



## Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 10:06 am GMT

PDB ID : 6S8H  
EMDB ID : EMD-10122  
Title : Cryo-EM structure of LptB2FG in complex with LPS  
Authors : Tang, X.D.; Chang, S.H.; Luo, Q.H.; Zhang, Z.Y.; Qiao, W.; Xu, C.H.; Zhang, C.B.; Niu, Y.; Yang, W.X.; Wang, T.; Zhang, Z.B.; Zhu, X.F.; Dong, C.J.; Zhang, X.; Dong, H.H.  
Deposited on : 2019-07-10  
Resolution : 3.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

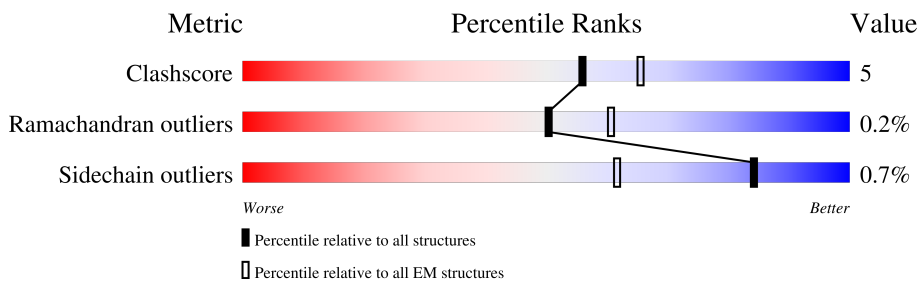
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	241	
1	B	241	
2	F	366	
3	G	360	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7818 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 Lipopolysaccharide ABC transporter, ATP-binding protein LptB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	239	1868	1168	342	353	5	0	0
1	B	238	1857	1162	338	352	5	0	0

- Molecule 2 is a protein called Lipopolysaccharide export system permease protein LptF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	239	1864	1233	303	313	15	0	0

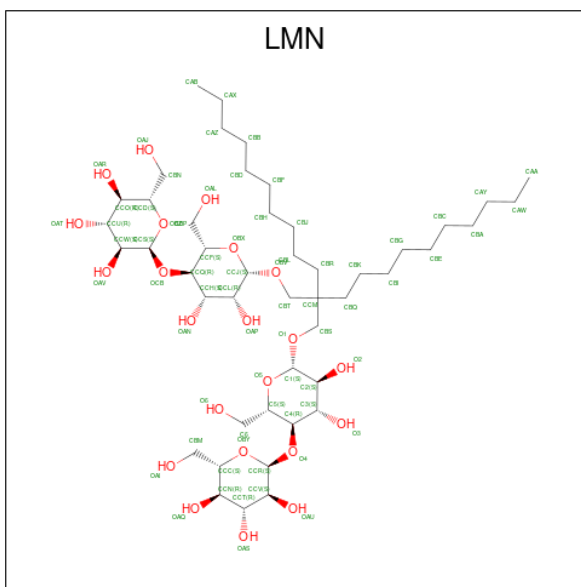
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	274	VAL	PHE	conflict	UNP P0AFA1

- Molecule 3 is a protein called Inner membrane protein yjgQ.

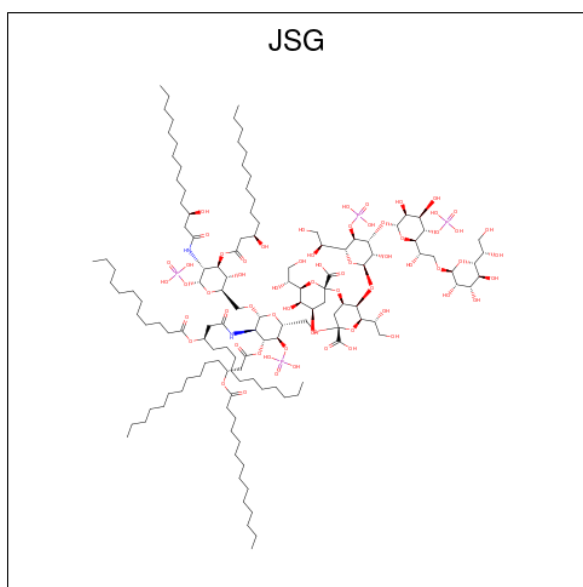
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	243	1876	1247	300	311	18	0	0

- Molecule 4 is Lauryl Maltose Neopentyl Glycol (three-letter code: LMN) (formula: C<sub>47</sub>H<sub>88</sub>O<sub>22</sub>) (labeled as "Ligand of Interest" by depositor).



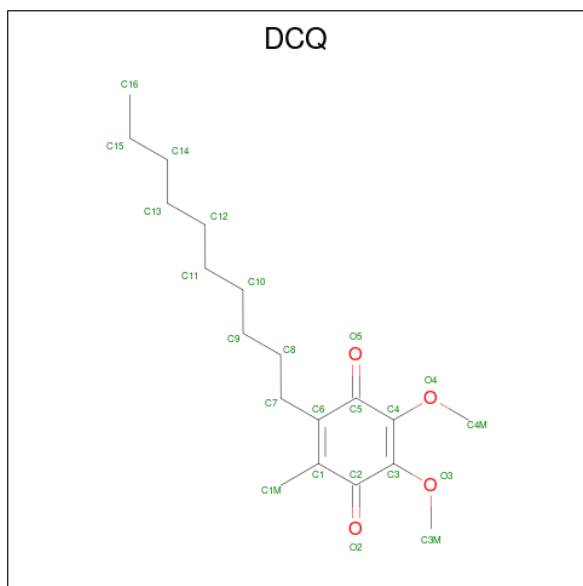
Mol	Chain	Residues	Atoms			AltConf
4	F	1	Total	C	O	0
			34	29	5	
4	G	1	Total	C	O	0
			35	29	6	

- Molecule 5 is (2 {R},4 {R},5 {R},6 {R})-6-[(1 {R})-1,2-bis(oxidanyl)ethyl]-2-[(2 {R},4 {R},5 {R},6 {R})-6-[(1 {R})-1,2-bis(oxidanyl)ethyl]-5-[(2 {S},3 {S},4 {R},5 {R},6 {R})-6-[(1 {S})-1,2-bis(oxidanyl)ethyl]-4-[(2 {R},3 {S},4 {R},5 {S},6 {R})-6-[(1 {S})-2-[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-[(1 {S})-1,2-bis(oxidanyl)ethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-1-oxidanyl-ethyl]-3,4-bis(oxidanyl)-5-phosphonooxy-oxan-2-yl]oxy-3-oxidanyl-5-phosphonooxy-oxan-2-yl]oxy-2-carboxy-2-[(2 {R},3 {S},4 {R},5 {R},6 {R})-5-[(3 {R})-3-dodecanoyloxytetradecanoyl]amino]-6-[(2 {R},3 {S},4 {R},5 {R},6 {R})-3-oxidanyl-5-[(3 {R})-3-oxidanyltetradecanoyl]amino]-4-[(3 {R})-3-oxidanyltetradecanoyl]oxy-6-phosphonooxy-oxan-2-yl]methoxy-3-phosphonooxy-4-[(3 {R})-3-tetradecanoyloxytetradecanoyl]oxy-oxan-2-yl]methoxy-oxan-4-yl]oxy-4,5-bis(oxidanyl)oxane-2-carboxylic acid (three-letter code: JSG) (formula:  $C_{131}H_{240}N_2O_{63}P_4$ ) (labeled as "Ligand of Interest" by depositor).



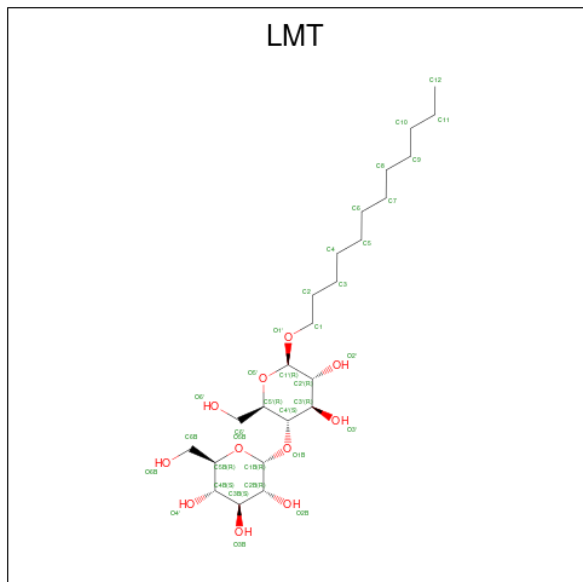
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	F	1	200	131	2	63	4	0

- Molecule 6 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (three-letter code: DCQ) (formula:  $C_{19}H_{30}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	F	1	23	19	4	0
6	G	1	23	19	4	0

- Molecule 7 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ) (labeled as "Ligand of Interest" by depositor).

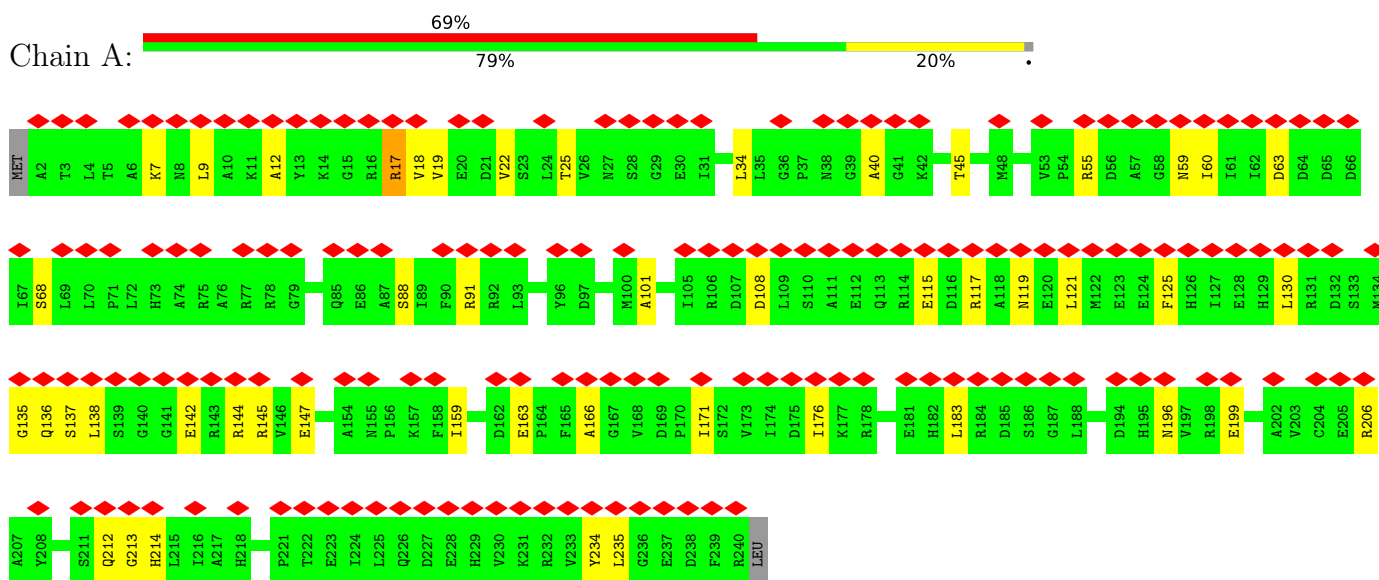


Mol	Chain	Residues	Atoms			AltConf
7	F	1	Total	C	O	0
			24	18	6	
7	G	1	Total	C	O	0
			14	13	1	

