



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:52 AM UTC

PDB ID : 8IFU / pdb_00008ifu
EMDB ID : EMD-35423
Title : HcCCR in NaCl
Authors : Zhang, M.F.
Deposited on : 2023-02-19
Resolution : 2.37 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

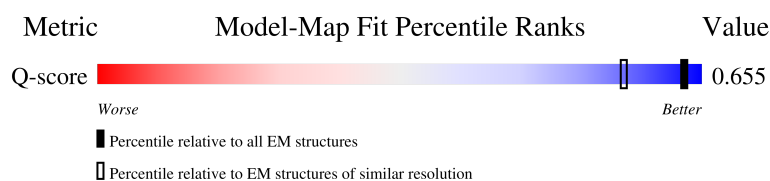
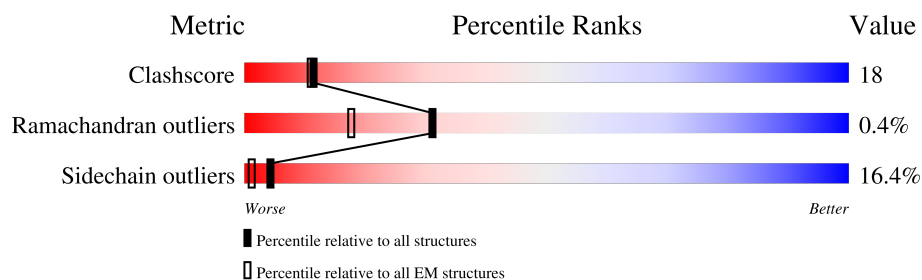
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.37 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	4742 (1.87 - 2.87)

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	265	 74% 18% 6%
1	B	265	 74% 19% 5%
1	C	265	 74% 19% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	L9Q	A	318	-	-	X	-
4	L9Q	A	319	-	-	X	-
4	L9Q	B	301	-	-	X	-
4	L9Q	B	319	-	-	X	-
4	L9Q	C	301	-	-	X	-
4	L9Q	C	302	-	-	X	-

2 Entry composition [i](#)

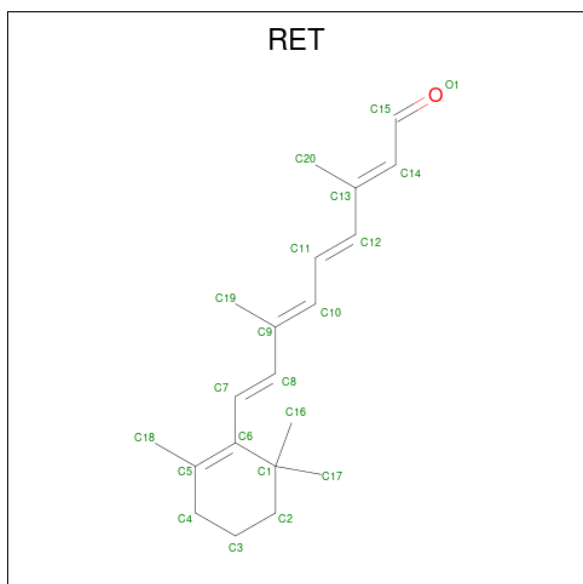
There are 5 unique types of molecules in this entry. The entry contains 6732 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HcCCR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	259	Total	C	N	O	S	0	0
			2095	1414	324	343	14		
1	B	259	Total	C	N	O	S	0	0
			2095	1414	324	343	14		
1	C	259	Total	C	N	O	S	0	0
			2095	1414	324	343	14		

- Molecule 2 is RETINAL (CCD ID: RET) (formula: $C_{20}H_{28}O$) (labeled as "Ligand of Interest" by depositor).

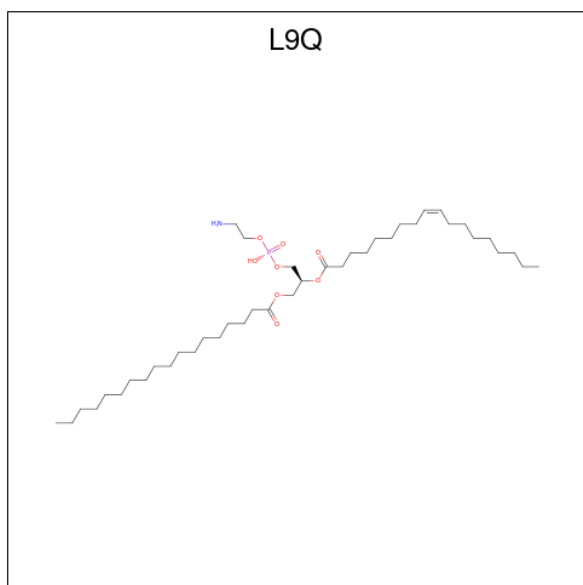


Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	C	0
			20	20	
2	B	1	Total	C	0
			20	20	
2	C	1	Total	C	0
			20	20	

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	16	Total	Na	0
			16	16	
3	B	16	Total	Na	0
			16	16	
3	C	16	Total	Na	0
			16	16	

- Molecule 4 is (1S)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(octadecanoyloxymethyl)ethyl (9Z)-octadec-9-enoate (CCD ID: L9Q) (formula: C₄₁H₈₀NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	C	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 5 is water.

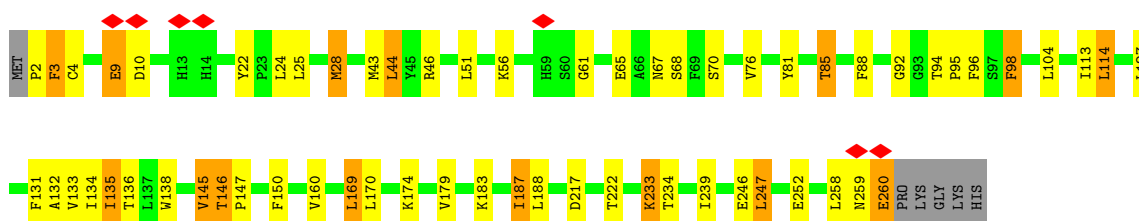
Mol	Chain	Residues	Atoms		AltConf
5	A	11	Total 11	O 11	0
5	B	11	Total 11	O 11	0
5	C	11	Total 11	O 11	0

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.

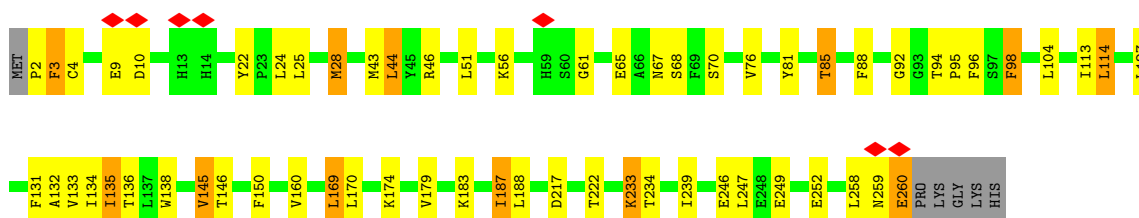
• Molecule 1: HcCCR

Chain A: 



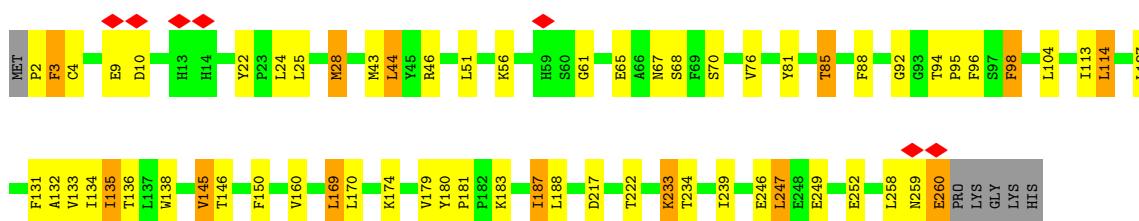
• Molecule 1: HcCCR

Chain B: 



• Molecule 1: HcCCR

Chain C: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	267000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.231	Depositor
Minimum map value	-0.815	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.22	Depositor
Map size ($\text{\AA}$)	273.6, 273.6, 273.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.57, 0.57, 0.57	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RET, L9Q, NA

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	1.08	0/2180	0.96	6/2973 (0.2%)
1	B	1.08	0/2180	0.96	7/2973 (0.2%)
1	C	1.08	0/2180	0.96	7/2973 (0.2%)
All	All	1.08	0/6540	0.96	20/8919 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	PHE	N-CA-C	-6.55	105.25	112.72
1	C	98	PHE	N-CA-C	-6.55	105.25	112.72
1	B	98	PHE	N-CA-C	-6.54	105.26	112.72
1	A	67	ASN	N-CA-C	-6.12	105.46	113.17
1	B	67	ASN	N-CA-C	-6.12	105.46	113.17
1	C	67	ASN	N-CA-C	-6.10	105.48	113.17
1	B	61	GLY	N-CA-C	-5.96	107.60	114.69
1	A	61	GLY	N-CA-C	-5.95	107.61	114.69
1	C	61	GLY	N-CA-C	-5.94	107.62	114.69
1	B	94	THR	N-CA-C	-5.92	102.65	110.40
1	A	94	THR	N-CA-C	-5.91	102.66	110.40
1	C	94	THR	N-CA-C	-5.91	102.66	110.40
1	C	150	PHE	N-CA-C	-5.16	106.76	113.16
1	A	150	PHE	N-CA-C	-5.15	106.77	113.16
1	A	92	GLY	N-CA-C	5.15	119.35	112.65
1	B	150	PHE	N-CA-C	-5.15	106.78	113.16
1	C	92	GLY	N-CA-C	5.14	119.33	112.65
1	B	92	GLY	N-CA-C	5.13	119.32	112.65
1	B	249	GLU	N-CA-C	-5.03	105.89	112.23
1	C	249	GLU	N-CA-C	-5.01	105.91	112.23

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	2095	0	2020	42	0
1	B	2095	0	2020	37	0
1	C	2095	0	2020	41	0
2	A	20	0	27	4	0
2	B	20	0	27	4	0
2	C	20	0	27	3	0
3	A	16	0	0	1	0
3	B	16	0	0	1	0
3	C	16	0	0	1	0
4	A	102	0	149	77	0
4	B	102	0	149	77	0
4	C	102	0	149	77	0
5	A	11	0	0	1	0
5	B	11	0	0	1	0
5	C	11	0	0	1	0
All	All	6732	0	6588	238	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 18.

