



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:45 PM UTC

PDB ID : 6HIJ / pdb_00006hij
EMDB ID : EMD-4256
Title : Cryo-EM structure of the human ABCG2-MZ29-Fab complex with cholesterol and PE lipids docked
Authors : Jackson, S.M.; Manolaridis, I.; Kowal, J.; Zechner, M.; Taylor, N.M.I.; Bause, M.; Bauer, S.; Bartholomaeus, R.; Stahlberg, H.; Bernhardt, G.; Koenig, B.; Buschauer, A.; Altmann, K.H.; Locher, K.P.
Deposited on : 2018-08-30
Resolution : 3.56 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:

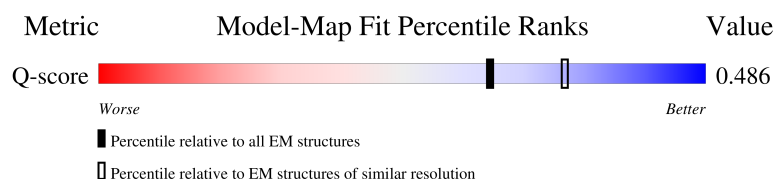
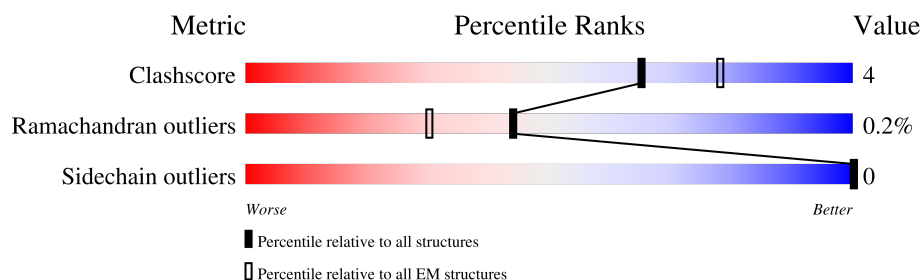
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.56 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	12750 (3.06 - 4.06)

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	655	
1	B	655	

2 Entry composition [i](#)

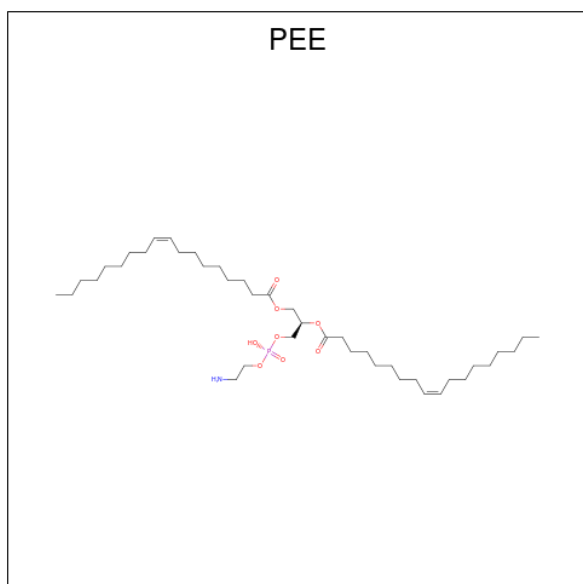
There are 4 unique types of molecules in this entry. The entry contains 9574 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-binding cassette sub-family G member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	572	Total	C	N	O	S	0	0
			4449	2888	733	799	29		
1	B	572	Total	C	N	O	S	0	0
			4449	2888	733	799	29		

- Molecule 2 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



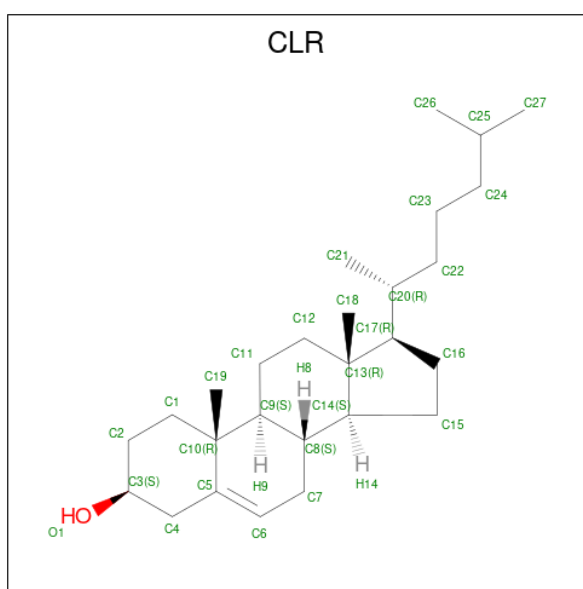
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
2	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
2	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
2	A	1	Total	C	N	O	P	0
			38	28	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			37	27	1	8	1	
2	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
2	B	1	Total	C	N	O	P	0
			38	28	1	8	1	
2	B	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



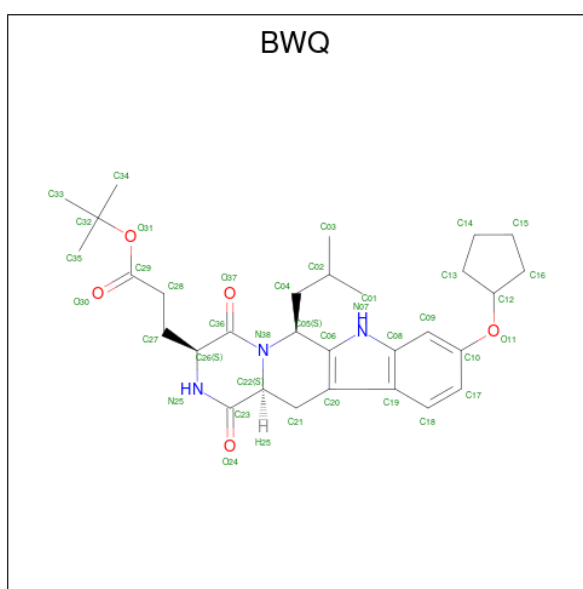
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	

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Mol	Chain	Residues	Atoms			AltConf
3	B	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	

- Molecule 4 is {tert}-butyl 3-[(2 {S},5 {S},8 {S})-14-cyclopentyloxy-2-(2-methylpropyl)-4,7-bis(oxidanylidene)-3,6,17-triazatetracyclo[8.7.0.0[^]{3,8}.0[^]{11,16}}]heptadeca-1(10),11,13,15-tetraen-5-yl]propanoate (CCD ID: BWQ) (formula: C₃₀H₄₁N₃O₅).

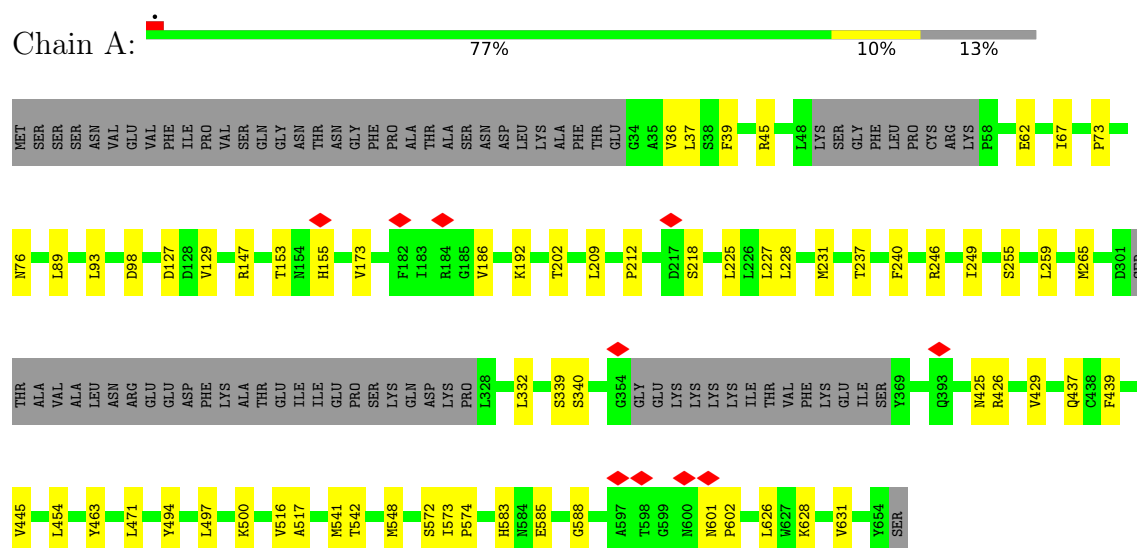


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			38	30	3	5	
4	B	1	Total	C	N	O	0
			38	30	3	5	

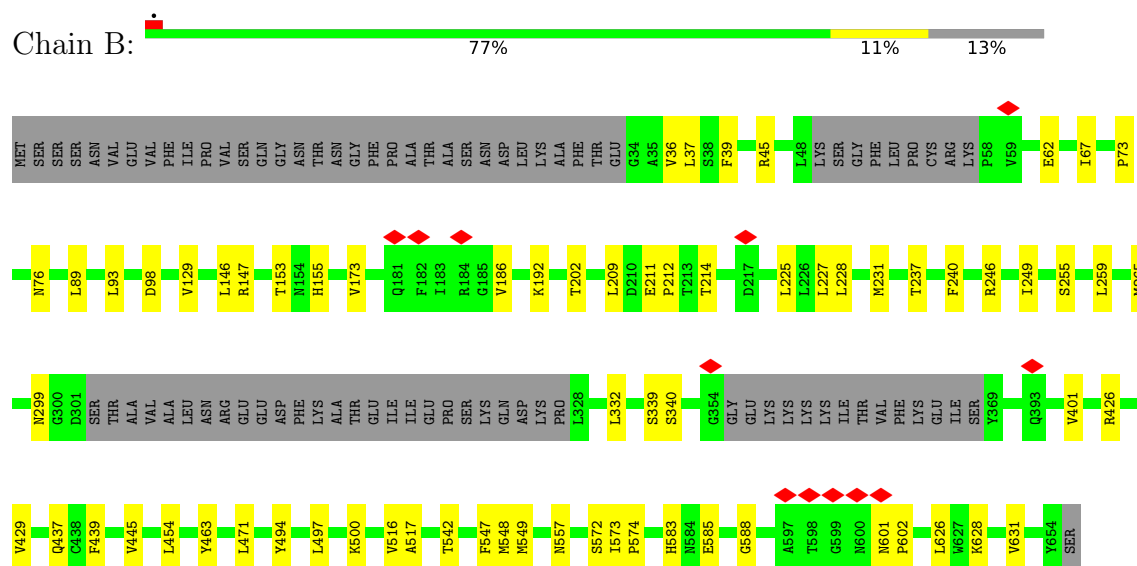
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ATP-binding cassette sub-family G member 2



• Molecule 1: ATP-binding cassette sub-family G member 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	402348	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 ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.209	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	259.84, 259.84, 259.84	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.812, 0.812, 0.812	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEE, BWQ, CLR

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	0.39	0/4542	0.64	4/6145 (0.1%)
1	B	0.39	0/4542	0.64	4/6145 (0.1%)
All	All	0.39	0/9084	0.64	8/12290 (0.1%)