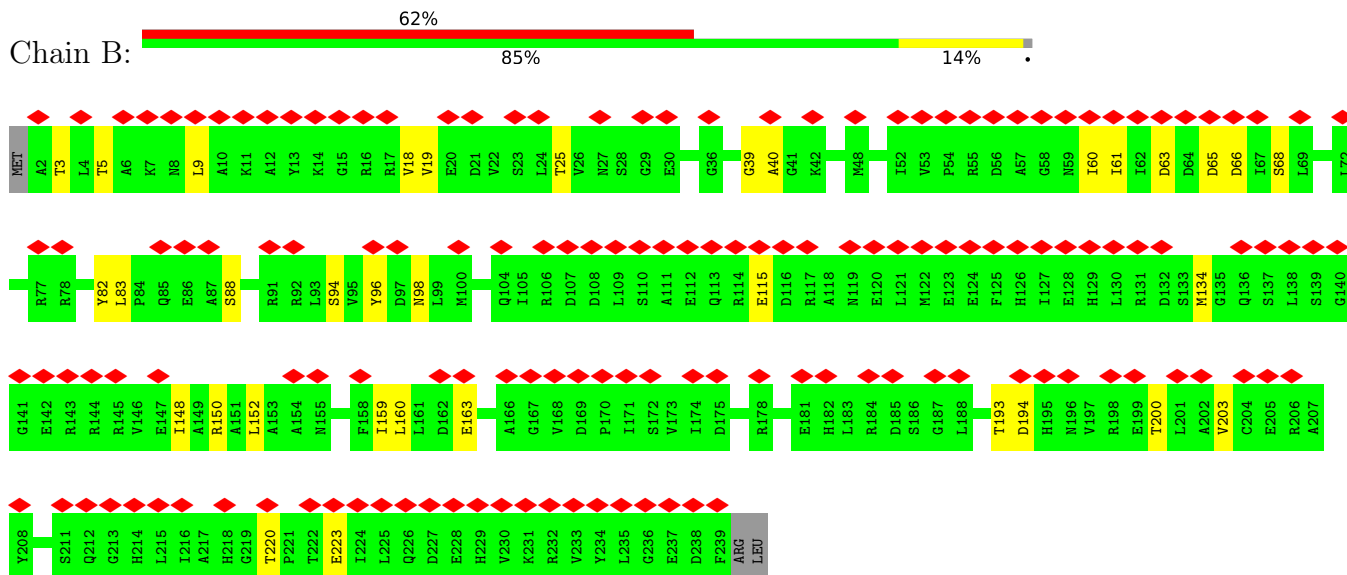
### 3 Residue-property plots

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: Lipopolysaccharide ABC transporter, ATP-binding protein LptB



- Molecule 1: Lipopolysaccharide ABC transporter, ATP-binding protein LptB



- Molecule 2: Lipopolysaccharide export system permease protein LptF





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	95887	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40, 40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.122	Depositor
Minimum map value	-0.083	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	182.52, 182.52, 182.52	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	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: LMT, LMN, JSG, DCQ

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	0.30	0/1895	0.59	2/2562 (0.1%)
1	B	0.30	0/1884	0.62	1/2548 (0.0%)
2	F	0.32	0/1899	0.67	1/2588 (0.0%)
3	G	0.32	0/1917	0.58	0/2589
All	All	0.31	0/7595	0.61	4/10287 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	160	LEU	CA-CB-CG	7.13	131.71	115.30
2	F	329	LEU	CA-CB-CG	6.51	130.27	115.30
1	A	130	LEU	CA-CB-CG	5.97	129.03	115.30
1	A	235	LEU	CA-CB-CG	5.22	127.30	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	TYR	Peptide
1	B	39	GLY	Peptide
1	B	40	ALA	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1868	0	1888	25	0
1	B	1857	0	1875	18	0
2	F	1864	0	2002	20	0
3	G	1876	0	1985	12	0
4	F	34	0	52	4	0
4	G	35	0	53	6	0
5	F	200	0	0	2	0
6	F	23	0	26	2	0
6	G	23	0	28	2	0
7	F	24	0	32	2	0
7	G	14	0	24	0	0
All	All	7818	0	7965	82	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 5.

All (82) 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)
2:F:248:GLN:HE21	2:F:263:ARG:HE	1.37	0.71
1:A:101:ALA:HB1	3:G:7:LEU:HG	1.81	0.62
1:A:25:THR:O	1:A:206:ARG:NH1	2.35	0.60
2:F:311:LEU:HD21	3:G:33:ILE:HG22	1.85	0.59
1:B:60:ILE:H	1:B:68:SER:HB2	1.68	0.58
3:G:22:THR:HG21	3:G:74:LEU:HD22	1.85	0.58
3:G:48:ASP:HA	3:G:52:ALA:HB3	1.85	0.58
1:A:40:ALA:HB1	1:A:212:GLN:H	1.68	0.58
1:B:3:THR:H	1:B:63:ASP:HB2	1.69	0.57
1:B:88:SER:O	1:B:150:ARG:NH2	2.38	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:250:SER:OG	3:G:251:ILE:N	2.38	0.55
1:A:115:GLU:O	1:A:119:ASN:ND2	2.40	0.55
1:A:12:ALA:HB2	1:A:17:ARG:HG3	1.90	0.54
1:B:65:ASP:N	1:B:65:ASP:OD1	2.41	0.54
1:A:63:ASP:OD1	1:A:63:ASP:N	2.40	0.53
1:B:83:LEU:HD21	1:B:148:ILE:HG12	1.89	0.53
1:A:125:PHE:O	1:A:145:ARG:NH2	2.43	0.52
1:A:91:ARG:HB3	1:A:136:GLN:HG2	1.93	0.51
1:B:194:ASP:OD1	1:B:194:ASP:N	2.44	0.51
4:F:401:LMN:HAWA	4:F:401:LMN:HABB	1.92	0.51
2:F:268:TRP:HA	2:F:271:THR:HG22	1.94	0.49
2:F:326:ASP:N	2:F:326:ASP:OD1	2.45	0.49
1:A:138:LEU:HB3	1:A:142:GLU:HB2	1.94	0.49
2:F:267:ASN:HA	2:F:270:ILE:HG22	1.93	0.49
2:F:89:HIS:HB3	2:F:93:LEU:HD12	1.95	0.49
3:G:277:SER:O	3:G:277:SER:OG	2.31	0.49
3:G:318:VAL:HG12	3:G:348:PHE:HZ	1.78	0.48
4:F:401:LMN:HAY	4:G:401:LMN:HBGA	1.96	0.48
1:B:9:LEU:HD11	1:B:60:ILE:HD11	1.96	0.48
1:B:94:SER:HA	1:B:134:MET:HA	1.96	0.48
1:B:163:GLU:HA	1:B:194:ASP:HB3	1.96	0.48
2:F:254:LEU:HD12	2:F:256:ASN:H	1.78	0.48
1:B:94:SER:O	1:B:98:ASN:ND2	2.48	0.47
1:A:22:VAL:HG22	1:A:214:HIS:HA	1.97	0.47
1:A:55:ARG:NH2	1:A:68:SER:OG	2.48	0.47
1:B:5:THR:HG23	1:B:25:THR:HG22	1.97	0.47
2:F:21:ILE:HG12	6:G:403:DCQ:H9A	1.96	0.47
6:F:403:DCQ:H1M	6:F:403:DCQ:H7	1.57	0.46
1:B:200:THR:HA	1:B:203:VAL:HG12	1.97	0.46
1:A:9:LEU:HD11	1:A:60:ILE:HD11	1.98	0.46
1:A:196:ASN:ND2	1:A:199:GLU:OE2	2.49	0.46
2:F:129:ASP:HB2	2:F:252:ARG:HH21	1.81	0.46
2:F:22:LEU:HA	2:F:25:ILE:HD12	1.98	0.46
1:B:152:LEU:HD13	1:B:159:ILE:HD11	1.98	0.45
4:F:401:LMN:HBI	4:G:401:LMN:HBA	1.99	0.45
3:G:74:LEU:HD21	4:G:401:LMN:HCL	1.97	0.45
1:B:18:VAL:HG23	1:B:19:VAL:HG12	1.98	0.45
1:B:82:TYR:HB3	2:F:90:ALA:HB1	1.98	0.45
1:A:137:SER:O	1:A:137:SER:OG	2.32	0.45
1:A:163:GLU:HB3	1:A:166:ALA:HB2	1.99	0.45
2:F:263:ARG:NH2	5:F:402:JSG:ODI	2.50	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:HD21	1:A:45:THR:HG23	1.98	0.45
7:F:404:LMT:O1B	7:F:404:LMT:O6'	2.30	0.43
2:F:249:MET:HG2	2:F:252:ARG:HD2	2.00	0.43
2:F:99:VAL:HG22	2:F:284:VAL:HG21	2.00	0.43
1:A:88:SER:OG	1:A:147:GLU:OE1	2.36	0.43
1:A:117:ARG:HH21	1:A:121:LEU:HD21	1.83	0.43
6:G:403:DCQ:H11A	6:G:403:DCQ:H8A	1.82	0.43
1:A:18:VAL:HG23	1:A:19:VAL:HG23	2.01	0.43
1:A:108:ASP:OD1	1:A:108:ASP:N	2.52	0.43
4:F:401:LMN:HBR	4:F:401:LMN:HBKA	1.72	0.43
1:A:144:ARG:HE	1:A:176:ILE:HD11	1.84	0.42
2:F:272:LEU:HA	2:F:275:THR:HG22	2.01	0.42
2:F:85:ILE:HA	2:F:88:MET:HB2	2.00	0.42
3:G:310:VAL:HA	3:G:313:ILE:HG22	2.00	0.42
2:F:14:SER:HB2	6:F:403:DCQ:H4MB	2.02	0.42
1:B:96:TYR:OH	1:B:115:GLU:OE1	2.37	0.42
1:A:135:GLY:HA2	1:A:138:LEU:HG	2.01	0.42
2:F:47:LEU:O	2:F:51:LEU:N	2.35	0.42
3:G:98:THR:OG1	3:G:99:ARG:N	2.53	0.41
1:B:220:THR:HB	1:B:223:GLU:HG3	2.02	0.41
1:A:7:LYS:HB2	1:A:59:ASN:HB3	2.02	0.41
1:A:159:ILE:HD13	1:A:183:LEU:HD21	2.03	0.41
7:F:404:LMT:H41	3:G:307:VAL:HG13	2.03	0.41
2:F:56:VAL:HA	2:F:59:MET:HG2	2.03	0.41
1:A:171:ILE:HD12	1:A:171:ILE:HA	1.95	0.41
2:F:124:SER:O	2:F:128:GLN:N	2.54	0.41
4:G:401:LMN:HCL	4:G:401:LMN:HBTA	1.83	0.40
4:G:401:LMN:HBFB	4:G:401:LMN:HBLA	1.71	0.40
5:F:402:JSG:OBU	5:F:402:JSG:OBY	2.39	0.40
1:B:61:ILE:HG22	1:B:66:ASP:HA	2.04	0.40
3:G:313:ILE:HD13	4:G:401:LMN:HBP	2.04	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	237/241 (98%)	208 (88%)	28 (12%)	1 (0%)	34	69
1	B	236/241 (98%)	212 (90%)	24 (10%)	0	100	100
2	F	235/366 (64%)	212 (90%)	22 (9%)	1 (0%)	34	69
3	G	237/360 (66%)	217 (92%)	20 (8%)	0	100	100
All	All	945/1208 (78%)	849 (90%)	94 (10%)	2 (0%)	50	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	47	LEU
1	A	213	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	200/202 (99%)	199 (100%)	1 (0%)	88	94
1	B	199/202 (98%)	198 (100%)	1 (0%)	88	94
2	F	206/307 (67%)	203 (98%)	3 (2%)	65	81
3	G	202/300 (67%)	201 (100%)	1 (0%)	88	94
All	All	807/1011 (80%)	801 (99%)	6 (1%)	84	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	B	193	THR
2	F	261	ARG
2	F	292	ARG
2	F	295	ARG
3	G	70	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	196	ASN
1	B	8	ASN
2	F	248	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 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	$\# Z  > 2$
5	JSG	F	402	-	203,206,206	1.08	17 (8%)	257,278,278	2.05	55 (21%)
6	DCQ	F	403	-	23,23,23	1.82	5 (21%)	26,29,29	2.45	7 (26%)
7	LMT	F	404	-	24,24,36	1.07	2 (8%)	29,29,47	1.03	1 (3%)
6	DCQ	G	403	-	23,23,23	1.61	6 (26%)	26,29,29	2.34	7 (26%)
4	LMN	F	401	-	34,34,72	1.01	3 (8%)	38,41,98	2.48	11 (28%)
7	LMT	G	402	-	13,13,36	0.40	0	12,12,47	0.87	0
4	LMN	G	401	-	35,35,72	0.98	2 (5%)	40,43,98	2.31	10 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	JSG	F	402	-	-	39/195/333/333	0/7/7/7
6	DCQ	F	403	-	-	5/14/38/38	0/1/1/1
7	LMT	F	404	-	-	6/15/35/61	0/1/1/2
6	DCQ	G	403	-	-	3/14/38/38	0/1/1/1
4	LMN	F	401	-	-	3/30/46/130	0/1/1/4
7	LMT	G	402	-	-	6/11/11/61	-
4	LMN	G	401	-	-	3/30/50/130	0/1/1/4