All (238) 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)
4:C:301:L9Q:C26	4:C:302:L9Q:C47	1.98	1.40
4:A:318:L9Q:C26	4:A:319:L9Q:C47	1.98	1.37
4:C:301:L9Q:H26A	4:C:302:L9Q:C48	1.55	1.35
4:A:318:L9Q:H26A	4:A:319:L9Q:C48	1.55	1.35
4:B:301:L9Q:C48	4:B:319:L9Q:H26A	1.55	1.33
4:B:301:L9Q:C47	4:B:319:L9Q:C26	1.98	1.33
4:B:301:L9Q:C47	4:B:319:L9Q:H26A	1.38	1.28
4:A:318:L9Q:C28	4:A:319:L9Q:H39	1.52	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:301:L9Q:H26A	4:C:302:L9Q:C47	1.39	1.24
4:A:319:L9Q:H43A	4:C:302:L9Q:C44	1.73	1.19
1:A:131:PHE:CZ	4:A:318:L9Q:H46	1.75	1.19
1:B:131:PHE:CZ	4:B:319:L9Q:H46	1.75	1.19
1:C:131:PHE:CZ	4:C:301:L9Q:H46	1.75	1.19
4:A:318:L9Q:C26	4:A:319:L9Q:C48	2.19	1.18
4:B:301:L9Q:H39	4:B:319:L9Q:C28	1.52	1.18
4:C:301:L9Q:C28	4:C:302:L9Q:H39	1.52	1.18
4:B:301:L9Q:C39	4:B:319:L9Q:C28	2.21	1.18
4:A:319:L9Q:C44	4:B:301:L9Q:H43A	1.72	1.17
4:A:318:L9Q:C26	4:A:319:L9Q:H48A	1.74	1.17
4:B:301:L9Q:C44	4:C:302:L9Q:H43A	1.73	1.17
4:A:318:L9Q:H26	4:A:319:L9Q:H47A	1.24	1.16
4:C:301:L9Q:C26	4:C:302:L9Q:H48A	1.74	1.16
4:B:301:L9Q:C48	4:B:319:L9Q:C26	2.19	1.16
4:C:301:L9Q:C26	4:C:302:L9Q:C48	2.19	1.15
4:C:301:L9Q:C26	4:C:302:L9Q:H47A	1.64	1.15
4:B:301:L9Q:H48A	4:B:319:L9Q:C26	1.74	1.15
4:C:301:L9Q:C28	4:C:302:L9Q:C39	2.21	1.14
4:A:318:L9Q:C26	4:A:319:L9Q:H47A	1.64	1.14
4:A:318:L9Q:H26A	4:A:319:L9Q:C47	1.38	1.14
4:A:318:L9Q:C28	4:A:319:L9Q:C39	2.21	1.13
4:C:301:L9Q:H26	4:C:302:L9Q:H47A	1.25	1.12
4:B:301:L9Q:H47A	4:B:319:L9Q:C26	1.64	1.12
4:C:301:L9Q:C24	4:C:302:L9Q:H48A	1.81	1.10
4:A:318:L9Q:H24	4:A:319:L9Q:H48A	1.33	1.10
4:B:301:L9Q:H48A	4:B:319:L9Q:C24	1.81	1.10
4:A:318:L9Q:C24	4:A:319:L9Q:H48A	1.81	1.09
4:B:301:L9Q:H47A	4:B:319:L9Q:H26	1.24	1.08
4:A:319:L9Q:C43	4:B:301:L9Q:H43A	1.86	1.05
4:B:301:L9Q:C43	4:C:302:L9Q:H43A	1.86	1.05
4:A:318:L9Q:H26A	4:A:319:L9Q:H48A	1.30	1.04
4:C:301:L9Q:H24	4:C:302:L9Q:H48A	1.33	1.04
4:A:319:L9Q:H43A	4:C:302:L9Q:C43	1.86	1.03
4:B:301:L9Q:H48A	4:B:319:L9Q:H24	1.33	1.02
1:A:131:PHE:CE2	4:A:318:L9Q:H46	1.97	0.99
1:C:131:PHE:CE2	4:C:301:L9Q:H46	1.97	0.99
4:C:301:L9Q:H26A	4:C:302:L9Q:H48A	1.30	0.99
1:B:131:PHE:CE2	4:B:319:L9Q:H46	1.97	0.98
4:A:319:L9Q:H44A	4:B:301:L9Q:C43	1.97	0.95
4:B:301:L9Q:H44A	4:C:302:L9Q:C43	1.97	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:318:L9Q:C25	4:A:319:L9Q:H48A	1.97	0.94
4:A:319:L9Q:C43	4:C:302:L9Q:H44A	1.97	0.94
4:C:301:L9Q:C25	4:C:302:L9Q:H48A	1.97	0.94
4:B:301:L9Q:H44A	4:C:302:L9Q:H43A	1.48	0.94
4:B:301:L9Q:H48A	4:B:319:L9Q:C25	1.97	0.94
4:A:319:L9Q:H43A	4:C:302:L9Q:H44A	1.48	0.91
4:B:301:L9Q:H48	1:C:134:ILE:HG21	1.52	0.90
1:A:134:ILE:HG21	4:C:302:L9Q:H48	1.52	0.90
4:B:301:L9Q:H48A	4:B:319:L9Q:H26A	1.30	0.89
4:A:319:L9Q:H44A	4:B:301:L9Q:H43A	1.48	0.89
4:A:319:L9Q:H48	1:B:134:ILE:HG21	1.52	0.88
4:A:319:L9Q:C43	4:C:302:L9Q:C44	2.51	0.88
4:A:319:L9Q:C44	4:B:301:L9Q:C43	2.51	0.86
4:B:301:L9Q:C44	4:C:302:L9Q:C43	2.51	0.86
4:A:319:L9Q:C41	4:C:302:L9Q:C42	2.54	0.84
4:A:319:L9Q:C42	4:B:301:L9Q:C41	2.54	0.83
1:C:131:PHE:CZ	4:C:301:L9Q:C46	2.61	0.83
1:B:135:ILE:HD11	1:C:76:VAL:HG22	1.61	0.83
3:B:307:NA:NA	5:B:409:HOH:O	1.52	0.83
3:A:306:NA:NA	5:A:409:HOH:O	1.52	0.83
1:A:135:ILE:HD11	1:B:76:VAL:HG22	1.61	0.83
4:B:301:L9Q:C48	1:C:134:ILE:HG21	2.09	0.82
3:C:308:NA:NA	5:C:409:HOH:O	1.52	0.82
1:B:131:PHE:CZ	4:B:319:L9Q:C46	2.61	0.82
1:A:134:ILE:HG21	4:C:302:L9Q:C48	2.09	0.82
4:A:319:L9Q:C48	1:B:134:ILE:HG21	2.09	0.81
1:A:76:VAL:HG22	1:C:135:ILE:HD11	1.61	0.81
1:A:131:PHE:CZ	4:A:318:L9Q:C46	2.61	0.80
4:A:318:L9Q:H26	4:A:319:L9Q:C47	1.91	0.80
4:A:319:L9Q:H48	1:B:134:ILE:CG2	2.11	0.80
1:A:134:ILE:CG2	4:C:302:L9Q:H48	2.11	0.80
4:B:301:L9Q:H48	1:C:134:ILE:CG2	2.11	0.79
4:B:301:L9Q:H37	4:C:302:L9Q:C40	2.12	0.79
4:A:319:L9Q:H37	4:B:301:L9Q:C40	2.12	0.79
4:C:301:L9Q:H24	4:C:302:L9Q:C48	2.13	0.78
4:B:301:L9Q:C42	4:C:302:L9Q:C41	2.54	0.77
4:C:301:L9Q:H26	4:C:302:L9Q:C47	1.91	0.77
4:B:301:L9Q:C48	4:B:319:L9Q:H24	2.13	0.77
4:A:319:L9Q:C40	4:C:302:L9Q:H37	2.12	0.76
4:A:318:L9Q:H24	4:A:319:L9Q:C48	2.13	0.76
1:A:2:PRO:HD2	4:A:319:L9Q:H2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:301:L9Q:C47	4:B:319:L9Q:H26	1.91	0.72
1:B:2:PRO:HD2	4:B:301:L9Q:H2	1.70	0.72
4:B:301:L9Q:H44A	4:C:302:L9Q:C44	2.20	0.71
1:C:2:PRO:HD2	4:C:302:L9Q:H2	1.70	0.71
4:A:319:L9Q:H44A	4:B:301:L9Q:C44	2.20	0.71
4:A:319:L9Q:C44	4:C:302:L9Q:H44A	2.20	0.70
4:A:319:L9Q:H43A	4:C:302:L9Q:C45	2.22	0.70
4:A:319:L9Q:C45	4:B:301:L9Q:H43A	2.22	0.69
4:A:319:L9Q:H23	1:C:135:ILE:HA	1.75	0.69
4:B:301:L9Q:C42	4:C:302:L9Q:H43A	2.23	0.69
4:B:301:L9Q:C45	4:C:302:L9Q:H43A	2.22	0.69
1:A:135:ILE:HA	4:B:301:L9Q:H23	1.75	0.68
4:A:318:L9Q:H28B	4:A:319:L9Q:H39	1.71	0.68
1:B:135:ILE:HA	4:C:302:L9Q:H23	1.75	0.68
4:A:319:L9Q:C42	4:B:301:L9Q:H43A	2.23	0.67
4:A:319:L9Q:H43A	4:C:302:L9Q:C42	2.23	0.67
4:A:319:L9Q:H43A	4:C:301:L9Q:C27	2.25	0.67
4:B:301:L9Q:C48	4:B:319:L9Q:H26	2.19	0.67
4:B:319:L9Q:C27	4:C:302:L9Q:H43A	2.25	0.67
4:B:301:L9Q:H45	4:C:302:L9Q:H43	1.77	0.66
4:A:319:L9Q:H45	4:B:301:L9Q:H43	1.77	0.66
4:A:318:L9Q:C27	4:B:301:L9Q:H43A	2.25	0.66
4:A:319:L9Q:H43	4:C:302:L9Q:H45	1.77	0.65
1:A:28:MET:HE1	1:A:222:THR:HG22	1.79	0.64
1:C:28:MET:HE1	1:C:222:THR:HG22	1.79	0.64
4:C:301:L9Q:H28B	4:C:302:L9Q:H39	1.71	0.63
1:B:28:MET:HE1	1:B:222:THR:HG22	1.79	0.63
4:A:318:L9Q:H26	4:A:319:L9Q:C48	2.19	0.63
4:A:319:L9Q:C41	4:C:301:L9Q:C28	2.77	0.62
1:A:138:TRP:HZ3	4:B:301:L9Q:H33A	1.65	0.62
1:B:138:TRP:HZ3	4:C:302:L9Q:H33A	1.65	0.62
4:A:318:L9Q:C28	4:B:301:L9Q:C41	2.77	0.62
4:A:319:L9Q:C43	4:C:302:L9Q:C45	2.79	0.61
4:A:319:L9Q:H33A	1:C:138:TRP:HZ3	1.65	0.61
1:B:135:ILE:HD13	4:C:302:L9Q:H23A	1.83	0.60
4:B:301:L9Q:H43A	4:C:302:L9Q:H43A	1.81	0.60
4:A:319:L9Q:C45	4:B:301:L9Q:C43	2.79	0.60
4:A:319:L9Q:H23A	1:C:135:ILE:HD13	1.83	0.60
4:B:301:L9Q:C45	4:C:302:L9Q:C43	2.79	0.60
1:A:135:ILE:HD13	4:B:301:L9Q:H23A	1.83	0.59
1:A:3:PHE:O	4:A:319:L9Q:H4A	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:319:L9Q:C28	4:C:302:L9Q:C41	2.77	0.59
1:B:3:PHE:O	4:B:301:L9Q:H4A	2.03	0.59
4:A:319:L9Q:H43A	4:B:301:L9Q:H43A	1.81	0.58
1:C:3:PHE:O	4:C:302:L9Q:H4A	2.03	0.58
4:C:301:L9Q:H26	4:C:302:L9Q:C48	2.19	0.58
4:B:301:L9Q:C37	4:C:302:L9Q:C40	2.82	0.57
4:B:301:L9Q:H39	4:B:319:L9Q:H28B	1.71	0.57
1:A:113:ILE:HD11	1:A:233:LYS:HD3	1.87	0.57
4:A:319:L9Q:C40	4:C:302:L9Q:C37	2.82	0.57
4:A:319:L9Q:C37	4:B:301:L9Q:C40	2.82	0.57
1:B:113:ILE:HD11	1:B:233:LYS:HD3	1.87	0.56
1:C:113:ILE:HD11	1:C:233:LYS:HD3	1.87	0.56
1:B:132:ALA:O	1:B:136:THR:HG23	2.07	0.55
1:C:132:ALA:O	1:C:136:THR:HG23	2.07	0.55
1:B:145:VAL:HG13	1:C:95:PRO:HB2	1.89	0.54
1:A:95:PRO:HB2	1:C:145:VAL:HG13	1.89	0.54
1:A:145:VAL:HG13	1:B:95:PRO:HB2	1.89	0.54
4:A:319:L9Q:C43	4:C:302:L9Q:H45	2.37	0.54
1:A:132:ALA:O	1:A:136:THR:HG23	2.07	0.54
4:A:319:L9Q:H43A	4:C:302:L9Q:H43A	1.81	0.54
4:A:319:L9Q:H45	4:B:301:L9Q:C43	2.37	0.54
4:B:301:L9Q:H45	4:C:302:L9Q:C43	2.37	0.53
1:B:136:THR:HB	2:B:302:RET:H182	1.91	0.52
1:C:136:THR:HB	2:C:303:RET:H182	1.91	0.52
1:B:187:ILE:HG22	1:B:239:ILE:HG23	1.91	0.52
1:A:136:THR:HB	2:A:301:RET:H182	1.91	0.51
1:A:187:ILE:HG22	1:A:239:ILE:HG23	1.91	0.51
1:C:187:ILE:HG22	1:C:239:ILE:HG23	1.91	0.51
4:A:319:L9Q:H20	4:B:301:L9Q:H47	1.94	0.50
1:A:81:TYR:O	1:A:85:THR:HG22	2.12	0.50
1:B:81:TYR:O	1:B:85:THR:HG22	2.12	0.50
4:B:301:L9Q:H20	4:C:302:L9Q:H47	1.94	0.49
4:A:319:L9Q:H47	4:C:302:L9Q:H20	1.94	0.49
1:C:81:TYR:O	1:C:85:THR:HG22	2.12	0.49
4:A:319:L9Q:H48B	1:B:134:ILE:HG21	1.94	0.48
1:A:134:ILE:HG21	4:C:302:L9Q:H48B	1.94	0.48
1:A:95:PRO:HB2	1:C:145:VAL:CG1	2.44	0.48
1:B:145:VAL:CG1	1:C:95:PRO:HB2	2.44	0.48
1:A:145:VAL:CG1	1:B:95:PRO:HB2	2.44	0.48
4:B:301:L9Q:H48B	1:C:134:ILE:HG21	1.94	0.48
2:C:303:RET:H191	2:C:303:RET:H11	1.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:301:L9Q:H21A	4:B:301:L9Q:H24A	1.65	0.46
2:B:302:RET:H191	2:B:302:RET:H11	1.48	0.46
2:B:302:RET:H11	2:B:302:RET:H203	1.81	0.46
4:A:319:L9Q:C20	4:B:301:L9Q:H47	2.47	0.45
1:C:259:ASN:O	1:C:260:GLU:C	2.59	0.45
4:C:302:L9Q:H18A	4:C:302:L9Q:H21A	1.72	0.45
1:B:138:TRP:CZ3	4:C:302:L9Q:H33A	2.49	0.45
4:B:301:L9Q:C20	4:C:302:L9Q:H47	2.47	0.45
4:C:302:L9Q:H28B	4:C:302:L9Q:H25A	1.70	0.45
1:A:138:TRP:CZ3	4:B:301:L9Q:H33A	2.49	0.45
1:A:259:ASN:O	1:A:260:GLU:C	2.59	0.44
2:C:303:RET:H171	2:C:303:RET:H7	1.40	0.44
4:A:319:L9Q:H47	4:C:302:L9Q:C20	2.47	0.44
1:B:179:VAL:HG12	1:B:258:LEU:HB3	1.99	0.44
1:C:179:VAL:HG12	1:C:258:LEU:HB3	1.99	0.44
1:B:259:ASN:O	1:B:260:GLU:C	2.59	0.44
4:B:319:L9Q:H12A	4:B:319:L9Q:H15A	1.81	0.44
1:A:179:VAL:HG12	1:A:258:LEU:HB3	1.99	0.44
1:A:247:LEU:HD23	1:A:247:LEU:HA	1.89	0.44
4:B:301:L9Q:H21A	4:B:301:L9Q:H18A	1.72	0.44
4:A:319:L9Q:H18A	4:A:319:L9Q:H21A	1.72	0.43
4:A:319:L9Q:H21A	4:A:319:L9Q:H24A	1.65	0.43
4:B:301:L9Q:H44A	4:C:302:L9Q:H44A	1.99	0.43
1:A:114:LEU:HD21	1:A:169:LEU:HD11	2.00	0.43
1:B:96:PHE:CE1	4:B:301:L9Q:O31	2.72	0.43
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.87	0.43
1:A:131:PHE:CE1	4:A:318:L9Q:H45A	2.53	0.43
2:B:302:RET:H7	2:B:302:RET:H171	1.40	0.43
1:B:131:PHE:CE1	4:B:319:L9Q:H45A	2.53	0.43
1:A:96:PHE:CE1	4:A:319:L9Q:O31	2.72	0.42
1:A:96:PHE:HE1	4:A:319:L9Q:O31	2.02	0.42
2:A:301:RET:H203	2:A:301:RET:H11	1.81	0.42
1:C:131:PHE:CE1	4:C:301:L9Q:H45A	2.53	0.42
4:C:301:L9Q:H12A	4:C:301:L9Q:H15A	1.81	0.42
4:A:319:L9Q:H33A	1:C:138:TRP:CZ3	2.49	0.42
4:A:319:L9Q:C23	1:C:135:ILE:HA	2.48	0.42
1:C:96:PHE:CE1	4:C:302:L9Q:O31	2.72	0.42
1:A:233:LYS:HE2	1:A:233:LYS:HB2	1.68	0.42
1:C:180:TYR:HA	1:C:181:PRO:HD3	1.90	0.42
1:A:22:TYR:HB3	1:A:88:PHE:O	2.20	0.42
1:A:258:LEU:HD23	1:A:258:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:PHE:HE1	4:B:301:L9Q:O31	2.02	0.42
4:C:302:L9Q:H21A	4:C:302:L9Q:H24A	1.65	0.42
1:B:22:TYR:HB3	1:B:88:PHE:O	2.20	0.42
1:B:114:LEU:HD21	1:B:169:LEU:HD11	2.00	0.42
1:C:114:LEU:HD21	1:C:169:LEU:HD11	2.00	0.42
1:B:258:LEU:HA	1:B:258:LEU:HD23	1.82	0.42
1:C:96:PHE:HE1	4:C:302:L9Q:O31	2.02	0.41
1:C:258:LEU:HA	1:C:258:LEU:HD23	1.82	0.41
2:A:301:RET:H11	2:A:301:RET:H191	1.48	0.41
1:C:247:LEU:HD23	1:C:247:LEU:HA	1.89	0.41
1:C:22:TYR:HB3	1:C:88:PHE:O	2.20	0.41
4:A:319:L9Q:H44A	4:C:302:L9Q:H44A	2.00	0.41
1:A:4:CYS:HB2	1:B:4:CYS:HB2	2.02	0.41
1:A:4:CYS:HB2	1:C:4:CYS:HB2	2.02	0.41
1:A:135:ILE:HA	4:B:301:L9Q:C23	2.48	0.41
1:B:4:CYS:HB2	1:C:4:CYS:HB2	2.02	0.41
1:B:44:LEU:HD23	1:B:44:LEU:HA	1.87	0.41
1:C:44:LEU:HD23	1:C:44:LEU:HA	1.87	0.41
1:A:146:THR:HA	1:A:147:PRO:HD3	1.82	0.41
1:B:145:VAL:HG13	1:C:95:PRO:CB	2.51	0.41
2:A:301:RET:H171	2:A:301:RET:H7	1.40	0.40
1:A:9:GLU:H	1:A:9:GLU:HG3	1.58	0.40
1:A:138:TRP:HB3	4:B:301:L9Q:H26A	2.03	0.40
4:A:318:L9Q:C28	4:A:319:L9Q:H47A	2.49	0.40
4:A:319:L9Q:H26A	1:C:138:TRP:HB3	2.03	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	257/265 (97%)	249 (97%)	7 (3%)	1 (0%)	30	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	257/265 (97%)	249 (97%)	7 (3%)	1 (0%)	30	40
1	C	257/265 (97%)	249 (97%)	7 (3%)	1 (0%)	30	40
All	All	771/795 (97%)	747 (97%)	21 (3%)	3 (0%)	31	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	B	51	LEU
1	C	51	LEU