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

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	572	SER	CA-C-N	9.73	126.37	120.24
1	B	572	SER	C-N-CA	9.73	126.37	120.24
1	A	572	SER	CA-C-N	9.72	126.37	120.24
1	A	572	SER	C-N-CA	9.72	126.37	120.24
1	B	445	VAL	CA-C-N	5.20	127.97	120.38
1	B	445	VAL	C-N-CA	5.20	127.97	120.38
1	A	445	VAL	CA-C-N	5.18	127.94	120.38
1	A	445	VAL	C-N-CA	5.18	127.94	120.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	601	ASN	Peptide
1	B	601	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4449	0	4532	36	0
1	B	4449	0	4532	39	0
2	A	160	0	219	4	0
2	B	160	0	219	2	0
3	A	140	0	228	2	0
3	B	140	0	228	3	0
4	A	38	0	0	0	0
4	B	38	0	0	0	0
All	All	9574	0	9958	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:VAL:HG21	1:A:497:LEU:HD21	1.81	0.62
1:B:429:VAL:HG21	1:B:497:LEU:HD21	1.81	0.62
1:A:76:ASN:HD22	1:A:255:SER:HB3	1.64	0.61
1:B:76:ASN:HD22	1:B:255:SER:HB3	1.65	0.61
1:A:426:ARG:NH1	1:A:585:GLU:OE2	2.35	0.60
1:B:500:LYS:HZ1	1:B:588:GLY:H	1.50	0.59
1:B:426:ARG:NH1	1:B:585:GLU:OE2	2.35	0.59
1:A:494:TYR:OH	1:A:500:LYS:O	2.22	0.58
1:A:500:LYS:HZ1	1:A:588:GLY:H	1.50	0.58
1:B:246:ARG:H	1:B:249:ILE:HD12	1.69	0.58
1:B:494:TYR:OH	1:B:500:LYS:O	2.22	0.57
1:A:246:ARG:H	1:A:249:ILE:HD12	1.69	0.57
1:A:218:SER:OG	1:B:299:ASN:ND2	2.37	0.57
1:B:401:VAL:HG22	2:B:709:PEE:H23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:708:PEE:H28	2:A:708:PEE:H53	1.90	0.53
1:B:147:ARG:HH21	1:B:202:THR:HG21	1.73	0.53
1:B:147:ARG:HH11	1:B:463:TYR:HE1	1.55	0.53
1:A:147:ARG:HH11	1:A:463:TYR:HE1	1.55	0.53
1:A:147:ARG:HH21	1:A:202:THR:HG21	1.73	0.52
1:B:225:LEU:HD23	1:B:228:LEU:HD12	1.91	0.52
1:A:37:LEU:HD21	1:A:93:LEU:HD22	1.92	0.52
1:A:225:LEU:HD23	1:A:228:LEU:HD12	1.91	0.52
1:A:516:VAL:HG23	1:A:573:ILE:HG22	1.92	0.52
1:B:516:VAL:HG23	1:B:573:ILE:HG22	1.92	0.51
1:B:37:LEU:HD21	1:B:93:LEU:HD22	1.92	0.51
1:B:471:LEU:HD21	3:B:703:CLR:H111	1.94	0.50
1:A:437:GLN:HE21	1:A:517:ALA:HB2	1.77	0.49
1:B:437:GLN:HE21	1:B:517:ALA:HB2	1.77	0.49
1:A:583:HIS:CD2	1:A:626:LEU:HB2	2.49	0.48
1:B:583:HIS:CD2	1:B:626:LEU:HB2	2.49	0.48
2:B:709:PEE:H13	2:B:709:PEE:H20	1.65	0.47
1:B:45:ARG:HB3	1:B:62:GLU:HG2	1.97	0.47
1:B:39:PHE:HE2	1:B:67:ILE:HG22	1.81	0.46
1:B:439:PHE:HE1	1:B:542:THR:HG23	1.81	0.46
1:A:439:PHE:HE1	1:A:542:THR:HG23	1.81	0.46
1:A:39:PHE:HE2	1:A:67:ILE:HG22	1.81	0.45
1:A:45:ARG:HB3	1:A:62:GLU:HG2	1.97	0.45
1:A:98:ASP:OD1	1:A:98:ASP:N	2.49	0.45
1:B:628:LYS:HA	1:B:631:VAL:HG22	1.98	0.45
1:A:628:LYS:HA	1:A:631:VAL:HG22	1.98	0.45
1:B:129:VAL:HB	1:B:454:LEU:HD13	1.99	0.45
1:B:548:MET:HB3	1:B:574:PRO:HD2	1.99	0.45
1:A:425:ASN:HD21	1:B:557:ASN:H	1.64	0.45
1:A:471:LEU:HD21	3:A:704:CLR:H111	1.98	0.44
1:A:129:VAL:HB	1:A:454:LEU:HD13	1.99	0.44
1:A:89:LEU:HD13	1:A:259:LEU:HD11	1.99	0.44
1:B:89:LEU:HD13	1:B:259:LEU:HD11	1.99	0.44
1:A:548:MET:HB3	1:A:574:PRO:HD2	1.99	0.44
1:B:209:LEU:HB2	1:B:240:PHE:HB3	1.99	0.44
1:A:209:LEU:HB2	1:A:240:PHE:HB3	1.99	0.44
1:A:541:MET:HE3	1:A:541:MET:HB3	1.86	0.44
1:B:98:ASP:N	1:B:98:ASP:OD1	2.49	0.44
3:B:703:CLR:H232	3:B:703:CLR:H211	1.80	0.43
1:A:265:MET:HE1	1:A:332:LEU:HB3	2.00	0.43
1:B:227:LEU:HG	1:B:231:MET:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:704:CLR:H232	3:A:704:CLR:H211	1.79	0.43
1:A:127:ASP:OD1	1:A:127:ASP:N	2.51	0.43
1:A:227:LEU:HG	1:A:231:MET:HE3	2.01	0.43
1:A:173:VAL:HG21	1:A:186:VAL:HG23	2.01	0.42
1:A:36:VAL:HG22	1:A:73:PRO:HD3	2.02	0.42
1:B:265:MET:HE1	1:B:332:LEU:HB3	2.01	0.42
1:B:192:LYS:HE2	1:B:212:PRO:HA	2.02	0.41
1:B:73:PRO:HA	1:B:237:THR:HG22	2.02	0.41
2:A:701:PEE:H20	2:A:701:PEE:H13	1.79	0.41
1:B:36:VAL:HG22	1:B:73:PRO:HD3	2.02	0.41
1:A:631:VAL:HG12	2:A:708:PEE:H57	2.03	0.41
2:A:708:PEE:H30	2:A:708:PEE:H23	1.85	0.41
1:A:192:LYS:HE2	1:A:212:PRO:HA	2.02	0.41
1:B:146:LEU:HD23	1:B:146:LEU:HA	1.91	0.41
1:B:173:VAL:HG21	1:B:186:VAL:HG23	2.01	0.41
1:A:153:THR:HG22	1:A:155:HIS:H	1.86	0.41
1:B:153:THR:HG22	1:B:155:HIS:H	1.86	0.40
1:A:73:PRO:HA	1:A:237:THR:HG22	2.02	0.40
1:B:211:GLU:HB3	1:B:214:THR:HG22	2.02	0.40
1:B:547:PHE:HB3	3:B:702:CLR:H273	2.03	0.40
1:A:339:SER:OG	1:A:340:SER:N	2.55	0.40
1:B:549:MET:HE3	1:B:549:MET:HB2	1.83	0.40
1:B:146:LEU:HD13	1:B:463:TYR:HB3	2.04	0.40
1:B:339:SER:OG	1:B:340:SER:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	564/655 (86%)	543 (96%)	20 (4%)	1 (0%)	43 73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	564/655 (86%)	543 (96%)	20 (4%)	1 (0%)	43	73
All	All	1128/1310 (86%)	1086 (96%)	40 (4%)	2 (0%)	44	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	602	PRO
1	B	602	PRO

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	487/560 (87%)	487 (100%)	0	100	100
1	B	487/560 (87%)	487 (100%)	0	100	100
All	All	974/1120 (87%)	974 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	222	ASN
1	A	299	ASN
1	A	425	ASN
1	A	437	GLN
1	A	583	HIS
1	B	76	ASN
1	B	141	GLN
1	B	222	ASN
1	B	299	ASN
1	B	437	GLN
1	B	583	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CLR	A	705	-	31,31,31	0.24	0	48,48,48	0.45	0
2	PEE	B	709	-	42,42,50	0.86	2 (4%)	45,47,55	0.65	0
3	CLR	B	702	-	31,31,31	0.26	0	48,48,48	0.54	0
2	PEE	A	707	-	36,36,50	0.77	2 (5%)	39,41,55	2.18	3 (7%)
3	CLR	A	704	-	31,31,31	0.23	0	48,48,48	0.46	0
2	PEE	B	708	-	37,37,50	0.83	2 (5%)	40,42,55	2.25	7 (17%)
2	PEE	A	701	-	42,42,50	0.85	2 (4%)	45,47,55	0.61	0
4	BWQ	B	710	-	42,42,42	3.42	15 (35%)	58,63,63	3.30	18 (31%)
3	CLR	B	701	-	31,31,31	0.22	0	48,48,48	0.42	0
3	CLR	B	705	-	31,31,31	0.24	0	48,48,48	0.45	0
3	CLR	A	703	-	31,31,31	0.26	0	48,48,48	0.54	0
3	CLR	B	703	-	31,31,31	0.23	0	48,48,48	0.43	0
2	PEE	B	707	-	41,41,50	0.82	2 (4%)	44,46,55	0.58	1 (2%)
3	CLR	B	704	-	31,31,31	0.24	0	48,48,48	0.45	0
3	CLR	A	702	-	31,31,31	0.21	0	48,48,48	0.43	0
2	PEE	A	708	-	41,41,50	0.82	2 (4%)	44,46,55	0.64	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BWQ	A	710	-	42,42,42	3.43	15 (35%)	58,63,63	3.27	18 (31%)
3	CLR	A	706	-	31,31,31	0.24	0	48,48,48	0.44	0
2	PEE	A	709	-	37,37,50	0.78	2 (5%)	40,42,55	2.14	3 (7%)
2	PEE	B	706	-	36,36,50	0.78	2 (5%)	39,41,55	2.18	3 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLR	A	705	-	-	1/10/68/68	0/4/4/4
2	PEE	B	709	-	-	15/46/46/54	-
3	CLR	B	702	-	-	3/10/68/68	0/4/4/4
2	PEE	A	707	-	-	12/40/40/54	-
3	CLR	A	704	-	-	2/10/68/68	0/4/4/4
2	PEE	B	708	-	-	10/41/41/54	-
2	PEE	A	701	-	-	14/46/46/54	-
4	BWQ	B	710	-	-	9/18/57/57	0/5/5/5
3	CLR	B	701	-	-	0/10/68/68	0/4/4/4
3	CLR	B	705	-	-	1/10/68/68	0/4/4/4
3	CLR	A	703	-	-	3/10/68/68	0/4/4/4
3	CLR	B	703	-	-	2/10/68/68	0/4/4/4
2	PEE	B	707	-	-	11/45/45/54	-
3	CLR	B	704	-	-	1/10/68/68	0/4/4/4
3	CLR	A	702	-	-	0/10/68/68	0/4/4/4
2	PEE	A	708	-	-	18/45/45/54	-
4	BWQ	A	710	-	-	5/18/57/57	0/5/5/5
3	CLR	A	706	-	-	1/10/68/68	0/4/4/4
2	PEE	A	709	-	-	12/41/41/54	-
2	PEE	B	706	-	-	12/40/40/54	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	710	BWQ	O37-C36	9.63	1.39	1.22
4	B	710	BWQ	O37-C36	9.60	1.39	1.22
4	A	710	BWQ	C23-N25	8.81	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	710	BWQ	C23-N25	8.58	1.46	1.33
4	B	710	BWQ	O24-C23	8.26	1.39	1.23
4	A	710	BWQ	O24-C23	8.23	1.39	1.23
4	A	710	BWQ	C06-N07	-8.16	1.29	1.38
4	B	710	BWQ	C06-N07	-8.14	1.29	1.38
4	A	710	BWQ	C36-N38	7.18	1.45	1.35
4	B	710	BWQ	C36-N38	7.00	1.45	1.35
4	B	710	BWQ	C19-C20	6.87	1.56	1.44
4	A	710	BWQ	C19-C20	6.84	1.56	1.44
4	B	710	BWQ	C08-N07	-3.87	1.31	1.38
4	A	710	BWQ	C08-N07	-3.85	1.31	1.38
4	B	710	BWQ	C18-C17	3.75	1.44	1.38
2	B	706	PEE	C18-C19	3.72	1.52	1.31
4	A	710	BWQ	C18-C17	3.69	1.44	1.38
2	A	709	PEE	C39-C38	3.67	1.52	1.31
2	B	708	PEE	C39-C38	3.66	1.52	1.31
2	B	707	PEE	C18-C19	3.66	1.52	1.31
2	A	707	PEE	C18-C19	3.62	1.52	1.31
2	A	708	PEE	C18-C19	3.62	1.52	1.31
2	B	709	PEE	C39-C38	3.61	1.52	1.31
2	A	701	PEE	C39-C38	3.58	1.52	1.31
2	B	709	PEE	C19-C18	3.52	1.51	1.29
2	A	701	PEE	C19-C18	3.50	1.51	1.29
4	A	710	BWQ	O31-C29	3.47	1.44	1.33
4	B	710	BWQ	O31-C29	3.25	1.43	1.33
2	A	708	PEE	C38-C39	3.09	1.52	1.29
2	B	707	PEE	C38-C39	3.08	1.52	1.29
4	B	710	BWQ	C21-C20	2.95	1.54	1.50
4	A	710	BWQ	C21-C20	2.83	1.53	1.50
4	B	710	BWQ	C06-C20	2.43	1.39	1.36
2	B	708	PEE	P-O4P	2.41	1.68	1.59
2	A	709	PEE	P-O4P	2.39	1.68	1.59
4	B	710	BWQ	O31-C32	-2.38	1.44	1.48
4	A	710	BWQ	O11-C10	2.33	1.42	1.38
4	B	710	BWQ	C09-C08	-2.26	1.36	1.39
4	B	710	BWQ	O11-C10	2.24	1.42	1.38
4	A	710	BWQ	C09-C08	-2.20	1.36	1.39
4	A	710	BWQ	C06-C20	2.16	1.39	1.36
4	A	710	BWQ	O31-C32	-2.13	1.44	1.48
2	A	707	PEE	P-O4P	2.13	1.67	1.59
2	B	706	PEE	P-O4P	2.12	1.67	1.59
4	A	710	BWQ	C18-C19	2.06	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	710	BWQ	C18-C19	2.00	1.43	1.39

