



Full wwPDB EM Validation Report ⓘ

Jul 15, 2026 – 02:19 PM JST

PDB ID : 9VOS / pdb_00009vos
EMDB ID : EMD-65226
Title : Cryo-EM Structure of GPR158 in Complex with RGS7-Gbeta5 and Nanobody Nb20
Authors : Laboute, T.; Zucca, S.; Sial, M.; Sharma, M.; Brunori, G.; Singh, S.; Singh, A.; Martemyanov, K.
Deposited on : 2025-07-02
Resolution : 4.30 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:

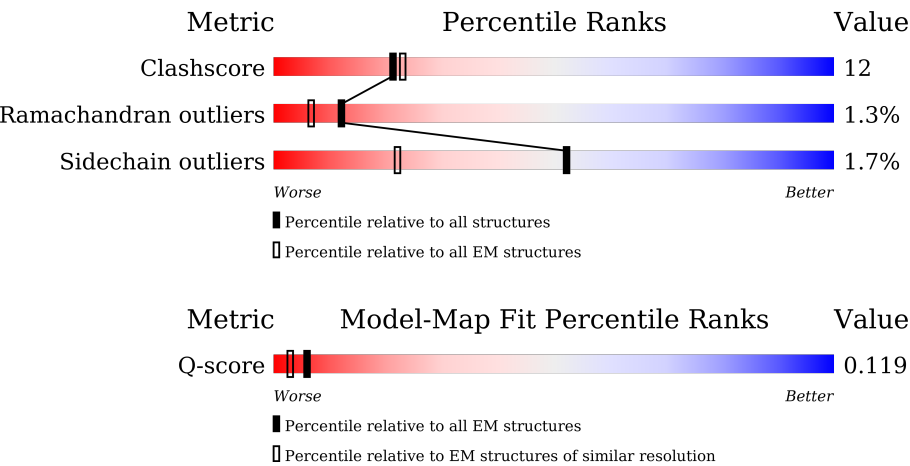
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.50

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 4.30 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	4585 (3.80 - 4.80)

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	781	26% 58% 17% • 23%
1	B	781	28% 57% 17% •• 24%
2	C	469	9% 34% 6% 59%
3	D	353	57% 79% 10% 10%

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Mol	Chain	Length	Quality of chain
4	H	150	74% 61% 19% 19%
4	I	150	70% 61% 18% 19%

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
6	PEE	A	811	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15903 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 Metabotropic glycine receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	590	Total	C	N	O	S	0	0
			4602	2982	773	817	30		
1	A	605	Total	C	N	O	S	0	0
			4714	3051	792	840	31		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	776	LEU	-	expression tag	UNP Q5T848
B	777	GLU	-	expression tag	UNP Q5T848
B	778	VAL	-	expression tag	UNP Q5T848
B	779	LEU	-	expression tag	UNP Q5T848
B	780	PHE	-	expression tag	UNP Q5T848
B	781	GLN	-	expression tag	UNP Q5T848
A	776	LEU	-	expression tag	UNP Q5T848
A	777	GLU	-	expression tag	UNP Q5T848
A	778	VAL	-	expression tag	UNP Q5T848
A	779	LEU	-	expression tag	UNP Q5T848
A	780	PHE	-	expression tag	UNP Q5T848
A	781	GLN	-	expression tag	UNP Q5T848

- Molecule 2 is a protein called Isoform 2 of Regulator of G-protein signaling 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	190	Total	C	N	O	S	0	0
			1568	1002	271	286	9		

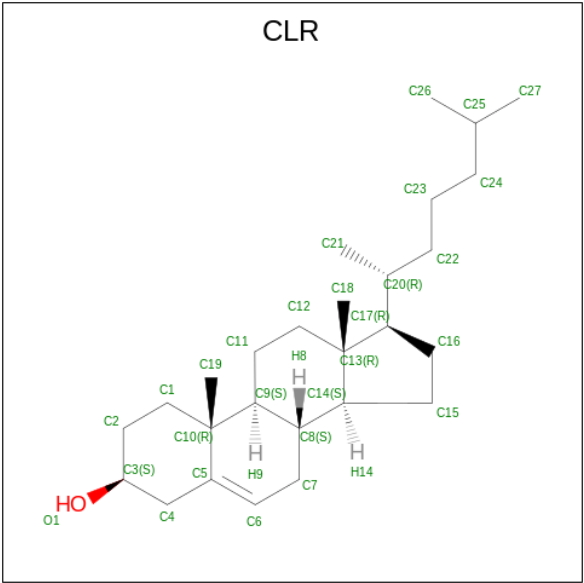
- Molecule 3 is a protein called Guanine nucleotide-binding protein subunit beta-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	316	Total	C	N	O	S	0	0
			2424	1510	423	468	23		

- Molecule 4 is a protein called Nb20.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	121	Total	C	N	O	S	0	0
			941	587	160	190	4		
4	I	121	Total	C	N	O	S	0	0
			940	587	159	190	4		

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



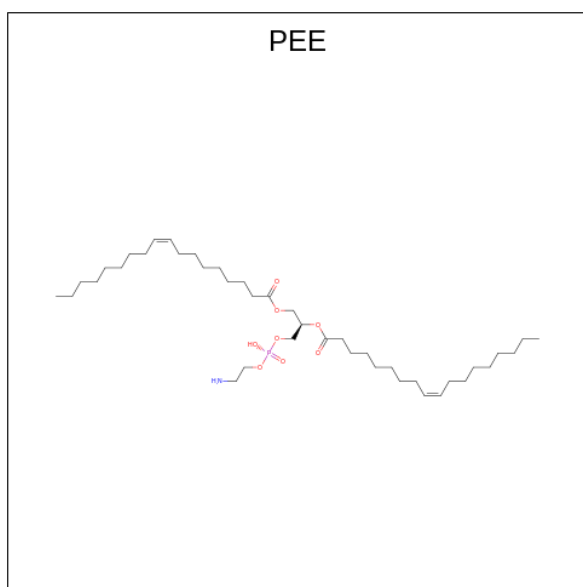
Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27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

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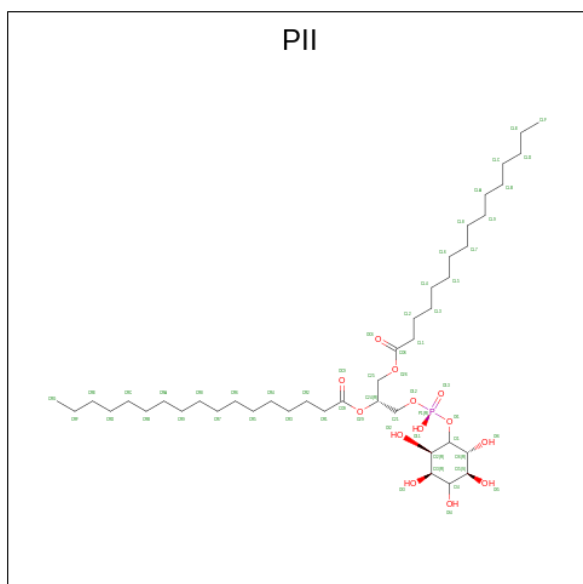
Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	
5	B	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27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

- 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).

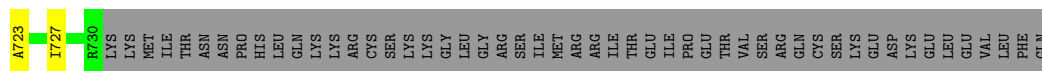


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			49	39	1	8	1	

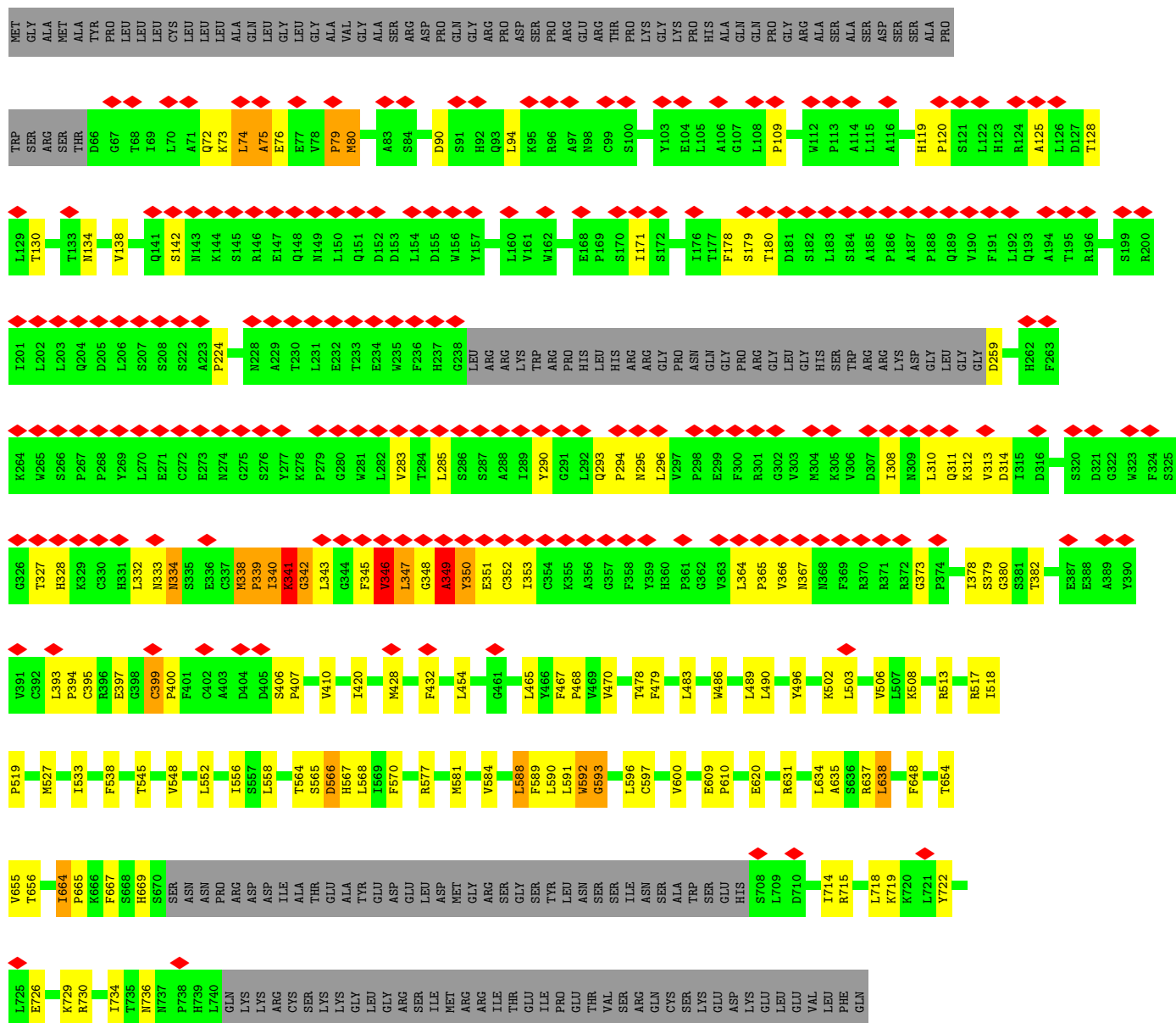
- Molecule 7 is 2-[(HYDROXY{[(2R,3R,5S,6R)-2,3,4,5,6-PENTAHYDROXYCYCLOHEXYL]OXY}PHOSPHORYL)OXY]-1-[(PALMITOYLOXY)METHYL]ETHYL HEPTADECANOATE (CCD ID: PII) (formula: $C_{42}H_{81}O_{13}P$) (labeled as "Ligand of Interest" by depositor).



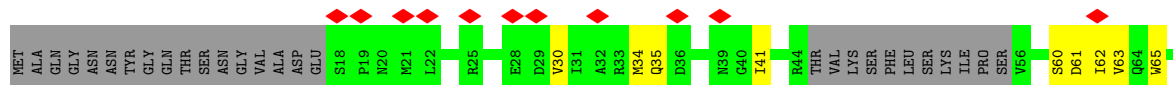
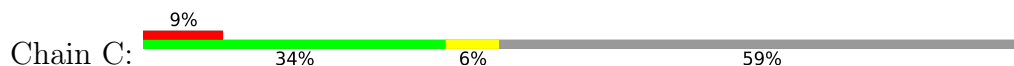
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	O	P	0
			49	35	13	1	

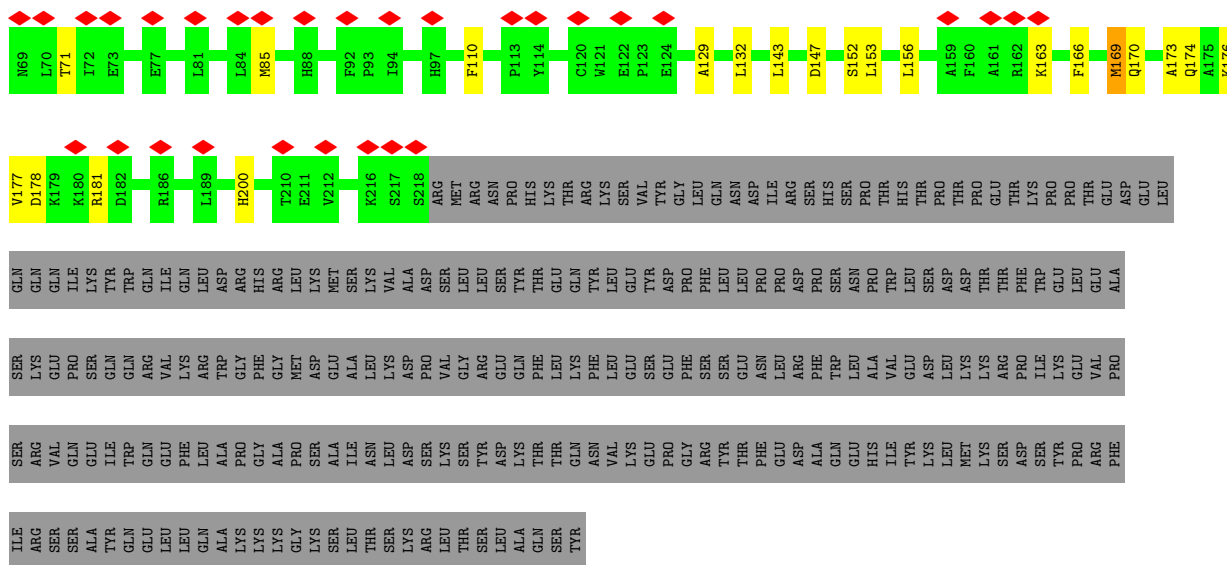


• Molecule 1: Metabotropic glycine receptor

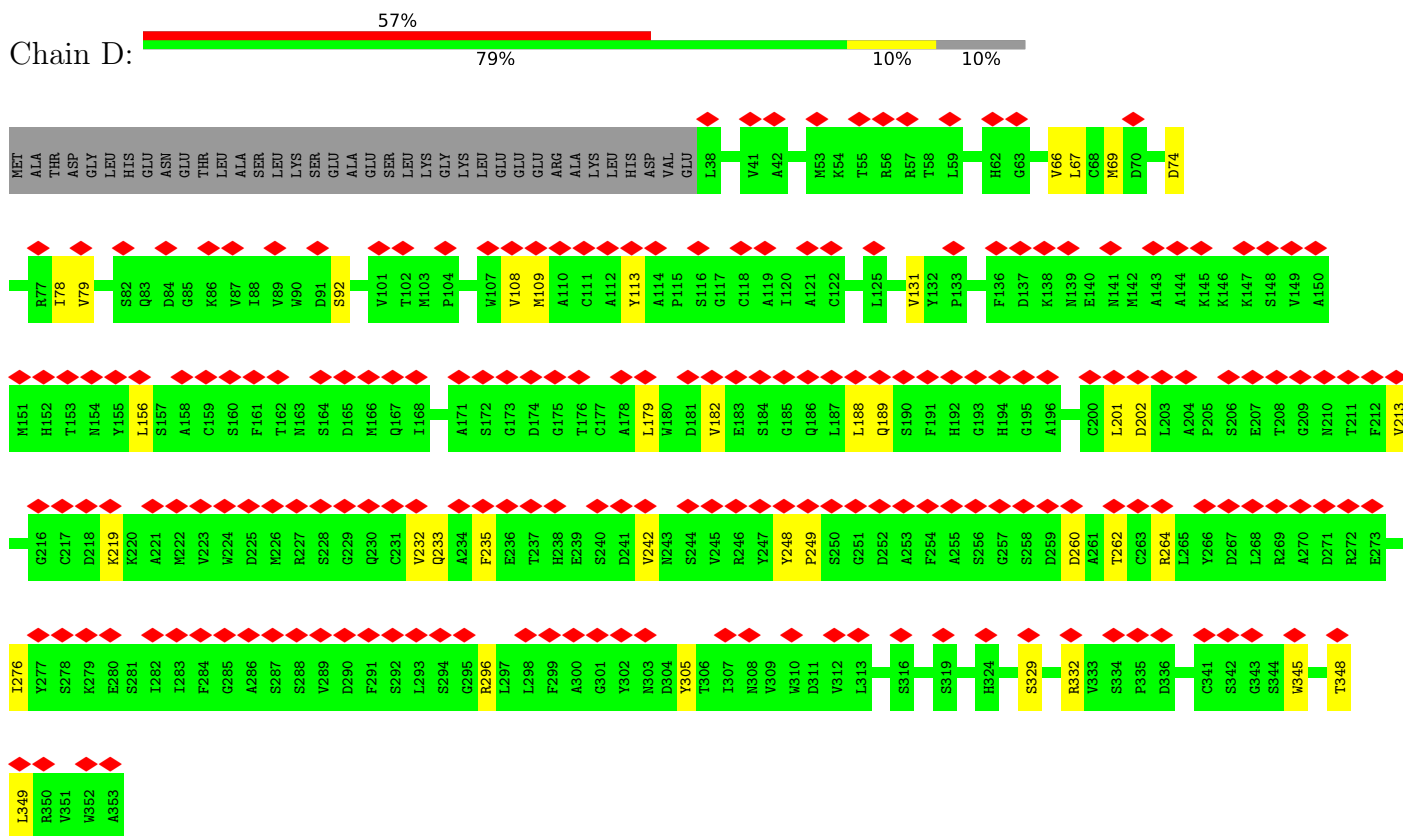


• Molecule 2: Isoform 2 of Regulator of G-protein signaling 7

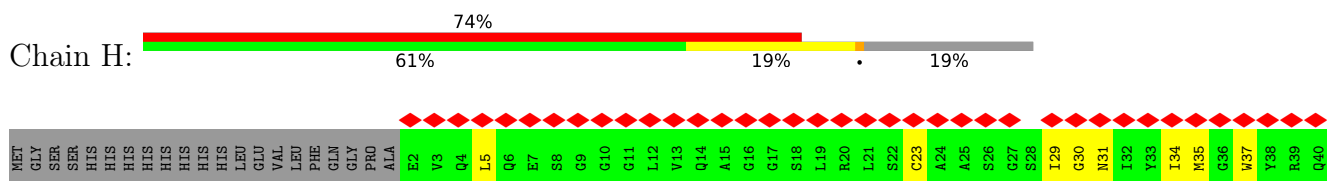




- Molecule 3: Guanine nucleotide-binding protein subunit beta-5

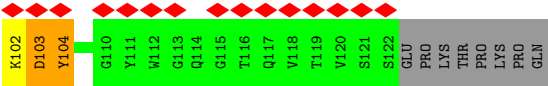
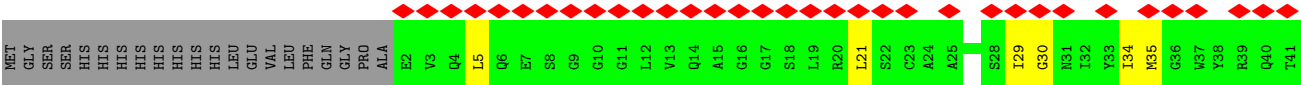