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	219/224 (98%)	183 (84%)	36 (16%)	2	2
1	B	219/224 (98%)	183 (84%)	36 (16%)	2	2
1	C	219/224 (98%)	183 (84%)	36 (16%)	2	2
All	All	657/672 (98%)	549 (84%)	108 (16%)	4	2

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE
1	A	9	GLU
1	A	10	ASP
1	A	24	LEU
1	A	25	LEU
1	A	28	MET
1	A	43	MET
1	A	44	LEU
1	A	46	ARG
1	A	56	LYS
1	A	65	GLU

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Mol	Chain	Res	Type
1	A	68	SER
1	A	70	SER
1	A	85	THR
1	A	98	PHE
1	A	104	LEU
1	A	114	LEU
1	A	127	LEU
1	A	133	VAL
1	A	135	ILE
1	A	145	VAL
1	A	146	THR
1	A	160	VAL
1	A	169	LEU
1	A	170	LEU
1	A	174	LYS
1	A	183	LYS
1	A	187	ILE
1	A	188	LEU
1	A	217	ASP
1	A	233	LYS
1	A	234	THR
1	A	246	GLU
1	A	247	LEU
1	A	252	GLU
1	A	260	GLU
1	B	3	PHE
1	B	9	GLU
1	B	10	ASP
1	B	24	LEU
1	B	25	LEU
1	B	28	MET
1	B	43	MET
1	B	44	LEU
1	B	46	ARG
1	B	56	LYS
1	B	65	GLU
1	B	68	SER
1	B	70	SER
1	B	85	THR
1	B	98	PHE
1	B	104	LEU
1	B	114	LEU

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Mol	Chain	Res	Type
1	B	127	LEU
1	B	133	VAL
1	B	135	ILE
1	B	145	VAL
1	B	146	THR
1	B	160	VAL
1	B	169	LEU
1	B	170	LEU
1	B	174	LYS
1	B	183	LYS
1	B	187	ILE
1	B	188	LEU
1	B	217	ASP
1	B	233	LYS
1	B	234	THR
1	B	246	GLU
1	B	247	LEU
1	B	252	GLU
1	B	260	GLU
1	C	3	PHE
1	C	9	GLU
1	C	10	ASP
1	C	24	LEU
1	C	25	LEU
1	C	28	MET
1	C	43	MET
1	C	44	LEU
1	C	46	ARG
1	C	56	LYS
1	C	65	GLU
1	C	68	SER
1	C	70	SER
1	C	85	THR
1	C	98	PHE
1	C	104	LEU
1	C	114	LEU
1	C	127	LEU
1	C	133	VAL
1	C	135	ILE
1	C	145	VAL
1	C	146	THR
1	C	160	VAL

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Mol	Chain	Res	Type
1	C	169	LEU
1	C	170	LEU
1	C	174	LYS
1	C	183	LYS
1	C	187	ILE
1	C	188	LEU
1	C	217	ASP
1	C	233	LYS
1	C	234	THR
1	C	246	GLU
1	C	247	LEU
1	C	252	GLU
1	C	260	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	14	HIS
1	A	125	HIS
1	A	259	ASN
1	B	13	HIS
1	B	14	HIS
1	B	259	ASN
1	C	13	HIS
1	C	14	HIS
1	C	259	ASN

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

Of 57 ligands modelled in this entry, 48 are monoatomic - leaving 9 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
4	L9Q	C	301	4	50,50,50	1.05	3 (6%)	53,55,55	1.11	3 (5%)
2	RET	B	302	-	20,20,21	0.79	0	27,27,28	5.56	17 (62%)
2	RET	C	303	-	20,20,21	0.79	0	27,27,28	5.57	17 (62%)
4	L9Q	A	319	4	50,50,50	1.04	3 (6%)	53,55,55	1.13	3 (5%)
4	L9Q	C	302	4	50,50,50	1.04	3 (6%)	53,55,55	1.13	3 (5%)
4	L9Q	B	319	4	50,50,50	1.05	3 (6%)	53,55,55	1.11	3 (5%)
2	RET	A	301	-	20,20,21	0.79	0	27,27,28	5.56	17 (62%)
4	L9Q	A	318	4	50,50,50	1.05	3 (6%)	53,55,55	1.11	3 (5%)
4	L9Q	B	301	4	50,50,50	1.03	3 (6%)	53,55,55	1.13	3 (5%)

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
4	L9Q	C	301	4	-	28/54/54/54	-
2	RET	B	302	-	-	0/13/30/31	0/1/1/1
2	RET	C	303	-	-	0/13/30/31	0/1/1/1
4	L9Q	A	319	4	-	27/54/54/54	-
4	L9Q	C	302	4	-	27/54/54/54	-
4	L9Q	B	319	4	-	28/54/54/54	-
2	RET	A	301	-	-	0/13/30/31	0/1/1/1
4	L9Q	A	318	4	-	28/54/54/54	-
4	L9Q	B	301	4	-	27/54/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	318	L9Q	O3-C11	4.14	1.45	1.33
4	B	319	L9Q	O3-C11	4.14	1.45	1.33
4	C	301	L9Q	O3-C11	4.13	1.45	1.33
4	C	302	L9Q	O3-C11	4.09	1.45	1.33
4	A	319	L9Q	O3-C11	4.09	1.45	1.33
4	A	318	L9Q	O2-C31	4.08	1.45	1.34
4	B	319	L9Q	O2-C31	4.08	1.45	1.34
4	C	301	L9Q	O2-C31	4.08	1.45	1.34
4	B	301	L9Q	O3-C11	4.06	1.45	1.33
4	A	319	L9Q	O2-C31	3.92	1.45	1.34
4	B	301	L9Q	O2-C31	3.92	1.45	1.34
4	C	302	L9Q	O2-C31	3.92	1.45	1.34
4	B	301	L9Q	C40-C39	3.70	1.52	1.31
4	C	302	L9Q	C40-C39	3.69	1.52	1.31
4	A	319	L9Q	C40-C39	3.69	1.52	1.31
4	B	319	L9Q	C40-C39	3.68	1.52	1.31
4	C	301	L9Q	C40-C39	3.68	1.52	1.31
4	A	318	L9Q	C40-C39	3.67	1.52	1.31

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	303	RET	C17-C1-C6	-17.95	82.09	110.24
2	B	302	RET	C17-C1-C6	-17.95	82.09	110.24
2	A	301	RET	C17-C1-C6	-17.95	82.10	110.24
2	C	303	RET	C11-C10-C9	-10.18	113.00	127.28
2	B	302	RET	C11-C10-C9	-10.17	113.01	127.28
2	A	301	RET	C11-C10-C9	-10.17	113.01	127.28
2	C	303	RET	C1-C6-C5	-8.86	110.53	122.64
2	B	302	RET	C1-C6-C5	-8.85	110.55	122.64
2	A	301	RET	C1-C6-C5	-8.84	110.55	122.64
2	B	302	RET	C17-C1-C16	-8.27	84.95	108.63
2	A	301	RET	C17-C1-C16	-8.27	84.95	108.63
2	C	303	RET	C17-C1-C16	-8.27	84.96	108.63
2	B	302	RET	C16-C1-C6	8.14	123.00	110.24
2	A	301	RET	C16-C1-C6	8.13	123.00	110.24
2	C	303	RET	C16-C1-C6	8.13	122.99	110.24
2	C	303	RET	C17-C1-C2	-6.07	85.66	108.95
2	A	301	RET	C17-C1-C2	-6.06	85.69	108.95
2	B	302	RET	C17-C1-C2	-6.06	85.69	108.95
2	C	303	RET	C3-C4-C5	-5.49	104.27	114.06
2	A	301	RET	C3-C4-C5	-5.48	104.29	114.06
2	B	302	RET	C3-C4-C5	-5.47	104.31	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	303	RET	C7-C8-C9	-5.23	118.50	126.23
2	A	301	RET	C7-C8-C9	-5.23	118.50	126.23
2	B	302	RET	C7-C8-C9	-5.20	118.53	126.23
2	C	303	RET	C4-C5-C6	-4.98	115.98	122.70
2	A	301	RET	C4-C5-C6	-4.97	115.98	122.70
2	B	302	RET	C4-C5-C6	-4.97	115.98	122.70
2	C	303	RET	C11-C12-C13	-4.67	113.57	126.36
2	A	301	RET	C11-C12-C13	-4.66	113.58	126.36
2	B	302	RET	C11-C12-C13	-4.66	113.59	126.36
4	A	319	L9Q	O2-C31-C32	4.14	120.43	111.48
4	C	302	L9Q	O2-C31-C32	4.13	120.41	111.48
4	B	301	L9Q	O2-C31-C32	4.12	120.40	111.48
4	C	301	L9Q	O2-C31-C32	3.99	120.12	111.48
4	B	319	L9Q	O2-C31-C32	3.99	120.12	111.48
4	A	318	L9Q	O2-C31-C32	3.98	120.10	111.48
2	C	303	RET	C16-C1-C2	2.98	120.39	108.95
2	B	302	RET	C16-C1-C2	2.98	120.38	108.95
2	A	301	RET	C16-C1-C2	2.98	120.38	108.95
4	A	318	L9Q	O3-C11-C12	2.87	120.60	111.83
4	C	301	L9Q	O3-C11-C12	2.87	120.59	111.83
4	B	319	L9Q	O3-C11-C12	2.87	120.58	111.83
4	B	301	L9Q	O3-C11-C12	2.76	120.24	111.83
4	C	302	L9Q	O3-C11-C12	2.75	120.22	111.83
4	A	319	L9Q	O3-C11-C12	2.75	120.21	111.83
2	B	302	RET	C7-C6-C5	2.51	127.34	121.56
2	C	303	RET	C7-C6-C5	2.51	127.33	121.56
2	A	301	RET	C7-C6-C5	2.51	127.33	121.56
2	B	302	RET	C18-C5-C4	2.42	118.75	113.60
2	C	303	RET	C18-C5-C4	2.42	118.75	113.60
2	A	301	RET	C18-C5-C4	2.41	118.73	113.60
2	C	303	RET	C1-C6-C7	2.38	122.09	115.65
2	A	301	RET	C1-C6-C7	2.37	122.08	115.65
2	B	302	RET	C1-C6-C7	2.37	122.08	115.65
4	B	319	L9Q	C2-O2-C31	-2.33	112.22	117.80
4	C	301	L9Q	C2-O2-C31	-2.32	112.23	117.80
2	C	303	RET	C3-C2-C1	-2.32	106.20	114.43
4	A	318	L9Q	C2-O2-C31	-2.32	112.24	117.80
2	B	302	RET	C3-C2-C1	-2.32	106.22	114.43
2	A	301	RET	C3-C2-C1	-2.32	106.22	114.43
2	A	301	RET	C2-C1-C6	2.20	113.64	110.44
2	C	303	RET	C2-C1-C6	2.20	113.63	110.44
2	B	302	RET	C2-C1-C6	2.19	113.62	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	302	L9Q	C2-O2-C31	-2.11	112.75	117.80
4	A	319	L9Q	C2-O2-C31	-2.11	112.76	117.80
4	B	301	L9Q	C2-O2-C31	-2.10	112.78	117.80
2	A	301	RET	C12-C13-C14	2.06	124.04	118.55
2	B	302	RET	C12-C13-C14	2.06	124.04	118.55
2	C	303	RET	C12-C13-C14	2.06	124.04	118.55

There are no chirality outliers.