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	402	JSG	OBW-CBP	4.11	1.47	1.42
6	F	403	DCQ	C1M-C1	-4.03	1.42	1.50
6	G	403	DCQ	C6-C1	3.94	1.42	1.35
6	F	403	DCQ	C6-C1	3.81	1.42	1.35
6	F	403	DCQ	C3-C2	-3.81	1.37	1.48
5	F	402	JSG	OCL-CCB	3.53	1.50	1.41
5	F	402	JSG	OBH-CBG	3.50	1.49	1.44
4	G	401	LMN	OBV-CCJ	3.48	1.46	1.40
6	G	403	DCQ	C7-C6	-3.21	1.43	1.51
5	F	402	JSG	ODA-CDB	3.15	1.45	1.40
6	F	403	DCQ	C7-C6	-3.10	1.43	1.51
4	G	401	LMN	OBX-CCJ	2.97	1.49	1.41
5	F	402	JSG	CBQ-CBP	2.92	1.56	1.52
5	F	402	JSG	OCL-CCF	2.89	1.48	1.44
6	G	403	DCQ	C3-C2	-2.89	1.40	1.48
5	F	402	JSG	OBW-CBV	2.82	1.48	1.44
4	F	401	LMN	CCL-CCJ	2.70	1.56	1.51
7	F	404	LMT	O3'-C3'	-2.66	1.36	1.43
5	F	402	JSG	OBD-CBC	2.54	1.51	1.43
7	F	404	LMT	O2'-C2'	-2.51	1.37	1.43
6	F	403	DCQ	C1-C2	-2.50	1.38	1.47
5	F	402	JSG	CBI-CBG	2.46	1.58	1.52
5	F	402	JSG	OCY-CCS	2.42	1.47	1.44
5	F	402	JSG	CAP-CAN	2.40	1.57	1.53
6	G	403	DCQ	C1M-C1	-2.37	1.45	1.50
5	F	402	JSG	ODL-CDF	2.25	1.47	1.44

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	401	LMN	OBV-CCJ	2.20	1.47	1.40
5	F	402	JSG	CDG-CDF	2.19	1.57	1.52
5	F	402	JSG	CBG-CBE	2.19	1.56	1.52
4	F	401	LMN	CBT-CCM	2.15	1.56	1.52
5	F	402	JSG	ODL-CDB	2.13	1.47	1.41
6	G	403	DCQ	C4-C5	-2.10	1.42	1.48
6	G	403	DCQ	C6-C5	-2.04	1.40	1.46
5	F	402	JSG	CDE-CDF	2.02	1.57	1.52
5	F	402	JSG	C8-CEW	2.01	1.56	1.51

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	401	LMN	CBR-CCM-CBQ	8.74	127.43	108.54
4	F	401	LMN	CBL-CBR-CCM	7.92	126.62	116.66
5	F	402	JSG	OFZ-CFM-CFL	7.79	121.96	106.65
5	F	402	JSG	CBI-CBG-CBE	7.59	127.48	114.18
4	F	401	LMN	CBR-CBL-CBJ	7.33	135.01	113.19
5	F	402	JSG	CEW-OFJ-CGB	7.14	135.37	117.79
5	F	402	JSG	CAV-O1-C1	-7.11	99.84	113.74
5	F	402	JSG	CFM-OFZ-CGN	6.80	134.53	117.79
5	F	402	JSG	CAP-OAQ-CEE	6.64	128.59	117.53
6	F	403	DCQ	C7-C6-C5	6.57	127.75	117.00
6	G	403	DCQ	C3M-O3-C3	6.55	139.67	116.47
5	F	402	JSG	C2-N2-C7	6.37	132.28	122.90
5	F	402	JSG	OFJ-CEW-C8	6.34	119.12	106.65
5	F	402	JSG	CAP-CAN-NAO	6.34	121.44	110.91
6	G	403	DCQ	C4M-O4-C4	6.24	138.59	116.47
6	F	403	DCQ	C4M-O4-C4	5.96	137.60	116.47
5	F	402	JSG	C8-C7-N2	-5.91	108.58	116.33
5	F	402	JSG	O3-C3-C4	5.89	120.03	108.25
6	F	403	DCQ	C3M-O3-C3	5.83	137.13	116.47
5	F	402	JSG	C1-C2-N2	5.64	120.72	111.00
5	F	402	JSG	CBQ-CBR-CBT	-4.98	105.97	110.84
5	F	402	JSG	C3-O3-CFK	4.86	125.62	117.53
5	F	402	JSG	CDH-CDG-CDF	4.25	120.76	112.17
5	F	402	JSG	CCU-ODA-CDB	4.08	121.71	113.74
5	F	402	JSG	OBL-CBK-CBI	3.99	119.76	111.07
4	F	401	LMN	CBQ-CBK-CBI	3.96	124.98	113.19
4	G	401	LMN	CCQ-CCH-CCL	-3.91	103.99	110.82
4	G	401	LMN	CBS-CCM-CBQ	-3.91	103.79	110.54
4	G	401	LMN	CBS-CCM-CBR	-3.87	103.86	110.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	401	LMN	CBT-OBV-CCJ	-3.84	103.38	113.36
6	G	403	DCQ	C7-C6-C5	3.81	123.24	117.00
5	F	402	JSG	CEZ-CEY-CEX	3.80	127.08	113.62
5	F	402	JSG	OFJ-CEW-CEX	3.75	117.88	107.10
5	F	402	JSG	CBK-CBI-CBG	3.58	119.41	112.17
4	F	401	LMN	CBK-CBQ-CCM	-3.55	112.20	116.66
4	F	401	LMN	CBJ-CBH-CBF	3.52	132.28	114.42
4	F	401	LMN	OBX-CCJ-OBV	3.45	116.92	109.40
5	F	402	JSG	OED-CDQ-CDP	-3.29	100.91	109.65
5	F	402	JSG	CBG-CBE-CBC	-3.29	103.69	110.55
7	F	404	LMT	C3'-C4'-C5'	-3.27	104.40	110.24
4	G	401	LMN	OBX-CCJ-CCL	-3.26	103.44	110.35
5	F	402	JSG	OBW-CBP-CBQ	-3.25	106.56	111.24
4	G	401	LMN	CBP-CCF-CCQ	-3.19	105.53	113.00
5	F	402	JSG	ODA-CCU-CCT	3.17	116.66	109.27
5	F	402	JSG	O5-C5-C6	3.04	112.79	106.67
5	F	402	JSG	OBH-CBG-CBE	3.01	114.07	108.84
4	F	401	LMN	CBS-CCM-CBR	2.98	115.69	110.54
4	F	401	LMN	OBX-CCF-CBP	2.91	113.67	106.44
5	F	402	JSG	CAN-NAO-CDO	-2.90	118.63	122.90
5	F	402	JSG	OAQ-CAP-CAN	2.86	113.26	107.91
5	F	402	JSG	CAV-CAT-CAR	-2.84	106.16	112.09
5	F	402	JSG	OFZ-CGN-CGP	2.76	117.44	111.50
5	F	402	JSG	C6-C5-C4	-2.75	106.52	113.33
5	F	402	JSG	CEI-CEH-CEG	-2.74	106.96	114.85
6	G	403	DCQ	C8-C7-C6	2.74	121.07	113.12
4	F	401	LMN	CBH-CBF-CBD	-2.71	100.65	114.42
6	G	403	DCQ	O5-C5-C6	-2.65	116.90	121.55
5	F	402	JSG	OCL-CCB-CCC	-2.64	104.77	110.35
4	G	401	LMN	CBJ-CBH-CBF	-2.60	101.23	114.42
5	F	402	JSG	C3-C2-N2	-2.59	106.61	110.91
4	G	401	LMN	OBX-CCF-CBP	-2.59	100.00	106.44
6	F	403	DCQ	O5-C5-C6	-2.53	117.11	121.55
5	F	402	JSG	CCB-OBF-CBE	2.50	124.16	117.96
5	F	402	JSG	CFU-CFT-CFS	-2.48	101.81	114.42
4	G	401	LMN	CBT-OBV-CCJ	-2.46	106.97	113.36
5	F	402	JSG	OFZ-CFM-CFN	2.45	114.14	107.10
5	F	402	JSG	OAU-CAL-CAN	-2.44	105.80	110.58
5	F	402	JSG	OAU-CAT-CAV	2.42	111.54	106.67
5	F	402	JSG	CDY-CDX-CDW	-2.37	102.38	114.42
5	F	402	JSG	O7-C7-C8	2.34	124.93	121.50
6	G	403	DCQ	C9-C8-C7	2.32	121.53	113.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	402	JSG	CCC-CCD-CCE	-2.29	106.43	111.66
6	F	403	DCQ	O4-C4-C5	2.29	124.31	116.56
5	F	402	JSG	CFO-CFN-CFM	2.29	122.92	114.64
6	F	403	DCQ	C9-C8-C7	2.26	121.32	113.19
5	F	402	JSG	OHN-PHK-OHM	2.25	116.25	107.64
6	G	403	DCQ	O4-C4-C5	2.25	124.17	116.56
5	F	402	JSG	CDE-CDD-CDC	-2.23	106.94	110.82
5	F	402	JSG	O3-C3-C2	2.19	112.01	107.91
6	F	403	DCQ	C6-C1-C2	2.17	120.90	119.18
5	F	402	JSG	CBX-CBV-CBT	-2.16	110.44	114.03
5	F	402	JSG	CGH-CGG-CGF	-2.12	103.65	114.42
4	F	401	LMN	CCH-CCQ-CCF	-2.11	107.86	109.97
5	F	402	JSG	OCX-PHK-OHL	-2.11	101.24	109.39
4	G	401	LMN	CBL-CBR-CCM	-2.10	114.02	116.66
5	F	402	JSG	OBO-CBM-CBP	-2.08	116.99	123.70
5	F	402	JSG	ODK-CDE-CDD	-2.06	105.58	110.35
5	F	402	JSG	CGR-CGQ-CGP	-2.04	105.85	113.19
5	F	402	JSG	OAZ-CAX-CBA	-2.04	117.14	123.70
5	F	402	JSG	OCJ-CCD-CCC	2.03	112.68	107.28
5	F	402	JSG	CFR-CFQ-CFP	-2.02	104.15	114.42