- Molecule 4: Nb20





• Molecule 4: Nb20



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91859	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.474	Depositor
Minimum map value	-0.311	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0457	Depositor
Map size (Å)	296.82, 296.82, 296.82	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.873, 0.873, 0.873	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PII, PEE, 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	0.32	1/4827 (0.0%)	0.70	24/6560 (0.4%)
1	B	0.33	3/4713 (0.1%)	0.64	14/6404 (0.2%)
2	C	0.15	0/1606	0.35	0/2170
3	D	0.12	0/2476	0.34	0/3350
4	H	0.13	0/961	0.37	0/1305
4	I	0.14	0/960	0.37	0/1303
All	All	0.27	4/15543 (0.0%)	0.57	38/21092 (0.2%)

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	5
1	B	0	5
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	79	PRO	N-CA	6.29	1.55	1.47
1	B	535	LEU	CA-C	-5.66	1.45	1.52
1	B	80	MET	N-CA	5.38	1.53	1.46
1	A	342	GLY	N-CA	5.34	1.50	1.45

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	ALA	CA-C-N	-14.19	100.11	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	ALA	C-N-CA	-14.19	100.11	122.67
1	B	78	VAL	CA-C-O	-11.15	105.01	119.95
1	A	338	MET	O-C-N	-9.80	112.40	121.32
1	B	80	MET	CA-C-N	9.26	136.43	120.68
1	B	80	MET	C-N-CA	9.26	136.43	120.68
1	A	348	GLY	N-CA-C	-8.87	102.92	115.43
1	A	350	TYR	CA-C-N	-8.55	105.21	121.54
1	A	350	TYR	C-N-CA	-8.55	105.21	121.54
1	A	80	MET	CA-C-N	8.25	134.70	120.68
1	A	80	MET	C-N-CA	8.25	134.70	120.68
1	B	79	PRO	CB-CA-C	7.75	124.35	111.56
1	B	349	ALA	CA-C-N	-7.75	108.40	122.50
1	B	349	ALA	C-N-CA	-7.75	108.40	122.50
1	B	535	LEU	N-CA-C	-7.28	95.29	110.80
1	A	592	TRP	N-CA-C	-7.14	103.43	112.93
1	B	211	PRO	N-CA-CB	6.86	110.55	103.00
1	B	350	TYR	N-CA-C	6.65	120.74	111.56
1	A	593	GLY	N-CA-C	-6.62	104.75	112.83
1	A	349	ALA	N-CA-CB	-6.50	99.50	110.49
1	B	78	VAL	CA-C-N	6.36	127.79	119.84
1	B	78	VAL	C-N-CA	6.36	127.79	119.84
1	A	224	PRO	N-CA-CB	6.16	110.11	103.33
1	A	339	PRO	N-CA-C	6.14	125.11	112.47
1	B	532	VAL	N-CA-C	-6.13	96.60	109.34
1	A	79	PRO	CA-C-N	5.85	132.71	121.54
1	A	79	PRO	C-N-CA	5.85	132.71	121.54
1	A	342	GLY	CA-C-N	-5.66	112.52	121.86
1	A	342	GLY	C-N-CA	-5.66	112.52	121.86
1	B	80	MET	CA-C-O	-5.58	112.53	120.51
1	A	346	VAL	CA-C-N	-5.50	113.56	121.98
1	A	346	VAL	C-N-CA	-5.50	113.56	121.98
1	A	341	LYS	CA-C-N	5.38	126.89	121.35
1	A	341	LYS	C-N-CA	5.38	126.89	121.35
1	B	78	VAL	CB-CA-C	-5.35	101.63	111.36
1	A	339	PRO	N-CA-CB	-5.31	97.67	103.25
1	A	342	GLY	CA-C-O	-5.24	116.03	121.63
1	A	347	LEU	N-CA-C	-5.18	106.88	114.39

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	338	MET	Mainchain
1	A	346	VAL	Mainchain
1	A	349	ALA	Peptide
1	A	74	LEU	Peptide
1	A	79	PRO	Peptide
1	B	329	LYS	Peptide
1	B	74	LEU	Peptide
1	B	78	VAL	Mainchain
1	B	79	PRO	Mainchain
1	B	80	MET	Mainchain

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	4714	0	4642	139	0
1	B	4602	0	4537	127	0
2	C	1568	0	1542	25	0
3	D	2424	0	2328	27	0
4	H	941	0	891	24	0
4	I	940	0	890	25	0
5	A	280	0	457	10	0
5	B	336	0	552	10	0
6	A	49	0	74	3	0
7	A	49	0	63	8	0
All	All	15903	0	15976	375	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 12.