All (165) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	318	L9Q	C1-O3P-P-O1P
4	A	318	L9Q	C1-O3P-P-O2P
4	A	318	L9Q	C1-O3P-P-O4P
4	A	318	L9Q	C4-O4P-P-O1P
4	A	318	L9Q	C32-C31-O2-C2
4	A	319	L9Q	C4-O4P-P-O1P
4	A	319	L9Q	C4-O4P-P-O3P
4	A	319	L9Q	O31-C31-O2-C2
4	A	319	L9Q	O4P-C4-C5-N
4	B	301	L9Q	C4-O4P-P-O1P
4	B	301	L9Q	C4-O4P-P-O3P
4	B	301	L9Q	O31-C31-O2-C2
4	B	301	L9Q	O4P-C4-C5-N
4	B	319	L9Q	C1-O3P-P-O1P
4	B	319	L9Q	C1-O3P-P-O2P
4	B	319	L9Q	C1-O3P-P-O4P
4	B	319	L9Q	C4-O4P-P-O1P
4	B	319	L9Q	C32-C31-O2-C2
4	C	301	L9Q	C1-O3P-P-O1P
4	C	301	L9Q	C1-O3P-P-O2P
4	C	301	L9Q	C1-O3P-P-O4P
4	C	301	L9Q	C4-O4P-P-O1P
4	C	301	L9Q	C32-C31-O2-C2
4	C	302	L9Q	C4-O4P-P-O1P
4	C	302	L9Q	C4-O4P-P-O3P
4	C	302	L9Q	O31-C31-O2-C2
4	C	302	L9Q	O4P-C4-C5-N
4	A	318	L9Q	O31-C31-O2-C2
4	B	319	L9Q	O31-C31-O2-C2
4	C	301	L9Q	O31-C31-O2-C2
4	A	319	L9Q	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
4	B	301	L9Q	C32-C31-O2-C2
4	C	302	L9Q	C32-C31-O2-C2
4	A	319	L9Q	C42-C43-C44-C45
4	B	301	L9Q	C42-C43-C44-C45
4	C	302	L9Q	C42-C43-C44-C45
4	A	319	L9Q	C18-C19-C20-C21
4	B	301	L9Q	C18-C19-C20-C21
4	C	302	L9Q	C18-C19-C20-C21
4	A	319	L9Q	C21-C22-C23-C24
4	B	301	L9Q	C21-C22-C23-C24
4	C	302	L9Q	C21-C22-C23-C24
4	C	301	L9Q	C32-C33-C34-C35
4	A	318	L9Q	C32-C33-C34-C35
4	B	319	L9Q	C32-C33-C34-C35
4	A	318	L9Q	C38-C39-C40-C41
4	B	319	L9Q	C38-C39-C40-C41
4	C	301	L9Q	C38-C39-C40-C41
4	A	318	L9Q	C12-C13-C14-C15
4	A	318	L9Q	C42-C43-C44-C45
4	B	319	L9Q	C12-C13-C14-C15
4	B	319	L9Q	C42-C43-C44-C45
4	C	301	L9Q	C12-C13-C14-C15
4	C	301	L9Q	C42-C43-C44-C45
4	A	318	L9Q	C34-C35-C36-C37
4	B	319	L9Q	C34-C35-C36-C37
4	C	301	L9Q	C34-C35-C36-C37
4	A	319	L9Q	C25-C26-C27-C28
4	B	301	L9Q	C25-C26-C27-C28
4	C	302	L9Q	C25-C26-C27-C28
4	A	318	L9Q	C14-C15-C16-C17
4	B	319	L9Q	C14-C15-C16-C17
4	C	301	L9Q	C14-C15-C16-C17
4	A	319	L9Q	C44-C45-C46-C47
4	B	301	L9Q	C44-C45-C46-C47
4	C	302	L9Q	C44-C45-C46-C47
4	A	319	L9Q	C12-C11-O3-C3
4	B	301	L9Q	C12-C11-O3-C3
4	C	302	L9Q	C12-C11-O3-C3
4	A	318	L9Q	C20-C21-C22-C23
4	B	319	L9Q	C20-C21-C22-C23
4	C	301	L9Q	C20-C21-C22-C23
4	A	318	L9Q	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
4	B	319	L9Q	C22-C23-C24-C25
4	C	301	L9Q	C22-C23-C24-C25
4	A	318	L9Q	C13-C14-C15-C16
4	B	319	L9Q	C13-C14-C15-C16
4	C	301	L9Q	C13-C14-C15-C16
4	A	318	L9Q	C24-C25-C26-C27
4	B	319	L9Q	C24-C25-C26-C27
4	C	301	L9Q	C24-C25-C26-C27
4	A	319	L9Q	O11-C11-O3-C3
4	B	301	L9Q	O11-C11-O3-C3
4	C	302	L9Q	O11-C11-O3-C3
4	A	319	L9Q	C43-C44-C45-C46
4	B	301	L9Q	C43-C44-C45-C46
4	C	302	L9Q	C43-C44-C45-C46
4	A	319	L9Q	C23-C24-C25-C26
4	B	301	L9Q	C23-C24-C25-C26
4	C	302	L9Q	C23-C24-C25-C26
4	A	319	L9Q	C34-C35-C36-C37
4	B	301	L9Q	C34-C35-C36-C37
4	C	302	L9Q	C34-C35-C36-C37
4	A	318	L9Q	C19-C20-C21-C22
4	B	319	L9Q	C19-C20-C21-C22
4	C	301	L9Q	C19-C20-C21-C22
4	A	318	L9Q	O3P-C1-C2-C3
4	B	319	L9Q	O3P-C1-C2-C3
4	C	301	L9Q	O3P-C1-C2-C3
4	A	319	L9Q	C19-C20-C21-C22
4	B	301	L9Q	C19-C20-C21-C22
4	C	302	L9Q	C19-C20-C21-C22
4	A	319	L9Q	C1-C2-C3-O3
4	B	301	L9Q	C1-C2-C3-O3
4	C	302	L9Q	C1-C2-C3-O3
4	C	302	L9Q	C45-C46-C47-C48
4	A	319	L9Q	C45-C46-C47-C48
4	B	301	L9Q	C45-C46-C47-C48
4	A	319	L9Q	C13-C14-C15-C16
4	B	301	L9Q	C13-C14-C15-C16
4	C	302	L9Q	C13-C14-C15-C16
4	A	318	L9Q	C25-C26-C27-C28
4	B	319	L9Q	C25-C26-C27-C28
4	C	301	L9Q	C25-C26-C27-C28
4	A	318	L9Q	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	319	L9Q	O3P-C1-C2-O2
4	C	301	L9Q	O3P-C1-C2-O2
4	A	319	L9Q	C32-C33-C34-C35
4	B	301	L9Q	C32-C33-C34-C35
4	C	302	L9Q	C32-C33-C34-C35
4	A	319	L9Q	C40-C41-C42-C43
4	B	301	L9Q	C40-C41-C42-C43
4	C	302	L9Q	C40-C41-C42-C43
4	A	318	L9Q	C18-C19-C20-C21
4	B	319	L9Q	C18-C19-C20-C21
4	C	301	L9Q	C18-C19-C20-C21
4	A	319	L9Q	C37-C38-C39-C40
4	B	301	L9Q	C37-C38-C39-C40
4	C	302	L9Q	C37-C38-C39-C40
4	A	319	L9Q	O2-C2-C3-O3
4	B	301	L9Q	O2-C2-C3-O3
4	C	302	L9Q	O2-C2-C3-O3
4	A	318	L9Q	C4-O4P-P-O3P
4	A	319	L9Q	C4-O4P-P-O2P
4	B	301	L9Q	C4-O4P-P-O2P
4	B	319	L9Q	C4-O4P-P-O3P
4	C	301	L9Q	C4-O4P-P-O3P
4	C	302	L9Q	C4-O4P-P-O2P
4	A	318	L9Q	C21-C22-C23-C24
4	B	319	L9Q	C21-C22-C23-C24
4	C	301	L9Q	C21-C22-C23-C24
4	B	301	L9Q	C41-C42-C43-C44
4	A	319	L9Q	C41-C42-C43-C44
4	C	302	L9Q	C41-C42-C43-C44
4	A	319	L9Q	O3-C11-C12-C13
4	B	301	L9Q	O3-C11-C12-C13
4	C	302	L9Q	O3-C11-C12-C13
4	A	319	L9Q	C38-C39-C40-C41
4	B	301	L9Q	C38-C39-C40-C41
4	C	302	L9Q	C38-C39-C40-C41
4	A	318	L9Q	O3-C11-C12-C13
4	B	319	L9Q	O3-C11-C12-C13
4	C	301	L9Q	O3-C11-C12-C13
4	A	318	L9Q	O2-C31-C32-C33
4	B	319	L9Q	O2-C31-C32-C33
4	C	301	L9Q	O2-C31-C32-C33
4	B	319	L9Q	O11-C11-C12-C13

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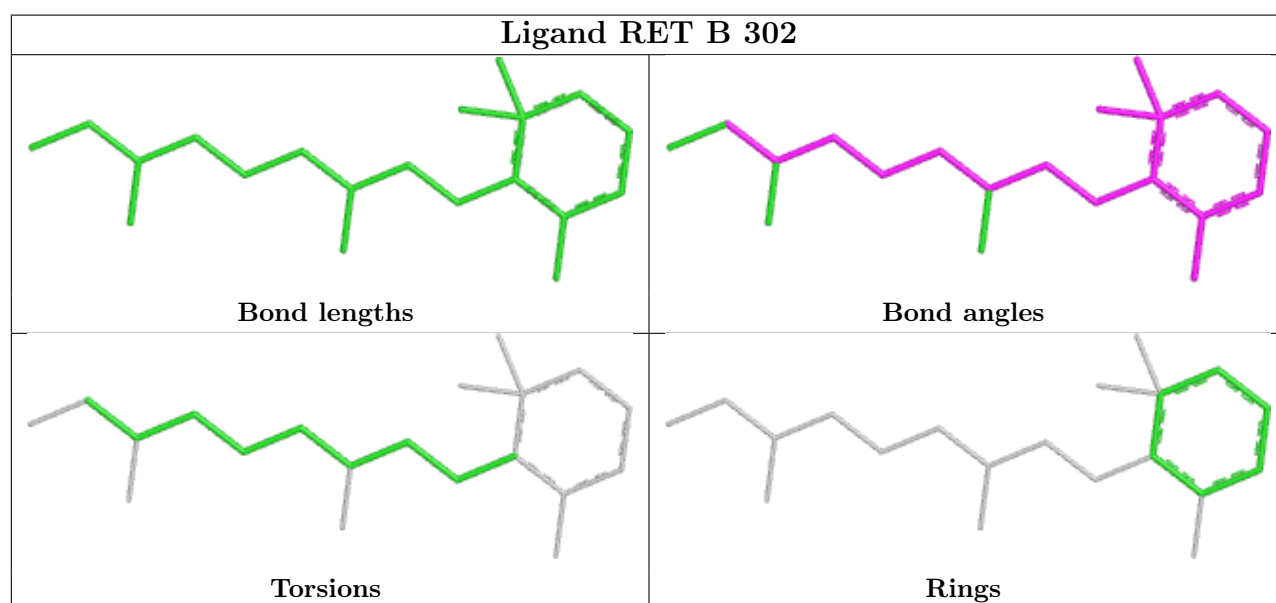
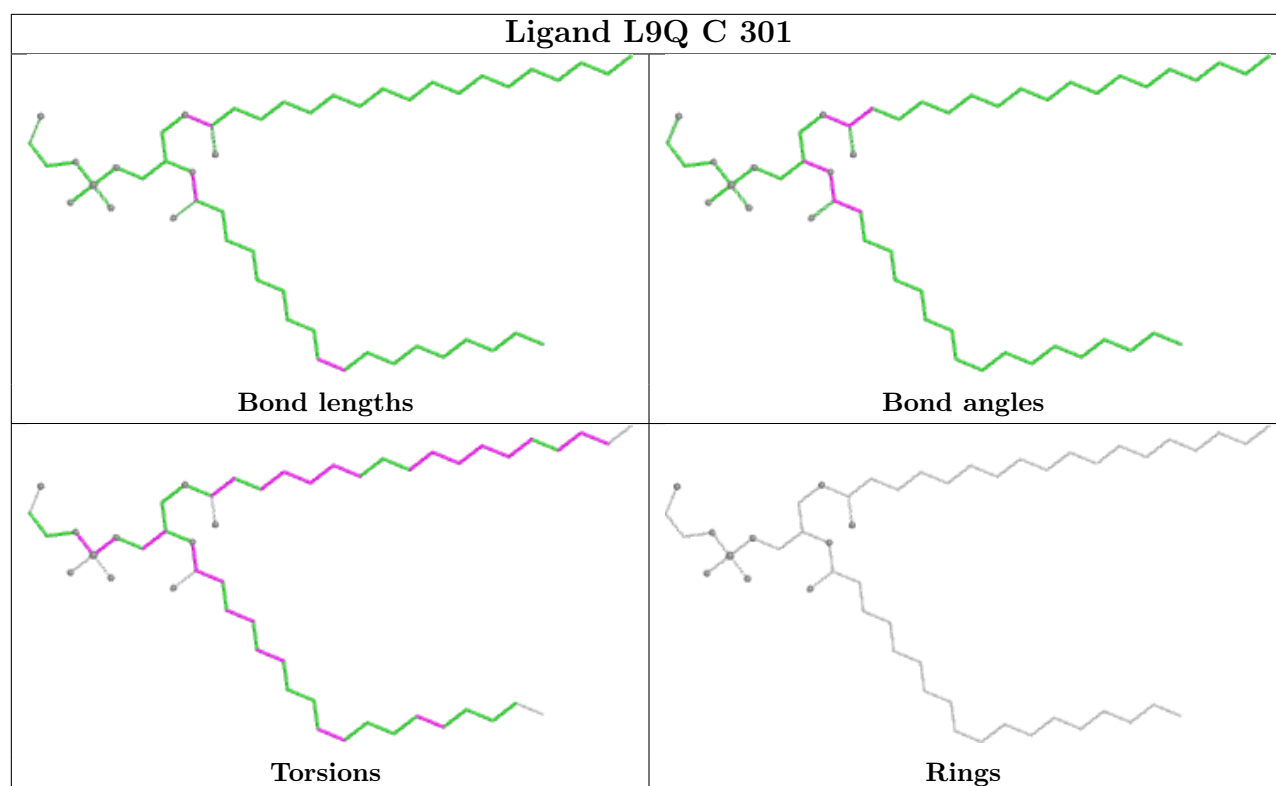
Mol	Chain	Res	Type	Atoms
4	C	301	L9Q	O11-C11-C12-C13
4	A	318	L9Q	O11-C11-C12-C13
4	B	319	L9Q	C15-C16-C17-C18
4	A	318	L9Q	C15-C16-C17-C18
4	C	301	L9Q	C15-C16-C17-C18
4	A	318	L9Q	O31-C31-C32-C33
4	B	319	L9Q	O31-C31-C32-C33
4	C	301	L9Q	O31-C31-C32-C33

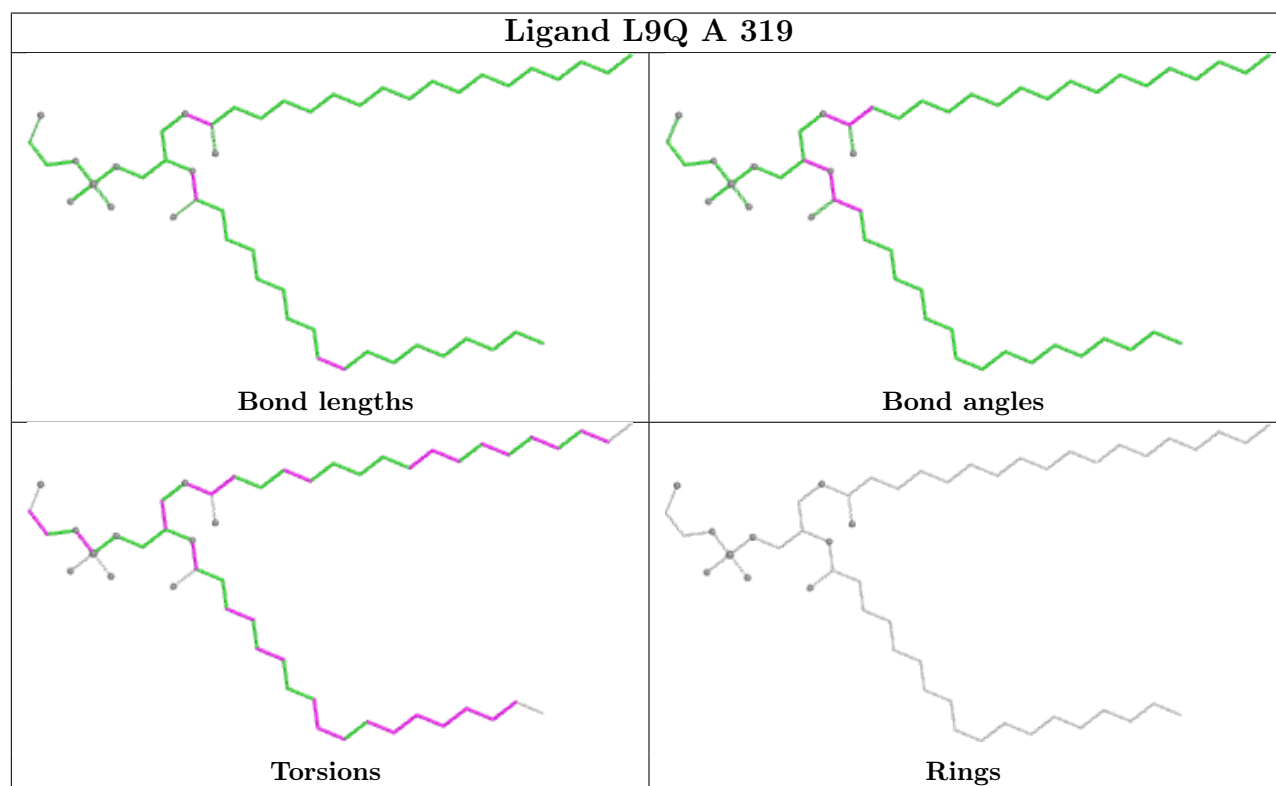
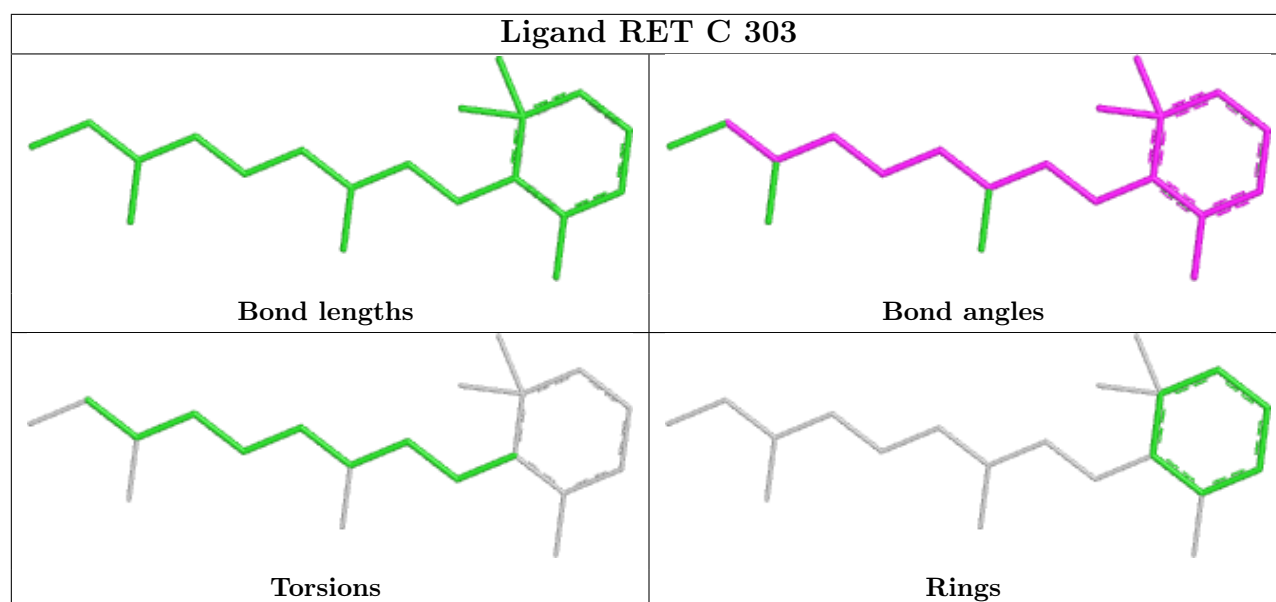
There are no ring outliers.

