



## Full wwPDB EM Validation Report ⓘ

Oct 29, 2022 – 12:30 PM EDT

PDB ID : 7USY  
EMDB ID : EMD-26743  
Title : Structure of C. elegans TMC-1 complex with ARRD-6  
Authors : Jeong, H.; Clark, S.; Gouaux, E.  
Deposited on : 2022-04-26  
Resolution : 3.54 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>.

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

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

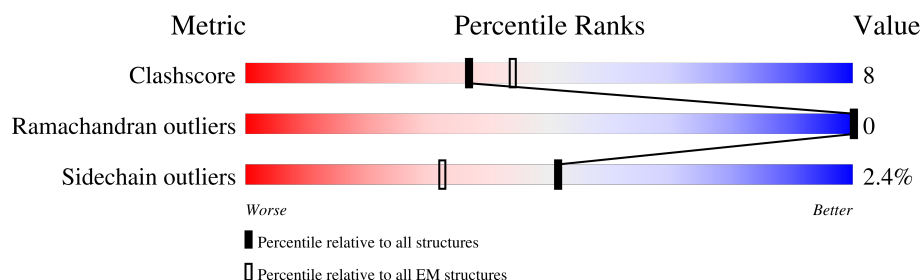
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.54 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	1285	<div> <div>10%</div> <div>37%</div> <div>9%</div> <div>53%</div> </div>
1	B	1285	<div> <div>10%</div> <div>37%</div> <div>10%</div> <div>53%</div> </div>
2	C	201	<div> <div>24%</div> <div>63%</div> <div>27%</div> <div>8%</div> </div>
2	E	201	<div> <div>20%</div> <div>75%</div> <div>16%</div> <div>8%</div> </div>
3	D	117	<div> <div>8%</div> <div>32%</div> <div>8%</div> <div>61%</div> </div>
3	F	117	<div> <div>9%</div> <div>32%</div> <div>6%</div> <div>61%</div> </div>
4	J	469	<div> <div>73%</div> <div>63%</div> <div>14%</div> <div>23%</div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16582 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 Transmembrane channel-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	602	Total	C	N	O	S	0	0
			4864	3206	816	815	27		
1	B	602	Total	C	N	O	S	0	0
			4864	3206	816	815	27		

- Molecule 2 is a protein called CALMyrin (Calcium and Integrin Binding protein) homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	184	Total	C	N	O	S	0	0
			1536	978	256	295	7		
2	E	184	Total	C	N	O	S	0	0
			1536	978	256	295	7		

- Molecule 3 is a protein called Transmembrane inner ear expressed protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	46	Total	C	N	O	S	0	0
			343	228	60	50	5		
3	F	46	Total	C	N	O	S	0	0
			343	228	60	50	5		

- Molecule 4 is a protein called ARRestin Domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	361	Total	C	N	O	S	0	0
			2878	1832	500	529	17		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

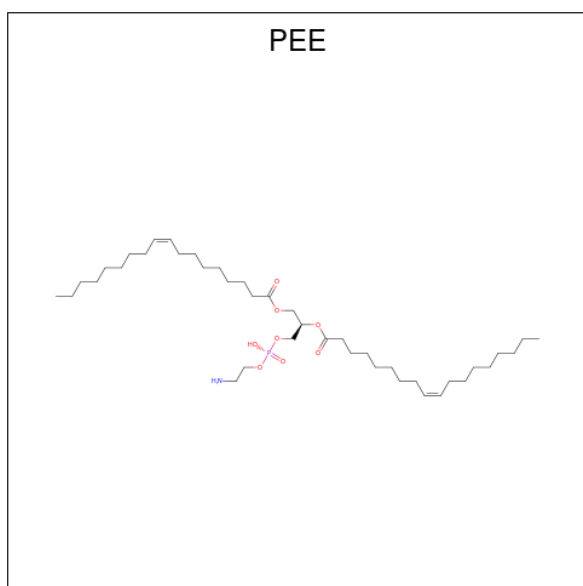
Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total	Ca	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
5	B	2	Total	Ca	0
			2	2	
5	C	2	Total	Ca	0
			2	2	
5	E	2	Total	Ca	0
			2	2	

- Molecule 6 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{78}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
6	B	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 7 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
7	B	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



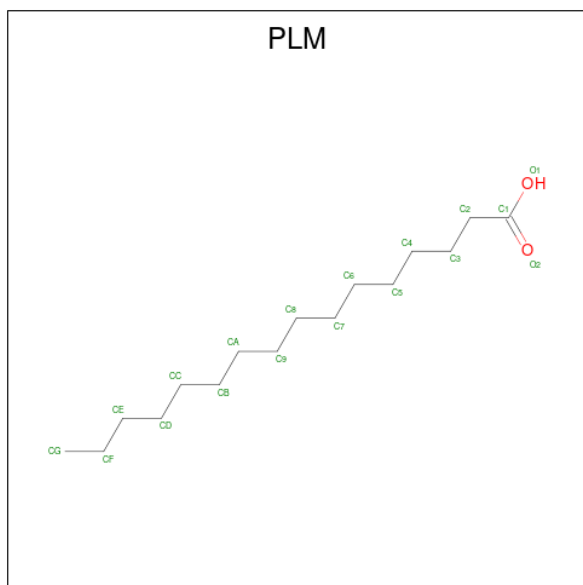
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 9 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

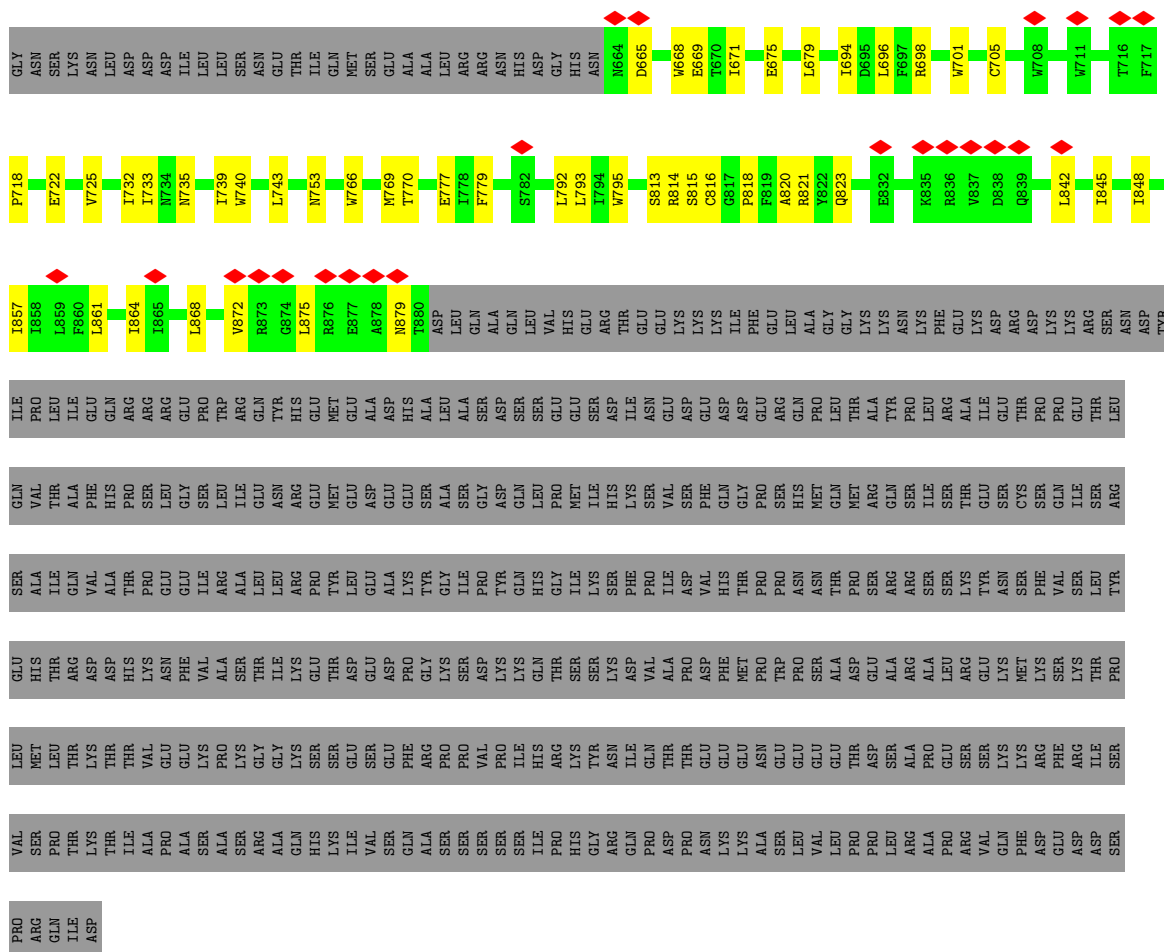


Mol	Chain	Residues	Atoms			AltConf
9	D	1	Total	C	O	0
			14	13	1	
9	F	1	Total	C	O	0
			14	13	1	

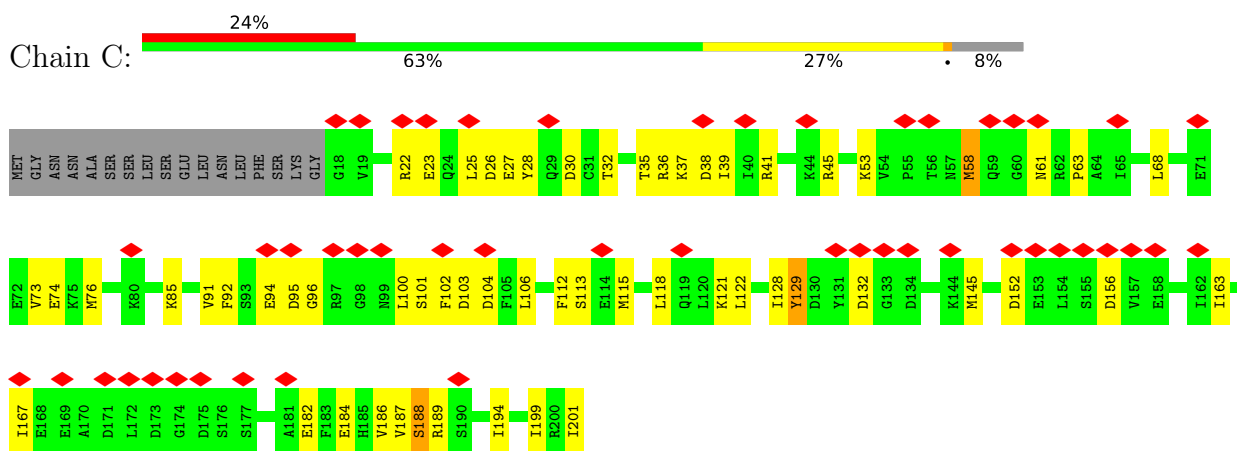




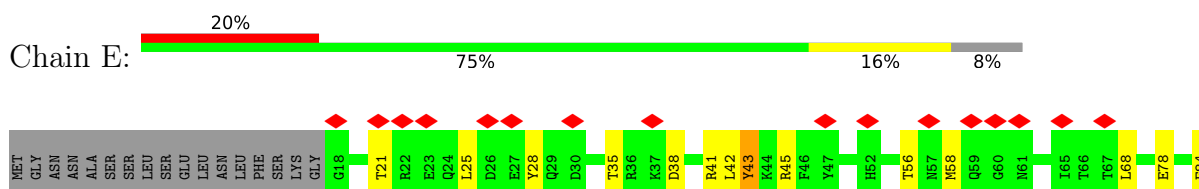


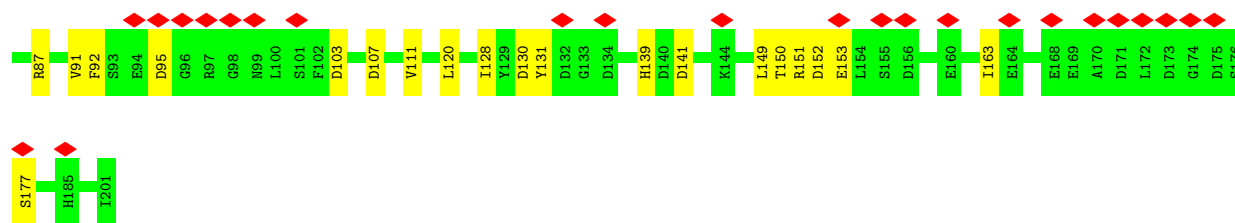


- Molecule 2: CALMyrin (Calcium and Integrin Binding protein) homolog

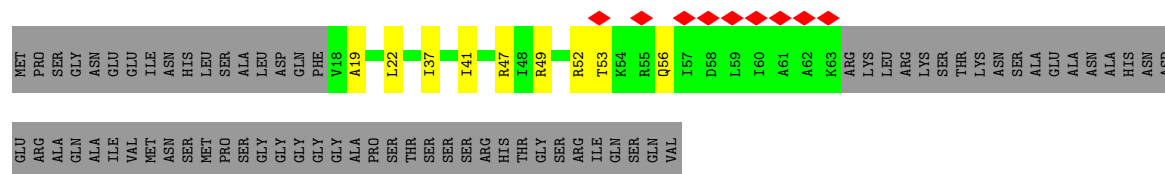


- Molecule 2: CALMyrin (Calcium and Integrin Binding protein) homolog

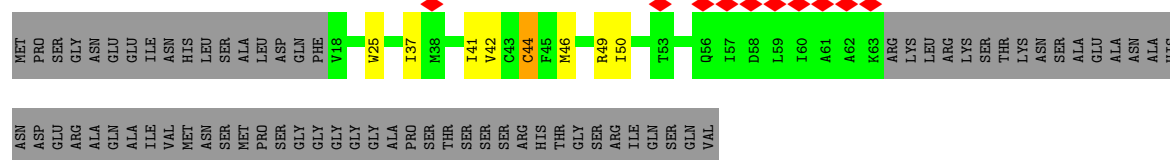




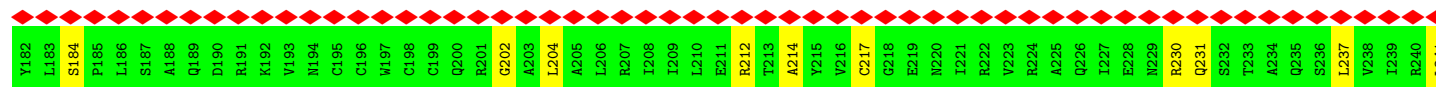
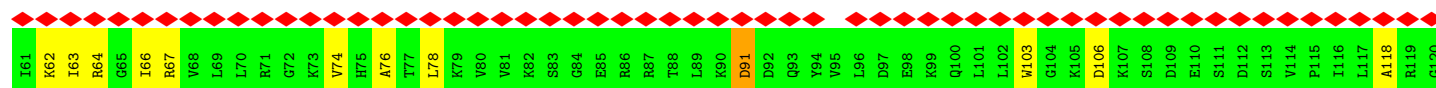
• Molecule 3: Transmembrane inner ear expressed protein



