359	ARG	LYS	engineered mutation	UNP Q10567
A	476	LYS	GLU	engineered mutation	UNP Q10567

- Molecule 2 is a protein called ADP-ribosylation factor 1.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
2	C	180	720	360	180	180	0	0
2	H	180	720	360	180	180	0	0
2	Z	180	720	360	180	180	0	0
2	D	180	720	360	180	180	0	0
2	F	180	720	360	180	180	0	0
2	Q	180	720	360	180	180	0	0

- Molecule 3 is a protein called AP-1 complex subunit gamma-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	G	585	2340	1170	585	585	0	0
3	E	585	2340	1170	585	585	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	596	GLU	-	expression tag	UNP P22892
G	597	ASN	-	expression tag	UNP P22892
G	598	LEU	-	expression tag	UNP P22892
G	599	TYR	-	expression tag	UNP P22892
G	600	PHE	-	expression tag	UNP P22892
G	601	GLN	-	expression tag	UNP P22892
E	596	GLU	-	expression tag	UNP P22892
E	597	ASN	-	expression tag	UNP P22892
E	598	LEU	-	expression tag	UNP P22892
E	599	TYR	-	expression tag	UNP P22892
E	600	PHE	-	expression tag	UNP P22892
E	601	GLN	-	expression tag	UNP P22892

- Molecule 4 is a protein called Protein Nef.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	L	10	40	20	10	10	0	0
4	N	137	548	274	137	137	0	0
4	I	10	40	20	10	10	0	0
4	K	137	548	274	137	137	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	207	GLY	-	expression tag	UNP Q90VU7
L	208	HIS	-	expression tag	UNP Q90VU7
L	209	HIS	-	expression tag	UNP Q90VU7
L	210	HIS	-	expression tag	UNP Q90VU7
L	211	HIS	-	expression tag	UNP Q90VU7
L	212	HIS	-	expression tag	UNP Q90VU7
L	213	HIS	-	expression tag	UNP Q90VU7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
N	207	GLY	-	expression tag	UNP Q90VU7
N	208	HIS	-	expression tag	UNP Q90VU7
N	209	HIS	-	expression tag	UNP Q90VU7
N	210	HIS	-	expression tag	UNP Q90VU7
N	211	HIS	-	expression tag	UNP Q90VU7
N	212	HIS	-	expression tag	UNP Q90VU7
N	213	HIS	-	expression tag	UNP Q90VU7
I	207	GLY	-	expression tag	UNP Q90VU7
I	208	HIS	-	expression tag	UNP Q90VU7
I	209	HIS	-	expression tag	UNP Q90VU7
I	210	HIS	-	expression tag	UNP Q90VU7
I	211	HIS	-	expression tag	UNP Q90VU7
I	212	HIS	-	expression tag	UNP Q90VU7
I	213	HIS	-	expression tag	UNP Q90VU7
K	207	GLY	-	expression tag	UNP Q90VU7
K	208	HIS	-	expression tag	UNP Q90VU7
K	209	HIS	-	expression tag	UNP Q90VU7
K	210	HIS	-	expression tag	UNP Q90VU7
K	211	HIS	-	expression tag	UNP Q90VU7
K	212	HIS	-	expression tag	UNP Q90VU7
K	213	HIS	-	expression tag	UNP Q90VU7

- Molecule 5 is a protein called AP-1 complex subunit mu-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	415	Total	C	N	O	0	0
			1660	830	415	415		
5	J	415	Total	C	N	O	0	0
			1660	830	415	415		

- Molecule 6 is a protein called AP-1 complex subunit sigma-3.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	S	142	Total	C	N	O	0	0
			568	284	142	142		
6	O	142	Total	C	N	O	0	0
			568	284	142	142		

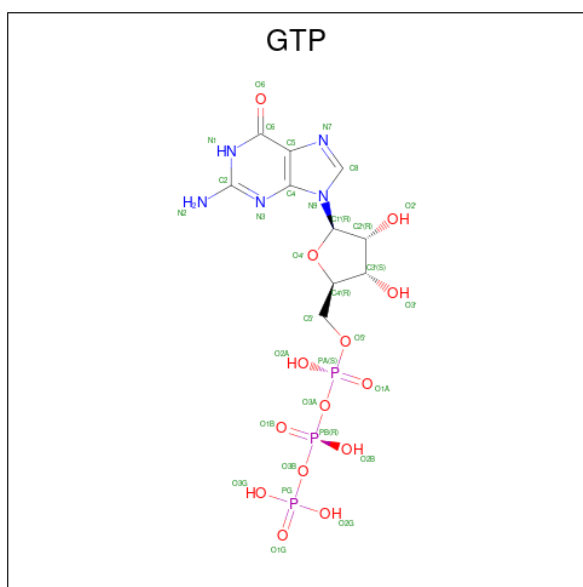
- Molecule 7 is a protein called HLA class I histocompatibility antigen, A alpha chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Y	18	Total	C	N	O	0	0
			72	36	18	18		
7	P	18	Total	C	N	O	0	0
			72	36	18	18		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	333	CYS	-	expression tag	UNP P04439
Y	345	SER	THR	engineered mutation	UNP P04439
Y	349	GLY	SER	engineered mutation	UNP P04439
Y	355	SER	GLY	engineered mutation	UNP P04439
Y	363	ALA	CYS	engineered mutation	UNP P04439
Y	366	HIS	-	expression tag	UNP P04439
Y	367	HIS	-	expression tag	UNP P04439
Y	368	HIS	-	expression tag	UNP P04439
Y	369	HIS	-	expression tag	UNP P04439
Y	370	HIS	-	expression tag	UNP P04439
Y	371	HIS	-	expression tag	UNP P04439
P	333	CYS	-	expression tag	UNP P04439
P	345	SER	THR	engineered mutation	UNP P04439
P	349	GLY	SER	engineered mutation	UNP P04439
P	355	SER	GLY	engineered mutation	UNP P04439
P	363	ALA	CYS	engineered mutation	UNP P04439
P	366	HIS	-	expression tag	UNP P04439
P	367	HIS	-	expression tag	UNP P04439
P	368	HIS	-	expression tag	UNP P04439
P	369	HIS	-	expression tag	UNP P04439
P	370	HIS	-	expression tag	UNP P04439
P	371	HIS	-	expression tag	UNP P04439

- Molecule 8 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
8	H	1	Total	C	N	O	P	0
			32	10	5	14	3	
8	Z	1	Total	C	N	O	P	0
			32	10	5	14	3	
8	D	1	Total	C	N	O	P	0
			32	10	5	14	3	
8	F	1	Total	C	N	O	P	0
			32	10	5	14	3	
8	Q	1	Total	C	N	O	P	0
			32	10	5	14	3	

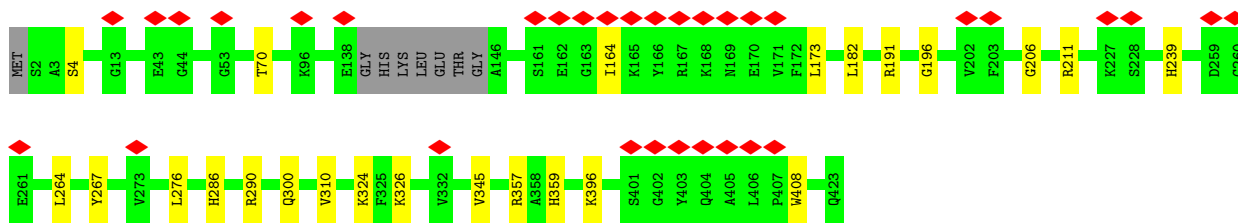
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
9	C	1	Total	Mg	0
			1	1	
9	H	1	Total	Mg	0
			1	1	
9	Z	1	Total	Mg	0
			1	1	
9	D	1	Total	Mg	0
			1	1	
9	F	1	Total	Mg	0
			1	1	

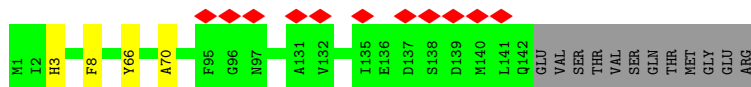
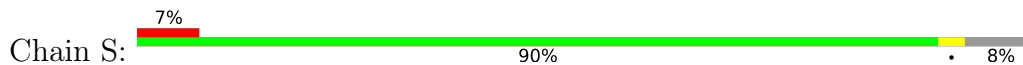
Continued on next page...

Continued from previous page...