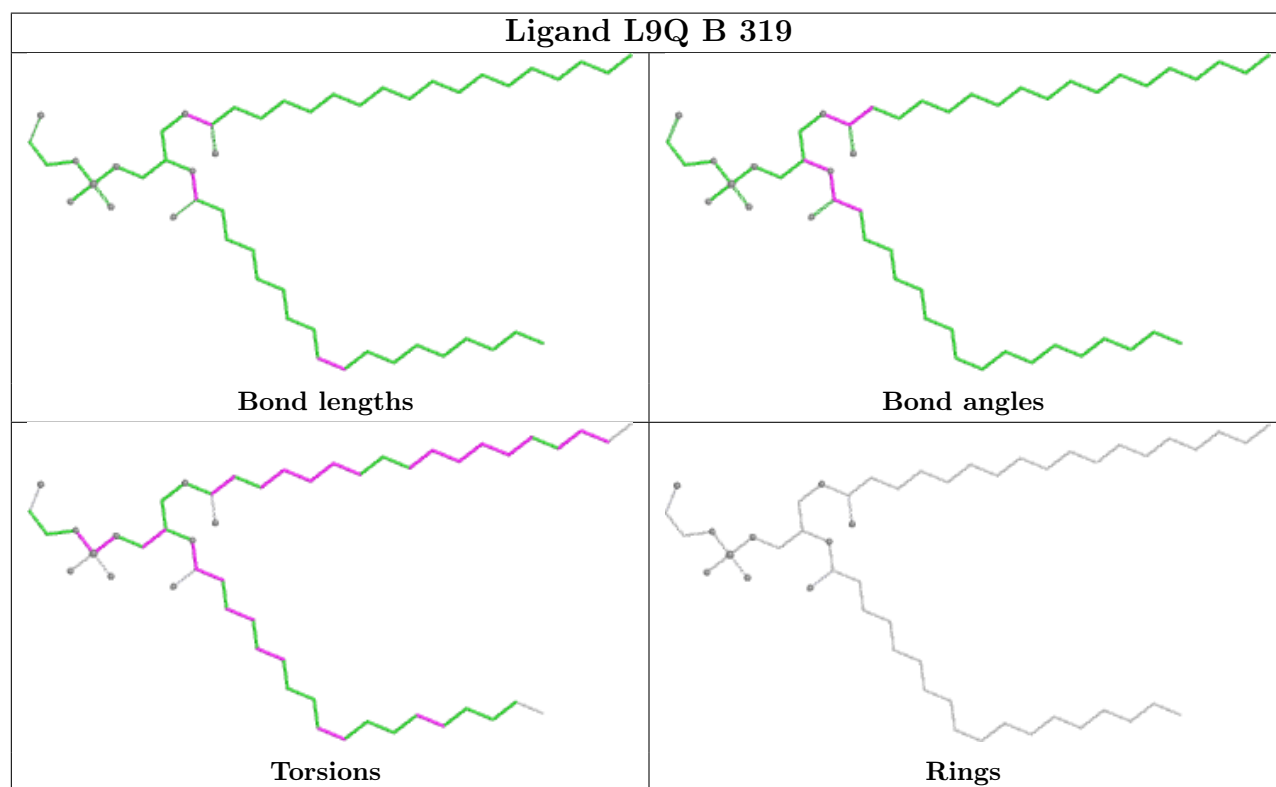
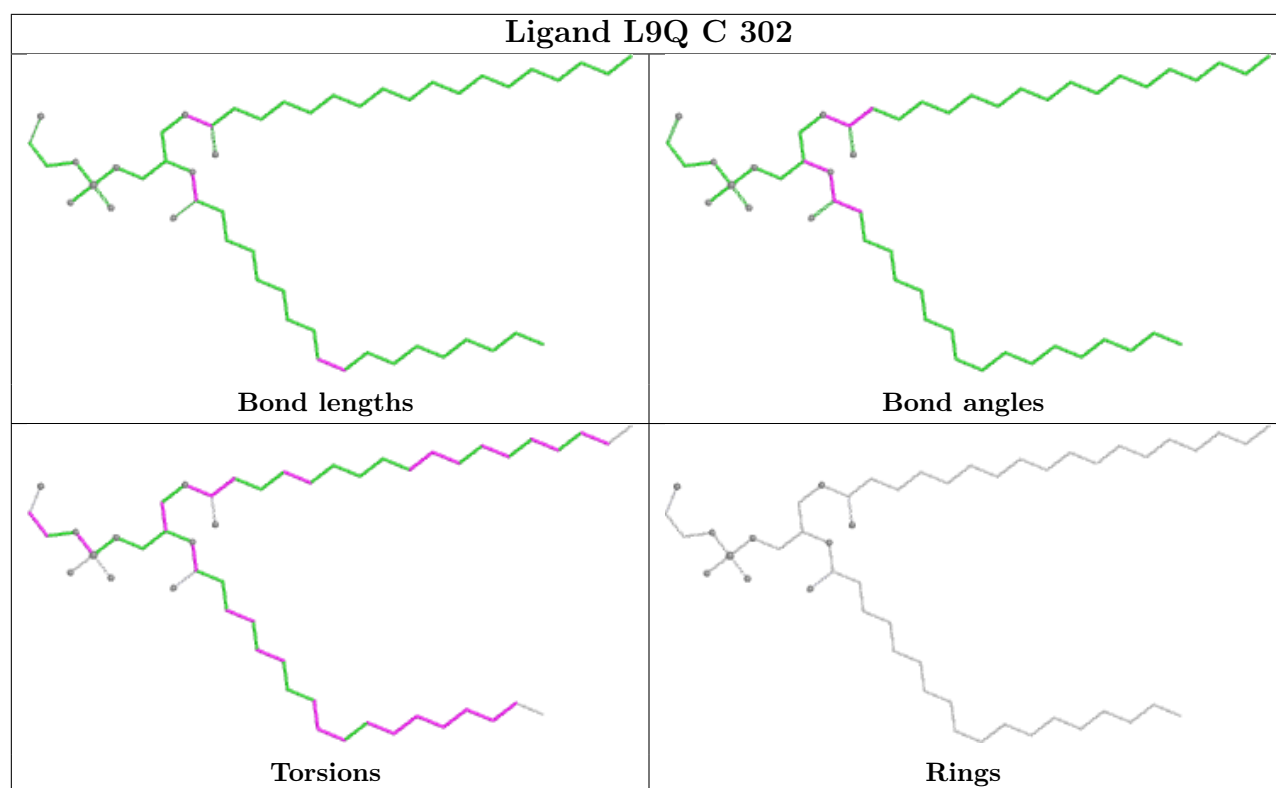
9 monomers are involved in 183 short contacts:

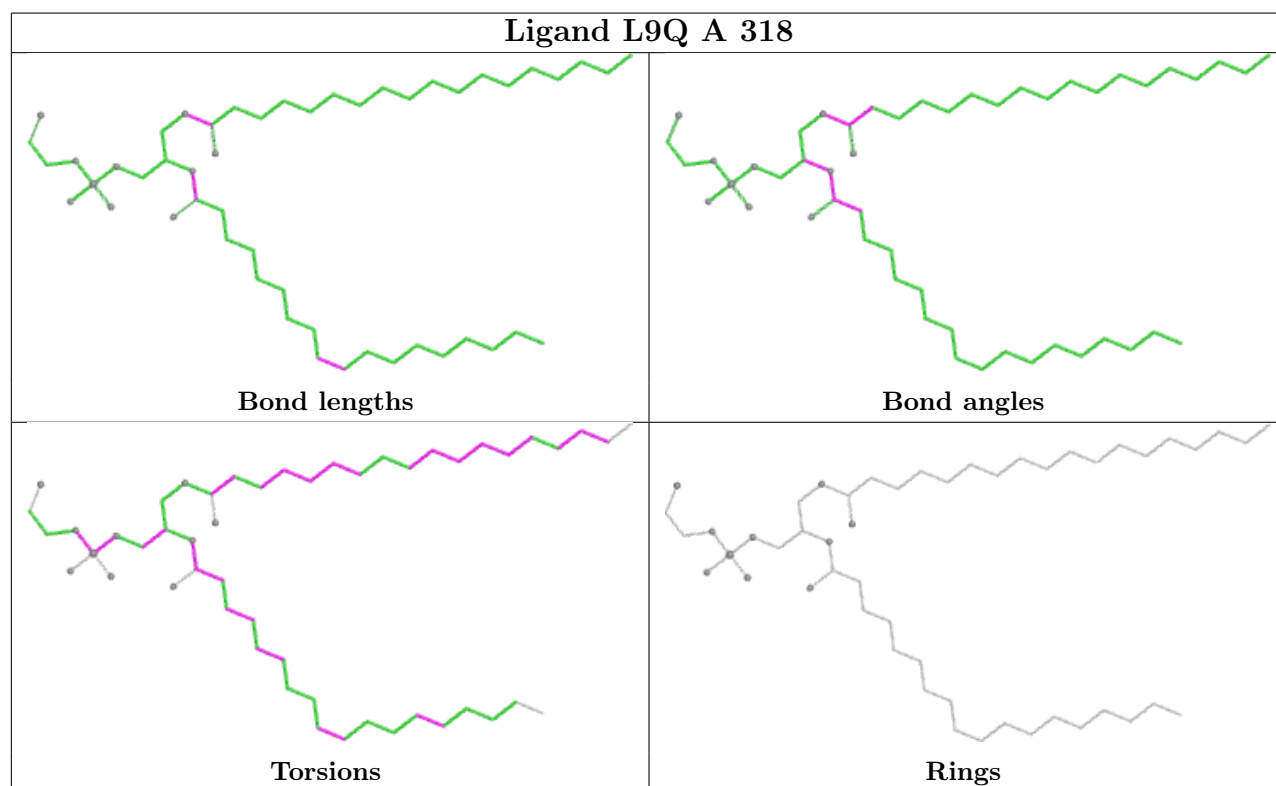
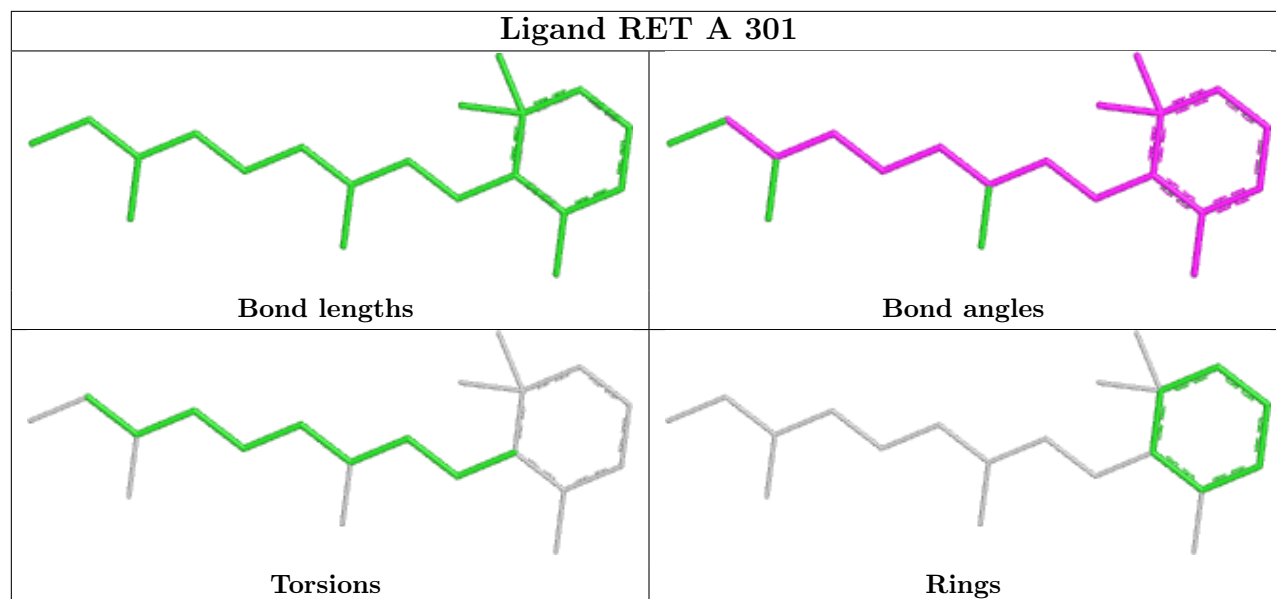
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	301	L9Q	24	0
2	B	302	RET	4	0
2	C	303	RET	3	0
4	A	319	L9Q	71	0
4	C	302	L9Q	70	0
4	B	319	L9Q	24	0
2	A	301	RET	4	0
4	A	318	L9Q	24	0
4	B	301	L9Q	70	0