All (375) 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:340:ILE:O	1:A:341:LYS:HD2	1.41	1.19
1:A:340:ILE:O	1:A:341:LYS:CD	2.02	1.06
1:A:343:LEU:HG	1:A:350:TYR:H	1.25	1.00
1:A:328:HIS:CE1	1:A:341:LYS:HG2	2.08	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:67:LEU:HD11	3:D:109:MET:HE2	1.58	0.85
1:A:332:LEU:HD22	1:A:340:ILE:N	1.94	0.83
1:B:341:LYS:HB2	1:B:349:ALA:HA	1.59	0.82
1:A:332:LEU:HD22	1:A:340:ILE:H	1.46	0.80
1:B:341:LYS:HA	1:B:349:ALA:C	2.08	0.78
1:A:343:LEU:HG	1:A:350:TYR:N	1.97	0.78
1:A:581:MET:HE3	1:A:581:MET:HA	1.67	0.77
4:H:5:LEU:HD22	4:H:23:CYS:SG	2.26	0.75
1:A:341:LYS:HG3	1:A:353:ILE:HG23	1.70	0.73
1:A:343:LEU:HG	1:A:349:ALA:HB3	1.71	0.72
1:A:343:LEU:HB2	1:A:347:LEU:HB2	1.71	0.72
1:A:718:LEU:CD1	2:C:169:MET:HE3	2.20	0.71
1:B:527:MET:HB3	5:B:802:CLR:H6	1.71	0.71
1:B:503:LEU:O	1:B:503:LEU:HD23	1.91	0.70
3:D:69:MET:HE1	3:D:332:ARG:HB2	1.73	0.70
1:A:340:ILE:O	1:A:341:LYS:HD3	1.91	0.70
1:A:454:LEU:HD13	1:A:527:MET:HE1	1.73	0.70
1:B:74:LEU:C	1:B:76:GLU:H	2.00	0.70
5:B:801:CLR:H122	5:B:802:CLR:H112	1.72	0.69
1:A:340:ILE:C	1:A:341:LYS:HD2	2.18	0.69
1:A:349:ALA:HB1	1:A:350:TYR:CD2	2.27	0.69
3:D:264:ARG:CZ	3:D:276:ILE:HG23	2.23	0.69
1:A:343:LEU:HG	1:A:349:ALA:CB	2.24	0.68
3:D:264:ARG:NH1	3:D:276:ILE:HG23	2.10	0.67
1:A:393:LEU:HD12	1:A:393:LEU:O	1.95	0.67
1:A:506:VAL:HG11	1:A:600:VAL:HG13	1.77	0.66
1:B:365:PRO:O	1:B:366:VAL:HG23	1.95	0.66
4:I:54:THR:HG23	4:I:55:VAL:H	1.60	0.66
1:A:341:LYS:C	1:A:349:ALA:O	2.38	0.66
1:B:301:ARG:O	1:B:303:VAL:HG23	1.95	0.65
1:A:343:LEU:CG	1:A:350:TYR:H	2.04	0.65
1:B:341:LYS:CB	1:B:349:ALA:HA	2.27	0.65
1:A:503:LEU:HD23	1:A:503:LEU:O	1.96	0.65
1:B:643:MET:HE2	1:B:643:MET:HA	1.80	0.63
4:I:29:ILE:HG22	4:I:30:GLY:H	1.62	0.63
4:I:73:ILE:HD11	4:I:82:VAL:HG22	1.80	0.63
1:A:328:HIS:ND1	1:A:341:LYS:HG2	2.13	0.63
1:A:342:GLY:C	1:A:351:GLU:H	2.07	0.63
1:A:634:LEU:O	1:A:638:LEU:HD13	1.98	0.63
1:B:308:ILE:HD13	1:B:310:LEU:HD23	1.80	0.62
1:B:350:TYR:O	1:B:351:GLU:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:GLY:O	1:A:351:GLU:N	2.31	0.62
1:B:310:LEU:HD12	1:B:310:LEU:O	2.01	0.61
1:A:332:LEU:HD11	1:A:350:TYR:O	2.00	0.61
1:B:455:LEU:O	1:B:455:LEU:HD23	2.01	0.61
1:A:343:LEU:CG	1:A:349:ALA:HB3	2.30	0.61
2:C:143:LEU:HD23	2:C:143:LEU:O	2.01	0.60
1:A:327:THR:HA	1:A:353:ILE:HD11	1.82	0.60
2:C:166:PHE:HA	2:C:169:MET:HE2	1.83	0.60
1:A:142:SER:HG	4:H:57:TRP:CD1	2.18	0.60
1:A:342:GLY:O	1:A:352:CYS:N	2.34	0.60
1:A:382:THR:O	1:A:393:LEU:HD13	2.02	0.60
1:A:259:ASP:N	1:A:290:TYR:HH	1.99	0.59
3:D:179:LEU:HD22	3:D:188:LEU:HD22	1.83	0.59
1:A:518:ILE:O	1:A:518:ILE:HG23	2.02	0.59
1:B:363:VAL:HG13	1:B:364:LEU:N	2.18	0.59
1:B:363:VAL:HG22	1:B:364:LEU:HG	1.85	0.59
1:B:285:LEU:HD12	1:B:310:LEU:HD21	1.86	0.58
1:B:342:GLY:HA2	1:B:347:LEU:HB3	1.85	0.58
4:H:34:ILE:HG22	4:H:35:MET:H	1.68	0.58
4:H:37:TRP:CD1	4:H:84:LEU:HD22	2.38	0.58
1:B:528:ARG:HG3	5:B:802:CLR:H42	1.85	0.58
1:A:465:LEU:HD23	1:A:465:LEU:O	2.03	0.58
1:B:171:ILE:HG23	1:B:308:ILE:HD11	1.85	0.58
1:B:78:VAL:O	1:B:79:PRO:O	2.21	0.57
1:A:590:LEU:C	1:A:592:TRP:H	2.13	0.57
1:B:455:LEU:HD23	1:B:455:LEU:C	2.29	0.57
1:A:349:ALA:HB1	1:A:350:TYR:CE2	2.40	0.57
3:D:66:VAL:HG11	3:D:349:LEU:HD11	1.85	0.57
1:A:454:LEU:HD12	1:A:454:LEU:O	2.05	0.57
1:A:592:TRP:O	1:A:593:GLY:C	2.48	0.57
1:B:176:ILE:HG22	1:B:306:VAL:HG12	1.87	0.56
4:I:73:ILE:CD1	4:I:82:VAL:HG22	2.35	0.56
1:A:310:LEU:HD12	1:A:310:LEU:O	2.05	0.56
1:A:74:LEU:C	1:A:76:GLU:H	2.13	0.56
3:D:329:SER:HG	3:D:345:TRP:CD1	2.24	0.56
1:A:285:LEU:HD22	1:A:310:LEU:HD11	1.87	0.55
1:A:332:LEU:HD13	1:A:339:PRO:HB2	1.89	0.55
1:A:577:ARG:HD2	5:A:805:CLR:H42	1.88	0.55
4:I:55:VAL:HG13	4:I:56:ARG:H	1.71	0.55
1:A:308:ILE:HD13	1:A:310:LEU:HD23	1.89	0.55
1:B:366:VAL:HG11	1:B:369:PHE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:PRO:HB2	1:B:340:ILE:HG23	1.87	0.54
4:I:34:ILE:HG22	4:I:35:MET:H	1.71	0.54
1:A:490:LEU:HD11	5:A:808:CLR:H271	1.89	0.54
1:B:714:ILE:HG23	1:A:714:ILE:CG2	2.37	0.54
5:B:801:CLR:H72	5:B:812:CLR:H9	1.90	0.54
1:B:510:PHE:CD1	1:B:603:VAL:HG13	2.43	0.54
1:A:600:VAL:HG12	1:A:600:VAL:O	2.07	0.54
1:B:162:TRP:HE1	1:B:201:ILE:HD13	1.73	0.54
1:A:454:LEU:HD11	1:A:502:LYS:HE2	1.89	0.54
1:B:507:LEU:C	1:B:507:LEU:HD23	2.32	0.53
1:A:558:LEU:O	1:A:558:LEU:HD12	2.07	0.53
2:C:34:MET:HE2	2:C:65:TRP:CE3	2.43	0.53
1:B:366:VAL:HG12	1:B:367:ASN:N	2.23	0.53
1:B:507:LEU:HD23	1:B:507:LEU:O	2.07	0.53
1:B:331:HIS:CE1	1:B:352:CYS:SG	3.01	0.53
1:A:138:VAL:HG12	4:H:57:TRP:CZ2	2.44	0.53
1:A:332:LEU:HB3	1:A:339:PRO:HB2	1.91	0.53
1:B:341:LYS:HA	1:B:349:ALA:O	2.08	0.52
1:A:486:TRP:HE1	1:A:545:THR:HG21	1.74	0.52
3:D:67:LEU:HD13	3:D:108:VAL:O	2.09	0.52
1:B:365:PRO:O	1:B:366:VAL:CG2	2.58	0.52
1:A:588:LEU:O	1:A:589:PHE:C	2.52	0.52
1:A:313:VAL:HG12	1:A:313:VAL:O	2.08	0.52
1:A:327:THR:HG22	1:A:327:THR:O	2.09	0.52
1:A:454:LEU:HD13	1:A:527:MET:CE	2.40	0.52
1:A:527:MET:HE2	1:A:527:MET:N	2.25	0.52
2:C:176:LYS:HD3	2:C:176:LYS:C	2.35	0.52
1:A:343:LEU:H	1:A:347:LEU:H	1.57	0.51
1:A:483:LEU:O	1:A:483:LEU:HD23	2.10	0.51
1:B:532:VAL:HG21	7:A:812:PII:H252	1.92	0.51
1:B:78:VAL:O	1:B:81:ASP:OD1	2.29	0.51
1:B:353:ILE:HG23	1:B:354:CYS:N	2.26	0.51
4:I:34:ILE:HG22	4:I:35:MET:N	2.26	0.51
4:I:48:LEU:O	4:I:67:VAL:HG22	2.10	0.51
4:H:34:ILE:HG22	4:H:35:MET:N	2.25	0.51
1:A:73:LYS:C	1:A:75:ALA:N	2.68	0.51
4:H:50:ALA:CA	4:H:67:VAL:HG11	2.41	0.51
1:A:581:MET:HE3	1:A:581:MET:CA	2.38	0.51
1:B:539:TRP:O	1:B:542:ILE:HG22	2.11	0.50
4:I:50:ALA:HB2	4:I:67:VAL:HG21	1.94	0.50
1:B:535:LEU:O	1:B:536:VAL:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:55:VAL:HG13	4:I:56:ARG:N	2.26	0.50
1:B:375:ASP:O	1:B:376:GLN:HG3	2.12	0.50
1:B:378:ILE:O	1:B:378:ILE:HG22	2.11	0.50
2:C:170:GLN:O	2:C:174:GLN:HG3	2.10	0.50
3:D:202:ASP:OD2	3:D:213:VAL:HG12	2.11	0.50
1:A:293:GLN:N	1:A:294:PRO:CD	2.75	0.50
1:A:729:LYS:O	1:A:734:ILE:HD12	2.12	0.50
3:D:188:LEU:HD23	3:D:189:GLN:HB2	1.93	0.50
1:B:495:VAL:HG23	1:B:496:TYR:N	2.27	0.50
4:I:21:LEU:HD12	4:I:86:MET:HE3	1.94	0.50
1:A:590:LEU:C	1:A:592:TRP:N	2.70	0.50
1:A:734:ILE:HG23	1:A:736:ASN:H	1.76	0.50
2:C:71:THR:HG23	2:C:71:THR:O	2.13	0.49
1:A:399:CYS:SG	1:A:400:PRO:HD3	2.53	0.49
1:B:328:HIS:O	1:B:329:LYS:C	2.56	0.49
4:I:43:GLY:N	4:I:44:PRO:HD3	2.28	0.49
1:B:638:LEU:HD22	1:B:643:MET:HE3	1.95	0.49
1:B:293:GLN:N	1:B:294:PRO:CD	2.76	0.49
1:B:345:PHE:CD2	1:B:346:VAL:HG22	2.47	0.49
1:A:467:PHE:N	1:A:468:PRO:CD	2.76	0.49
3:D:262:THR:HB	3:D:264:ARG:NH1	2.28	0.49
1:B:542:ILE:HD11	5:B:804:CLR:H213	1.95	0.49
1:B:600:VAL:O	1:B:600:VAL:HG12	2.12	0.48
1:B:376:GLN:HB2	1:B:394:PRO:HB3	1.95	0.48
1:A:631:ARG:O	1:A:635:ALA:HB2	2.14	0.48
1:B:651:THR:O	1:B:655:VAL:HG12	2.14	0.48
1:A:664:ILE:N	1:A:665:PRO:CD	2.77	0.48
1:A:73:LYS:O	1:A:75:ALA:N	2.47	0.48
3:D:66:VAL:HG21	3:D:349:LEU:CD1	2.44	0.48
4:I:58:THR:O	4:I:59:LYS:C	2.57	0.48
1:A:581:MET:HA	1:A:581:MET:CE	2.42	0.48
1:B:411:GLN:OE1	1:B:411:GLN:N	2.47	0.48
1:B:79:PRO:O	1:B:81:ASP:N	2.38	0.47
4:I:103:ASP:O	4:I:104:TYR:CD2	2.67	0.47
1:B:467:PHE:HA	1:B:470:VAL:HG22	1.95	0.47
1:A:332:LEU:HD21	1:A:340:ILE:C	2.40	0.47
4:H:47:GLU:C	4:H:48:LEU:HD12	2.40	0.47
1:B:384:ASP:HB3	1:B:394:PRO:HA	1.97	0.47
1:B:370:ARG:HE	1:B:375:ASP:HB3	1.80	0.47
7:A:812:PII:HR72	7:A:812:PII:HR41	1.59	0.47
3:D:67:LEU:HD11	3:D:109:MET:CE	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:MET:HE2	1:B:525:ARG:HG3	1.96	0.47
1:B:534:LEU:HD23	1:B:534:LEU:HA	1.69	0.47
1:A:109:PRO:HG3	1:A:347:LEU:HG	1.96	0.47
1:A:332:LEU:HB3	1:A:339:PRO:CB	2.44	0.47
1:B:587:PHE:CD1	1:B:587:PHE:C	2.92	0.47
1:B:626:ILE:HG22	1:B:630:ILE:CD1	2.45	0.47
1:B:638:LEU:CD2	1:B:643:MET:HE3	2.44	0.47
1:B:74:LEU:C	1:B:76:GLU:N	2.67	0.47
1:A:730:ARG:HG3	2:C:181:ARG:NH2	2.30	0.47
2:C:129:ALA:HB2	2:C:156:LEU:HD23	1.95	0.47
1:B:330:CYS:O	1:B:331:HIS:C	2.57	0.46
7:A:812:PII:HL41	7:A:812:PII:HL11	1.76	0.46
4:H:82:VAL:HG23	4:H:82:VAL:O	2.14	0.46
1:B:410:VAL:HG22	1:B:568:LEU:HD13	1.96	0.46
1:A:178:PHE:O	1:A:180:THR:N	2.48	0.46
4:H:29:ILE:HG23	4:H:30:GLY:N	2.30	0.46
7:A:812:PII:H24	7:A:812:PII:O13	2.15	0.46
3:D:219:LYS:O	3:D:219:LYS:CG	2.63	0.46
4:H:35:MET:HE3	4:H:37:TRP:HD1	1.80	0.46
1:B:115:LEU:HD23	1:B:346:VAL:HG23	1.98	0.46
1:A:517:ARG:HB3	1:A:519:PRO:HD3	1.96	0.46
1:B:278:LYS:N	1:B:279:PRO:HD3	2.31	0.46
3:D:296:ARG:O	3:D:296:ARG:HD3	2.16	0.46
1:B:73:LYS:C	1:B:75:ALA:N	2.73	0.46
1:A:130:THR:O	1:A:134:ASN:OD1	2.32	0.46
1:A:407:PRO:HA	1:A:567:HIS:O	2.15	0.46
5:A:804:CLR:H161	5:A:805:CLR:H71	1.98	0.46
2:C:35:GLN:OE1	2:C:110:PHE:CE2	2.69	0.46
4:H:43:GLY:N	4:H:44:PRO:HD3	2.31	0.46
4:H:49:VAL:C	4:H:67:VAL:HG11	2.41	0.46
1:B:76:GLU:O	1:B:79:PRO:HD3	2.16	0.46
1:A:365:PRO:O	1:A:366:VAL:HG23	2.15	0.46
1:A:552:LEU:HA	1:A:556:ILE:O	2.15	0.46
1:B:72:GLN:O	1:B:75:ALA:HB2	2.16	0.45
1:B:503:LEU:HD22	1:B:596:LEU:HB3	1.97	0.45
5:B:802:CLR:H162	5:B:802:CLR:H221	1.39	0.45
1:A:125:ALA:CB	1:A:310:LEU:HD13	2.46	0.45
1:B:620:GLU:CD	1:B:620:GLU:O	2.59	0.45
1:A:533:ILE:HG23	6:A:811:PEE:H35	1.98	0.45
1:B:329:LYS:O	1:B:330:CYS:HB3	2.15	0.45
1:B:376:GLN:CB	1:B:394:PRO:HB3	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ILE:HD12	1:B:453:ILE:H	1.82	0.45
1:B:662:LEU:HD12	1:B:662:LEU:N	2.31	0.45
1:A:669:HIS:CE1	5:A:803:CLR:H21	2.51	0.45
1:B:530:LEU:HD12	1:B:530:LEU:HA	1.73	0.45
1:B:308:ILE:CD1	1:B:310:LEU:HD23	2.45	0.45
5:B:802:CLR:H213	5:B:802:CLR:H232	1.72	0.45
1:A:342:GLY:HA2	1:A:349:ALA:N	2.31	0.45
1:B:337:CYS:HB3	1:B:392:CYS:HB2	1.86	0.45
1:A:90:ASP:OD2	1:A:94:LEU:HD21	2.16	0.45
1:A:410:VAL:HG11	1:A:570:PHE:HB3	1.98	0.45
1:A:637:ARG:O	1:A:638:LEU:C	2.60	0.45
3:D:345:TRP:CD1	3:D:345:TRP:N	2.85	0.45
3:D:79:VAL:HG11	3:D:113:TYR:HD1	1.82	0.45
1:B:77:GLU:C	1:B:79:PRO:HD3	2.42	0.45
1:B:630:ILE:HG23	1:B:634:LEU:HD13	1.98	0.45
1:A:74:LEU:C	1:A:76:GLU:N	2.73	0.45
1:A:428:MET:HE1	1:A:470:VAL:HG21	1.99	0.45
1:A:489:LEU:H	1:A:489:LEU:HD12	1.82	0.45
2:C:30:VAL:HG21	2:C:85:MET:CE	2.47	0.45
2:C:41:ILE:HD11	2:C:61:ASP:HB3	1.99	0.45
1:B:525:ARG:HA	1:B:525:ARG:HD3	1.74	0.45
1:A:478:THR:O	1:A:479:PHE:HB3	2.16	0.44
2:C:132:LEU:HD23	2:C:153:LEU:HD13	1.98	0.44
4:I:54:THR:HG23	4:I:55:VAL:N	2.30	0.44
1:A:564:THR:O	1:A:568:LEU:HB2	2.18	0.44
2:C:200:HIS:O	2:C:200:HIS:ND1	2.50	0.44
1:A:378:ILE:HG22	1:A:378:ILE:O	2.17	0.44
1:A:379:SER:C	1:A:394:PRO:HD2	2.42	0.44
2:C:174:GLN:O	2:C:178:ASP:OD1	2.36	0.44
1:B:382:THR:OG1	1:B:393:LEU:HB3	2.17	0.44
1:A:171:ILE:CD1	1:A:308:ILE:HD11	2.46	0.44
1:B:178:PHE:O	1:B:180:THR:N	2.50	0.44
3:D:305:TYR:N	3:D:305:TYR:CD1	2.86	0.44
1:B:278:LYS:N	1:B:279:PRO:CD	2.81	0.44
1:B:623:ILE:HD12	1:B:654:THR:OG1	2.17	0.44
7:A:812:PII:HR61	7:A:812:PII:HR91	1.65	0.44
4:H:52:ILE:O	4:H:53:ARG:HB2	2.17	0.44
4:I:5:LEU:HD23	4:I:5:LEU:H	1.83	0.44
1:B:330:CYS:HB2	1:B:352:CYS:HA	1.98	0.44
1:B:327:THR:O	1:B:328:HIS:C	2.60	0.43
1:B:715:ARG:O	1:B:715:ARG:HD3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ASN:O	1:A:334:ASN:C	2.61	0.43
1:A:366:VAL:HG12	1:A:367:ASN:N	2.33	0.43
5:A:804:CLR:H71	5:A:805:CLR:H41	1.99	0.43
1:B:187:ALA:N	1:B:188:PRO:HD3	2.32	0.43
1:B:328:HIS:CD2	1:B:328:HIS:H	2.35	0.43
1:B:327:THR:N	1:B:365:PRO:HG3	2.33	0.43
1:A:503:LEU:HD23	1:A:503:LEU:C	2.44	0.43
2:C:147:ASP:C	2:C:147:ASP:OD1	2.61	0.43
3:D:78:ILE:HD12	3:D:92:SER:HB3	2.00	0.43
1:A:334:ASN:HB2	1:A:366:VAL:HG21	2.00	0.43
4:I:35:MET:HE1	4:I:52:ILE:HD11	2.01	0.43
1:B:637:ARG:O	1:B:638:LEU:O	2.36	0.43
1:A:328:HIS:ND1	1:A:341:LYS:CG	2.81	0.43
1:A:506:VAL:HG11	1:A:600:VAL:CG1	2.47	0.43
3:D:232:VAL:HG23	3:D:233:GLN:CD	2.44	0.43
4:H:54:THR:CG2	4:H:59:LYS:HA	2.48	0.43
1:B:638:LEU:O	1:B:639:GLN:HG3	2.18	0.43
1:B:714:ILE:HG23	1:A:714:ILE:HG21	2.00	0.43
1:A:517:ARG:O	1:A:518:ILE:C	2.61	0.43
1:A:577:ARG:HH11	5:A:805:CLR:H42	1.83	0.43
5:A:805:CLR:H222	5:A:805:CLR:H162	1.66	0.43
2:C:163:LYS:O	2:C:163:LYS:CG	2.67	0.43
3:D:248:TYR:CD1	3:D:249:PRO:HD2	2.53	0.43
1:A:600:VAL:O	1:A:600:VAL:CG1	2.66	0.43
1:B:723:ALA:O	1:B:727:ILE:HG13	2.19	0.43
1:A:395:CYS:SG	1:A:395:CYS:O	2.76	0.43
1:B:428:MET:HE3	1:B:466:TYR:HB3	2.01	0.43
1:A:490:LEU:HG	5:A:808:CLR:H261	2.01	0.43
4:H:70:ARG:O	4:H:71:PHE:C	2.62	0.43
4:I:52:ILE:CG2	4:I:73:ILE:HG23	2.49	0.43
1:B:177:THR:HG23	1:B:305:LYS:O	2.19	0.42
1:B:342:GLY:H	1:B:351:GLU:H	1.65	0.42
1:B:345:PHE:CE2	1:B:346:VAL:HG22	2.53	0.42
1:B:448:ARG:HA	1:B:448:ARG:NE	2.34	0.42
1:A:715:ARG:O	1:A:719:LYS:HG3	2.19	0.42
6:A:811:PEE:H38	7:A:812:PII:HL	2.01	0.42
7:A:812:PII:HR92	7:A:812:PII:HH1	1.23	0.42
4:H:46:ARG:O	4:H:47:GLU:HB2	2.19	0.42
4:I:102:LYS:O	4:I:103:ASP:OD2	2.36	0.42
6:A:811:PEE:H12	7:A:812:PII:OI3	2.18	0.42
2:C:152:SER:O	2:C:156:LEU:HD13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLY:HA2	1:A:397:GLU:HB3	2.02	0.42
1:A:513:ARG:O	1:A:513:ARG:HG3	2.19	0.42
5:A:805:CLR:H191	5:A:805:CLR:H8	1.86	0.42
1:A:283:VAL:HG22	1:A:311:GLN:HB2	2.01	0.42
4:I:70:ARG:O	4:I:71:PHE:C	2.62	0.42
1:B:460:PHE:CD1	1:B:460:PHE:C	2.97	0.42
1:A:119:HIS:HB2	1:A:120:PRO:HD3	2.02	0.42
1:B:347:LEU:HA	1:B:347:LEU:HD12	1.80	0.42
5:B:802:CLR:H182	5:B:802:CLR:H8	1.74	0.42
1:A:295:ASN:C	1:A:296:LEU:HD12	2.45	0.42
1:A:341:LYS:HG3	1:A:353:ILE:CG2	2.44	0.42
1:B:530:LEU:O	1:B:532:VAL:N	2.48	0.42
1:A:345:PHE:O	1:A:346:VAL:CG2	2.68	0.42
4:H:31:ASN:CG	4:H:31:ASN:O	2.63	0.42
4:H:50:ALA:HB2	4:H:67:VAL:HB	2.02	0.42
4:I:46:ARG:O	4:I:47:GLU:HG2	2.20	0.42
1:B:193:GLN:HA	1:B:201:ILE:HD12	2.02	0.42
1:A:719:LYS:HG2	2:C:173:ALA:HB1	2.01	0.42
4:H:35:MET:HE1	4:H:73:ILE:HD13	2.02	0.42
1:B:645:MET:SD	1:B:646:LEU:N	2.93	0.41
1:A:125:ALA:O	1:A:128:THR:HG22	2.20	0.41
1:A:420:ILE:HD12	1:A:648:PHE:CD2	2.55	0.41
4:H:54:THR:O	4:H:55:VAL:HB	2.20	0.41
1:B:379:SER:HB2	1:B:394:PRO:HD3	2.03	0.41
5:B:802:CLR:H183	5:B:802:CLR:H20	1.77	0.41
1:A:171:ILE:HD12	1:A:308:ILE:HD11	2.02	0.41
1:A:552:LEU:HD12	1:A:552:LEU:C	2.45	0.41
1:A:722:TYR:CG	2:C:174:GLN:HG2	2.54	0.41
1:B:267:PRO:O	1:B:268:PRO:C	2.63	0.41
1:A:343:LEU:CD1	1:A:349:ALA:CB	2.98	0.41
4:H:58:THR:O	4:H:59:LYS:C	2.63	0.41
1:B:311:GLN:O	1:B:312:LYS:C	2.62	0.41
1:B:370:ARG:HG3	1:B:373:GLY:O	2.20	0.41
1:B:623:ILE:HG13	1:B:624:SER:N	2.35	0.41
5:B:812:CLR:H211	5:B:812:CLR:H232	1.64	0.41
1:A:655:VAL:HG13	1:A:656:THR:N	2.35	0.41
1:A:715:ARG:HG2	2:C:169:MET:SD	2.60	0.41
3:D:74:ASP:O	3:D:74:ASP:CG	2.64	0.41
3:D:131:VAL:HG21	3:D:182:VAL:HG23	2.01	0.41
3:D:242:VAL:O	3:D:242:VAL:HG23	2.20	0.41
4:H:54:THR:HG21	4:H:57:TRP:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:TYR:O	1:B:442:ARG:HB2	2.20	0.41
1:A:72:GLN:O	1:A:75:ALA:HB2	2.21	0.41
3:D:109:MET:HG3	3:D:156:LEU:O	2.20	0.41
1:B:284:THR:HA	1:B:308:ILE:O	2.21	0.41
1:B:335:SER:C	1:B:337:CYS:N	2.79	0.41
1:B:366:VAL:CG1	1:B:367:ASN:N	2.83	0.41
1:B:401:PHE:CD1	1:B:401:PHE:C	2.98	0.41
1:A:565:SER:O	1:A:566:ASP:OD1	2.38	0.41
1:A:609:GLU:HB3	1:A:610:PRO:HD3	2.02	0.41
2:C:60:SER:O	2:C:63:VAL:HG22	2.20	0.41
3:D:348:THR:C	3:D:349:LEU:HD12	2.46	0.41
1:B:161:VAL:HG21	1:B:176:ILE:HG12	2.02	0.41
1:B:301:ARG:HG3	1:B:302:GLY:H	1.85	0.41
1:B:311:GLN:HG2	1:B:313:VAL:HG22	2.03	0.41
1:B:328:HIS:N	1:B:365:PRO:HG2	2.36	0.41
1:B:455:LEU:C	1:B:455:LEU:CD2	2.94	0.41
1:A:347:LEU:HA	1:A:347:LEU:HD23	1.49	0.41
1:A:364:LEU:O	1:A:364:LEU:HG	2.21	0.41
1:A:496:TYR:CZ	1:A:620:GLU:CD	2.99	0.41
1:A:722:TYR:HD2	2:C:177:VAL:HG11	1.85	0.41
1:B:157:TYR:O	1:B:161:VAL:HG23	2.20	0.41
1:B:420:ILE:HG23	1:B:648:PHE:CD1	2.56	0.41
1:B:486:TRP:HE1	1:B:545:THR:CG2	2.34	0.41
1:A:130:THR:O	1:A:134:ASN:CG	2.64	0.41
1:A:312:LYS:C	1:A:314:ASP:H	2.29	0.41
5:A:805:CLR:H8	5:A:805:CLR:H182	1.72	0.40
1:B:119:HIS:HB2	1:B:120:PRO:HD3	2.03	0.40
1:B:193:GLN:HG3	1:B:201:ILE:HD13	2.03	0.40
1:A:637:ARG:O	1:A:638:LEU:O	2.39	0.40
1:B:539:TRP:NE1	1:A:581:MET:HE2	2.36	0.40
2:C:62:ILE:HD12	2:C:62:ILE:H	1.85	0.40
4:H:63:TYR:CD1	4:H:67:VAL:HG23	2.56	0.40
4:I:5:LEU:HD23	4:I:5:LEU:N	2.36	0.40
1:A:364:LEU:HD13	1:A:373:GLY:H	1.86	0.40
2:C:30:VAL:HG21	2:C:85:MET:HE2	2.04	0.40
3:D:201:LEU:HD12	3:D:201:LEU:C	2.47	0.40
4:I:67:VAL:O	4:I:67:VAL:HG12	2.22	0.40
4:I:103:ASP:O	4:I:103:ASP:CG	2.64	0.40
1:B:161:VAL:HG22	1:B:176:ILE:HG23	2.04	0.40
1:B:341:LYS:CA	1:B:349:ALA:HA	2.51	0.40
1:B:363:VAL:HG13	1:B:364:LEU:H	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:TYR:O	1:A:726:GLU:HB2	2.20	0.40
4:I:52:ILE:HG23	4:I:73:ILE:HG23	2.02	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	595/781 (76%)	467 (78%)	118 (20%)	10 (2%)	7	35
1	B	578/781 (74%)	453 (78%)	114 (20%)	11 (2%)	6	32
2	C	186/469 (40%)	171 (92%)	15 (8%)	0	100	100
3	D	314/353 (89%)	304 (97%)	10 (3%)	0	100	100
4	H	119/150 (79%)	84 (71%)	34 (29%)	1 (1%)	16	52
4	I	119/150 (79%)	86 (72%)	30 (25%)	3 (2%)	4	26
All	All	1911/2684 (71%)	1565 (82%)	321 (17%)	25 (1%)	12	41

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	75	ALA
1	B	79	PRO
1	B	638	LEU
1	A	75	ALA
1	A	399	CYS
1	A	406	SER
1	A	638	LEU
1	B	179	SER
1	A	80	MET
1	A	179	SER

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Mol	Chain	Res	Type
1	A	341	LYS
1	A	566	ASP
4	H	55	VAL
1	A	340	ILE
4	I	77	ASP
4	I	104	TYR
1	B	210	ALA
1	B	351	GLU
1	B	80	MET
1	B	414	LYS
1	B	556	ILE
1	A	334	ASN
4	I	53	ARG
1	B	78	VAL
1	B	532	VAL

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	502/677 (74%)	489 (97%)	13 (3%)	40	60
1	B	490/677 (72%)	479 (98%)	11 (2%)	45	64
2	C	169/425 (40%)	168 (99%)	1 (1%)	78	80
3	D	264/295 (90%)	262 (99%)	2 (1%)	73	77
4	H	100/126 (79%)	100 (100%)	0	100	100
4	I	99/126 (79%)	98 (99%)	1 (1%)	68	76
All	All	1624/2326 (70%)	1596 (98%)	28 (2%)	52	67

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	74	LEU
1	B	80	MET
1	B	123	HIS

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Mol	Chain	Res	Type
1	B	330	CYS
1	B	532	VAL
1	B	533	ILE
1	B	534	LEU
1	B	535	LEU
1	B	538	PHE
1	B	597	CYS
1	B	619	ASN
1	A	341	LYS
1	A	432	PHE
1	A	508	LYS
1	A	538	PHE
1	A	548	VAL
1	A	584	VAL
1	A	588	LEU
1	A	591	LEU
1	A	596	LEU
1	A	597	CYS
1	A	654	THR
1	A	664	ILE
1	A	667	PHE
2	C	169	MET
3	D	235	PHE
3	D	260	ASP
4	I	103	ASP

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

Mol	Chain	Res	Type
1	B	92	HIS
1	B	143	ASN
1	B	652	HIS
1	B	669	HIS
1	A	331	HIS
1	A	561	GLN
1	A	571	ASN
2	C	97	HIS
2	C	174	GLN
4	I	14	GLN