• Molecule 3: Transmembrane inner ear expressed protein



• Molecule 4: ARRestin Domain protein



ASN	GLY	SER	VAL	ARG	ARG	ARG	SER	ILE	LEU	VAL	ALA	ASN	ASN	PRO	CYS	LEU	ALA	MET	ARG	ASP	GLU	SER	MET	ASP	GLU	LYS	LEU	MET	THR	THR	ASN	GLY	CYS	ASN	SER	GLU	GLY	ASP	PRO	PRO	LEU	VAL	ALA																
G368	GLN	VAL	TYR	ASP	GLY	GLY	GLU	GLU	GLU	ILE	ASN	LYS	GLU	E382	E383	I384	V385	L386	Y387	R388	P389	V390	Y391	V392	K393	L394	A395	D396	R397	R398	I399	G400	SER	PRO	HIS	VAL	SER	LYS	ASP	PHE	ARG	SER	GLY	SER	PHE	THR	ARG	ILE	ALA	ASP	SER	SER	LEU	ALA	LEU	VAL	THR	GLU	PRO
Y308	A309	L310	R311	V312	C313	M314	E315	D316	E317	K318	G319	N320	E321	C322	L323	H324	I325	D326	F327	P328	L329	T330	V331	A332	T333	I334	P335	Y336	R337	I338	P339	N340	A341	P342	P343	P344	P345	V346	D347	Y348	D349	F350	C351	S352	N353	H354	V355	E356	G357	G358	K359	Y360	V361	S362	P363	E364	F365	R366	L367

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99248	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	66.937	Depositor
Minimum map value	-42.398	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.0	Depositor
Map size ( $\text{\AA}$ )	335.6, 335.6, 335.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.839, 0.839, 0.839	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, PLM, NAG, PEE, CA

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	0.26	0/4987	0.50	0/6763
1	B	0.26	0/4987	0.47	0/6763
2	C	0.25	0/1569	0.50	0/2111
2	E	0.26	0/1569	0.52	0/2111
3	D	0.24	0/347	0.56	0/471
3	F	0.24	0/347	0.53	0/471
4	J	0.25	0/2938	0.52	0/3979
All	All	0.25	0/16744	0.50	0/22669

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

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	4864	0	4941	84	0
1	B	4864	0	4941	90	0
2	C	1536	0	1484	39	0
2	E	1536	0	1484	20	0
3	D	343	0	377	5	0
3	F	343	0	378	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	2878	0	2908	40	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	E	2	0	0	0	0
6	A	42	0	58	4	0
6	B	42	0	58	4	0
7	A	35	0	44	3	0
7	B	35	0	44	0	0
8	A	14	0	13	0	0
8	B	14	0	13	1	0
9	D	14	0	22	4	0
9	F	14	0	22	1	0
All	All	16582	0	16787	278	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 8.