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	401	LMN	OBX-CCJ-OBV-CBT
4	F	401	LMN	CCL-CCJ-OBV-CBT
4	G	401	LMN	OBX-CCJ-OBV-CBT
5	F	402	JSG	C7-C8-CEW-CEX
5	F	402	JSG	OAU-CAL-OAM-PHG
5	F	402	JSG	CBE-CBG-CBI-CBK
5	F	402	JSG	CBE-CBG-CBI-OBJ
5	F	402	JSG	OBN-CBM-CBP-OBD
5	F	402	JSG	CFL-CFM-OFZ-CGN
5	F	402	JSG	CGP-CGN-OFZ-CFM
5	F	402	JSG	CCE-OCK-PHO-OHQ
5	F	402	JSG	OGO-CGN-OFZ-CFM
7	F	404	LMT	O5'-C5'-C6'-O6'
5	F	402	JSG	CFN-CFM-OFZ-CGN
6	F	403	DCQ	C3-C4-O4-C4M
6	G	403	DCQ	C3-C4-O4-C4M
4	F	401	LMN	CBJ-CBL-CBR-CCM

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	F	402	JSG	CAN-CAP-OAQ-CEE
6	F	403	DCQ	C5-C4-O4-C4M
6	G	403	DCQ	C5-C4-O4-C4M
7	F	404	LMT	C3-C4-C5-C6
5	F	402	JSG	CBC-CBE-OBF-CCB
5	F	402	JSG	C3-C2-N2-C7
7	F	404	LMT	C2-C3-C4-C5
7	G	402	LMT	C6-C7-C8-C9
7	F	404	LMT	C4'-C5'-C6'-O6'
5	F	402	JSG	OCL-CCB-OBF-CBE
7	G	402	LMT	C2-C1-O1'-C1'
7	G	402	LMT	C1-C2-C3-C4
5	F	402	JSG	CAR-CAP-OAQ-CEE
7	G	402	LMT	C3-C4-C5-C6
7	G	402	LMT	C2-C3-C4-C5
5	F	402	JSG	CCT-CCU-ODA-CDB
4	G	401	LMN	CBJ-CBL-CBR-CCM
4	G	401	LMN	CCL-CCJ-OBV-CBT
5	F	402	JSG	CBG-CBE-OBF-CCB
7	F	404	LMT	C1-C2-C3-C4
5	F	402	JSG	C2-C3-O3-CFK
7	F	404	LMT	O1'-C1-C2-C3
5	F	402	JSG	CFK-CFL-CFM-CFN
7	G	402	LMT	C7-C8-C9-C10
5	F	402	JSG	CCE-CCD-OCJ-CCO
5	F	402	JSG	C4-C3-O3-CFK
5	F	402	JSG	OFJ-CEW-CEX-CEY
5	F	402	JSG	C8-CEW-OFJ-CGB
5	F	402	JSG	CAP-CAN-NAO-CDO
6	F	403	DCQ	C2-C3-O3-C3M
6	G	403	DCQ	C2-C3-O3-C3M
5	F	402	JSG	OBO-CBM-CBP-CBQ
5	F	402	JSG	CCC-CCD-OCJ-CCO
5	F	402	JSG	CDQ-CDR-CDS-CDT
5	F	402	JSG	CCR-OCX-PHK-OHL
5	F	402	JSG	OFZ-CGN-CGP-CGQ
5	F	402	JSG	OBO-CBM-CBP-OBQ
5	F	402	JSG	C5-C6-O6-CBA
5	F	402	JSG	OBN-CBM-CBP-OBW
5	F	402	JSG	C4-O4-PHC-OHF
5	F	402	JSG	CAL-OAM-PHG-OHJ
5	F	402	JSG	CCE-OCK-PHO-OHR

*Continued on next page...*

*Continued from previous page...*

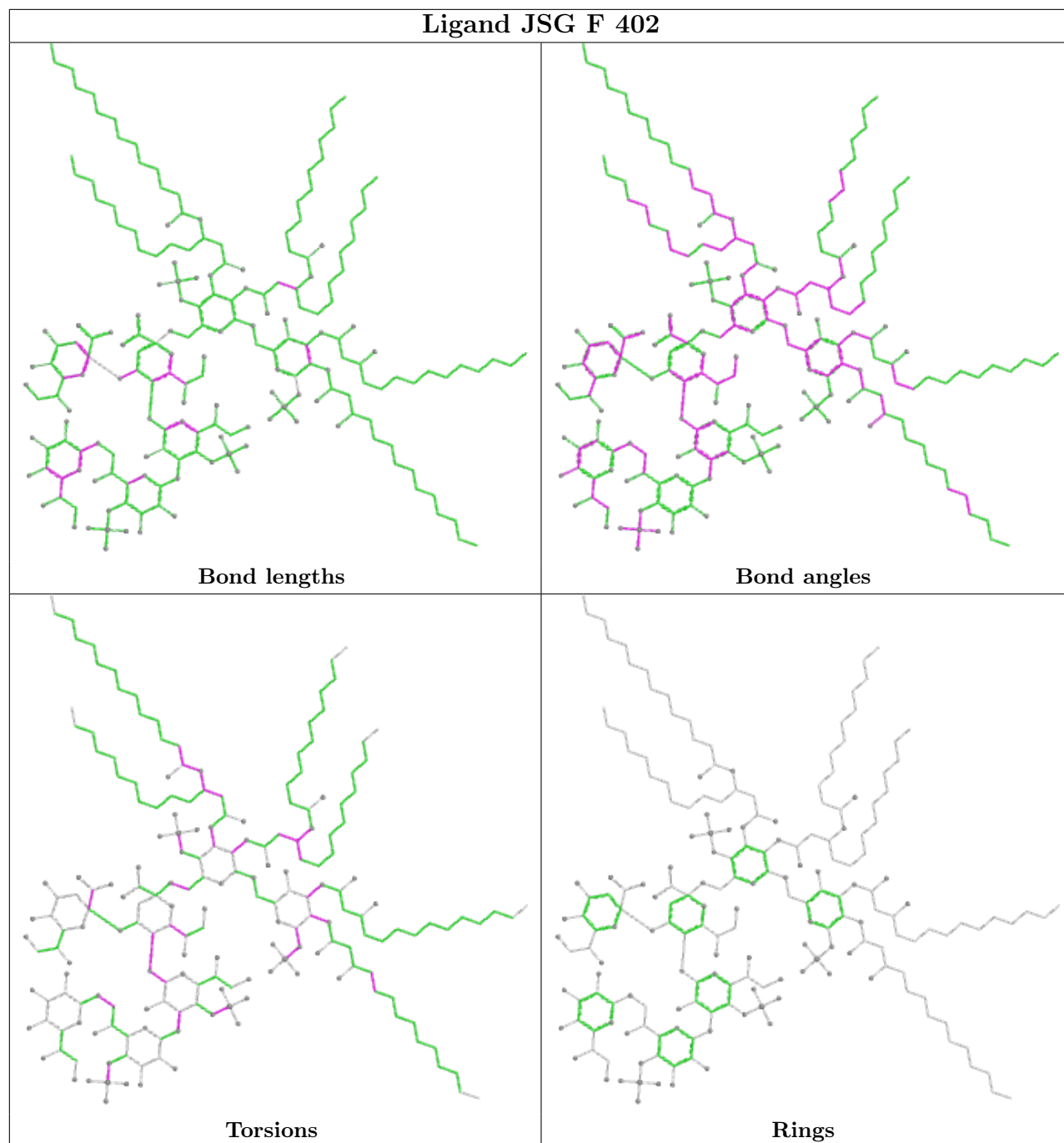
Mol	Chain	Res	Type	Atoms
5	F	402	JSG	CCR-OCX-PHK-OHM
5	F	402	JSG	CCR-OCX-PHK-OHN
5	F	402	JSG	OGO-CGN-CGP-CGQ
5	F	402	JSG	C1-C2-N2-C7
6	F	403	DCQ	C4-C3-O3-C3M
6	F	403	DCQ	C6-C7-C8-C9

