



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:45 PM UTC

PDB ID : 7USY / pdb_00007usy
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

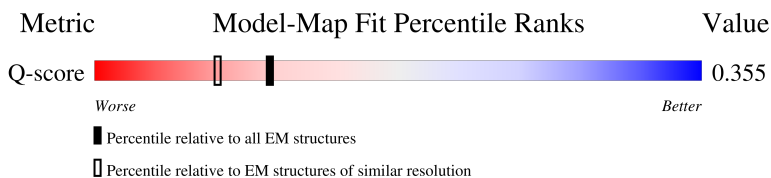
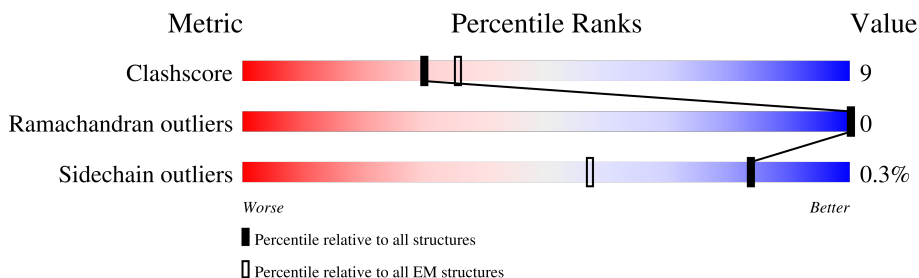
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.54 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12891 (3.04 - 4.04)

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	1285	10% 37% 10% 53%
1	B	1285	10% 37% 10% 53%
2	C	201	24% 65% 27% 8%
2	E	201	20% 75% 17% 8%

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Mol	Chain	Length	Quality of chain
3	D	117	8%31%9%61%
3	F	117	9%32%8%61%
4	J	469	73%62%15%23%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 16602 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 (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

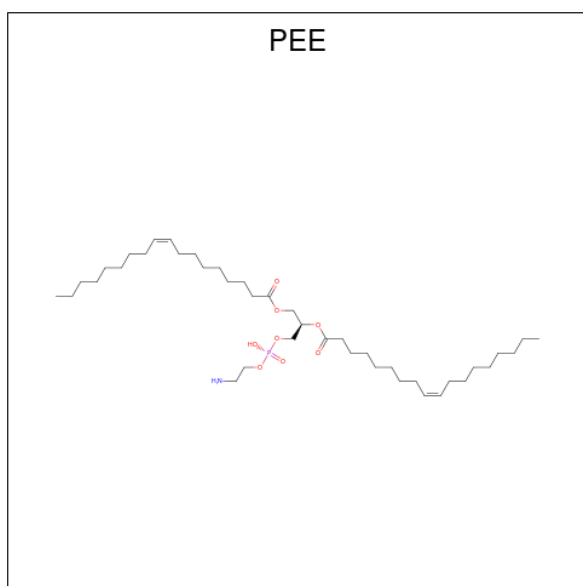
Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total	Ca	0
			2	2	

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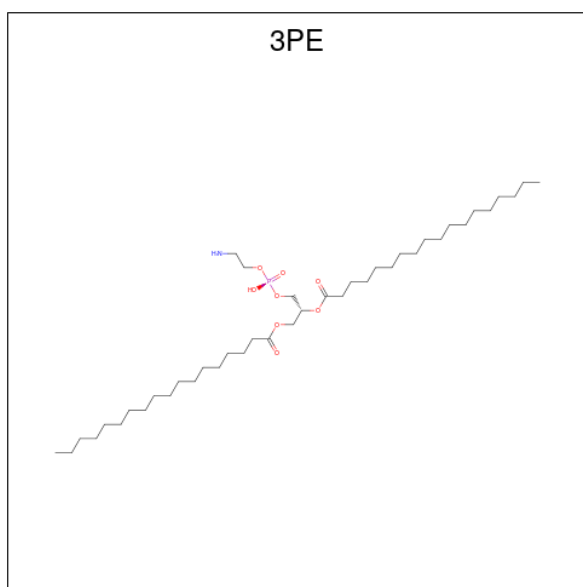
Mol	Chain	Residues	Atoms		AltConf
5	B	2	Total	Ca	0
			2	2	
5	C	2	Total	Ca	0
			2	2	
5	E	2	Total	Ca	0
			2	2	

- Molecule 6 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: 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 (CCD ID: 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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



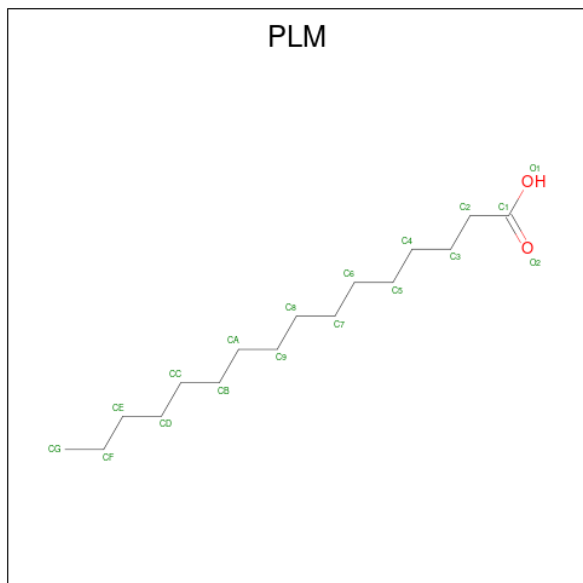
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	

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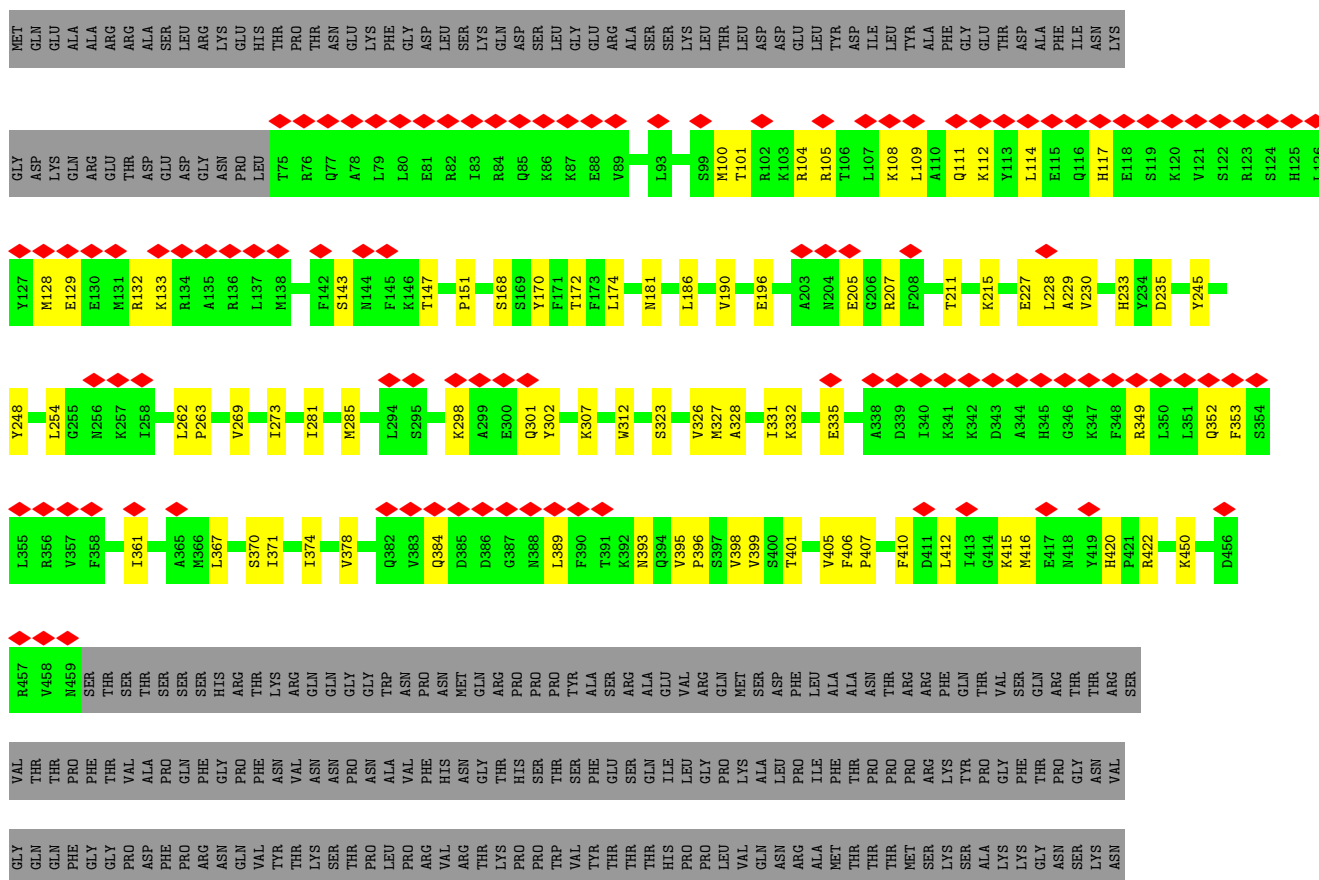
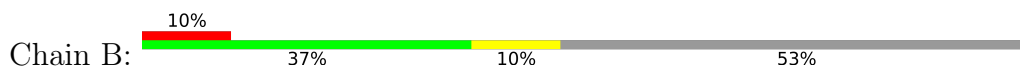
Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	N	O	0
			14	8	1	5	

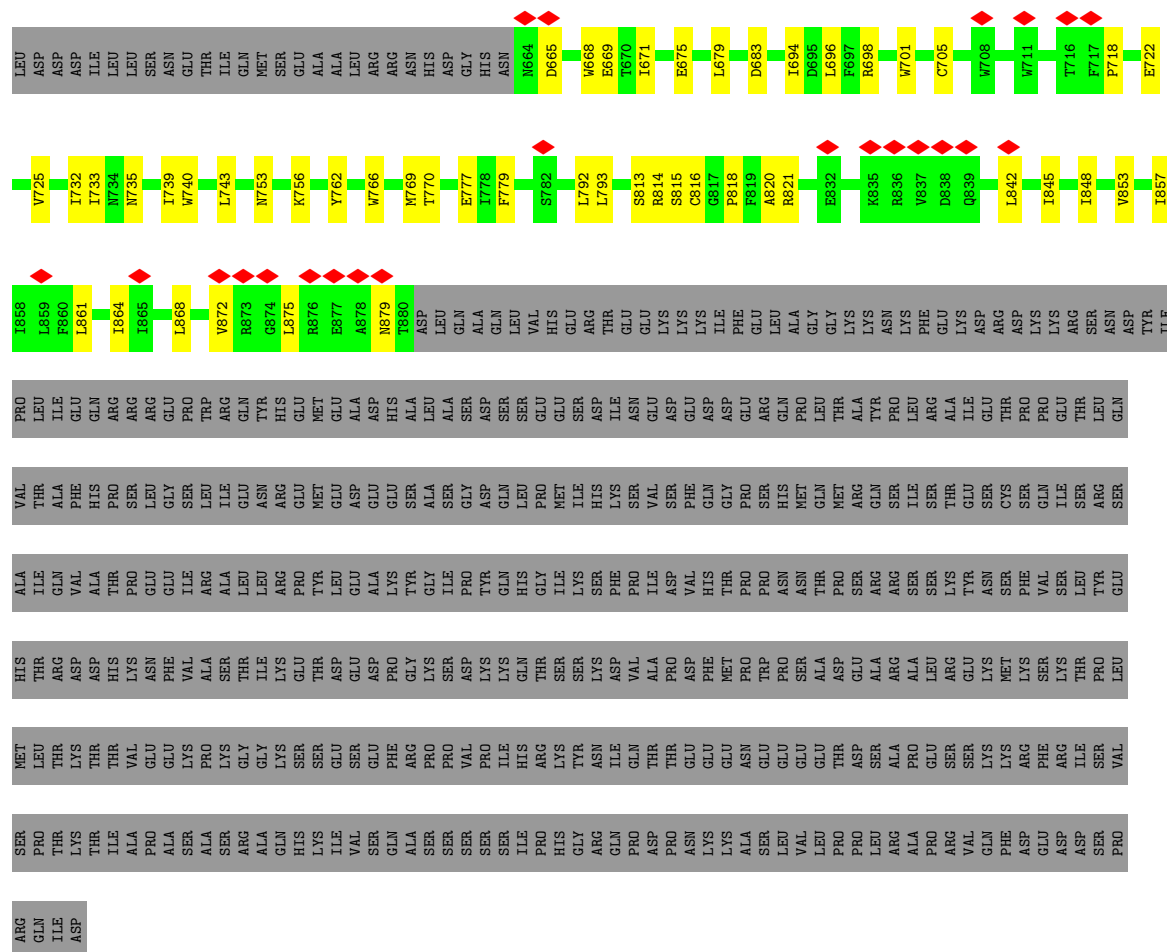
- Molecule 9 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