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	710	BWQ	C08-N07-C06	16.93	123.16	108.53
4	B	710	BWQ	C08-N07-C06	16.90	123.13	108.53
2	B	708	PEE	O4P-P-O1P	-8.58	74.95	108.94
2	B	706	PEE	O4P-P-O1P	-8.30	76.05	108.94
2	B	708	PEE	O2P-P-O1P	-8.29	73.87	112.44
2	A	707	PEE	O4P-P-O1P	-8.17	76.54	108.94
4	B	710	BWQ	C20-C06-N07	-7.93	103.12	110.22
2	A	707	PEE	O3P-P-O1P	-7.85	77.81	108.94
4	A	710	BWQ	C20-C06-N07	-7.79	103.25	110.22
2	A	709	PEE	O3P-P-O1P	-7.77	78.14	108.94
4	B	710	BWQ	C05-C06-N07	7.72	132.23	124.05
2	B	706	PEE	O3P-P-O1P	-7.70	78.43	108.94
2	A	709	PEE	O4P-P-O1P	-7.55	79.03	108.94
2	A	709	PEE	O2P-P-O1P	-7.50	77.57	112.44
4	A	710	BWQ	C05-C06-N07	7.26	131.74	124.05
2	B	706	PEE	O2P-P-O1P	-6.85	80.59	112.44
2	A	707	PEE	O2P-P-O1P	-6.82	80.70	112.44
2	B	708	PEE	O3P-P-O1P	-5.35	87.75	108.94
4	A	710	BWQ	C10-O11-C12	-4.74	110.60	119.18
4	B	710	BWQ	C21-C20-C06	-4.58	116.20	121.71
4	B	710	BWQ	O31-C29-C28	4.54	118.60	110.67
4	B	710	BWQ	C21-C20-C19	4.43	136.89	130.85
4	A	710	BWQ	C21-C20-C06	-4.38	116.44	121.71
4	A	710	BWQ	C21-C20-C19	4.31	136.73	130.85
4	B	710	BWQ	C08-C19-C20	-4.22	103.00	106.84
4	A	710	BWQ	C19-C08-N07	-4.09	103.62	108.23
4	A	710	BWQ	C08-C19-C20	-4.07	103.14	106.84
4	B	710	BWQ	C10-O11-C12	-3.95	112.03	119.18
4	B	710	BWQ	C19-C08-N07	-3.89	103.85	108.23
4	B	710	BWQ	C22-C21-C20	-3.83	103.80	108.84
4	A	710	BWQ	C28-C27-C26	-3.79	106.18	113.16
4	A	710	BWQ	C23-C22-N38	-3.61	105.74	113.29
4	B	710	BWQ	C18-C19-C20	3.53	139.75	133.73
4	A	710	BWQ	C18-C19-C20	3.52	139.73	133.73
4	B	710	BWQ	O37-C36-N38	-3.31	118.41	123.06
4	A	710	BWQ	O31-C29-C28	3.30	116.43	110.67
4	B	710	BWQ	C23-C22-N38	-3.15	106.70	113.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	710	BWQ	C26-N25-C23	-2.91	119.53	125.83
4	A	710	BWQ	C26-N25-C23	-2.76	119.86	125.83
4	A	710	BWQ	O37-C36-N38	-2.58	119.43	123.06
2	B	708	PEE	O2-C2-C1	2.47	117.22	108.34
4	B	710	BWQ	C02-C04-C05	-2.37	109.92	115.10
2	B	708	PEE	O3-C3-C2	2.29	114.99	108.40
2	B	707	PEE	C37-C38-C39	-2.27	113.31	130.48
4	A	710	BWQ	C08-C09-C10	2.22	122.20	118.03
4	B	710	BWQ	C26-C36-N38	2.21	121.29	115.86
4	B	710	BWQ	C08-C09-C10	2.20	122.17	118.03
4	B	710	BWQ	C27-C28-C29	-2.18	107.02	113.21
4	A	710	BWQ	C26-C36-N38	2.11	121.02	115.86
2	A	708	PEE	C37-C38-C39	-2.08	114.75	130.48
4	A	710	BWQ	C22-C21-C20	-2.07	106.11	108.84
2	B	708	PEE	C2-O2-C10	2.06	122.74	117.80
4	A	710	BWQ	C02-C04-C05	-2.04	110.64	115.10
2	B	708	PEE	O2P-P-O4P	2.02	116.73	107.57

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	PEE	C4-O4P-P-O2P
2	A	707	PEE	C4-O4P-P-O1P
2	A	708	PEE	C17-C18-C19-C20
2	A	708	PEE	C1-O3P-P-O2P
2	A	708	PEE	C1-O3P-P-O4P
2	A	708	PEE	C37-C38-C39-C40
2	A	709	PEE	O2-C2-C3-O3
2	A	709	PEE	C1-O3P-P-O2P
2	B	706	PEE	C1-O3P-P-O1P
2	B	706	PEE	C4-O4P-P-O3P
2	B	706	PEE	C5-C4-O4P-P
2	B	707	PEE	C37-C38-C39-C40
2	B	708	PEE	C1-O3P-P-O1P
2	B	708	PEE	C4-O4P-P-O3P
2	B	708	PEE	C4-O4P-P-O1P
2	B	709	PEE	C4-O4P-P-O3P
2	B	709	PEE	C4-O4P-P-O2P
4	A	710	BWQ	C13-C12-O11-C10
4	A	710	BWQ	C16-C12-O11-C10
4	B	710	BWQ	C16-C12-O11-C10

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Mol	Chain	Res	Type	Atoms
4	B	710	BWQ	C28-C29-O31-C32
4	B	710	BWQ	O30-C29-O31-C32
2	B	709	PEE	C11-C12-C13-C14
3	B	702	CLR	C17-C20-C22-C23
2	B	706	PEE	C17-C18-C19-C20
2	B	707	PEE	C17-C18-C19-C20
3	B	702	CLR	C21-C20-C22-C23
3	A	703	CLR	C17-C20-C22-C23
4	B	710	BWQ	C33-C32-O31-C29
4	B	710	BWQ	C35-C32-O31-C29
4	B	710	BWQ	C34-C32-O31-C29
3	B	705	CLR	C20-C22-C23-C24
3	A	706	CLR	C20-C22-C23-C24
2	A	708	PEE	C10-C11-C12-C13
3	A	704	CLR	C22-C23-C24-C25
3	A	705	CLR	C20-C22-C23-C24
3	B	703	CLR	C22-C23-C24-C25
3	B	704	CLR	C20-C22-C23-C24
3	A	704	CLR	C20-C22-C23-C24
2	B	709	PEE	C16-C17-C18-C19
2	B	709	PEE	C37-C38-C39-C40
3	B	703	CLR	C20-C22-C23-C24
2	B	708	PEE	C11-C12-C13-C14
2	A	701	PEE	C12-C13-C14-C15
2	A	708	PEE	C32-C33-C34-C35
2	B	707	PEE	C33-C34-C35-C36
2	A	708	PEE	C14-C15-C16-C17
2	A	707	PEE	C17-C18-C19-C20
2	B	709	PEE	C12-C13-C14-C15
2	A	709	PEE	O3P-C1-C2-C3
2	A	701	PEE	C15-C16-C17-C18
3	B	702	CLR	C22-C23-C24-C25
3	A	703	CLR	C21-C20-C22-C23
2	A	709	PEE	O3P-C1-C2-O2
2	B	706	PEE	C13-C14-C15-C16
2	A	708	PEE	C16-C17-C18-C19
2	A	708	PEE	C2-C1-O3P-P
2	A	701	PEE	C11-C12-C13-C14
2	A	707	PEE	O3P-C1-C2-O2
2	B	706	PEE	O3P-C1-C2-O2
4	B	710	BWQ	C09-C10-O11-C12
4	B	710	BWQ	C17-C10-O11-C12

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Mol	Chain	Res	Type	Atoms
2	A	707	PEE	O2-C2-C3-O3
2	B	709	PEE	C10-C11-C12-C13
4	B	710	BWQ	C13-C12-O11-C10
2	A	708	PEE	O3P-C1-C2-C3
2	A	701	PEE	C16-C17-C18-C19
2	A	707	PEE	C1-C2-C3-O3
2	A	709	PEE	C1-C2-C3-O3
2	A	709	PEE	C5-C4-O4P-P
2	A	701	PEE	C37-C38-C39-C40
4	A	710	BWQ	C09-C10-O11-C12
2	A	708	PEE	C12-C13-C14-C15
2	B	706	PEE	O2-C2-C3-O3
2	B	707	PEE	O2-C2-C3-O3
4	A	710	BWQ	C17-C10-O11-C12
2	B	706	PEE	O3P-C1-C2-C3
2	A	707	PEE	C35-C36-C37-C38
2	A	708	PEE	O3P-C1-C2-O2
2	A	701	PEE	C31-C32-C33-C34
2	A	709	PEE	C38-C39-C40-C41
2	B	706	PEE	C1-C2-C3-O3
4	A	710	BWQ	C02-C04-C05-C06
2	A	701	PEE	C4-O4P-P-O3P
2	A	701	PEE	O4P-C4-C5-N
2	A	707	PEE	C1-O3P-P-O2P
2	A	707	PEE	C1-O3P-P-O1P
2	A	709	PEE	C1-O3P-P-O4P
2	A	709	PEE	C4-O4P-P-O2P
2	B	708	PEE	C4-O4P-P-O2P
2	B	709	PEE	O4P-C4-C5-N
2	B	708	PEE	C36-C37-C38-C39
2	B	706	PEE	C35-C36-C37-C38
2	B	707	PEE	C16-C17-C18-C19
2	A	709	PEE	C32-C33-C34-C35
2	B	707	PEE	C32-C33-C34-C35
2	A	708	PEE	O3-C30-C31-C32
2	A	708	PEE	C36-C37-C38-C39
2	A	707	PEE	C10-C11-C12-C13
2	A	708	PEE	C19-C20-C21-C22
2	A	708	PEE	C18-C19-C20-C21
2	B	708	PEE	C38-C39-C40-C41
2	B	706	PEE	C18-C19-C20-C21
3	A	703	CLR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
2	B	709	PEE	C31-C32-C33-C34
2	A	707	PEE	C18-C19-C20-C21
2	A	709	PEE	C36-C37-C38-C39
2	B	707	PEE	C18-C19-C20-C21
2	A	708	PEE	C13-C14-C15-C16
2	A	707	PEE	O3P-C1-C2-C3
2	A	701	PEE	C36-C37-C38-C39
2	B	709	PEE	C38-C39-C40-C41
2	B	708	PEE	C1-C2-O2-C10
2	B	709	PEE	C36-C37-C38-C39
2	A	709	PEE	C31-C32-C33-C34
2	B	708	PEE	C1-C2-C3-O3
2	A	701	PEE	O3-C30-C31-C32
2	A	701	PEE	C38-C39-C40-C41
2	B	706	PEE	C16-C17-C18-C19
2	A	707	PEE	C14-C15-C16-C17
2	A	708	PEE	C33-C34-C35-C36
2	B	709	PEE	O2-C10-C11-C12
2	B	708	PEE	C12-C13-C14-C15
2	B	707	PEE	O2-C10-C11-C12
2	B	709	PEE	O3-C30-C31-C32
2	B	707	PEE	C2-C1-O3P-P
2	A	701	PEE	O2-C10-C11-C12
2	B	709	PEE	O4-C10-C11-C12
2	B	707	PEE	C1-C2-C3-O3
2	B	709	PEE	O5-C30-C31-C32
2	A	701	PEE	O5-C30-C31-C32
2	B	707	PEE	O4-C10-C11-C12

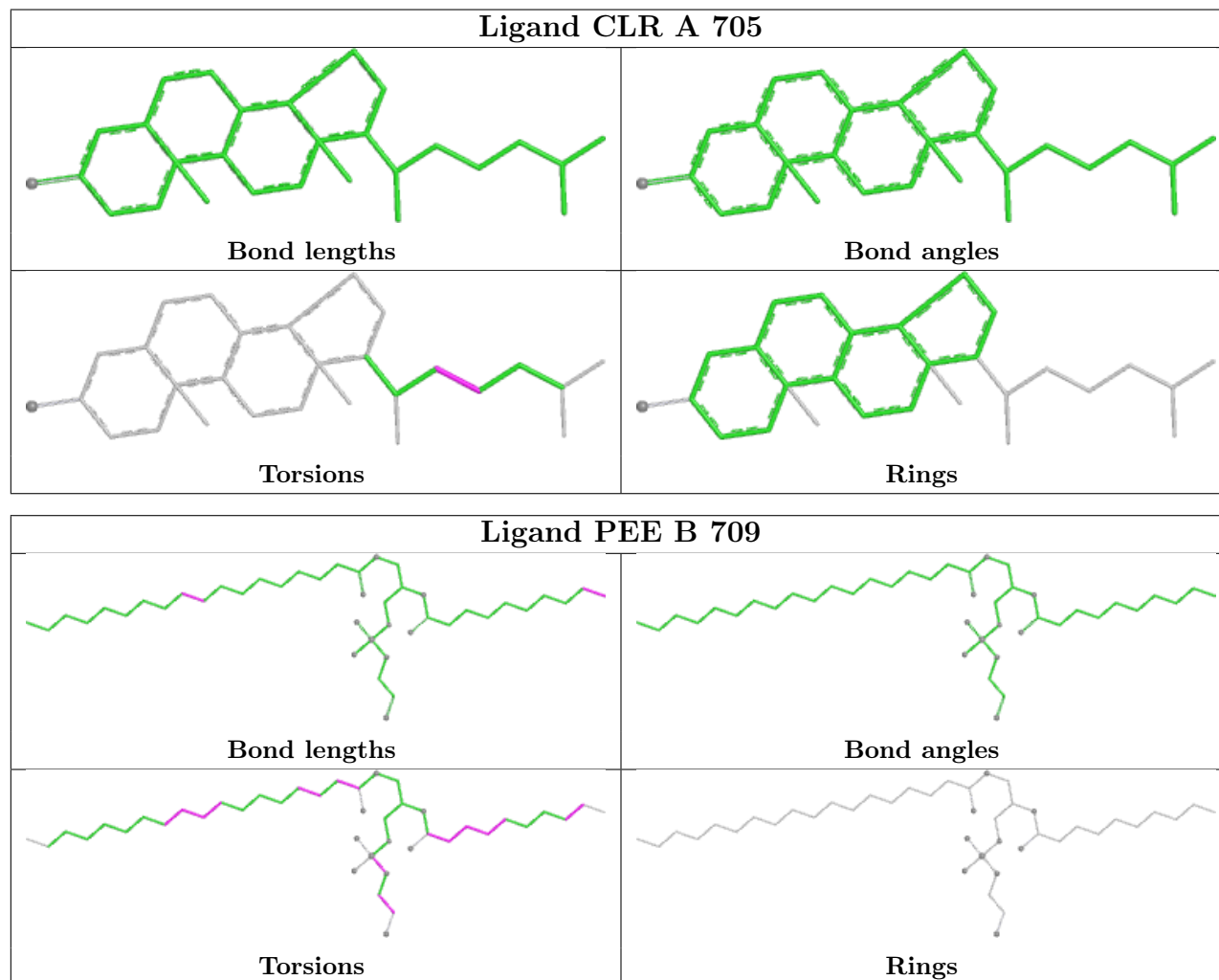
There are no ring outliers.