All (278) 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)
3:F:44:CYS:SG	9:F:201:PLM:C1	2.38	1.11
9:D:201:PLM:C9	9:D:201:PLM:CD	2.48	0.92
1:A:868:LEU:HD23	1:A:871:LEU:HD12	1.49	0.92
9:D:201:PLM:CD	9:D:201:PLM:H92	2.05	0.85
1:A:378:VAL:HG11	1:A:446:ALA:HB1	1.64	0.79
4:J:63:ILE:HG12	4:J:156:ILE:HG12	1.67	0.77
1:B:407:PRO:O	1:B:410:PHE:HB2	1.85	0.76
1:B:245:TYR:HE1	1:B:818:PRO:HD2	1.50	0.74
1:A:814:ARG:HH22	1:A:823:GLN:HA	1.53	0.73
1:B:740:TRP:HA	1:B:743:LEU:HD23	1.69	0.73
1:B:698:ARG:NH2	1:B:718:PRO:O	2.21	0.73
4:J:212:ARG:NH1	4:J:214:ALA:O	2.21	0.72
1:B:349:ARG:HB2	1:B:352:GLN:HG3	1.73	0.71
4:J:53:VAL:HG23	4:J:126:PHE:HE2	1.56	0.69
1:B:769:MET:O	3:F:49:ARG:NH1	2.26	0.69
2:C:73:VAL:HG21	2:C:100:LEU:HD23	1.75	0.69
1:B:147:THR:HG21	2:E:35:THR:HG21	1.74	0.68
1:B:105:ARG:HA	1:B:108:LYS:HE2	1.75	0.67
4:J:260:MET:HE1	4:J:262:CYS:HB2	1.77	0.67
1:A:324:ASN:OD1	1:A:776:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:201:PLM:CD	9:D:201:PLM:H91	2.24	0.67
1:A:188:ALA:HB2	1:A:273:ILE:HD11	1.77	0.66
4:J:204:LEU:HB2	4:J:231:GLN:HE22	1.60	0.66
1:B:245:TYR:CE1	1:B:818:PRO:HD2	2.29	0.66
1:A:175:ARG:HG2	6:A:1303:PEE:H7	1.76	0.66
1:B:248:TYR:HB3	1:B:262:LEU:HD21	1.78	0.66
4:J:351:CYS:O	4:J:388:ARG:NH2	2.29	0.66
1:B:104:ARG:O	1:B:108:LYS:HG3	1.97	0.65
1:B:701:TRP:O	1:B:705:CYS:HB2	1.97	0.65
2:C:186:VAL:HG13	2:C:187:VAL:HG13	1.79	0.64
2:E:91:VAL:HG21	2:E:128:ILE:HA	1.79	0.64
2:C:38:ASP:OD1	2:C:41:ARG:NH2	2.30	0.64
1:B:196:GLU:OE2	1:B:215:LYS:NZ	2.29	0.64
2:C:91:VAL:HG21	2:C:128:ILE:HA	1.79	0.64
1:B:813:SER:OG	1:B:816:CYS:SG	2.54	0.64
1:A:210:ARG:NH1	1:A:251:ASP:OD2	2.30	0.63
4:J:140:GLU:HA	4:J:145:THR:HG22	1.80	0.63
1:A:214:ARG:HD3	1:A:816:CYS:HA	1.81	0.63
2:C:129:TYR:HE1	2:C:145:MET:HG3	1.64	0.62
4:J:33:SER:HB3	4:J:56:GLU:HB3	1.80	0.62
4:J:74:VAL:HG22	4:J:146:ILE:HG12	1.82	0.61
1:B:328:ALA:O	1:B:332:LYS:HG3	2.01	0.60
1:A:298:LYS:CB	1:A:880:THR:HA	2.32	0.60
1:B:398:VAL:O	1:B:401:THR:HG22	2.02	0.60
1:A:407:PRO:O	1:A:410:PHE:HB2	2.01	0.60
1:B:422:ARG:C	1:B:422:ARG:HD3	2.23	0.60
1:B:374:ILE:HG12	1:B:399:VAL:HG22	1.83	0.59
1:A:213:THR:HG23	1:A:214:ARG:HG3	1.84	0.59
1:A:426:ARG:HD2	1:A:781:ALA:HB1	1.85	0.59
1:B:263:PRO:HG3	1:B:818:PRO:HB2	1.85	0.59
1:B:186:LEU:O	1:B:190:VAL:HG23	2.03	0.59
2:E:150:THR:HG22	2:E:153:GLU:H	1.67	0.58
3:F:37:ILE:O	3:F:41:ILE:HG12	2.03	0.58
2:C:74:GLU:HG3	2:C:85:LYS:HD2	1.86	0.58
1:A:124:SER:O	1:A:128:MET:HG2	2.03	0.58
1:B:395:VAL:HG13	1:B:396:PRO:HD3	1.86	0.58
1:A:679:LEU:HD23	1:A:738:MET:CE	2.34	0.57
1:B:181:ASN:HD21	1:B:753:ASN:HB3	1.68	0.57
1:B:420:HIS:HD2	1:B:422:ARG:HB3	1.69	0.57
3:D:53:THR:OG1	3:D:56:GLN:OE1	2.23	0.57
3:D:37:ILE:O	3:D:41:ILE:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LYS:HG2	1:A:789:LEU:HD21	1.87	0.56
2:C:45:ARG:HD3	2:C:201:ILE:HD11	1.87	0.56
2:C:163:ILE:O	2:C:167:ILE:HG12	2.05	0.56
1:A:722:GLU:N	1:A:722:GLU:OE2	2.39	0.56
1:B:326:VAL:HG21	2:E:151:ARG:HD2	1.88	0.56
2:C:94:GLU:HG3	2:C:96:GLY:H	1.71	0.56
2:C:182:GLU:O	2:C:186:VAL:HG12	2.06	0.56
1:A:186:LEU:O	1:A:190:VAL:HG23	2.05	0.56
1:B:105:ARG:HH22	1:B:109:LEU:HD22	1.70	0.56
1:B:416:MET:SD	1:B:416:MET:N	2.79	0.55
1:B:367:LEU:O	1:B:371:ILE:HG13	2.07	0.55
2:E:111:VAL:HG23	2:E:120:LEU:HG	1.88	0.55
1:A:417:GLU:HB3	1:A:419:TYR:CE2	2.41	0.55
1:A:679:LEU:HD23	1:A:738:MET:HE2	1.89	0.55
1:B:671:ILE:O	1:B:675:GLU:HG2	2.06	0.55
1:A:297:SER:O	2:C:189:ARG:NH1	2.39	0.54
2:C:58:MET:SD	2:C:63:PRO:HG3	2.48	0.54
2:C:115:MET:SD	2:C:115:MET:N	2.81	0.54
4:J:241:LEU:O	4:J:264:VAL:N	2.38	0.54
2:C:122:LEU:HD13	2:C:184:GLU:HG3	1.90	0.54
1:B:735:ASN:O	1:B:739:ILE:HG12	2.08	0.54
1:A:206:GLY:O	1:A:210:ARG:HG3	2.06	0.54
1:A:245:TYR:HD2	1:A:266:TYR:CZ	2.26	0.53
4:J:363:PRO:HA	4:J:366:ARG:HE	1.73	0.53
4:J:53:VAL:HG23	4:J:126:PHE:CE2	2.41	0.53
1:B:770:THR:HG22	3:F:50:ILE:HD12	1.90	0.53
1:A:214:ARG:NH1	1:A:248:TYR:O	2.42	0.53
1:B:174:LEU:HD13	1:B:732:ILE:HD12	1.91	0.53
1:A:147:THR:HG21	2:C:35:THR:HG21	1.91	0.53
1:A:687:THR:HG21	1:A:760:LEU:HD11	1.90	0.52
2:C:118:LEU:HD22	2:C:194:ILE:HD11	1.92	0.52
1:B:668:TRP:NE1	1:B:669:GLU:OE1	2.43	0.51
1:B:845:ILE:HD12	1:B:848:ILE:HD12	1.92	0.51
2:C:112:PHE:HB3	2:C:199:ILE:HB	1.92	0.51
2:C:113:SER:O	2:C:121:LYS:NZ	2.31	0.51
1:A:214:ARG:HH12	1:A:249:SER:HA	1.75	0.51
1:B:374:ILE:O	1:B:378:VAL:HG23	2.10	0.51
1:A:867:PHE:CZ	1:A:871:LEU:HD11	2.45	0.51
1:B:285:MET:HE1	1:B:793:LEU:HD22	1.93	0.51
3:D:47:ARG:HH12	3:D:49:ARG:HB2	1.76	0.51
1:A:263:PRO:HB2	1:A:828:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:58:MET:O	2:E:58:MET:HG2	2.12	0.50
1:A:455:ARG:NH2	1:A:665:ASP:OD2	2.44	0.50
1:B:420:HIS:CD2	1:B:422:ARG:HB3	2.46	0.50
1:B:205:GLU:OE2	8:B:1305:NAG:O7	2.30	0.50
1:A:140:ARG:NH1	2:C:26:ASP:OD1	2.39	0.50
1:B:331:ILE:O	1:B:335:GLU:HG2	2.12	0.50
1:A:249:SER:OG	1:A:251:ASP:OD1	2.30	0.50
1:B:248:TYR:HB2	1:B:818:PRO:HD3	1.94	0.50
1:A:226:ASP:N	1:A:226:ASP:OD1	2.44	0.49
1:A:207:ARG:O	1:A:211:THR:OG1	2.22	0.49
1:A:868:LEU:O	1:A:871:LEU:HB2	2.13	0.49
1:A:868:LEU:HA	1:A:871:LEU:HB2	1.94	0.49
1:B:396:PRO:HA	1:B:679:LEU:HD13	1.94	0.49
1:B:814:ARG:HD3	1:B:820:ALA:O	2.12	0.49
1:A:740:TRP:HA	1:A:743:LEU:HD23	1.94	0.49
2:C:28:TYR:HD2	2:C:39:ILE:HD12	1.77	0.49
1:A:683:ASP:OD2	1:A:756:LYS:NZ	2.33	0.49
1:B:170:TYR:HB2	1:B:725:VAL:HG13	1.94	0.49
4:J:76:ALA:HB3	4:J:91:ASP:OD1	2.13	0.49
2:C:63:PRO:O	2:C:101:SER:OG	2.31	0.49
2:E:87:ARG:NH2	2:E:130:ASP:O	2.44	0.49
1:B:100:MET:HG2	2:E:103:ASP:HB3	1.95	0.49
1:B:665:ASP:O	1:B:815:SER:OG	2.29	0.49
1:A:146:LYS:HG3	6:A:1303:PEE:H17	1.95	0.48
1:A:245:TYR:CE2	1:A:818:PRO:HD2	2.49	0.48
1:B:733:ILE:HG12	1:B:792:LEU:HD13	1.95	0.48
1:B:117:HIS:ND1	1:B:117:HIS:O	2.46	0.48
1:A:717:PHE:N	1:A:718:PRO:HD2	2.27	0.48
1:A:404:HIS:HE2	1:A:687:THR:HG1	1.58	0.48
1:A:671:ILE:O	1:A:675:GLU:HG2	2.14	0.48
2:C:28:TYR:O	2:C:32:THR:OG1	2.28	0.48
6:B:1303:PEE:H25	6:B:1303:PEE:H32	1.60	0.48
1:A:263:PRO:HG3	1:A:818:PRO:HB2	1.95	0.48
4:J:316:ASP:OD1	4:J:320:ASN:N	2.35	0.48
2:C:61:ASN:ND2	4:J:184:SER:OG	2.46	0.48
4:J:149:TYR:HB3	4:J:167:TYR:HD1	1.79	0.48
4:J:67:ARG:HH21	4:J:106:ASP:HA	1.78	0.47
1:A:174:LEU:HD13	1:A:732:ILE:HD12	1.95	0.47
1:A:876:ARG:O	1:A:880:THR:HG23	2.15	0.47
3:D:52:ARG:HB3	3:D:56:GLN:NE2	2.29	0.47
1:A:797:LEU:HA	1:A:800:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:SER:HB2	1:B:406:PHE:CE2	2.49	0.47
2:C:23:GLU:O	2:C:27:GLU:HG2	2.15	0.47
2:E:43:TYR:OH	2:E:56:THR:O	2.31	0.47
1:B:254:LEU:HD13	1:B:262:LEU:HB2	1.97	0.46
1:B:151:PRO:HB3	6:B:1303:PEE:H67	1.97	0.46
1:B:128:MET:O	1:B:132:ARG:HD3	2.15	0.46
2:E:95:ASP:N	2:E:95:ASP:OD1	2.48	0.46
4:J:66:ILE:HG22	4:J:103:TRP:HB3	1.97	0.46
1:B:230:VAL:HG13	1:B:235:ASP:HB2	1.96	0.46
4:J:230:ARG:HA	4:J:275:ASN:HA	1.98	0.46
1:B:143:SER:O	1:B:147:THR:HG23	2.16	0.46
1:B:207:ARG:O	1:B:211:THR:HG23	2.16	0.46
1:A:702:ILE:HG21	1:A:720:TYR:CE1	2.51	0.46
4:J:365:PHE:HE1	4:J:387:TYR:HB3	1.80	0.46
2:E:38:ASP:OD1	2:E:41:ARG:NH1	2.45	0.46
2:C:132:ASP:N	2:C:132:ASP:OD1	2.49	0.45
4:J:212:ARG:NH2	4:J:336:TYR:HE1	2.14	0.45
1:B:861:LEU:HA	1:B:864:ILE:HG22	1.99	0.45
2:E:43:TYR:HD1	2:E:43:TYR:O	2.00	0.45
1:B:312:TRP:HZ3	1:B:326:VAL:HG23	1.81	0.45
2:C:63:PRO:HB3	2:C:102:PHE:HD2	1.82	0.45
1:A:396:PRO:HG3	1:A:678:LYS:HE3	1.98	0.45
1:B:395:VAL:CG1	1:B:396:PRO:HD3	2.47	0.45
1:B:696:LEU:HD22	1:B:766:TRP:HH2	1.81	0.45
4:J:66:ILE:CG2	4:J:103:TRP:HB3	2.46	0.45
4:J:237:LEU:HB2	4:J:269:SER:HB3	1.99	0.45
4:J:264:VAL:HG13	4:J:355:VAL:HG23	1.98	0.45
2:C:100:LEU:HD12	2:C:104:ASP:HB2	1.99	0.45
1:A:296:GLY:HA2	2:C:189:ARG:HA	1.98	0.45
1:A:303:ILE:O	1:A:307:LYS:HG2	2.17	0.45
1:B:722:GLU:OE2	1:B:722:GLU:N	2.50	0.45
1:A:165:SER:O	1:A:165:SER:OG	2.31	0.44
1:A:290:ARG:HB2	1:A:291:MET:SD	2.56	0.44
1:A:720:TYR:HD2	1:A:773:VAL:HG11	1.83	0.44
2:C:76:MET:HE3	2:C:76:MET:HB3	1.88	0.44
2:C:92:PHE:O	2:C:104:ASP:HB3	2.17	0.44
3:D:19:ALA:HB3	3:D:22:LEU:HB2	1.99	0.44
1:B:112:LYS:HA	1:B:112:LYS:HD3	1.74	0.44
6:B:1303:PEE:H20	6:B:1303:PEE:H26	1.64	0.44
2:C:95:ASP:OD1	2:C:95:ASP:N	2.50	0.44
2:E:107:ASP:O	2:E:111:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:ALA:HB1	1:B:298:LYS:CB	2.47	0.44
6:A:1303:PEE:H60	6:A:1303:PEE:H54	1.76	0.44
1:B:269:VAL:O	1:B:273:ILE:HG12	2.17	0.44
7:A:1304:3PE:H282	7:A:1304:3PE:H342	1.99	0.44
1:A:842:LEU:O	1:A:846:ARG:HG2	2.18	0.43
1:A:858:ILE:O	1:A:862:ILE:HG12	2.18	0.43
1:B:227:GLU:O	1:B:228:LEU:HB3	2.18	0.43
1:B:101:THR:HA	1:B:104:ARG:HD3	2.00	0.43
1:A:701:TRP:O	1:A:705:CYS:HB2	2.18	0.43
4:J:62:LYS:O	4:J:156:ILE:HG23	2.18	0.43
1:A:814:ARG:NH1	1:A:822:TYR:O	2.50	0.43
3:F:42:VAL:HG22	3:F:46:MET:SD	2.58	0.43
1:A:100:MET:HG2	2:C:103:ASP:HB3	1.99	0.43
1:B:450:LYS:HD2	1:B:450:LYS:HA	1.87	0.43
1:B:108:LYS:O	1:B:111:GLN:HG2	2.18	0.43
6:B:1303:PEE:H54	6:B:1303:PEE:H60	1.84	0.43
1:A:262:LEU:HB3	1:A:263:PRO:HD3	1.99	0.43
1:A:420:HIS:HB3	1:A:423:THR:HG22	2.00	0.43
2:C:25:LEU:HD13	2:C:36:ARG:HD3	2.00	0.43
2:C:53:LYS:NZ	2:C:68:LEU:HA	2.34	0.43
1:A:179:PHE:HB2	6:A:1303:PEE:H8	2.01	0.42
1:B:129:GLU:O	1:B:133:LYS:HG2	2.19	0.42
1:A:363:ILE:HD11	1:A:413:ILE:HG21	2.01	0.42
1:B:349:ARG:H	1:B:352:GLN:HE21	1.67	0.42
2:C:58:MET:O	2:C:58:MET:HG3	2.18	0.42
1:B:186:LEU:HD23	1:B:186:LEU:HA	1.84	0.42
4:J:365:PHE:CE1	4:J:387:TYR:HB3	2.54	0.42
1:A:444:ILE:HD13	1:A:802:PRO:HG2	2.00	0.42
1:B:401:THR:O	1:B:405:VAL:N	2.52	0.42
4:J:290:LEU:HA	4:J:291:PRO:HD3	1.91	0.42
4:J:302:ARG:HE	4:J:302:ARG:HB3	1.71	0.42
1:A:375:ILE:O	1:A:378:VAL:HG12	2.20	0.42
7:A:1304:3PE:H12	9:D:201:PLM:H22	2.02	0.42
1:B:384:GLN:HE21	1:B:384:GLN:HB3	1.72	0.42
2:E:139:HIS:ND1	2:E:163:ILE:HG21	2.34	0.42
4:J:64:ARG:HB2	4:J:155:ASP:OD2	2.19	0.42
4:J:78:LEU:HD13	4:J:256:GLU:HB2	2.00	0.42
1:A:422:ARG:HE	1:A:783:ARG:NH1	2.18	0.42
1:B:352:GLN:OE1	1:B:353:PHE:N	2.53	0.42
1:B:857:ILE:HD13	1:B:857:ILE:HA	1.85	0.42
4:J:40:LYS:HA	4:J:40:LYS:HD2	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:118:ALA:O	4:J:122:HIS:NE2	2.41	0.42
4:J:177:SER:OG	4:J:334:ILE:O	2.23	0.42
1:A:677:VAL:HG22	1:A:749:LEU:HD13	2.01	0.42
1:A:679:LEU:HD23	1:A:738:MET:HE1	2.00	0.42
4:J:293:VAL:HG12	4:J:355:VAL:HG21	2.00	0.42
1:A:696:LEU:HA	1:A:771:CYS:SG	2.60	0.42
1:B:412:LEU:O	1:B:415:LYS:HB2	2.20	0.42
4:J:64:ARG:NH2	4:J:157:PRO:HA	2.34	0.42
1:B:777:GLU:HG2	1:B:779:PHE:CZ	2.55	0.42
1:A:735:ASN:O	1:A:739:ILE:HG12	2.20	0.41
1:B:233:HIS:NE2	1:B:393:ASN:HB2	2.36	0.41
1:B:307:LYS:HZ1	1:B:332:LYS:C	2.23	0.41
2:E:42:LEU:HD23	2:E:42:LEU:HA	1.82	0.41
2:E:45:ARG:NH1	2:E:78:GLU:OE2	2.53	0.41
1:A:313:ASP:OD1	1:A:315:THR:OG1	2.37	0.41
1:A:143:SER:O	1:A:147:THR:HG23	2.20	0.41
1:A:455:ARG:HD2	1:A:455:ARG:HA	1.85	0.41
1:A:709:TRP:HD1	1:A:713:ILE:HG21	1.85	0.41
1:A:112:LYS:HA	1:A:112:LYS:HD3	1.72	0.41
7:A:1304:3PE:H371	7:A:1304:3PE:H3A2	1.69	0.41
2:C:39:ILE:HD13	2:C:106:LEU:HD11	2.03	0.41
1:A:811:SER:HA	1:A:812:PRO:HD3	1.95	0.41
2:C:92:PHE:HE2	2:C:128:ILE:HD11	1.86	0.41
1:A:148:TYR:HE1	2:C:37:LYS:HB2	1.86	0.41
1:B:302:TYR:N	1:B:302:TYR:CD1	2.89	0.41
1:B:361:ILE:HD13	1:B:361:ILE:HA	1.91	0.41
1:A:868:LEU:HD22	1:B:872:VAL:HG21	2.03	0.41
1:A:879:ASN:O	1:A:880:THR:C	2.59	0.41
2:E:21:THR:O	2:E:25:LEU:HG	2.20	0.41
2:E:84:PHE:HZ	2:E:149:LEU:HB2	1.86	0.41
4:J:64:ARG:HH21	4:J:157:PRO:HA	1.84	0.41
1:A:359:ALA:HB3	1:A:417:GLU:OE1	2.20	0.41
1:A:382:GLN:H	1:A:382:GLN:HG2	1.71	0.41
1:A:777:GLU:OE2	1:A:777:GLU:N	2.54	0.41
1:B:233:HIS:CE1	1:B:389:LEU:HB3	2.56	0.41
1:B:821:ARG:HG2	1:B:821:ARG:HH11	1.86	0.41
2:E:131:TYR:HB2	2:E:141:ASP:OD1	2.21	0.41
4:J:204:LEU:HB2	4:J:231:GLN:NE2	2.30	0.41
1:B:114:LEU:HD12	1:B:114:LEU:HA	1.83	0.40
1:B:168:SER:O	1:B:172:THR:HG23	2.22	0.40
1:B:868:LEU:O	1:B:872:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:202:GLY:O	4:J:231:GLN:NE2	2.48	0.40
4:J:217:CYS:HA	4:J:290:LEU:HD22	2.02	0.40
1:B:842:LEU:HA	1:B:845:ILE:HG22	2.03	0.40
2:E:92:PHE:CE1	2:E:111:VAL:HG11	2.56	0.40
1:A:875:LEU:HB2	1:B:875:LEU:CD2	2.52	0.40
1:B:228:LEU:HD13	3:F:25:TRP:HB2	2.03	0.40
1:B:298:LYS:CB	1:B:879:ASN:HD21	2.34	0.40
1:B:694:ILE:O	1:B:698:ARG:HB3	2.20	0.40
2:C:184:GLU:O	2:C:188:SER:HB2	2.22	0.40
1:A:239:ARG:HG3	1:A:674:GLN:NE2	2.37	0.40
1:B:323:SER:O	1:B:327:MET:HG2	2.22	0.40
4:J:44:TYR:HE1	4:J:171:ILE:HG21	1.87	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	598/1285 (46%)	577 (96%)	21 (4%)	0	100	100
1	B	598/1285 (46%)	579 (97%)	19 (3%)	0	100	100
2	C	182/201 (90%)	181 (100%)	1 (0%)	0	100	100
2	E	182/201 (90%)	178 (98%)	4 (2%)	0	100	100
3	D	44/117 (38%)	43 (98%)	1 (2%)	0	100	100
3	F	44/117 (38%)	42 (96%)	2 (4%)	0	100	100
4	J	357/469 (76%)	345 (97%)	12 (3%)	0	100	100
All	All	2005/3675 (55%)	1945 (97%)	60 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	517/1150 (45%)	507 (98%)	10 (2%)	57	80
1	B	517/1150 (45%)	505 (98%)	12 (2%)	50	77
2	C	171/185 (92%)	164 (96%)	7 (4%)	30	64
2	E	171/185 (92%)	166 (97%)	5 (3%)	42	72
3	D	35/96 (36%)	35 (100%)	0	100	100
3	F	35/96 (36%)	34 (97%)	1 (3%)	42	72
4	J	323/419 (77%)	315 (98%)	8 (2%)	47	76
All	All	1769/3281 (54%)	1726 (98%)	43 (2%)	51	76