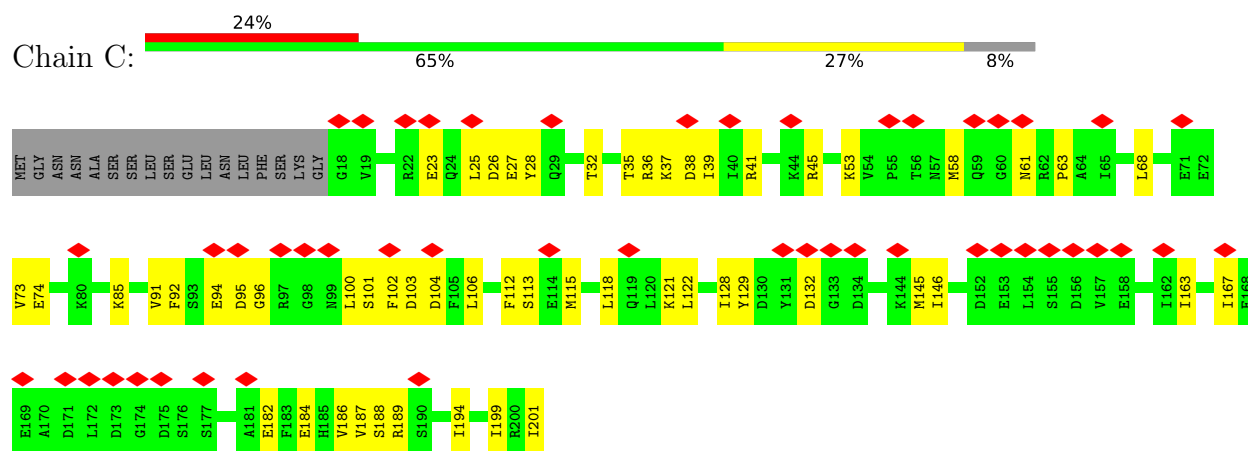
Mol	Chain	Residues	Atoms			AltConf
9	D	1	Total	C	O	0
			14	13	1	
9	D	1	Total	C	O	0
			10	9	1	
9	F	1	Total	C	O	0
			14	13	1	
9	F	1	Total	C	O	0
			10	9	1	

- Molecule 1: Transmembrane channel-like protein 1

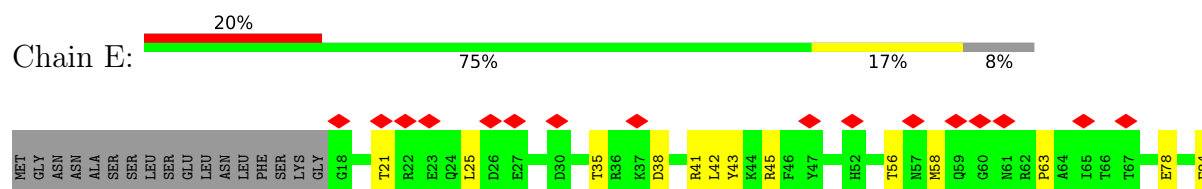


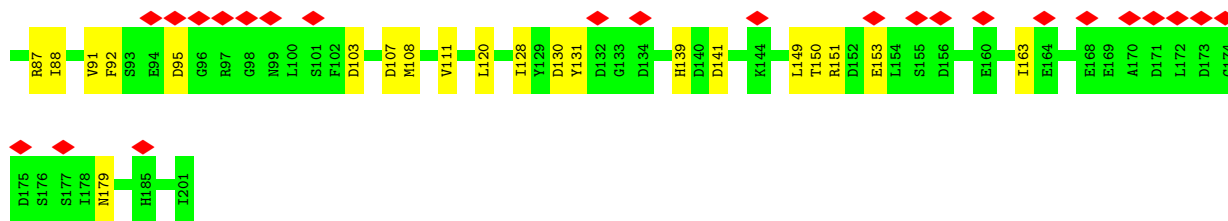


• Molecule 2: CALMyrin (Calcium and Integrin Binding protein) homolog

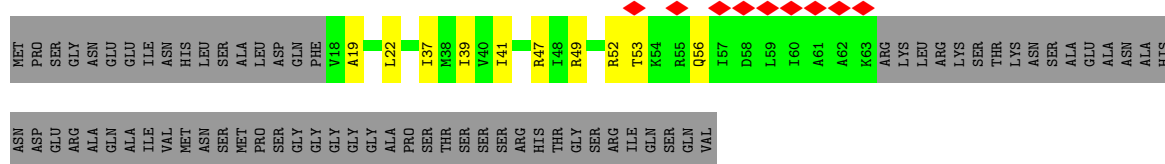


• Molecule 2: CALMyrin (Calcium and Integrin Binding protein) homolog

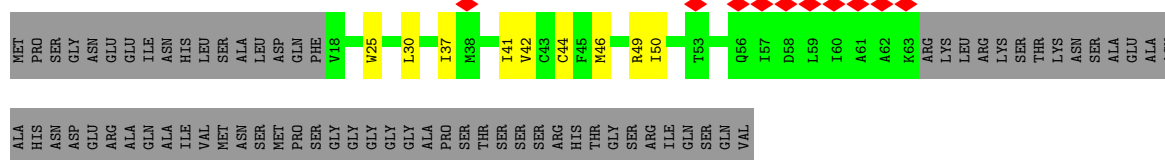




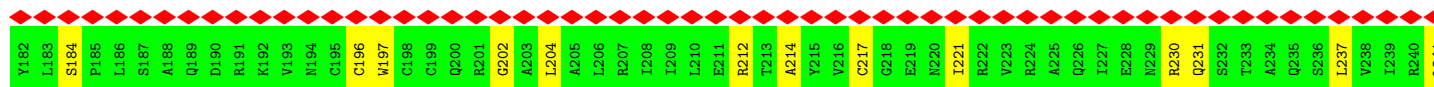
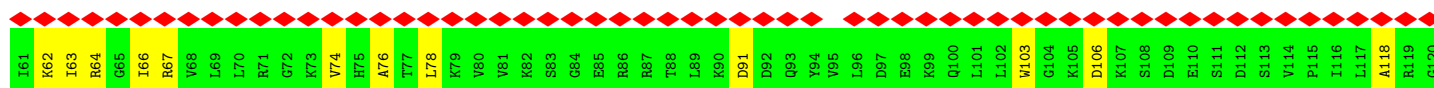
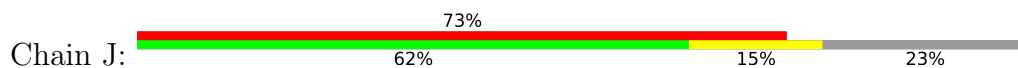
• Molecule 3: Transmembrane inner ear expressed protein



• Molecule 3: Transmembrane inner ear expressed protein



• Molecule 4: ARRestin Domain protein



ASN	GLY	ASN	GLN	G368	◆	Y308
SER	VAL	SER	VAL	GLN	◆	A309
ARG	ARG	ARG	TYR	TYR	◆	L310
ARG	ARG	ASP	ASP	ASP	◆	R311
SER	GLU	SER	GLU	GLU	◆	V312
ILE	ILE	ILE	GLY	GLY	◆	G313
LEU	LEU	LEU	GLU	GLU	◆	M314
VAL	VAL	VAL	GLU	GLU	◆	E315
ALA	ALA	ALA	ILE	ILE	◆	D316
SER	SER	SER	ASN	ASN	◆	E317
ASN	ASN	ASN	LYS	LYS	◆	K318
PRO	PRO	PRO	GLU	GLU	◆	G319
CYS	CYS	CYS	E362	E362	◆	N320
LEU	LEU	LEU	E363	E363	◆	E321
ALA	ALA	ALA	I364	I364	◆	C322
MET	MET	MET	V365	V365	◆	L323
ARG	ARG	ASP	L366	L366	◆	H324
ASP	GLU	GLU	Y367	Y367	◆	I325
SER	SER	SER	R368	R368	◆	D326
MET	MET	MET	P369	P369	◆	F327
ASP	ASP	ASP	V390	V390	◆	P328
GLU	GLU	LYS	G391	G391	◆	L329
LYS	LEU	LEU	V392	V392	◆	T330
MET	MET	MET	K393	K393	◆	V331
MET	MET	THR	K393	K393	◆	A332
THR	THR	ASN	L394	L394	◆	T333
ASN	ASN	GLY	A395	A395	◆	I334
GLY	GLY	CYS	D396	D396	◆	P335
CYS	CYS	SER	R397	R397	◆	Y336
GLU	GLU	GLU	R398	R398	◆	R337
GLY	GLY	GLY	I399	I399	◆	I338
GLY	GLY	ASP	G400	G400	◆	P339
PRO	PRO	PRO	SER	SER	◆	N340
LEU	LEU	LEU	PRO	PRO	◆	A341
VAL	VAL	VAL	HIS	HIS	◆	P342
ALA	ALA	VAL	VAL	VAL	◆	P343
		SER	SER	SER	◆	P344
		LYS	LYS	LYS	◆	P345
		ASP	ASP	ASP	◆	V346
		PHE	PHE	PHE	◆	D347
		ARG	THR	THR	◆	T348
		ARG	ARG	ARG	◆	D349
		ILE	ILE	ILE	◆	F350
		ALA	ALA	ALA	◆	C351
		ASP	ASP	ASP	◆	S352
		SER	SER	SER	◆	N353
		SER	LEU	LEU	◆	H354
		ALA	ALA	ALA	◆	V355
		LEU	LEU	LEU	◆	E356
		VAL	VAL	VAL	◆	G357
		THR	THR	THR	◆	G358
		GLU	GLU	GLU	◆	K359
		PRO	PRO	PRO	◆	Y360
					◆	V361
					◆	S362
					◆	P363
					◆	E364
					◆	F365
					◆	R366
					◆	I367

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT	Depositor
Number of particles used	99248, 99248, 99248, 99248	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.00	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	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, NAG, PEE, CA, PLM

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	0.15	0/4987	0.43	5/6763 (0.1%)
1	B	0.15	0/4987	0.37	2/6763 (0.0%)
2	C	0.10	0/1569	0.32	0/2111
2	E	0.12	0/1569	0.35	0/2111
3	D	0.17	0/347	0.40	0/471
3	F	0.15	0/347	0.35	0/471
4	J	0.15	0/2938	0.42	2/3979 (0.1%)
All	All	0.15	0/16744	0.39	9/22669 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	340	ASN	CA-C-N	8.56	133.70	120.68
4	J	340	ASN	C-N-CA	8.56	133.70	120.68
1	A	870	SER	N-CA-C	-8.31	102.17	111.14
1	A	810	MET	CA-C-N	8.04	132.79	121.61
1	A	810	MET	C-N-CA	8.04	132.79	121.61
1	B	301	GLN	CB-CA-C	-5.81	109.86	116.54
1	A	301	GLN	CB-CA-C	-5.60	110.10	116.54
1	B	853	VAL	N-CA-C	-5.40	107.56	112.96
1	A	396	PRO	CA-N-CD	-5.32	104.56	112.00