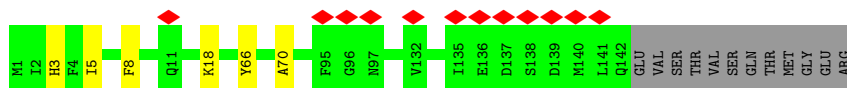
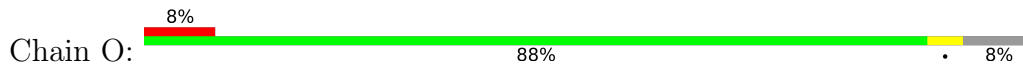
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
9	Q	1	1	1	0



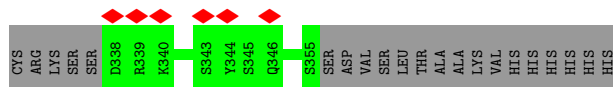
• Molecule 6: AP-1 complex subunit sigma-3



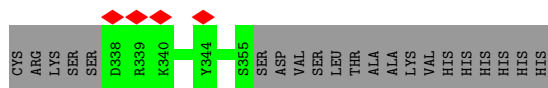
• Molecule 6: AP-1 complex subunit sigma-3



• Molecule 7: HLA class I histocompatibility antigen, A alpha chain



• Molecule 7: HLA class I histocompatibility antigen, A alpha chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of subtomograms used	5094	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF was estimated on a per-tilt basis in IMOD (4.11) using CTFPLOTTER. The results were used as input to NOVACTF during 3DCTF correction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	123	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	42000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	13.122	Depositor
Minimum map value	-11.100	Depositor
Average map value	0.056	Depositor
Map value standard deviation	1.403	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	302.4, 302.4, 302.4	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.1, 2.1, 2.1	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.22	0/2279	0.39	0/2847
1	B	0.22	0/2279	0.39	0/2847
2	C	0.23	0/719	0.46	0/897
2	D	0.23	0/719	0.46	0/897
2	F	0.23	0/719	0.46	0/897
2	H	0.23	0/719	0.46	0/897
2	Q	0.23	0/719	0.46	0/897
2	Z	0.23	0/719	0.46	0/897
3	E	0.22	0/2339	0.39	0/2922
3	G	0.22	0/2339	0.39	0/2922
4	I	0.24	0/39	0.46	0/47
4	K	0.24	0/545	0.44	0/676
4	L	0.23	0/39	0.45	0/47
4	N	0.24	0/545	0.44	0/676
5	J	0.24	0/1658	0.51	0/2069
5	M	0.24	0/1658	0.51	0/2069
6	O	0.22	0/567	0.44	0/707
6	S	0.22	0/567	0.44	0/707
7	P	0.23	0/71	0.50	0/87
7	Y	0.24	0/71	0.50	0/87
All	All	0.23	0/19310	0.44	0/24092

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	2280	0	564	0	0
1	B	2280	0	564	0	0
2	C	720	0	204	1	0
2	D	720	0	204	0	0
2	F	720	0	204	1	0
2	H	720	0	204	1	0
2	Q	720	0	204	1	0
2	Z	720	0	204	1	0
3	E	2340	0	621	0	0
3	G	2340	0	621	0	0
4	I	40	0	10	0	0
4	K	548	0	139	2	0
4	L	40	0	10	0	0
4	N	548	0	139	2	0
5	J	1660	0	437	12	0
5	M	1660	0	437	11	0
6	O	568	0	153	3	0
6	S	568	0	153	2	0
7	P	72	0	23	0	0
7	Y	72	0	23	0	0
8	C	32	0	12	1	0
8	D	32	0	12	1	0
8	F	32	0	12	1	0
8	H	32	0	12	1	0
8	Q	32	0	12	1	0
8	Z	32	0	12	1	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	F	1	0	0	0	0
9	H	1	0	0	0	0
9	Q	1	0	0	0	0
9	Z	1	0	0	0	0
All	All	19534	0	5190	43	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 2.

All (43) 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)
5:J:164:ILE:O	5:J:206:GLY:N	2.34	0.60
5:M:164:ILE:O	5:M:206:GLY:N	2.34	0.57
6:O:3:HIS:N	6:O:70:ALA:O	2.38	0.55
8:H:1001:GTP:H2'	8:H:1001:GTP:N3	2.27	0.50
8:Q:1001:GTP:H2'	8:Q:1001:GTP:N3	2.27	0.50
5:J:196:GLY:N	5:J:267:TYR:O	2.45	0.50
5:J:182:LEU:N	5:J:191:ARG:O	2.44	0.49
5:M:196:GLY:N	5:M:267:TYR:O	2.45	0.49
8:Z:1001:GTP:N3	8:Z:1001:GTP:H2'	2.27	0.49
8:D:1001:GTP:H2'	8:D:1001:GTP:N3	2.27	0.49
8:C:1001:GTP:N3	8:C:1001:GTP:H2'	2.27	0.49
6:S:3:HIS:N	6:S:70:ALA:O	2.38	0.49
8:F:1001:GTP:H2'	8:F:1001:GTP:N3	2.27	0.49
5:J:324:LYS:N	5:J:359:HIS:O	2.42	0.48
5:M:173:LEU:N	5:M:408:TRP:O	2.39	0.48
5:M:182:LEU:N	5:M:191:ARG:O	2.44	0.48
5:J:211:ARG:N	5:J:396:LYS:O	2.48	0.46
4:K:134:ARG:N	4:K:145:LEU:O	2.41	0.46
5:J:326:LYS:O	5:J:357:ARG:N	2.49	0.46
5:M:211:ARG:N	5:M:396:LYS:O	2.48	0.46
5:J:173:LEU:N	5:J:408:TRP:O	2.38	0.46
5:M:326:LYS:O	5:M:357:ARG:N	2.49	0.45
4:N:134:ARG:N	4:N:145:LEU:O	2.41	0.45
5:M:239:HIS:N	5:M:264:LEU:O	2.50	0.44
5:M:235:ASP:N	5:M:268:ARG:O	2.43	0.44
5:M:324:LYS:N	5:M:359:HIS:O	2.42	0.44
5:J:310:VAL:O	5:J:345:VAL:N	2.42	0.43
5:J:239:HIS:N	5:J:264:LEU:O	2.50	0.43
4:K:128:THR:N	4:K:135:TYR:O	2.52	0.43
6:S:8:PHE:O	6:S:66:TYR:N	2.44	0.42
5:J:4:SER:N	5:J:70:THR:O	2.53	0.42
2:Z:71:GLN:O	2:Z:75:ARG:N	2.52	0.42
4:N:128:THR:N	4:N:135:TYR:O	2.52	0.42
5:M:4:SER:N	5:M:70:THR:O	2.52	0.41
2:Q:71:GLN:O	2:Q:75:ARG:N	2.52	0.41
2:C:71:GLN:O	2:C:75:ARG:N	2.52	0.41
2:H:71:GLN:O	2:H:75:ARG:N	2.52	0.41
2:F:71:GLN:O	2:F:75:ARG:N	2.52	0.41
5:J:276:LEU:O	5:J:300:GLN:N	2.54	0.41
5:J:286:HIS:N	5:J:290:ARG:O	2.46	0.41
6:O:8:PHE:O	6:O:66:TYR:N	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:286:HIS:N	5:M:290:ARG:O	2.46	0.40
6:O:5:ILE:O	6:O:18:LYS:N	2.53	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	568/949 (60%)	557 (98%)	11 (2%)	0	100	100
1	B	568/949 (60%)	557 (98%)	11 (2%)	0	100	100
2	C	178/181 (98%)	177 (99%)	1 (1%)	0	100	100
2	D	178/181 (98%)	177 (99%)	1 (1%)	0	100	100
2	F	178/181 (98%)	177 (99%)	1 (1%)	0	100	100
2	H	178/181 (98%)	177 (99%)	1 (1%)	0	100	100
2	Q	178/181 (98%)	177 (99%)	1 (1%)	0	100	100
2	Z	178/181 (98%)	177 (99%)	1 (1%)	0	100	100
3	E	583/601 (97%)	579 (99%)	4 (1%)	0	100	100
3	G	583/601 (97%)	579 (99%)	4 (1%)	0	100	100
4	I	8/213 (4%)	8 (100%)	0	0	100	100
4	K	131/213 (62%)	131 (100%)	0	0	100	100
4	L	8/213 (4%)	8 (100%)	0	0	100	100
4	N	131/213 (62%)	131 (100%)	0	0	100	100
5	J	411/423 (97%)	409 (100%)	2 (0%)	0	100	100
5	M	411/423 (97%)	409 (100%)	2 (0%)	0	100	100
6	O	140/154 (91%)	139 (99%)	1 (1%)	0	100	100
6	S	140/154 (91%)	139 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	P	16/39 (41%)	16 (100%)	0	0	100	100
7	Y	16/39 (41%)	16 (100%)	0	0	100	100
All	All	4782/6270 (76%)	4740 (99%)	42 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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
8	GTP	Z	1001	9	26,34,34	1.11	2 (7%)	32,54,54	1.56	7 (21%)
8	GTP	F	1001	9	26,34,34	1.11	2 (7%)	32,54,54	1.56	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GTP	H	1001	9	26,34,34	1.11	2 (7%)	32,54,54	1.56	7 (21%)
8	GTP	C	1001	9	26,34,34	1.11	2 (7%)	32,54,54	1.56	7 (21%)
8	GTP	Q	1001	9	26,34,34	1.11	2 (7%)	32,54,54	1.56	7 (21%)
8	GTP	D	1001	9	26,34,34	1.11	2 (7%)	32,54,54	1.56	7 (21%)

