



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:26 PM UTC

PDB ID : 7SHE / pdb_00007she
EMDB ID : EMD-25125
Title : Cryo-EM structure of human GPR158
Authors : Patil, D.N.; Singh, S.; Singh, A.K.; Martemyanov, K.A.
Deposited on : 2021-10-08
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

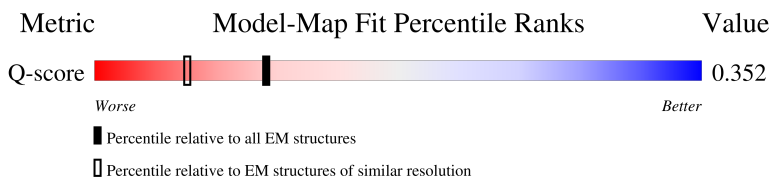
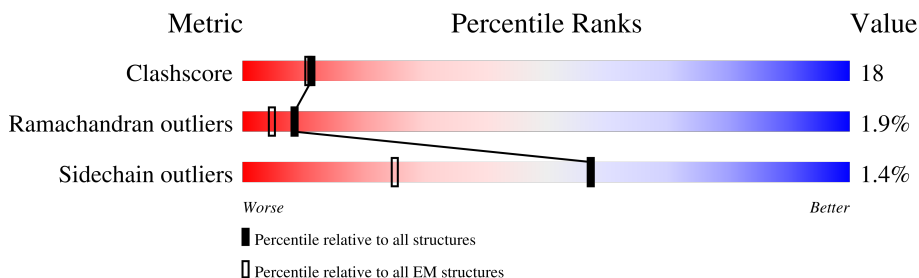
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	
1	B	781	

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	CLR	A	803	X	-	-	-
4	CLR	B	802	X	-	-	-
4	CLR	B	808	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8990 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.

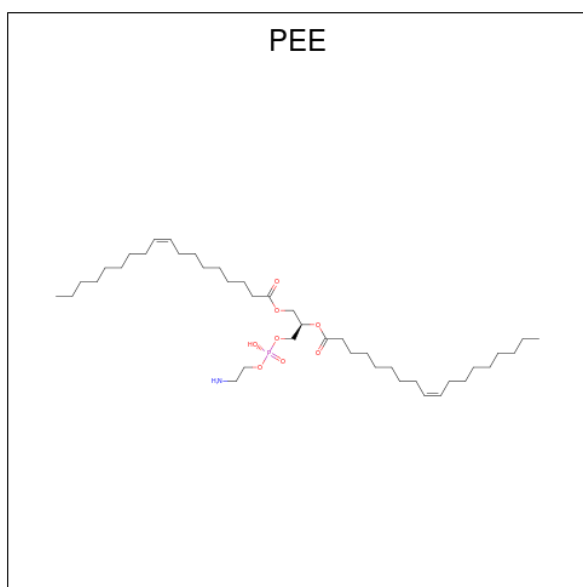
- Molecule 1 is a protein called G-protein coupled receptor 158.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	541	Total	C	N	O	S	0	0
			4131	2678	695	728	30		
1	B	540	Total	C	N	O	S	0	0
			4136	2681	698	727	30		

There are 12 discrepancies between the modelled and reference sequences:

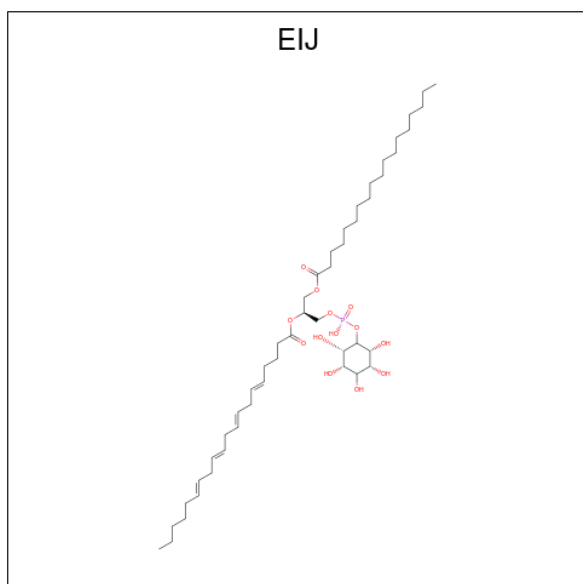
Chain	Residue	Modelled	Actual	Comment	Reference
A	776	LEU	-	expression tag	UNP Q5T848
A	777	GLU	-	expression tag	UNP Q5T848
A	778	VAL	-	expression tag	UNP Q5T848
A	779	LEU	-	expression tag	UNP Q5T848
A	780	PHE	-	expression tag	UNP Q5T848
A	781	GLN	-	expression tag	UNP Q5T848
B	776	LEU	-	expression tag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

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



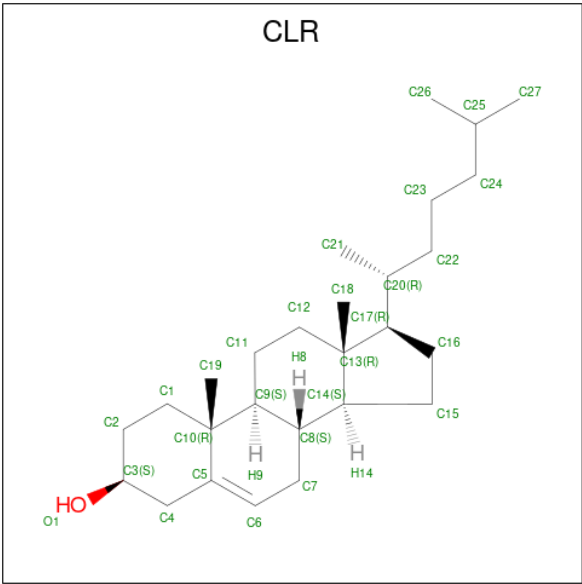
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 3 is (2S)-1-{[(S)-hydroxy{[(1s,2R,3R,4R,5S,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}-3-(octadecanoyloxy)propan-2-yl (5E,8E,11E,14E)-icosa-5,8,11,14-tetraenoate (CCD ID: EIJ) (formula: C₄₇H₈₃O₁₃P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			56	42	13	1	

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).



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

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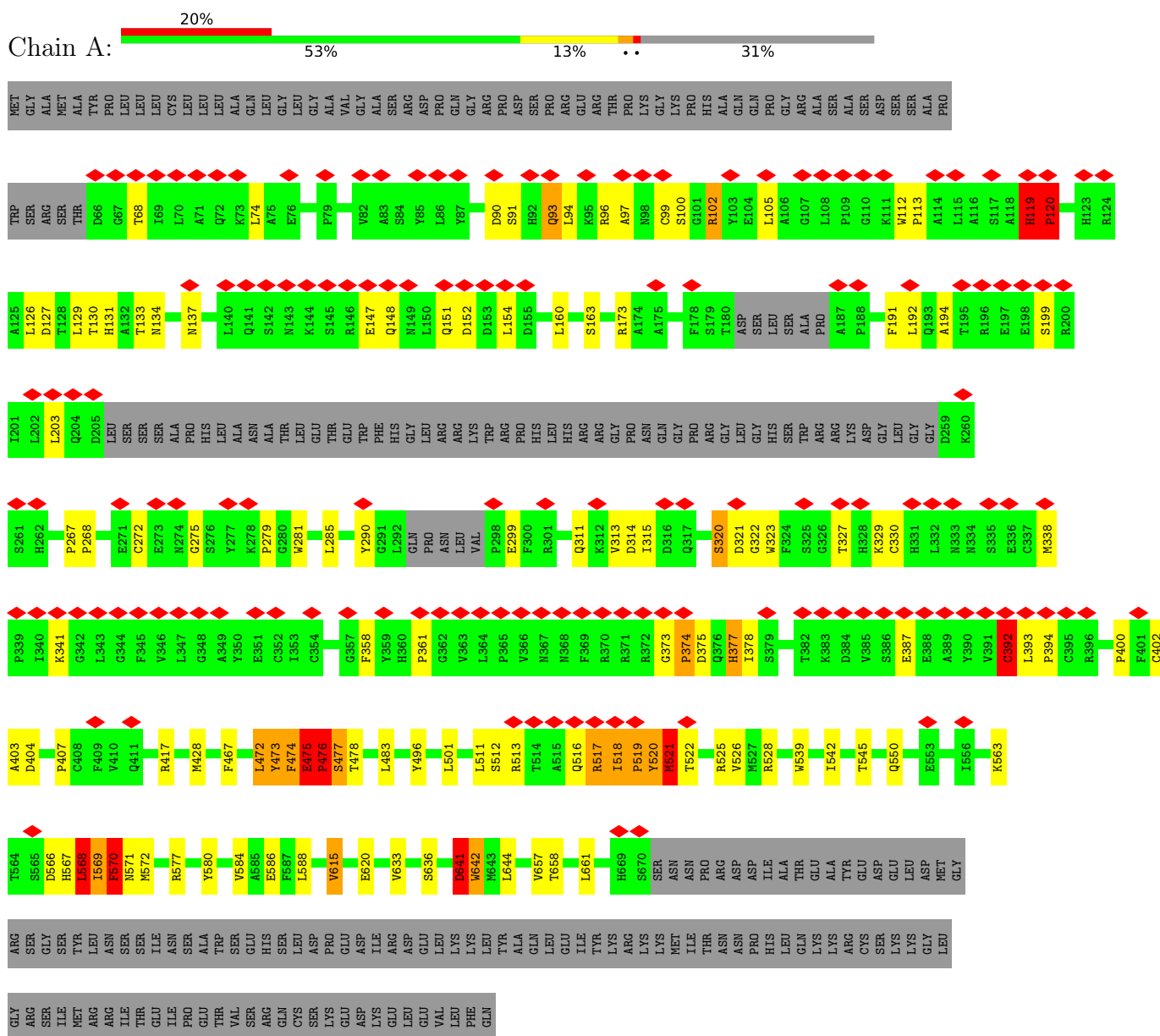
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Mol	Chain	Residues	Atoms			AltConf
4	B	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	B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

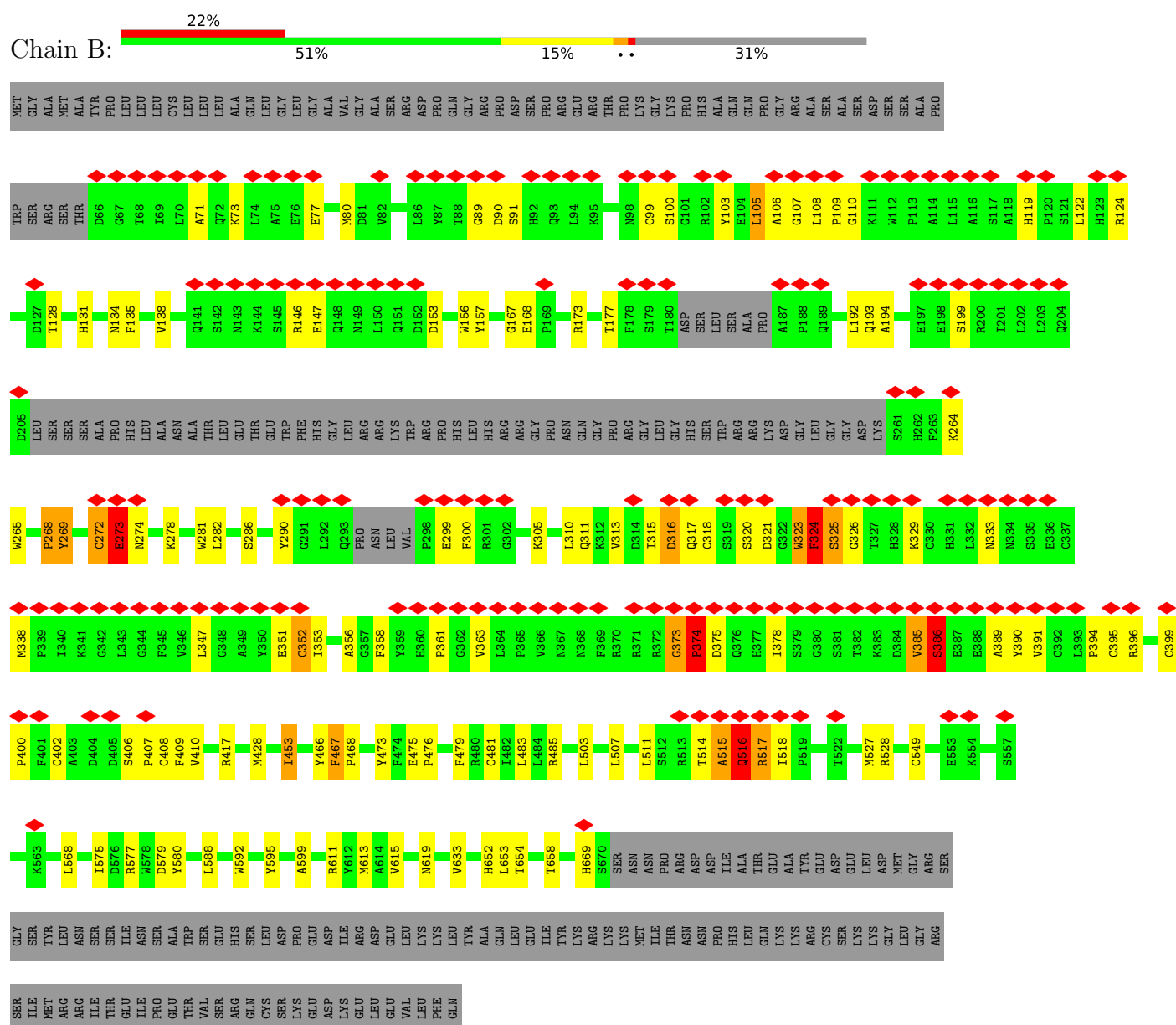
3 Residue-property plots

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: G-protein coupled receptor 158