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	88	0
1	B	4864	0	4941	96	0
2	C	1536	0	1484	38	0
2	E	1536	0	1484	23	0
3	D	343	0	376	7	0
3	F	343	0	376	5	0
4	J	2878	0	2908	45	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	7	0
7	B	35	0	44	3	0
8	A	14	0	13	0	0
8	B	14	0	13	1	0
9	D	24	0	36	10	0
9	F	24	0	36	6	0
All	All	16602	0	16812	304	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (304) 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)
7:A:1304:3PE:C25	9:D:202:PLM:H41	1.93	0.98
7:A:1304:3PE:H251	9:D:202:PLM:H41	1.49	0.93
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:679:LEU:HD23	1:A:738:MET:HE2	1.60	0.84
3:D:39:ILE:HG23	9:D:202:PLM:H22	1.63	0.81
1:A:378:VAL:HG11	1:A:446:ALA:HB1	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1304:3PE:H252	9:D:202:PLM:H41	1.63	0.77
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
4:J:260:MET:HE1	4:J:262:CYS:HB2	1.68	0.74
2:E:88:ILE:HG22	2:E:108:MET:HE2	1.69	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
1:A:324:ASN:OD1	1:A:776:ARG:NH1	2.27	0.67
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
1:B:422:ARG:C	1:B:422:ARG:HD3	2.23	0.64
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
1:B:766:TRP:HZ2	9:F:202:PLM:H32	1.63	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
3:D:39:ILE:CG2	9:D:202:PLM:H22	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ALA:HA	1:A:291:MET:HE2	1.82	0.60
2:E:58:MET:HE2	2:E:63:PRO:HG3	1.82	0.60
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: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
7:A:1304:3PE:H231	9:D:202:PLM:H21	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: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
1:A:284:LYS:HG2	1:A:789:LEU:HD21	1.87	0.56
7:B:1304:3PE:H261	9:F:202:PLM:H61	1.87	0.56
1:B:762:TYR:CE2	9:F:201:PLM:H92	2.39	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:A:207:ARG:O	1:A:211:THR:OG1	2.22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:241:LEU:O	4:J:264:VAL:N	2.38	0.54
1:A:679:LEU:HD23	1:A:738:MET:CE	2.34	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
4:J:136:PRO:O	4:J:148:TYR:OH	2.25	0.53
1:A:687:THR:HG21	1:A:760:LEU:HD11	1.90	0.52
1:B:281:ILE:HG22	1:B:285:MET:HE2	1.91	0.52
2:C:118:LEU:HD22	2:C:194:ILE:HD11	1.92	0.52
1:B:100:MET:HE2	1:B:104:ARG:HH11	1.74	0.52
4:J:314:MET:HE1	4:J:323:LEU:HD12	1.91	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
7:B:1304:3PE:O32	9:F:201:PLM:HC2	2.11	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
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:B:665:ASP:O	1:B:815:SER:OG	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:769:MET:HE3	1:A:769:MET:HA	1.93	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: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: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
1:B:285:MET:HE1	1:B:793:LEU:HD22	1.95	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:B:307:LYS:HZ1	1:B:332:LYS:C	2.23	0.47
1:A:797:LEU:HA	1:A:800:THR:HG22	1.96	0.47
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
4:J:221:ILE:O	4:J:282:SER:OG	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:879:ASN:O	1:A:880:THR:C	2.59	0.45
7:B:1304:3PE:H11	9:F:201:PLM:H52	1.96	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:A:451:MET:HE2	1:A:668:TRP:HB3	1.99	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:683:ASP:OD2	1:B:756:LYS:NZ	2.31	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: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
9:F:202:PLM:C1	9:F:202:PLM:H51	2.48	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
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:A:327:MET:HE3	1:A:331:ILE:HG12	2.00	0.44
1:B:269:VAL:O	1:B:273:ILE:HG12	2.17	0.44
1:A:683:ASP:OD2	1:A:756:LYS:NZ	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:227:GLU:C	1:A:229:ALA:H	2.27	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
2:C:132:ASP:OD1	2:C:132:ASP:N	2.49	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:227:GLU:C	1:B:229:ALA:H	2.27	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
2:E:179:ASN:C	2:E:179:ASN:OD1	2.63	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
7:A:1304:3PE:H12	9:D:201:PLM:H22	2.01	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:152:TRP:CE3	1:A:761:MET:HE3	2.54	0.42
1:A:375:ILE:O	1:A:378:VAL:HG12	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:VAL:HG22	1:A:749:LEU:HD13	2.01	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
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
4:J:344:PRO:O	4:J:345:PRO:C	2.63	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
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:196:CYS:O	4:J:197:TRP:C	2.64	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	516 (100%)	1 (0%)	87	85
1	B	517/1150 (45%)	517 (100%)	0	100	100
2	C	171/185 (92%)	170 (99%)	1 (1%)	78	80
2	E	171/185 (92%)	171 (100%)	0	100	100
3	D	35/96 (36%)	35 (100%)	0	100	100
3	F	35/96 (36%)	33 (94%)	2 (6%)	18	46
4	J	323/419 (77%)	322 (100%)	1 (0%)	86	83
All	All	1769/3281 (54%)	1764 (100%)	5 (0%)	84	83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	879	ASN
2	C	146	ILE
3	F	30	LEU
3	F	44	CYS
4	J	129	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	144	ASN
1	A	181	ASN
1	A	731	HIS
1	A	736	GLN
1	A	753	ASN
1	B	420	HIS
1	B	879	ASN
2	C	24	GLN
2	C	29	GLN

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Mol	Chain	Res	Type
4	J	75	HIS
4	J	194	ASN
4	J	235	GLN
4	J	275	ASN
4	J	286	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	$\# Z > 2$
7	3PE	B	1304	-	34,34,50	1.05	4 (11%)	37,39,55	1.14	2 (5%)
9	PLM	F	202	3	8,9,17	0.53	0	7,8,17	0.91	0
6	PEE	A	1303	-	41,41,50	1.27	6 (14%)	44,46,55	1.21	6 (13%)
6	PEE	B	1303	-	41,41,50	1.28	6 (14%)	44,46,55	1.25	6 (13%)
8	NAG	B	1305	-	14,14,15	0.46	0	19,19,21	0.76	0
9	PLM	D	202	3	8,9,17	0.41	0	7,8,17	1.07	0
9	PLM	F	201	3	12,13,17	0.27	0	11,12,17	0.87	0
7	3PE	A	1304	-	34,34,50	1.05	4 (11%)	37,39,55	1.17	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	A	1305	-	14,14,15	0.47	0	19,19,21	0.75	0
9	PLM	D	201	3	12,13,17	0.27	0	11,12,17	0.88	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
7	3PE	B	1304	-	-	16/38/38/54	-
9	PLM	F	202	3	-	2/7/7/15	-
6	PEE	A	1303	-	-	24/45/45/54	-
6	PEE	B	1303	-	-	20/45/45/54	-
8	NAG	B	1305	-	-	2/6/22/26	0/1/1/1
9	PLM	D	202	3	-	1/7/7/15	-
9	PLM	F	201	3	-	6/11/11/15	-
7	3PE	A	1304	-	-	16/38/38/54	-
8	NAG	A	1305	-	-	0/6/22/26	0/1/1/1
9	PLM	D	201	3	-	3/11/11/15	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1303	PEE	C18-C19	3.79	1.53	1.31
6	A	1303	PEE	C18-C19	3.78	1.53	1.31
6	B	1303	PEE	C39-C38	3.78	1.53	1.31
6	A	1303	PEE	C39-C38	3.77	1.53	1.31
7	A	1304	3PE	O21-C2	-2.73	1.40	1.46
6	B	1303	PEE	O2-C2	-2.67	1.40	1.46
6	A	1303	PEE	O2-C2	-2.66	1.40	1.46
7	B	1304	3PE	O21-C2	-2.66	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	-2.22	1.40	1.45
7	B	1304	3PE	O31-C3	-2.16	1.40	1.45
6	B	1303	PEE	O2-C10	2.15	1.40	1.34
7	B	1304	3PE	O21-C21	2.14	1.40	1.34
6	B	1303	PEE	O3-C3	-2.13	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1304	3PE	O21-C21	2.12	1.40	1.34
7	A	1304	3PE	O31-C3	-2.09	1.40	1.45
6	A	1303	PEE	O2-C10	2.07	1.40	1.34

All (16) 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	111.48
7	A	1304	3PE	O21-C21-C22	4.10	120.34	111.48
7	B	1304	3PE	O21-C21-C22	4.08	120.31	111.48
6	A	1303	PEE	O2-C10-C11	3.83	119.77	111.48
7	A	1304	3PE	O31-C31-C32	2.82	120.42	111.83
6	B	1303	PEE	O3-C30-C31	2.82	120.42	111.83
7	B	1304	3PE	O31-C31-C32	2.58	119.71	111.83
6	A	1303	PEE	O3-C30-C31	2.54	119.57	111.83
6	A	1303	PEE	C17-C18-C19	-2.10	109.10	124.83
6	B	1303	PEE	C40-C39-C38	-2.06	109.42	124.83
6	A	1303	PEE	C37-C38-C39	-2.06	109.43	124.83
6	B	1303	PEE	C17-C18-C19	-2.05	109.45	124.83
6	B	1303	PEE	C37-C38-C39	-2.05	109.46	124.83
6	A	1303	PEE	C20-C19-C18	-2.02	109.70	124.83
6	B	1303	PEE	C20-C19-C18	-2.01	109.76	124.83
6	A	1303	PEE	C40-C39-C38	-2.01	109.78	124.83

There are no chirality outliers.

All (90) 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	C1-O3P-P-O4P
6	A	1303	PEE	C4-O4P-P-O3P
6	A	1303	PEE	C4-O4P-P-O2P
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
7	A	1304	3PE	C1-O11-P-O14
7	A	1304	3PE	C11-O13-P-O11
7	A	1304	3PE	C11-O13-P-O12
7	A	1304	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
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
9	F	201	PLM	O2-C1-C2-C3
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	C37-C38-C39-C40
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	B	1303	PEE	C39-C40-C41-C42
6	A	1303	PEE	O2-C2-C3-O3
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	C31-C30-O3-C3
6	A	1303	PEE	C11-C12-C13-C14
7	A	1304	3PE	C23-C24-C25-C26
7	B	1304	3PE	C25-C26-C27-C28
6	A	1303	PEE	C12-C13-C14-C15
6	B	1303	PEE	C17-C18-C19-C20
6	A	1303	PEE	O5-C30-O3-C3
7	A	1304	3PE	C21-C22-C23-C24
9	D	201	PLM	C6-C7-C8-C9
7	B	1304	3PE	C37-C38-C39-C3A
6	B	1303	PEE	C12-C13-C14-C15
6	A	1303	PEE	C35-C36-C37-C38
7	A	1304	3PE	C33-C34-C35-C36
6	A	1303	PEE	C1-C2-C3-O3
6	B	1303	PEE	C1-C2-C3-O3
7	B	1304	3PE	C21-C22-C23-C24
6	B	1303	PEE	C35-C36-C37-C38
7	A	1304	3PE	C37-C38-C39-C3A
7	B	1304	3PE	C33-C34-C35-C36
9	D	201	PLM	C7-C8-C9-CA
6	A	1303	PEE	C30-C31-C32-C33
6	B	1303	PEE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
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	C31-C32-C33-C34
7	B	1304	3PE	C32-C33-C34-C35
6	A	1303	PEE	C11-C10-O2-C2
6	A	1303	PEE	C14-C15-C16-C17
6	B	1303	PEE	O3P-C1-C2-C3
6	A	1303	PEE	O4-C10-O2-C2
6	B	1303	PEE	O3P-C1-C2-O2
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	C1-O11-P-O13
6	A	1303	PEE	C32-C33-C34-C35
7	A	1304	3PE	C35-C36-C37-C38
6	B	1303	PEE	C34-C35-C36-C37
9	F	201	PLM	C9-CA-CB-CC
7	B	1304	3PE	C35-C36-C37-C38
6	A	1303	PEE	C37-C38-C39-C40
6	A	1303	PEE	C39-C40-C41-C42
7	B	1304	3PE	C1-C2-C3-O31
9	F	201	PLM	C7-C8-C9-CA
7	B	1304	3PE	C26-C27-C28-C29
6	B	1303	PEE	C36-C37-C38-C39
6	A	1303	PEE	O3P-C1-C2-C3
6	B	1303	PEE	C38-C39-C40-C41
6	A	1303	PEE	C38-C39-C40-C41
6	A	1303	PEE	C36-C37-C38-C39
7	A	1304	3PE	C26-C27-C28-C29
9	F	202	PLM	C1-C2-C3-C4
9	D	202	PLM	C6-C7-C8-C9
9	F	202	PLM	C4-C5-C6-C7
7	B	1304	3PE	O21-C2-C3-O31

There are no ring outliers.

9 monomers are involved in 27 short contacts:

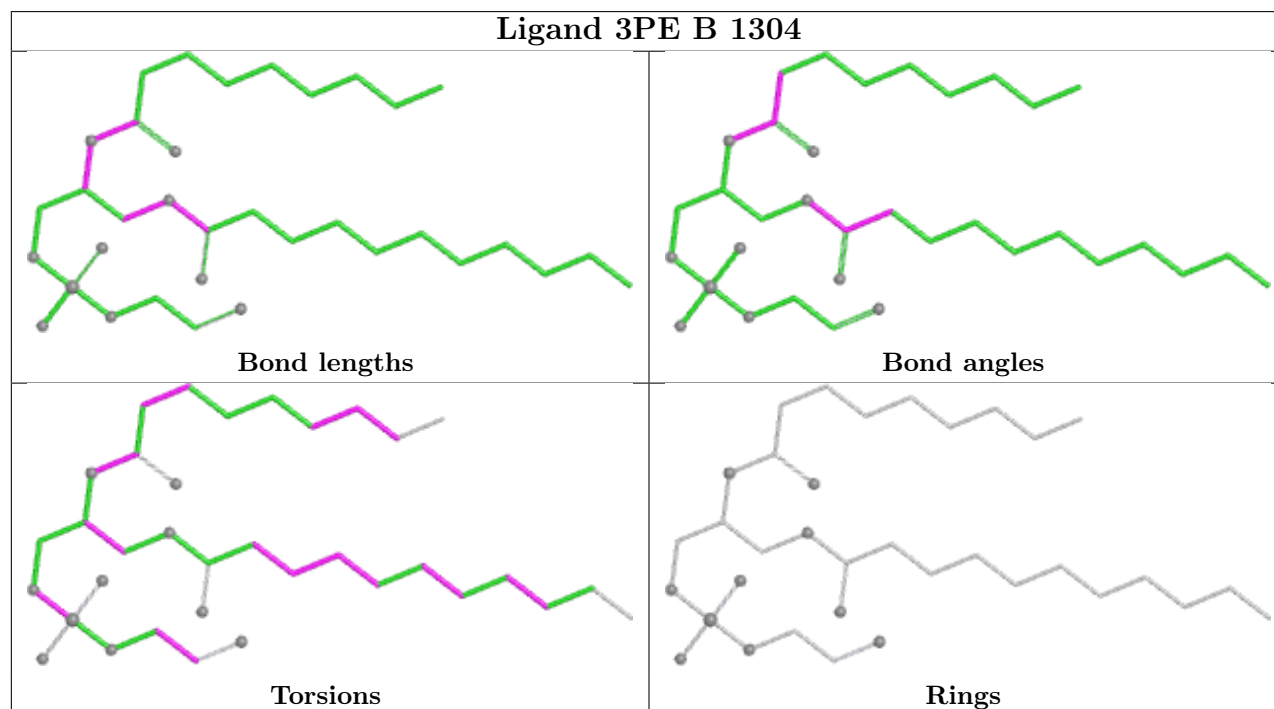
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1304	3PE	3	0
9	F	202	PLM	3	0
6	A	1303	PEE	4	0