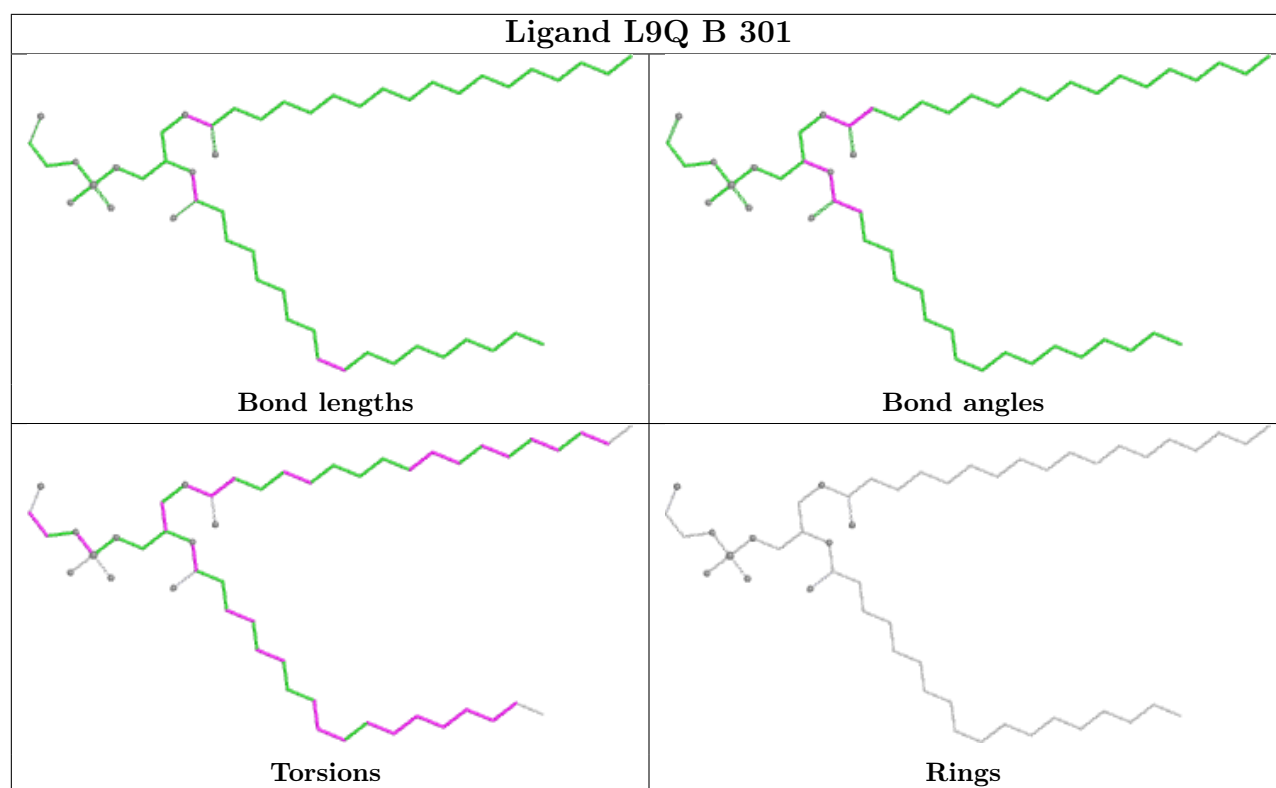
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

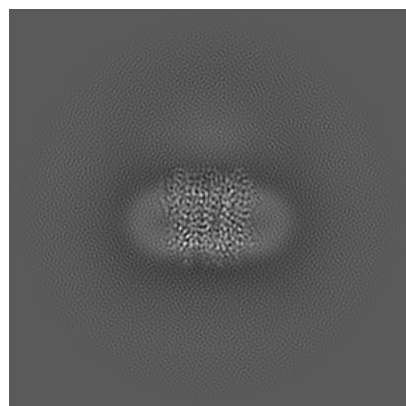
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35423. These allow visual inspection of the internal detail of the map and identification of artifacts.

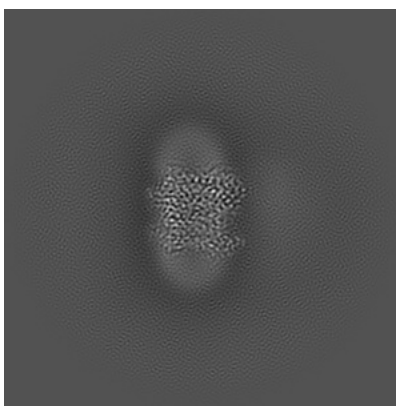
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

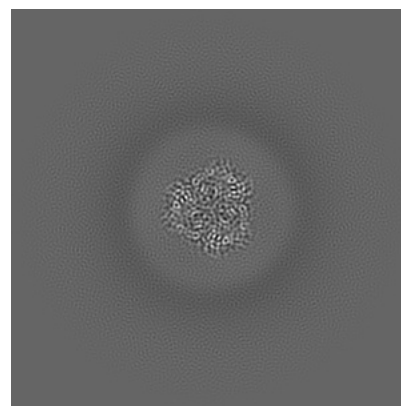
6.1.1 Primary map



X

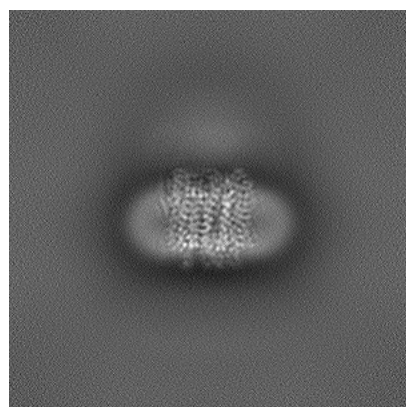


Y

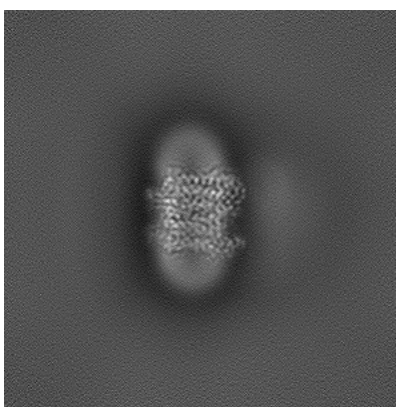


Z

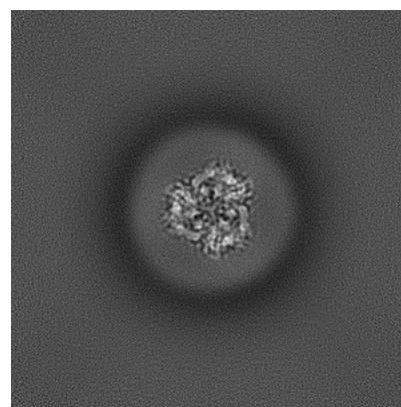
6.1.2 Raw map



X



Y

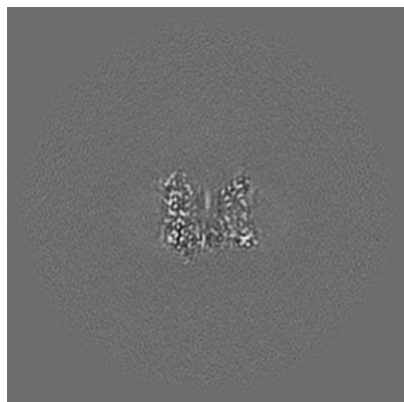


Z

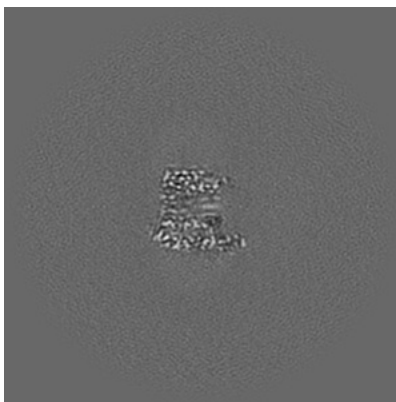
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

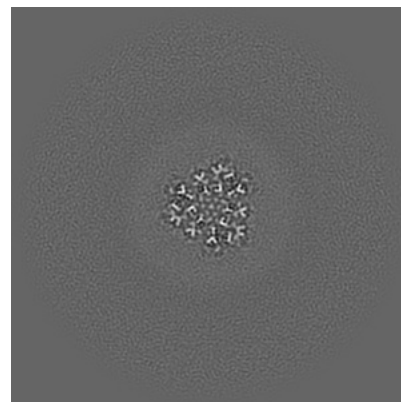
6.2.1 Primary map



X Index: 240

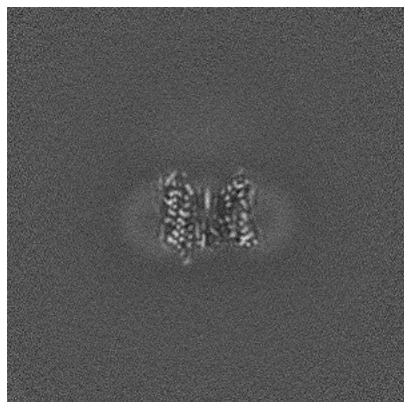


Y Index: 240

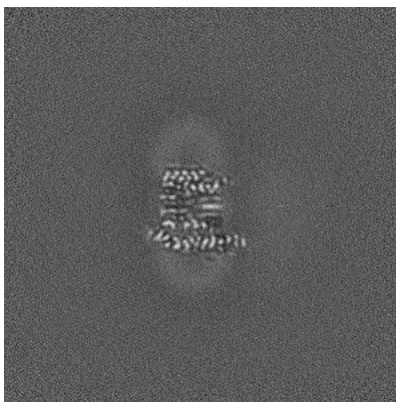


Z Index: 240

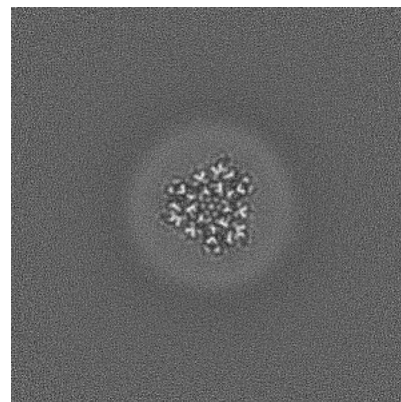
6.2.2 Raw map



X Index: 240



Y Index: 240

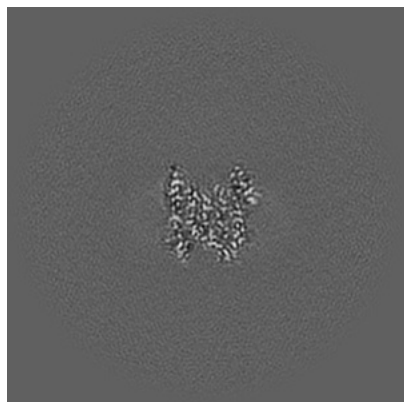


Z Index: 240

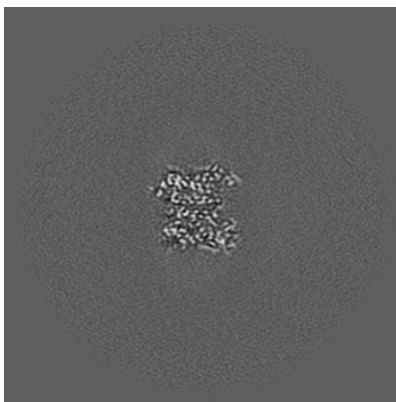
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

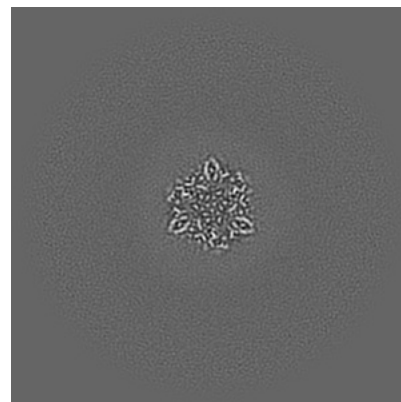
6.3.1 Primary map



X Index: 259

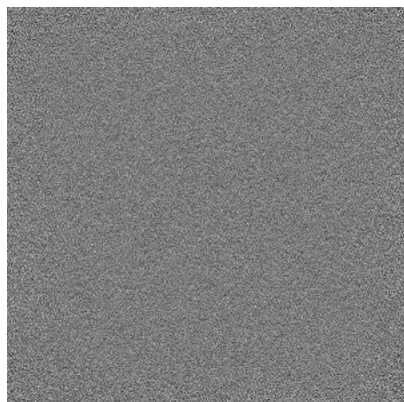


Y Index: 260

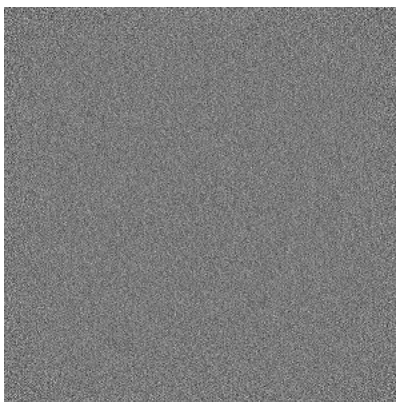


Z Index: 199

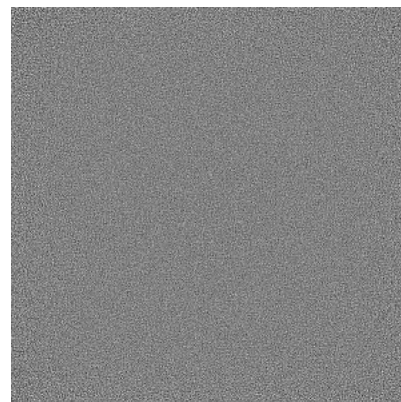
6.3.2 Raw map



X Index: 0



Y Index: 0

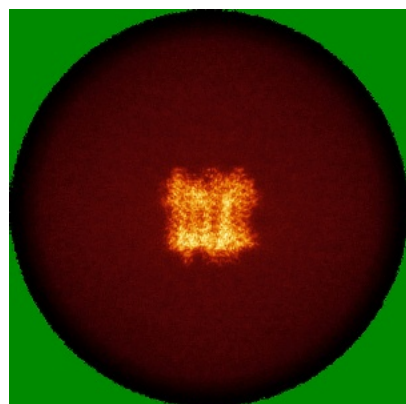


Z Index: 0

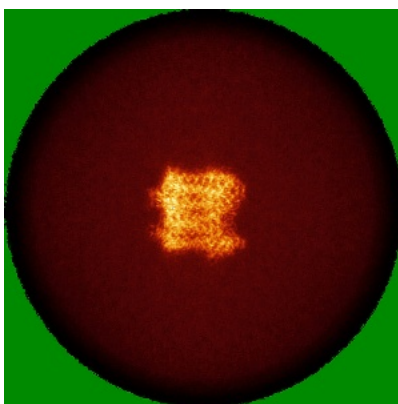
The images above show the largest variance slices of the map in three orthogonal directions.