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 ⓘ

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	CLR	B	810	-	31,31,31	0.35	0	48,48,48	0.61	0
5	CLR	A	802	-	31,31,31	0.36	0	48,48,48	1.73	4 (8%)
5	CLR	A	804	-	31,31,31	0.35	0	48,48,48	0.79	0
5	CLR	A	803	-	31,31,31	0.39	0	48,48,48	0.89	2 (4%)
5	CLR	B	801	-	31,31,31	0.88	2 (6%)	48,48,48	1.32	4 (8%)
5	CLR	B	807	-	31,31,31	0.38	0	48,48,48	0.78	1 (2%)
6	PEE	A	811	-	48,48,50	0.89	2 (4%)	51,53,55	1.12	3 (5%)
5	CLR	A	809	-	31,31,31	0.37	0	48,48,48	0.66	0
5	CLR	B	803	-	31,31,31	0.36	0	48,48,48	0.85	1 (2%)
5	CLR	A	808	-	31,31,31	0.39	0	48,48,48	0.66	0
5	CLR	A	806	-	31,31,31	0.36	0	48,48,48	0.69	0
5	CLR	B	805	-	31,31,31	0.36	0	48,48,48	0.56	0
5	CLR	A	810	-	31,31,31	0.36	0	48,48,48	0.65	0
5	CLR	B	802	-	31,31,31	0.91	1 (3%)	48,48,48	1.95	11 (22%)
7	PII	A	812	-	49,49,56	1.30	7 (14%)	59,61,68	0.99	4 (6%)
5	CLR	A	805	-	31,31,31	1.05	3 (9%)	48,48,48	1.61	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CLR	B	811	-	31,31,31	0.37	0	48,48,48	0.52	0
5	CLR	B	804	-	31,31,31	0.39	0	48,48,48	0.84	1 (2%)
5	CLR	B	809	-	31,31,31	0.35	0	48,48,48	0.64	0
5	CLR	A	801	-	31,31,31	0.36	0	48,48,48	1.99	5 (10%)
5	CLR	B	812	-	31,31,31	0.94	1 (3%)	48,48,48	1.40	7 (14%)
5	CLR	B	808	-	31,31,31	0.40	0	48,48,48	0.61	1 (2%)
5	CLR	A	807	-	31,31,31	0.37	0	48,48,48	1.61	4 (8%)
5	CLR	B	806	-	31,31,31	0.40	0	48,48,48	0.64	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
5	CLR	B	810	-	-	6/10/68/68	0/4/4/4
5	CLR	A	802	-	-	8/10/68/68	0/4/4/4
5	CLR	A	804	-	-	6/10/68/68	0/4/4/4
5	CLR	A	803	-	-	6/10/68/68	0/4/4/4
5	CLR	B	807	-	-	6/10/68/68	0/4/4/4
5	CLR	B	801	-	-	7/10/68/68	0/4/4/4
6	PEE	A	811	-	1/1/4/8	21/52/52/54	-
5	CLR	A	809	-	-	7/10/68/68	0/4/4/4
5	CLR	B	803	-	-	6/10/68/68	0/4/4/4
5	CLR	A	808	-	-	4/10/68/68	0/4/4/4
5	CLR	A	806	-	-	1/10/68/68	0/4/4/4
5	CLR	B	805	-	-	3/10/68/68	0/4/4/4
5	CLR	A	810	-	-	6/10/68/68	0/4/4/4
5	CLR	B	802	-	-	10/10/68/68	0/4/4/4
7	PII	A	812	-	-	22/44/68/75	0/1/1/1
5	CLR	A	805	-	-	5/10/68/68	0/4/4/4
5	CLR	B	811	-	-	4/10/68/68	0/4/4/4
5	CLR	B	804	-	-	6/10/68/68	0/4/4/4
5	CLR	B	809	-	-	0/10/68/68	0/4/4/4
5	CLR	A	801	-	-	6/10/68/68	0/4/4/4
5	CLR	B	812	-	-	9/10/68/68	0/4/4/4
5	CLR	B	808	-	-	8/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLR	A	807	-	-	5/10/68/68	0/4/4/4
5	CLR	B	806	-	-	6/10/68/68	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	811	PEE	C18-C19	3.62	1.52	1.31
6	A	811	PEE	C39-C38	3.61	1.52	1.31
7	A	812	PII	CRB-CRA	-3.09	1.34	1.51
7	A	812	PII	CRE-CRD	-3.09	1.34	1.51
7	A	812	PII	CR8-CR7	-3.01	1.34	1.51
5	A	805	CLR	C10-C9	-2.94	1.51	1.56
7	A	812	PII	O29-CO9	2.84	1.42	1.34
5	B	801	CLR	C10-C9	-2.83	1.51	1.56
5	B	812	CLR	C10-C9	-2.66	1.51	1.56
7	A	812	PII	O26-CO6	2.65	1.41	1.33
5	A	805	CLR	C13-C14	-2.51	1.50	1.55
5	B	802	CLR	C13-C14	-2.35	1.50	1.55
7	A	812	PII	O29-C24	-2.30	1.40	1.46
7	A	812	PII	P1-OI1	2.23	1.66	1.60
5	B	801	CLR	C13-C14	-2.07	1.51	1.55
5	A	805	CLR	C13-C17	-2.01	1.51	1.55

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	801	CLR	C7-C8-C9	9.31	120.99	109.71
5	A	802	CLR	C13-C17-C20	7.05	130.53	119.49
5	B	802	CLR	C8-C7-C6	-6.78	102.99	112.73
5	A	801	CLR	C7-C8-C14	6.35	120.11	110.91
5	A	807	CLR	C16-C17-C20	6.15	121.67	112.15
5	A	807	CLR	C13-C17-C20	5.96	128.82	119.49
5	A	802	CLR	C16-C17-C20	5.77	121.08	112.15
6	A	811	PEE	C3-C2-C1	5.54	124.89	111.79
5	A	802	CLR	C17-C13-C14	-5.02	94.12	100.07
5	B	802	CLR	C3-C4-C5	-4.85	103.80	112.03
5	A	801	CLR	C14-C8-C9	4.63	115.29	109.09
5	B	802	CLR	C13-C14-C8	-4.36	107.92	114.38
5	A	805	CLR	C13-C14-C8	-4.34	107.95	114.38
5	A	807	CLR	C17-C13-C14	-4.20	95.10	100.07
5	A	805	CLR	C13-C17-C20	-4.16	112.97	119.49
5	B	802	CLR	C13-C17-C20	-3.89	113.39	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	801	CLR	C21-C20-C17	3.80	118.74	112.92
5	B	804	CLR	C16-C17-C20	3.72	117.90	112.15
5	B	812	CLR	C4-C5-C10	3.57	121.16	116.42
7	A	812	PII	O29-CO9-CR1	3.42	118.88	111.50
5	A	805	CLR	C4-C5-C10	3.30	120.80	116.42
5	B	802	CLR	C7-C6-C5	-3.17	119.21	125.06
5	B	801	CLR	C11-C9-C10	-3.11	108.99	113.08
6	A	811	PEE	O2-C2-C1	3.10	119.61	108.40
5	A	805	CLR	C7-C8-C9	2.85	113.17	109.71
5	B	801	CLR	C21-C20-C22	-2.85	105.90	110.36
5	A	803	CLR	C16-C17-C20	2.84	116.55	112.15
5	B	812	CLR	C13-C17-C20	-2.83	115.06	119.49
5	A	805	CLR	C17-C13-C14	2.79	103.38	100.07
5	B	812	CLR	C9-C10-C5	-2.74	105.36	109.65
5	B	802	CLR	C19-C10-C9	-2.70	108.46	111.68
5	A	801	CLR	C16-C17-C20	2.65	116.25	112.15
5	B	801	CLR	C18-C13-C14	-2.62	106.83	111.71
5	A	805	CLR	C10-C9-C8	-2.60	108.83	112.73
5	B	812	CLR	C10-C5-C6	-2.60	118.93	122.90
5	B	807	CLR	C16-C17-C20	2.59	116.16	112.15
5	A	807	CLR	C16-C17-C13	2.56	106.93	103.84
5	B	812	CLR	C11-C12-C13	-2.52	108.47	112.78
5	B	802	CLR	C2-C3-C4	-2.48	106.90	110.31
7	A	812	PII	CI6-CI1-CI2	2.46	114.40	110.85
7	A	812	PII	O26-CO6-CL1	2.45	119.60	111.91
5	A	802	CLR	C13-C14-C8	2.44	118.00	114.38
5	A	805	CLR	C11-C9-C10	-2.44	109.87	113.08
5	B	812	CLR	C7-C8-C9	2.39	112.61	109.71
5	B	802	CLR	C14-C8-C9	-2.38	105.90	109.09
5	B	808	CLR	C16-C17-C20	2.31	115.72	112.15
5	A	803	CLR	C22-C20-C17	2.24	114.91	110.28
5	B	812	CLR	C8-C7-C6	-2.24	109.51	112.73
5	A	801	CLR	C22-C20-C17	2.19	114.82	110.28
6	A	811	PEE	C2-O2-C10	2.16	123.11	117.79
5	B	803	CLR	C16-C17-C20	2.15	115.48	112.15
5	B	802	CLR	C9-C10-C5	2.15	113.02	109.65
5	B	802	CLR	C11-C9-C10	-2.11	110.29	113.08
5	B	802	CLR	C4-C5-C10	2.07	119.17	116.42
7	A	812	PII	CI3-CI2-CI1	2.05	114.37	109.68

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	811	PEE	C2

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	802	CLR	C13-C17-C20-C21
5	B	804	CLR	C13-C17-C20-C21
5	B	804	CLR	C16-C17-C20-C22
7	A	812	PII	C21-O12-P1-OI1
7	A	812	PII	C21-O12-P1-O13
7	A	812	PII	C24-C21-O12-P1
7	A	812	PII	OC6-CO6-O26-C25
5	B	804	CLR	C16-C17-C20-C21
5	A	803	CLR	C16-C17-C20-C21
5	A	802	CLR	C13-C17-C20-C21
5	A	803	CLR	C13-C17-C20-C21
5	A	805	CLR	C13-C17-C20-C21
5	B	804	CLR	C13-C17-C20-C22
5	A	802	CLR	C13-C17-C20-C22
7	A	812	PII	CL1-CO6-O26-C25
5	B	802	CLR	C21-C20-C22-C23
5	B	812	CLR	C21-C20-C22-C23
5	B	802	CLR	C16-C17-C20-C21
5	B	807	CLR	C16-C17-C20-C21
5	A	805	CLR	C16-C17-C20-C21
5	B	807	CLR	C13-C17-C20-C21
5	B	802	CLR	C16-C17-C20-C22
5	B	802	CLR	C13-C17-C20-C22
5	B	807	CLR	C13-C17-C20-C22
5	B	812	CLR	C13-C17-C20-C22
5	A	803	CLR	C13-C17-C20-C22
5	A	805	CLR	C13-C17-C20-C22
7	A	812	PII	CR6-CR7-CR8-CR9
7	A	812	PII	CR9-CRA-CRB-CRC
5	B	807	CLR	C16-C17-C20-C22
5	A	803	CLR	C16-C17-C20-C22
5	A	805	CLR	C16-C17-C20-C22
5	B	812	CLR	C13-C17-C20-C21
5	B	801	CLR	C16-C17-C20-C22
5	A	807	CLR	C16-C17-C20-C22
7	A	812	PII	CL1-CL2-CL3-CL4
5	B	812	CLR	C17-C20-C22-C23
7	A	812	PII	CR4-CR5-CR6-CR7

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Mol	Chain	Res	Type	Atoms
5	B	801	CLR	C21-C20-C22-C23
5	B	801	CLR	C17-C20-C22-C23
5	A	810	CLR	C17-C20-C22-C23
6	A	811	PEE	C31-C30-O3-C3
5	B	806	CLR	C22-C23-C24-C25
5	A	802	CLR	C16-C17-C20-C21
5	B	806	CLR	C13-C17-C20-C22
5	B	808	CLR	C13-C17-C20-C22
5	A	807	CLR	C13-C17-C20-C22
5	B	802	CLR	C17-C20-C22-C23
7	A	812	PII	CL3-CL4-CL5-CL6
6	A	811	PEE	O2-C2-C3-O3
5	B	812	CLR	C20-C22-C23-C24
5	A	807	CLR	C16-C17-C20-C21
5	A	807	CLR	C13-C17-C20-C21
6	A	811	PEE	O5-C30-O3-C3
5	B	805	CLR	C21-C20-C22-C23
5	B	802	CLR	C20-C22-C23-C24
5	B	804	CLR	C22-C23-C24-C25
5	B	807	CLR	C22-C23-C24-C25
5	B	810	CLR	C20-C22-C23-C24
6	A	811	PEE	C17-C18-C19-C20
5	A	808	CLR	C20-C22-C23-C24
5	A	809	CLR	C20-C22-C23-C24
5	B	808	CLR	C16-C17-C20-C21
5	A	804	CLR	C13-C17-C20-C21
5	B	811	CLR	C17-C20-C22-C23
5	B	806	CLR	C16-C17-C20-C21
5	B	806	CLR	C13-C17-C20-C21
5	B	808	CLR	C13-C17-C20-C21
5	A	801	CLR	C22-C23-C24-C25
5	B	811	CLR	C21-C20-C22-C23
5	B	808	CLR	C22-C23-C24-C25
5	B	803	CLR	C20-C22-C23-C24
5	B	806	CLR	C20-C22-C23-C24
5	B	801	CLR	C13-C17-C20-C21
5	A	802	CLR	C23-C24-C25-C27
5	A	803	CLR	C23-C24-C25-C26
5	B	812	CLR	C16-C17-C20-C21
7	A	812	PII	CR2-CR3-CR4-CR5
6	A	811	PEE	C14-C15-C16-C17
7	A	812	PII	CR7-CR8-CR9-CRA

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Mol	Chain	Res	Type	Atoms
5	A	809	CLR	C23-C24-C25-C26
6	A	811	PEE	O4P-C4-C5-N
7	A	812	PII	CRA-CRB-CRC-CRD
5	B	803	CLR	C22-C23-C24-C25
7	A	812	PII	CR1-CR2-CR3-CR4
5	A	802	CLR	C21-C20-C22-C23
5	A	802	CLR	C23-C24-C25-C26
5	A	803	CLR	C23-C24-C25-C27
6	A	811	PEE	C13-C14-C15-C16
6	A	811	PEE	C12-C13-C14-C15
5	A	802	CLR	C17-C20-C22-C23
7	A	812	PII	CL5-CL6-CL7-CL8
5	B	812	CLR	C16-C17-C20-C22
5	A	804	CLR	C16-C17-C20-C22
6	A	811	PEE	C39-C40-C41-C42
6	A	811	PEE	C42-C43-C44-C45
5	B	802	CLR	C23-C24-C25-C26
5	B	808	CLR	C23-C24-C25-C26
6	A	811	PEE	C36-C37-C38-C39
5	A	805	CLR	C22-C23-C24-C25
6	A	811	PEE	C4-O4P-P-O3P
5	A	809	CLR	C22-C23-C24-C25
7	A	812	PII	O12-C21-C24-C25
5	A	809	CLR	C23-C24-C25-C27
7	A	812	PII	CR3-CR4-CR5-CR6
5	B	811	CLR	C22-C23-C24-C25
5	A	810	CLR	C22-C23-C24-C25
5	A	810	CLR	C21-C20-C22-C23
5	A	807	CLR	C20-C22-C23-C24
7	A	812	PII	CL4-CL5-CL6-CL7
5	A	806	CLR	C21-C20-C22-C23
5	B	802	CLR	C23-C24-C25-C27
5	B	808	CLR	C23-C24-C25-C27
5	A	801	CLR	C16-C17-C20-C21
5	A	801	CLR	C13-C17-C20-C21
5	A	808	CLR	C23-C24-C25-C26
5	A	801	CLR	C16-C17-C20-C22
5	A	801	CLR	C13-C17-C20-C22
5	B	805	CLR	C22-C23-C24-C25
5	B	801	CLR	C16-C17-C20-C21
7	A	812	PII	CR8-CR9-CRA-CRB
5	B	810	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
5	B	810	CLR	C16-C17-C20-C21
5	B	810	CLR	C13-C17-C20-C21
6	A	811	PEE	C22-C23-C24-C25
5	B	810	CLR	C13-C17-C20-C22
6	A	811	PEE	C32-C33-C34-C35
5	A	802	CLR	C20-C22-C23-C24
5	A	804	CLR	C16-C17-C20-C21
5	A	808	CLR	C23-C24-C25-C27
5	A	804	CLR	C21-C20-C22-C23
6	A	811	PEE	O3P-C1-C2-O2
5	B	801	CLR	C13-C17-C20-C22
5	B	805	CLR	C23-C24-C25-C26
6	A	811	PEE	C4-O4P-P-O2P
5	A	810	CLR	C23-C24-C25-C26
5	B	808	CLR	C20-C22-C23-C24
7	A	812	PII	O12-C21-C24-O29
5	B	808	CLR	C16-C17-C20-C22
5	B	803	CLR	C13-C17-C20-C22
5	B	803	CLR	C13-C17-C20-C21
5	B	812	CLR	C23-C24-C25-C26
7	A	812	PII	O29-CO9-CR1-CR2
6	A	811	PEE	C38-C39-C40-C41
6	A	811	PEE	C40-C41-C42-C43
5	B	803	CLR	C16-C17-C20-C22
5	A	810	CLR	C23-C24-C25-C27
5	B	811	CLR	C20-C22-C23-C24
5	B	807	CLR	C23-C24-C25-C27
7	A	812	PII	CRB-CRC-CRD-CRE
5	B	810	CLR	C22-C23-C24-C25
6	A	811	PEE	C30-C31-C32-C33
5	A	810	CLR	C20-C22-C23-C24
5	B	812	CLR	C23-C24-C25-C27
5	A	804	CLR	C13-C17-C20-C22
5	A	808	CLR	C21-C20-C22-C23
5	B	806	CLR	C16-C17-C20-C22
5	A	804	CLR	C23-C24-C25-C27
5	B	801	CLR	C22-C23-C24-C25
6	A	811	PEE	C20-C21-C22-C23
5	B	804	CLR	C20-C22-C23-C24
5	A	809	CLR	C13-C17-C20-C21
5	A	809	CLR	C16-C17-C20-C22
5	B	803	CLR	C16-C17-C20-C21