- Molecule 1: G-protein coupled receptor 158



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	263237	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.034	Depositor
Minimum map value	-1.445	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.593	Depositor
Map size ($\text{\AA}$)	349.2, 349.2, 349.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.873, 0.873, 0.873	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.17	24/4233 (0.6%)	1.24	60/5761 (1.0%)
1	B	0.41	5/4240 (0.1%)	1.14	37/5772 (0.6%)
All	All	0.88	29/8473 (0.3%)	1.19	97/11533 (0.8%)

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	1	6
1	B	0	4
All	All	1	10

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	642	TRP	C-O	-25.21	0.90	1.24
1	A	570	PHE	C-O	-23.89	0.95	1.23
1	A	476	PRO	C-O	-23.63	0.93	1.24
1	A	374	PRO	N-CA	21.36	1.69	1.47
1	B	374	PRO	N-CA	17.36	1.69	1.47
1	A	569	ILE	C-O	-17.18	1.02	1.24
1	A	571	ASN	C-O	-17.02	1.03	1.23
1	A	120	PRO	N-CD	17.00	1.71	1.47
1	A	477	SER	C-O	-16.54	1.01	1.23
1	A	568	LEU	C-O	-14.70	1.07	1.24
1	A	474	PHE	C-O	-14.52	1.06	1.24
1	A	473	TYR	C-O	-13.60	1.06	1.24
1	A	373	GLY	C-N	13.55	1.44	1.33
1	A	475	GLU	C-O	-11.57	1.09	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	477	SER	CA-CB	-10.69	1.37	1.53
1	A	476	PRO	N-CD	-7.50	1.37	1.47
1	A	475	GLU	C-N	7.37	1.51	1.33
1	B	268	PRO	C-N	-7.33	1.24	1.33
1	A	642	TRP	CA-C	-6.42	1.44	1.52
1	B	269	TYR	C-O	-6.41	1.15	1.23
1	A	472	LEU	C-N	-6.28	1.25	1.34
1	A	476	PRO	N-CA	-6.24	1.39	1.47
1	A	477	SER	CA-C	-5.92	1.45	1.53
1	A	642	TRP	C-N	-5.91	1.25	1.33
1	B	80	MET	C-O	-5.77	1.16	1.24
1	A	521	MET	C-O	-5.15	1.18	1.24
1	A	569	ILE	CA-CB	-5.15	1.48	1.54
1	B	373	GLY	C-N	5.09	1.45	1.33
1	A	473	TYR	CZ-OH	-5.00	1.27	1.38

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	390	TYR	N-CA-C	38.49	160.85	113.50
1	A	516	GLN	N-CA-C	32.09	152.37	113.23
1	A	403	ALA	N-CA-C	26.21	139.54	110.97
1	B	391	VAL	N-CA-CB	-20.27	87.74	110.65
1	B	389	ALA	N-CA-C	19.93	136.84	109.54
1	A	474	PHE	CA-C-O	-19.25	98.75	120.69
1	A	373	GLY	CA-C-N	18.08	141.97	121.00
1	A	373	GLY	C-N-CA	18.08	141.97	121.00
1	B	385	VAL	CB-CA-C	-18.07	86.02	110.42
1	B	100	SER	N-CA-CB	-17.72	83.49	110.42
1	B	373	GLY	CA-C-N	17.01	141.10	119.84
1	B	373	GLY	C-N-CA	17.01	141.10	119.84
1	A	516	GLN	CB-CA-C	-15.36	85.62	111.26
1	A	402	CYS	N-CA-C	14.79	132.34	112.68
1	A	403	ALA	N-CA-CB	-13.56	90.12	109.91
1	B	99	CYS	CB-CA-C	-13.22	88.83	111.30
1	B	385	VAL	N-CA-C	13.15	127.23	107.77
1	A	320	SER	N-CA-C	-12.49	84.20	110.80
1	A	322	GLY	N-CA-C	11.91	141.40	113.18
1	B	99	CYS	N-CA-C	-11.25	88.19	107.99
1	B	323	TRP	CB-CA-C	-11.21	88.85	109.37
1	B	517	ARG	N-CA-C	11.04	127.56	109.02
1	A	568	LEU	CA-C-N	11.00	138.64	122.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	568	LEU	C-N-CA	11.00	138.64	122.91
1	B	374	PRO	CA-N-CD	-10.99	96.61	112.00
1	B	390	TYR	N-CA-CB	-10.91	94.50	110.53
1	A	374	PRO	CA-N-CD	-10.89	96.76	112.00
1	A	323	TRP	N-CA-CB	10.76	127.76	110.97
1	A	519	PRO	N-CA-C	10.04	133.14	112.47
1	A	323	TRP	N-CA-C	-9.90	95.17	108.24
1	B	390	TYR	CB-CA-C	-9.48	92.04	109.29
1	A	642	TRP	N-CA-C	-9.38	101.52	113.72
1	B	325	SER	N-CA-C	-9.06	92.17	108.02
1	B	300	PHE	N-CA-C	8.99	124.06	113.18
1	B	389	ALA	CB-CA-C	-8.90	91.08	111.83
1	A	474	PHE	N-CA-C	-8.75	95.84	109.76
1	A	571	ASN	CA-CB-CG	8.68	121.28	112.60
1	A	120	PRO	CA-N-CD	-8.64	99.90	112.00
1	B	517	ARG	N-CA-CB	-8.64	93.70	111.15
1	A	475	GLU	N-CA-C	8.56	128.73	109.81
1	B	269	TYR	CB-CA-C	8.32	129.98	111.09
1	A	475	GLU	O-C-N	-8.22	111.86	121.32
1	A	93	GLN	N-CA-C	-8.14	102.23	112.90
1	B	324	PHE	N-CA-C	8.08	128.00	110.80
1	A	571	ASN	CB-CA-C	-8.02	95.94	109.65
1	A	321	ASP	N-CA-CB	-7.98	99.97	111.54
1	A	476	PRO	CA-C-N	7.83	134.91	121.29
1	A	476	PRO	C-N-CA	7.83	134.91	121.29
1	B	386	SER	N-CA-C	-7.79	94.21	110.80
1	A	517	ARG	N-CA-CB	-7.77	99.75	111.56
1	A	477	SER	CB-CA-C	-7.57	94.42	111.30
1	B	324	PHE	CB-CA-C	-7.49	95.52	110.42
1	A	119	HIS	C-N-CD	-7.28	95.16	125.00
1	B	268	PRO	CA-C-N	-7.24	110.00	121.87
1	B	268	PRO	C-N-CA	-7.24	110.00	121.87
1	A	475	GLU	N-CA-CB	-7.24	97.49	110.37
1	A	517	ARG	N-CA-C	-7.22	97.30	108.42
1	A	570	PHE	CA-C-O	-7.14	112.03	120.60
1	A	570	PHE	N-CA-CB	-7.08	98.46	111.13
1	B	269	TYR	N-CA-CB	-7.07	100.39	111.56
1	B	272	CYS	N-CA-C	6.85	121.38	112.89
1	A	377	HIS	CA-C-N	6.82	134.25	121.97
1	A	377	HIS	C-N-CA	6.82	134.25	121.97
1	A	120	PRO	N-CA-C	-6.68	98.71	112.47
1	B	272	CYS	CB-CA-C	-6.68	96.04	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	GLU	N-CA-CB	-6.62	99.30	110.49
1	A	404	ASP	N-CA-C	-6.50	99.78	108.74
1	A	392	CYS	CA-C-O	-6.49	111.58	119.43
1	B	300	PHE	N-CA-CB	-6.48	99.52	110.41
1	A	374	PRO	CB-CA-C	6.38	117.15	110.00
1	A	102	ARG	CA-C-N	-6.27	107.82	121.87
1	A	102	ARG	C-N-CA	-6.27	107.82	121.87
1	A	641	ASP	O-C-N	-6.21	113.90	122.46
1	A	474	PHE	CB-CA-C	6.20	119.95	109.84
1	B	516	GLN	CA-C-N	6.12	135.30	121.53
1	B	516	GLN	C-N-CA	6.12	135.30	121.53
1	A	473	TYR	CA-C-N	6.04	130.13	121.50
1	A	473	TYR	C-N-CA	6.04	130.13	121.50
1	A	568	LEU	N-CA-C	-5.87	97.58	108.02
1	B	105	LEU	N-CA-C	-5.72	106.94	114.04
1	A	519	PRO	N-CD-CG	-5.71	94.63	103.20
1	A	120	PRO	N-CA-CB	5.67	109.21	103.25
1	B	321	ASP	N-CA-C	5.55	122.62	110.80
1	A	475	GLU	CA-C-N	5.49	126.70	119.84
1	A	475	GLU	C-N-CA	5.49	126.70	119.84
1	A	642	TRP	CA-C-O	-5.41	113.09	119.05
1	A	476	PRO	N-CD-CG	-5.31	95.24	103.20
1	B	515	ALA	CB-CA-C	5.28	121.15	110.38
1	A	403	ALA	CB-CA-C	-5.14	103.05	110.96
1	A	517	ARG	O-C-N	-5.13	118.38	123.46
1	A	119	HIS	CB-CA-C	5.13	120.27	110.17
1	A	404	ASP	N-CA-CB	5.08	119.69	111.21
1	A	519	PRO	N-CA-CB	-5.05	97.94	103.25
1	A	567	HIS	CA-C-N	5.03	130.00	122.86
1	A	567	HIS	C-N-CA	5.03	130.00	122.86
1	B	516	GLN	CB-CA-C	-5.02	100.44	110.42
1	B	385	VAL	O-C-N	-5.01	117.96	123.18

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	402	CYS	CA

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	472	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	474	PHE	Mainchain
1	A	566	ASP	Mainchain
1	A	570	PHE	Mainchain
1	A	641	ASP	Mainchain
1	A	642	TRP	Mainchain
1	B	268	PRO	Mainchain
1	B	278	LYS	Peptide
1	B	352	CYS	Peptide
1	B	467	PHE	Peptide