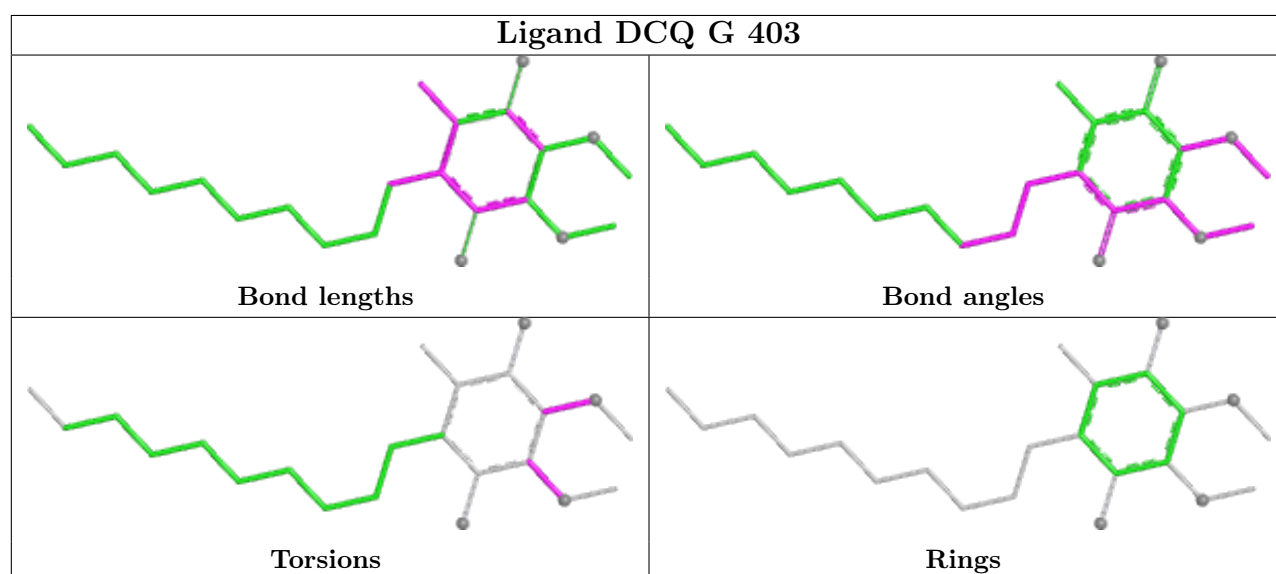
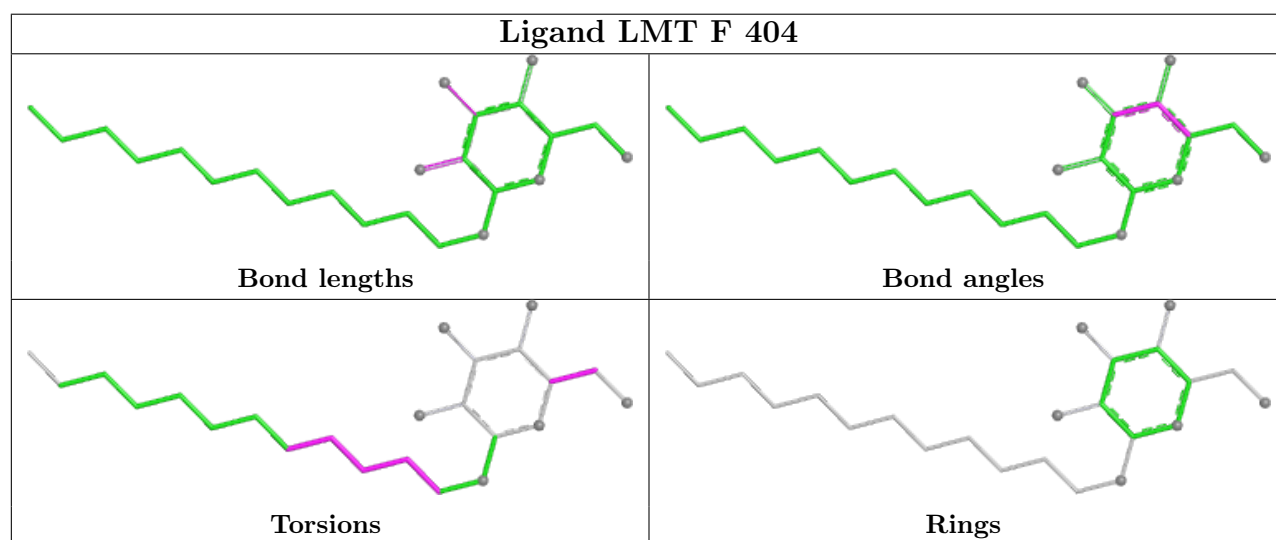
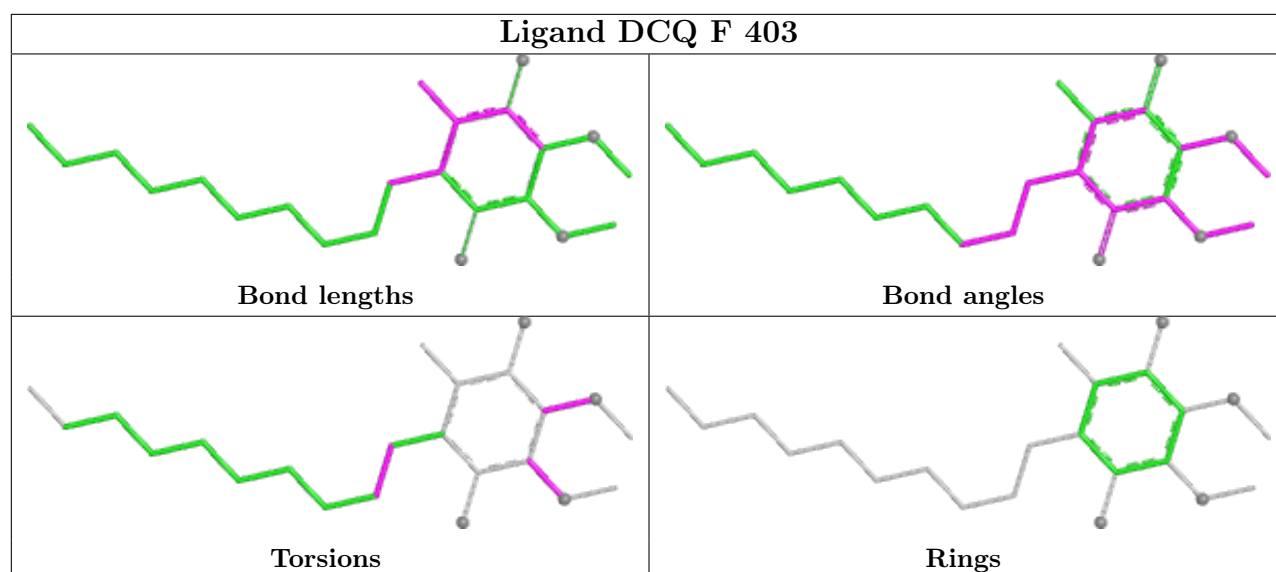
There are no ring outliers.

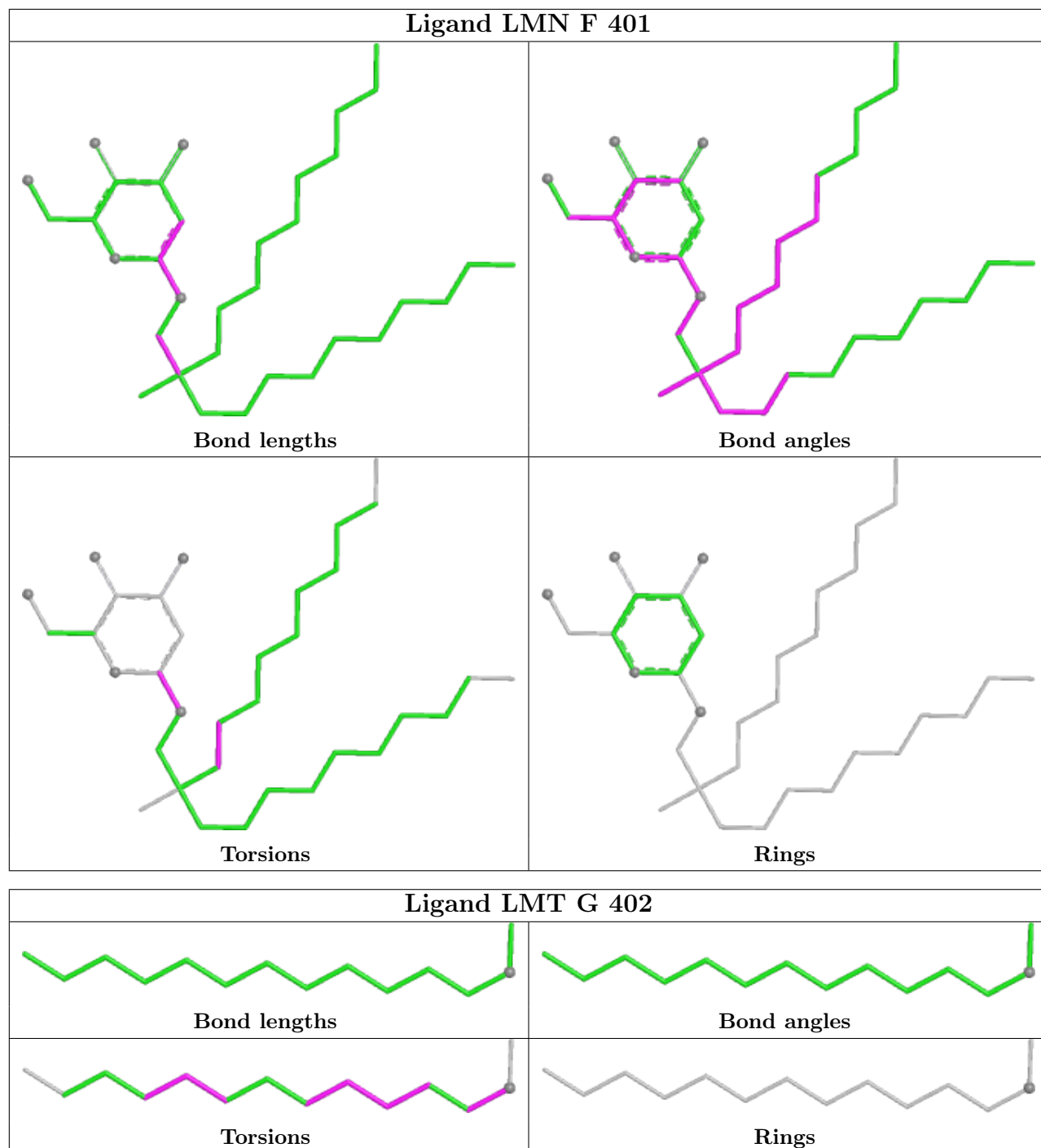
6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	402	JSG	2	0
6	F	403	DCQ	2	0
7	F	404	LMT	2	0
6	G	403	DCQ	2	0
4	F	401	LMN	4	0
4	G	401	LMN	6	0