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	MET
1	A	169	SER
1	A	181	ASN
1	A	201	SER
1	A	245	TYR
1	A	313	ASP
1	A	708	TRP
1	A	709	TRP
1	A	795	TRP
1	A	879	ASN
1	B	117	HIS
1	B	132	ARG
1	B	140	ARG
1	B	224	HIS
1	B	226	ASP
1	B	245	TYR
1	B	253	PHE
1	B	352	GLN
1	B	364	CYS
1	B	384	GLN

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Mol	Chain	Res	Type
1	B	795	TRP
1	B	823	GLN
2	C	22	ARG
2	C	30	ASP
2	C	58	MET
2	C	129	TYR
2	C	152	ASP
2	C	156	ASP
2	C	188	SER
2	E	28	TYR
2	E	43	TYR
2	E	68	LEU
2	E	152	ASP
2	E	177	SER
3	F	44	CYS
4	J	34	PHE
4	J	41	ASP
4	J	44	TYR
4	J	91	ASP
4	J	128	PHE
4	J	129	ASP
4	J	139	LEU
4	J	279	LYS

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	731	HIS
1	A	879	ASN
1	B	420	HIS
1	B	879	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	B	1305	-	14,14,15	0.46	0	19,19,21	0.73	0
7	3PE	B	1304	-	34,34,50	1.03	4 (11%)	37,39,55	1.13	2 (5%)
8	NAG	A	1305	-	14,14,15	0.47	0	19,19,21	0.73	0
6	PEE	B	1303	-	41,41,50	1.26	6 (14%)	44,46,55	1.23	2 (4%)
9	PLM	F	201	-	13,13,17	0.32	0	12,12,17	0.92	0
6	PEE	A	1303	-	41,41,50	1.25	6 (14%)	44,46,55	1.20	3 (6%)
7	3PE	A	1304	-	34,34,50	1.03	4 (11%)	37,39,55	1.16	2 (5%)
9	PLM	D	201	3	13,13,17	0.32	0	12,12,17	0.91	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	B	1305	-	-	2/6/22/26	0/1/1/1
7	3PE	B	1304	-	-	16/38/38/54	-
8	NAG	A	1305	-	-	0/6/22/26	0/1/1/1
6	PEE	B	1303	-	-	21/45/45/54	-
9	PLM	F	201	-	-	5/10/11/15	-
6	PEE	A	1303	-	-	25/45/45/54	-
7	3PE	A	1304	-	-	16/38/38/54	-
9	PLM	D	201	3	-	3/10/11/15	-



All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1303	PEE	C18-C19	3.70	1.53	1.31
6	A	1303	PEE	C18-C19	3.69	1.53	1.31
6	B	1303	PEE	C39-C38	3.69	1.53	1.31
6	A	1303	PEE	C39-C38	3.68	1.53	1.31
7	A	1304	3PE	O21-C2	-2.56	1.40	1.46
6	B	1303	PEE	O2-C2	-2.51	1.40	1.46
6	A	1303	PEE	O2-C2	-2.50	1.40	1.46
7	B	1304	3PE	O21-C2	-2.50	1.40	1.46
7	A	1304	3PE	O31-C31	2.44	1.40	1.33
6	B	1303	PEE	O3-C30	2.44	1.40	1.33
7	B	1304	3PE	O31-C31	2.41	1.40	1.33
6	A	1303	PEE	O3-C30	2.33	1.40	1.33
6	A	1303	PEE	O3-C3	-2.17	1.40	1.45
6	B	1303	PEE	O2-C10	2.14	1.40	1.34
7	B	1304	3PE	O21-C21	2.13	1.40	1.34
7	B	1304	3PE	O31-C3	-2.11	1.40	1.45
7	A	1304	3PE	O21-C21	2.11	1.40	1.34
6	B	1303	PEE	O3-C3	-2.08	1.40	1.45
6	A	1303	PEE	O2-C10	2.06	1.40	1.34
7	A	1304	3PE	O31-C3	-2.04	1.40	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1303	PEE	O2-C10-C11	4.18	120.52	111.50
7	A	1304	3PE	O21-C21-C22	4.10	120.34	111.50
7	B	1304	3PE	O21-C21-C22	4.09	120.31	111.50
6	A	1303	PEE	O2-C10-C11	3.84	119.77	111.50
7	A	1304	3PE	O31-C31-C32	2.71	120.42	111.91
6	B	1303	PEE	O3-C30-C31	2.71	120.42	111.91
7	B	1304	3PE	O31-C31-C32	2.49	119.71	111.91
6	A	1303	PEE	O3-C30-C31	2.44	119.57	111.91
6	A	1303	PEE	C17-C18-C19	-2.04	109.10	124.73

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1303	PEE	C1-O3P-P-O2P
6	A	1303	PEE	C1-O3P-P-O1P
6	A	1303	PEE	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
6	A	1303	PEE	C4-O4P-P-O1P
6	A	1303	PEE	O4P-C4-C5-N
6	B	1303	PEE	O2-C2-C3-O3
6	B	1303	PEE	C1-O3P-P-O1P
6	B	1303	PEE	O4P-C4-C5-N
6	B	1303	PEE	C37-C38-C39-C40
7	A	1304	3PE	C1-O11-P-O14
7	A	1304	3PE	O13-C11-C12-N
7	A	1304	3PE	O11-C1-C2-O21
7	A	1304	3PE	C22-C21-O21-C2
7	B	1304	3PE	C1-O11-P-O12
7	B	1304	3PE	C1-O11-P-O13
7	B	1304	3PE	C1-O11-P-O14
7	B	1304	3PE	O13-C11-C12-N
7	B	1304	3PE	O22-C21-O21-C2
7	A	1304	3PE	O22-C21-O21-C2
7	B	1304	3PE	C22-C21-O21-C2
6	B	1303	PEE	C31-C30-O3-C3
6	B	1303	PEE	O5-C30-O3-C3
8	B	1305	NAG	C8-C7-N2-C2
8	B	1305	NAG	O7-C7-N2-C2
6	A	1303	PEE	C1-O3P-P-O4P
6	A	1303	PEE	C4-O4P-P-O3P
7	A	1304	3PE	C11-O13-P-O11
9	F	201	PLM	C6-C7-C8-C9
9	F	201	PLM	C4-C5-C6-C7
9	D	201	PLM	C9-CA-CB-CC
6	A	1303	PEE	C11-C12-C13-C14
6	A	1303	PEE	O2-C2-C3-O3
7	B	1304	3PE	C25-C26-C27-C28
6	A	1303	PEE	C12-C13-C14-C15
6	B	1303	PEE	C39-C40-C41-C42
7	A	1304	3PE	C23-C24-C25-C26
9	D	201	PLM	C6-C7-C8-C9
6	B	1303	PEE	C12-C13-C14-C15
6	A	1303	PEE	C31-C30-O3-C3
7	A	1304	3PE	C33-C34-C35-C36
6	A	1303	PEE	C35-C36-C37-C38
7	A	1304	3PE	C21-C22-C23-C24
7	B	1304	3PE	C37-C38-C39-C3A
6	B	1303	PEE	C35-C36-C37-C38
6	B	1303	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
6	A	1303	PEE	O5-C30-O3-C3
7	A	1304	3PE	C1-O11-P-O13
7	B	1304	3PE	C21-C22-C23-C24
7	A	1304	3PE	C37-C38-C39-C3A
6	A	1303	PEE	C1-C2-C3-O3
6	B	1303	PEE	C1-C2-C3-O3
7	B	1304	3PE	C33-C34-C35-C36
6	A	1303	PEE	C30-C31-C32-C33
9	D	201	PLM	C7-C8-C9-CA
6	B	1303	PEE	C11-C12-C13-C14
7	B	1304	3PE	C31-C32-C33-C34
6	B	1303	PEE	C14-C15-C16-C17
9	F	201	PLM	C5-C6-C7-C8
7	A	1304	3PE	O11-C1-C2-C3
7	B	1304	3PE	C32-C33-C34-C35
6	A	1303	PEE	C14-C15-C16-C17
6	A	1303	PEE	C11-C10-O2-C2
6	A	1303	PEE	O4-C10-O2-C2
6	B	1303	PEE	C4-O4P-P-O3P
6	B	1303	PEE	C4-O4P-P-O1P
7	A	1304	3PE	C1-O11-P-O12
7	A	1304	3PE	C11-O13-P-O12
6	B	1303	PEE	O3P-C1-C2-C3
6	B	1303	PEE	O3P-C1-C2-O2
6	A	1303	PEE	C32-C33-C34-C35
7	A	1304	3PE	C35-C36-C37-C38
7	B	1304	3PE	C11-O13-P-O11
7	B	1304	3PE	C1-C2-C3-O31
6	B	1303	PEE	C34-C35-C36-C37
7	B	1304	3PE	C35-C36-C37-C38
9	F	201	PLM	C9-CA-CB-CC
6	A	1303	PEE	C37-C38-C39-C40
6	A	1303	PEE	C39-C40-C41-C42
9	F	201	PLM	C7-C8-C9-CA
7	B	1304	3PE	C26-C27-C28-C29
6	A	1303	PEE	O3P-C1-C2-C3
6	B	1303	PEE	C36-C37-C38-C39
6	B	1303	PEE	C38-C39-C40-C41
6	A	1303	PEE	C36-C37-C38-C39
6	A	1303	PEE	C38-C39-C40-C41
7	A	1304	3PE	C26-C27-C28-C29
6	B	1303	PEE	C4-O4P-P-O2P