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	4131	0	3987	136	0
1	B	4136	0	3995	140	0
2	A	51	0	82	4	0
3	A	56	0	0	4	0
4	A	308	0	504	55	0
4	B	308	0	506	76	0
All	All	8990	0	9074	325	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 (325) 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:B:103:TYR:HE1	1:B:106:ALA:CB	1.20	1.52
1:A:374:PRO:CA	1:A:374:PRO:N	1.69	1.49
1:B:580:TYR:CD2	4:B:805:CLR:H151	1.51	1.46
1:B:374:PRO:N	1:B:374:PRO:CA	1.69	1.46
1:A:120:PRO:N	1:A:120:PRO:CD	1.71	1.45
1:A:513:ARG:CD	1:A:518:ILE:HD11	1.44	1.44
1:B:103:TYR:CE1	1:B:106:ALA:HB2	1.54	1.43
1:A:513:ARG:HD2	1:A:518:ILE:CD1	1.56	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:TYR:CE1	1:B:106:ALA:CB	2.09	1.31
1:A:407:PRO:O	1:A:568:LEU:HD12	1.10	1.27
1:A:475:GLU:OE1	1:A:476:PRO:HD2	1.39	1.22
1:A:407:PRO:O	1:A:568:LEU:CD1	1.87	1.22
1:B:577:ARG:NH2	4:B:806:CLR:H22	1.53	1.21
1:A:580:TYR:HE2	4:A:809:CLR:H112	1.05	1.17
1:B:103:TYR:HE1	1:B:106:ALA:HB3	1.11	1.16
1:B:580:TYR:CD2	4:B:805:CLR:C15	2.27	1.16
1:B:588:LEU:HD22	4:B:801:CLR:H212	1.19	1.13
4:A:806:CLR:H152	4:A:807:CLR:H12	1.33	1.11
1:B:580:TYR:CE2	4:B:805:CLR:H151	1.86	1.10
1:B:580:TYR:HD2	4:B:805:CLR:C15	1.63	1.09
4:A:808:CLR:H191	4:B:807:CLR:H122	1.37	1.07
1:A:119:HIS:C	1:A:120:PRO:CD	2.26	1.06
1:A:580:TYR:HE2	4:A:809:CLR:C11	1.69	1.05
1:A:563:LYS:CD	1:A:569:ILE:HG22	1.86	1.04
1:B:652:HIS:O	4:B:804:CLR:C26	2.07	1.03
1:A:577:ARG:HH21	4:A:810:CLR:H192	1.18	1.02
1:B:588:LEU:HD22	4:B:801:CLR:C21	1.90	1.01
1:A:580:TYR:CE2	4:A:809:CLR:H112	1.95	1.01
1:B:528:ARG:HD2	4:B:807:CLR:H193	1.40	1.00
1:A:513:ARG:CG	1:A:518:ILE:HG13	1.91	0.99
1:A:513:ARG:HG2	1:A:518:ILE:HG13	1.46	0.98
1:B:103:TYR:CD1	1:B:106:ALA:HB2	1.98	0.98
1:A:513:ARG:CD	1:A:518:ILE:CD1	2.28	0.96
1:B:577:ARG:HH21	4:B:806:CLR:H22	1.13	0.96
1:B:105:LEU:HB3	1:B:324:PHE:CE1	2.01	0.94
1:B:652:HIS:O	4:B:804:CLR:H262	1.68	0.94
1:A:341:LYS:HA	1:A:375:ASP:CB	1.98	0.93
1:B:483:LEU:CD1	4:B:811:CLR:H213	2.00	0.91
1:B:105:LEU:CB	1:B:324:PHE:CE1	2.55	0.90
1:A:520:TYR:CE1	1:A:526:VAL:CG2	2.54	0.90
1:B:580:TYR:HD2	4:B:805:CLR:H151	1.09	0.90
1:A:475:GLU:OE1	1:A:476:PRO:CD	2.20	0.90
1:B:105:LEU:CB	1:B:324:PHE:HE1	1.85	0.90
1:A:563:LYS:HD2	1:A:569:ILE:HG22	1.53	0.89
1:B:549:CYS:SG	4:B:810:CLR:H11	2.14	0.88
1:A:513:ARG:CG	1:A:518:ILE:CG1	2.51	0.88
1:B:577:ARG:NH2	4:B:806:CLR:H192	1.89	0.88
1:A:513:ARG:CG	1:A:518:ILE:CD1	2.53	0.86
1:A:520:TYR:CE1	1:A:526:VAL:HG22	2.11	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ARG:CG	1:A:518:ILE:HD11	2.07	0.84
4:A:808:CLR:C19	4:B:807:CLR:H122	2.07	0.84
1:A:374:PRO:HG3	1:A:400:PRO:HB3	1.56	0.84
1:A:407:PRO:HA	1:A:568:LEU:HD11	1.59	0.84
1:B:103:TYR:CE1	1:B:106:ALA:HB3	1.92	0.84
1:B:105:LEU:HB3	1:B:324:PHE:CD1	2.13	0.83
1:B:375:ASP:O	1:B:396:ARG:CB	2.25	0.83
1:A:520:TYR:HE1	1:A:526:VAL:CG2	1.91	0.83
1:A:320:SER:O	1:A:327:THR:N	2.11	0.83
1:B:577:ARG:HH21	4:B:806:CLR:C2	1.92	0.83
1:B:324:PHE:O	1:B:324:PHE:CG	2.32	0.82
1:B:577:ARG:HH21	4:B:806:CLR:H192	1.43	0.82
1:B:273:GLU:CD	1:B:274:ASN:H	1.89	0.81
1:A:517:ARG:HG2	1:A:519:PRO:HG3	1.60	0.80
1:B:595:TYR:CE2	4:B:801:CLR:O1	2.35	0.80
1:A:545:THR:HG22	4:A:806:CLR:H151	1.62	0.80
1:B:669:HIS:ND1	4:B:804:CLR:O1	1.77	0.80
1:B:333:ASN:ND2	1:B:352:CYS:SG	2.55	0.80
1:B:269:TYR:O	1:B:281:TRP:HA	1.83	0.79
1:A:580:TYR:CE2	4:A:809:CLR:C11	2.61	0.79
4:A:806:CLR:H152	4:A:807:CLR:C1	2.12	0.79
1:A:513:ARG:HG3	1:A:518:ILE:HG13	1.64	0.78
1:B:105:LEU:HB2	1:B:324:PHE:HE1	1.48	0.78
1:B:619:ASN:ND2	4:B:803:CLR:H213	1.98	0.77
1:B:483:LEU:CD1	4:B:811:CLR:C21	2.62	0.77
1:A:577:ARG:NH2	4:A:810:CLR:H192	1.99	0.77
1:B:580:TYR:HD2	4:B:805:CLR:C16	1.98	0.77
1:A:520:TYR:HE1	1:A:526:VAL:HG23	1.50	0.76
1:A:520:TYR:CE1	1:A:526:VAL:HG23	2.20	0.76
4:A:803:CLR:H182	4:A:803:CLR:H72	1.67	0.76
1:A:539:TRP:HA	4:B:806:CLR:H272	1.67	0.75
1:B:453:ILE:HD11	4:B:808:CLR:H6	1.69	0.75
1:A:528:ARG:HB3	4:A:804:CLR:H193	1.70	0.74
4:B:802:CLR:H182	4:B:802:CLR:H72	1.68	0.73
3:A:802:EIJ:O18	4:A:808:CLR:H21	1.88	0.72
1:A:513:ARG:HG3	1:A:518:ILE:CG1	2.18	0.72
1:A:580:TYR:CE2	4:A:809:CLR:C12	2.72	0.72
1:A:513:ARG:HG2	1:A:518:ILE:CG1	2.16	0.71
1:A:528:ARG:HB3	4:A:804:CLR:C19	2.20	0.71
1:A:341:LYS:CB	1:A:375:ASP:CB	2.69	0.71
1:A:545:THR:CG2	4:A:806:CLR:H151	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ILE:HD12	4:B:809:CLR:H11	1.73	0.70
1:A:341:LYS:CA	1:A:375:ASP:CB	2.69	0.70
1:A:588:LEU:HD22	4:A:808:CLR:H212	1.74	0.70
1:A:314:ASP:HB3	1:A:361:PRO:HG2	1.74	0.70
1:B:479:PHE:HE2	4:B:811:CLR:H122	1.56	0.69
1:B:317:GLN:NE2	1:B:320:SER:OG	2.18	0.69
1:A:130:THR:O	1:A:134:ASN:ND2	2.26	0.68
1:B:105:LEU:HD23	1:B:324:PHE:CD1	2.27	0.68
1:A:563:LYS:HD3	1:A:569:ILE:HG22	1.75	0.68
1:A:615:VAL:HB	4:A:811:CLR:H182	1.77	0.67
1:A:147:GLU:HG2	1:A:148:GLN:H	1.59	0.67
1:B:615:VAL:HG11	4:B:803:CLR:H122	1.76	0.67
1:A:580:TYR:HE2	4:A:809:CLR:C12	2.08	0.66
1:B:577:ARG:HH22	4:B:806:CLR:H22	1.56	0.66
1:A:580:TYR:CD2	4:A:809:CLR:H121	2.31	0.66
1:A:377:HIS:CB	1:A:393:LEU:HA	2.26	0.66
1:B:71:ALA:HB2	1:B:329:LYS:HE3	1.78	0.66
1:B:194:ALA:HB3	1:B:199:SER:HA	1.77	0.66
1:A:615:VAL:HB	4:A:811:CLR:C18	2.25	0.65
4:A:804:CLR:H192	4:A:804:CLR:O1	1.96	0.65
1:B:527:MET:CE	4:B:808:CLR:H72	2.26	0.65
1:A:119:HIS:C	1:A:120:PRO:HD3	2.22	0.63
4:B:801:CLR:H242	4:B:801:CLR:H211	1.79	0.63
1:A:580:TYR:CE2	4:A:809:CLR:H121	2.33	0.63
1:B:105:LEU:CD2	1:B:324:PHE:CE1	2.81	0.63
1:B:483:LEU:HD11	4:B:811:CLR:H213	1.78	0.62
1:B:619:ASN:ND2	4:B:803:CLR:C21	2.61	0.62
1:B:89:GLY:O	1:B:91:SER:N	2.33	0.62
1:B:669:HIS:CE1	4:B:804:CLR:H1	2.06	0.62
1:A:194:ALA:HB3	1:A:199:SER:HA	1.81	0.61
1:B:324:PHE:O	1:B:324:PHE:CD2	2.53	0.61
1:B:128:THR:HA	1:B:131:HIS:CE1	2.35	0.61
1:B:417:ARG:NH2	1:B:473:TYR:O	2.34	0.61
1:A:542:ILE:HG21	4:B:806:CLR:H222	1.83	0.60
1:B:479:PHE:CE2	4:B:811:CLR:H122	2.35	0.60
1:A:154:LEU:HD11	1:A:191:PHE:HZ	1.67	0.60
1:B:528:ARG:CD	4:B:807:CLR:H193	2.24	0.60
1:B:669:HIS:CE1	4:B:804:CLR:O1	2.52	0.60
4:B:811:CLR:C24	4:B:811:CLR:H211	2.32	0.59
1:A:191:PHE:HE1	1:A:203:LEU:HD13	1.67	0.59
1:B:105:LEU:HD23	1:B:324:PHE:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:CYS:HA	1:B:325:SER:HB3	1.85	0.59
2:A:801:PEE:O2P	3:A:802:EIJ:O52	2.21	0.58
1:A:154:LEU:HD11	1:A:191:PHE:CZ	2.38	0.58
1:B:105:LEU:HD21	1:B:329:LYS:HE2	1.86	0.58
1:A:112:TRP:HZ2	1:A:267:PRO:HA	1.68	0.58
4:A:809:CLR:H272	4:A:809:CLR:H211	1.85	0.58
1:B:315:ILE:HG12	1:B:356:ALA:HA	1.85	0.58
1:A:513:ARG:HG2	1:A:518:ILE:CD1	2.30	0.58
1:A:131:HIS:HA	1:A:134:ASN:HD22	1.67	0.58
1:A:152:ASP:OD1	1:B:146:ARG:NH2	2.36	0.58
1:B:193:GLN:HB3	1:B:199:SER:HB2	1.84	0.58
1:B:317:GLN:HE21	1:B:320:SER:HG	1.50	0.58
1:B:290:TYR:HA	1:B:299:GLU:HG2	1.85	0.58
1:B:577:ARG:CZ	4:B:806:CLR:H192	2.34	0.58
1:A:512:SER:OG	1:A:519:PRO:HD3	2.04	0.57
1:A:68:THR:HG22	1:A:330:CYS:H	1.69	0.57
1:B:654:THR:O	1:B:658:THR:OG1	2.23	0.57
1:A:74:LEU:HD21	1:A:105:LEU:HD12	1.87	0.57
1:A:563:LYS:CE	1:A:569:ILE:HG22	2.35	0.57
4:A:809:CLR:H272	4:A:809:CLR:C21	2.35	0.56
1:B:385:VAL:O	1:B:386:SER:CB	2.51	0.56
1:B:483:LEU:HD13	4:B:811:CLR:H213	1.88	0.56
1:B:483:LEU:HD12	4:B:811:CLR:C21	2.34	0.56
1:A:417:ARG:NH2	1:A:641:ASP:OD1	2.39	0.56
4:A:808:CLR:C19	4:B:807:CLR:C12	2.83	0.56
1:A:572:MET:HE1	1:A:636:SER:HA	1.88	0.56
1:B:588:LEU:CD2	4:B:801:CLR:C21	2.77	0.56
1:B:326:GLY:H	1:B:329:LYS:HG3	1.71	0.55
1:A:476:PRO:O	1:A:476:PRO:HG2	2.06	0.55
1:A:377:HIS:HA	1:A:393:LEU:HA	1.89	0.55