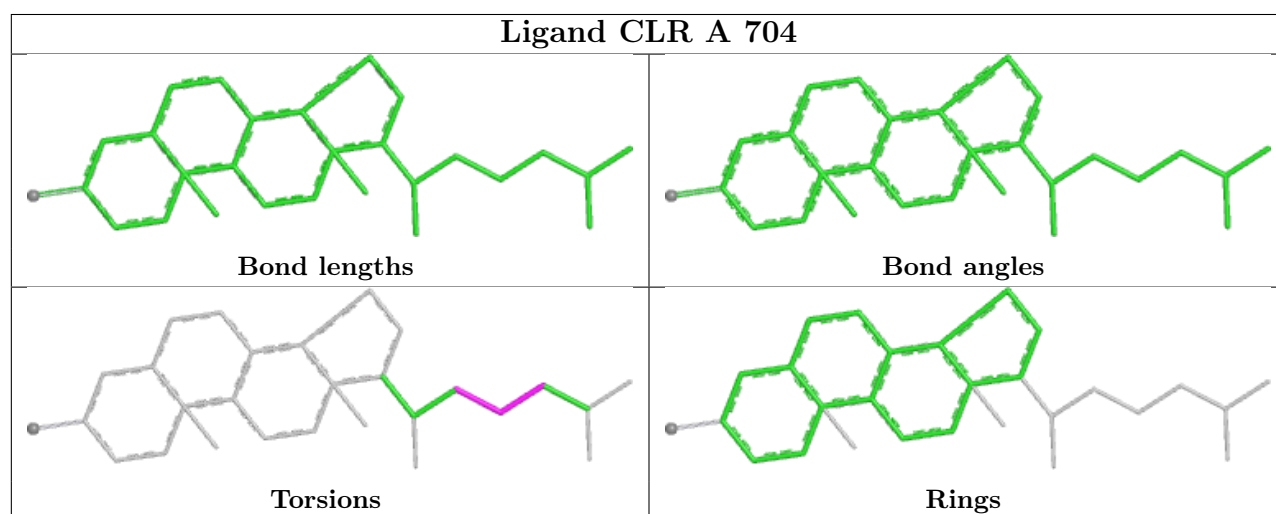
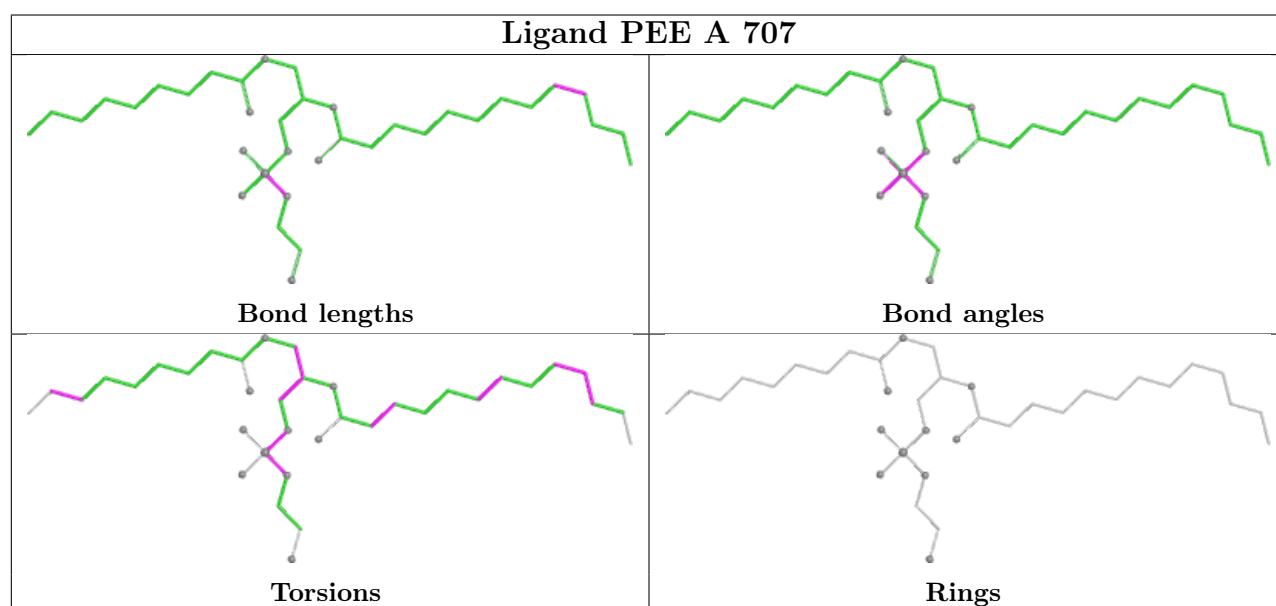
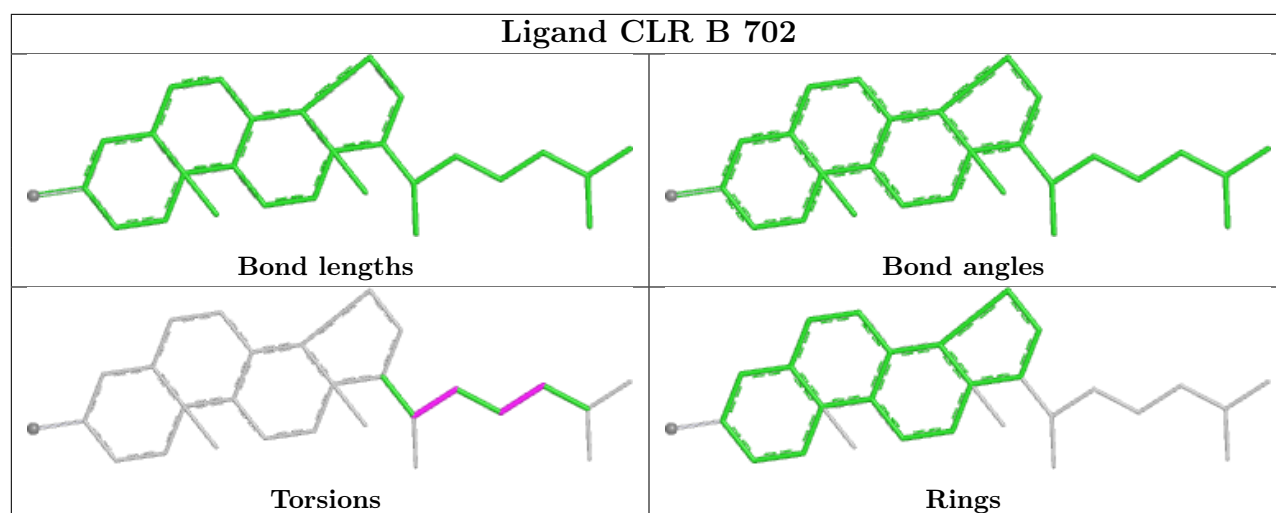
6 monomers are involved in 11 short contacts:

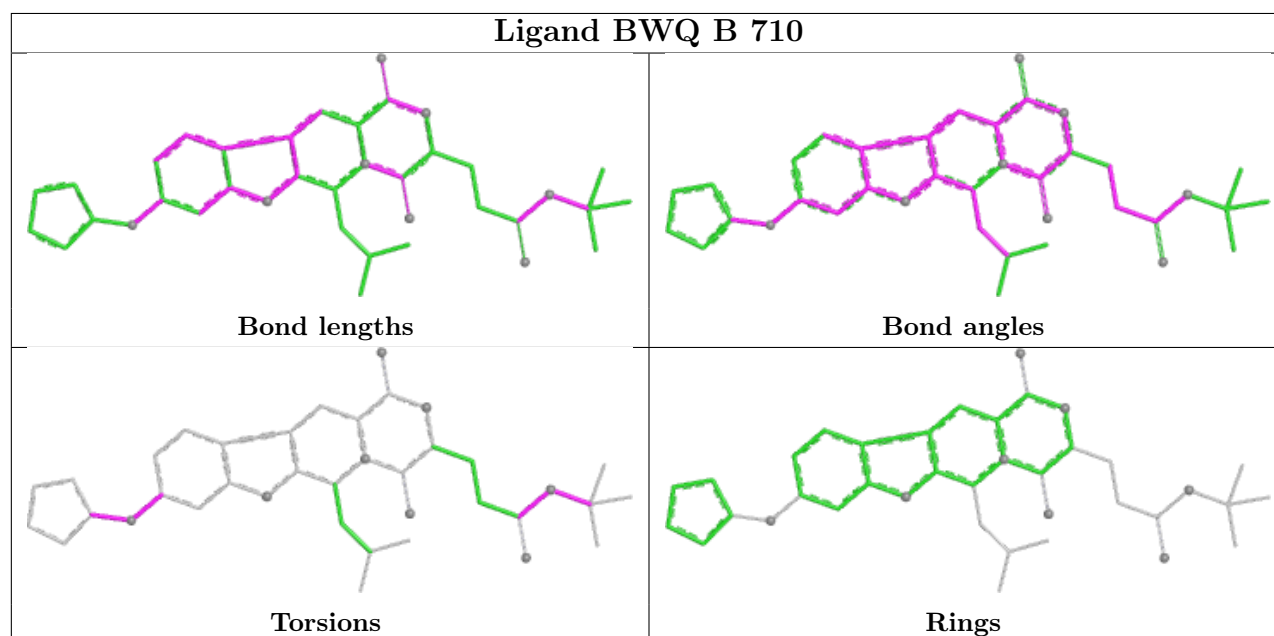
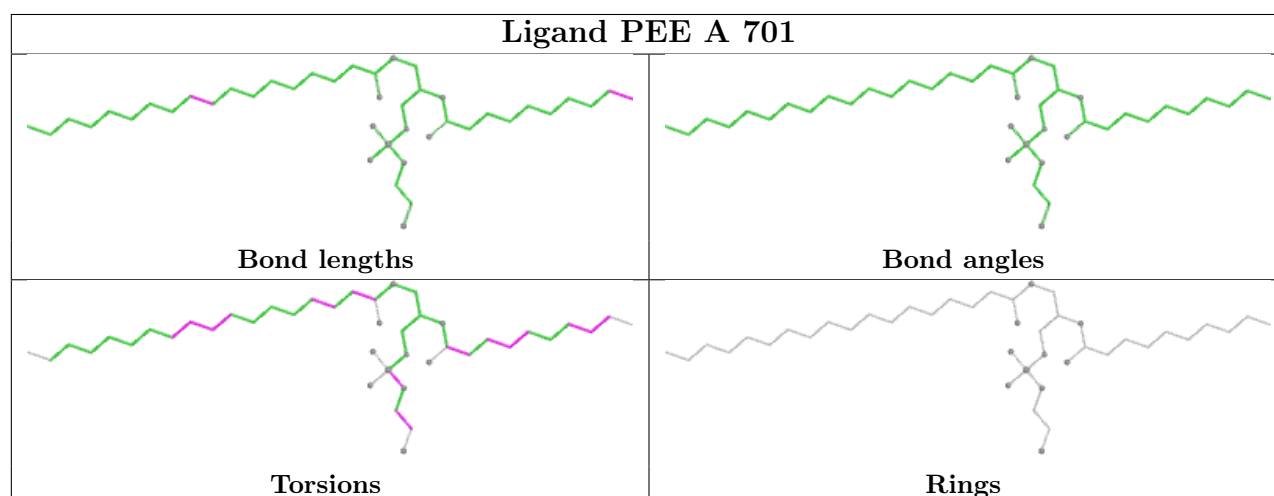
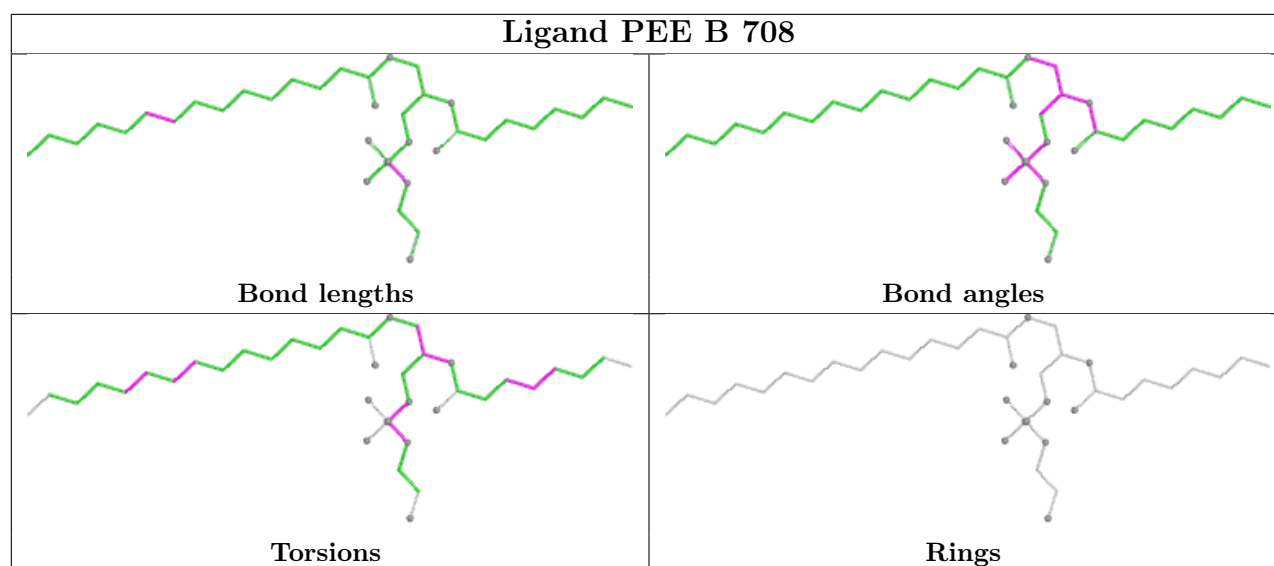
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	709	PEE	2	0
3	B	702	CLR	1	0
3	A	704	CLR	2	0
2	A	701	PEE	1	0
3	B	703	CLR	2	0
2	A	708	PEE	3	0