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
8	GTP	Z	1001	9	-	4/18/38/38	0/3/3/3
8	GTP	F	1001	9	-	4/18/38/38	0/3/3/3
8	GTP	H	1001	9	-	4/18/38/38	0/3/3/3
8	GTP	C	1001	9	-	4/18/38/38	0/3/3/3
8	GTP	Q	1001	9	-	4/18/38/38	0/3/3/3
8	GTP	D	1001	9	-	4/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	1001	GTP	C5-C6	-3.99	1.39	1.47
8	C	1001	GTP	C5-C6	-3.99	1.39	1.47
8	D	1001	GTP	C5-C6	-3.99	1.39	1.47
8	F	1001	GTP	C5-C6	-3.99	1.39	1.47
8	Q	1001	GTP	C5-C6	-3.99	1.39	1.47
8	Z	1001	GTP	C5-C6	-3.99	1.39	1.47
8	F	1001	GTP	C2-N3	2.22	1.38	1.33
8	C	1001	GTP	C2-N3	2.22	1.38	1.33
8	D	1001	GTP	C2-N3	2.22	1.38	1.33
8	Q	1001	GTP	C2-N3	2.22	1.38	1.33
8	Z	1001	GTP	C2-N3	2.22	1.38	1.33
8	H	1001	GTP	C2-N3	2.22	1.38	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1001	GTP	C5-C6-N1	3.35	119.87	113.95
8	Z	1001	GTP	C5-C6-N1	3.35	119.86	113.95
8	Q	1001	GTP	C5-C6-N1	3.35	119.86	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	1001	GTP	C5-C6-N1	3.35	119.86	113.95
8	C	1001	GTP	C5-C6-N1	3.35	119.86	113.95
8	D	1001	GTP	C5-C6-N1	3.35	119.86	113.95
8	F	1001	GTP	PA-O3A-PB	-3.26	121.63	132.83
8	Z	1001	GTP	PA-O3A-PB	-3.26	121.63	132.83
8	H	1001	GTP	PA-O3A-PB	-3.26	121.63	132.83
8	D	1001	GTP	PA-O3A-PB	-3.26	121.63	132.83
8	C	1001	GTP	PA-O3A-PB	-3.26	121.64	132.83
8	Q	1001	GTP	PA-O3A-PB	-3.26	121.64	132.83
8	H	1001	GTP	C3'-C2'-C1'	3.24	105.85	100.98
8	Z	1001	GTP	C3'-C2'-C1'	3.23	105.85	100.98
8	D	1001	GTP	C3'-C2'-C1'	3.23	105.85	100.98
8	C	1001	GTP	C3'-C2'-C1'	3.23	105.84	100.98
8	F	1001	GTP	C3'-C2'-C1'	3.23	105.84	100.98
8	Q	1001	GTP	C3'-C2'-C1'	3.23	105.84	100.98
8	H	1001	GTP	C2-N1-C6	-3.04	119.51	125.10
8	Z	1001	GTP	C2-N1-C6	-3.04	119.51	125.10
8	D	1001	GTP	C2-N1-C6	-3.03	119.51	125.10
8	Q	1001	GTP	C2-N1-C6	-3.03	119.51	125.10
8	C	1001	GTP	C2-N1-C6	-3.03	119.51	125.10
8	F	1001	GTP	C2-N1-C6	-3.03	119.51	125.10
8	D	1001	GTP	PB-O3B-PG	-2.98	122.60	132.83
8	H	1001	GTP	PB-O3B-PG	-2.98	122.60	132.83
8	Q	1001	GTP	PB-O3B-PG	-2.98	122.60	132.83
8	C	1001	GTP	PB-O3B-PG	-2.98	122.61	132.83
8	Z	1001	GTP	PB-O3B-PG	-2.98	122.61	132.83
8	F	1001	GTP	PB-O3B-PG	-2.98	122.61	132.83
8	Q	1001	GTP	C8-N7-C5	2.92	108.56	102.99
8	H	1001	GTP	C8-N7-C5	2.92	108.56	102.99
8	F	1001	GTP	C8-N7-C5	2.92	108.56	102.99
8	D	1001	GTP	C8-N7-C5	2.92	108.55	102.99
8	C	1001	GTP	C8-N7-C5	2.92	108.55	102.99
8	Z	1001	GTP	C8-N7-C5	2.92	108.55	102.99
8	H	1001	GTP	O6-C6-C5	-2.25	119.98	124.37
8	Q	1001	GTP	O6-C6-C5	-2.25	119.98	124.37
8	C	1001	GTP	O6-C6-C5	-2.25	119.98	124.37
8	Z	1001	GTP	O6-C6-C5	-2.25	119.98	124.37
8	D	1001	GTP	O6-C6-C5	-2.25	119.98	124.37
8	F	1001	GTP	O6-C6-C5	-2.25	119.99	124.37

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1001	GTP	O4'-C4'-C5'-O5'
8	H	1001	GTP	O4'-C4'-C5'-O5'
8	Z	1001	GTP	O4'-C4'-C5'-O5'
8	D	1001	GTP	O4'-C4'-C5'-O5'
8	F	1001	GTP	O4'-C4'-C5'-O5'
8	Q	1001	GTP	O4'-C4'-C5'-O5'
8	C	1001	GTP	C3'-C4'-C5'-O5'
8	H	1001	GTP	C3'-C4'-C5'-O5'
8	Z	1001	GTP	C3'-C4'-C5'-O5'
8	D	1001	GTP	C3'-C4'-C5'-O5'
8	F	1001	GTP	C3'-C4'-C5'-O5'
8	Q	1001	GTP	C3'-C4'-C5'-O5'
8	C	1001	GTP	PB-O3A-PA-O5'
8	H	1001	GTP	PB-O3A-PA-O5'
8	Z	1001	GTP	PB-O3A-PA-O5'
8	D	1001	GTP	PB-O3A-PA-O5'
8	F	1001	GTP	PB-O3A-PA-O5'
8	Q	1001	GTP	PB-O3A-PA-O5'
8	C	1001	GTP	PA-O3A-PB-O1B
8	H	1001	GTP	PA-O3A-PB-O1B
8	Z	1001	GTP	PA-O3A-PB-O1B
8	D	1001	GTP	PA-O3A-PB-O1B
8	F	1001	GTP	PA-O3A-PB-O1B
8	Q	1001	GTP	PA-O3A-PB-O1B

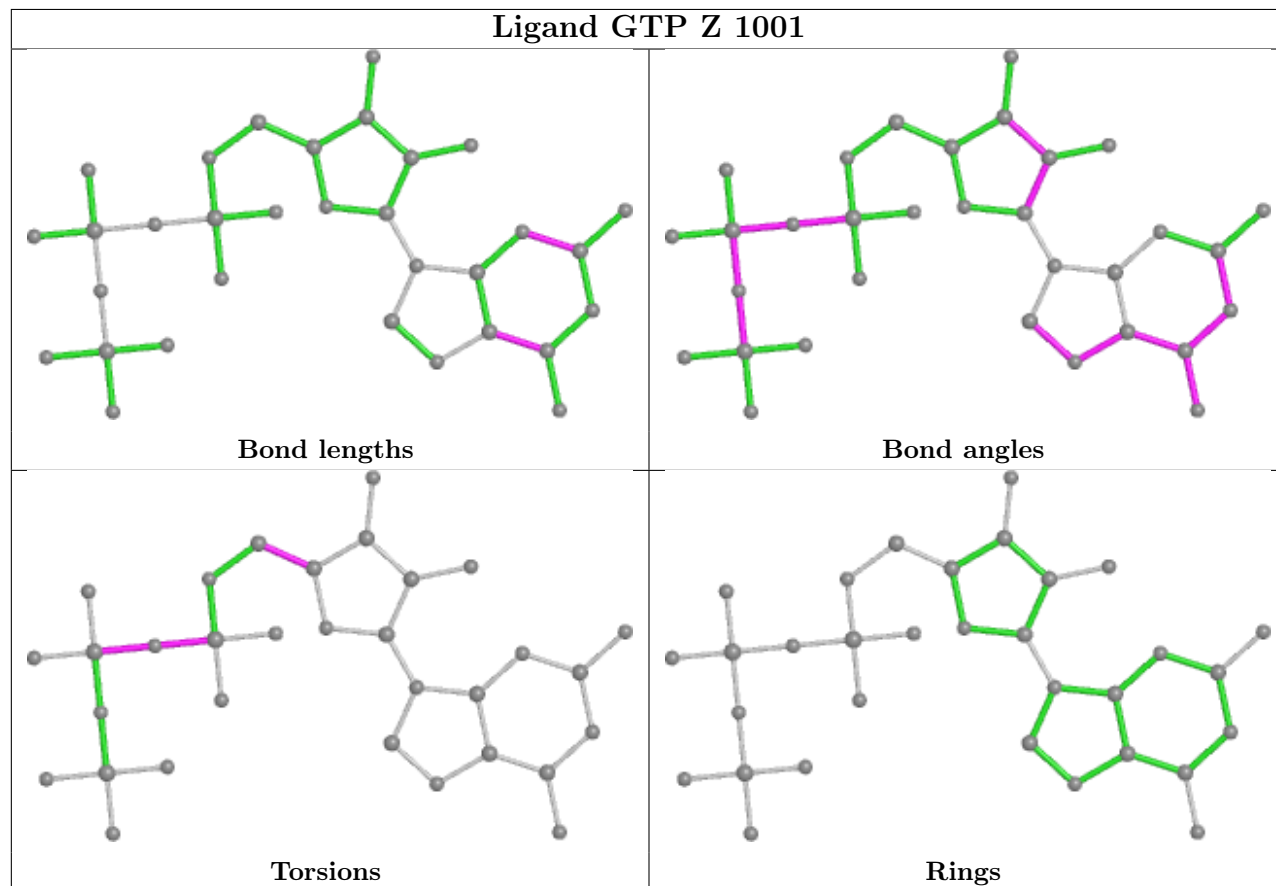
There are no ring outliers.