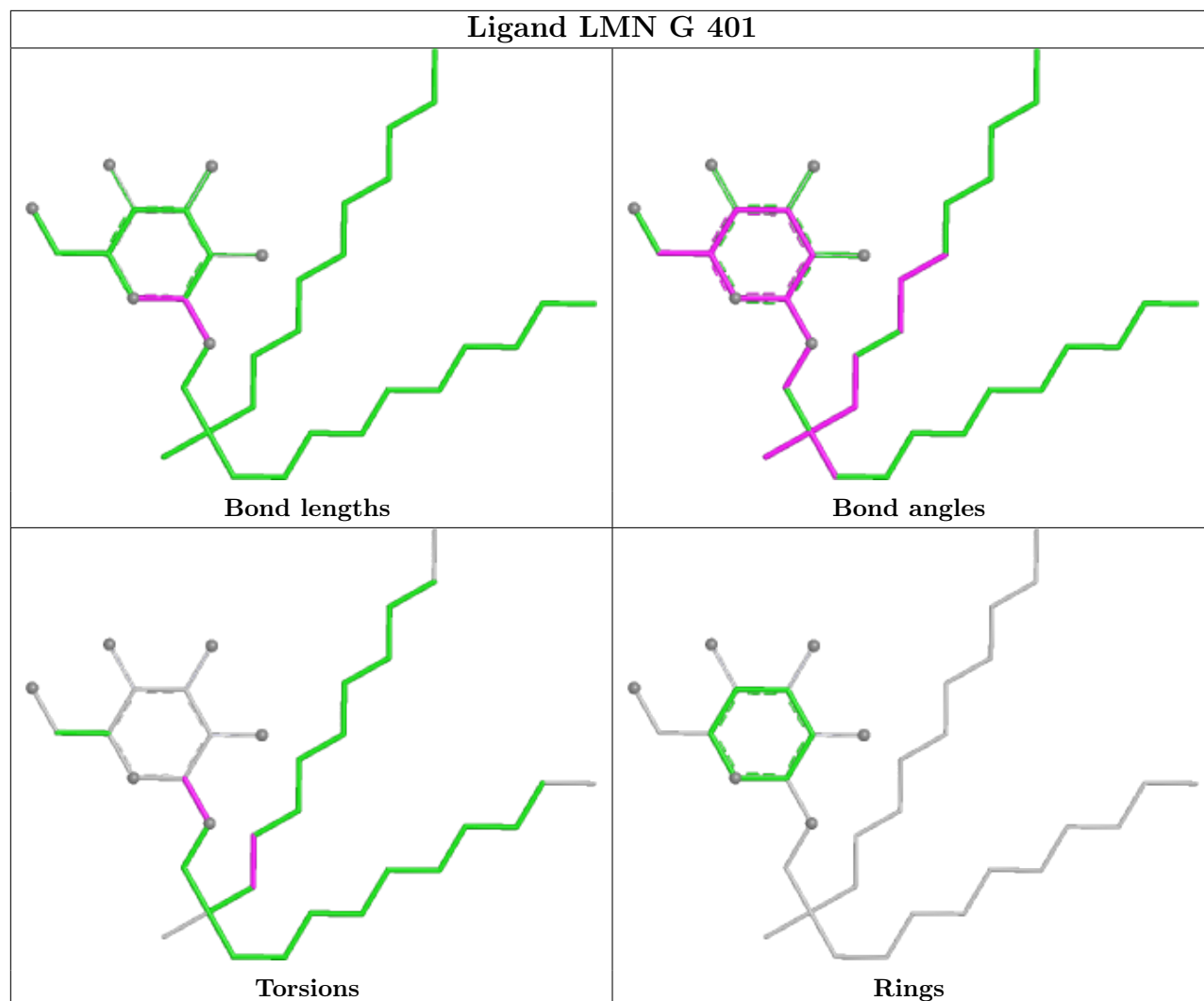
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

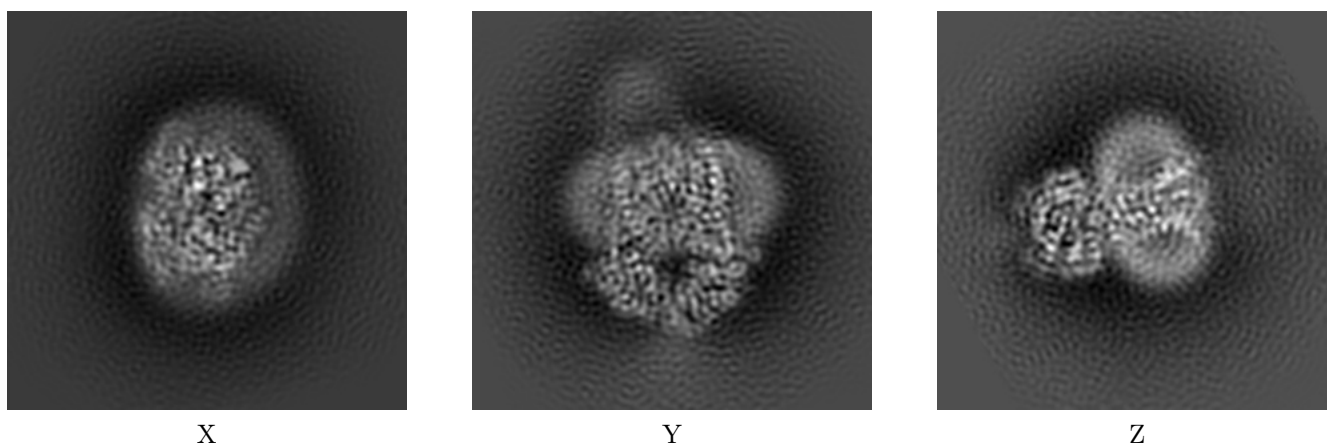
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10122. 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](#)

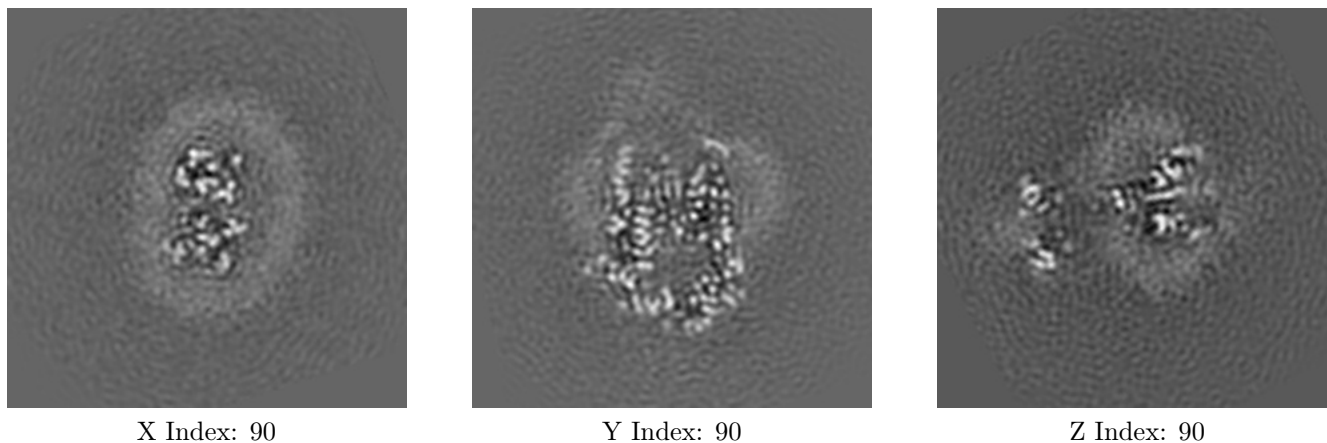
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

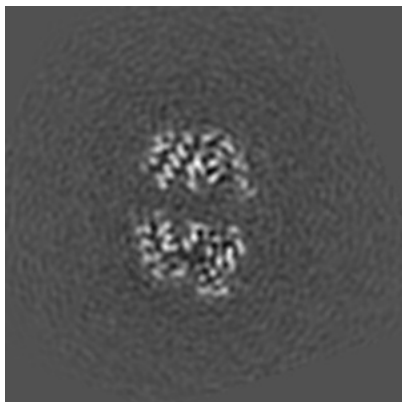
#### 6.2.1 Primary map



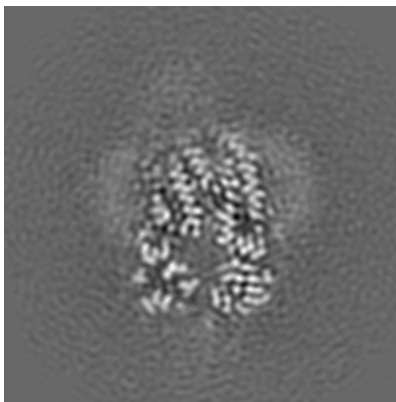
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

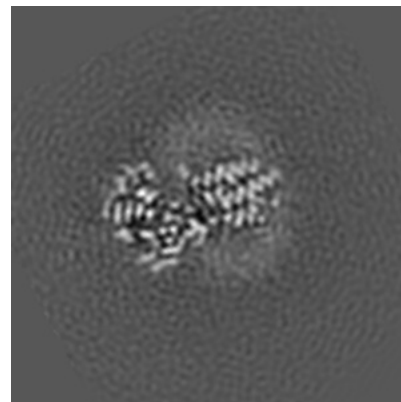
### 6.3.1 Primary map



X Index: 62



Y Index: 85

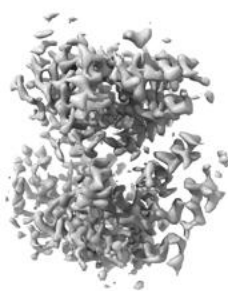


Z Index: 109

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

## 6.4 Orthogonal surface views [i](#)

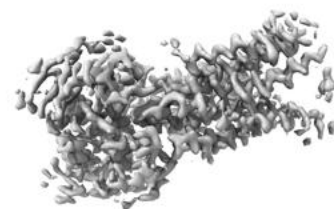
### 6.4.1 Primary map



X



Y



Z

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.