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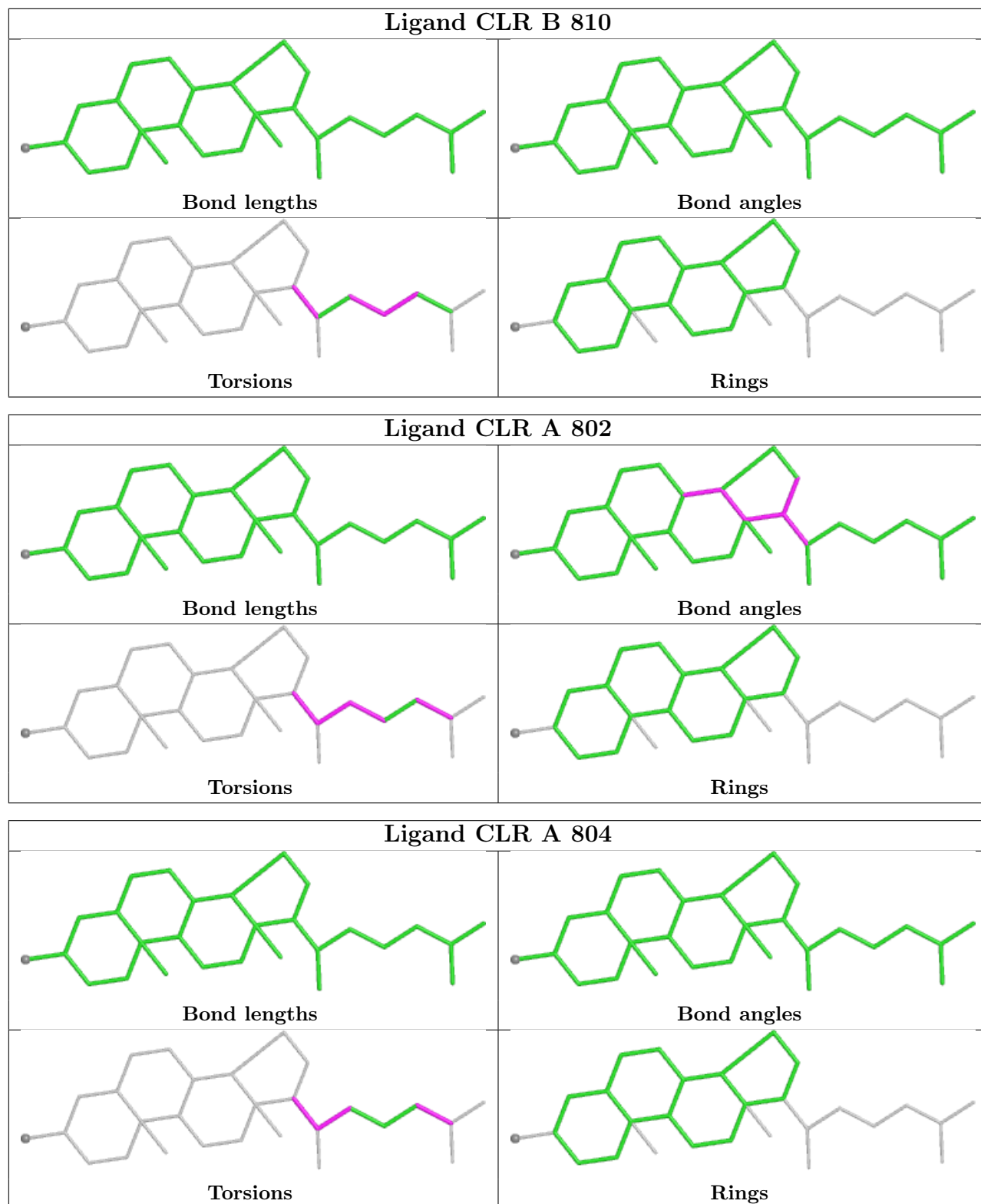
Mol	Chain	Res	Type	Atoms
6	A	811	PEE	C21-C22-C23-C24
5	A	809	CLR	C13-C17-C20-C22
5	B	802	CLR	C22-C23-C24-C25
5	A	801	CLR	C20-C22-C23-C24

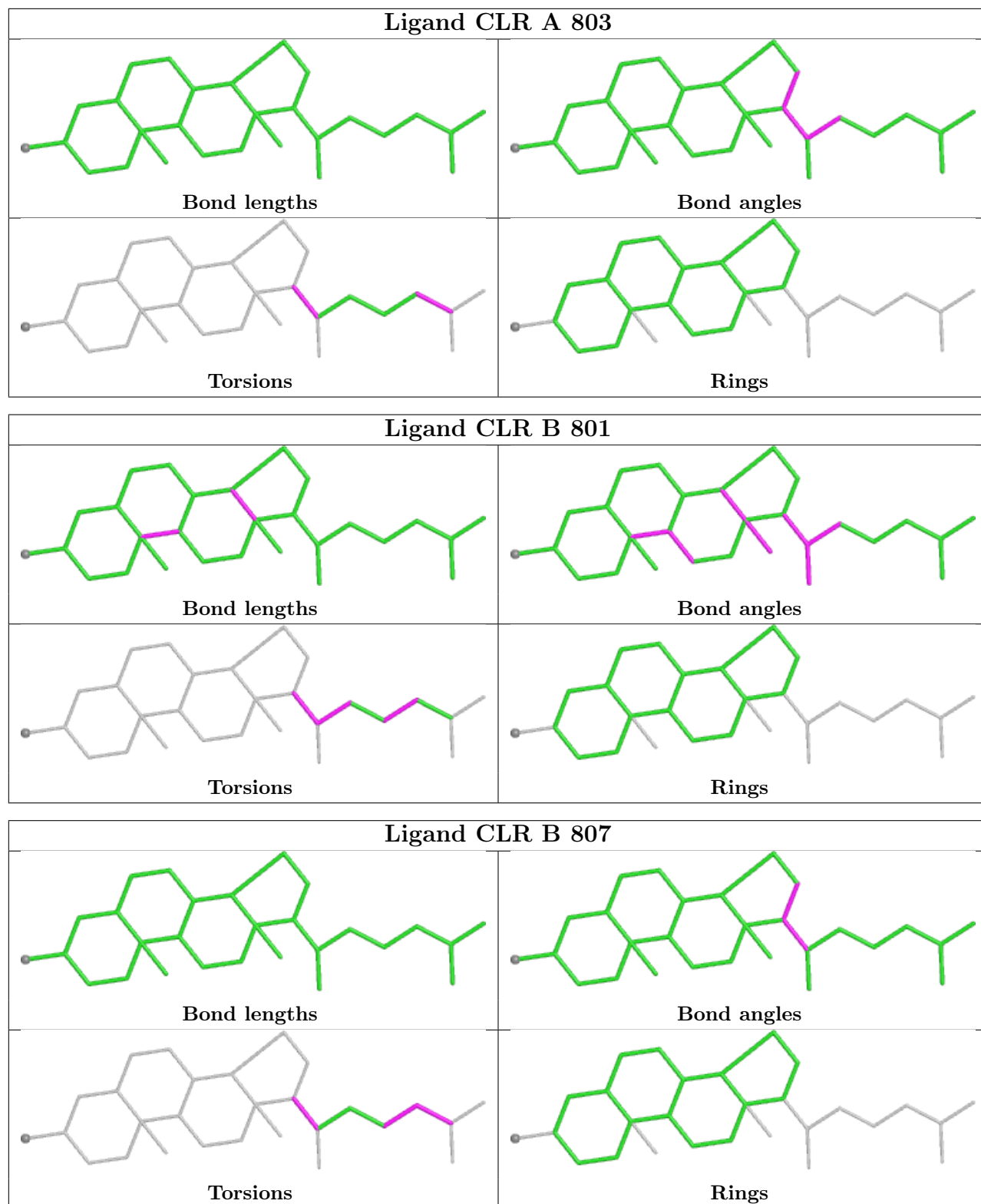
There are no ring outliers.

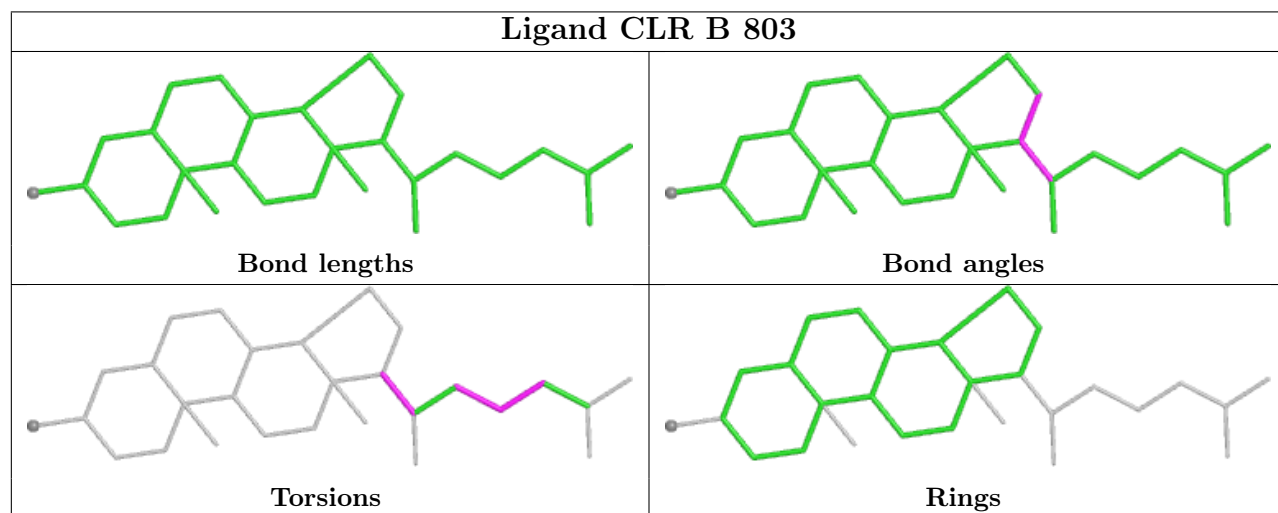
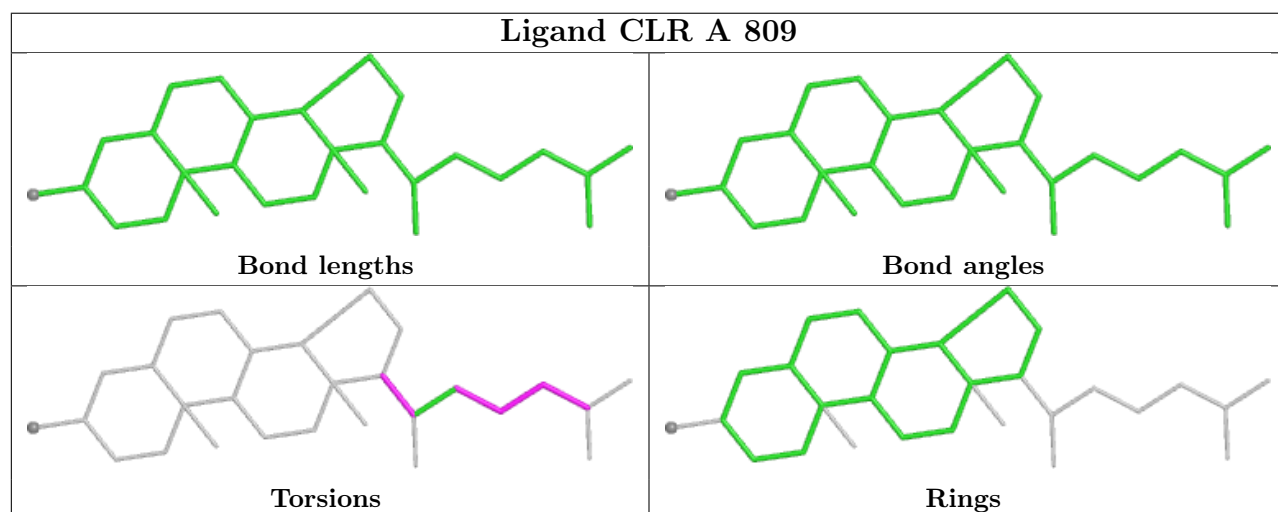
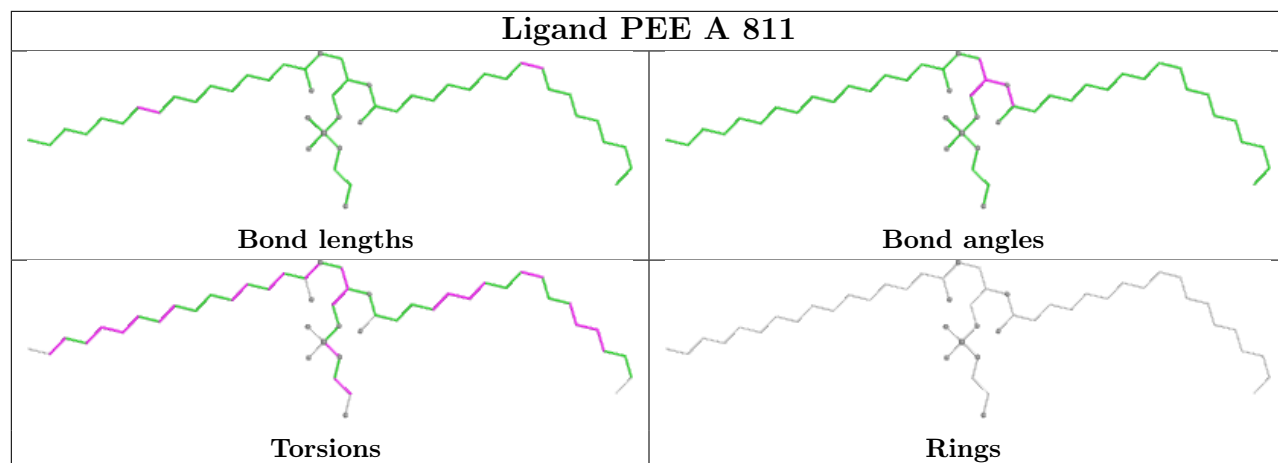
10 monomers are involved in 29 short contacts:

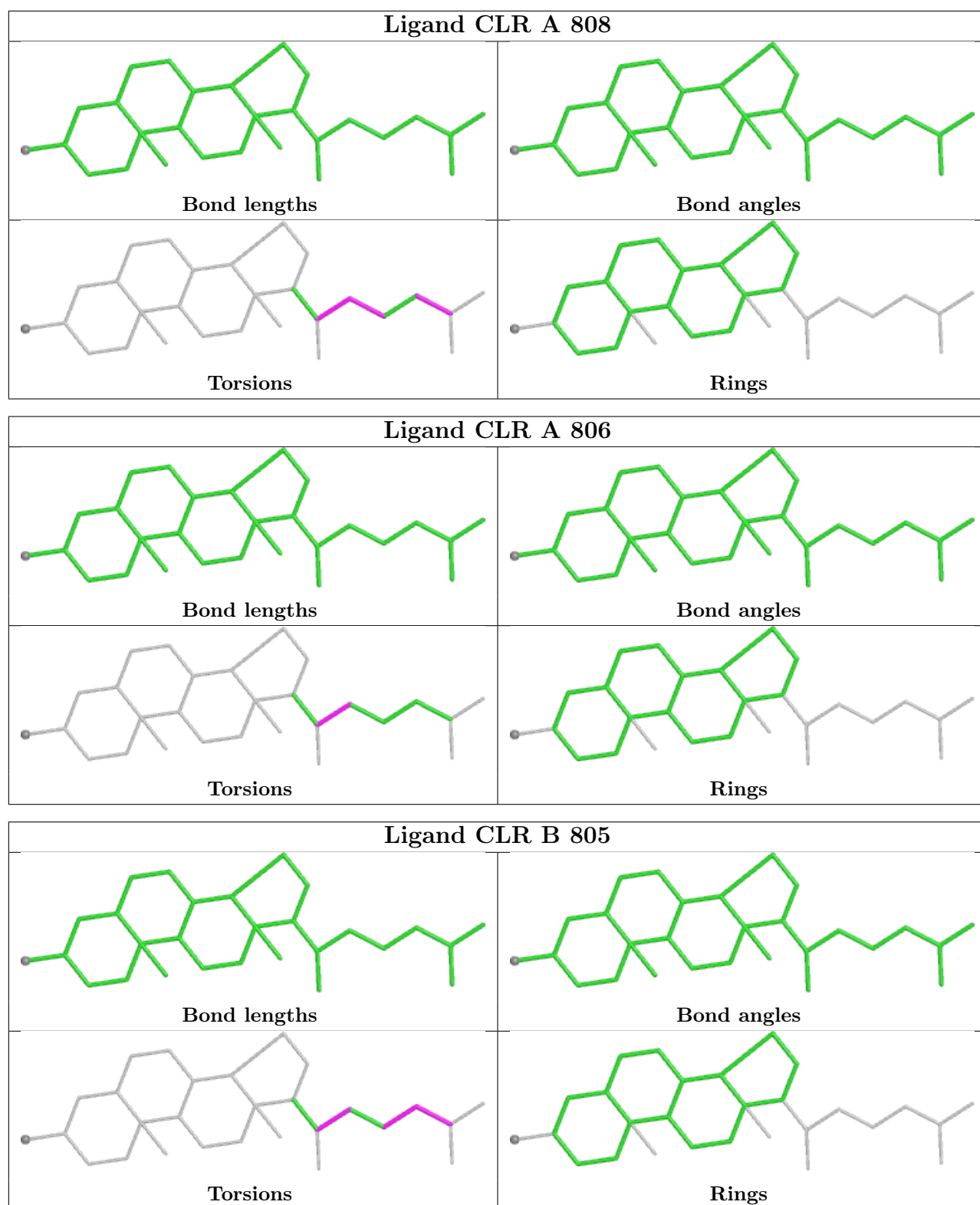
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	804	CLR	2	0
5	A	803	CLR	1	0
5	B	801	CLR	2	0
6	A	811	PEE	3	0
5	A	808	CLR	2	0
5	B	802	CLR	7	0
7	A	812	PII	8	0
5	A	805	CLR	7	0
5	B	804	CLR	1	0
5	B	812	CLR	2	0

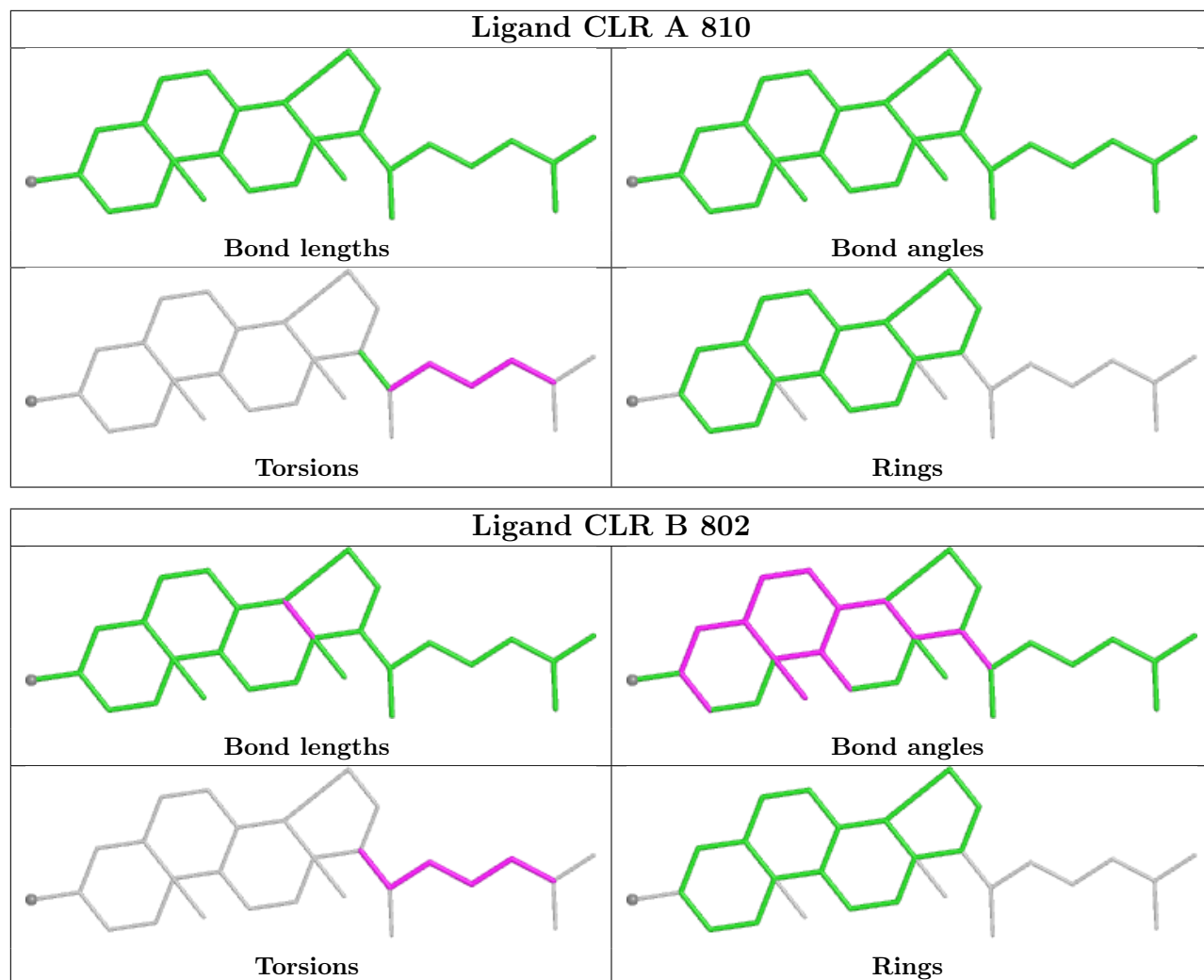
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