1:A:513:ARG:HD2	1:A:518:ILE:HD11	0.64	0.55
4:B:801:CLR:H213	4:B:801:CLR:H183	1.88	0.55
1:A:392:CYS:O	1:A:392:CYS:SG	2.63	0.55
4:A:810:CLR:H183	4:A:810:CLR:H212	1.89	0.54
1:A:407:PRO:C	1:A:568:LEU:CD1	2.73	0.54
1:A:127:ASP:HA	1:A:130:THR:HG22	1.89	0.54
1:B:311:GLN:NE2	1:B:358:PHE:O	2.40	0.54
1:B:549:CYS:SG	4:B:810:CLR:C1	2.93	0.54
1:B:105:LEU:HB2	1:B:324:PHE:CE1	2.32	0.54
1:B:315:ILE:HG21	1:B:356:ALA:HA	1.90	0.54
1:B:527:MET:HE3	4:B:808:CLR:H72	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:809:CLR:H213	4:A:809:CLR:C27	2.38	0.54
1:A:580:TYR:CD2	4:A:809:CLR:C12	2.90	0.53
1:B:105:LEU:CD2	1:B:329:LYS:HE2	2.38	0.53
1:B:323:TRP:O	1:B:325:SER:N	2.34	0.53
1:B:669:HIS:HD1	4:B:804:CLR:H1	0.55	0.52
1:A:521:MET:HE2	1:A:522:THR:H	1.75	0.52
1:B:124:ARG:NH2	1:B:167:GLY:O	2.43	0.52
4:B:811:CLR:H211	4:B:811:CLR:H242	1.89	0.52
1:A:374:PRO:CG	1:A:400:PRO:HB3	2.35	0.51
1:A:528:ARG:CB	4:A:804:CLR:H193	2.39	0.51
1:A:407:PRO:CA	1:A:568:LEU:HD11	2.38	0.51
4:A:809:CLR:C21	4:A:809:CLR:C27	2.88	0.51
1:A:661:LEU:HD21	4:A:812:CLR:H193	1.93	0.51
1:B:374:PRO:HB3	1:B:400:PRO:HA	1.92	0.51
1:A:68:THR:HA	1:A:329:LYS:HA	1.92	0.51
1:A:584:VAL:O	1:A:588:LEU:HG	2.10	0.51
4:A:806:CLR:H8	4:A:807:CLR:H21	1.92	0.51
1:B:408:CYS:SG	1:B:409:PHE:N	2.78	0.51
1:B:515:ALA:O	1:B:516:GLN:CB	2.59	0.51
1:B:399:CYS:SG	1:B:408:CYS:HB3	2.50	0.51
1:B:428:MET:HE2	1:B:466:TYR:HB3	1.93	0.50
1:B:515:ALA:O	1:B:516:GLN:HB2	2.10	0.50
1:B:177:THR:HG23	1:B:305:LYS:NZ	2.27	0.50
1:B:575:ILE:HG23	1:B:579:ASP:HB2	1.92	0.50
1:B:653:LEU:HD22	4:B:803:CLR:H241	1.92	0.50
1:B:272:CYS:O	1:B:273:GLU:C	2.54	0.50
1:B:580:TYR:HD2	4:B:805:CLR:H161	1.77	0.50
4:B:806:CLR:H181	4:B:806:CLR:H221	1.94	0.50
1:A:570:PHE:O	1:A:570:PHE:CD2	2.66	0.49
4:A:808:CLR:H182	4:B:807:CLR:H17	1.94	0.49
4:A:809:CLR:H213	4:A:809:CLR:H273	1.93	0.49
1:B:264:LYS:HZ2	1:B:286:SER:HB3	1.76	0.49
1:A:633:VAL:HG22	4:A:809:CLR:H191	1.93	0.49
1:B:347:LEU:HA	1:B:351:GLU:HA	1.94	0.49
1:B:269:TYR:HB3	1:B:282:LEU:O	2.12	0.49
1:A:191:PHE:CE1	1:A:203:LEU:HD13	2.47	0.48
1:A:290:TYR:HA	1:A:299:GLU:HA	1.93	0.48
1:B:592:TRP:CD1	4:B:801:CLR:H6	2.49	0.48
1:A:417:ARG:HG2	1:A:473:TYR:HE1	1.78	0.48
4:B:801:CLR:H213	4:B:801:CLR:C18	2.43	0.48
1:B:122:LEU:HD12	1:B:265:TRP:HH2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:808:CLR:H222	4:A:808:CLR:C18	2.43	0.48
4:B:801:CLR:C21	4:B:801:CLR:H242	2.40	0.48
4:A:809:CLR:H222	4:A:809:CLR:C18	2.44	0.48
1:B:134:ASN:O	1:B:138:VAL:HG23	2.13	0.48
1:A:320:SER:O	1:A:327:THR:OG1	2.28	0.48
4:A:803:CLR:H72	4:A:803:CLR:C18	2.42	0.48
1:A:569:ILE:O	1:A:569:ILE:HG13	2.12	0.47
1:A:119:HIS:HD2	1:A:313:VAL:HG22	1.79	0.47
1:A:588:LEU:HD22	4:A:808:CLR:C21	2.43	0.47
1:A:550:GLN:HB2	1:B:577:ARG:HH11	1.79	0.47
1:B:615:VAL:CG1	4:B:803:CLR:H122	2.44	0.47
1:A:112:TRP:HE3	1:A:113:PRO:HD3	1.80	0.47
1:B:310:LEU:HD12	1:B:313:VAL:HG21	1.97	0.47
1:B:511:LEU:O	1:B:514:THR:OG1	2.32	0.47
1:A:133:THR:O	1:A:137:ASN:N	2.47	0.46
4:A:808:CLR:H25	4:A:810:CLR:H262	1.98	0.46
1:B:107:GLY:O	1:B:110:GLY:N	2.49	0.46
4:A:803:CLR:H232	4:A:803:CLR:H161	1.98	0.46
4:B:802:CLR:H72	4:B:802:CLR:C18	2.42	0.46
1:B:373:GLY:HA3	1:B:374:PRO:HD3	1.73	0.46
1:B:410:VAL:HG22	1:B:568:LEU:HD13	1.98	0.46
1:A:173:ARG:HE	1:A:192:LEU:HB2	1.81	0.46
1:A:377:HIS:CA	1:A:393:LEU:HA	2.46	0.45
1:A:417:ARG:HG2	1:A:473:TYR:CE1	2.51	0.45
1:B:108:LEU:HD23	1:B:326:GLY:HA3	1.97	0.45
1:B:503:LEU:HD13	1:B:613:MET:HE3	1.99	0.45
1:B:73:LYS:O	1:B:77:GLU:HG2	2.17	0.45
1:B:517:ARG:HG3	1:B:518:ILE:H	1.81	0.45
1:A:496:TYR:OH	1:A:658:THR:OG1	2.30	0.45
4:B:811:CLR:C21	4:B:811:CLR:H242	2.46	0.45
1:B:315:ILE:HG23	1:B:315:ILE:O	2.17	0.45
1:B:316:ASP:OD1	1:B:323:TRP:N	2.49	0.45
1:A:550:GLN:HG3	1:B:577:ARG:HD2	1.99	0.44
1:A:586:GLU:HG3	2:A:801:PEE:H81	1.98	0.44
1:B:507:LEU:HD13	1:B:599:ALA:HB1	1.99	0.44
2:A:801:PEE:H60	2:A:801:PEE:H55	1.75	0.44
1:A:279:PRO:O	1:A:311:GLN:NE2	2.50	0.44
3:A:802:EIJ:O45	3:A:802:EIJ:O54	2.35	0.44
1:A:90:ASP:O	1:A:94:LEU:HG	2.17	0.44
4:B:806:CLR:H221	4:B:806:CLR:C18	2.47	0.44
4:A:803:CLR:C16	4:A:803:CLR:C23	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:ILE:O	1:A:569:ILE:CG1	2.64	0.44
1:A:657:VAL:HG11	4:A:812:CLR:H183	2.00	0.44
4:A:809:CLR:H221	4:A:809:CLR:H162	1.83	0.44
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.82	0.44
1:A:160:LEU:O	1:A:163:SER:OG	2.27	0.44
4:B:806:CLR:C18	4:B:806:CLR:C22	2.96	0.44
4:B:808:CLR:H213	4:B:808:CLR:H161	1.84	0.43
1:A:281:TRP:HE3	1:A:311:GLN:HE22	1.65	0.43
1:A:374:PRO:HB3	1:A:400:PRO:HA	2.00	0.43
1:B:361:PRO:HG2	1:B:363:VAL:HG22	1.98	0.43
1:B:467:PHE:N	1:B:468:PRO:HD2	2.34	0.43
1:B:549:CYS:SG	4:B:810:CLR:C2	3.06	0.43
1:A:475:GLU:OE1	1:A:475:GLU:CA	2.67	0.43
1:B:633:VAL:HG22	4:B:805:CLR:H12	2.01	0.43
4:B:801:CLR:H221	4:B:801:CLR:C12	2.48	0.43
1:A:112:TRP:HA	1:A:112:TRP:CE3	2.54	0.43
1:A:129:LEU:HD23	1:A:285:LEU:HD22	1.99	0.43
1:A:569:ILE:HD13	1:A:569:ILE:HG21	1.61	0.43
4:A:809:CLR:H273	4:A:809:CLR:H221	2.01	0.43
1:A:477:SER:OG	1:A:478:THR:N	2.48	0.43
1:A:93:GLN:O	1:A:94:LEU:C	2.61	0.43
3:A:802:EIJ:O18	4:A:808:CLR:C2	2.65	0.43
1:B:173:ARG:HH12	1:B:192:LEU:HD13	1.84	0.43
1:B:475:GLU:HG2	1:B:476:PRO:HD2	2.00	0.43
1:B:406:SER:HB3	1:B:407:PRO:HD3	2.00	0.43
1:B:481:CYS:SG	1:B:485:ARG:NH1	2.91	0.43
1:A:315:ILE:HD11	1:A:358:PHE:HB2	2.01	0.42
1:B:153:ASP:O	1:B:156:TRP:HB2	2.19	0.42
4:B:806:CLR:H221	4:B:806:CLR:H162	1.81	0.42
4:B:809:CLR:H263	4:B:809:CLR:H231	1.93	0.42
1:A:483:LEU:HD13	4:A:807:CLR:C15	2.49	0.42
4:B:808:CLR:H161	4:B:808:CLR:H231	2.01	0.42
4:A:809:CLR:H211	4:A:809:CLR:H232	1.84	0.42
1:A:475:GLU:OE1	1:A:475:GLU:C	2.62	0.42
4:A:808:CLR:H191	4:B:807:CLR:C12	2.27	0.42
1:B:352:CYS:O	1:B:353:ILE:C	2.63	0.42
1:B:395:CYS:HB3	1:B:402:CYS:HA	2.01	0.42
1:A:160:LEU:HD12	1:B:135:PHE:HE1	1.84	0.42
1:A:518:ILE:O	1:A:518:ILE:CG2	2.67	0.42
2:A:801:PEE:H34	2:A:801:PEE:H39	1.89	0.42
1:B:147:GLU:OE2	1:B:157:TYR:OH	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:SER:O	1:A:94:LEU:HB2	2.20	0.42
1:B:108:LEU:HB3	1:B:109:PRO:HD3	2.01	0.42
1:B:316:ASP:CG	1:B:317:GLN:H	2.26	0.42
4:B:808:CLR:H14	4:B:808:CLR:H212	2.02	0.42
4:A:808:CLR:H221	4:A:808:CLR:H162	1.85	0.42
1:B:611:ARG:NH1	4:B:803:CLR:H3	2.35	0.42
1:B:592:TRP:HD1	4:B:801:CLR:H6	1.84	0.42
1:A:126:LEU:HD13	1:A:285:LEU:HD11	2.02	0.41
1:A:496:TYR:CZ	1:A:620:GLU:HG3	2.55	0.41
1:A:511:LEU:HD23	1:A:511:LEU:HA	1.91	0.41
1:A:563:LYS:HE3	1:A:569:ILE:CG2	2.50	0.41
1:B:105:LEU:HD21	1:B:329:LYS:CE	2.51	0.41
1:A:428:MET:HE1	1:A:467:PHE:CZ	2.56	0.41
1:B:517:ARG:CG	1:B:518:ILE:H	2.33	0.41
1:A:112:TRP:CZ2	1:A:268:PRO:HD3	2.55	0.41
1:A:501:LEU:HB3	1:A:526:VAL:HG13	2.03	0.41
1:A:525:ARG:HA	1:A:525:ARG:HD2	1.85	0.41
4:A:808:CLR:H183	4:B:807:CLR:H221	2.03	0.41
4:B:804:CLR:H272	4:B:804:CLR:H232	1.91	0.41
1:A:96:ARG:O	1:A:275:GLY:HA2	2.21	0.41
1:A:644:LEU:HD23	1:A:644:LEU:HA	1.92	0.41
1:B:124:ARG:NH2	1:B:168:GLU:HG3	2.36	0.41
1:A:407:PRO:HA	1:A:568:LEU:CD1	2.42	0.41
4:A:809:CLR:H222	4:A:809:CLR:H183	2.02	0.41
1:A:520:TYR:CZ	1:A:526:VAL:HG22	2.53	0.40
1:A:151:GLN:HE21	1:B:146:ARG:HH12	1.70	0.40
4:A:808:CLR:H222	4:A:808:CLR:H183	2.04	0.40
1:B:375:ASP:C	1:B:396:ARG:CB	2.94	0.40
1:B:518:ILE:HG23	1:B:518:ILE:O	2.20	0.40
1:B:107:GLY:O	1:B:110:GLY:C	2.64	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	533/781 (68%)	449 (84%)	75 (14%)	9 (2%)	7	28
1	B	532/781 (68%)	446 (84%)	75 (14%)	11 (2%)	5	24
All	All	1065/1562 (68%)	895 (84%)	150 (14%)	20 (2%)	8	26