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

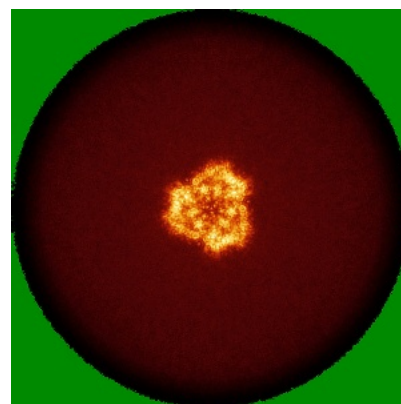
6.4.1 Primary map



X

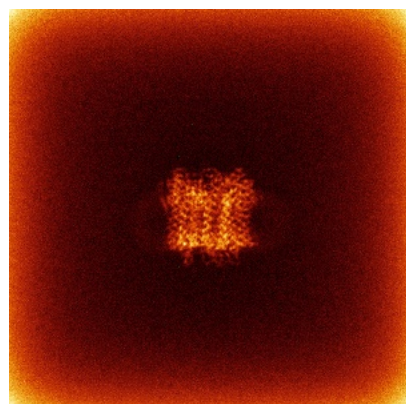


Y

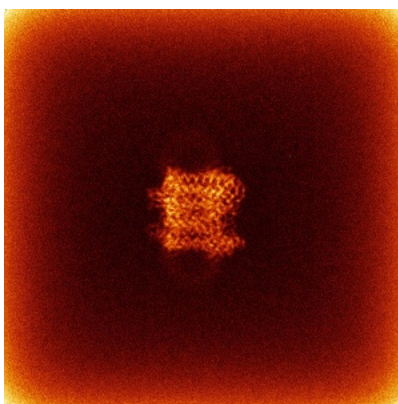


Z

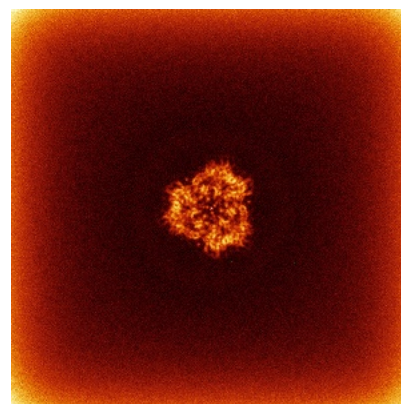
6.4.2 Raw map



X



Y

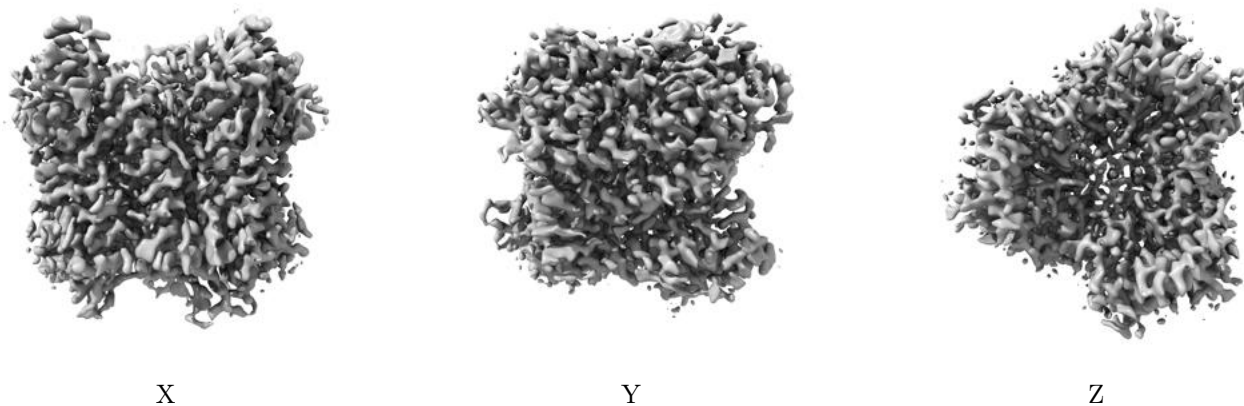


Z

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.

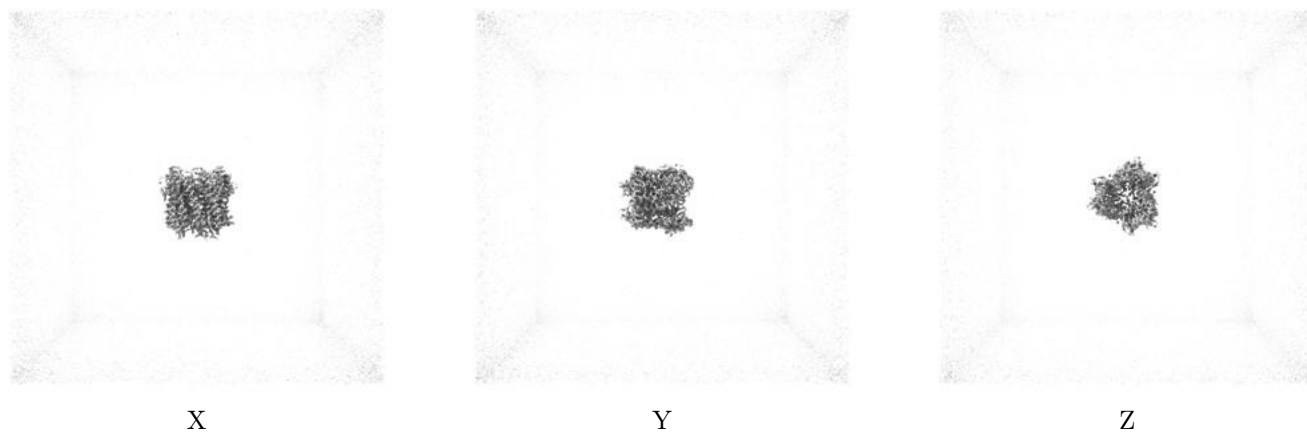
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.22. 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.

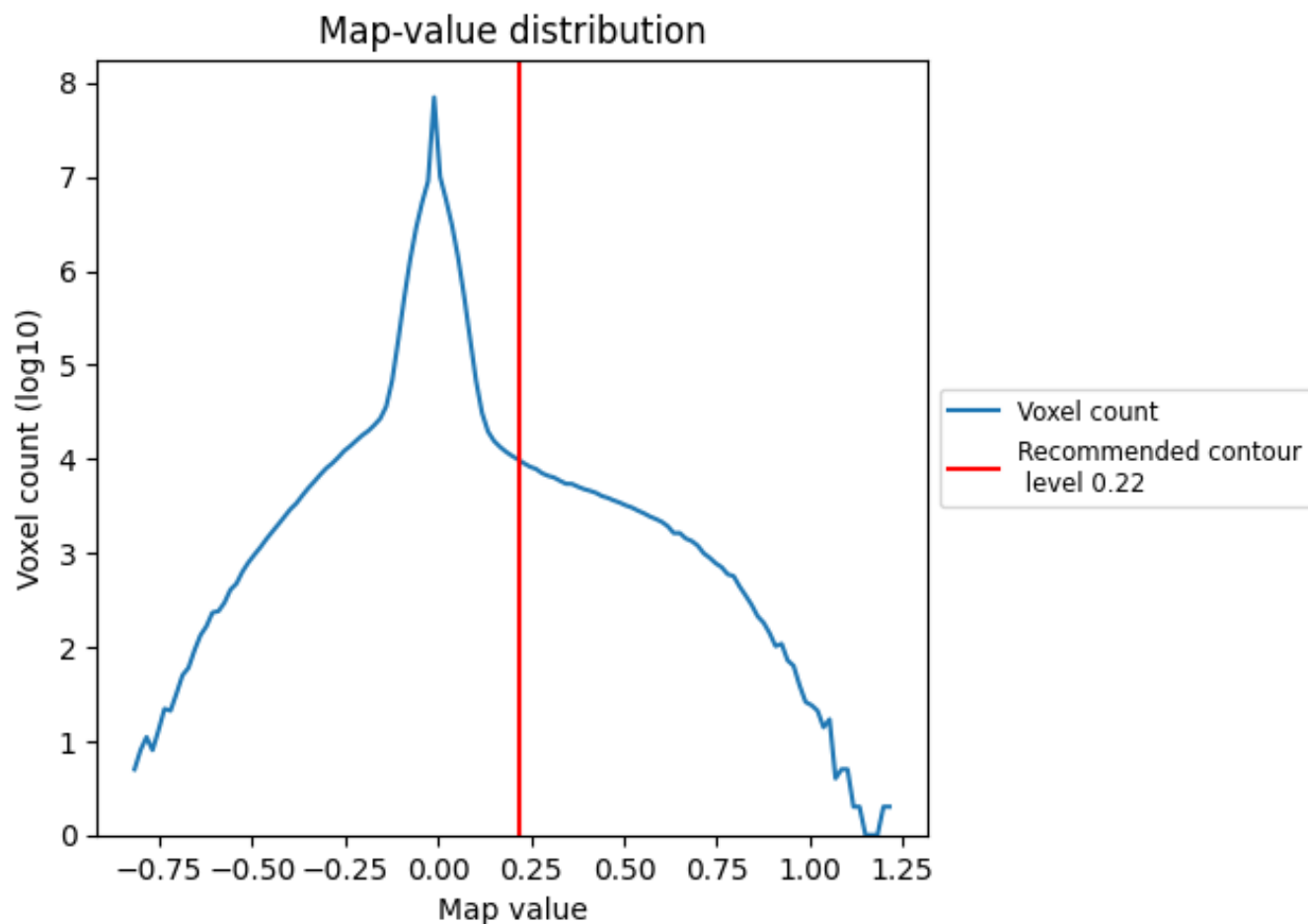
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

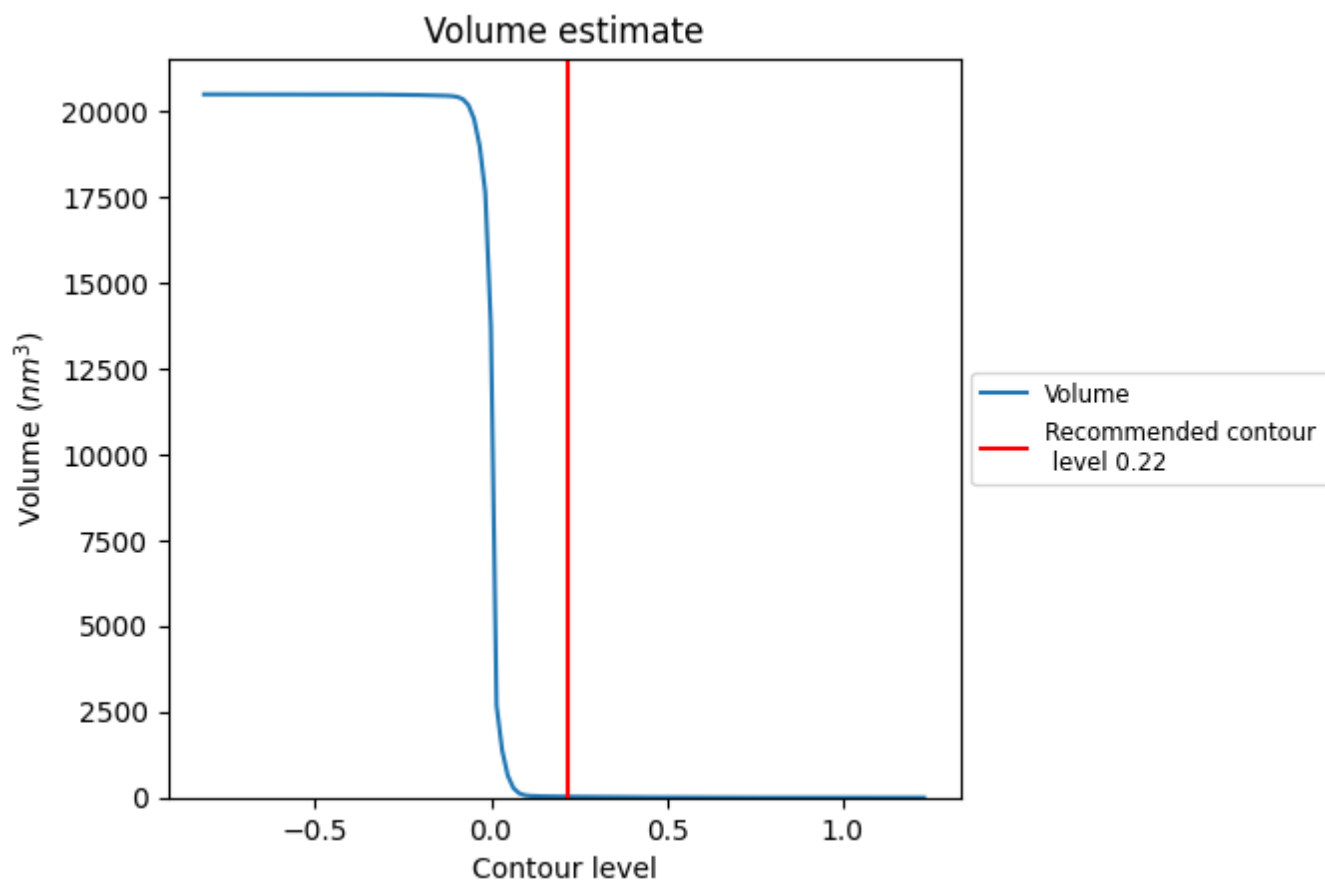
This section contains the results of statistical analysis of the map.

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.