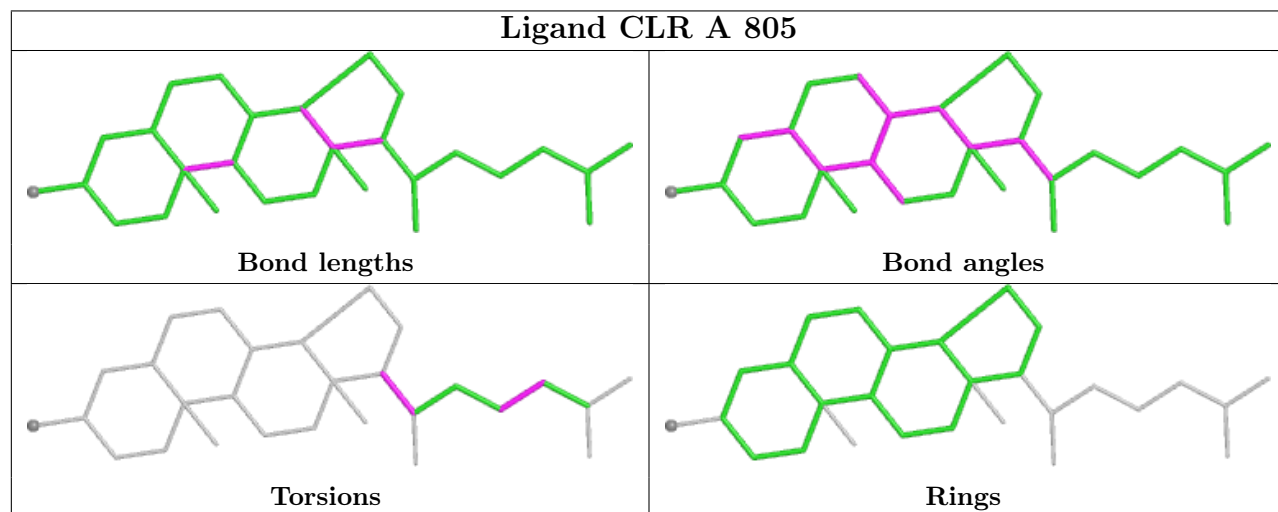
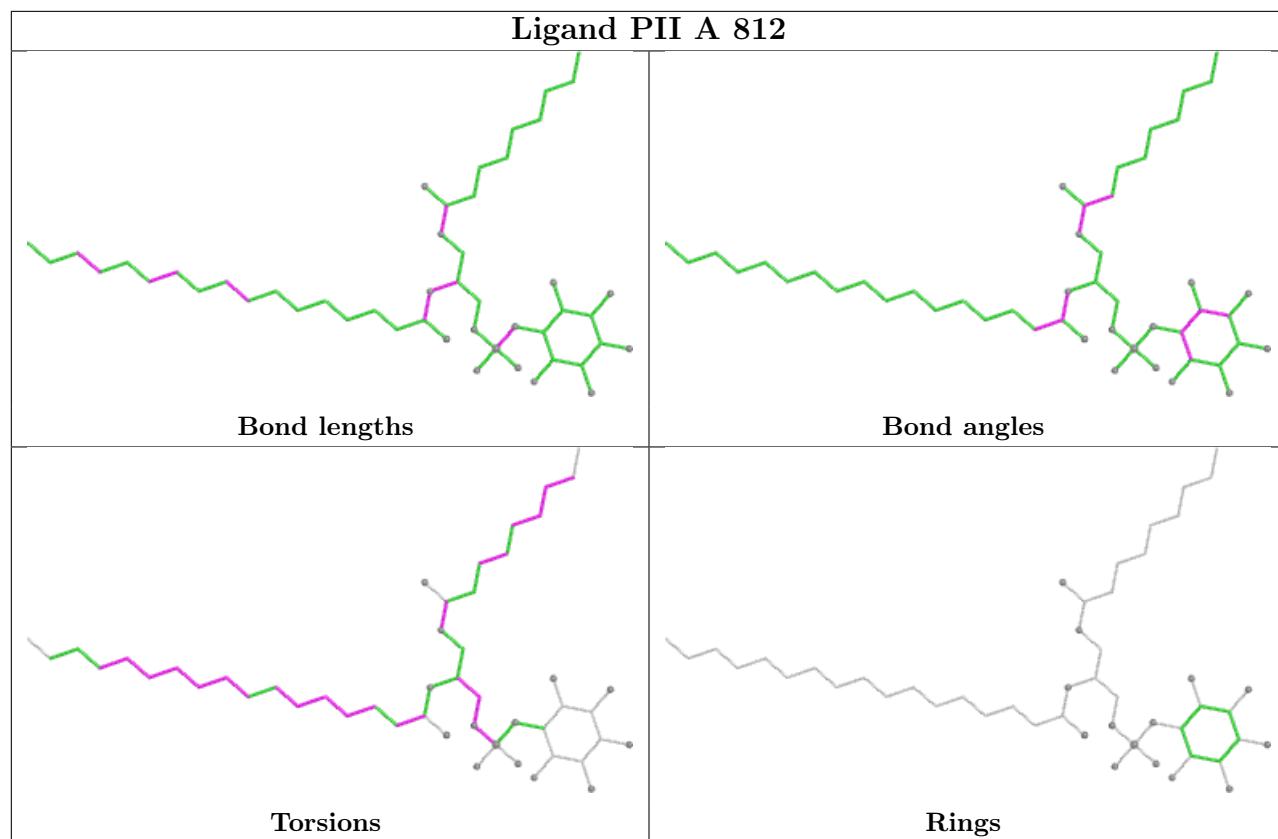


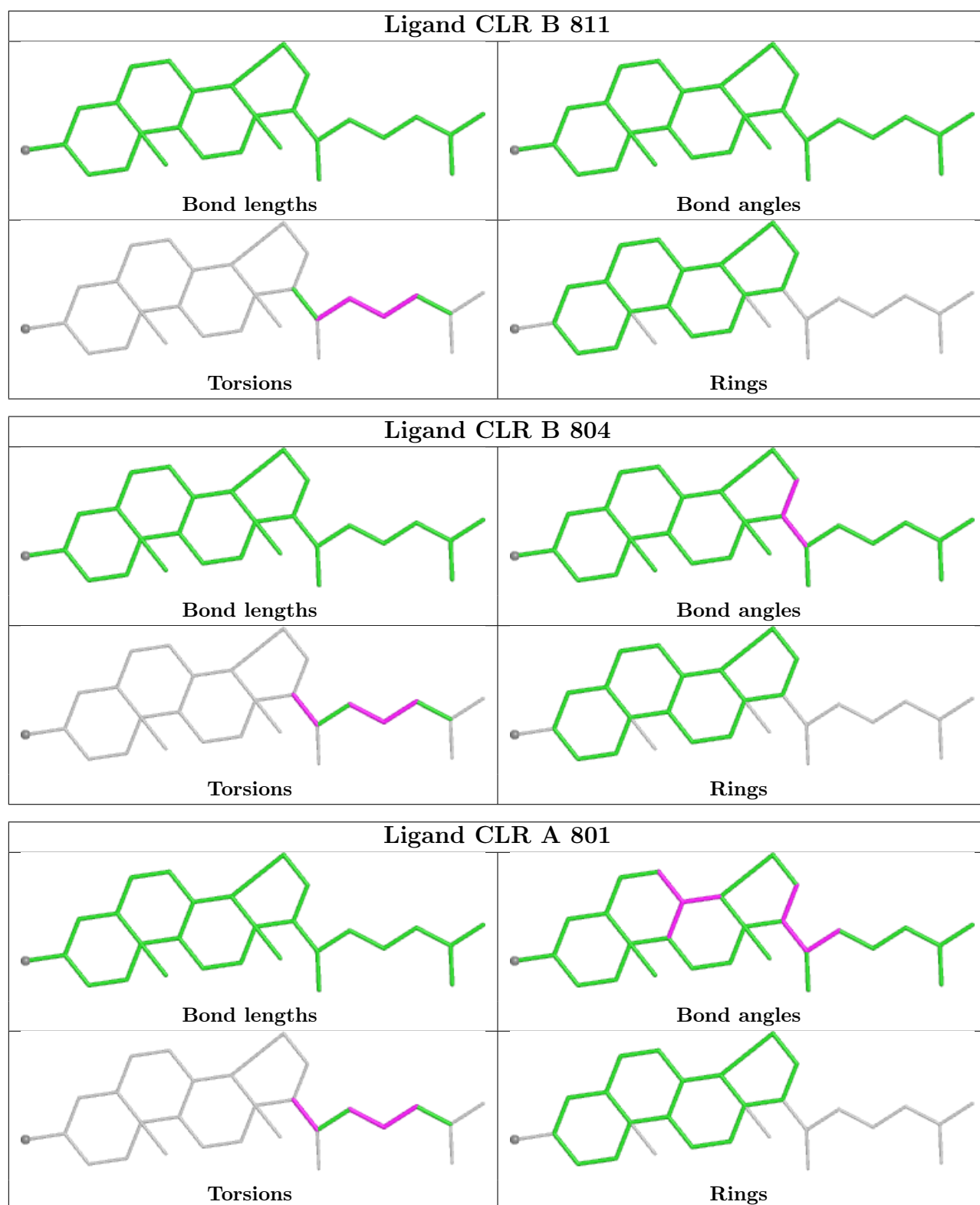


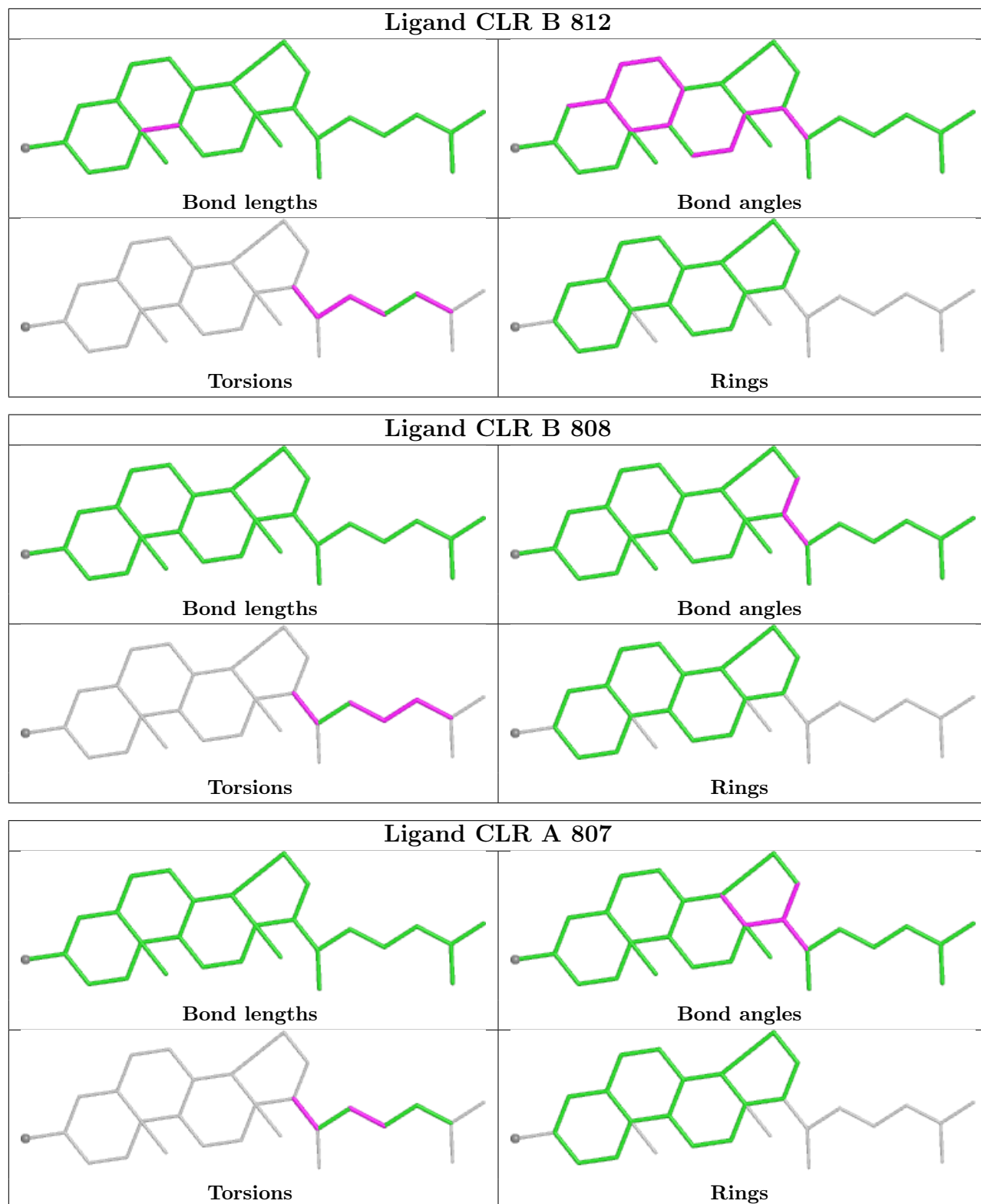


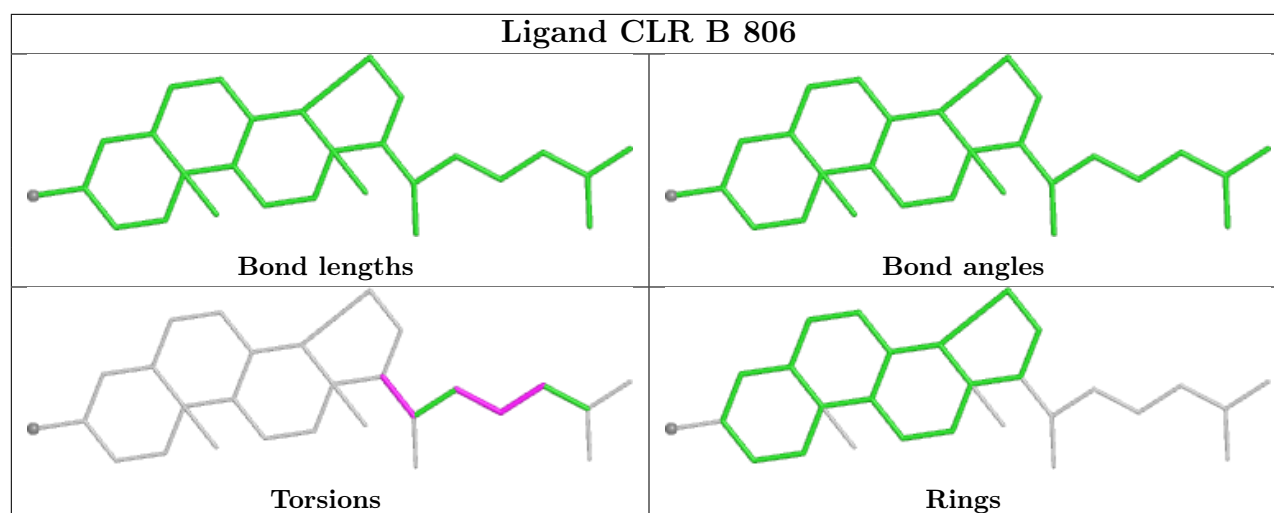












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	208:SER	C	222:SER	N	12.33
1	B	211:PRO	C	224:HIS	N	11.26
1	B	203:LEU	C	204:GLN	N	5.84
1	B	340:ILE	C	341:LYS	N	4.75
1	A	738:PRO	C	739:HIS	N	3.17

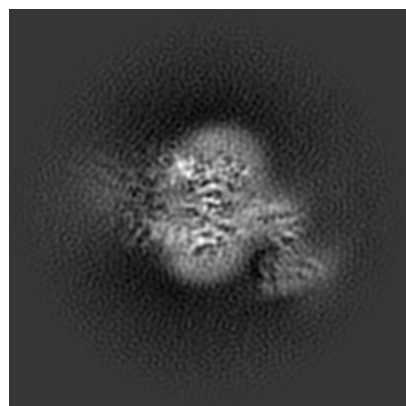
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65226. These allow visual inspection of the internal detail of the map and identification of artifacts.