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	A	338	MET
1	A	378	ILE
1	A	394	PRO
1	B	90	ASP
1	B	273	GLU
1	B	324	PHE
1	B	338	MET
1	B	386	SER
1	B	394	PRO
1	A	97	ALA
1	A	272	CYS
1	B	374	PRO
1	B	378	ILE
1	B	516	GLN
1	A	120	PRO
1	B	316	ASP
1	A	387	GLU
1	B	119	HIS
1	A	99	CYS

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	424/677 (63%)	413 (97%)	11 (3%)	40	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	426/677 (63%)	425 (100%)	1 (0%)	87	85
All	All	850/1354 (63%)	838 (99%)	12 (1%)	57	70

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	SER
1	A	102	ARG
1	A	120	PRO
1	A	392	CYS
1	A	475	GLU
1	A	476	PRO
1	A	518	ILE
1	A	520	TYR
1	A	521	MET
1	A	568	LEU
1	A	615	VAL
1	B	453	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	561	GLN
1	A	608	HIS
1	B	333	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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$
4	CLR	B	801	-	31,31,31	1.19	3 (9%)	48,48,48	2.65	18 (37%)
4	CLR	A	805	-	31,31,31	0.28	0	48,48,48	0.33	0
4	CLR	A	813	-	31,31,31	0.28	0	48,48,48	0.34	0
4	CLR	B	805	-	31,31,31	0.29	0	48,48,48	0.34	0
4	CLR	A	807	-	31,31,31	0.29	0	48,48,48	0.33	0
4	CLR	B	806	-	31,31,31	0.28	0	48,48,48	0.34	0
4	CLR	A	808	-	31,31,31	0.28	0	48,48,48	0.38	0
4	CLR	A	803	-	31,31,31	0.30	0	48,48,48	0.67	1 (2%)
4	CLR	A	812	-	31,31,31	0.29	0	48,48,48	0.32	0
4	CLR	B	807	-	31,31,31	0.28	0	48,48,48	0.32	0
4	CLR	B	810	-	31,31,31	0.29	0	48,48,48	0.33	0
4	CLR	B	804	-	31,31,31	0.27	0	48,48,48	0.36	0
4	CLR	A	810	-	31,31,31	0.28	0	48,48,48	0.33	0
4	CLR	A	806	-	31,31,31	0.30	0	48,48,48	0.33	0
2	PEE	A	801	-	50,50,50	1.15	6 (12%)	53,55,55	1.02	2 (3%)
4	CLR	A	809	-	31,31,31	0.27	0	48,48,48	0.39	0
4	CLR	A	804	-	31,31,31	0.29	0	48,48,48	0.35	0
4	CLR	A	811	-	31,31,31	0.29	0	48,48,48	0.32	0
4	CLR	B	809	-	31,31,31	0.29	0	48,48,48	0.32	0
4	CLR	B	802	-	31,31,31	0.29	0	48,48,48	0.67	1 (2%)
3	EIJ	A	802	-	56,56,61	1.48	7 (12%)	65,68,73	1.33	6 (9%)
4	CLR	B	808	-	31,31,31	0.29	0	48,48,48	0.32	0
4	CLR	B	811	-	31,31,31	0.29	0	48,48,48	0.32	0
4	CLR	B	803	-	31,31,31	0.28	0	48,48,48	0.33	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
4	CLR	B	801	-	-	6/10/68/68	0/4/4/4
4	CLR	A	805	-	-	8/10/68/68	0/4/4/4
4	CLR	A	813	-	-	3/10/68/68	0/4/4/4
4	CLR	B	805	-	-	2/10/68/68	0/4/4/4
4	CLR	A	807	-	-	2/10/68/68	0/4/4/4
4	CLR	B	806	-	-	7/10/68/68	0/4/4/4
4	CLR	A	808	-	-	4/10/68/68	0/4/4/4
4	CLR	A	803	-	1/1/10/11	5/10/68/68	0/4/4/4
4	CLR	A	812	-	-	3/10/68/68	0/4/4/4
4	CLR	B	807	-	-	3/10/68/68	0/4/4/4
4	CLR	B	810	-	-	5/10/68/68	0/4/4/4
4	CLR	B	804	-	-	4/10/68/68	0/4/4/4
4	CLR	A	810	-	-	4/10/68/68	0/4/4/4
4	CLR	A	806	-	-	7/10/68/68	0/4/4/4
2	PEE	A	801	-	-	32/54/54/54	-
4	CLR	A	809	-	-	7/10/68/68	0/4/4/4
4	CLR	A	804	-	-	8/10/68/68	0/4/4/4
4	CLR	A	811	-	-	8/10/68/68	0/4/4/4
4	CLR	B	809	-	-	4/10/68/68	0/4/4/4
4	CLR	B	802	-	1/1/10/11	6/10/68/68	0/4/4/4
3	EIJ	A	802	-	-	28/51/75/80	0/1/1/1
4	CLR	B	808	-	1/1/10/11	8/10/68/68	0/4/4/4
4	CLR	B	811	-	-	1/10/68/68	0/4/4/4
4	CLR	B	803	-	-	8/10/68/68	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	EIJ	C13-C12	4.24	1.55	1.31
3	A	802	EIJ	C10-C09	4.24	1.55	1.31
3	A	802	EIJ	C07-C06	3.96	1.54	1.31
3	A	802	EIJ	C04-C03	3.80	1.53	1.31
2	A	801	PEE	C18-C19	3.75	1.53	1.31
2	A	801	PEE	C39-C38	3.74	1.52	1.31
3	A	802	EIJ	O19-C17	3.25	1.43	1.34
3	A	802	EIJ	O22-C23	2.83	1.41	1.33
4	B	801	CLR	C8-C14	-2.81	1.48	1.53
2	A	801	PEE	O2-C2	-2.60	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	PEE	O3-C30	2.32	1.40	1.33
3	A	802	EIJ	C16-C17	2.28	1.57	1.50
2	A	801	PEE	O3-C3	-2.21	1.40	1.45
4	B	801	CLR	C7-C8	-2.14	1.49	1.53
2	A	801	PEE	O2-C10	2.11	1.40	1.34
4	B	801	CLR	C13-C14	-2.05	1.51	1.55

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	CLR	C17-C13-C14	-6.33	92.83	100.10
4	B	801	CLR	C4-C5-C10	5.98	124.08	116.42
4	B	801	CLR	C11-C9-C10	5.50	119.86	113.08
4	B	801	CLR	C7-C8-C14	-5.19	103.58	110.93
4	B	801	CLR	C4-C5-C6	-4.82	114.04	120.57
3	A	802	EIJ	C51-C49-C47	4.63	118.96	110.83
4	B	801	CLR	C3-C4-C5	4.38	119.04	112.05
4	B	801	CLR	O1-C3-C4	-4.28	100.08	109.71
3	A	802	EIJ	O19-C17-C16	4.27	120.73	111.48
2	A	801	PEE	O2-C10-C11	4.24	120.66	111.48
4	B	801	CLR	C12-C13-C17	4.10	122.64	116.60
4	B	801	CLR	C2-C3-C4	3.75	115.57	110.29
4	B	801	CLR	C11-C12-C13	3.73	119.03	112.74
4	B	801	CLR	C19-C10-C1	3.65	114.99	109.43
3	A	802	EIJ	C53-C51-C49	3.63	117.19	110.83
4	B	801	CLR	C7-C8-C9	3.51	113.77	109.72
4	B	801	CLR	C12-C11-C9	3.43	118.96	113.14
3	A	802	EIJ	C49-C47-C46	3.12	116.76	109.68
4	B	801	CLR	C1-C2-C3	2.92	114.35	110.48
3	A	802	EIJ	O22-C23-C25	2.77	120.29	111.83
4	B	801	CLR	C16-C17-C13	-2.76	100.59	103.84
2	A	801	PEE	O3-C30-C31	2.71	120.09	111.83
4	B	801	CLR	C10-C9-C8	2.43	116.27	112.71
3	A	802	EIJ	C02-C03-C04	-2.38	112.08	126.42
4	B	801	CLR	C12-C13-C14	2.27	110.64	107.25
4	B	801	CLR	C23-C22-C20	-2.16	109.04	115.08
4	B	802	CLR	C13-C14-C8	2.11	117.41	114.41
4	A	803	CLR	C13-C14-C8	2.08	117.36	114.41

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	803	CLR	C8
4	B	802	CLR	C8
4	B	808	CLR	C17

All (173) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	PEE	C4-O4P-P-O3P
2	A	801	PEE	C4-O4P-P-O2P
2	A	801	PEE	C4-O4P-P-O1P
4	A	812	CLR	C21-C20-C22-C23
4	B	806	CLR	C21-C20-C22-C23
4	B	808	CLR	C16-C17-C20-C22
4	A	803	CLR	C13-C17-C20-C22
4	B	803	CLR	C13-C17-C20-C22
4	B	804	CLR	C13-C17-C20-C22
4	B	810	CLR	C21-C20-C22-C23
4	A	803	CLR	C13-C17-C20-C21
4	B	803	CLR	C13-C17-C20-C21
4	B	802	CLR	C21-C20-C22-C23
4	B	804	CLR	C13-C17-C20-C21
4	A	813	CLR	C17-C20-C22-C23
4	B	806	CLR	C17-C20-C22-C23
4	A	804	CLR	C21-C20-C22-C23
4	A	805	CLR	C21-C20-C22-C23
4	A	811	CLR	C13-C17-C20-C22
4	B	801	CLR	C13-C17-C20-C22
4	A	813	CLR	C21-C20-C22-C23
4	A	803	CLR	C16-C17-C20-C21
4	B	803	CLR	C16-C17-C20-C21
4	B	804	CLR	C16-C17-C20-C21
4	B	808	CLR	C16-C17-C20-C21
4	A	806	CLR	C13-C17-C20-C22
2	A	801	PEE	C31-C30-O3-C3
4	B	805	CLR	C20-C22-C23-C24
4	A	810	CLR	C17-C20-C22-C23
4	A	812	CLR	C17-C20-C22-C23
2	A	801	PEE	C31-C32-C33-C34
4	A	805	CLR	C22-C23-C24-C25
4	B	808	CLR	C20-C22-C23-C24
4	B	806	CLR	C16-C17-C20-C21
4	A	811	CLR	C13-C17-C20-C21
2	A	801	PEE	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
3	A	802	EIJ	C14-C15-C16-C17
2	A	801	PEE	O5-C30-O3-C3
4	A	811	CLR	C20-C22-C23-C24
4	A	809	CLR	C13-C17-C20-C22
4	B	810	CLR	C17-C20-C22-C23
4	A	807	CLR	C22-C23-C24-C25
4	B	802	CLR	C22-C23-C24-C25
4	B	810	CLR	C22-C23-C24-C25
4	A	804	CLR	C20-C22-C23-C24
4	B	803	CLR	C20-C22-C23-C24
4	B	811	CLR	C22-C23-C24-C25
4	A	809	CLR	C13-C17-C20-C21
4	A	808	CLR	C20-C22-C23-C24
4	B	801	CLR	C16-C17-C20-C22
4	A	808	CLR	C13-C17-C20-C22
4	A	810	CLR	C21-C20-C22-C23
4	B	807	CLR	C20-C22-C23-C24
4	A	808	CLR	C13-C17-C20-C21
4	B	803	CLR	C16-C17-C20-C22
4	B	806	CLR	C13-C17-C20-C22
3	A	802	EIJ	C25-C23-O22-C21
4	A	806	CLR	C20-C22-C23-C24
4	A	807	CLR	C20-C22-C23-C24
4	A	813	CLR	C22-C23-C24-C25
4	A	808	CLR	C16-C17-C20-C21
4	A	809	CLR	C16-C17-C20-C21
4	B	806	CLR	C13-C17-C20-C21
4	A	811	CLR	C16-C17-C20-C21
4	A	806	CLR	C13-C17-C20-C21
4	A	804	CLR	C23-C24-C25-C27
4	B	806	CLR	C23-C24-C25-C27
3	A	802	EIJ	O24-C23-O22-C21
4	B	801	CLR	C16-C17-C20-C21
4	A	803	CLR	C16-C17-C20-C22
4	B	801	CLR	C23-C24-C25-C26
4	B	810	CLR	C23-C24-C25-C26
3	A	802	EIJ	C23-C25-C26-C27
4	B	804	CLR	C16-C17-C20-C22
4	A	804	CLR	C23-C24-C25-C26
4	B	801	CLR	C23-C24-C25-C27
4	B	807	CLR	C23-C24-C25-C26
4	B	810	CLR	C23-C24-C25-C27