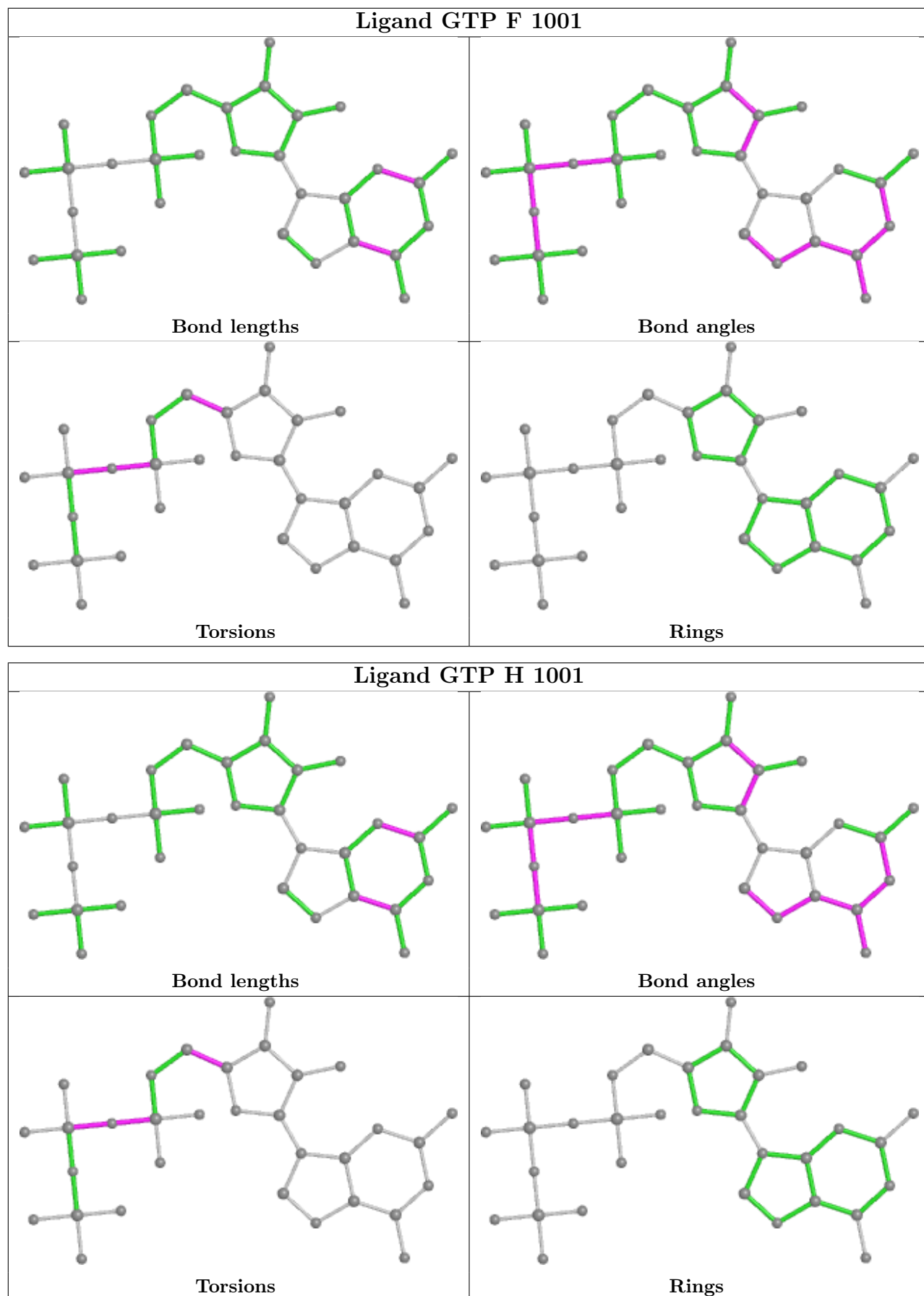
6 monomers are involved in 6 short contacts:

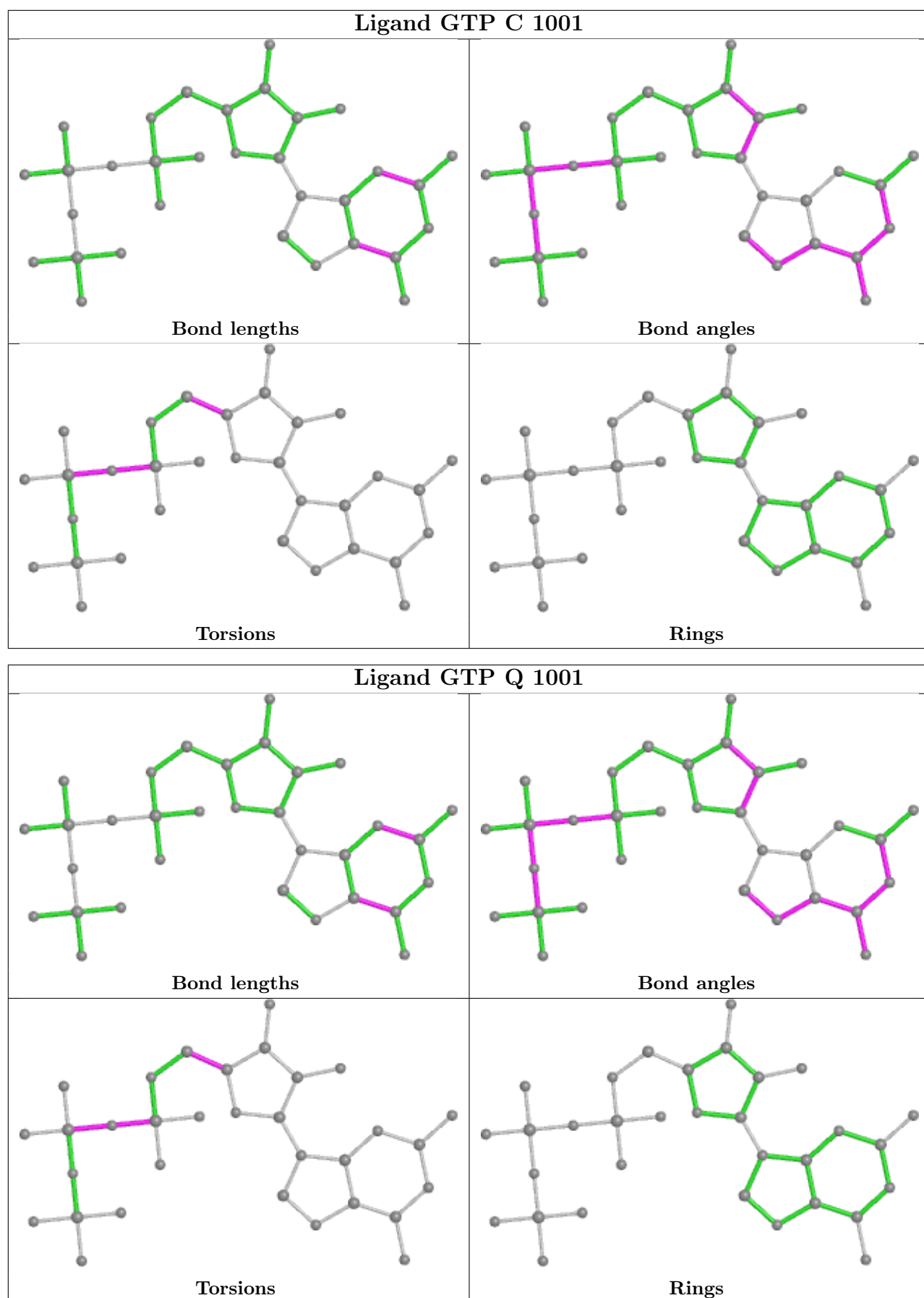
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	Z	1001	GTP	1	0
8	F	1001	GTP	1	0
8	H	1001	GTP	1	0
8	C	1001	GTP	1	0
8	Q	1001	GTP	1	0
8	D	1001	GTP	1	0

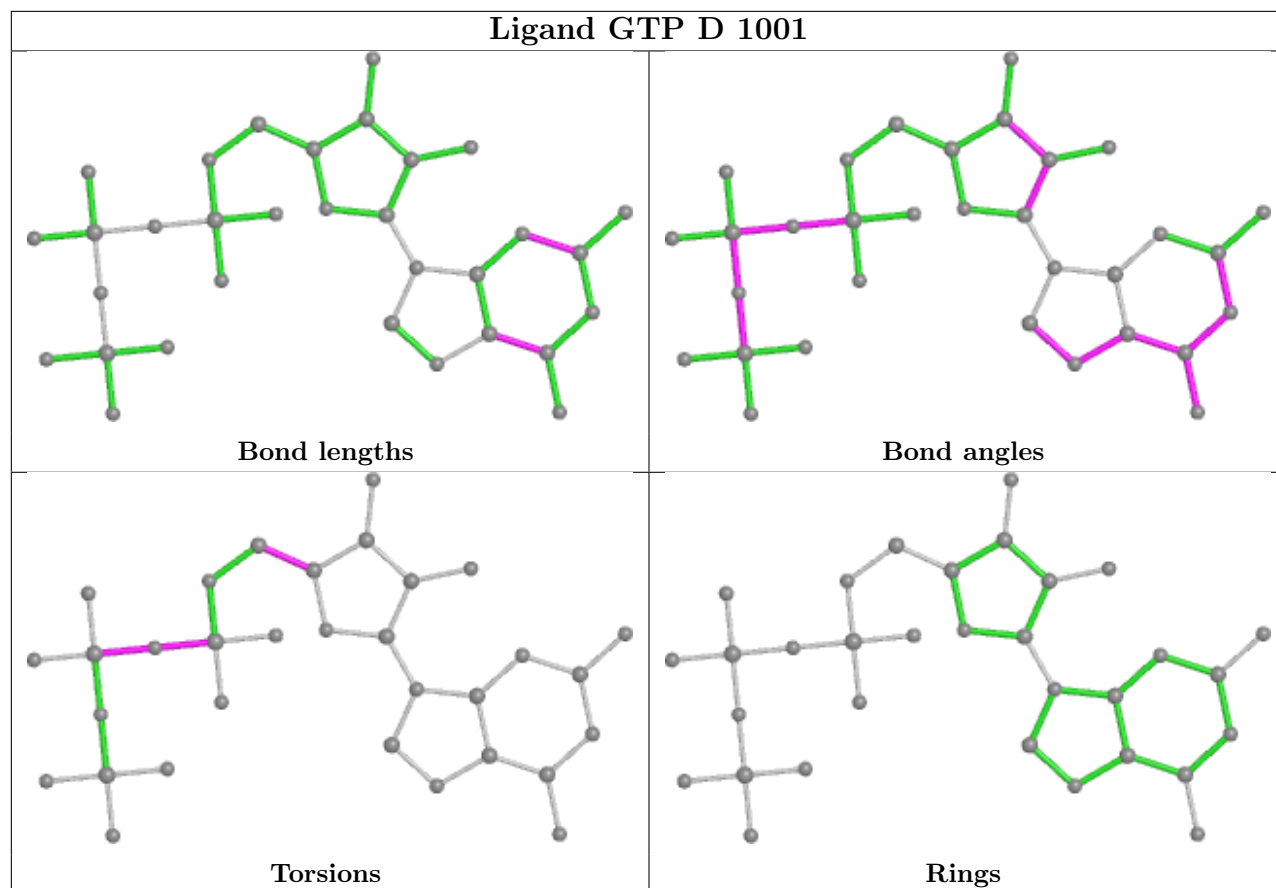
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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-27185. 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](#)