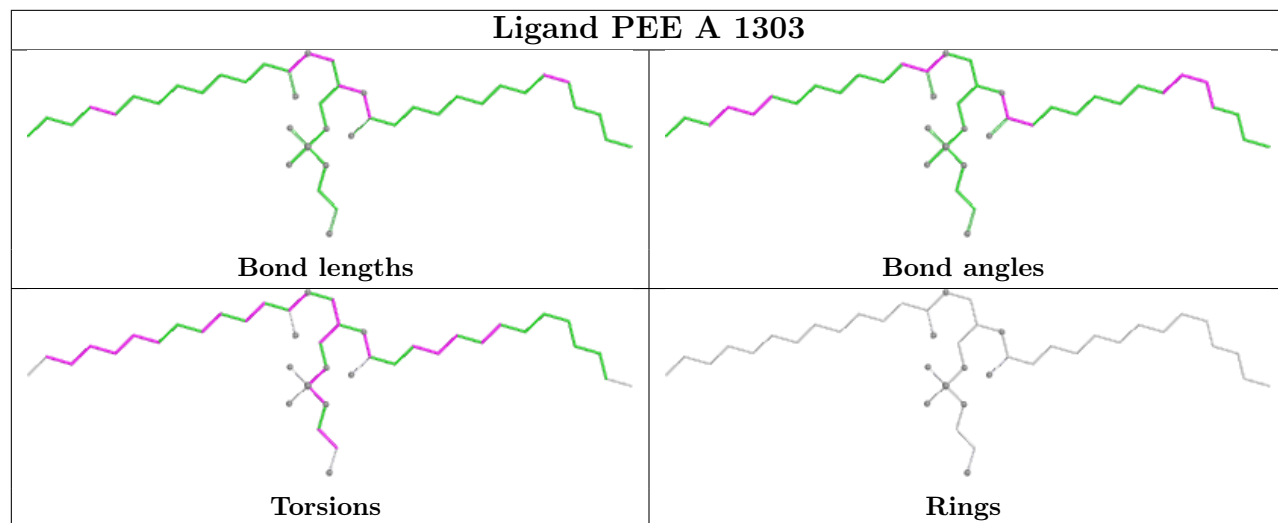
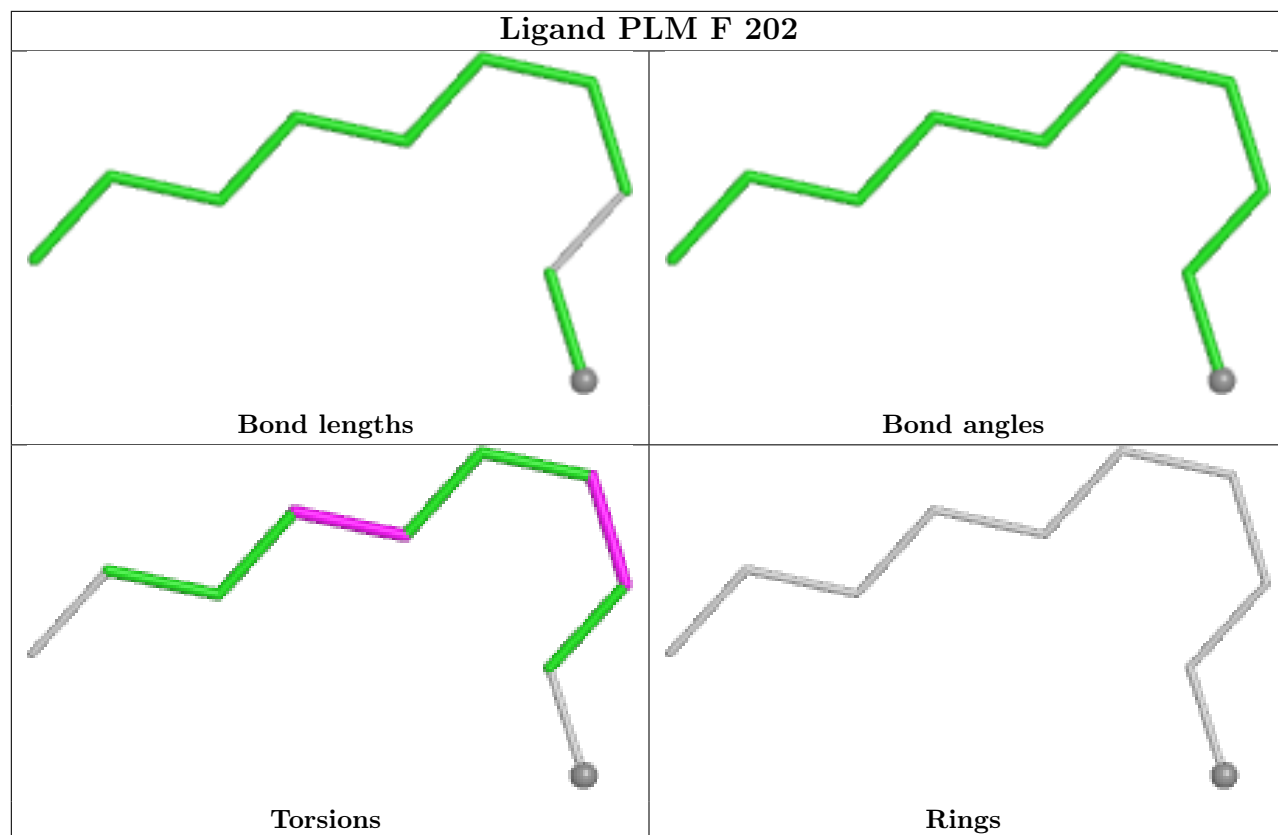
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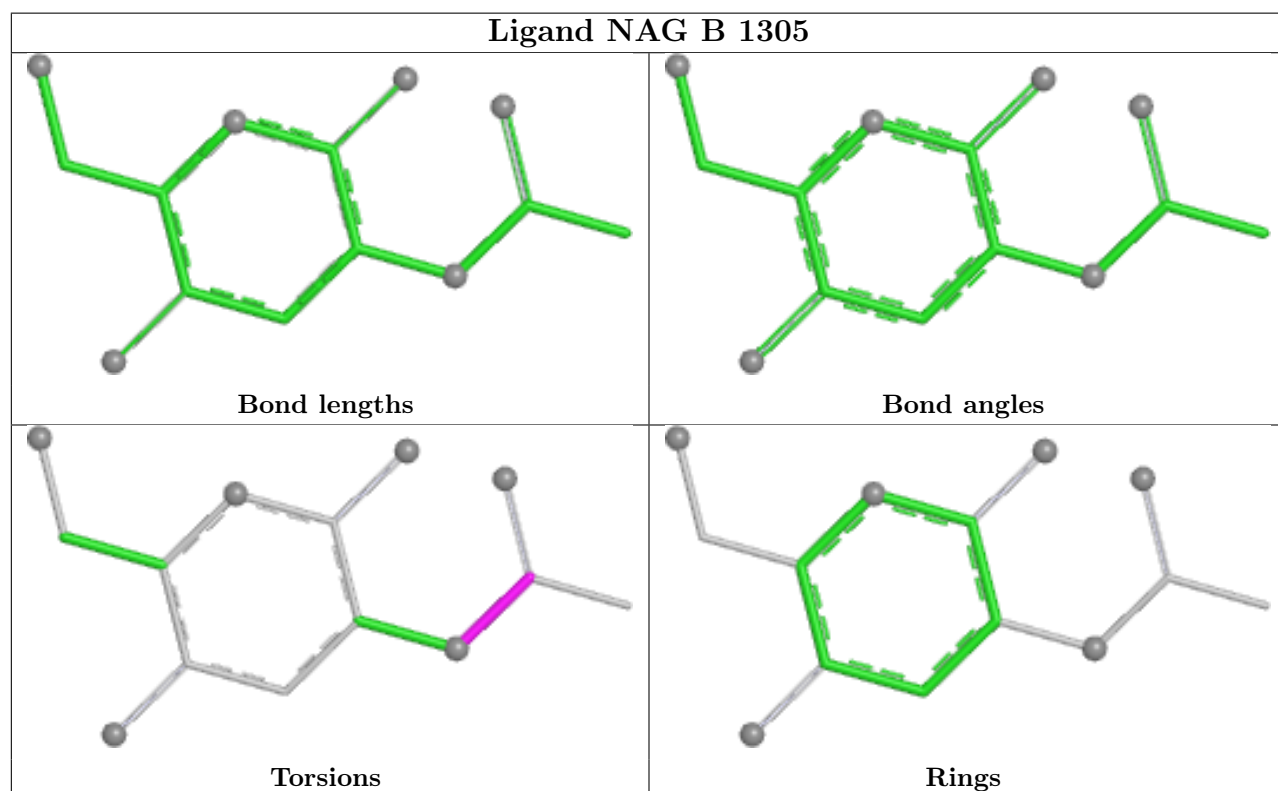
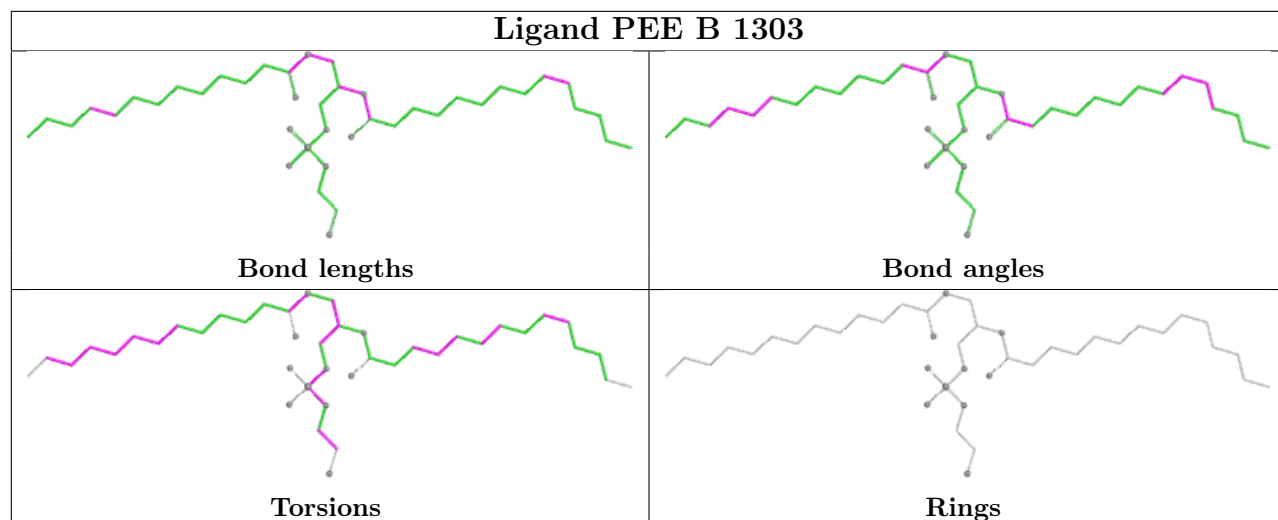
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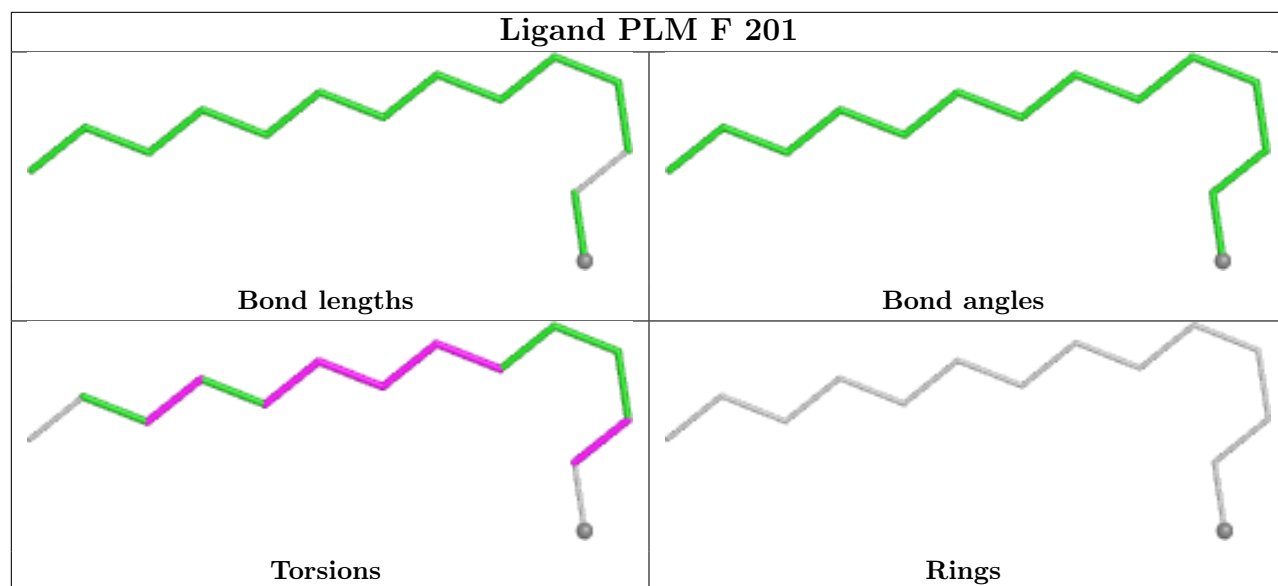
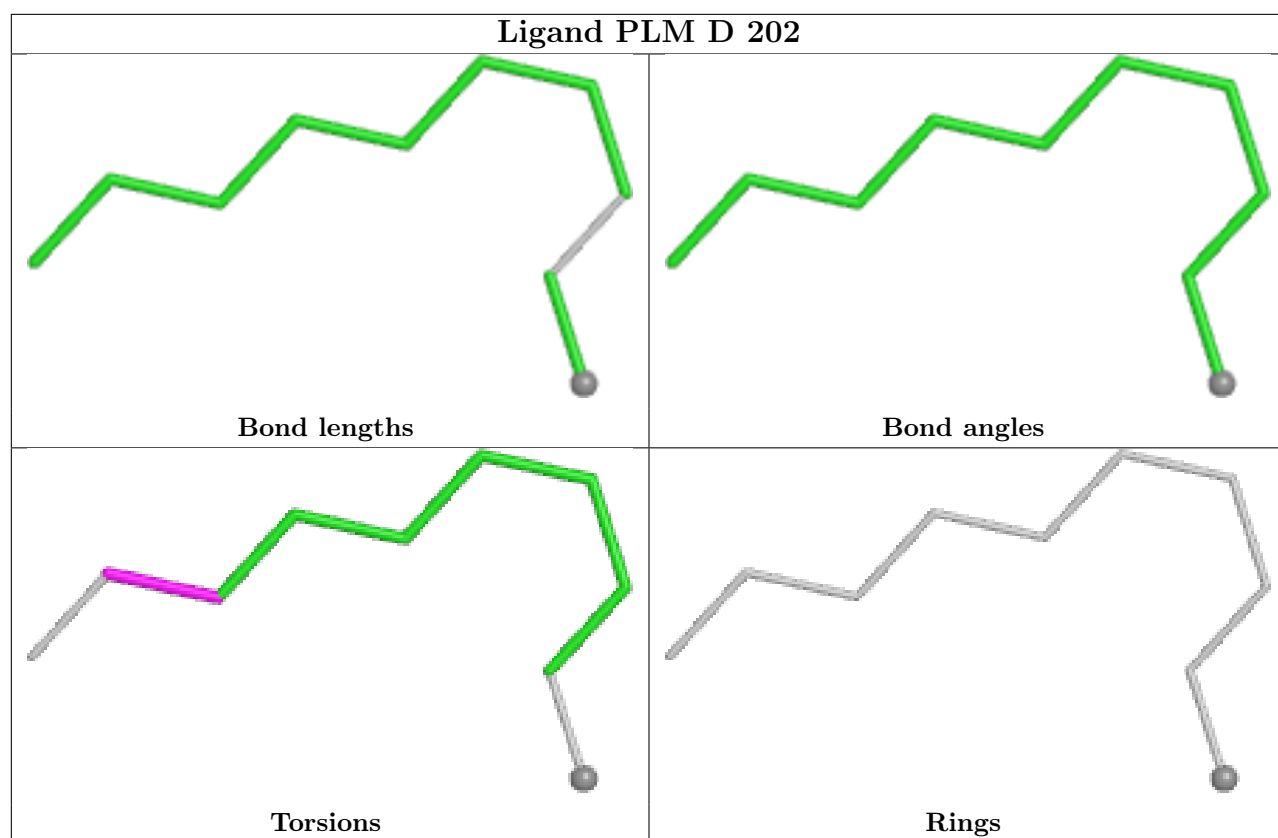
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1303	PEE	4	0
8	B	1305	NAG	1	0
9	D	202	PLM	6	0
9	F	201	PLM	3	0
7	A	1304	3PE	7	0
9	D	201	PLM	4	0