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Mol	Chain	Res	Type	Atoms
4	A	806	CLR	C23-C24-C25-C26
4	B	807	CLR	C23-C24-C25-C27
3	A	802	EIJ	C16-C17-O19-C20
2	A	801	PEE	C32-C33-C34-C35
4	B	808	CLR	C23-C24-C25-C26
4	A	806	CLR	C16-C17-C20-C21
4	A	811	CLR	C16-C17-C20-C22
3	A	802	EIJ	O18-C17-O19-C20
4	B	806	CLR	C23-C24-C25-C26
4	A	805	CLR	C13-C17-C20-C22
4	B	808	CLR	C13-C17-C20-C22
2	A	801	PEE	C11-C12-C13-C14
2	A	801	PEE	C10-C11-C12-C13
2	A	801	PEE	C19-C20-C21-C22
4	A	806	CLR	C23-C24-C25-C27
4	A	809	CLR	C23-C24-C25-C26
4	B	808	CLR	C23-C24-C25-C27
3	A	802	EIJ	C31-C32-C33-C34
3	A	802	EIJ	C27-C28-C29-C30
4	A	811	CLR	C22-C23-C24-C25
2	A	801	PEE	C36-C37-C38-C39
2	A	801	PEE	C43-C44-C45-C46
3	A	802	EIJ	C32-C33-C34-C35
3	A	802	EIJ	C36-C37-C38-C39
4	A	806	CLR	C16-C17-C20-C22
4	A	812	CLR	C22-C23-C24-C25
4	B	803	CLR	C23-C24-C25-C26
3	A	802	EIJ	C25-C26-C27-C28
2	A	801	PEE	C1-C2-C3-O3
4	A	805	CLR	C16-C17-C20-C21
4	A	805	CLR	C13-C17-C20-C21
4	B	808	CLR	C13-C17-C20-C21
4	B	803	CLR	C21-C20-C22-C23
4	A	804	CLR	C16-C17-C20-C21
2	A	801	PEE	C33-C34-C35-C36
4	A	804	CLR	C13-C17-C20-C22
4	B	803	CLR	C23-C24-C25-C27
4	A	804	CLR	C13-C17-C20-C21
2	A	801	PEE	C38-C39-C40-C41
4	B	809	CLR	C20-C22-C23-C24
2	A	801	PEE	C44-C45-C46-C47
4	A	805	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
2	A	801	PEE	C22-C23-C24-C25
3	A	802	EIJ	O19-C20-C21-O22
3	A	802	EIJ	C04-C05-C06-C07
3	A	802	EIJ	C09-C10-C11-C12
3	A	802	EIJ	C34-C35-C36-C37
4	A	804	CLR	C16-C17-C20-C22
4	A	809	CLR	C23-C24-C25-C27
4	B	801	CLR	C20-C22-C23-C24
4	B	802	CLR	C13-C17-C20-C22
3	A	802	EIJ	C01-C02-C03-C04
4	A	809	CLR	C20-C22-C23-C24
4	B	802	CLR	C13-C17-C20-C21
2	A	801	PEE	O3P-C1-C2-O2
2	A	801	PEE	C34-C35-C36-C37
3	A	802	EIJ	C29-C30-C31-C32
4	A	811	CLR	C23-C24-C25-C27
3	A	802	EIJ	C26-C27-C28-C29
4	A	805	CLR	C20-C22-C23-C24
4	A	803	CLR	C20-C22-C23-C24
3	A	802	EIJ	C08-C09-C10-C11
2	A	801	PEE	O3P-C1-C2-C3
2	A	801	PEE	C16-C17-C18-C19
4	B	802	CLR	C16-C17-C20-C22
3	A	802	EIJ	O19-C20-C40-O41
2	A	801	PEE	C42-C43-C44-C45
2	A	801	PEE	O2-C2-C3-O3
3	A	802	EIJ	C40-C20-C21-O22
3	A	802	EIJ	C40-O41-P42-O43
3	A	802	EIJ	C40-O41-P42-O45
3	A	802	EIJ	C21-C20-C40-O41
4	B	808	CLR	C17-C20-C22-C23
4	A	809	CLR	C22-C23-C24-C25
4	B	802	CLR	C16-C17-C20-C21
2	A	801	PEE	C39-C40-C41-C42
2	A	801	PEE	C18-C19-C20-C21
2	A	801	PEE	C21-C22-C23-C24
3	A	802	EIJ	C10-C11-C12-C13
4	A	810	CLR	C13-C17-C20-C21
3	A	802	EIJ	C28-C29-C30-C31
3	A	802	EIJ	C30-C31-C32-C33
3	A	802	EIJ	C05-C06-C07-C08
2	A	801	PEE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
2	A	801	PEE	C12-C13-C14-C15
4	B	809	CLR	C13-C17-C20-C21
4	B	809	CLR	C16-C17-C20-C22
4	A	805	CLR	C23-C24-C25-C26
2	A	801	PEE	O4-C10-O2-C2
2	A	801	PEE	C14-C15-C16-C17
4	B	809	CLR	C22-C23-C24-C25
4	B	805	CLR	C23-C24-C25-C27
4	A	810	CLR	C23-C24-C25-C26
4	A	811	CLR	C23-C24-C25-C26
2	A	801	PEE	C11-C10-O2-C2

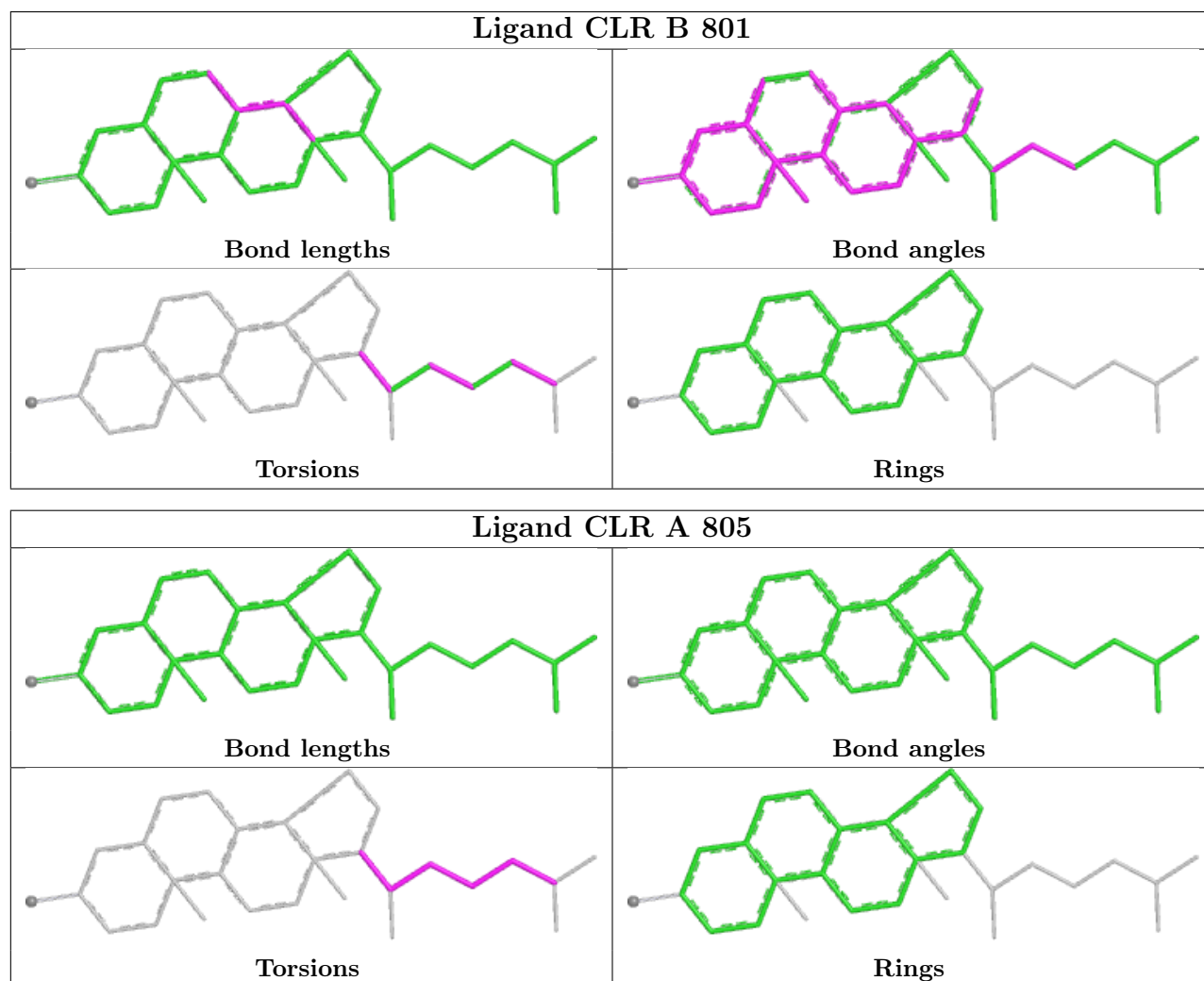
There are no ring outliers.

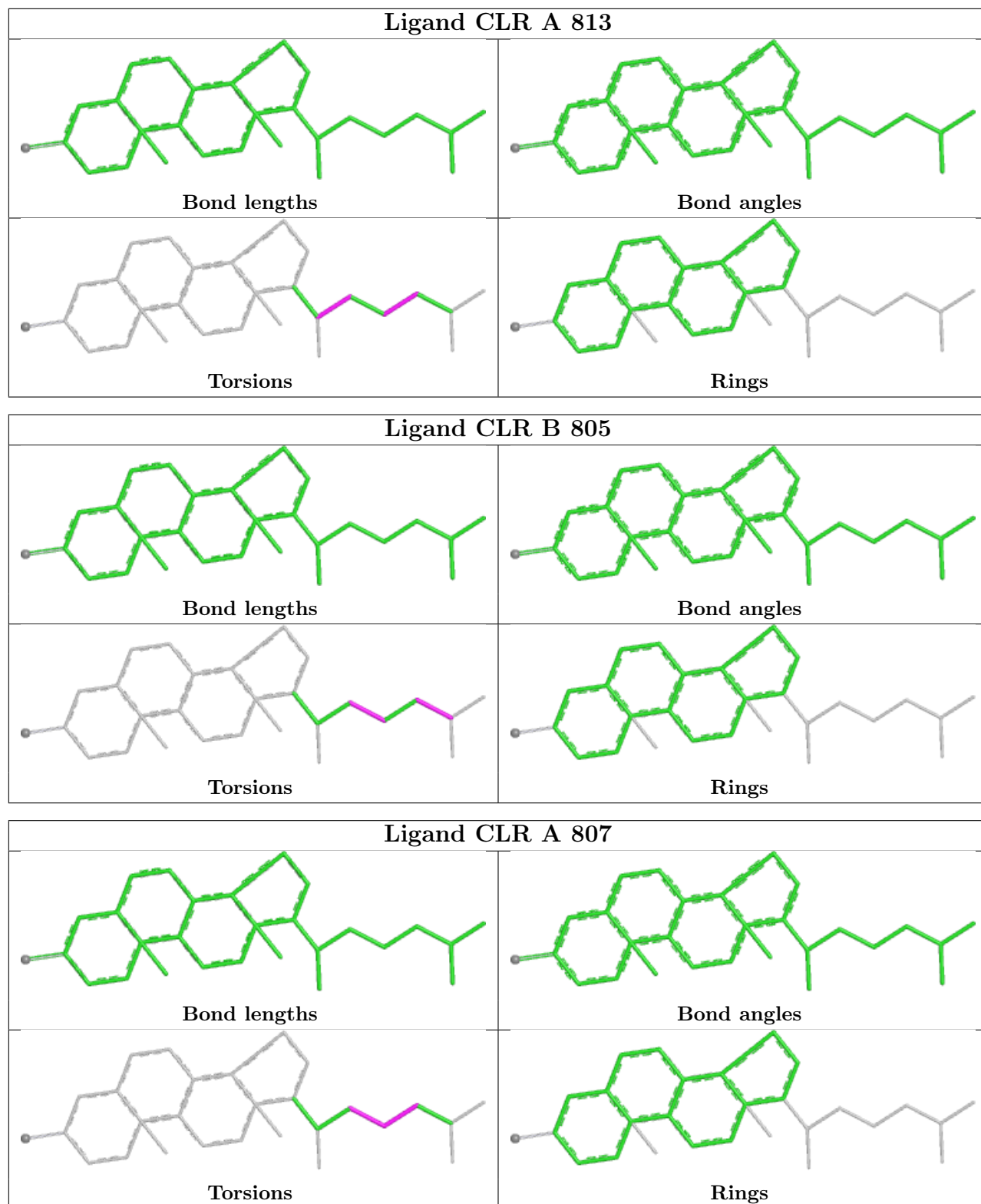
22 monomers are involved in 130 short contacts:

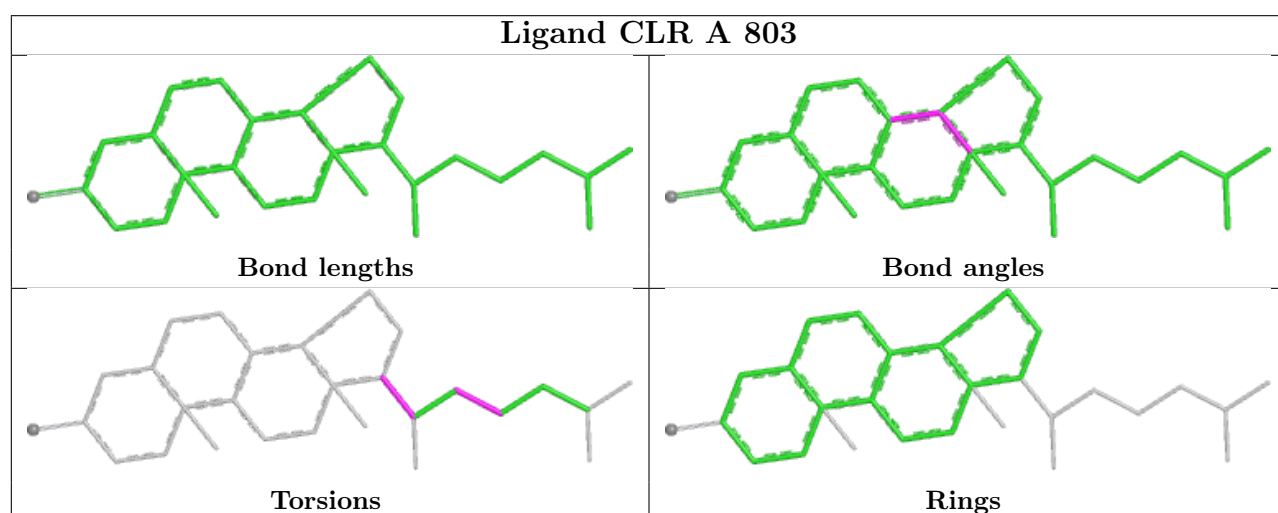
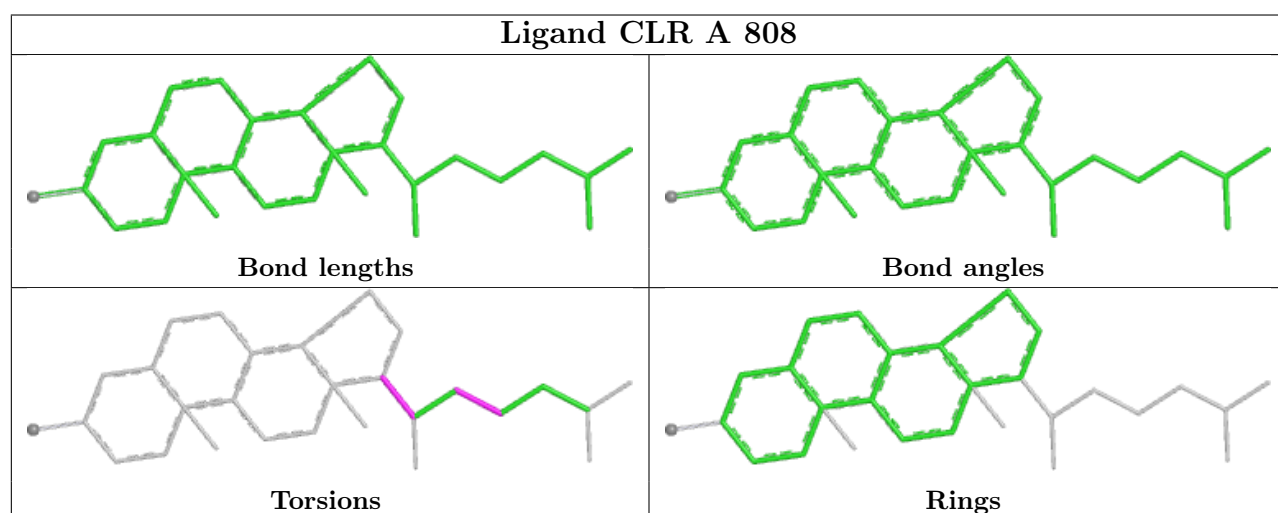
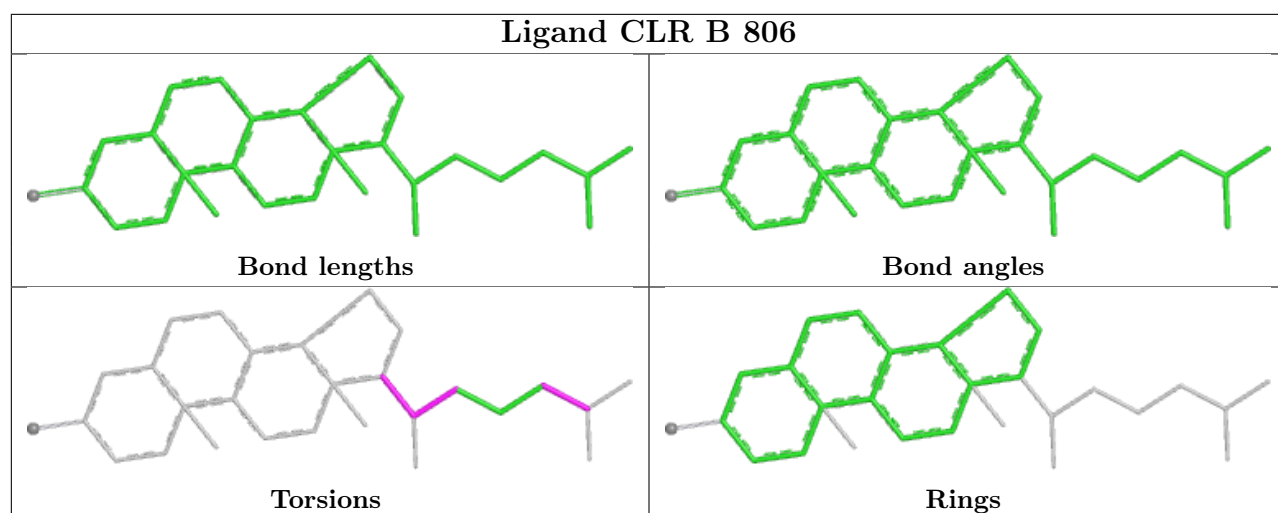
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	801	CLR	11	0
4	B	805	CLR	8	0
4	A	807	CLR	4	0
4	B	806	CLR	13	0
4	A	808	CLR	14	0
4	A	803	CLR	4	0
4	A	812	CLR	2	0
4	B	807	CLR	8	0
4	B	810	CLR	3	0
4	B	804	CLR	7	0
4	A	810	CLR	4	0
4	A	806	CLR	5	0
2	A	801	PEE	4	0
4	A	809	CLR	20	0
4	A	804	CLR	4	0
4	A	811	CLR	2	0
4	B	809	CLR	2	0
4	B	802	CLR	2	0
3	A	802	EIJ	4	0
4	B	808	CLR	6	0
4	B	811	CLR	10	0
4	B	803	CLR	6	0

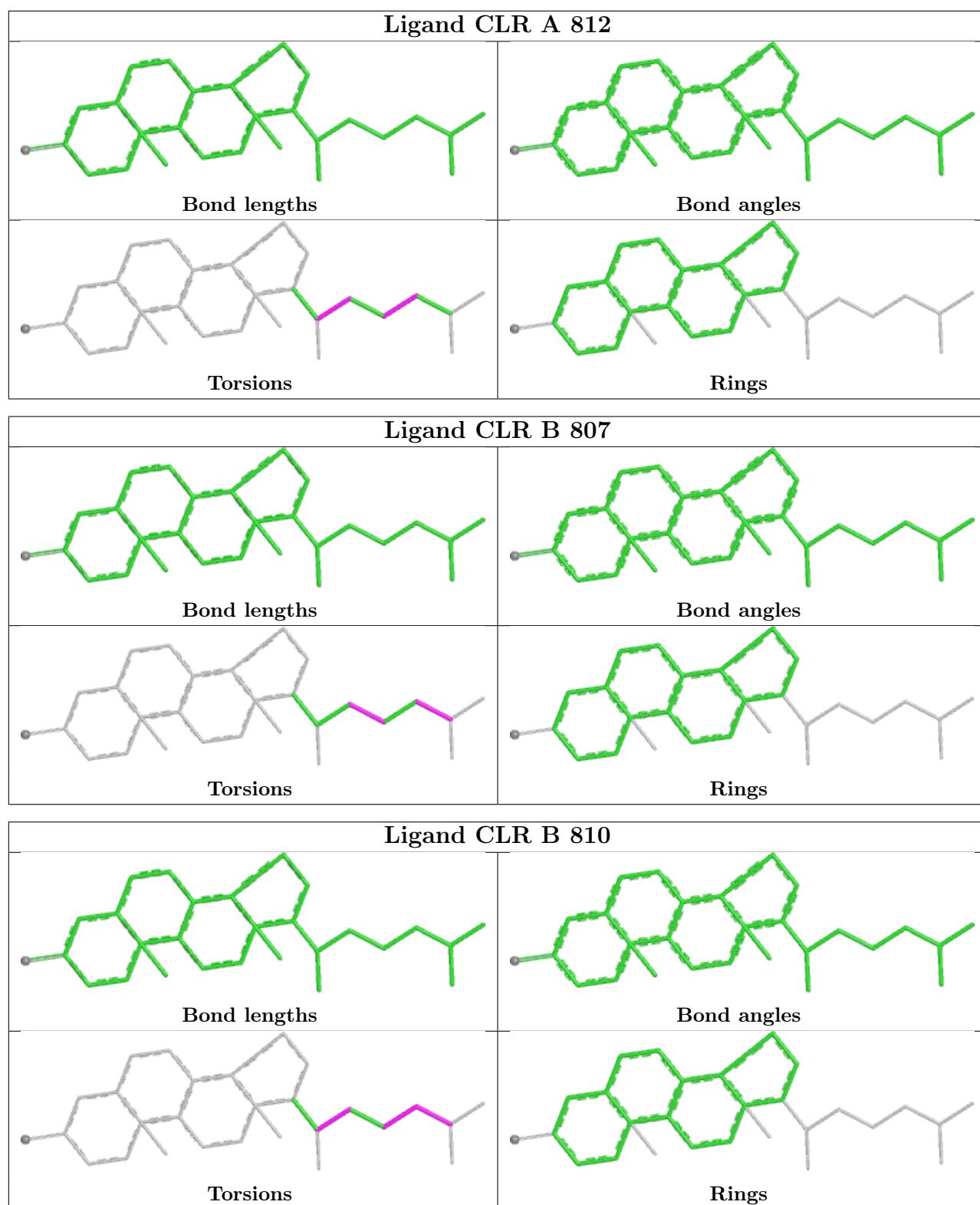
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

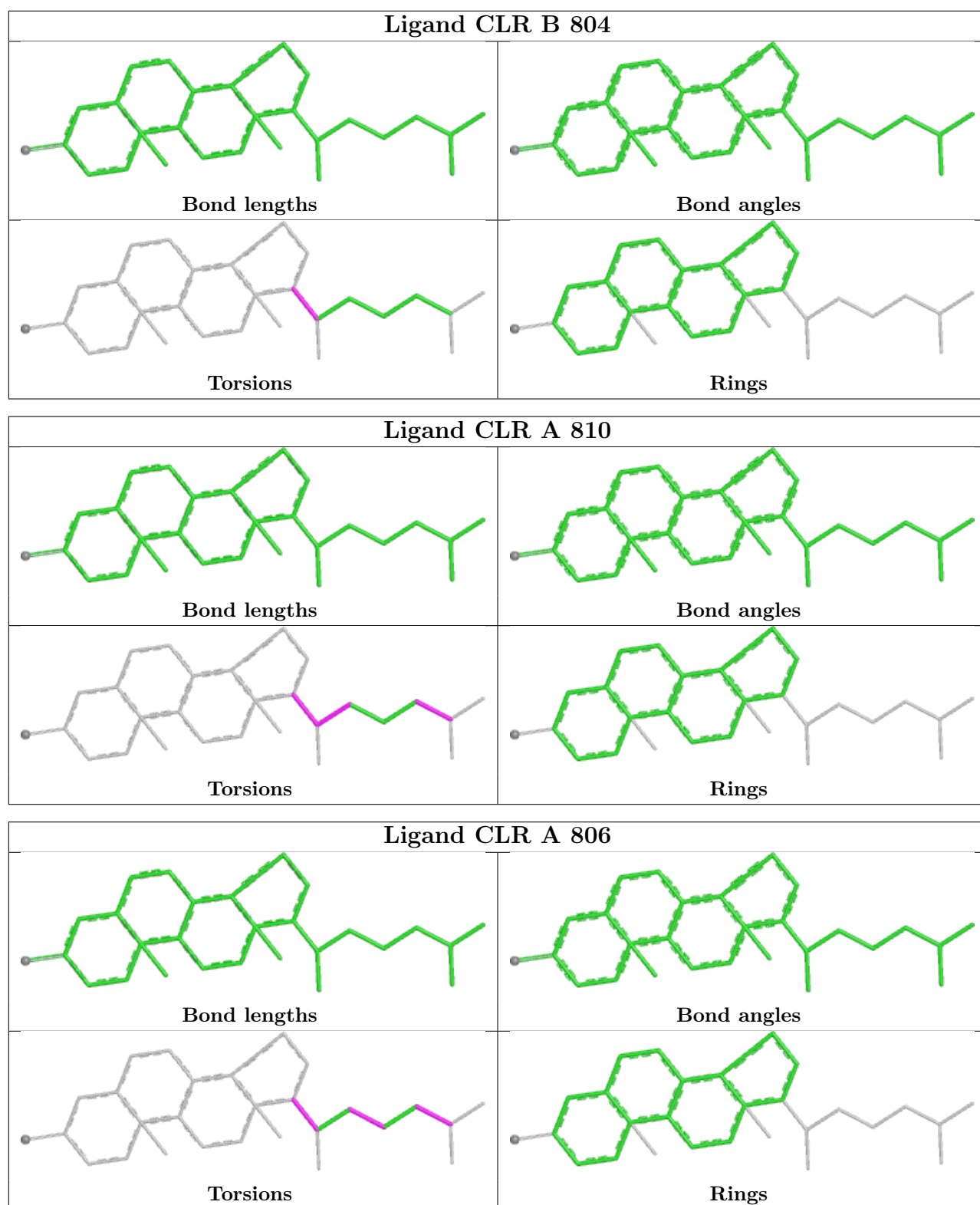
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