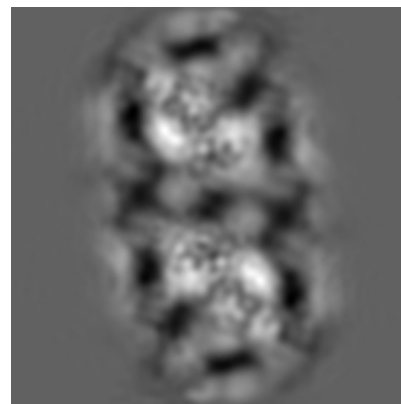
6.1.1 Primary map



X



Y

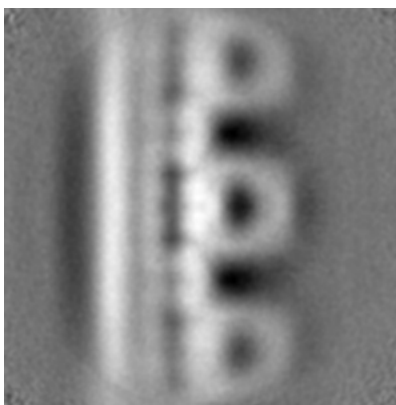


Z

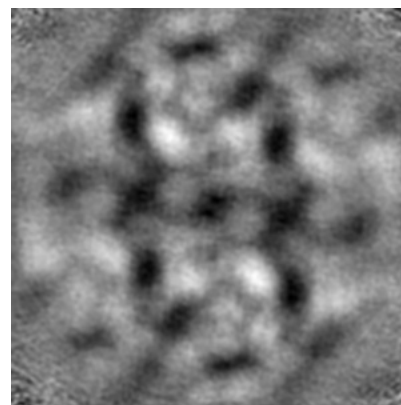
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

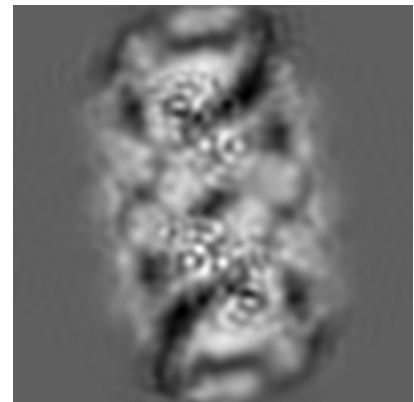
6.2.1 Primary map



X Index: 72

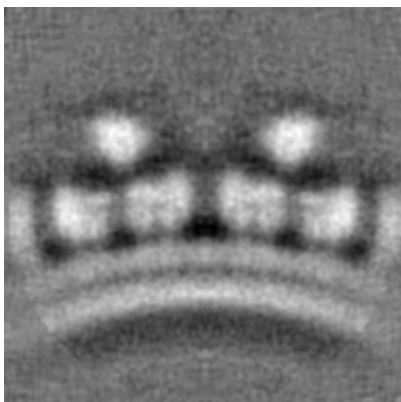


Y Index: 72

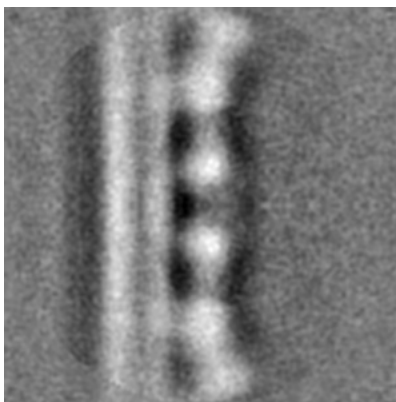


Z Index: 72

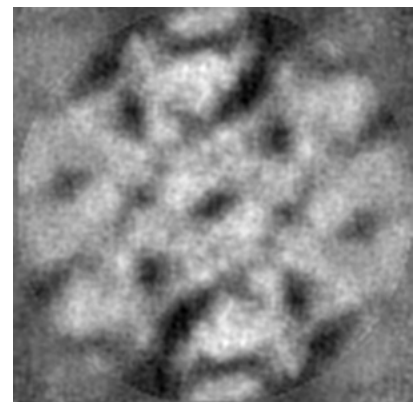
6.2.2 Raw map



X Index: 72



Y Index: 72



Z Index: 72

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

6.3 Largest variance slices [i](#)

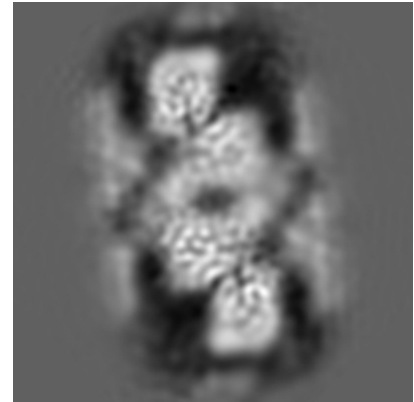
6.3.1 Primary map



X Index: 69

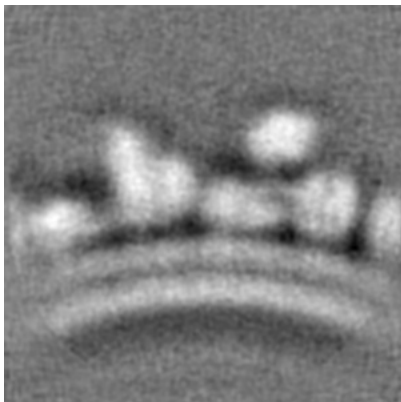


Y Index: 99

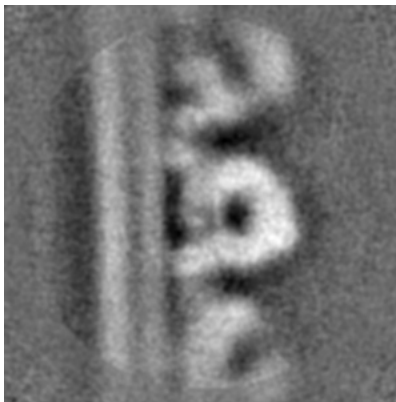


Z Index: 76

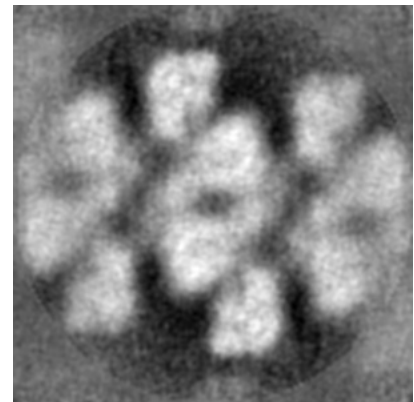
6.3.2 Raw map



X Index: 64



Y Index: 99



Z Index: 77

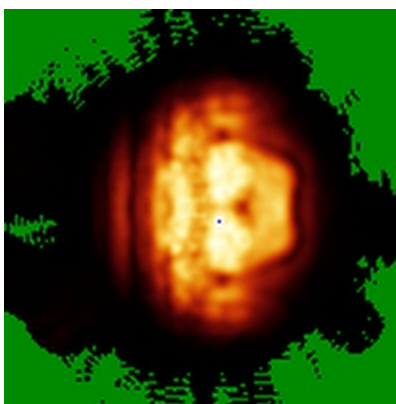
The images above show the largest variance slices of the map in three orthogonal directions.