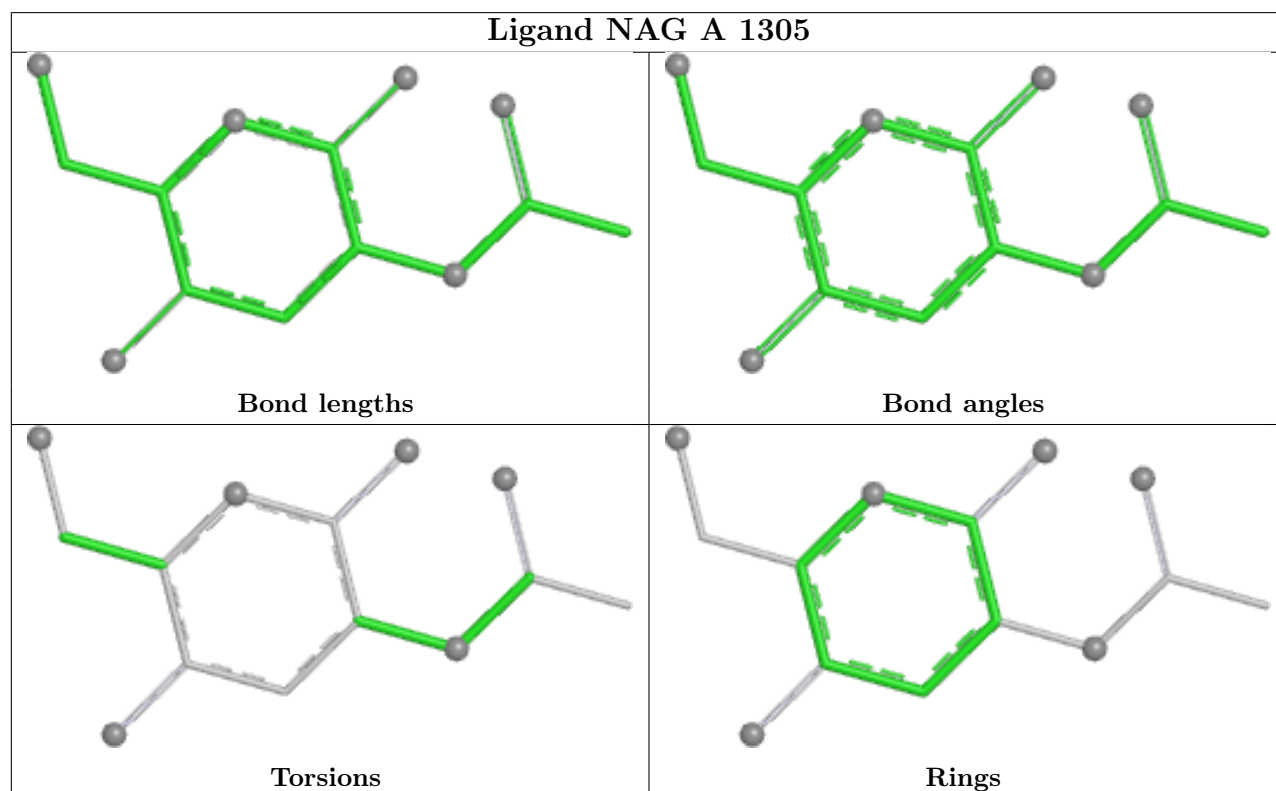
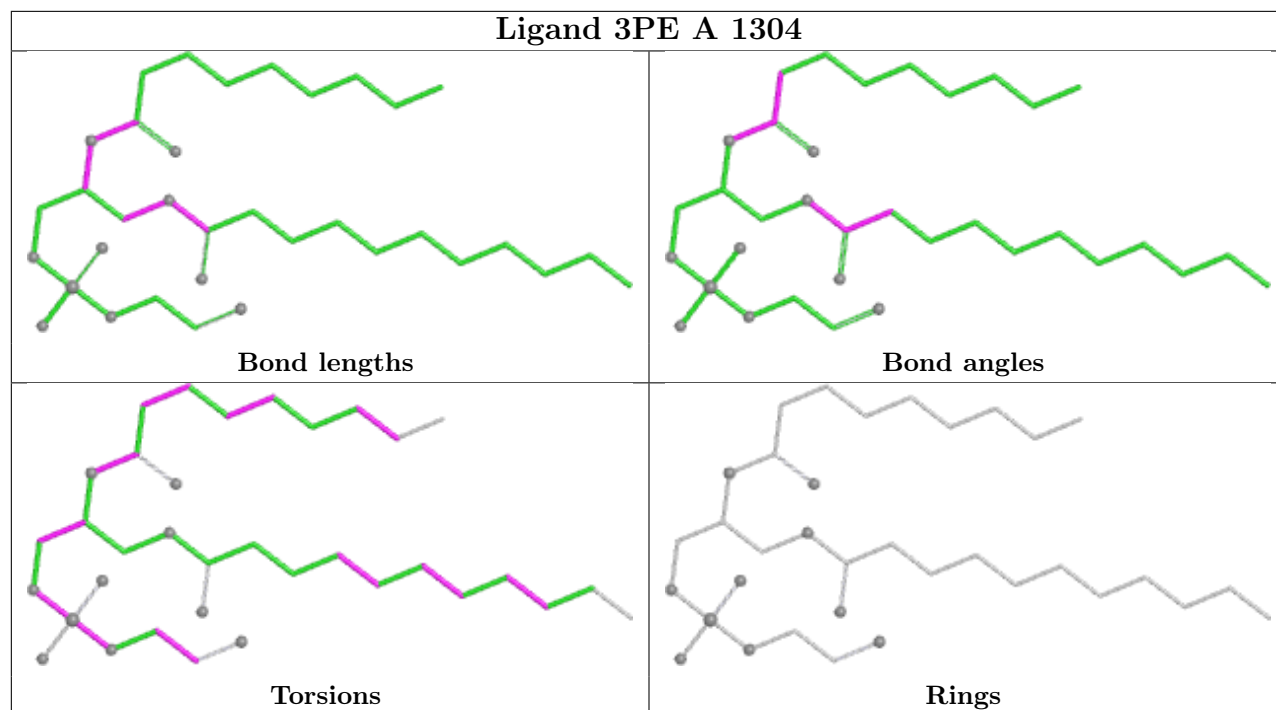
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

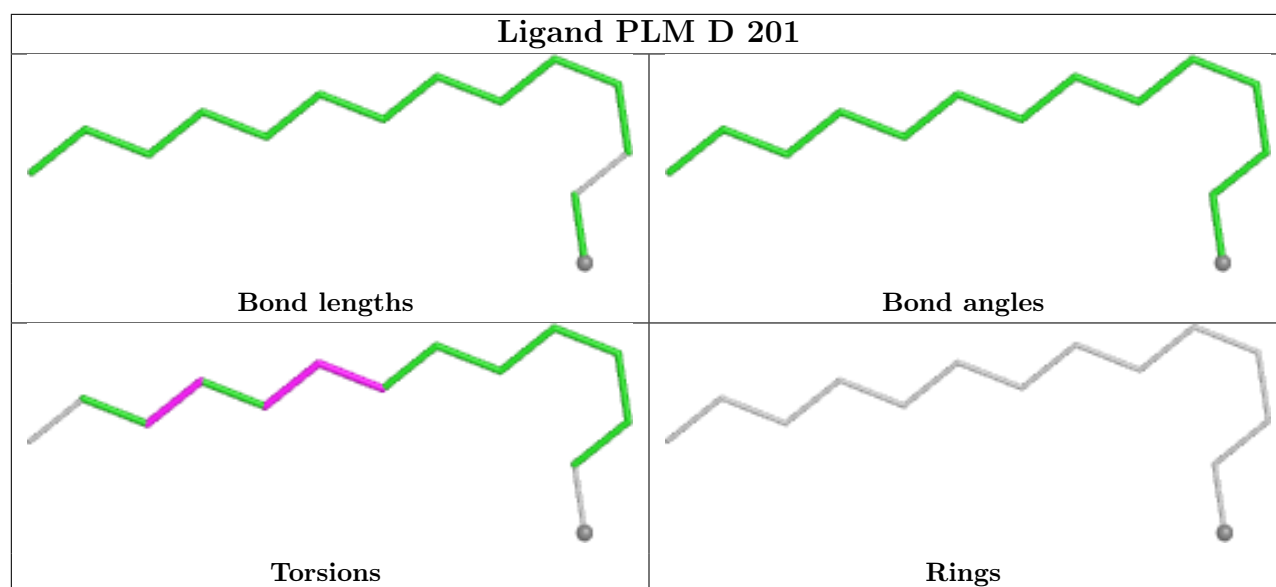












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

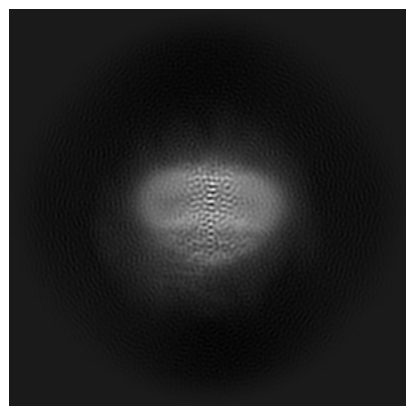
6 Map visualisation [i](#)

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.