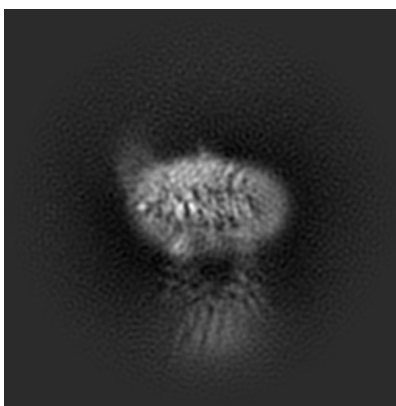
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

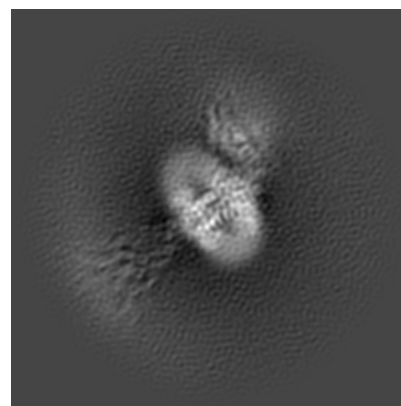
6.1.1 Primary map



X

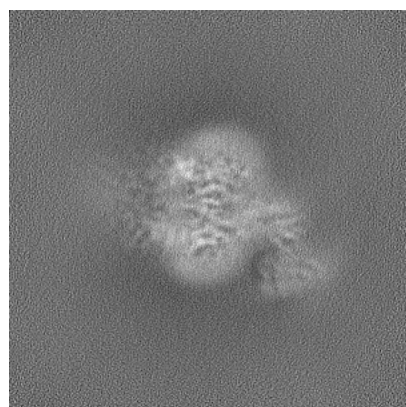


Y

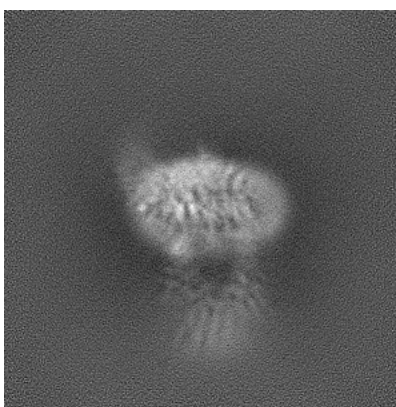


Z

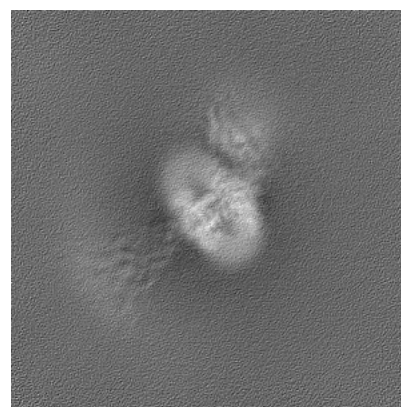
6.1.2 Raw map



X



Y

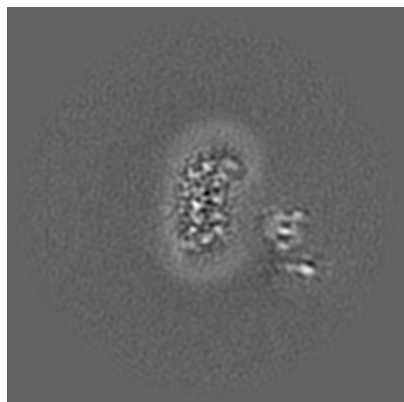


Z

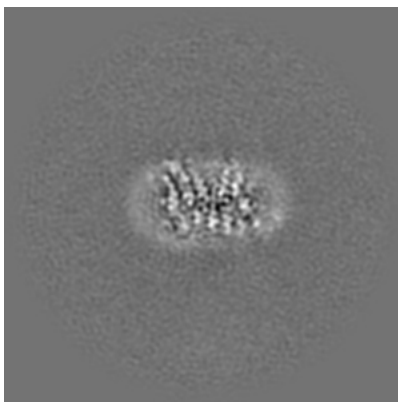
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

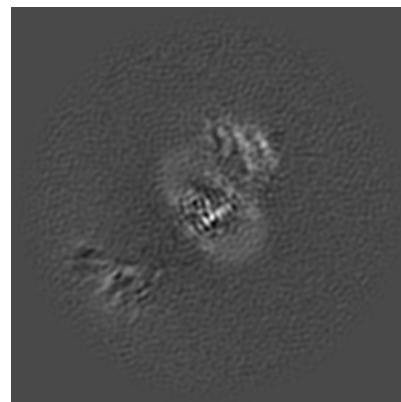
6.2.1 Primary map



X Index: 170

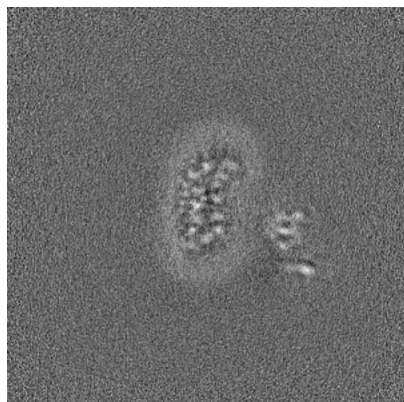


Y Index: 170

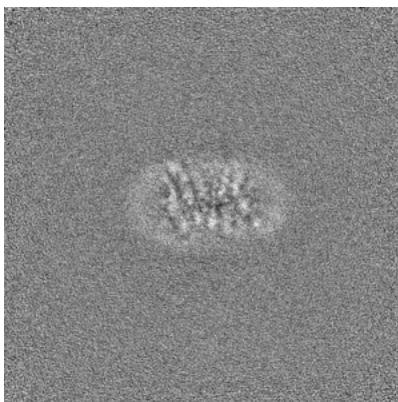


Z Index: 170

6.2.2 Raw map



X Index: 170



Y Index: 170

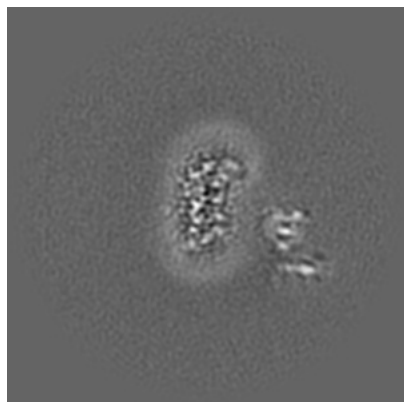


Z Index: 170

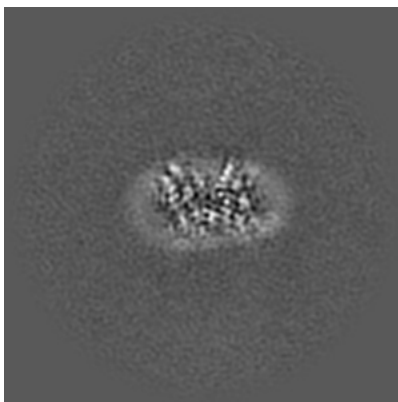
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

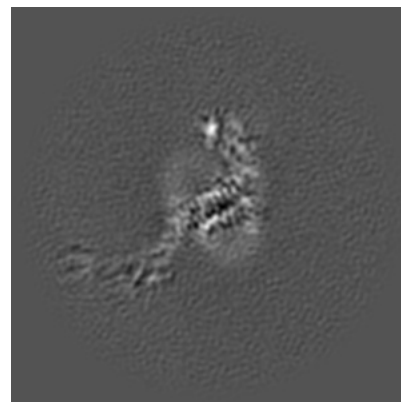
6.3.1 Primary map



X Index: 171

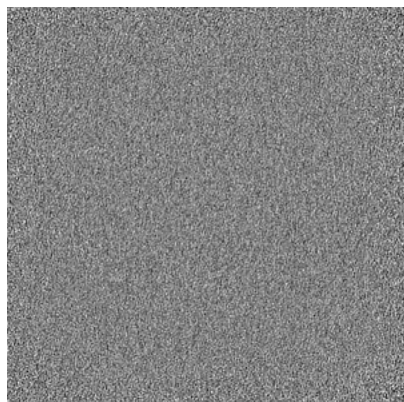


Y Index: 173

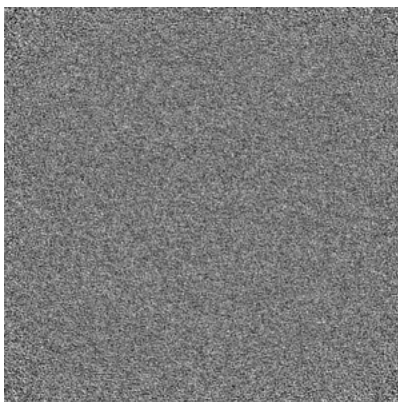


Z Index: 149

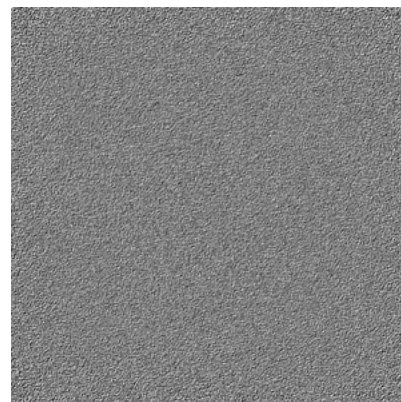
6.3.2 Raw map



X Index: 0



Y Index: 0

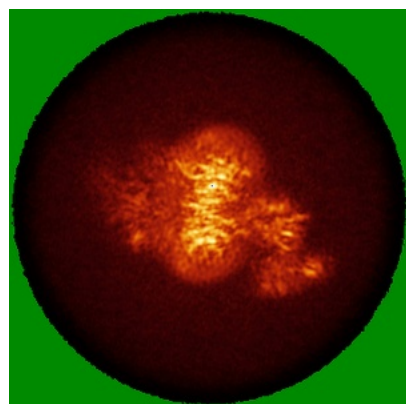


Z Index: 0

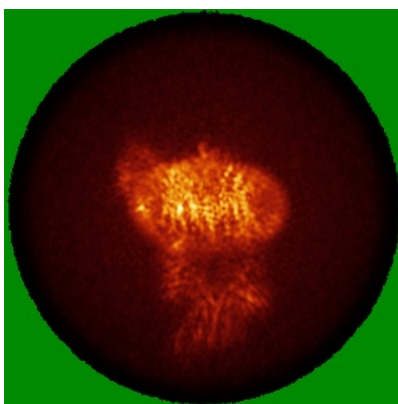
The images above show the largest variance slices of the map in three orthogonal directions.

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

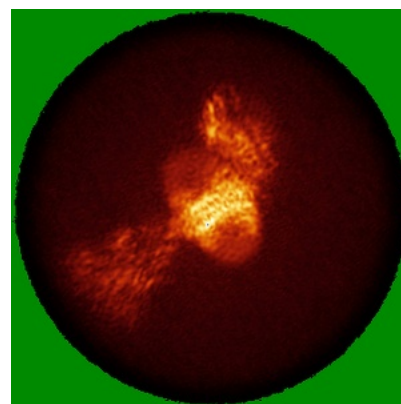
6.4.1 Primary map



X

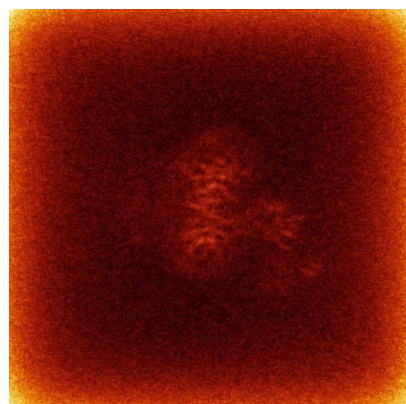


Y

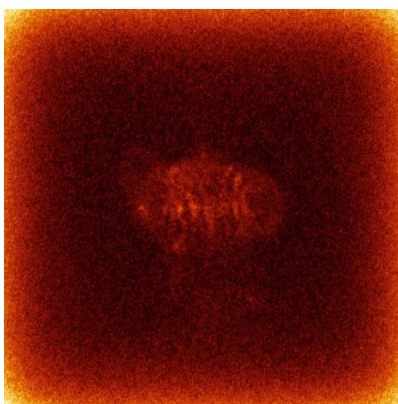


Z

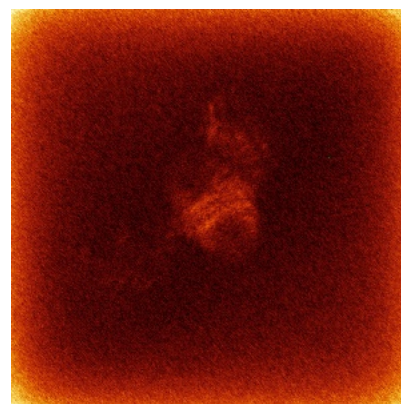
6.4.2 Raw map



X



Y

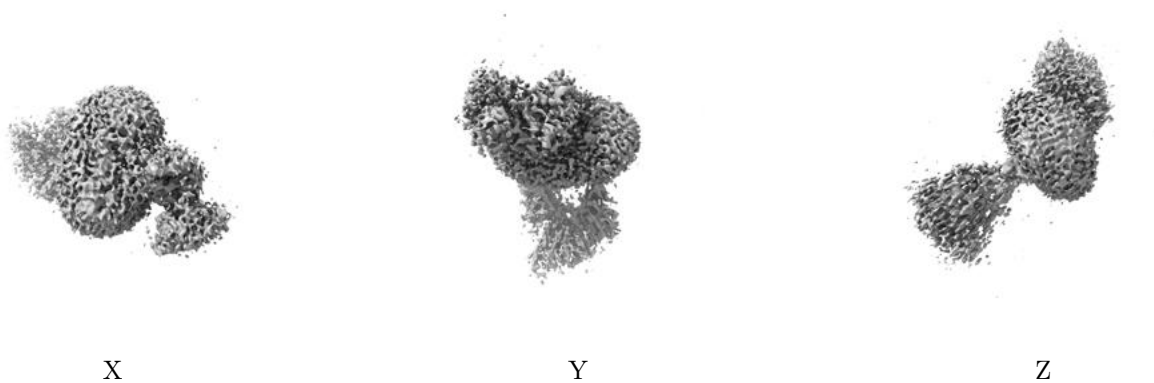


Z

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.

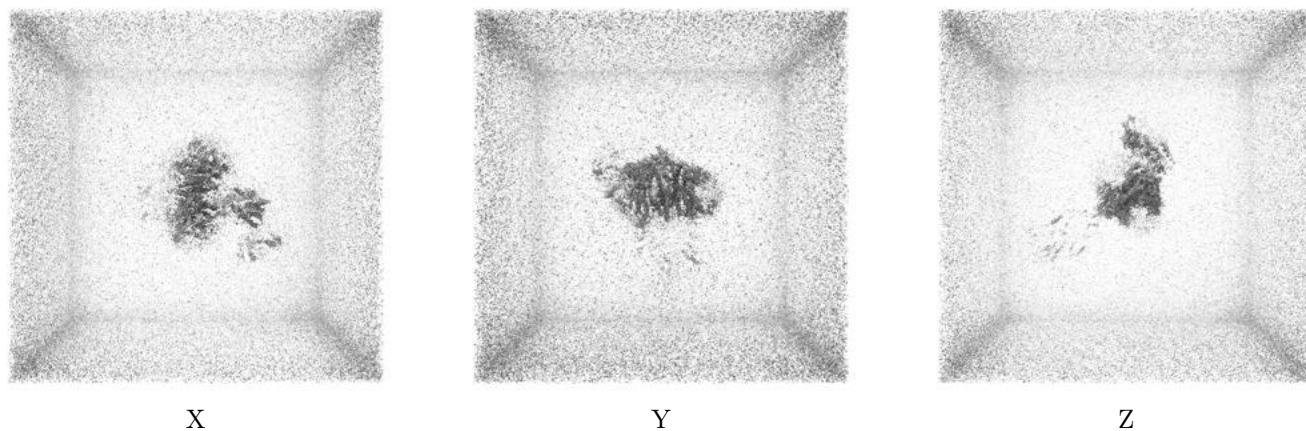
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0457. 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.

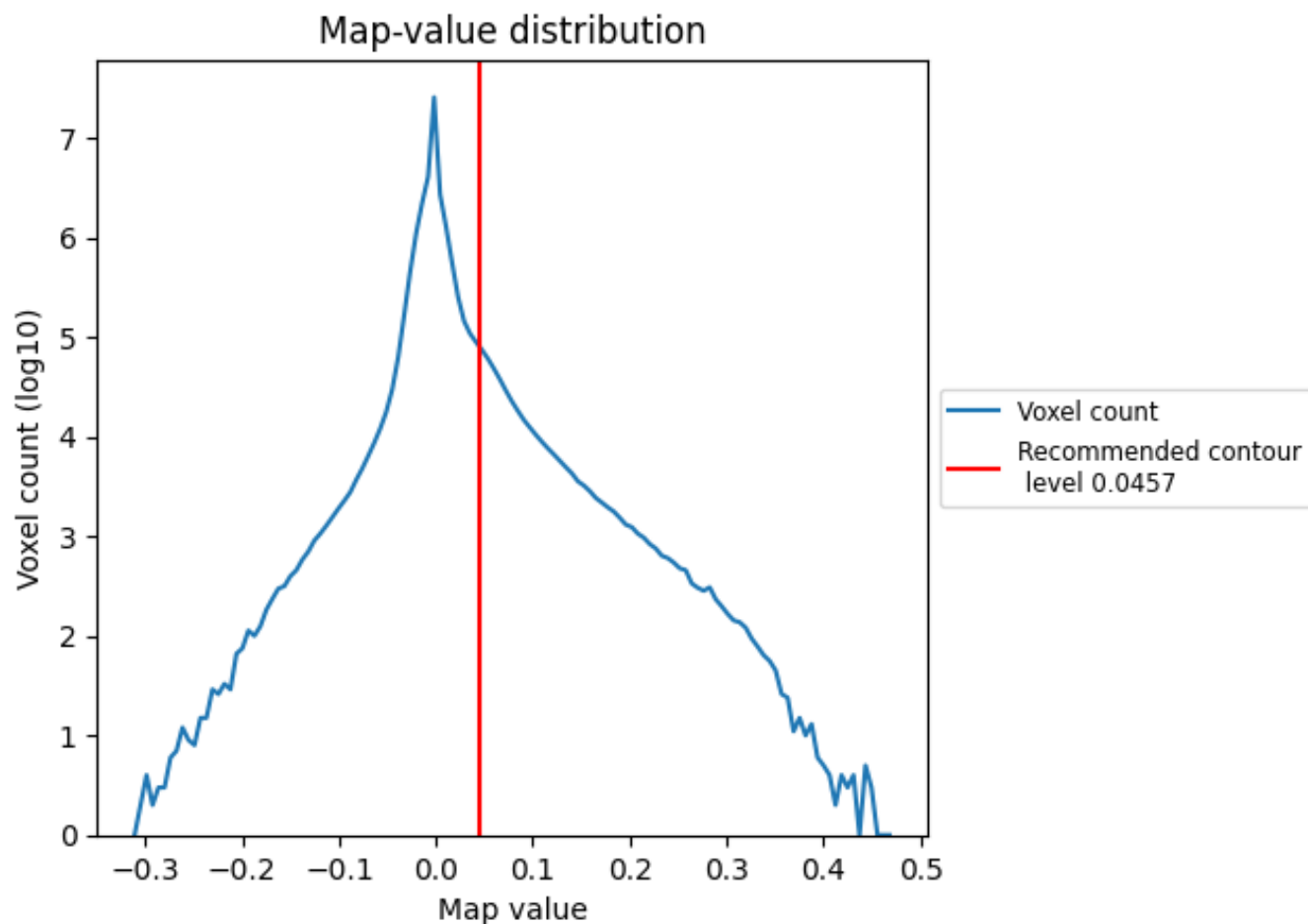
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

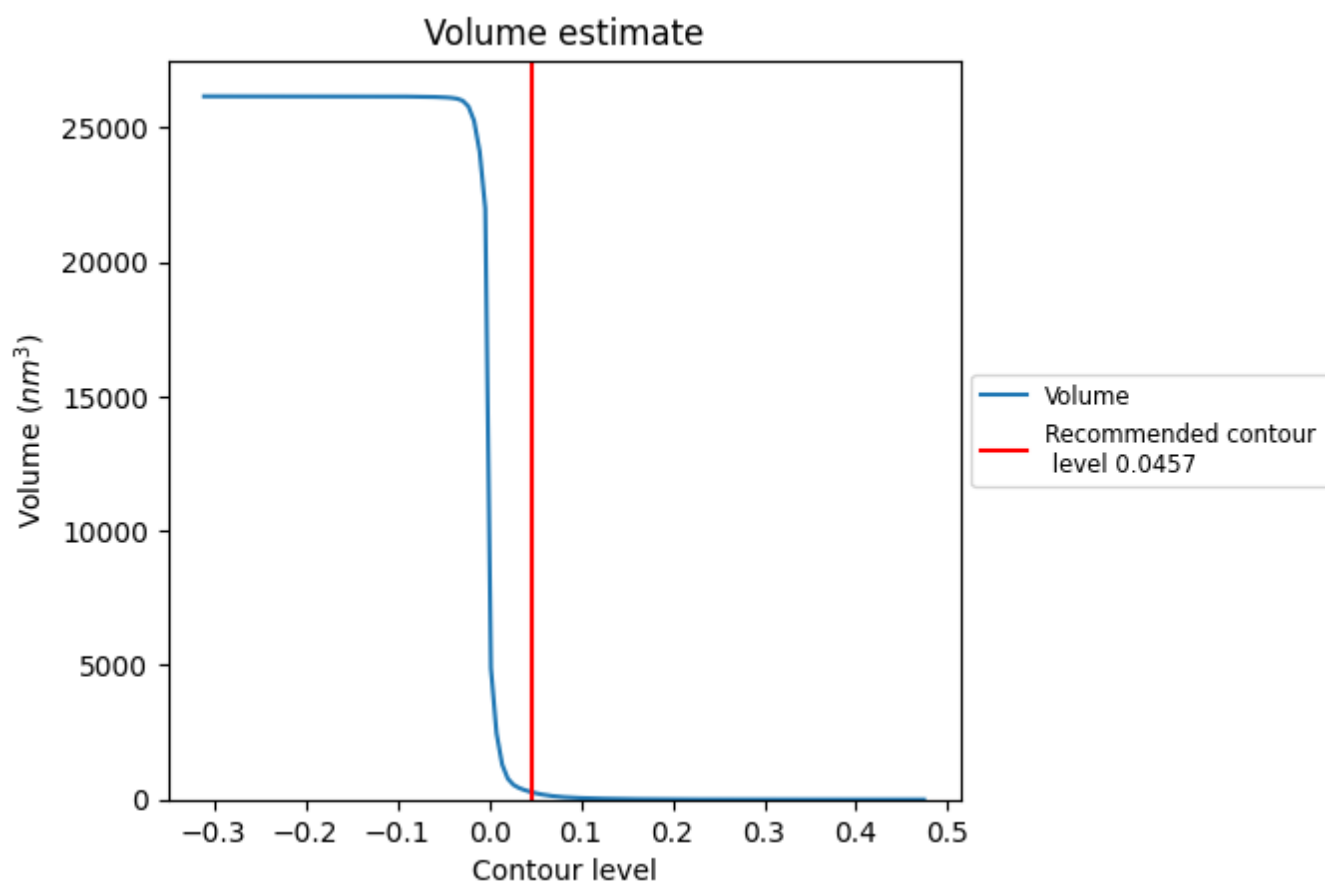
This section contains the results of statistical analysis of the map.