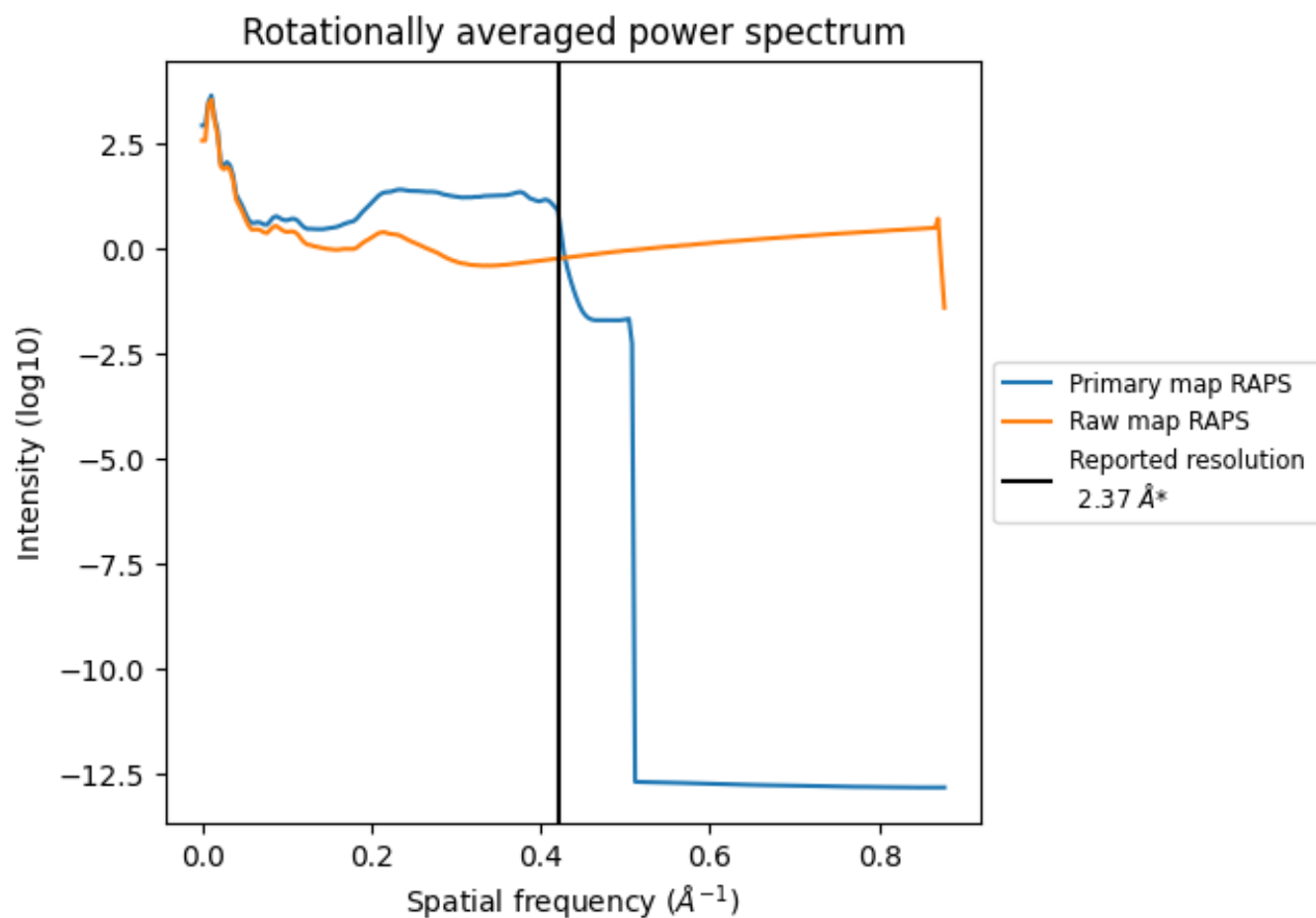
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 25 nm³; this corresponds to an approximate mass of 23 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 ⓘ

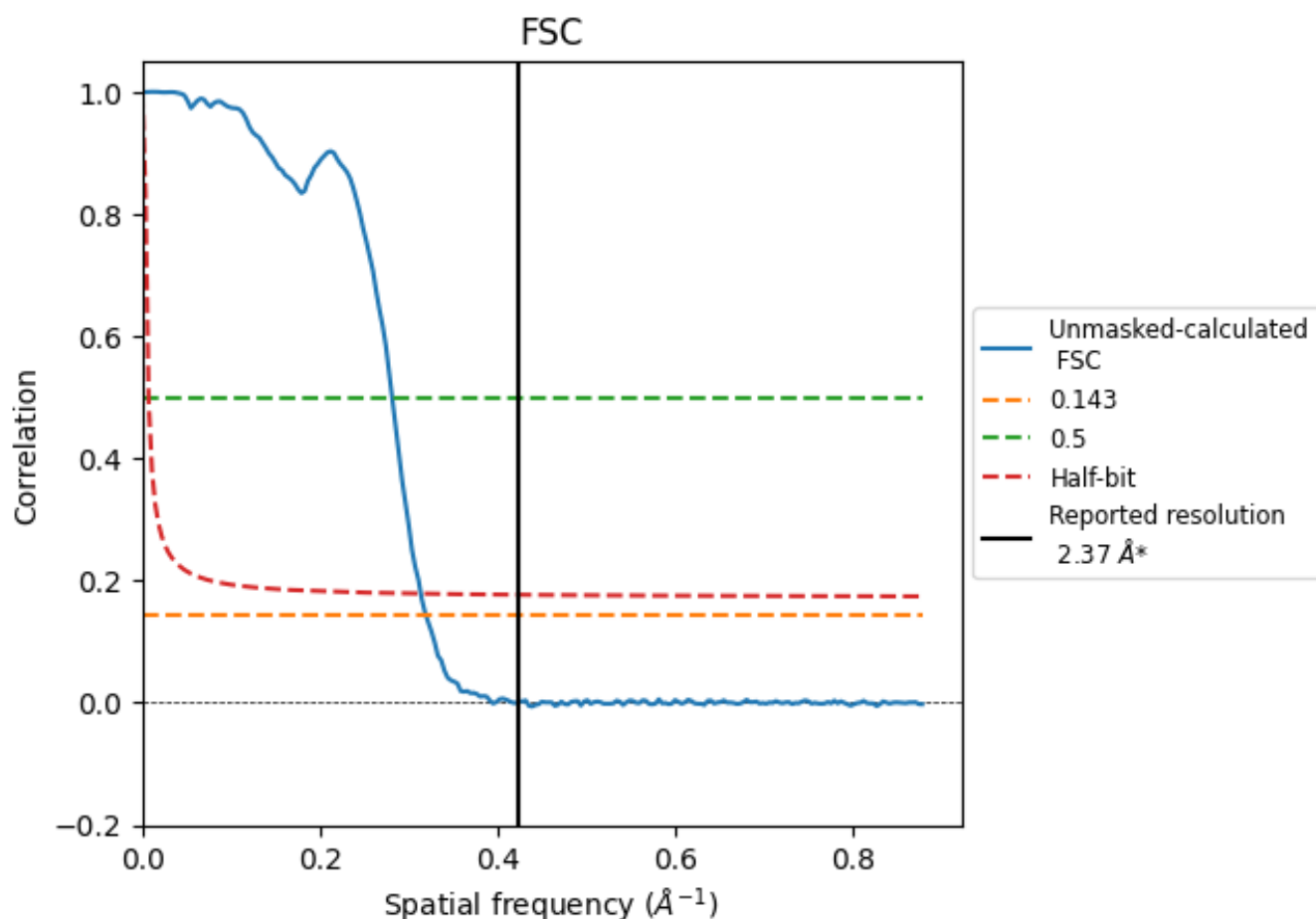


*Reported resolution corresponds to spatial frequency of 0.422 Å⁻¹

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 0.422 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

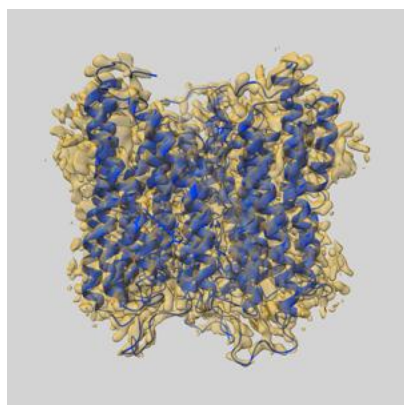
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.37	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.13	3.55	3.19

*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 3.13 differs from the reported value 2.37 by more than 10 %

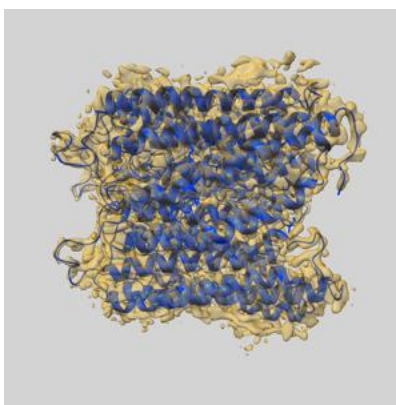
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35423 and PDB model 8IFU. Per-residue inclusion information can be found in section [3](#) on page [7](#).

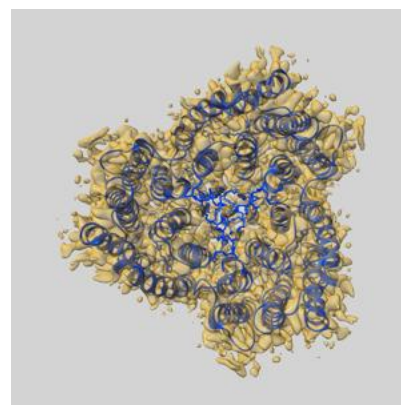
9.1 Map-model overlay [i](#)



X



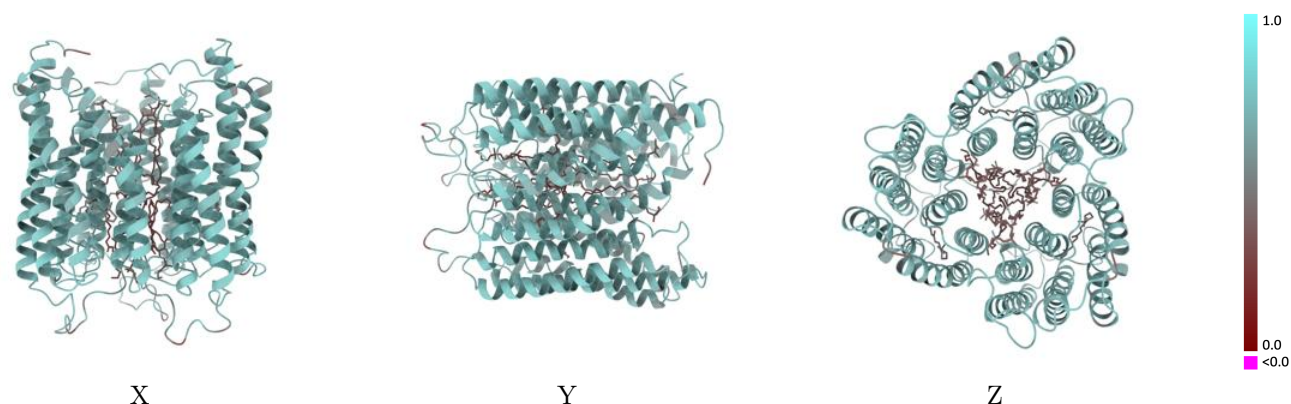
Y



Z

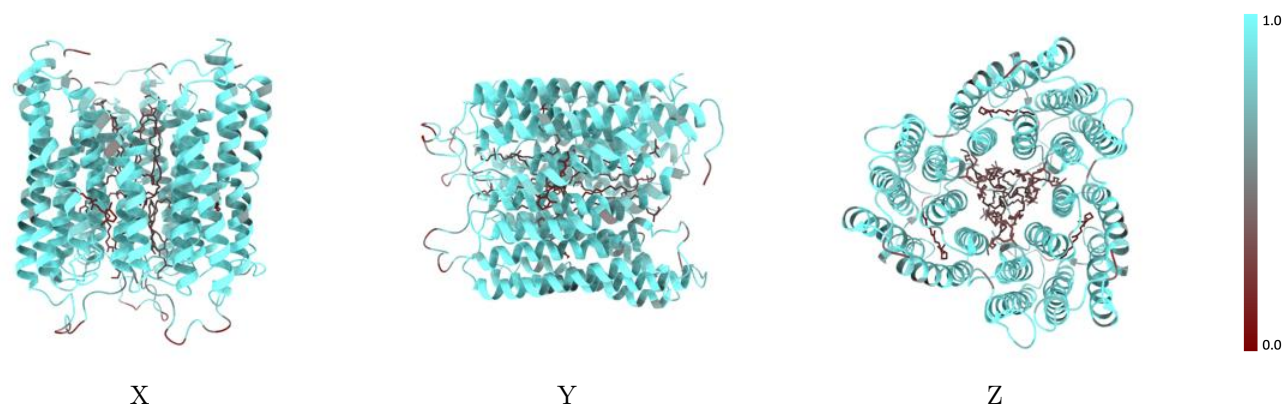
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



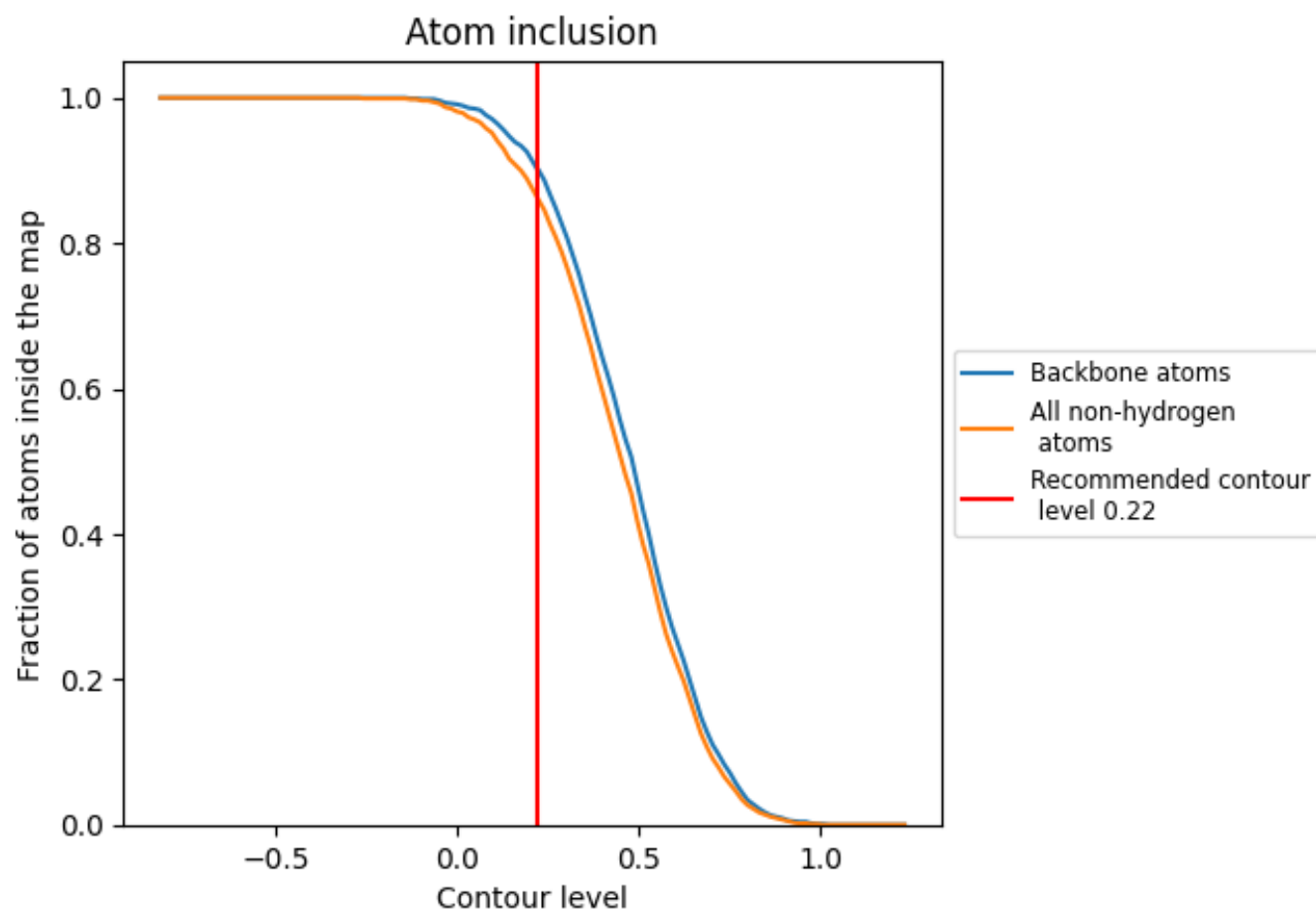
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 86% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8630	0.6550
A	0.8630	0.6550
B	0.8640	0.6550
C	0.8640	0.6560