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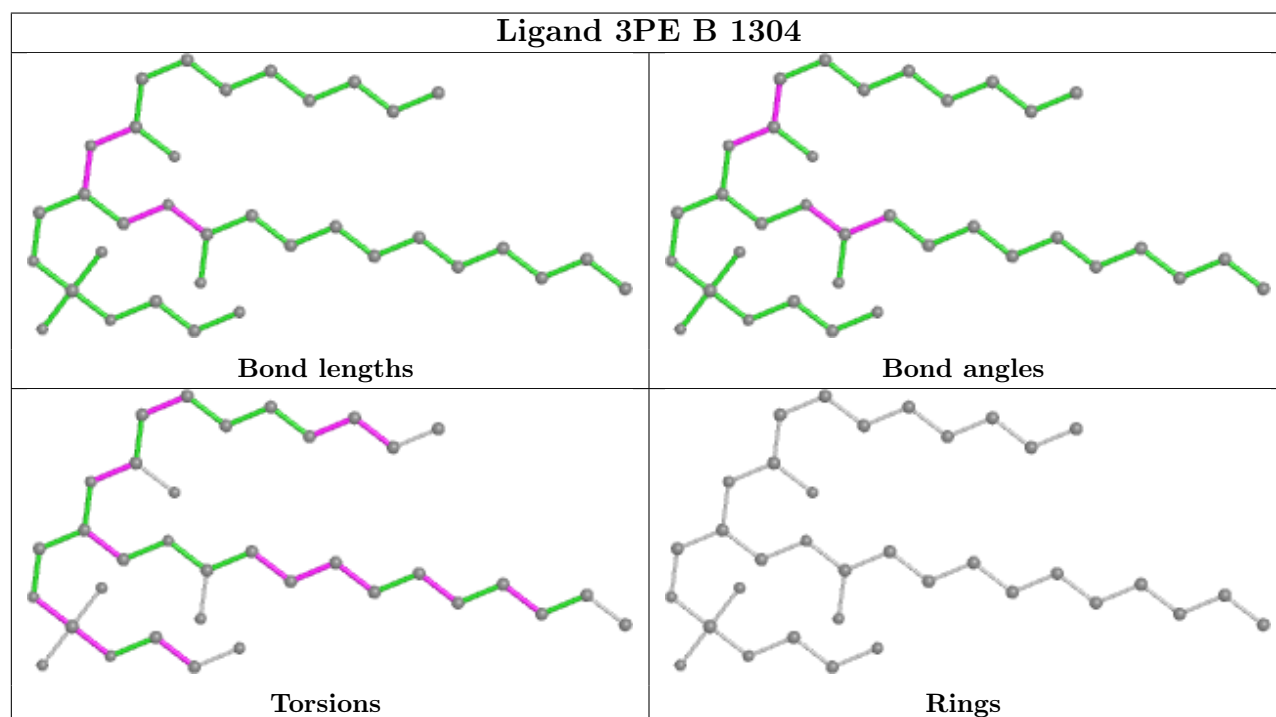
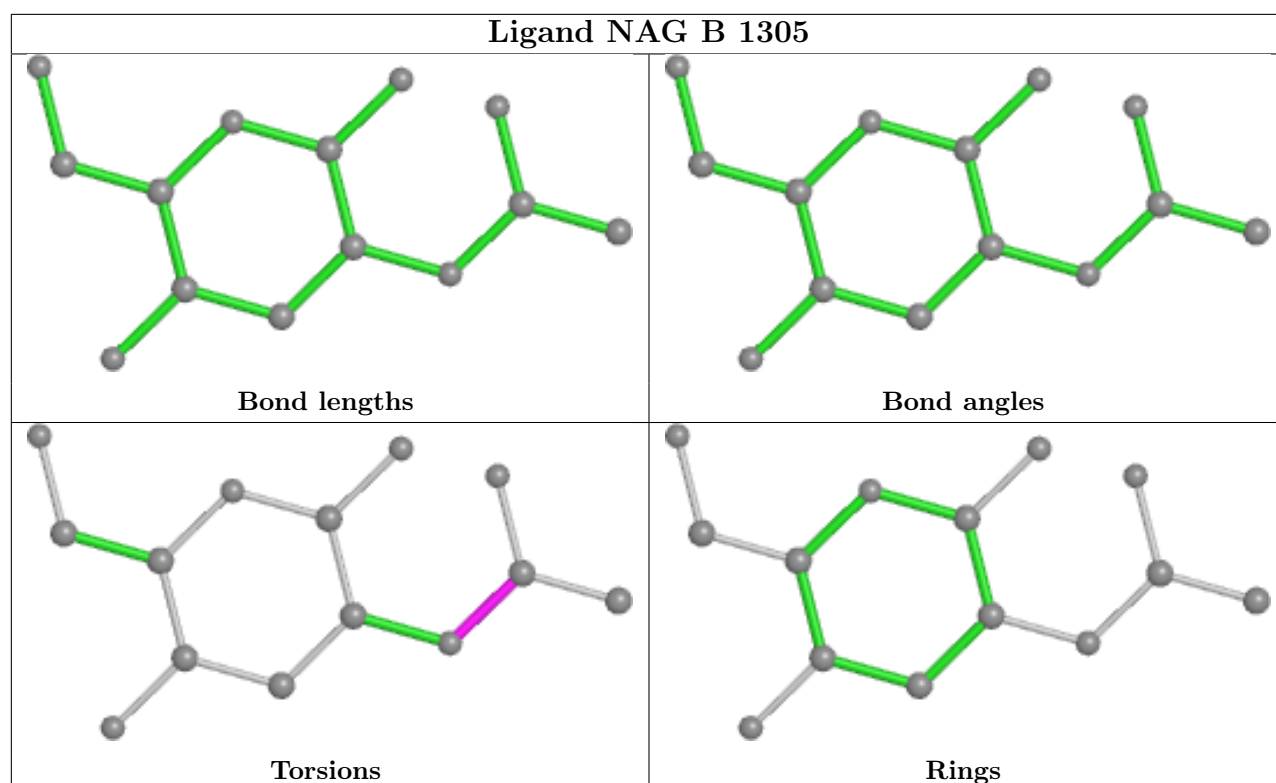
Mol	Chain	Res	Type	Atoms
6	A	1303	PEE	C16-C17-C18-C19

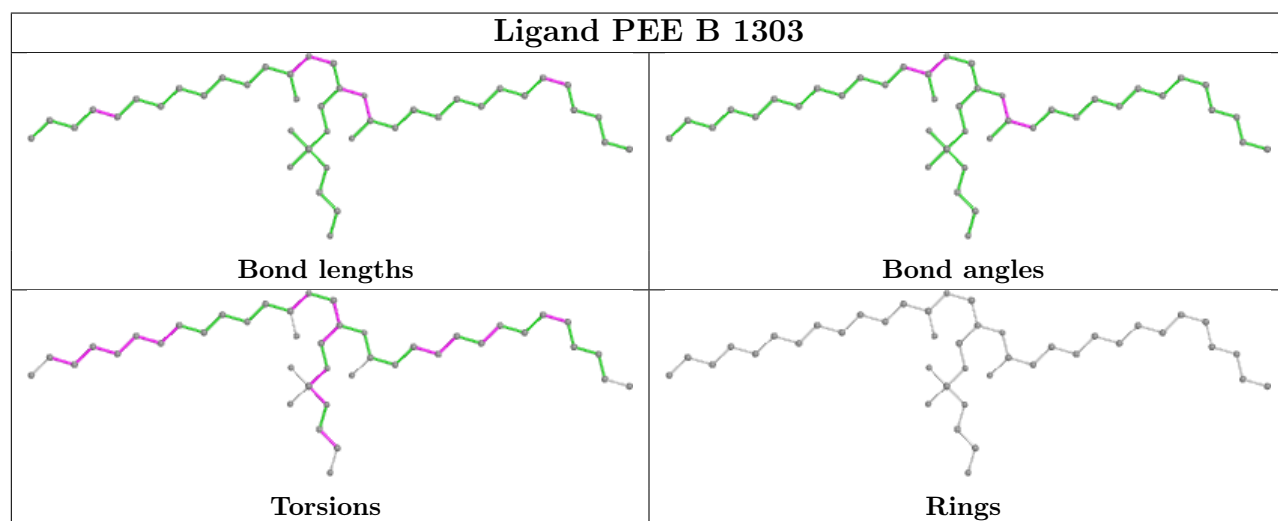
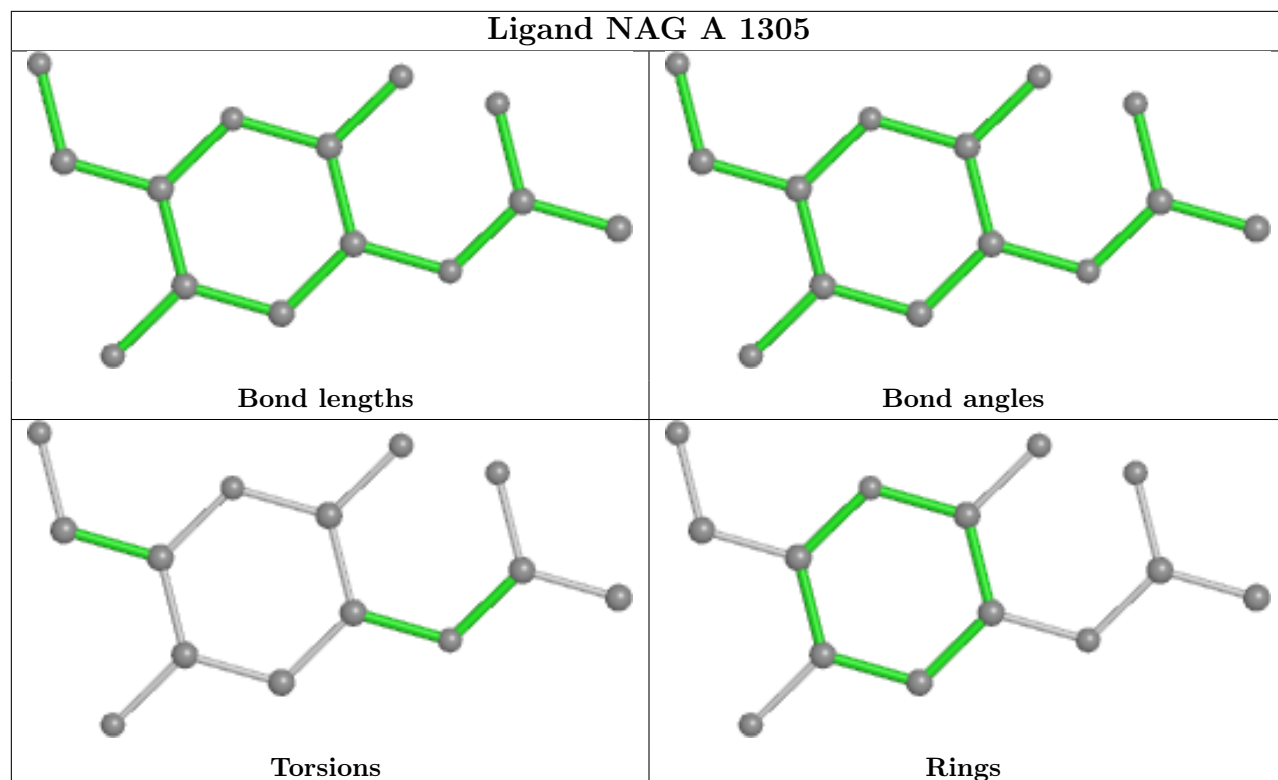
There are no ring outliers.

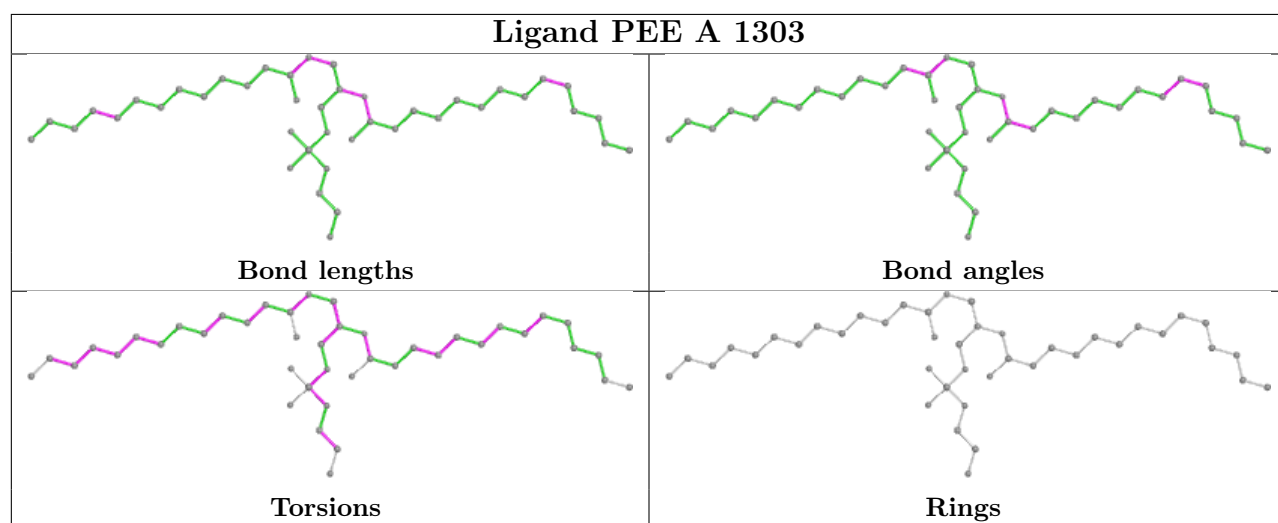
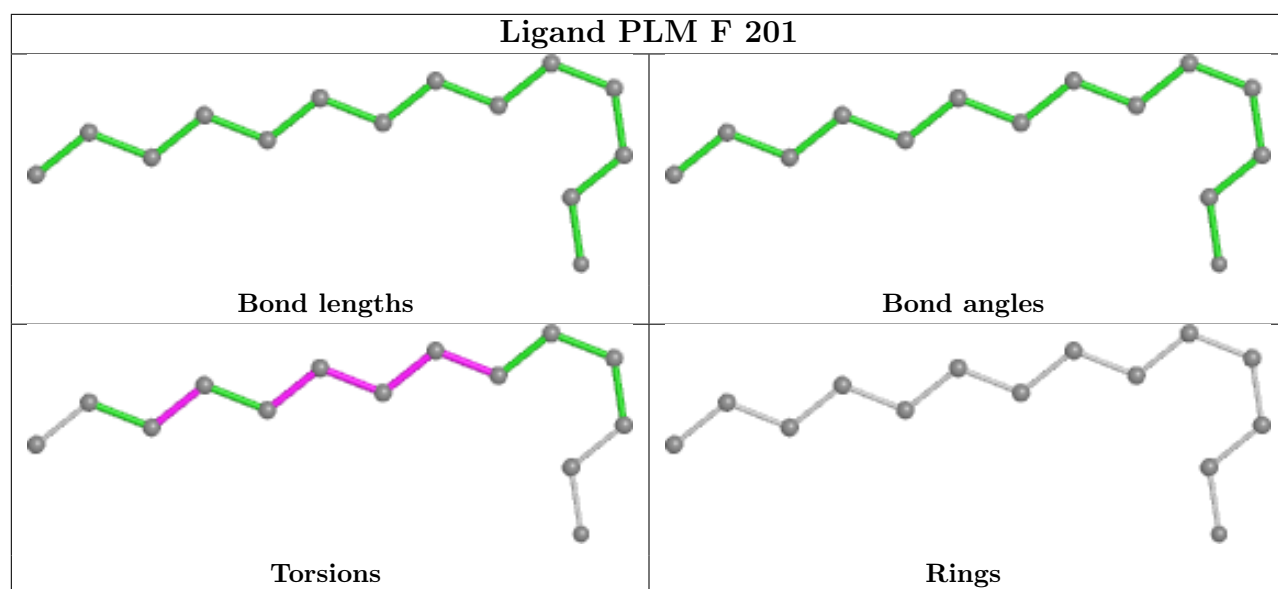
6 monomers are involved in 16 short contacts:

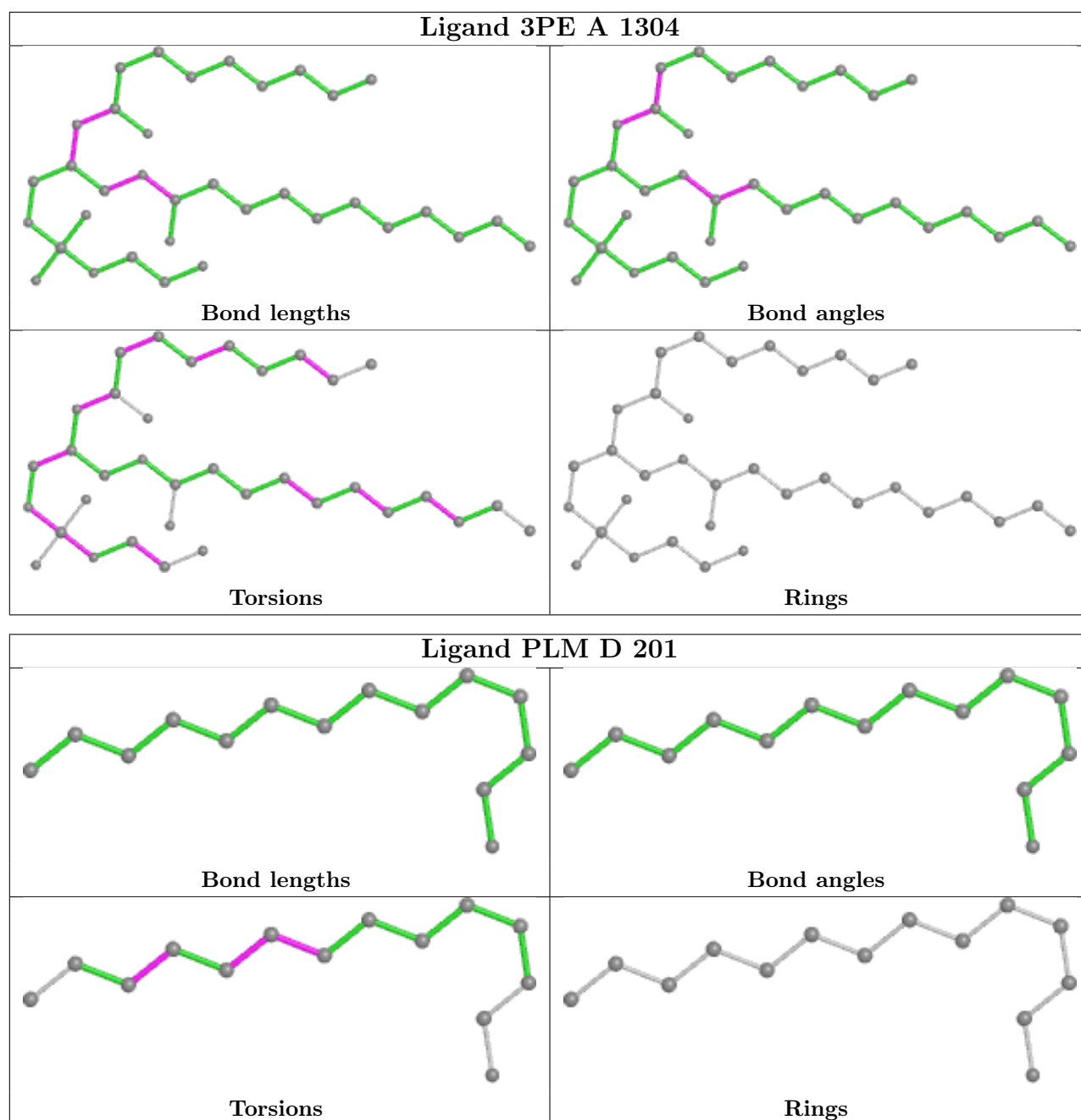
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1305	NAG	1	0
6	B	1303	PEE	4	0
9	F	201	PLM	1	0
6	A	1303	PEE	4	0
7	A	1304	3PE	3	0
9	D	201	PLM	4	0

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.



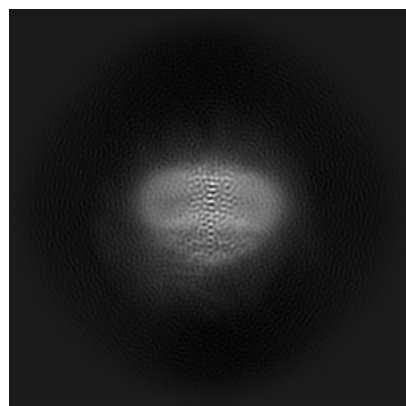
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26743. These allow visual inspection of the internal detail of the map and identification of artifacts.

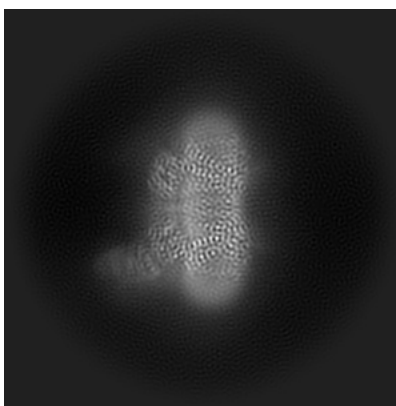
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

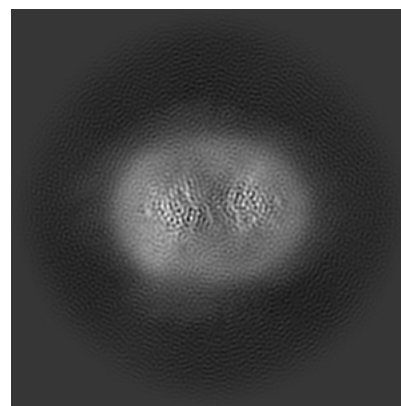
#### 6.1.1 Primary map



X

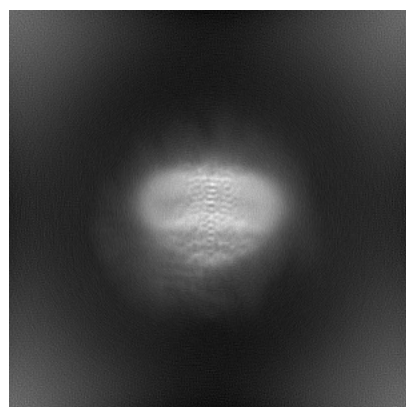


Y

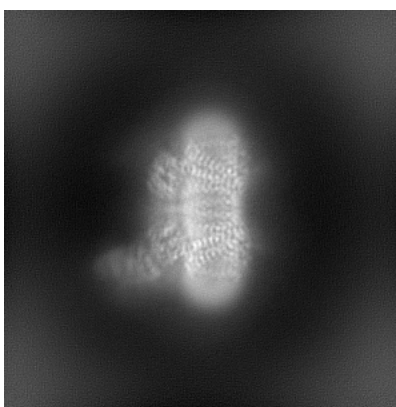


Z

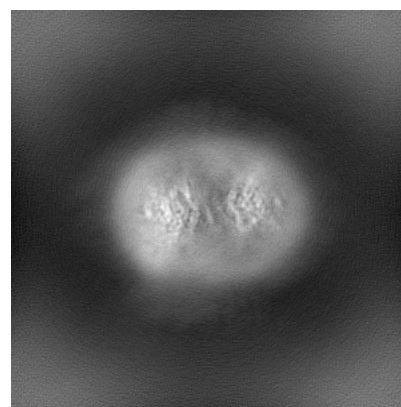
#### 6.1.2 Raw map



X



Y

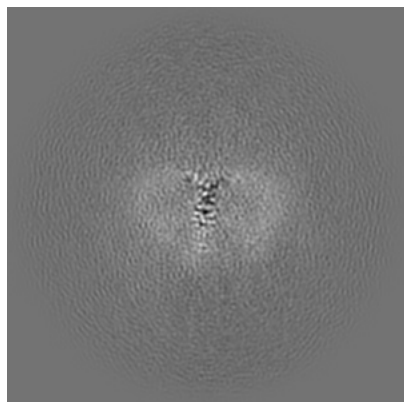


Z

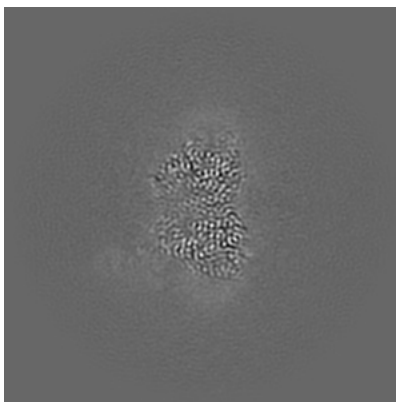
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

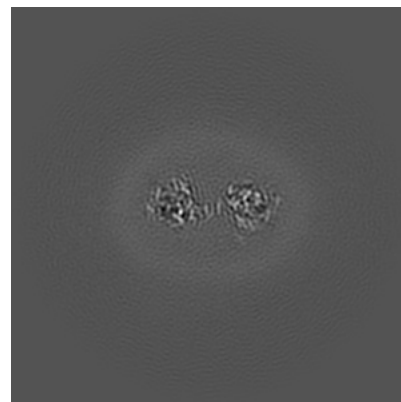
### 6.2.1 Primary map



X Index: 200

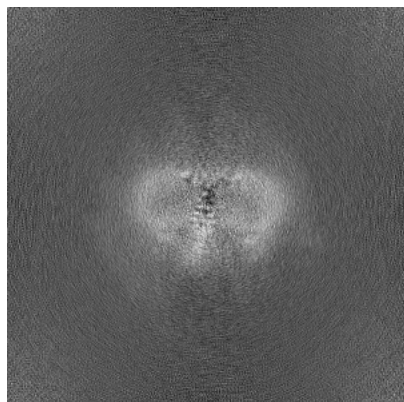


Y Index: 200

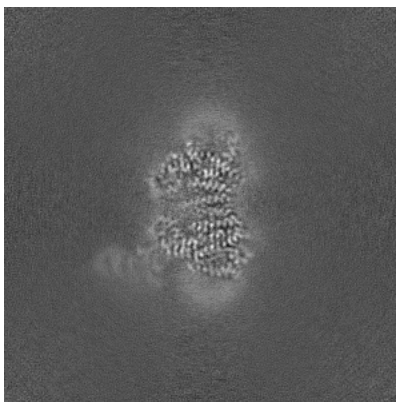


Z Index: 200

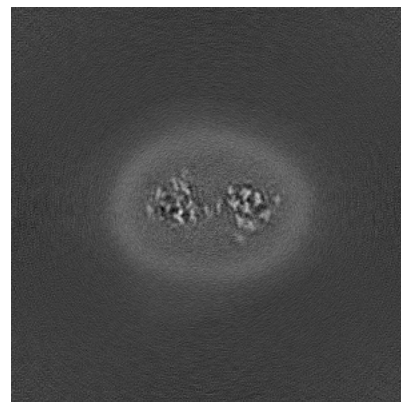
### 6.2.2 Raw map



X Index: 200



Y Index: 200

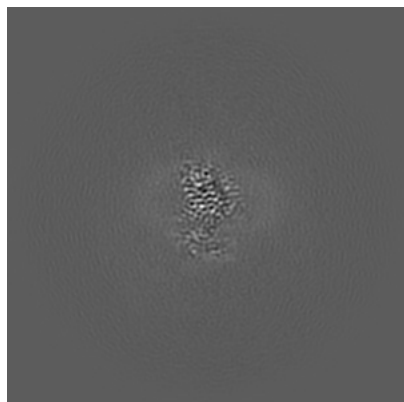


Z Index: 200

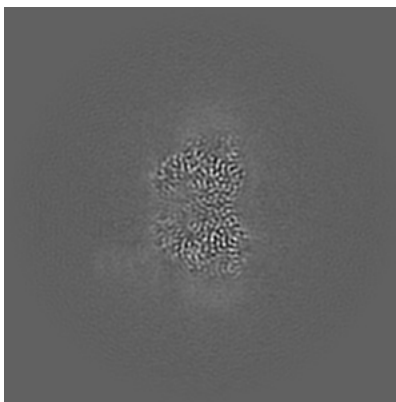
The images above show central slices of the map in three orthogonal directions.