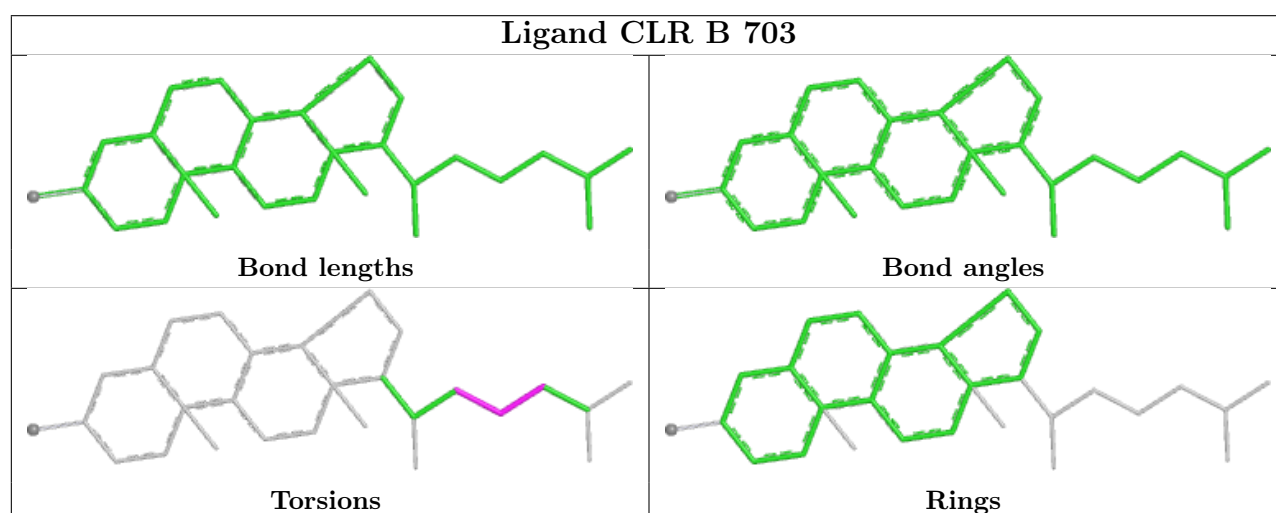
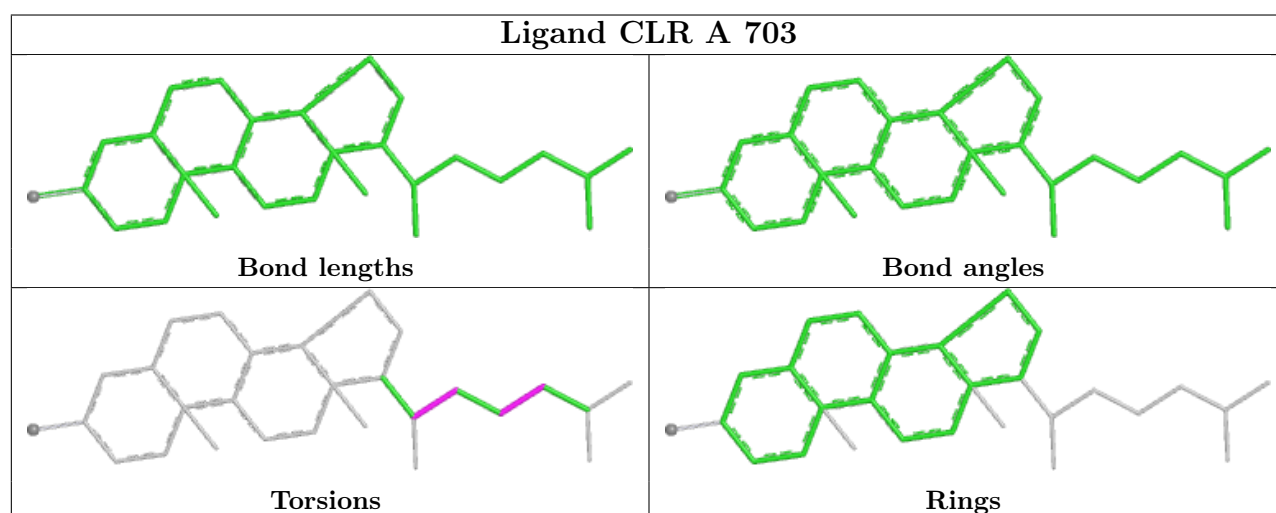
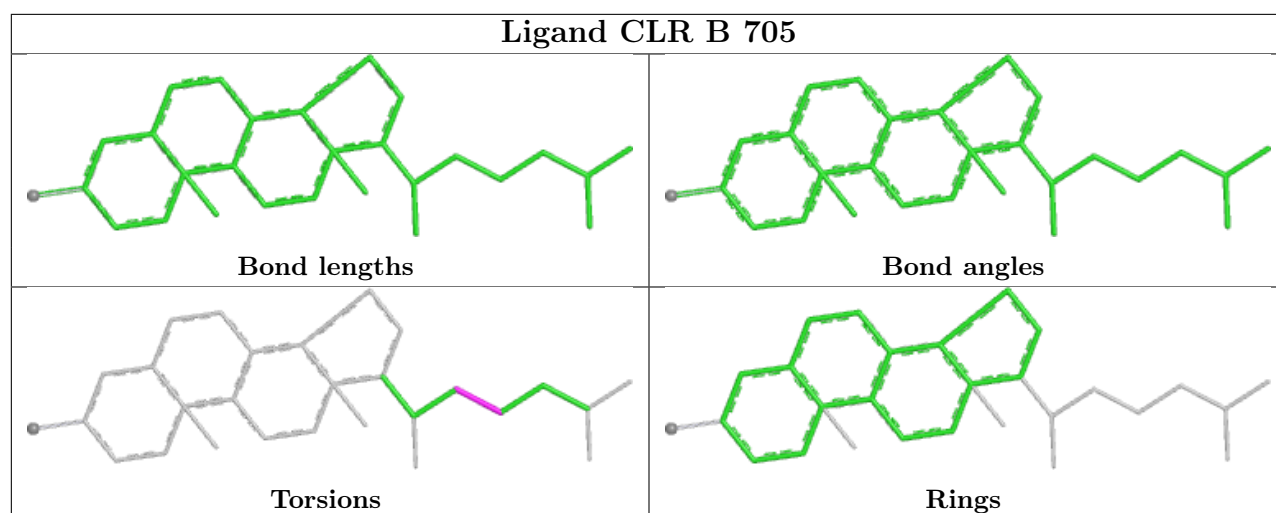
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

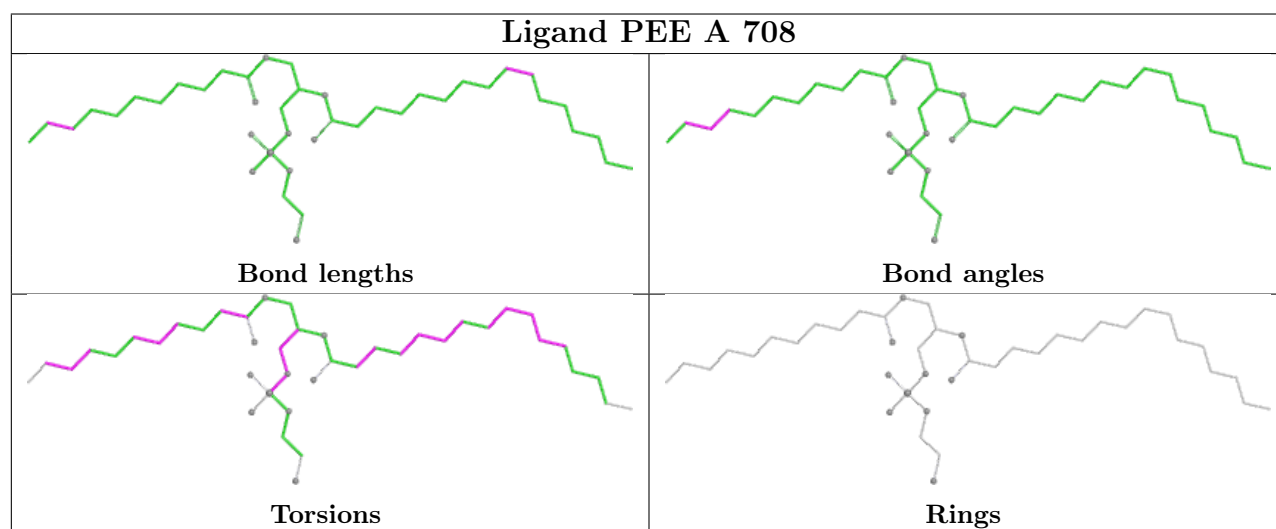
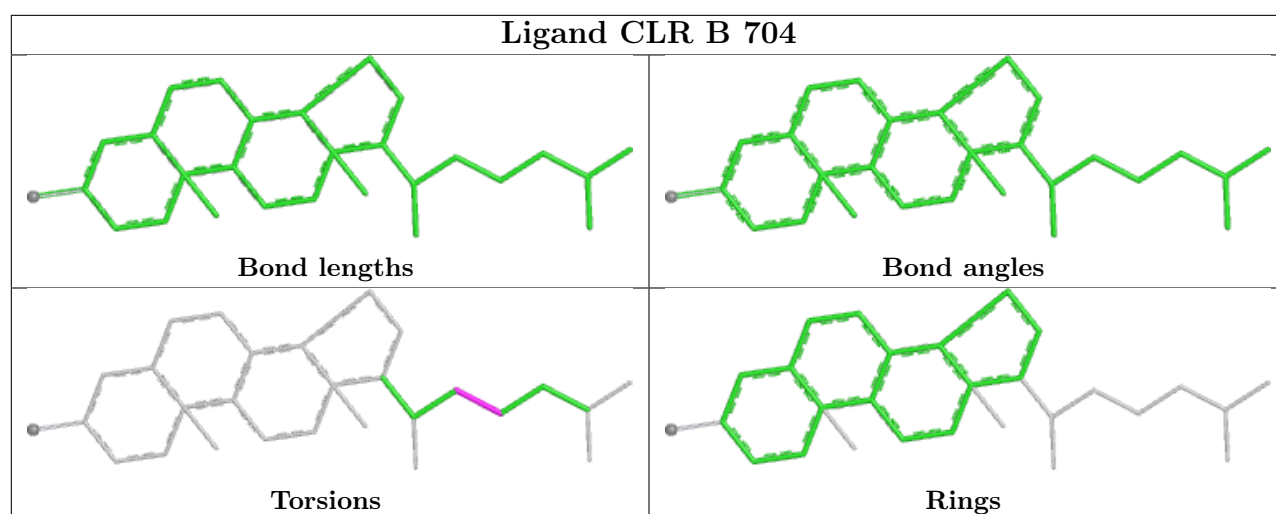
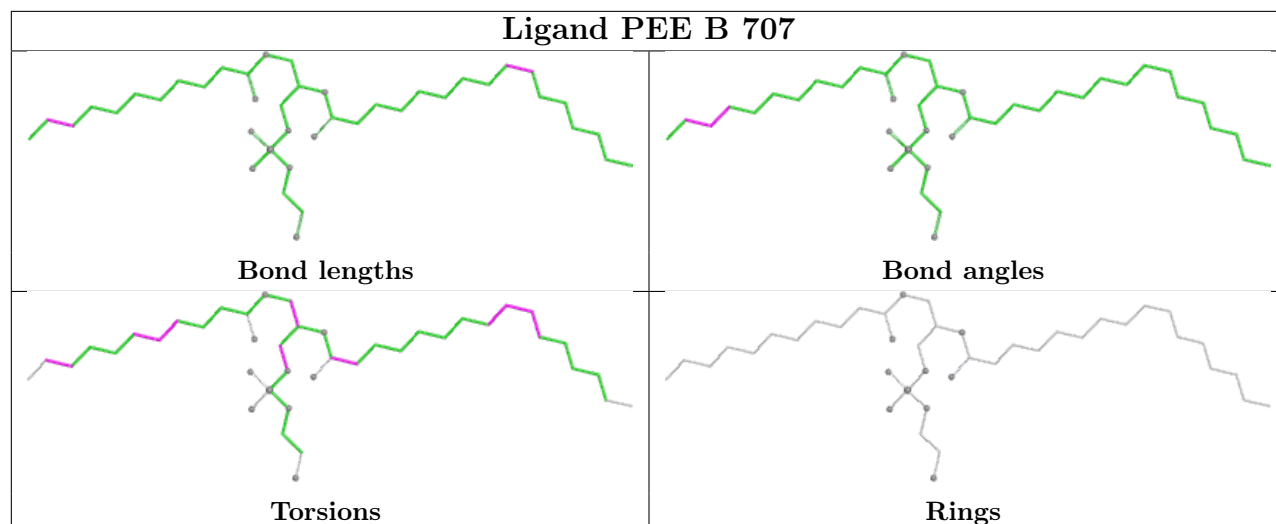
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