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

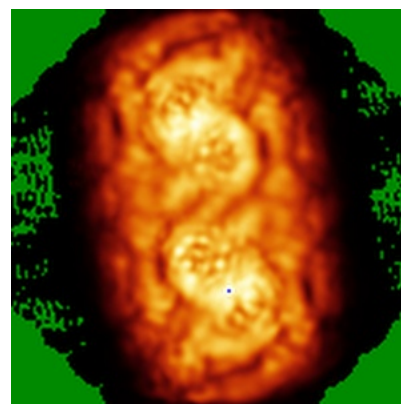
6.4.1 Primary map



X

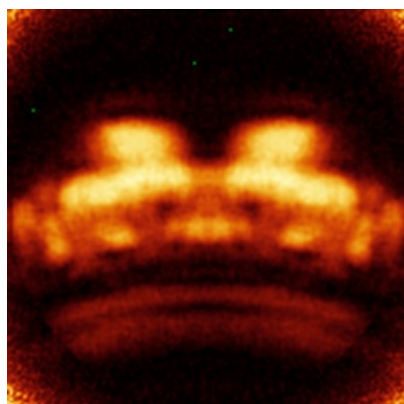


Y

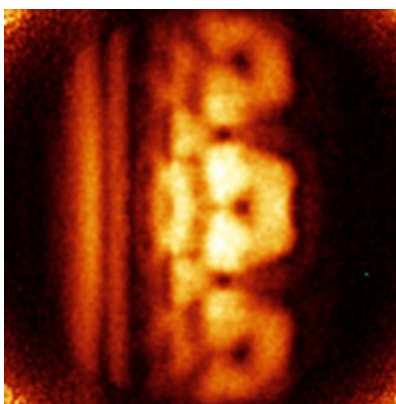


Z

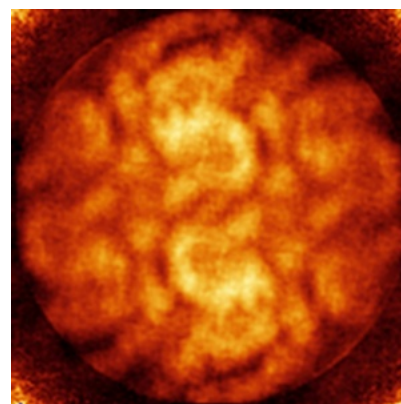
6.4.2 Raw map



X



Y

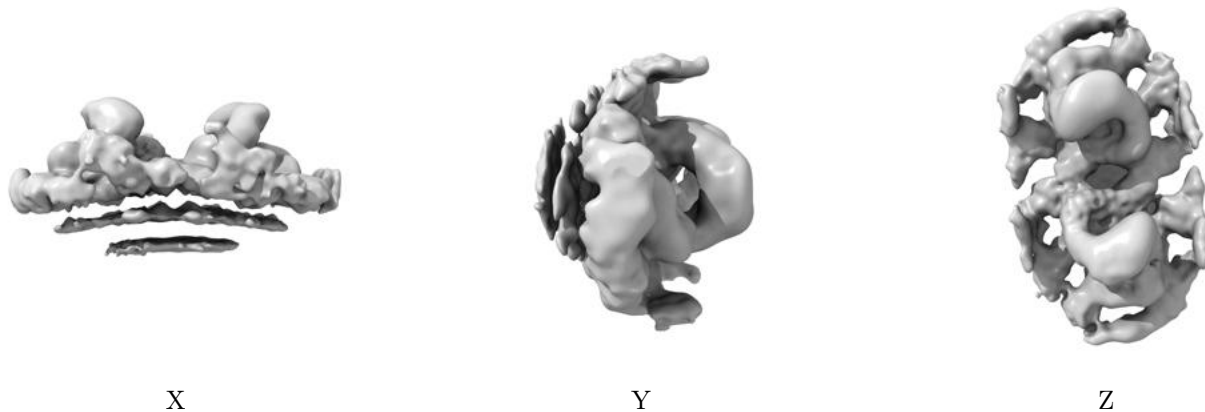


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

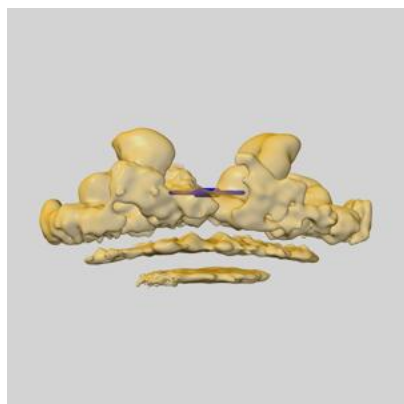
6.6 Mask visualisation [i](#)

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

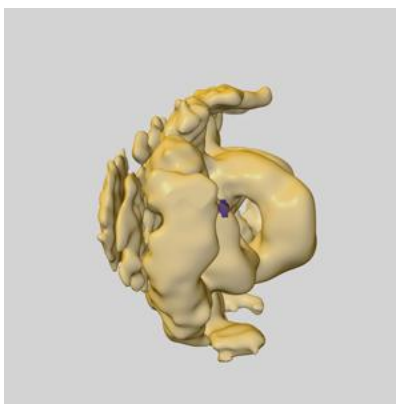
A mask typically either:

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

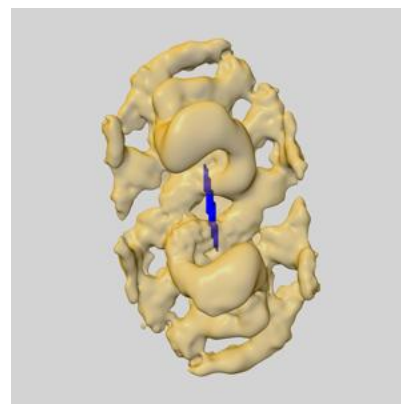
6.6.1 emd_27185_msk_1.map [i](#)



X



Y

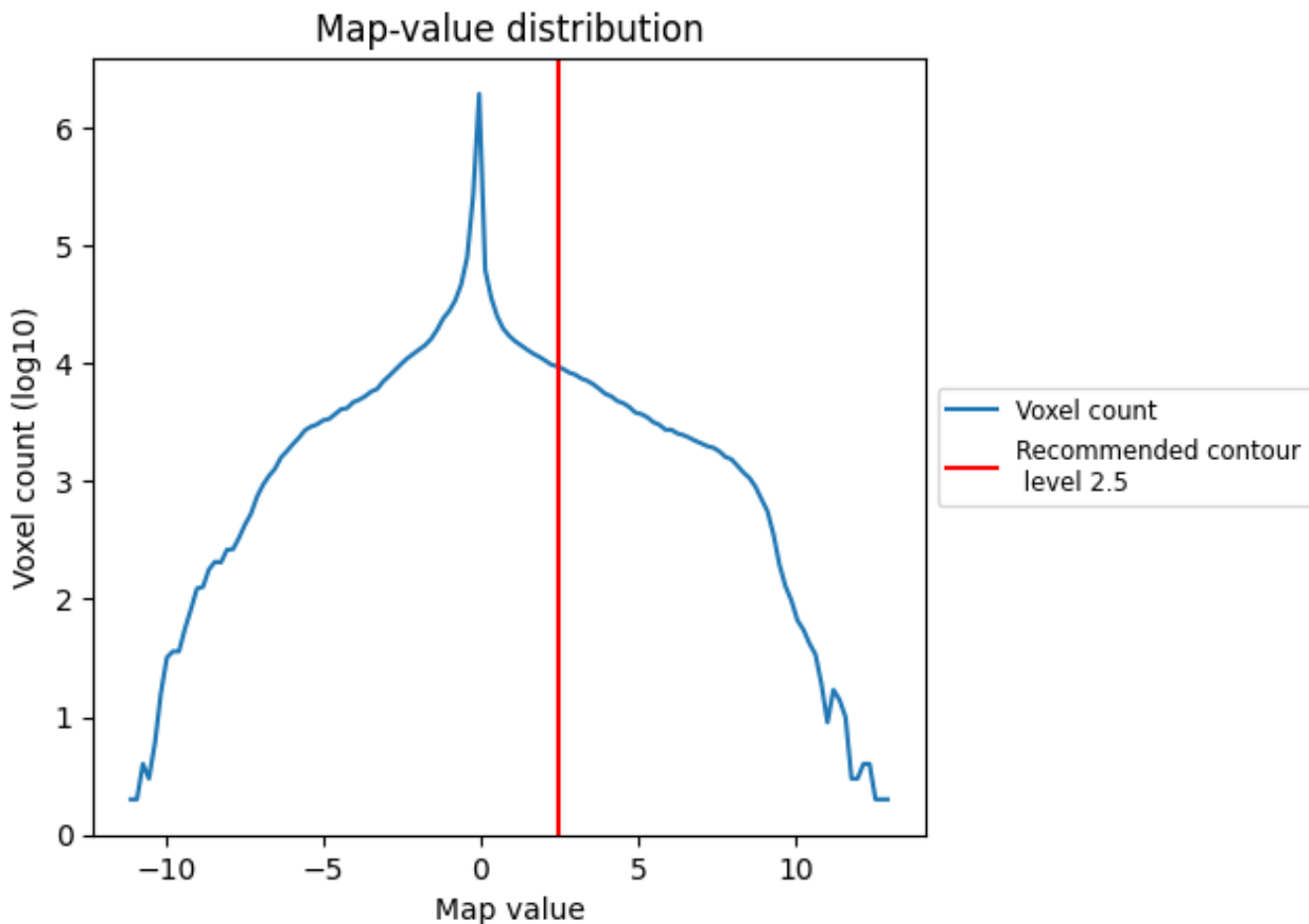


Z

7 Map analysis [i](#)

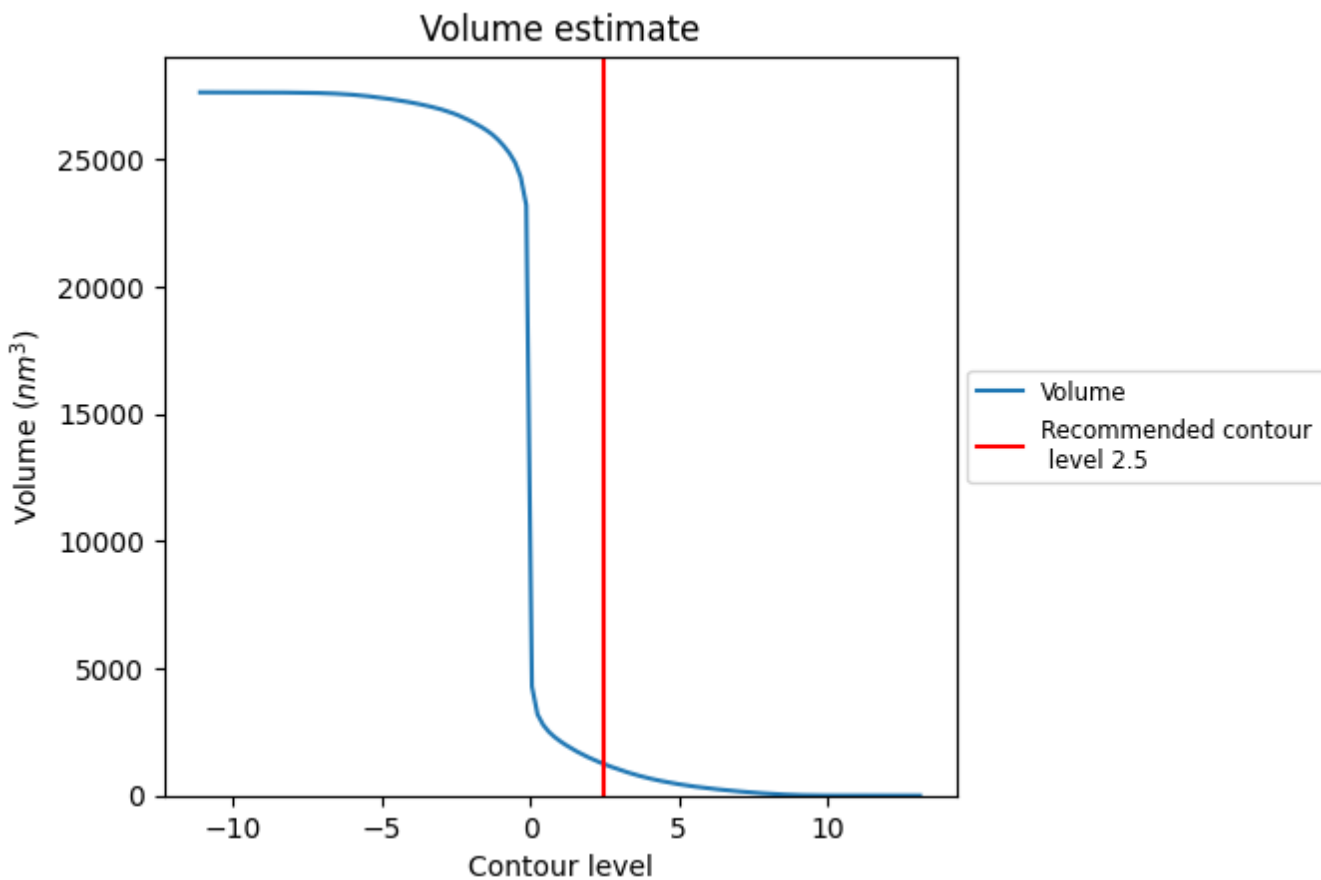
This section contains the results of statistical analysis of the map.