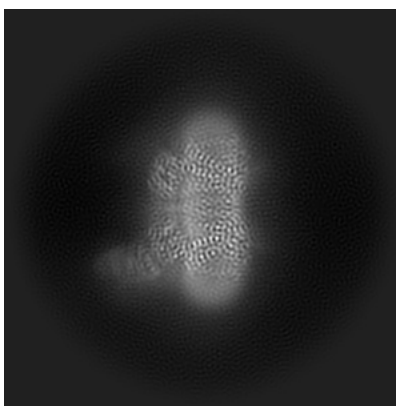
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

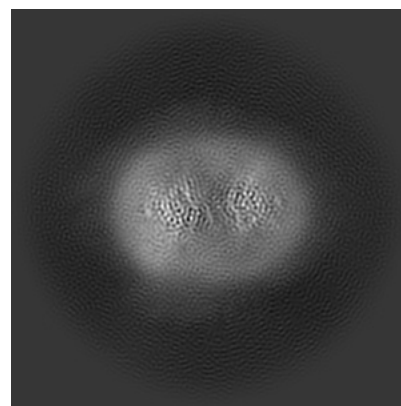
6.1.1 Primary map



X

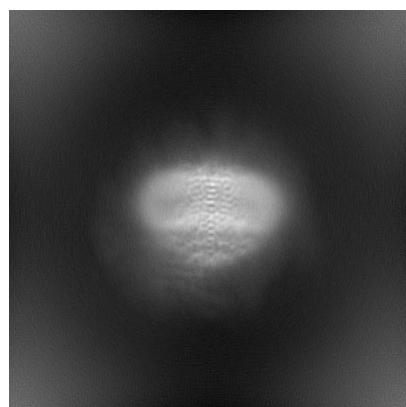


Y

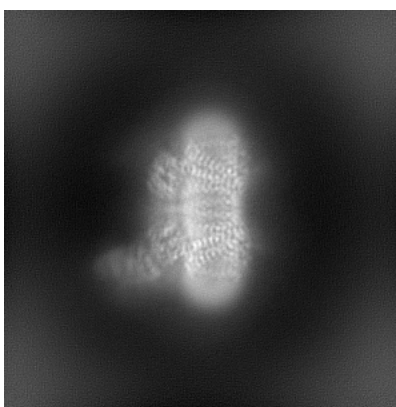


Z

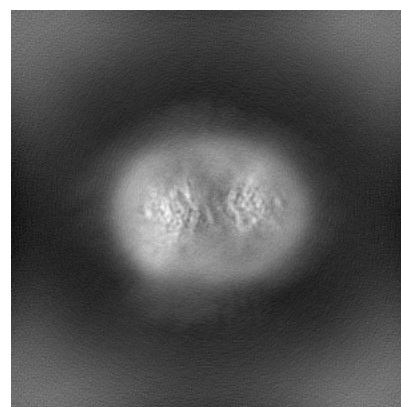
6.1.2 Raw map



X



Y

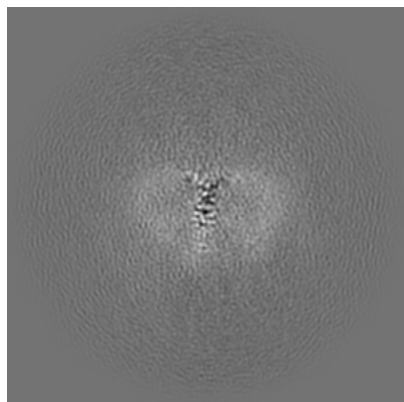


Z

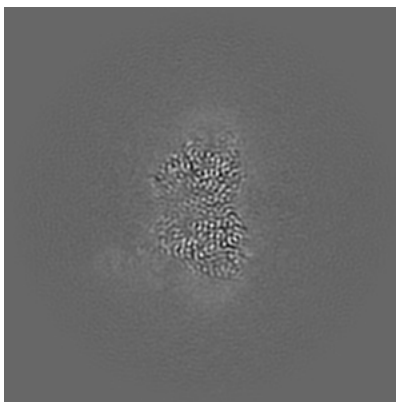
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

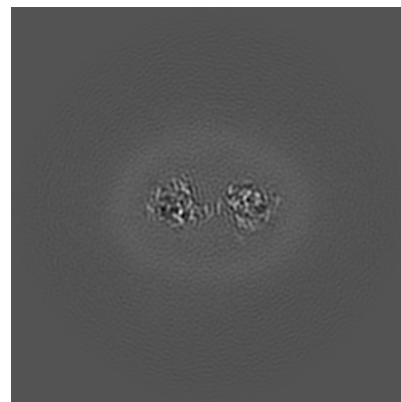
6.2.1 Primary map



X Index: 200

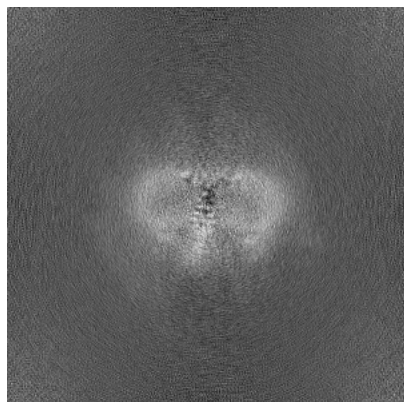


Y Index: 200

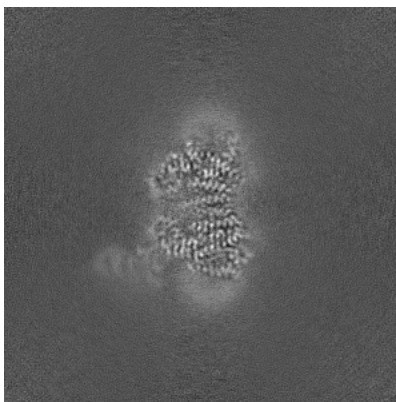


Z Index: 200

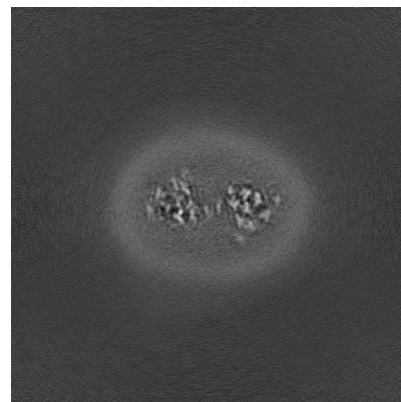
6.2.2 Raw map



X Index: 200



Y Index: 200

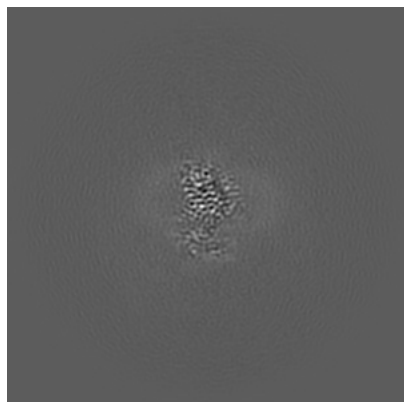


Z Index: 200

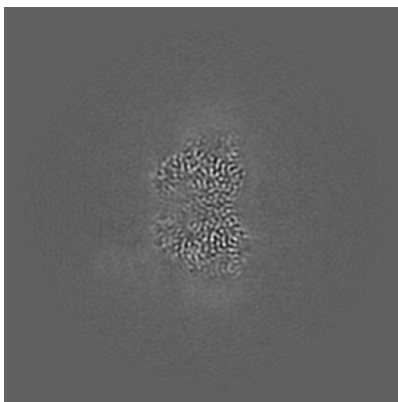
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

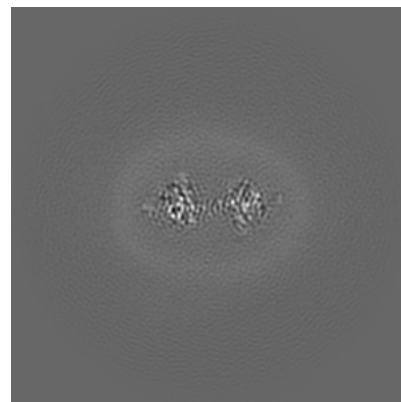
6.3.1 Primary map



X Index: 169

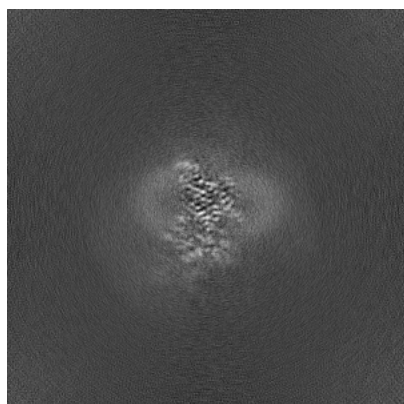


Y Index: 202

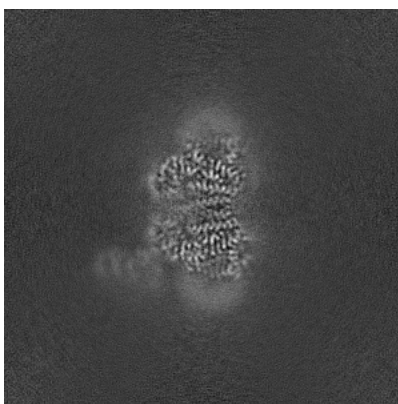


Z Index: 207

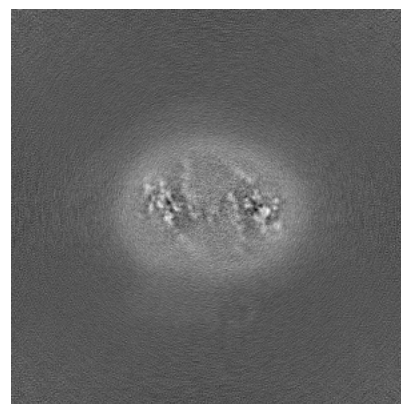
6.3.2 Raw map



X Index: 165



Y Index: 202

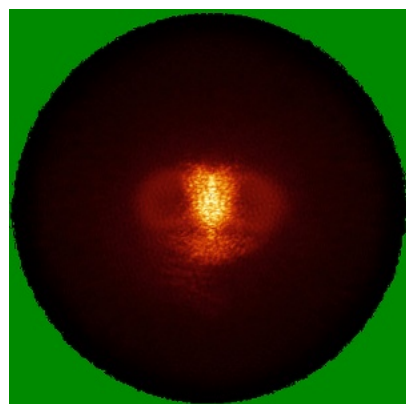


Z Index: 186

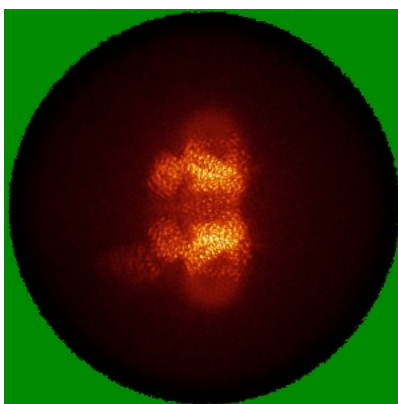
The images above show the largest variance slices of the map in three orthogonal directions.