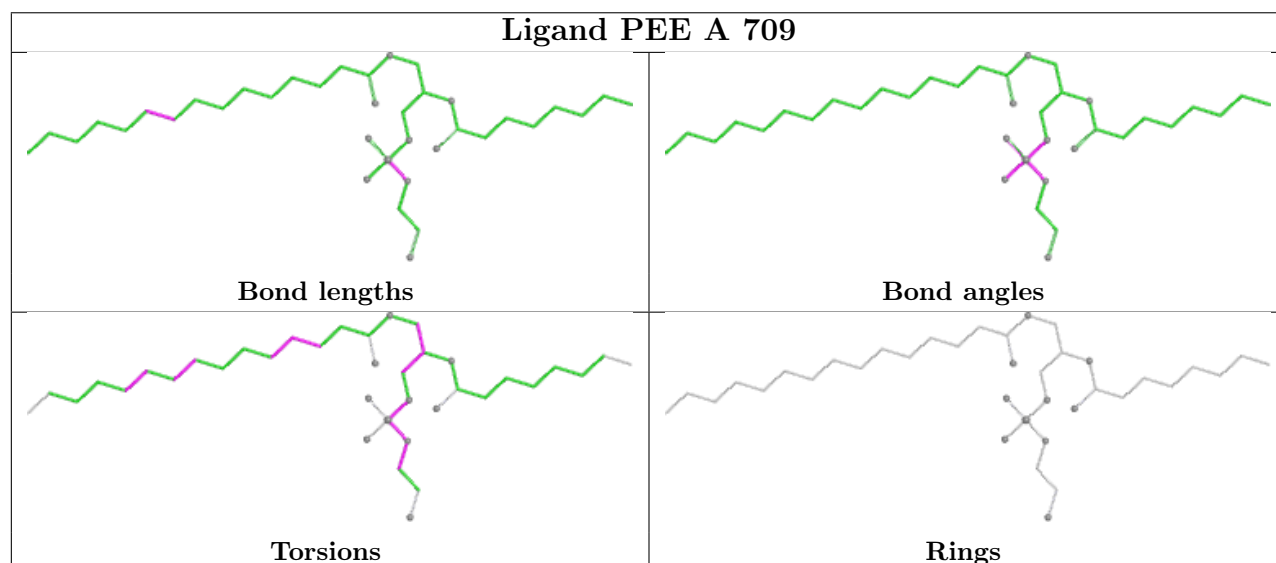
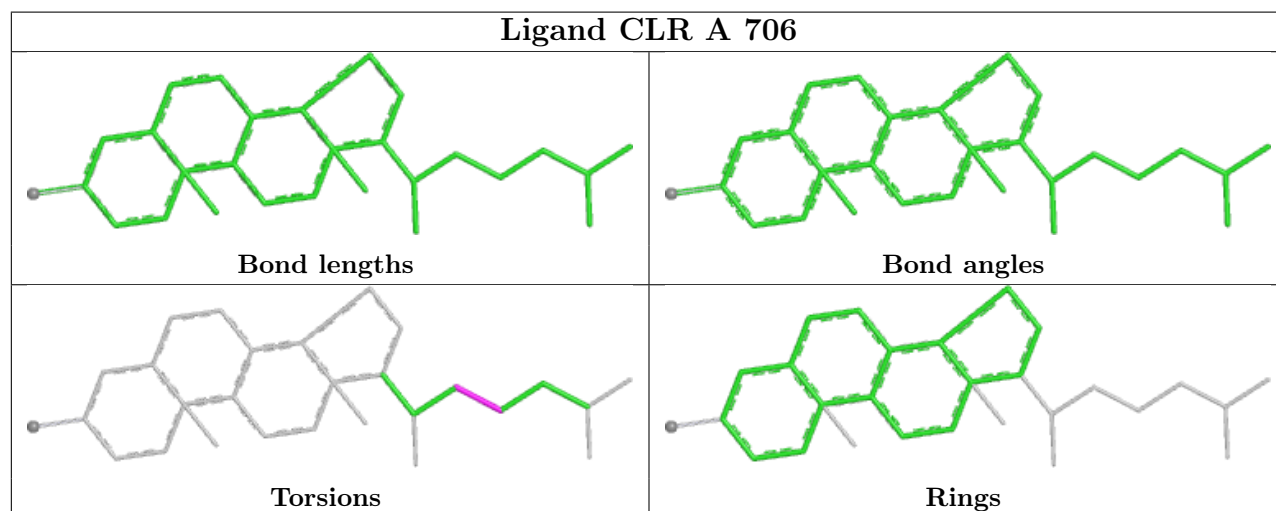
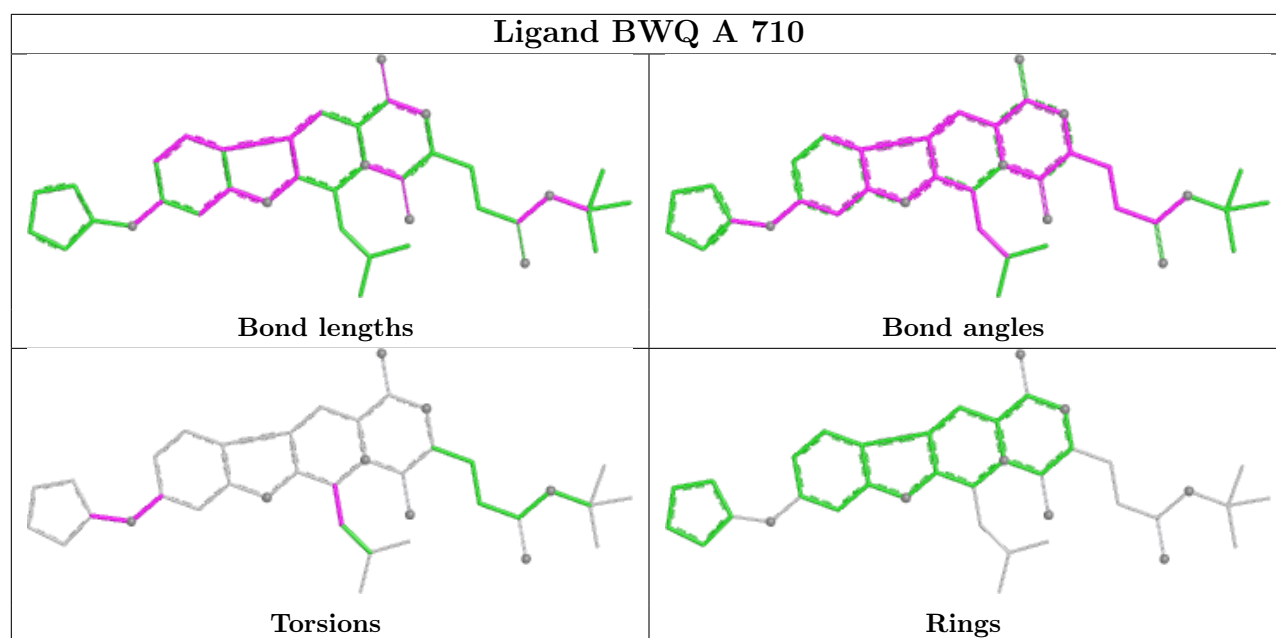


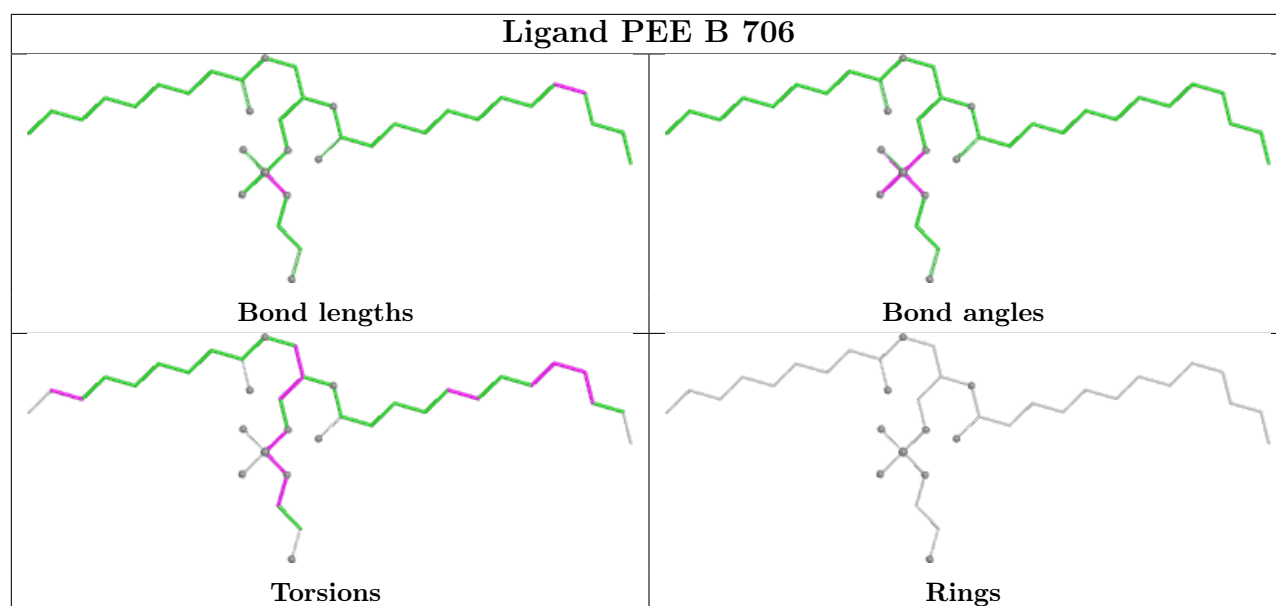












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

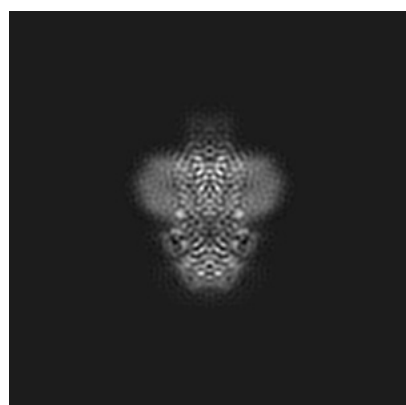
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4256. These allow visual inspection of the internal detail of the map and identification of artifacts.

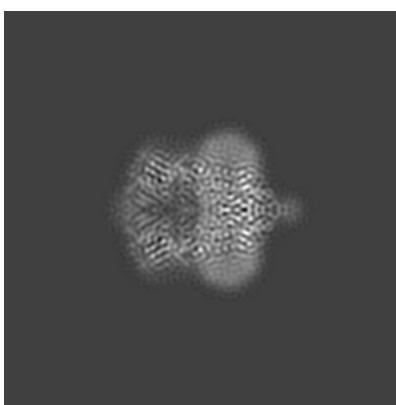
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

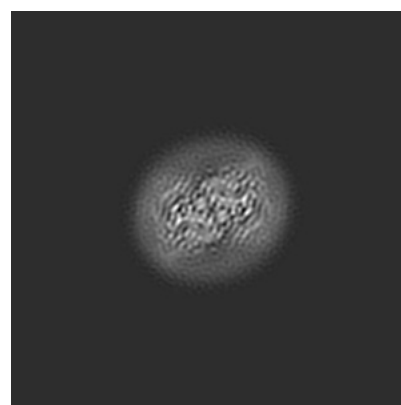
6.1.1 Primary map



X



Y



Z

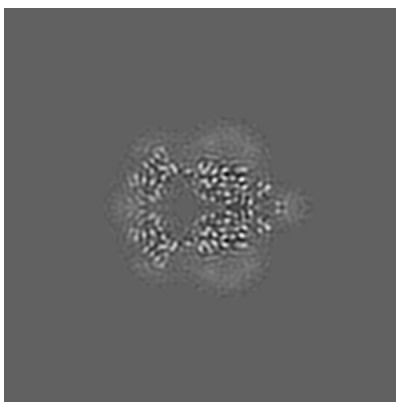
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

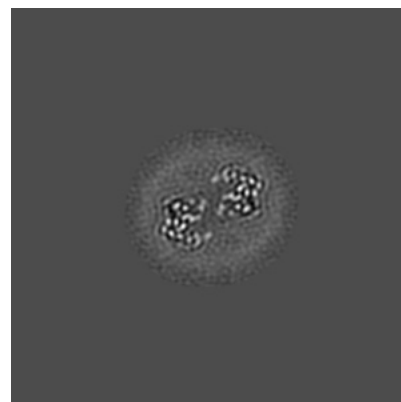
6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

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

6.3 Largest variance slices [i](#)

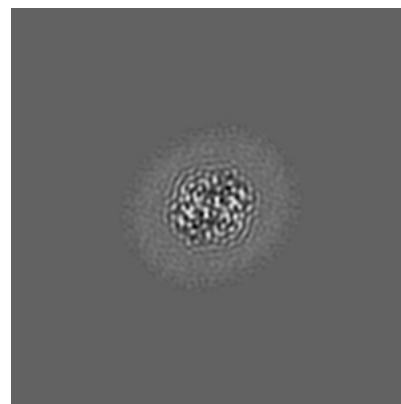
6.3.1 Primary map



X Index: 179



Y Index: 153

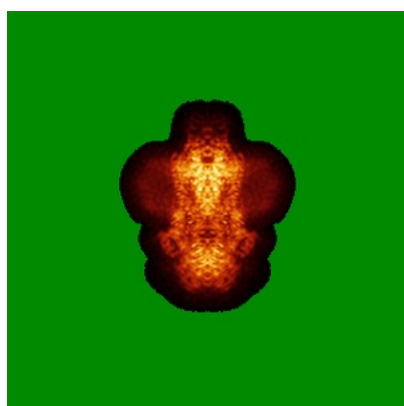


Z Index: 191

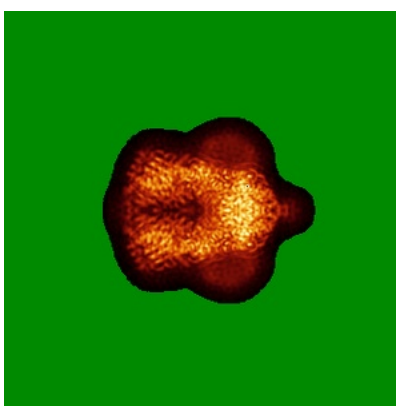
The images above show the largest variance slices of the map in three orthogonal directions.