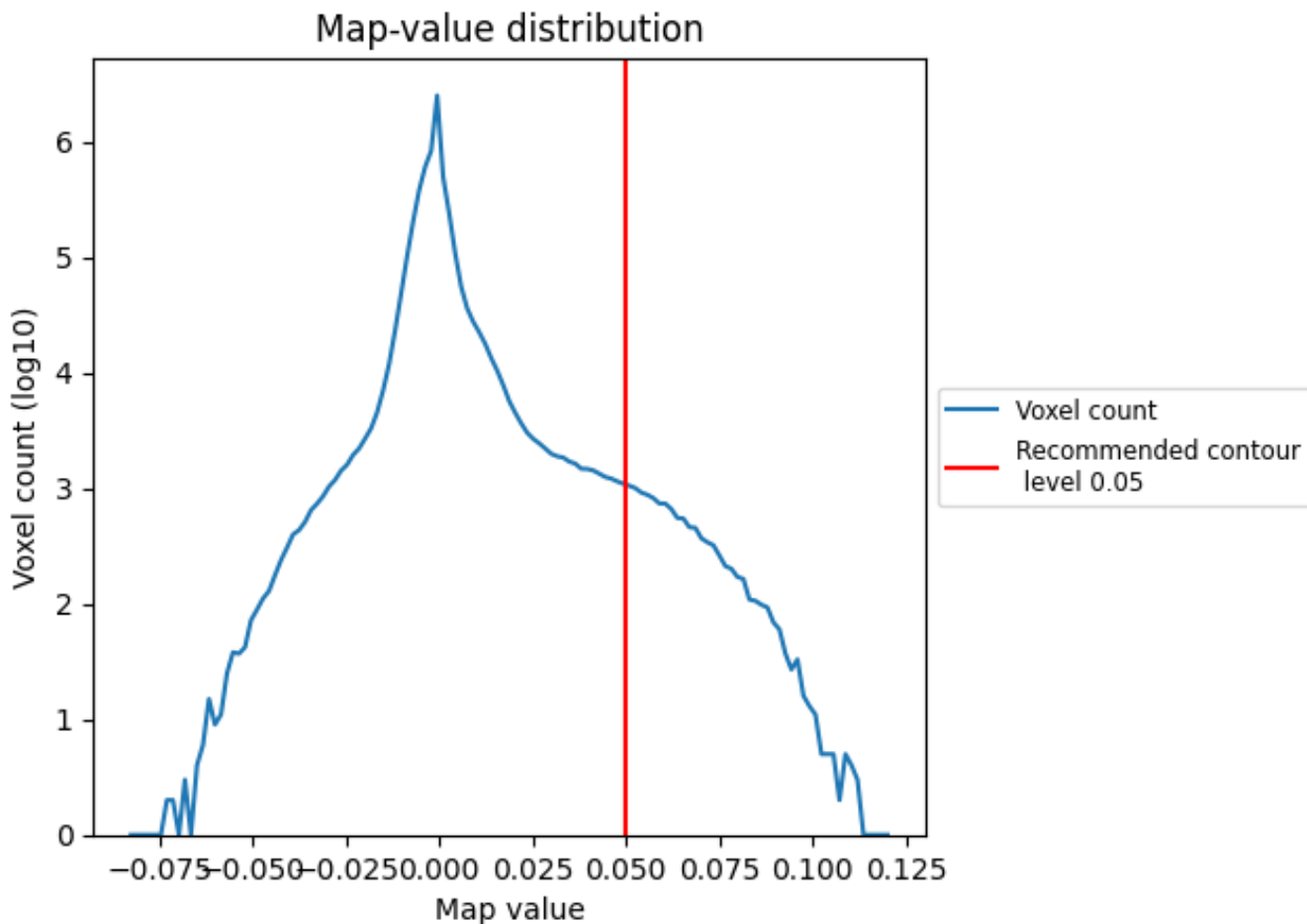
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

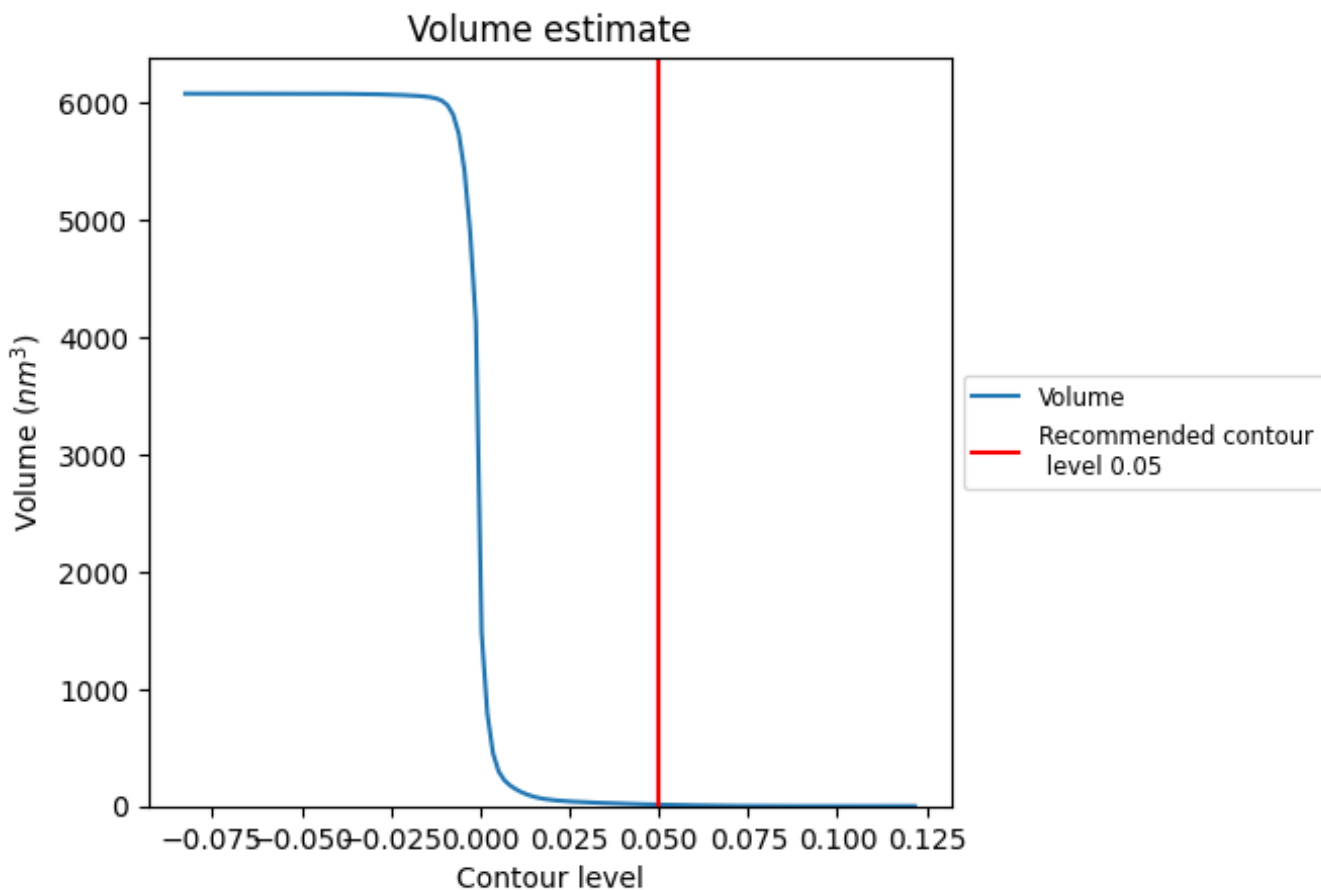
This section contains the results of statistical analysis of the map.

### 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.

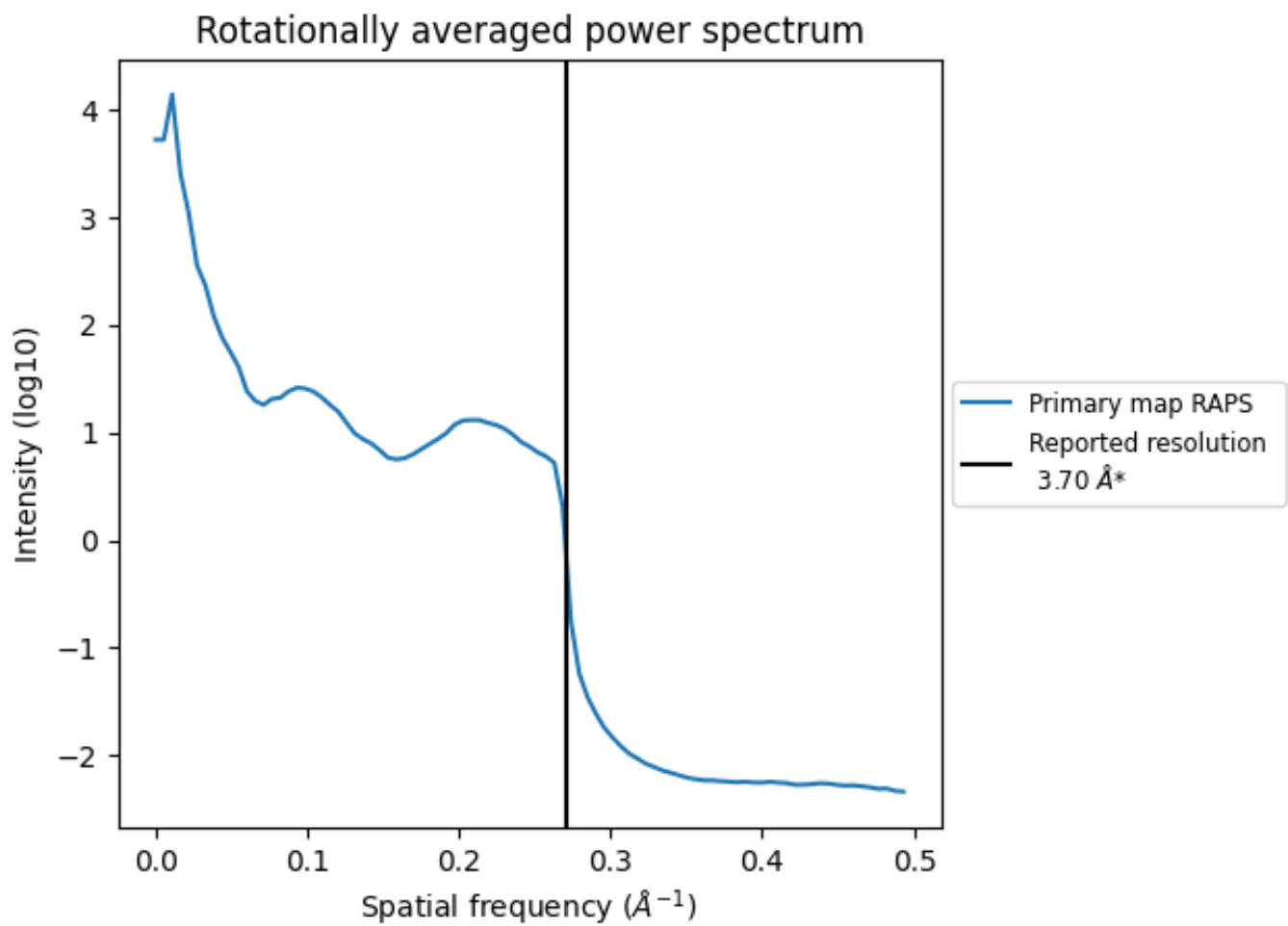
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 13  $\text{nm}^3$ ; this corresponds to an approximate mass of 11 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  $0.270 \text{\AA}^{-1}$