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

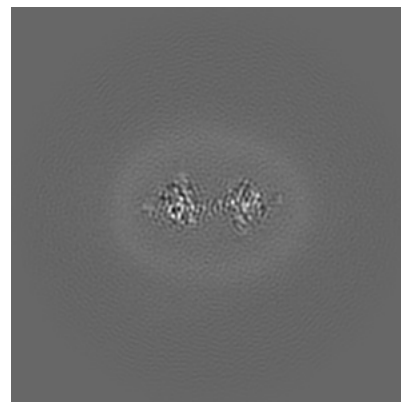
### 6.3.1 Primary map



X Index: 169

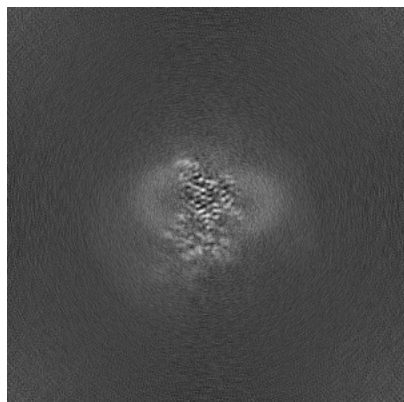


Y Index: 202

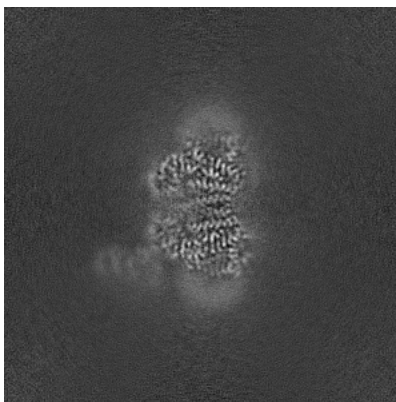


Z Index: 207

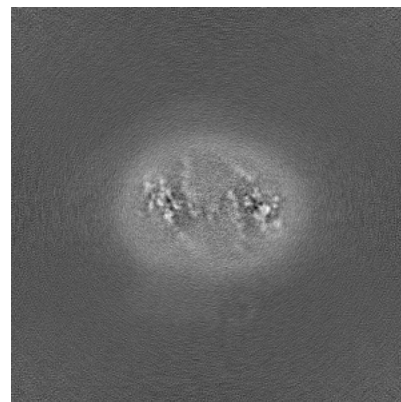
### 6.3.2 Raw map



X Index: 165



Y Index: 202

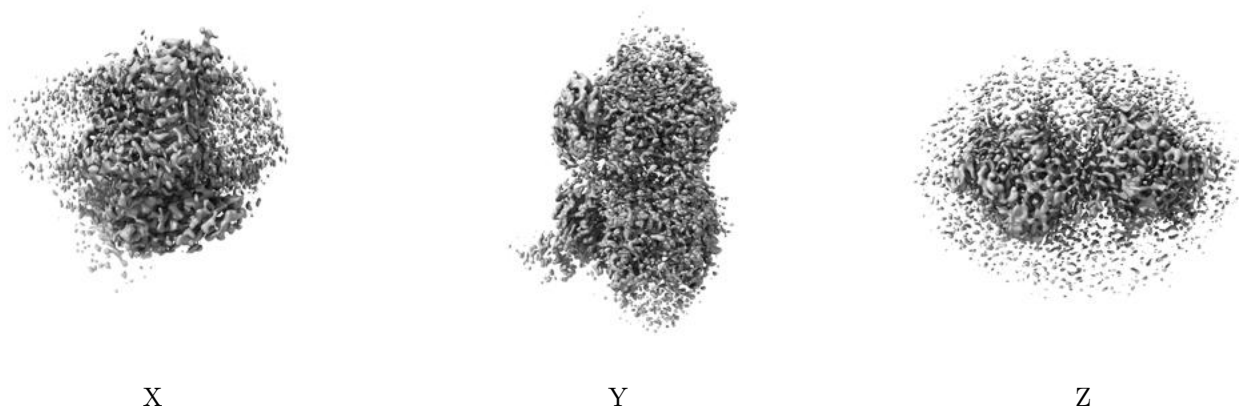


Z Index: 186

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

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

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

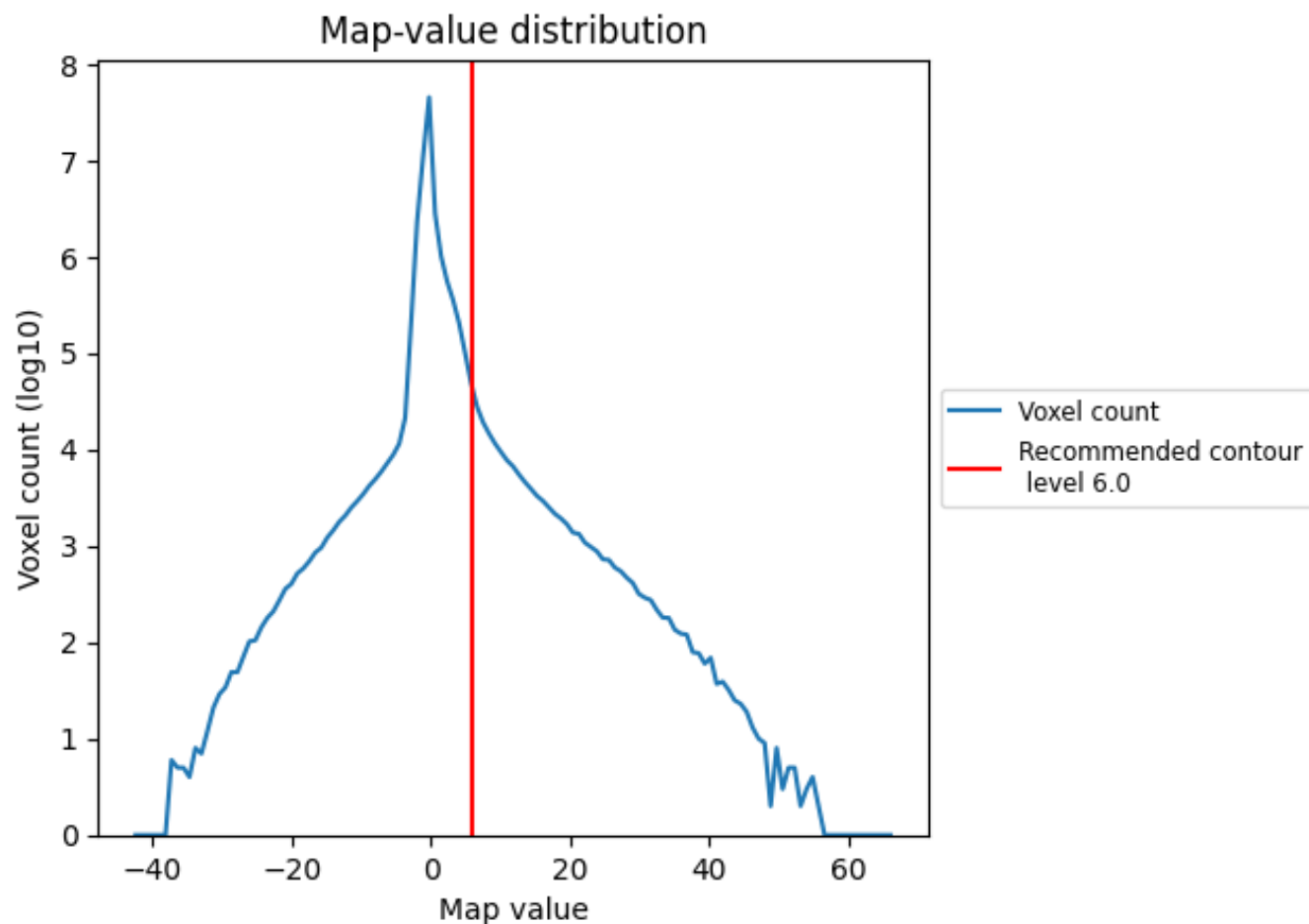
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

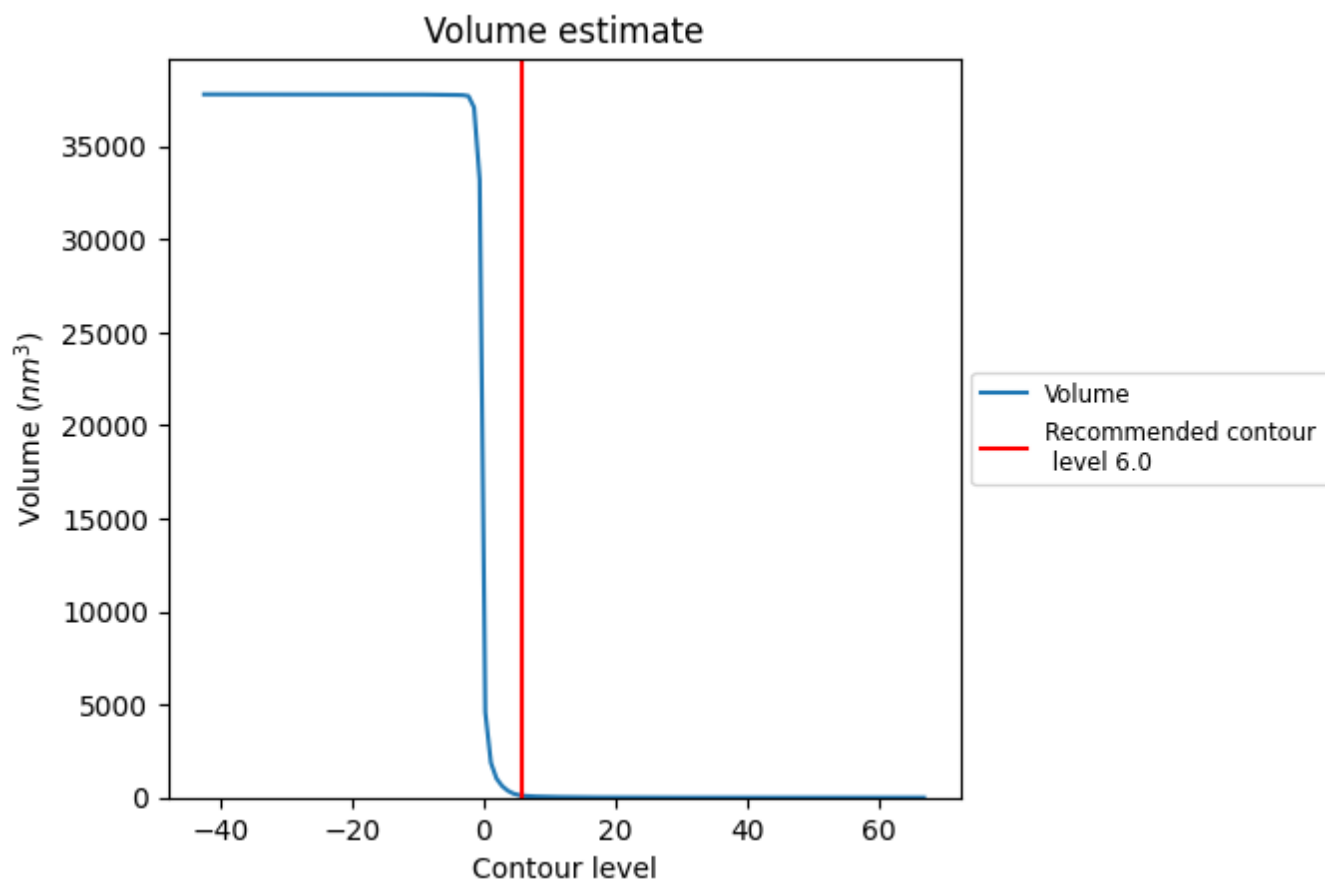
This section contains the results of statistical analysis of the map.

### 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.

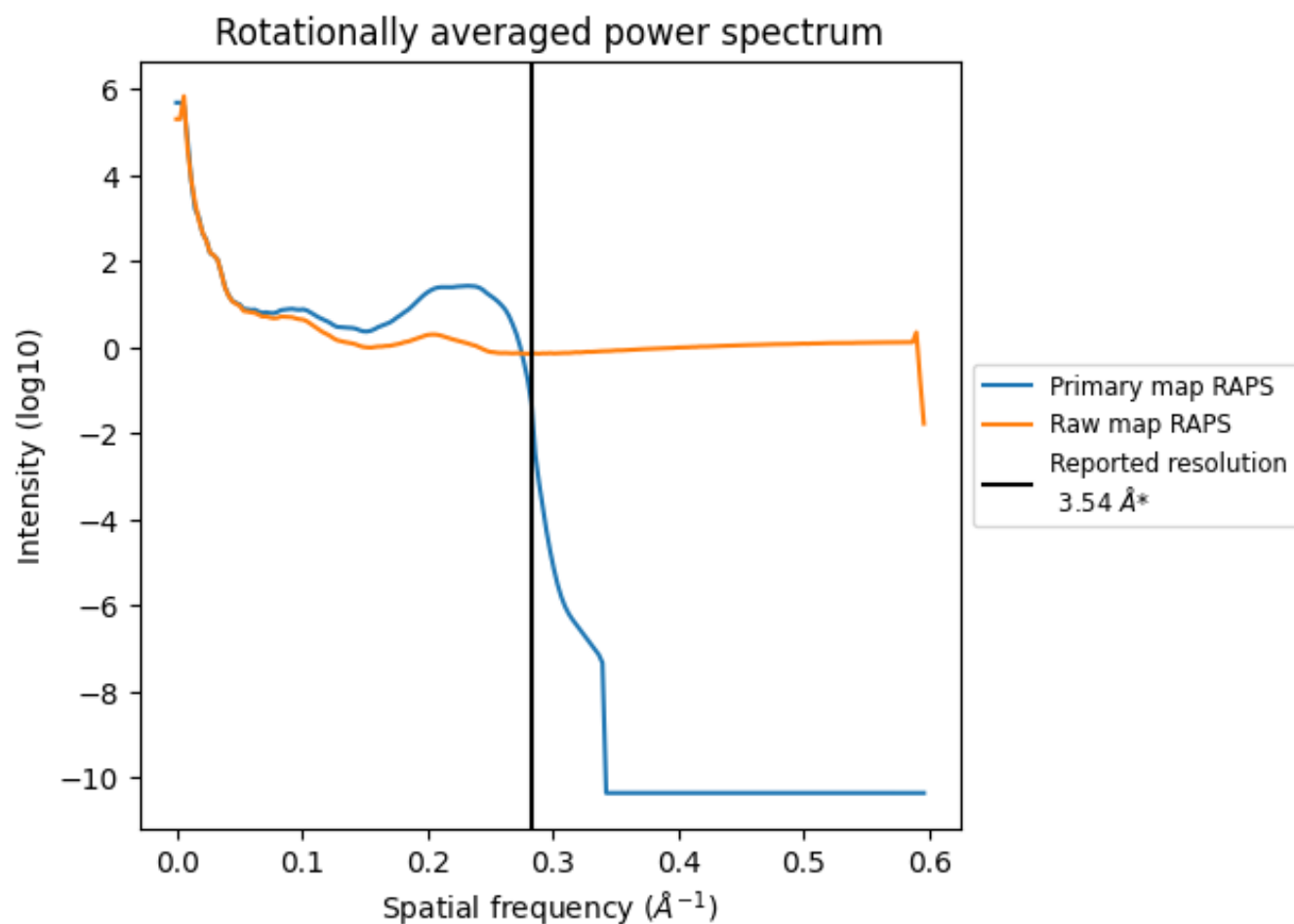
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105  $\text{nm}^3$ ; this corresponds to an approximate mass of 94 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 ⓘ