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

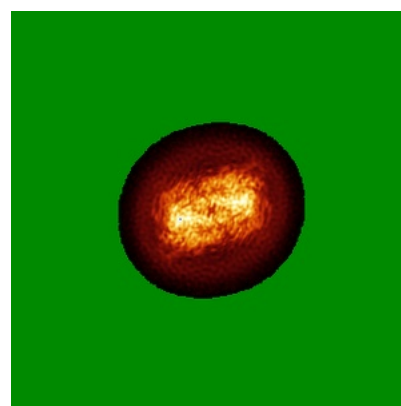
6.4.1 Primary map



X



Y

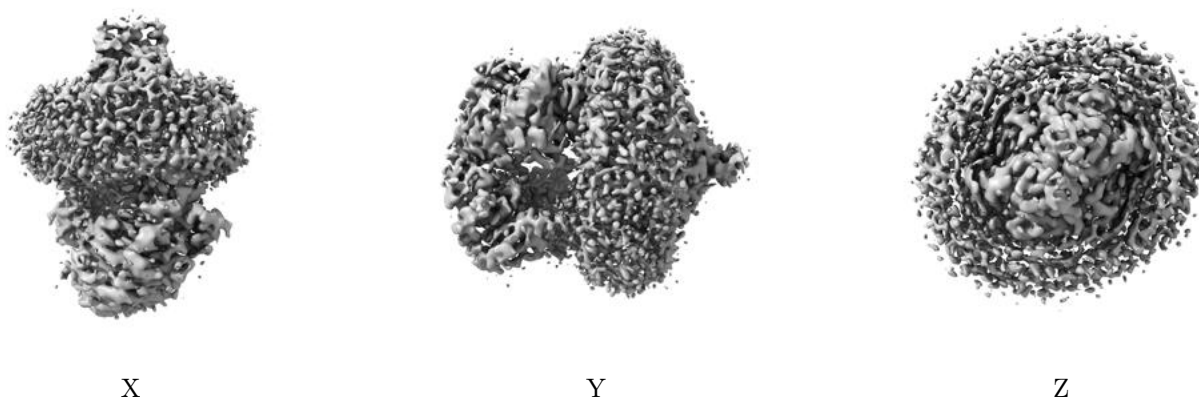


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

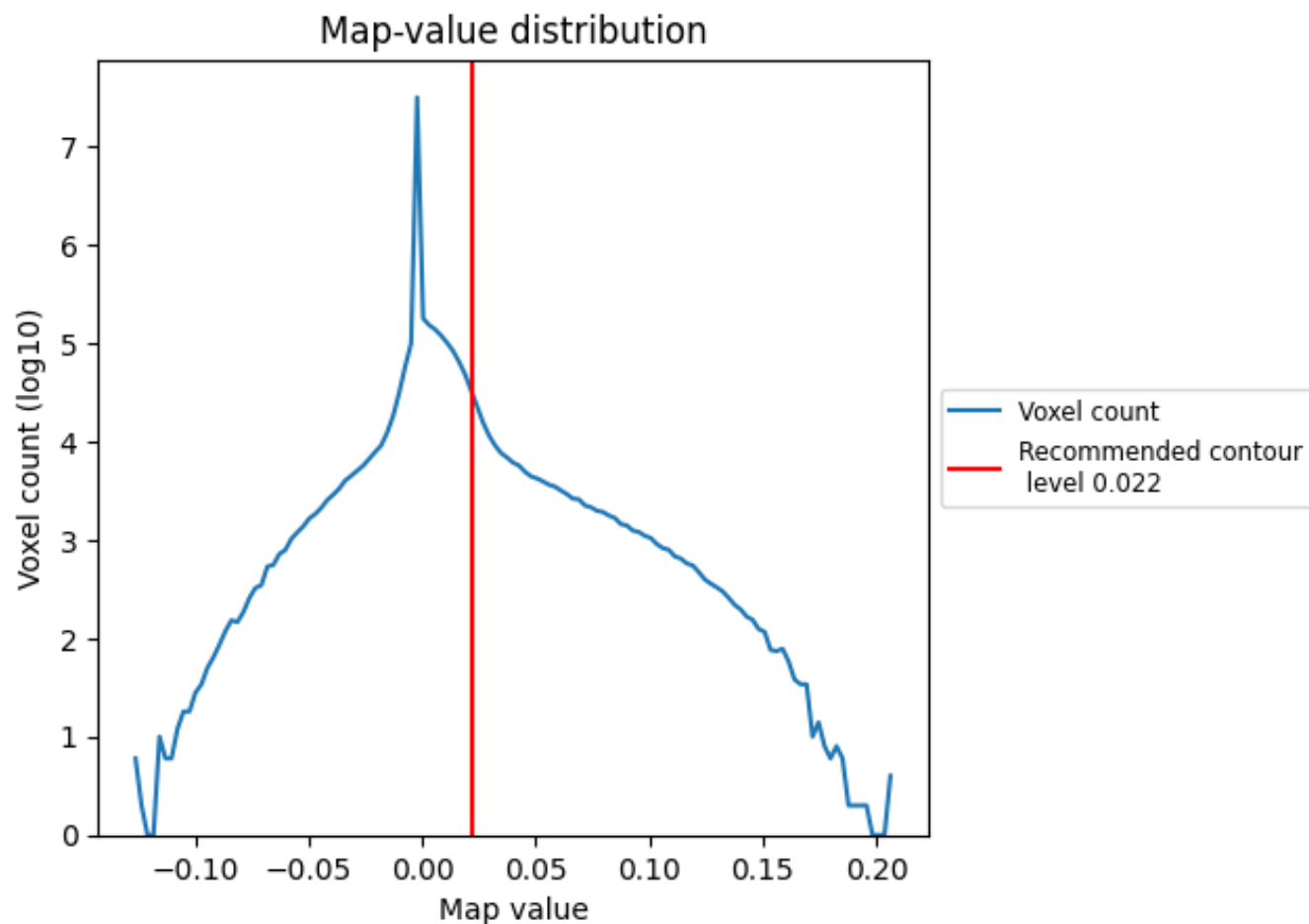
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

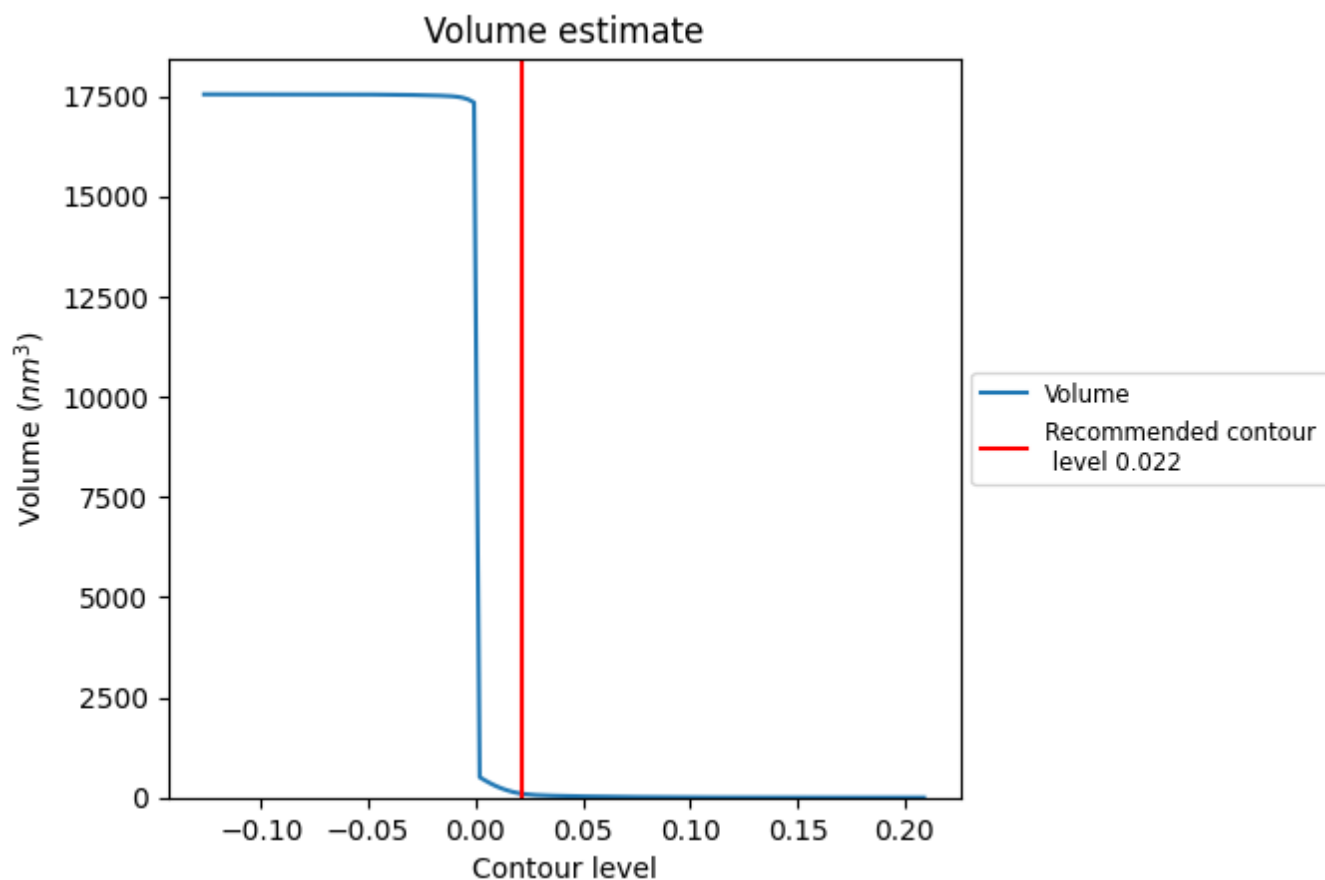
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

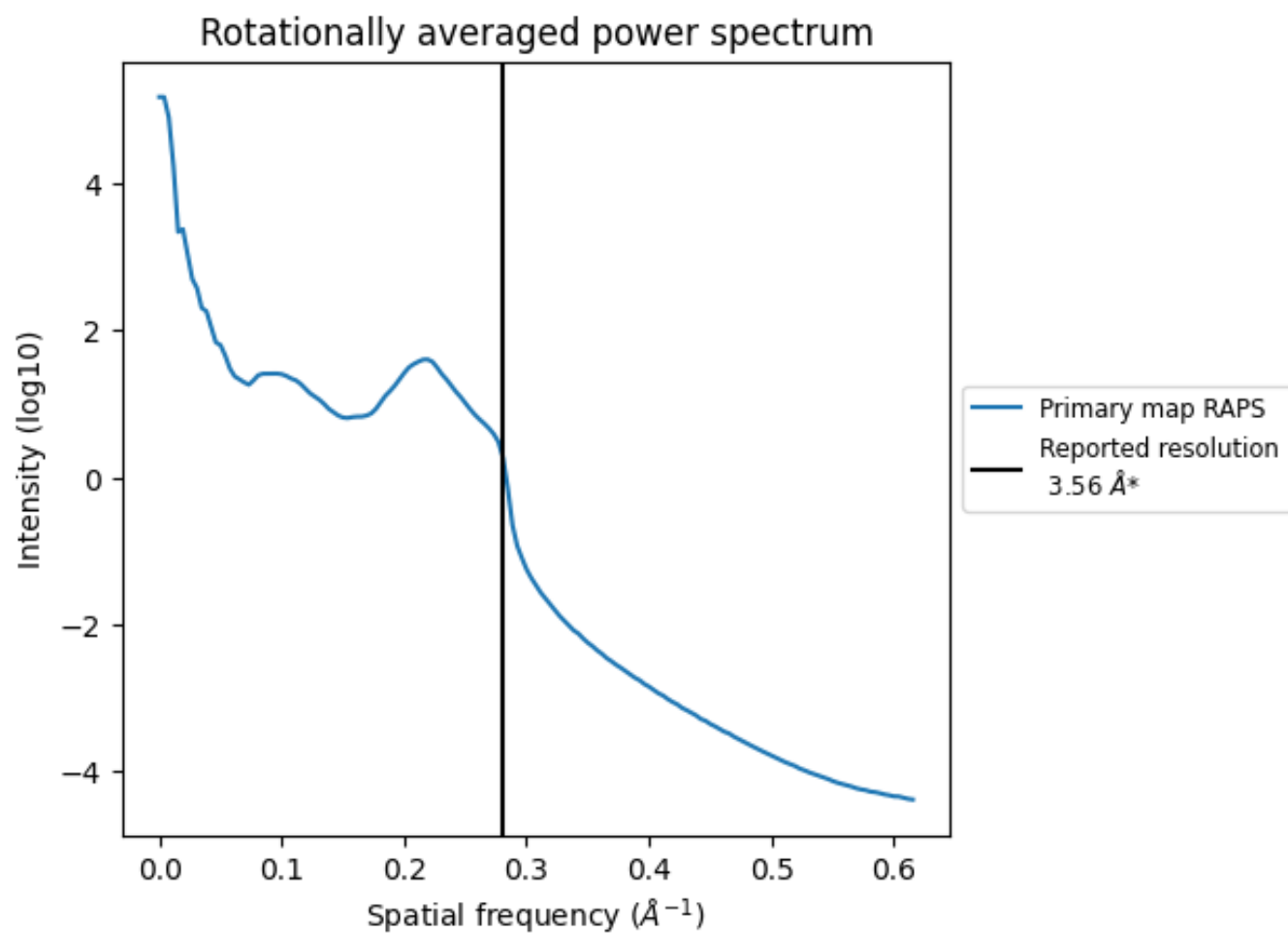
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 94 nm^3 ; this corresponds to an approximate mass of 85 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 ⓘ