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.

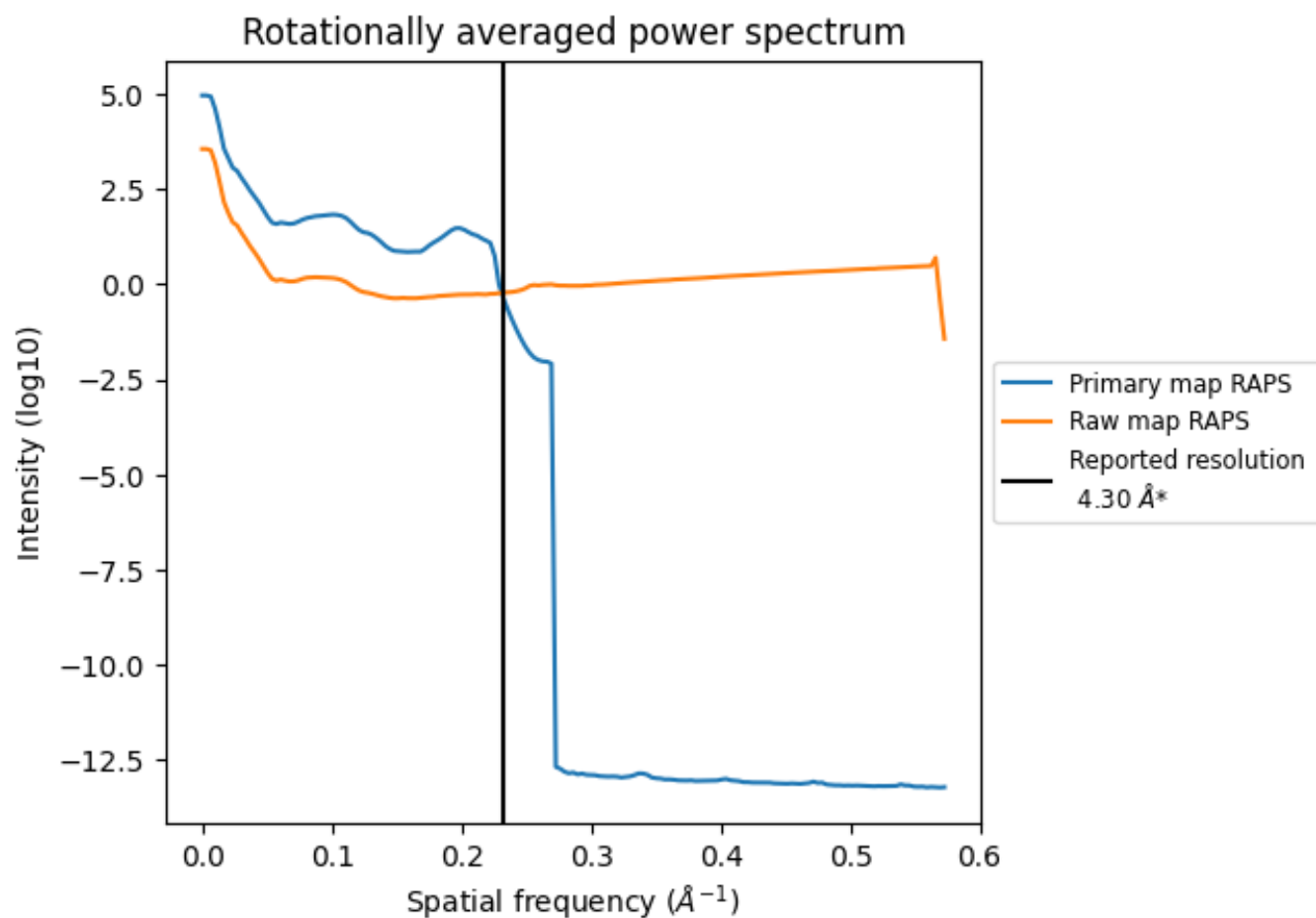
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 281 nm³; this corresponds to an approximate mass of 254 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 ⓘ

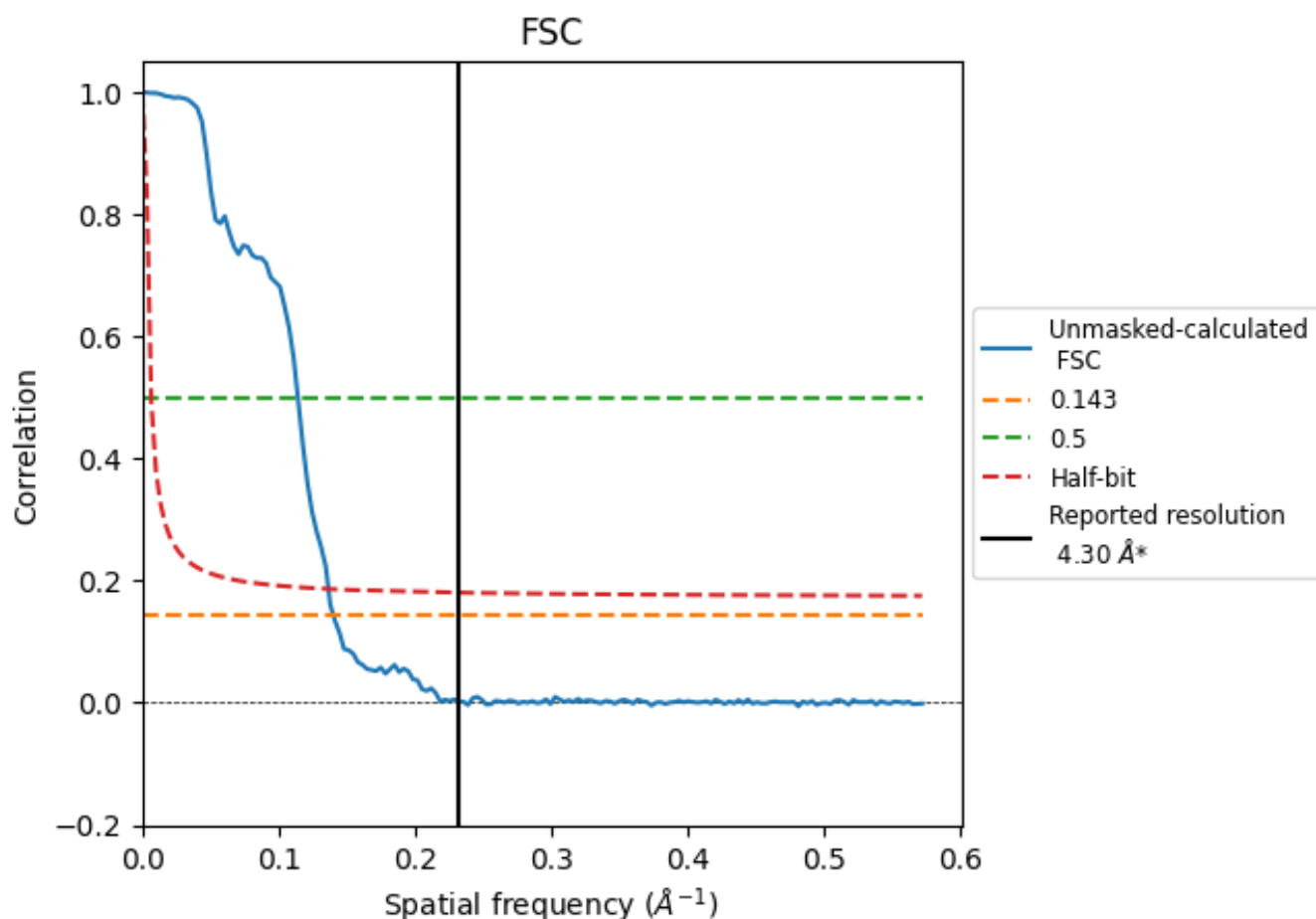


*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

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 0.233 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

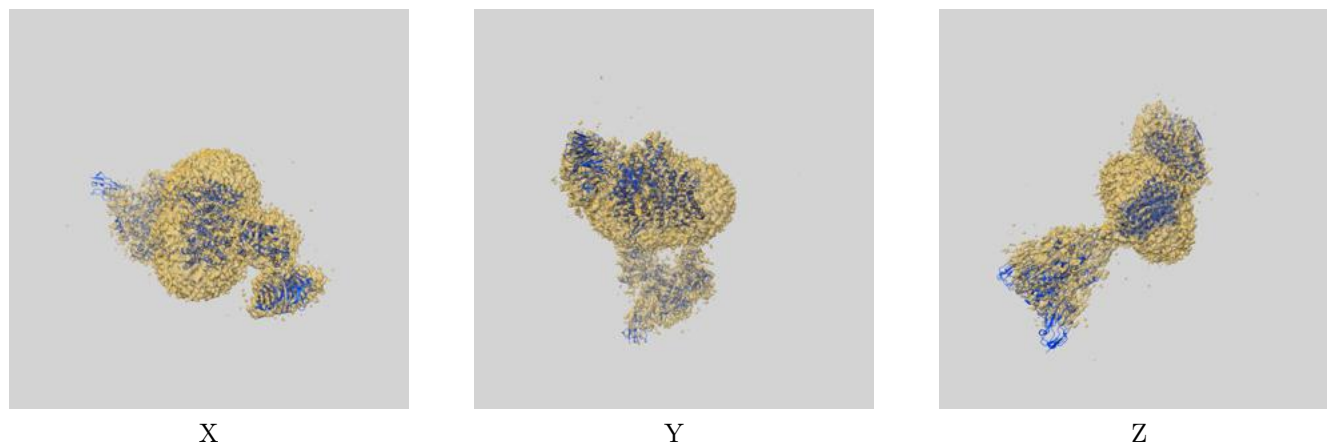
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.12	8.75	7.32

*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 7.12 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

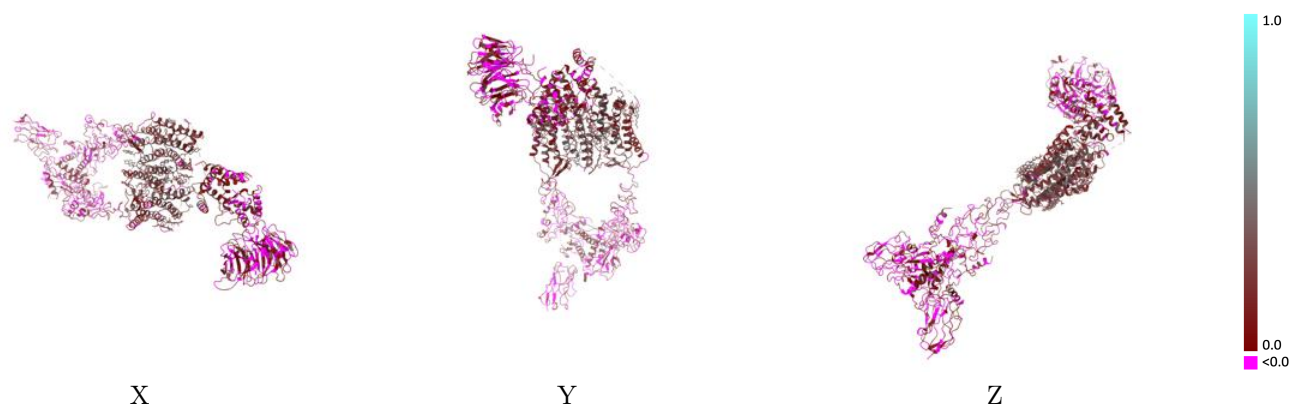
This section contains information regarding the fit between EMDB map EMD-65226 and PDB model 9VOS. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



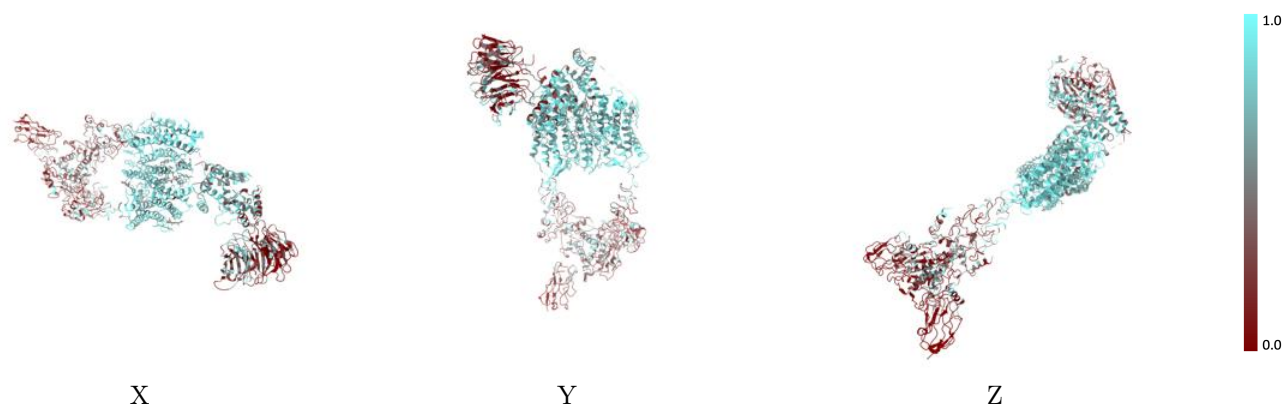
The images above show the 3D surface view of the map at the recommended contour level 0.0457 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



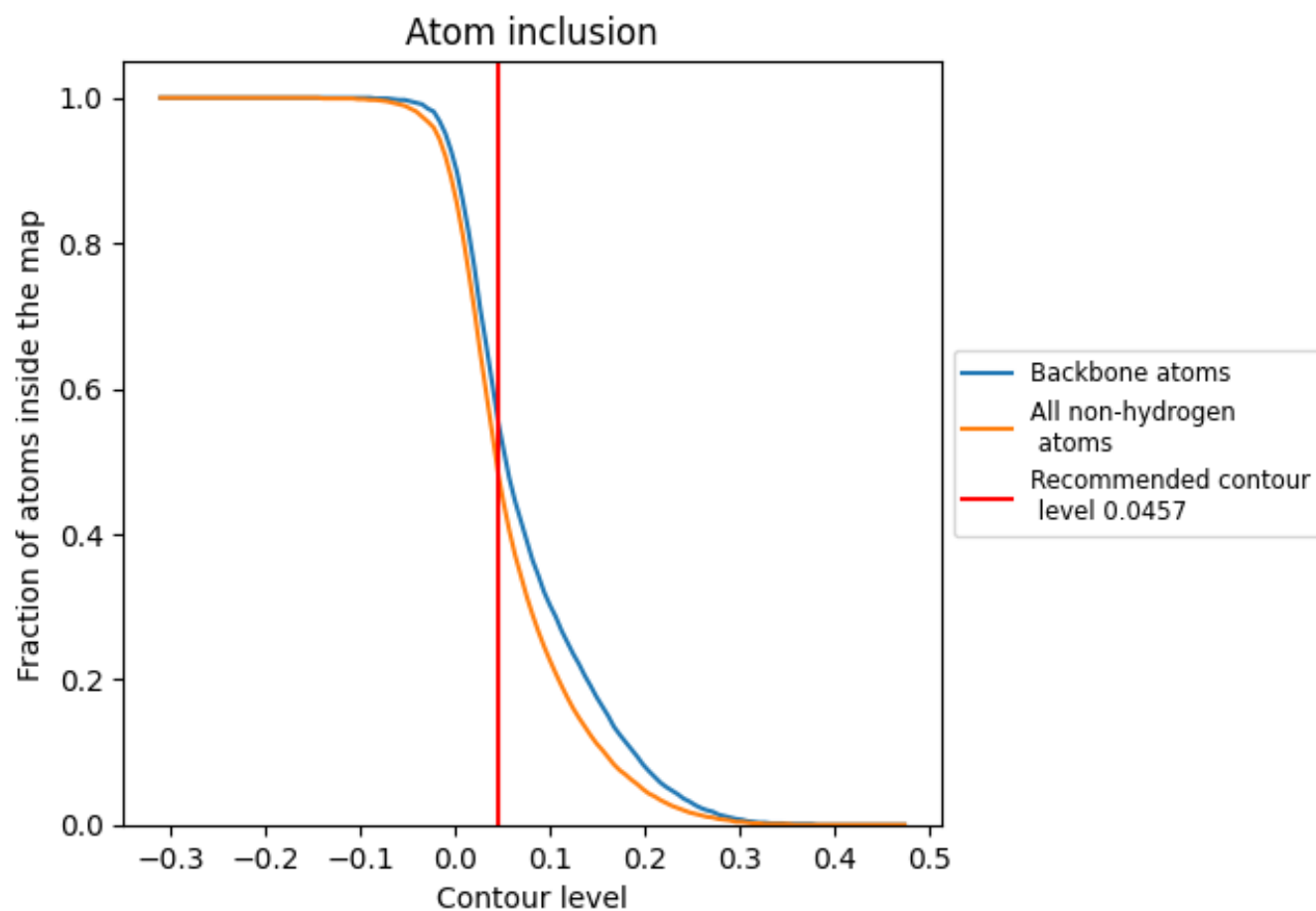
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0457).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 48% 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 (0.0457) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4810	0.1190
A	0.5730	0.1570
B	0.5570	0.1620
C	0.6370	0.1100
D	0.3260	0.0350
H	0.0860	0.0520
I	0.1180	-0.0150

1.0
0.0
-0.0