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

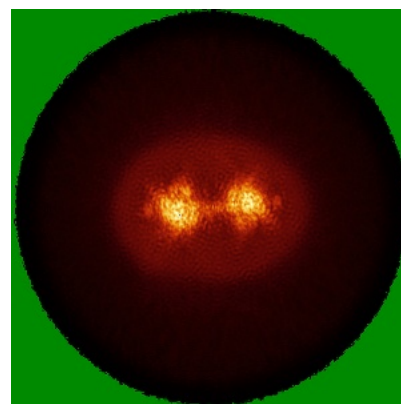
6.4.1 Primary map



X

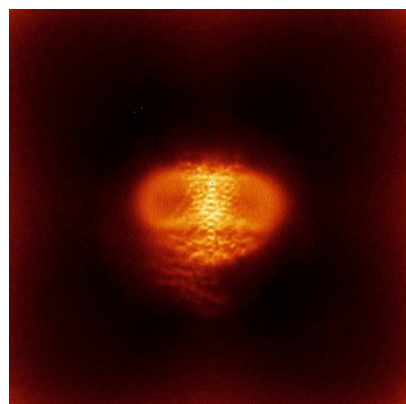


Y

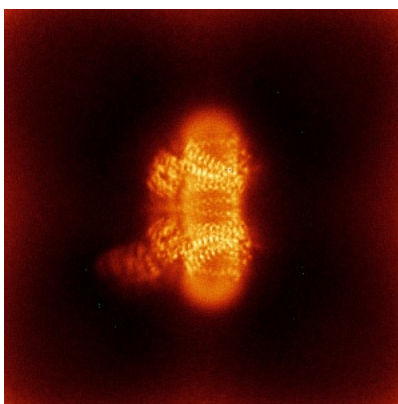


Z

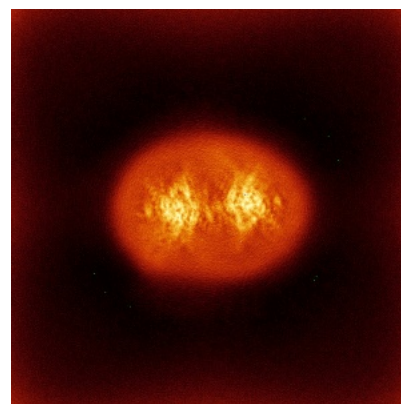
6.4.2 Raw map



X



Y

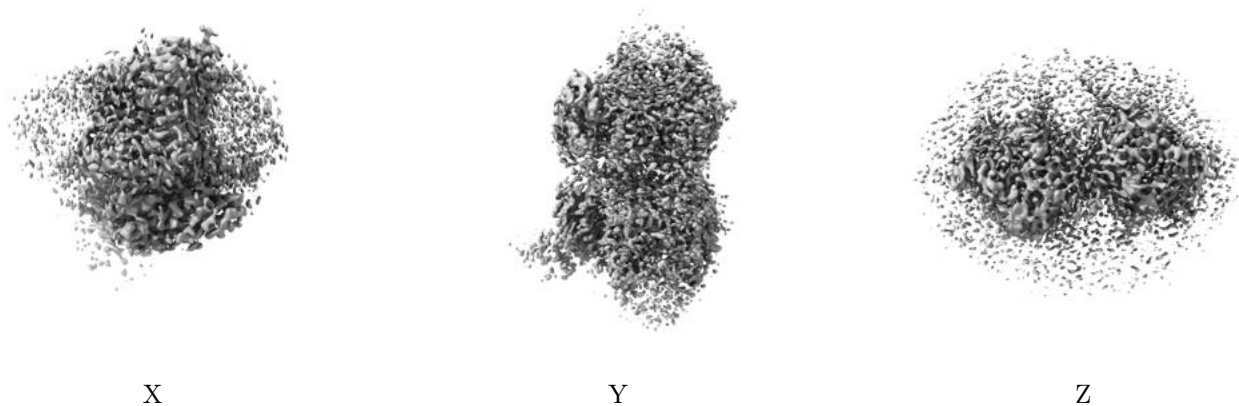


Z

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.

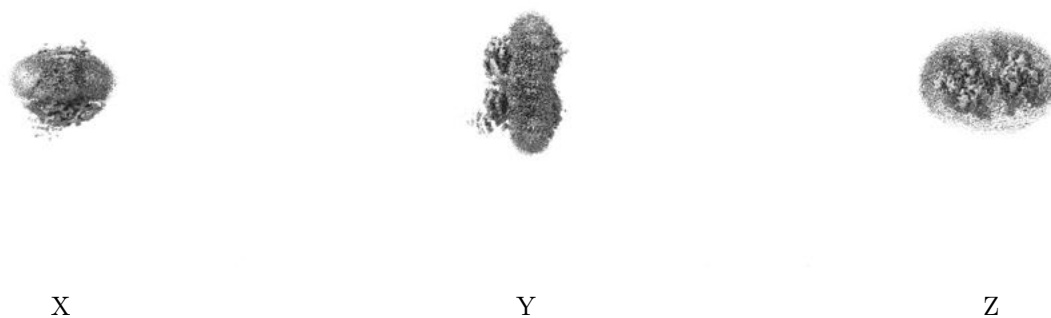
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.0. 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.

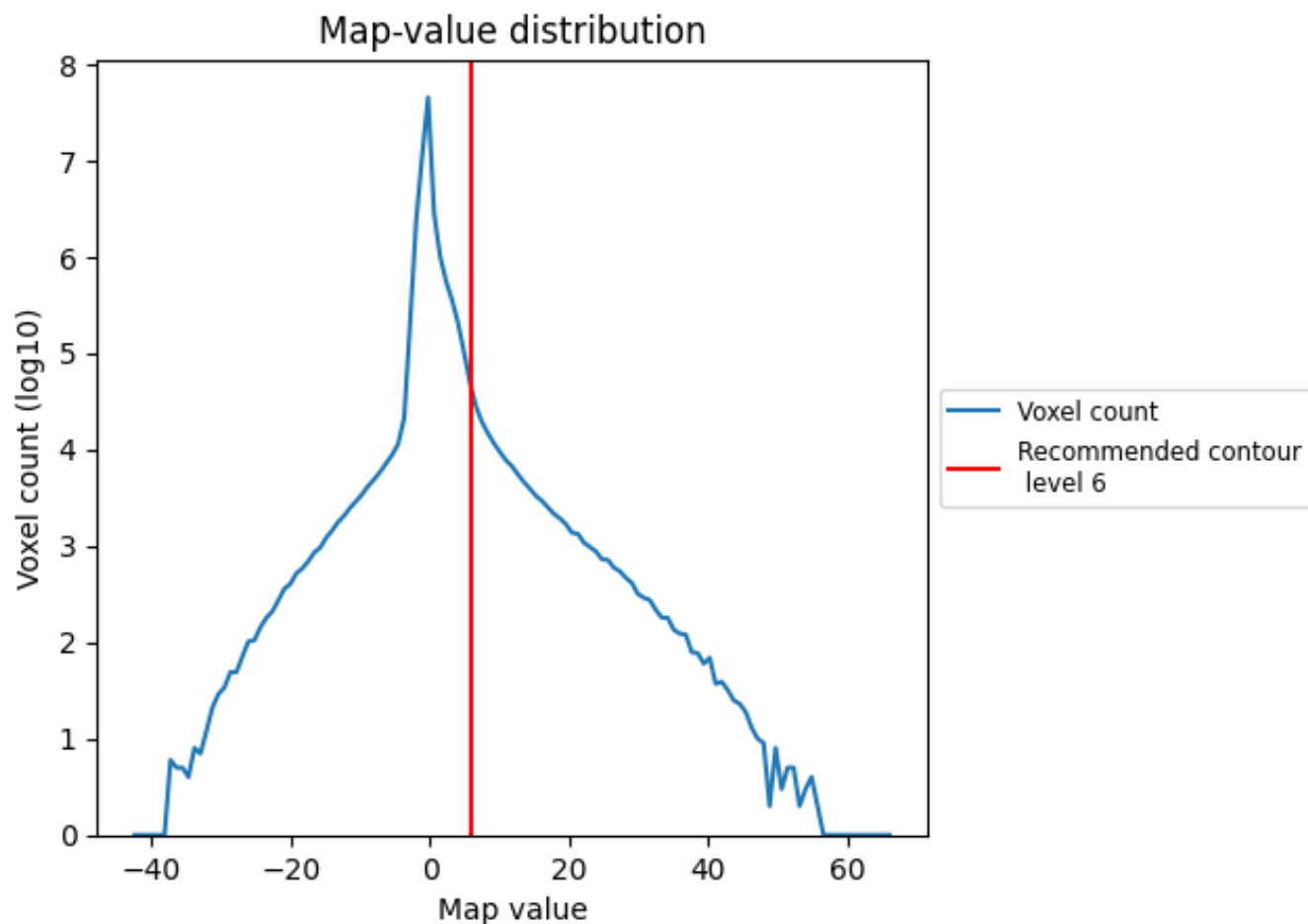
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

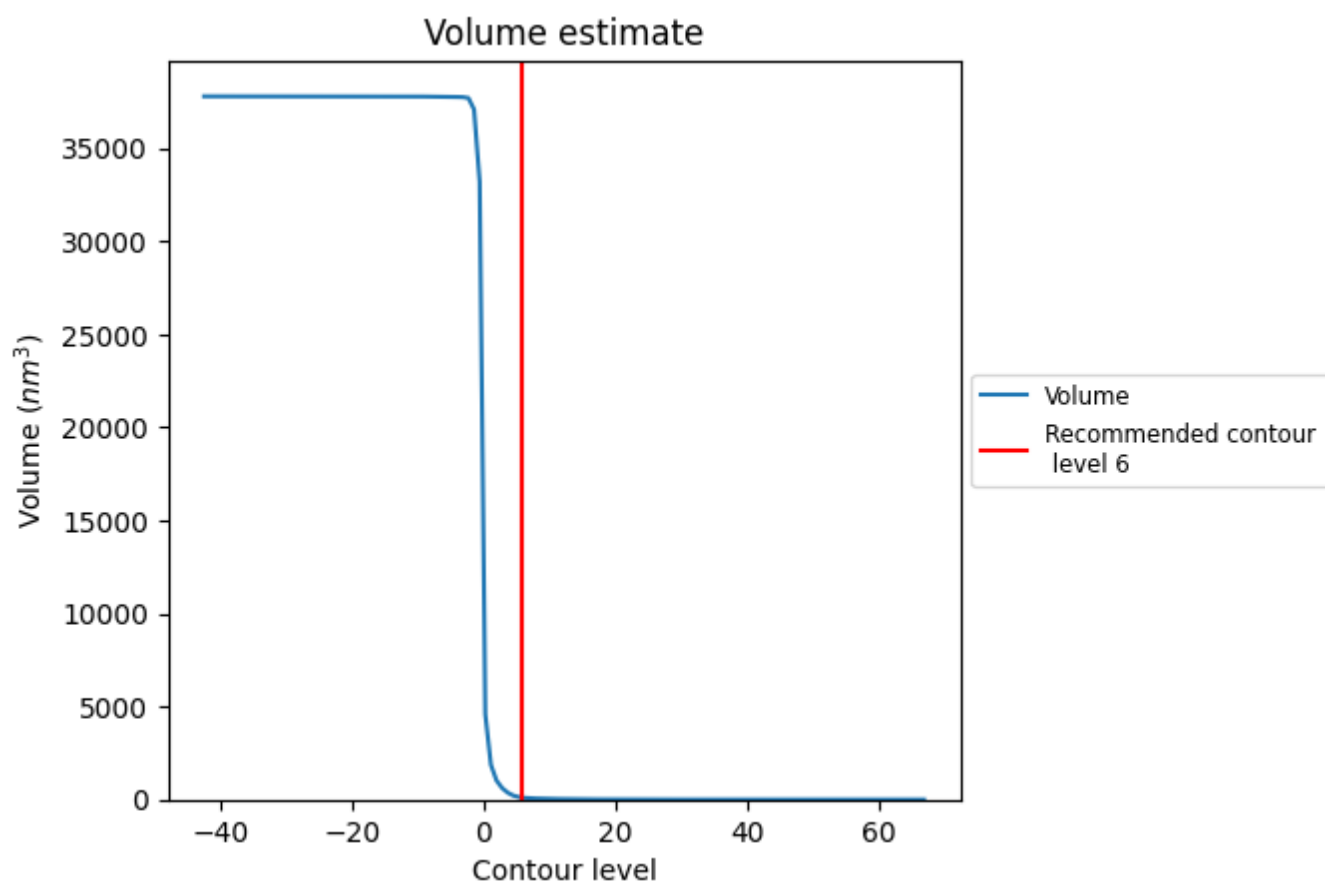
This section contains the results of statistical analysis of the map.

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.

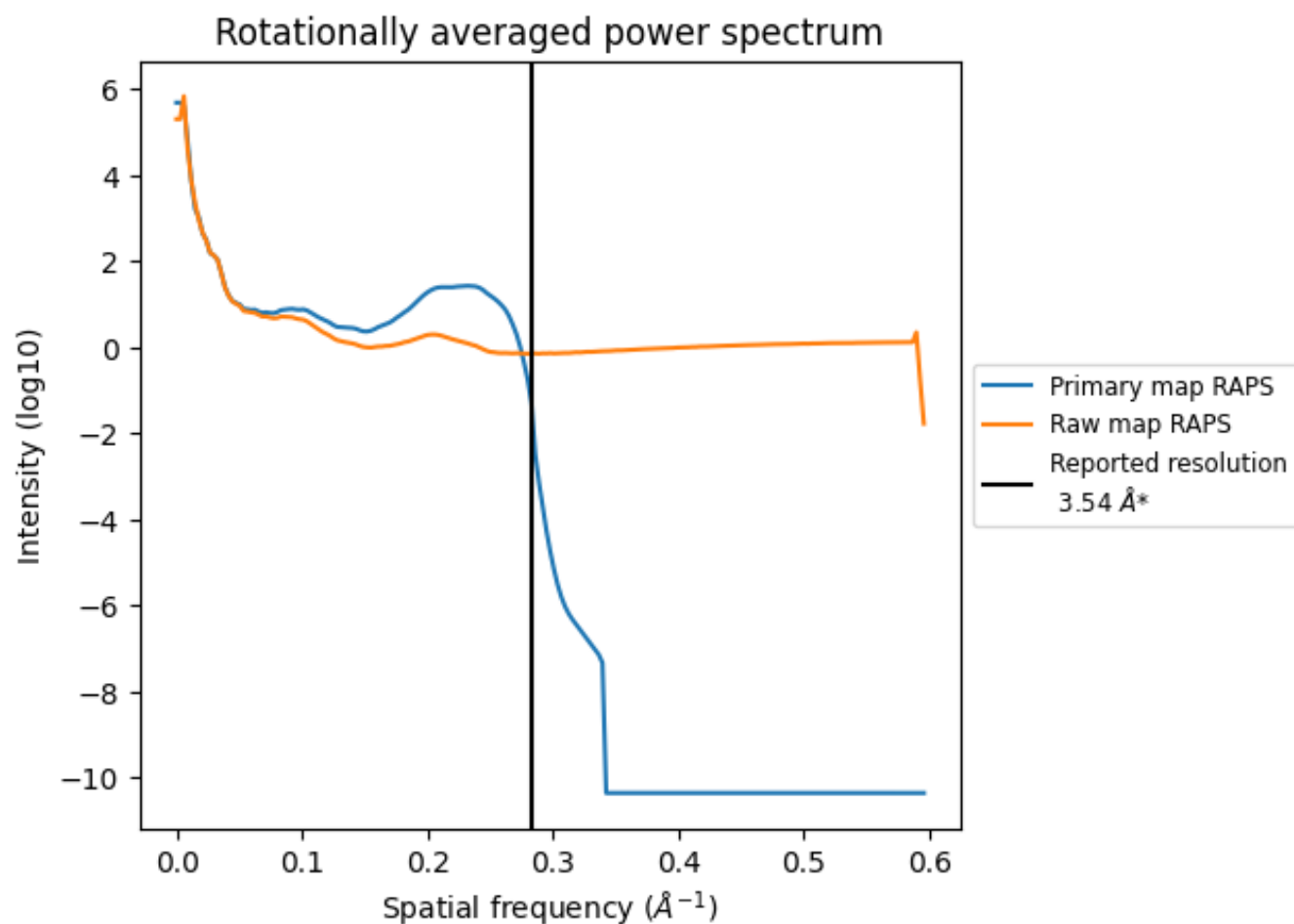
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 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 ⓘ