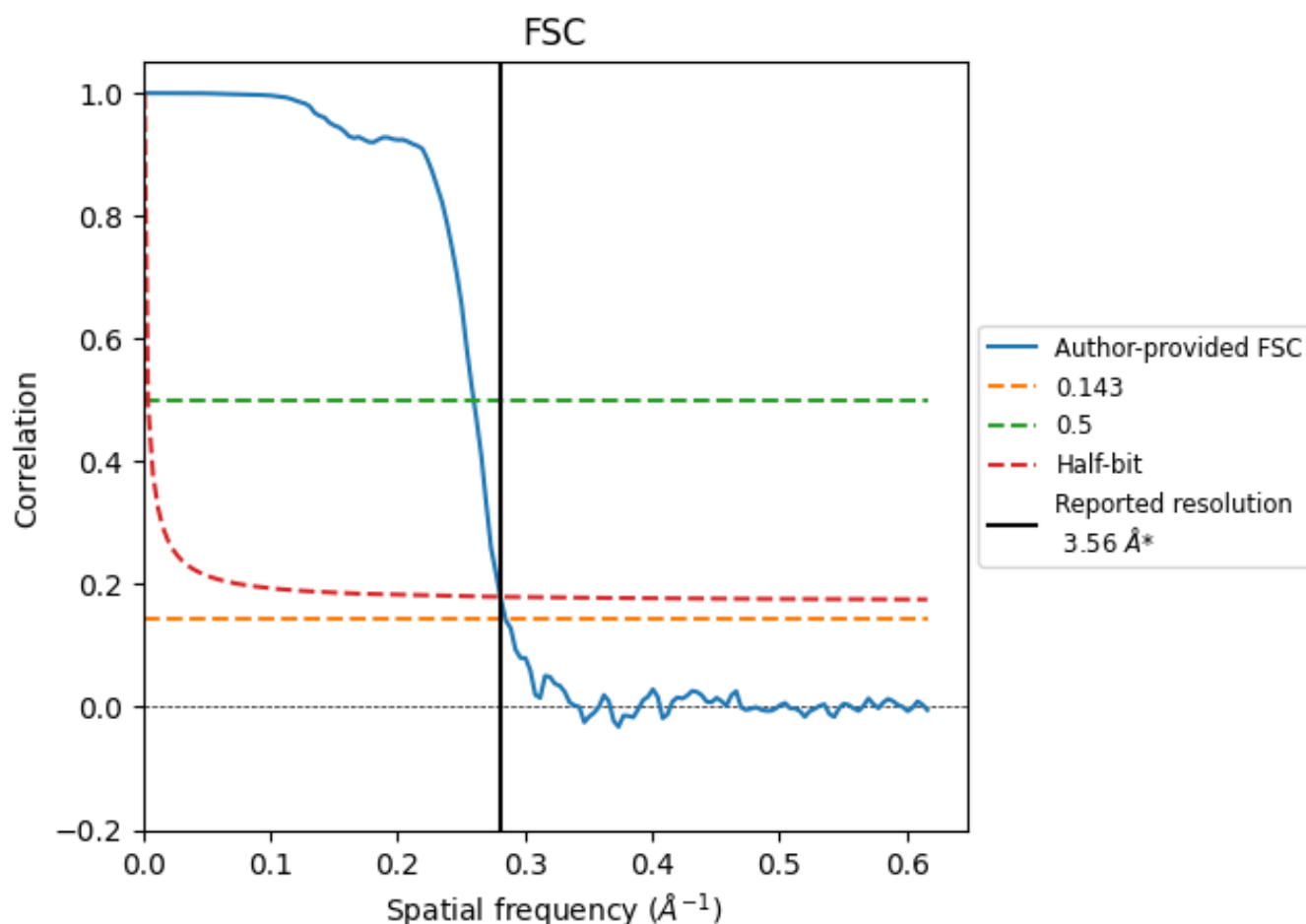


*Reported resolution corresponds to spatial frequency of 0.281 Å⁻¹

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 0.281 Å⁻¹

8.2 Resolution estimates [i](#)

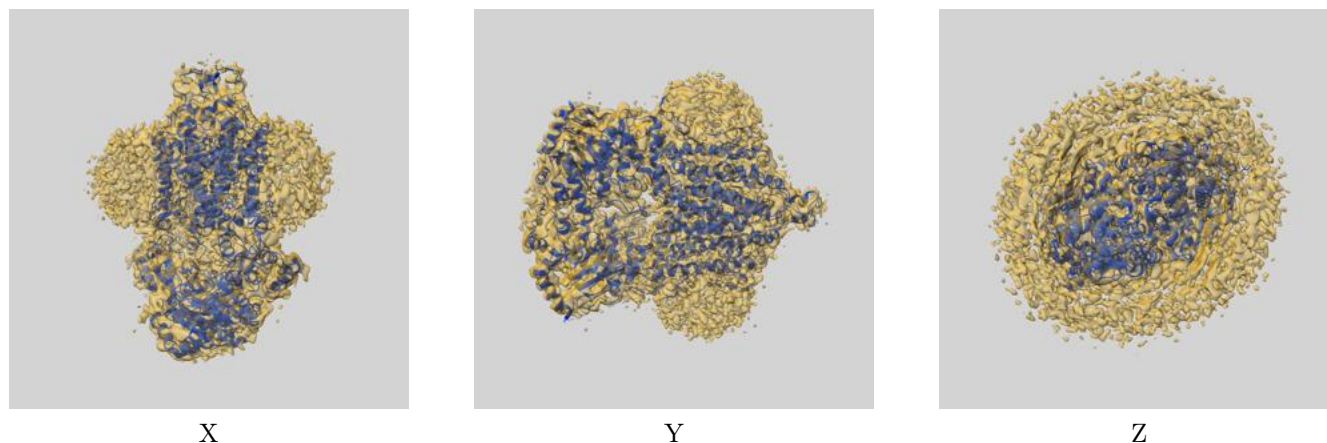
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.56	-	-
Author-provided FSC curve	3.51	3.85	3.56
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

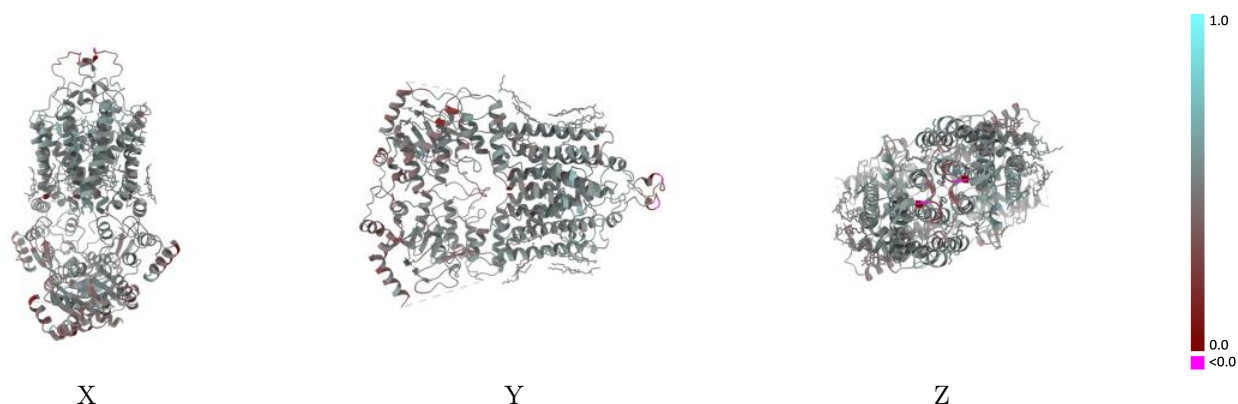
This section contains information regarding the fit between EMDB map EMD-4256 and PDB model 6HIJ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



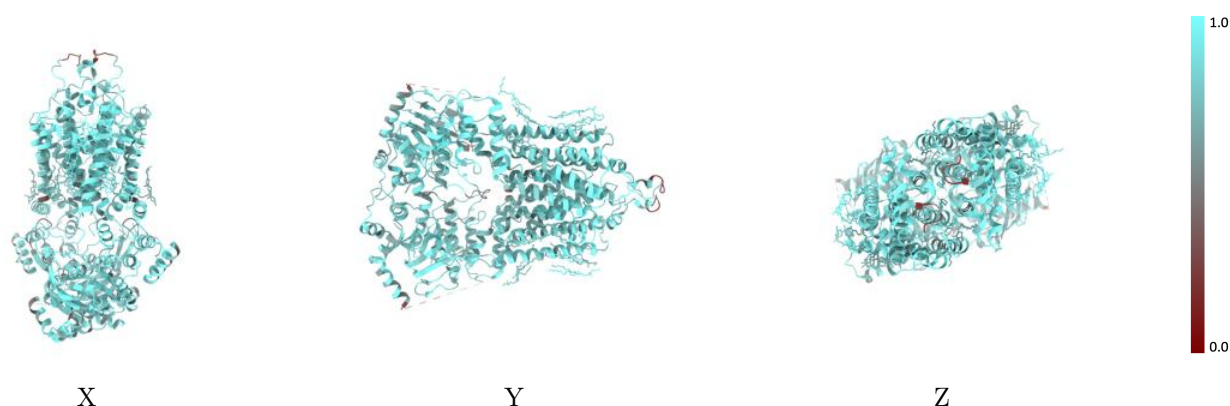
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



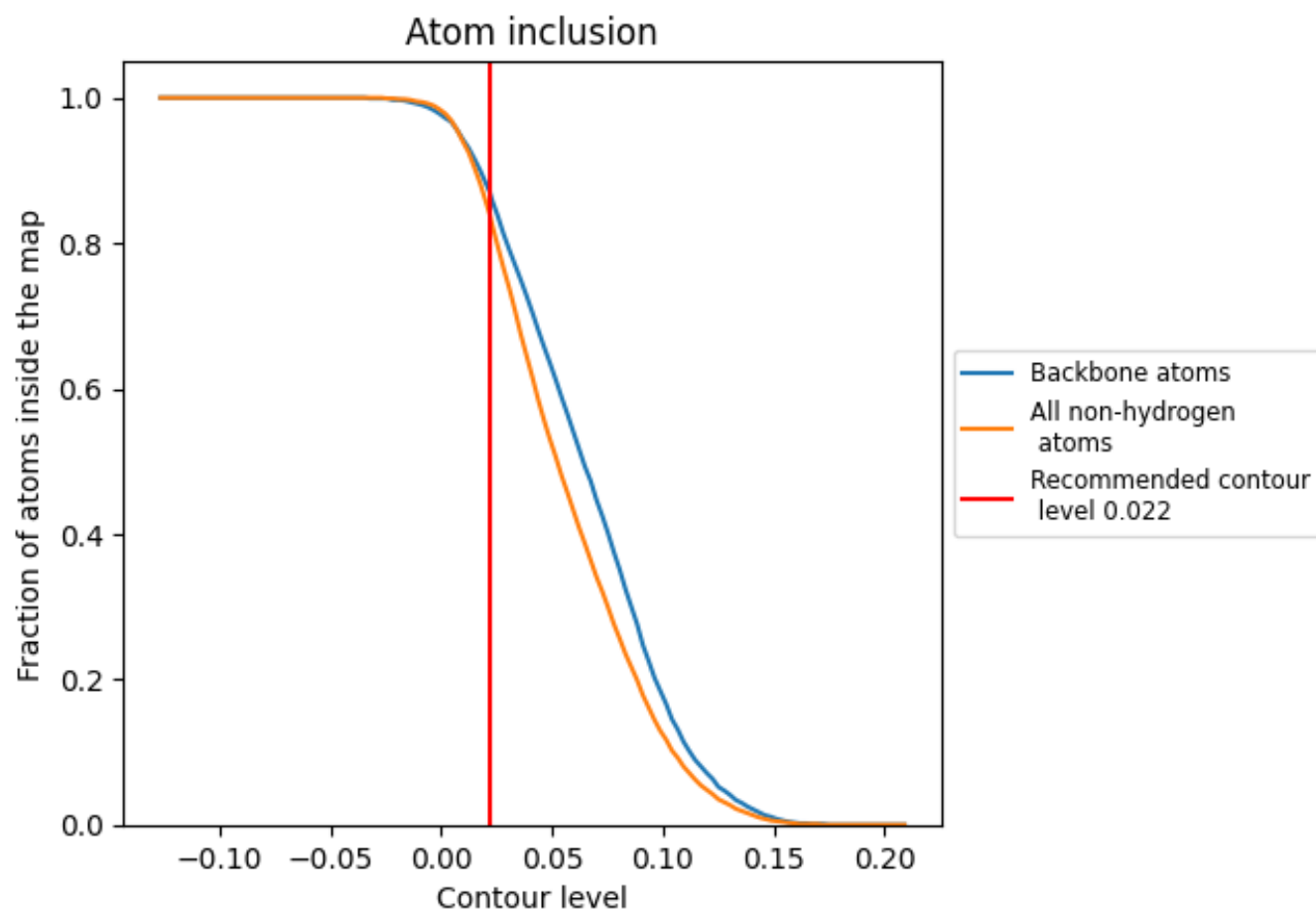
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8390	0.4860
A	0.8370	0.4860
B	0.8400	0.4870