## 8 Fourier-Shell correlation

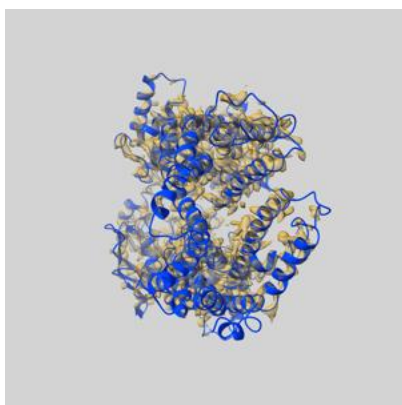
This section was not generated. No FSC curve or half-maps provided.



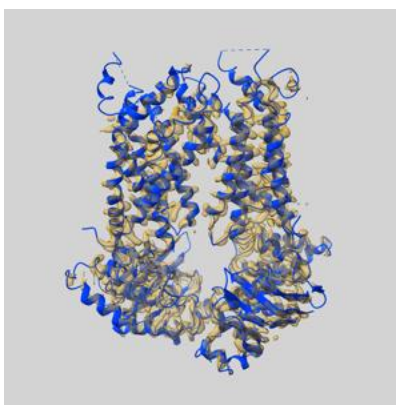
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10122 and PDB model 6S8H. Per-residue inclusion information can be found in section 3 on page 7.

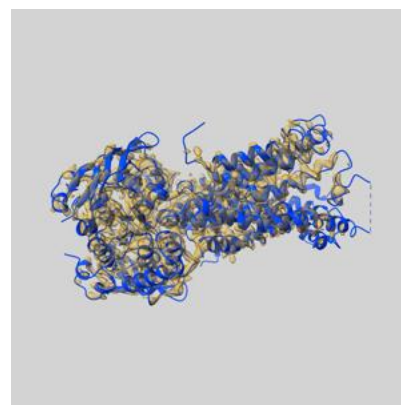
### 9.1 Map-model overlay [i](#)



X



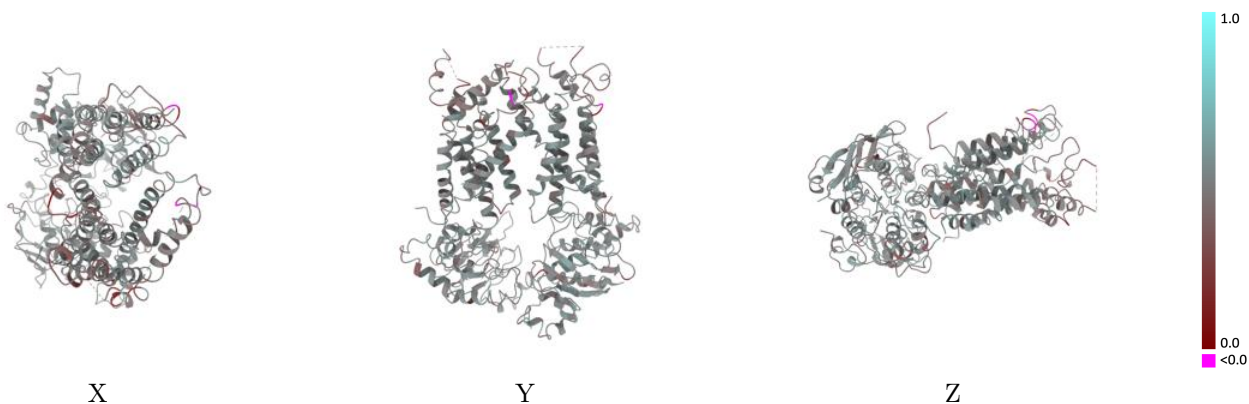
Y



Z

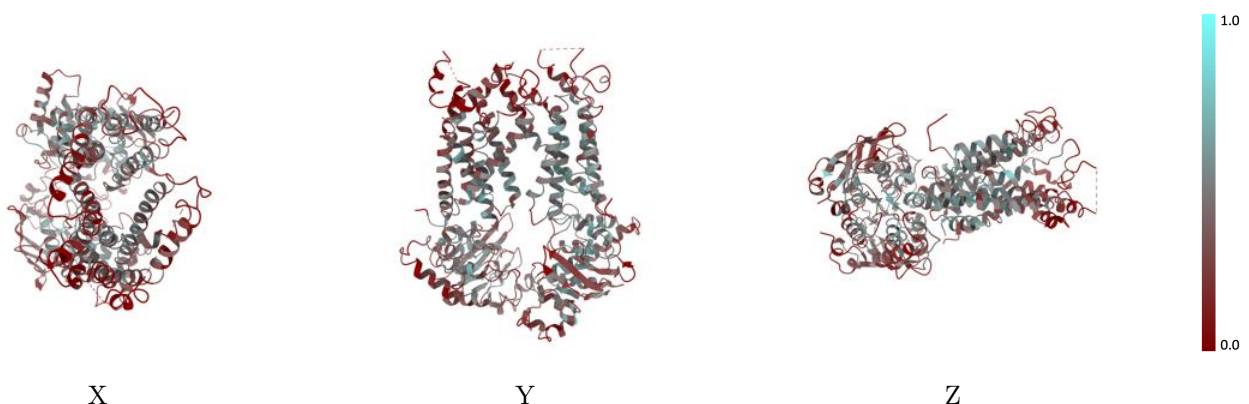
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



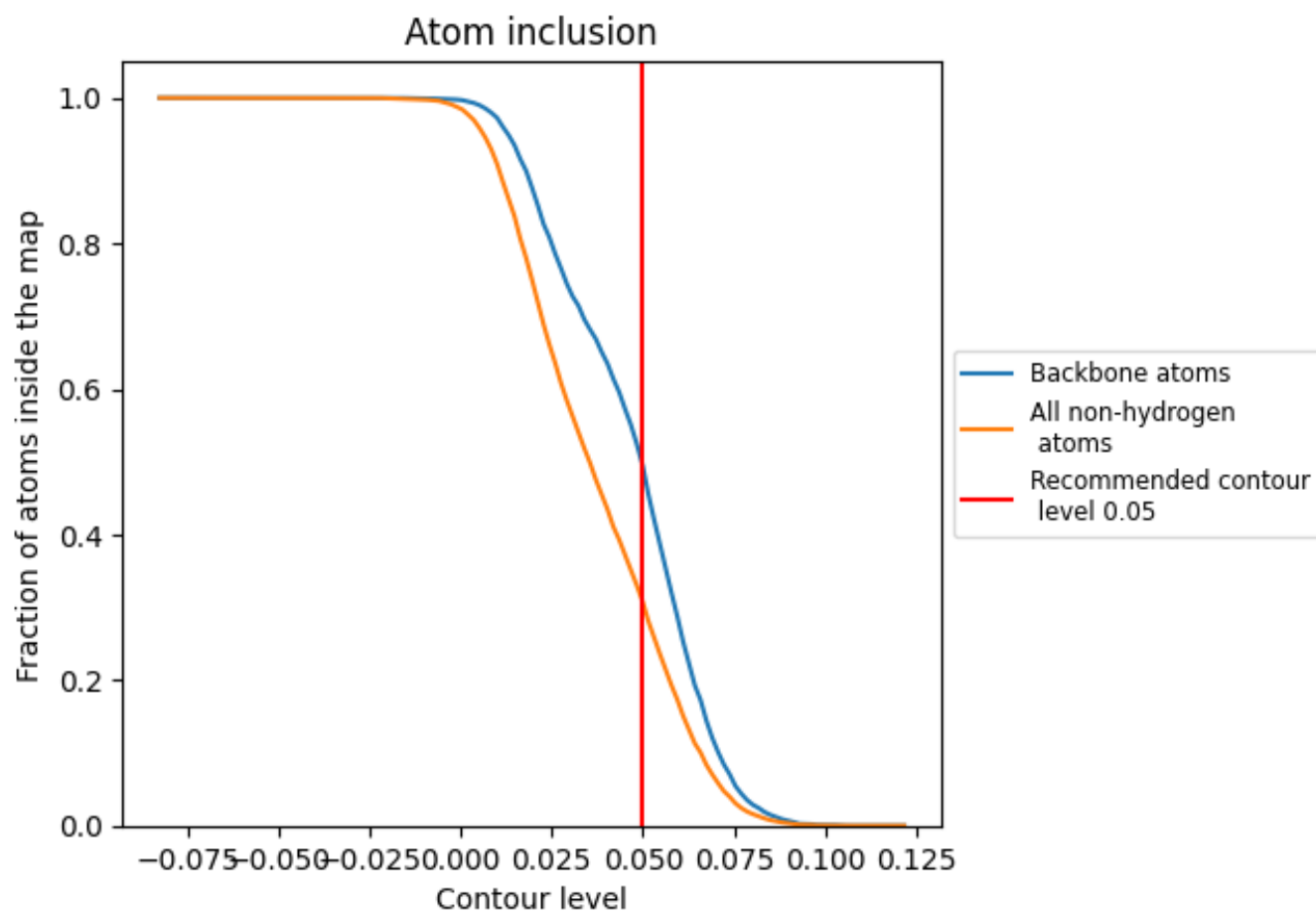
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 49% of all backbone atoms, 31% of all non-hydrogen atoms, are inside the map.

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

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3069	 0.4700
A	 0.2970	 0.4850
B	 0.3339	 0.4900
F	 0.3132	 0.4570
G	 0.2839	 0.4490