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.

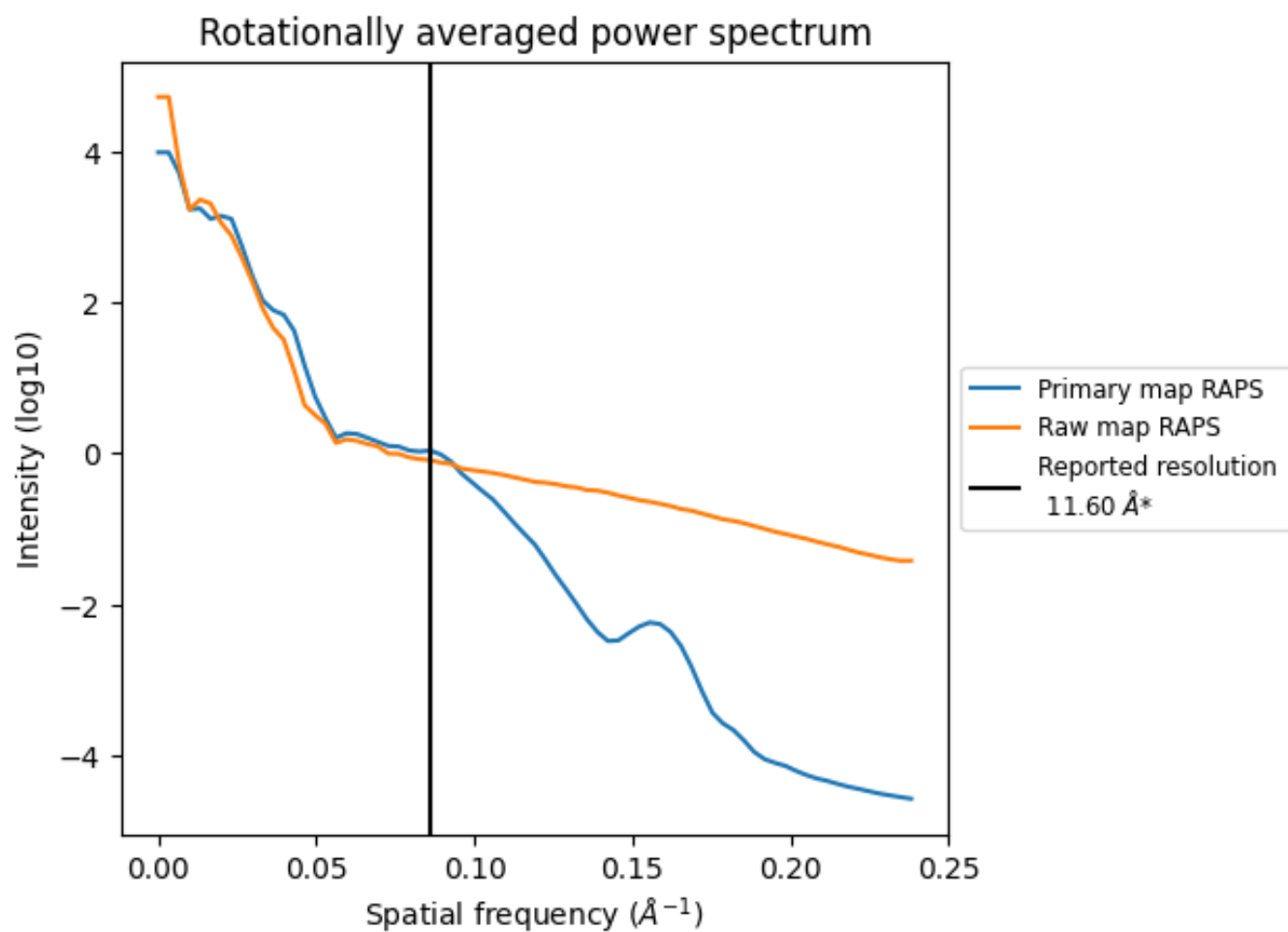
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1237 nm³; this corresponds to an approximate mass of 1118 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

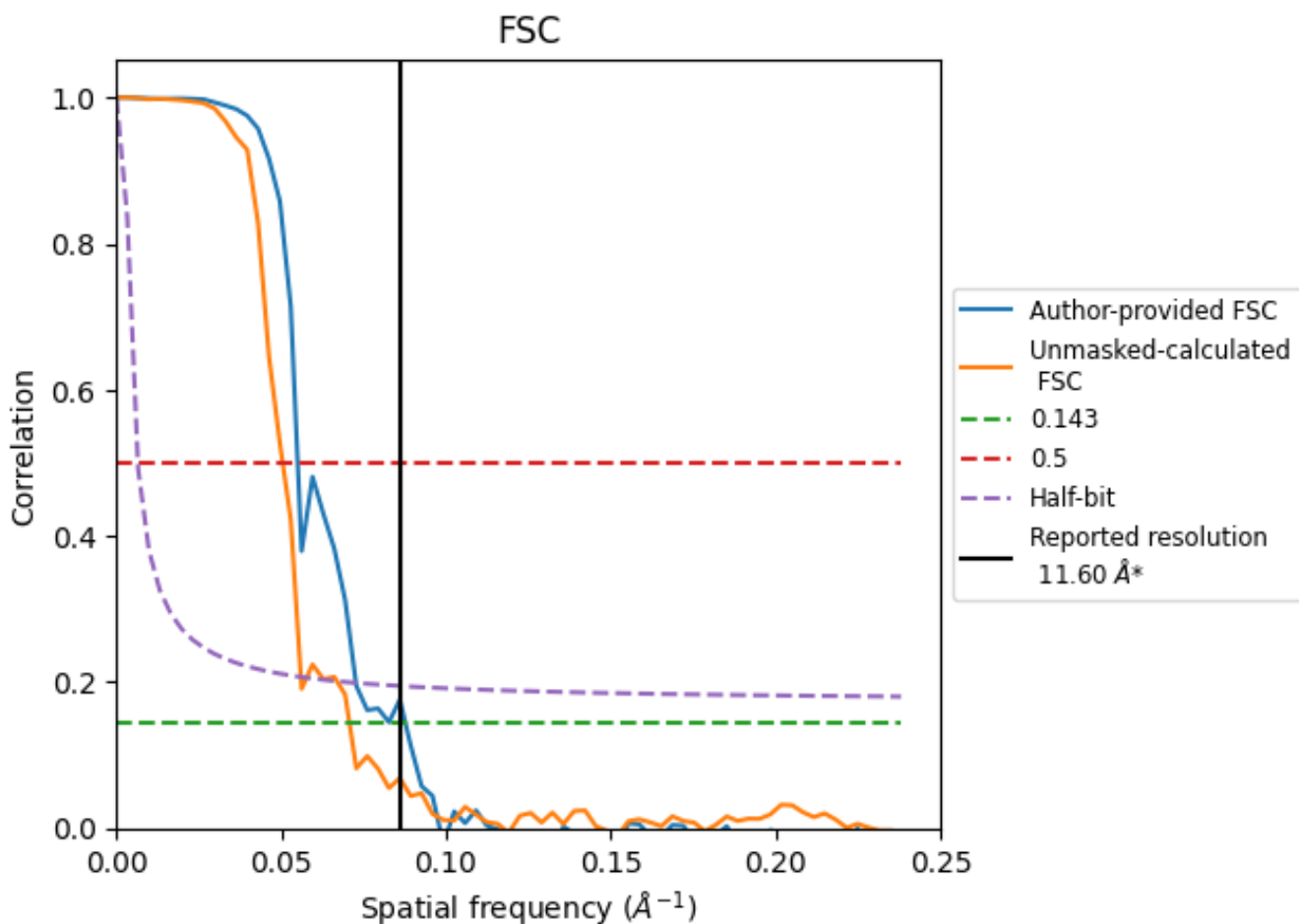


*Reported resolution corresponds to spatial frequency of 0.086 Å⁻¹

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 0.086 Å⁻¹

8.2 Resolution estimates [i](#)

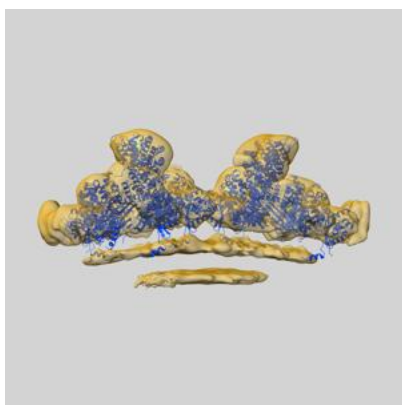
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	11.60	-	-
Author-provided FSC curve	11.40	18.18	13.76
Unmasked-calculated*	14.14	19.80	17.86

*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 14.14 differs from the reported value 11.6 by more than 10 %

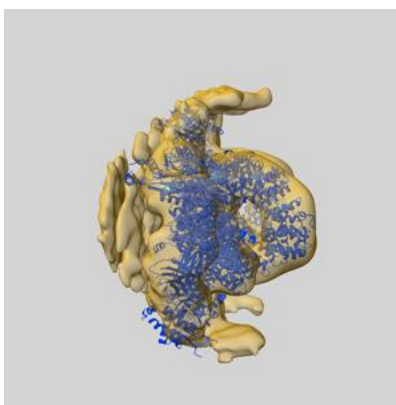
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27185 and PDB model 8D4G. Per-residue inclusion information can be found in section 3 on page 10.