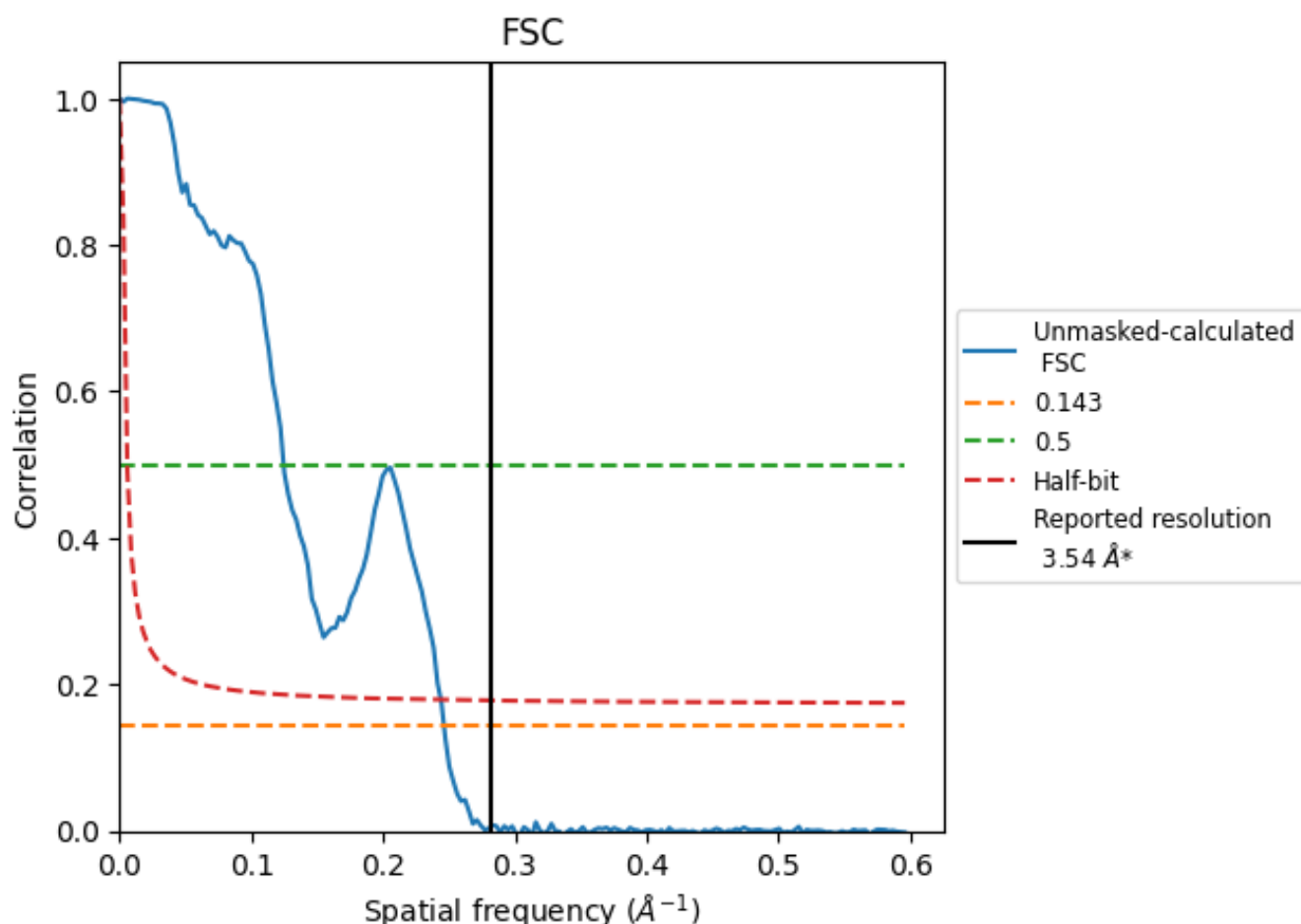


\*Reported resolution corresponds to spatial frequency of 0.282 Å<sup>-1</sup>

## 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 0.282 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

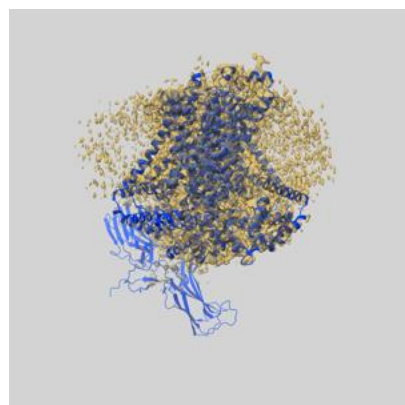
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.54	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.06	8.03	4.10

\*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 4.06 differs from the reported value 3.54 by more than 10 %

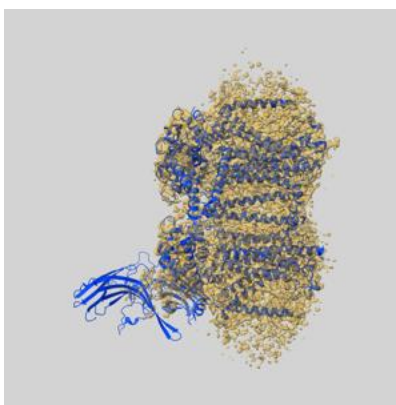
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26743 and PDB model 7USY. Per-residue inclusion information can be found in section 3 on page 7.

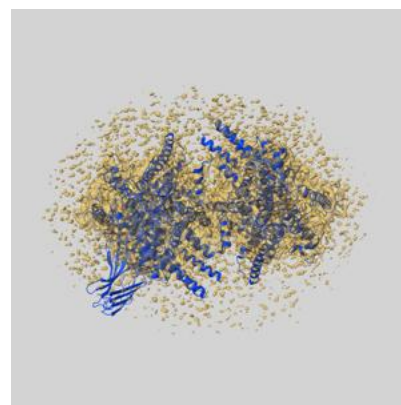
### 9.1 Map-model overlay [i](#)



X



Y



Z

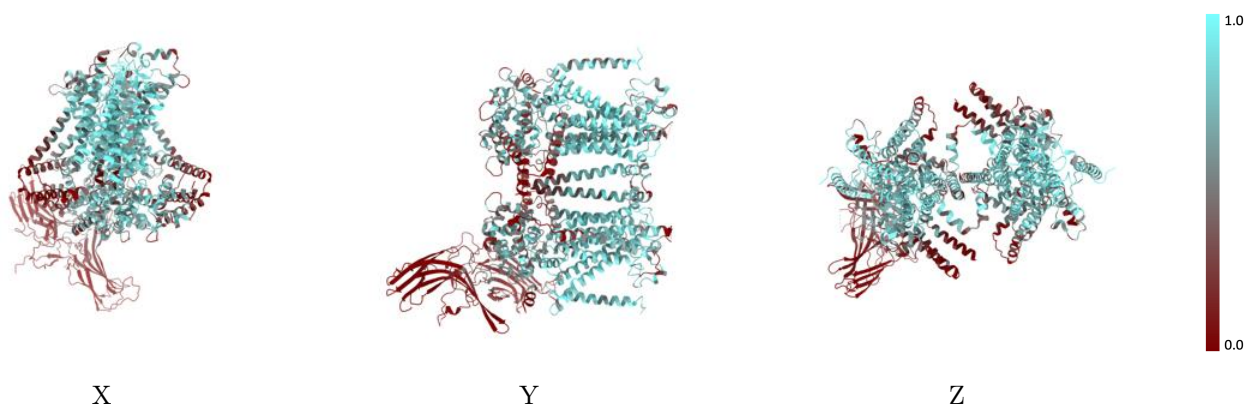
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



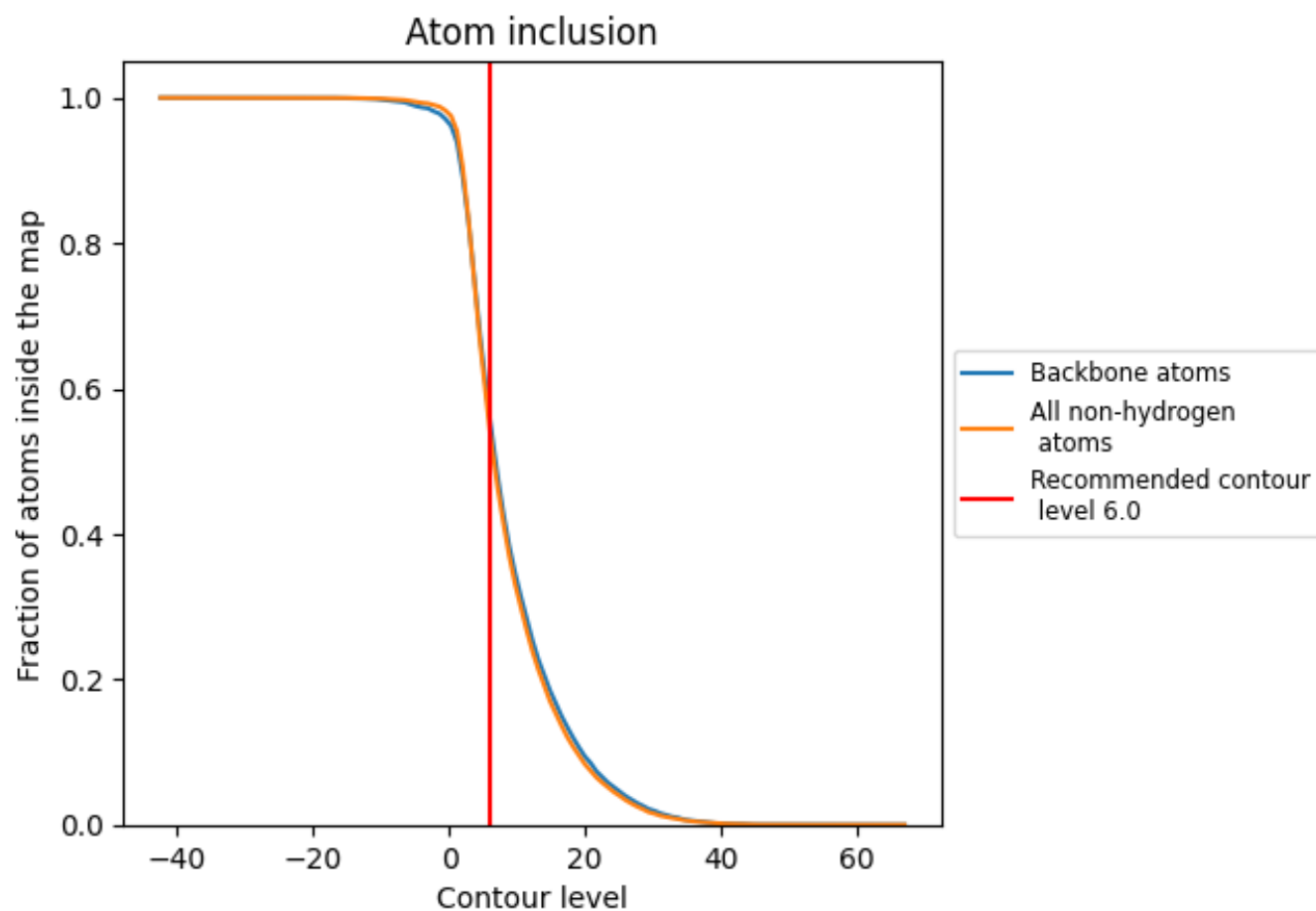
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.0).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 54% 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 (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5409	<div></div> 0.3550
A	<div></div> 0.6526	<div></div> 0.3880
B	<div></div> 0.6608	<div></div> 0.3820
C	<div></div> 0.5899	<div></div> 0.3800
D	<div></div> 0.6638	<div></div> 0.4150
E	<div></div> 0.6198	<div></div> 0.3880
F	<div></div> 0.6149	<div></div> 0.4000
J	<div></div> 0.0488	<div></div> 0.2080

1.0

0.0

<0.0