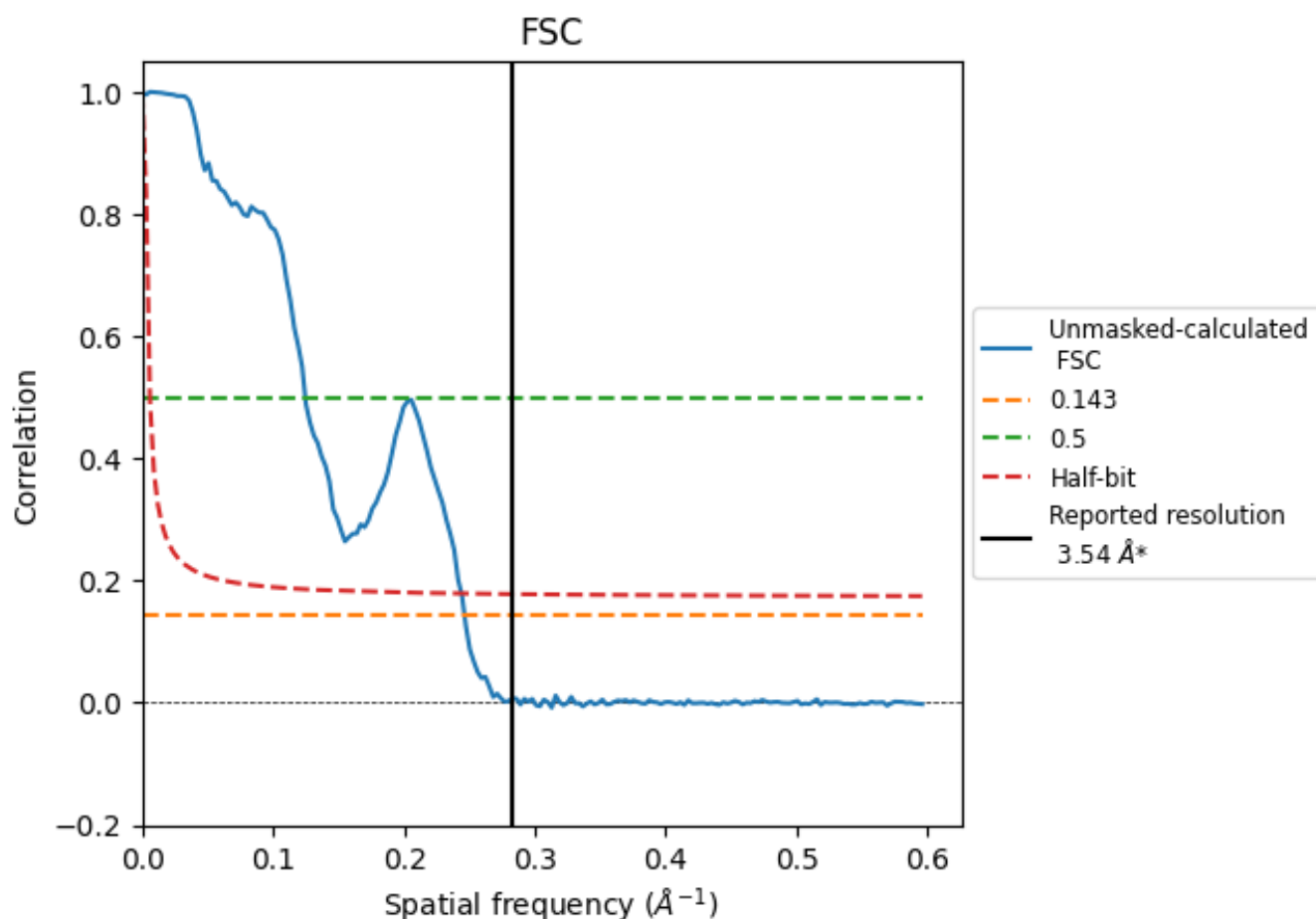


*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

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 0.282 Å⁻¹

8.2 Resolution estimates [i](#)

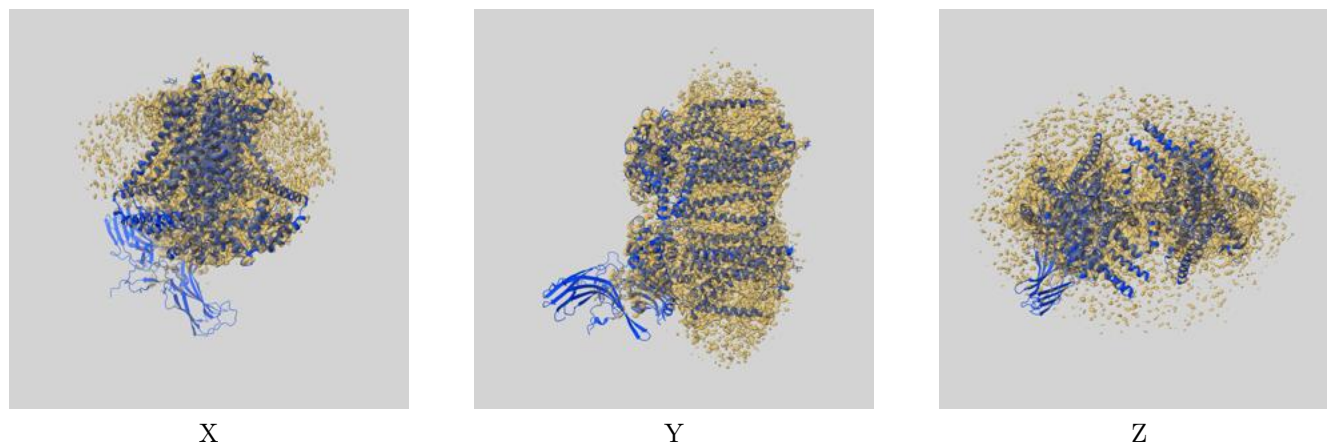
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.06	8.03	4.10

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

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 8.

9.1 Map-model overlay [i](#)



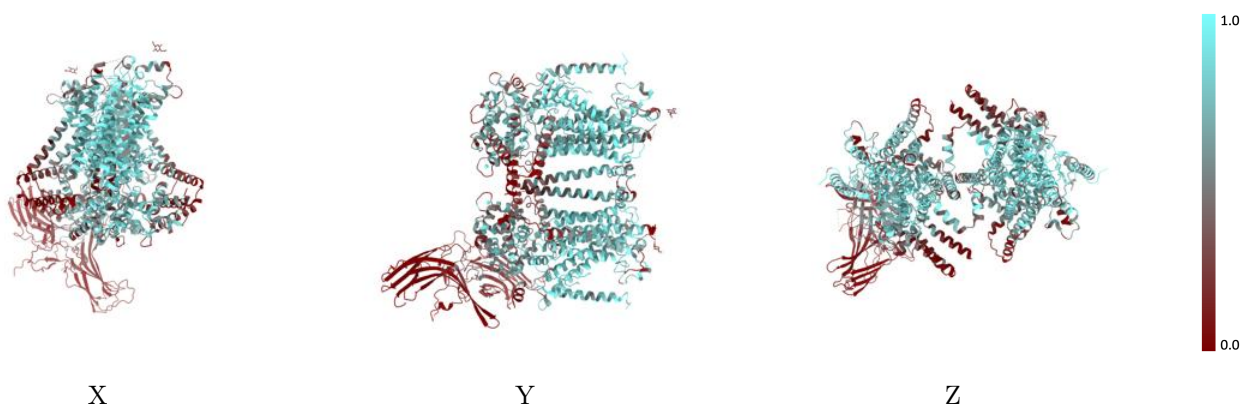
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



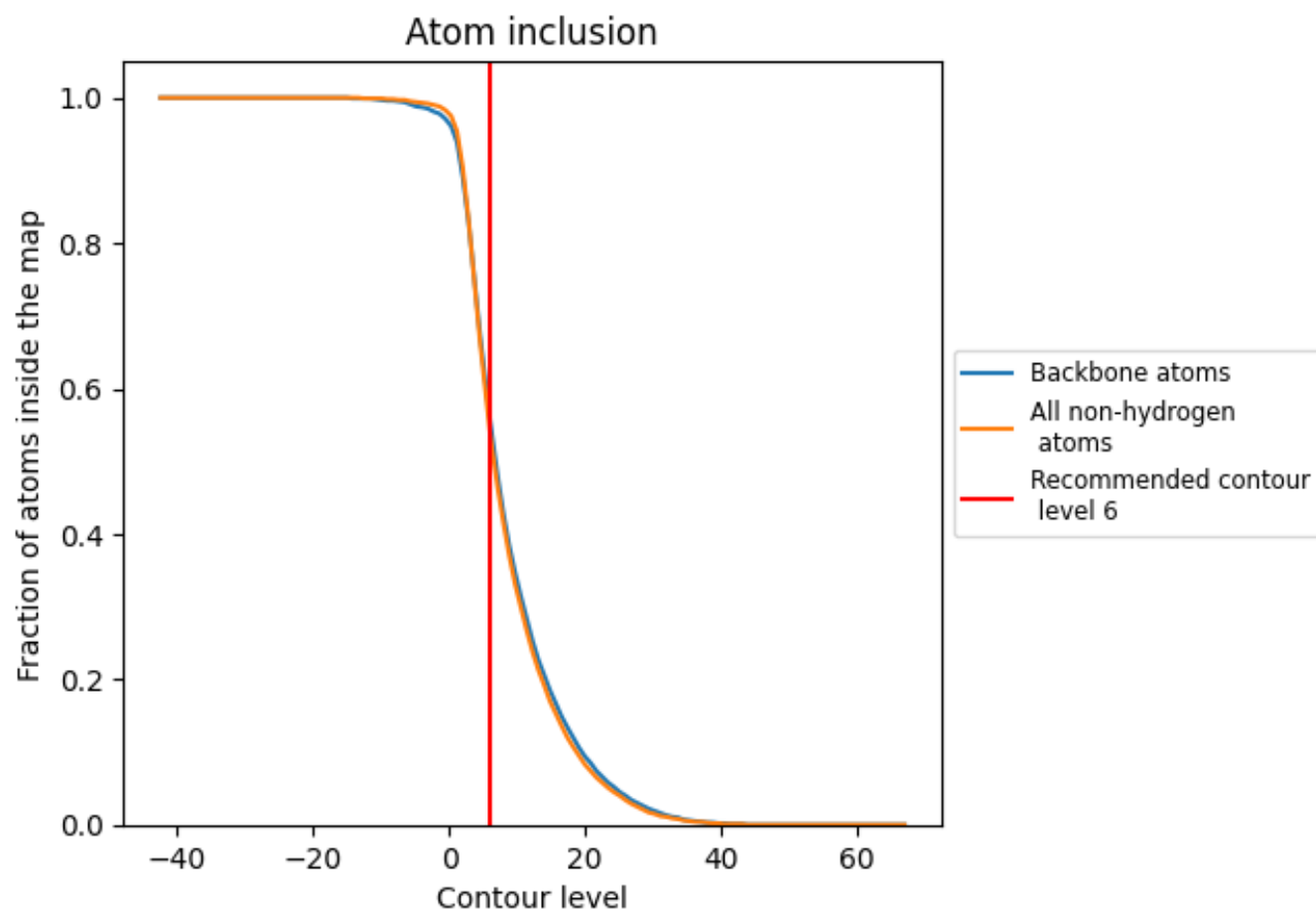
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5410	0.3550
A	0.6530	0.3880
B	0.6610	0.3820
C	0.5900	0.3800
D	0.6730	0.4190
E	0.6200	0.3880
F	0.6120	0.4020
J	0.0490	0.2080

1.0

0.0

<0.0