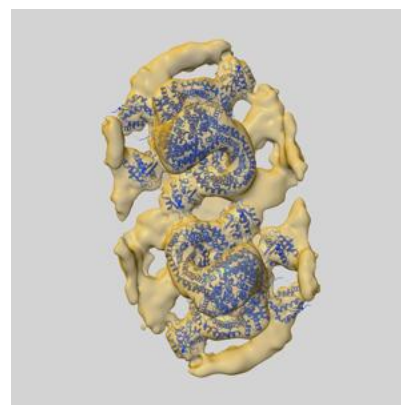
9.1 Map-model overlay [i](#)



X



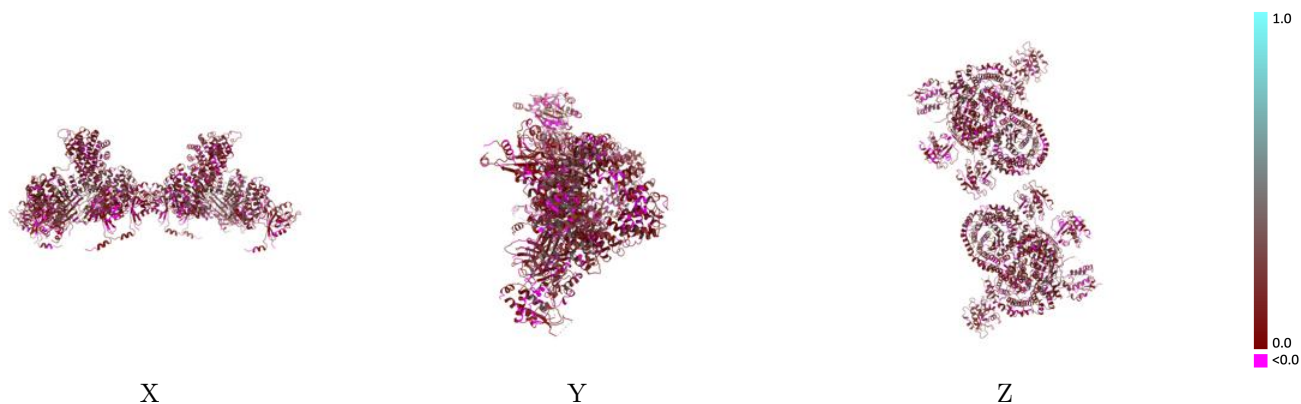
Y



Z

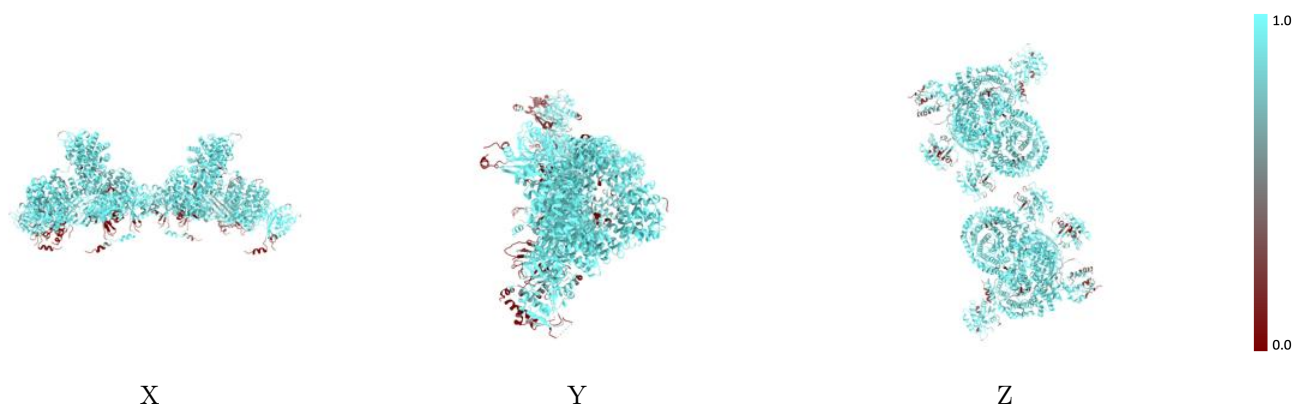
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



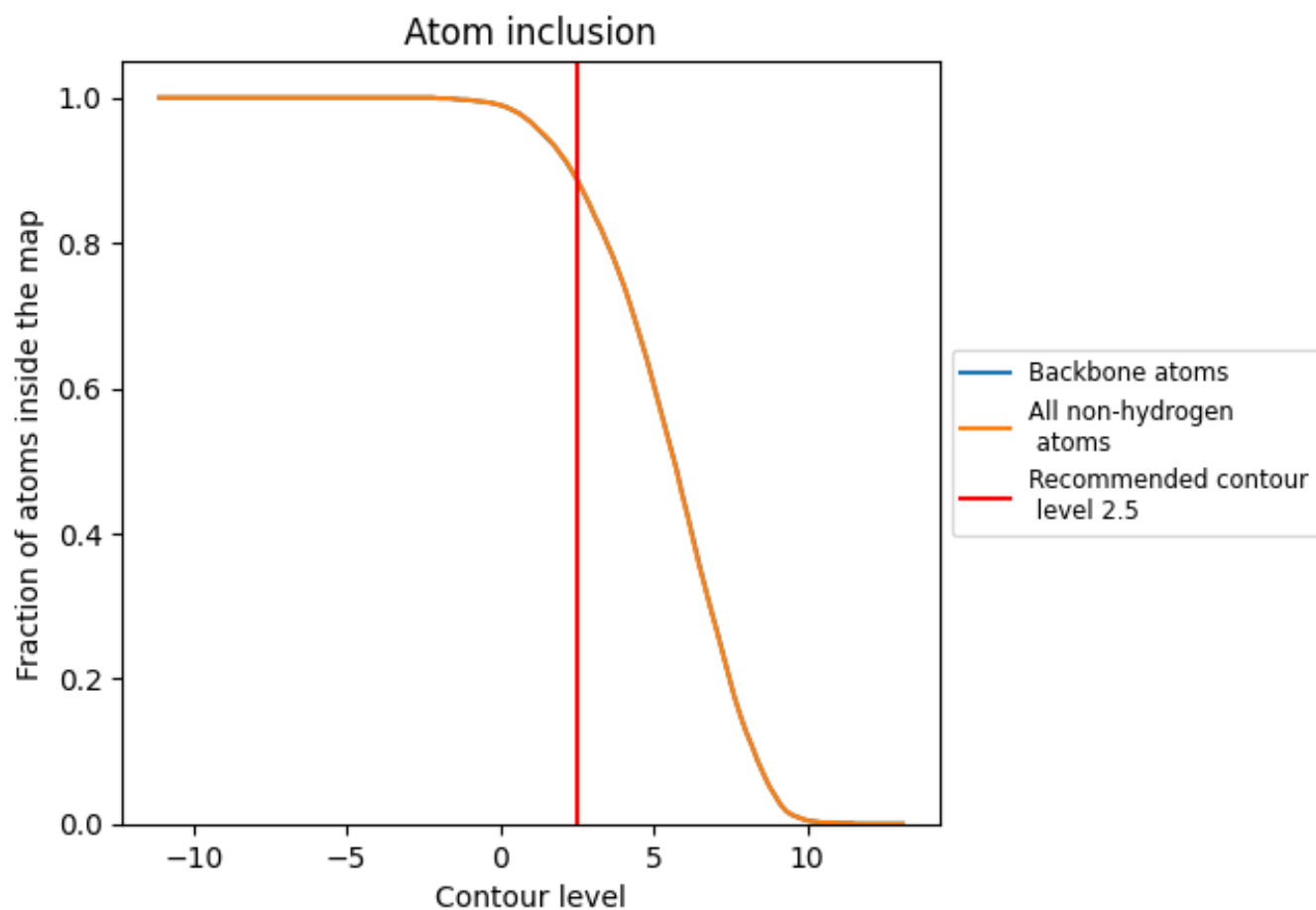
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8880	 0.1350
A	 0.9570	 0.1400
B	 0.9620	 0.1460
C	 0.8390	 0.1320
D	 0.8410	 0.1100
E	 0.9660	 0.1240
F	 0.8540	 0.0820
G	 0.9620	 0.1470
H	 0.8470	 0.0860
I	 0.9000	 0.1590
J	 0.8980	 0.1770
K	 0.6350	 0.1030
L	 0.9000	 0.1760
M	 0.9030	 0.1850
N	 0.6500	 0.1080
O	 0.8940	 0.1840
P	 0.6670	 0.0230
Q	 0.6800	 0.0590
S	 0.9150	 0.1970
Y	 0.5970	 0.0210
Z	 0.6840	 0.0700