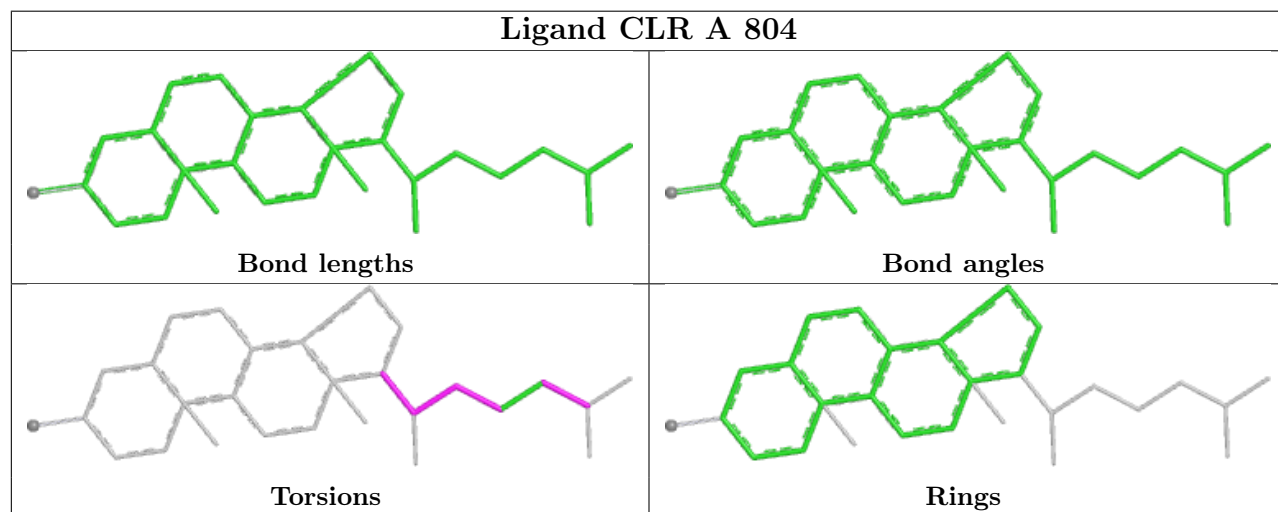
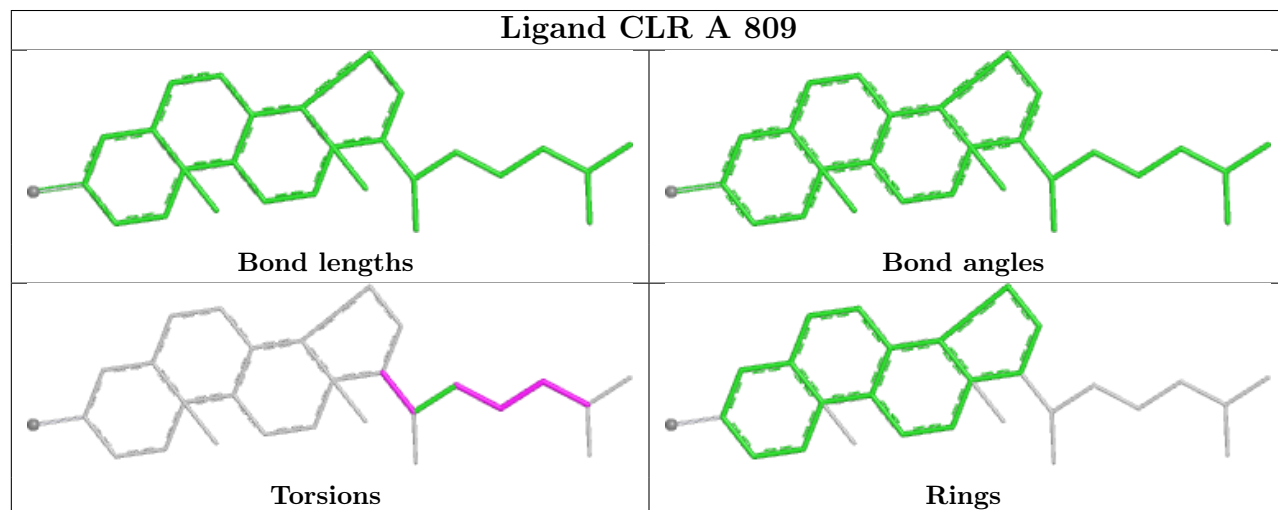
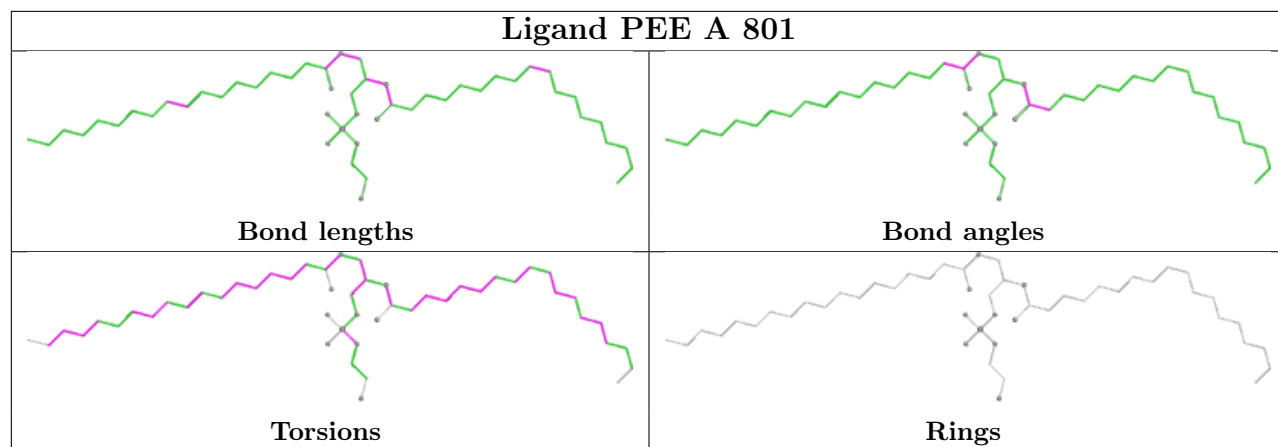


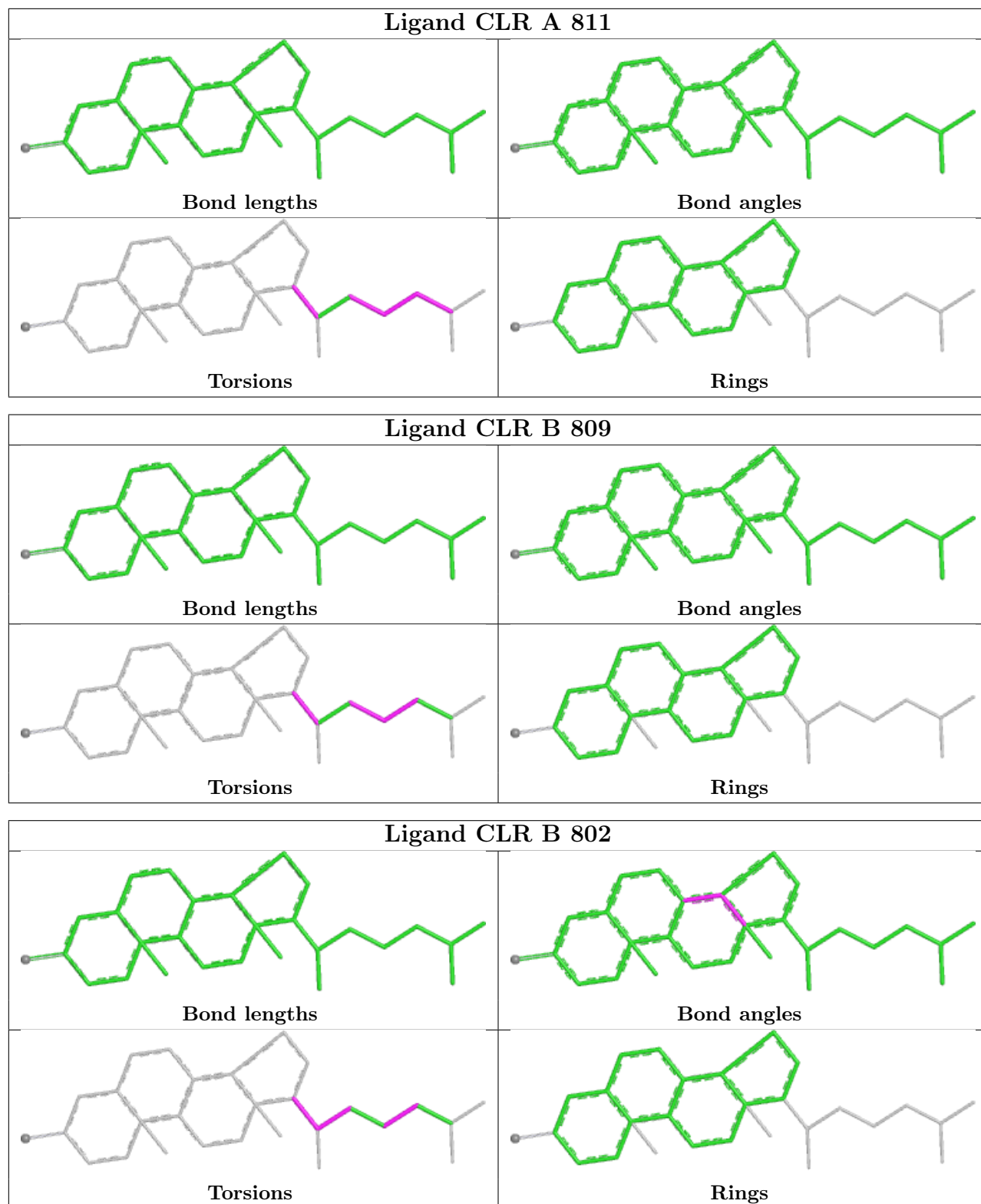


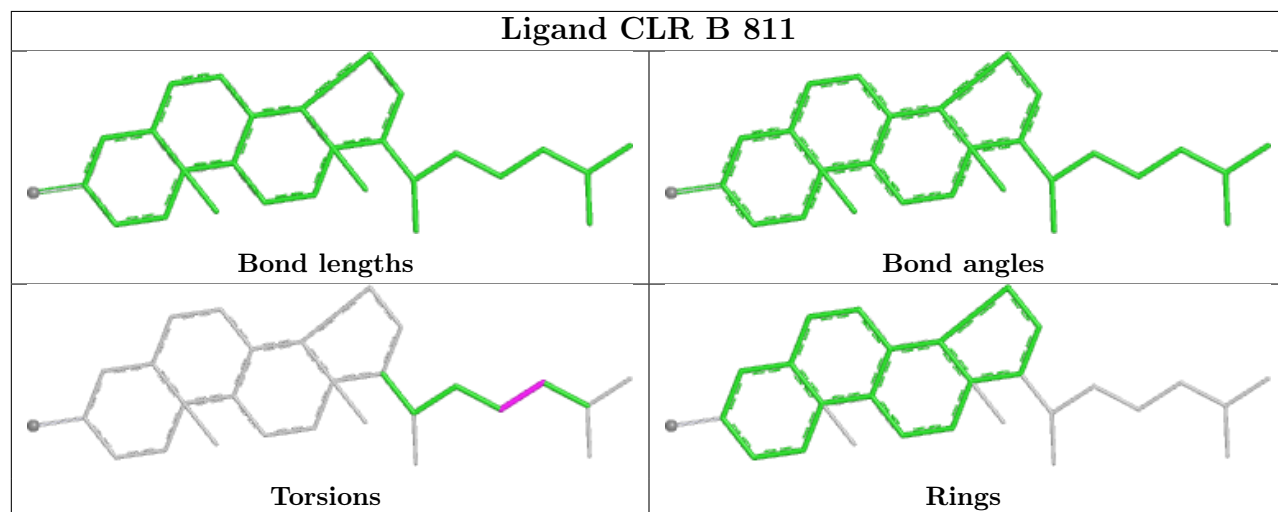
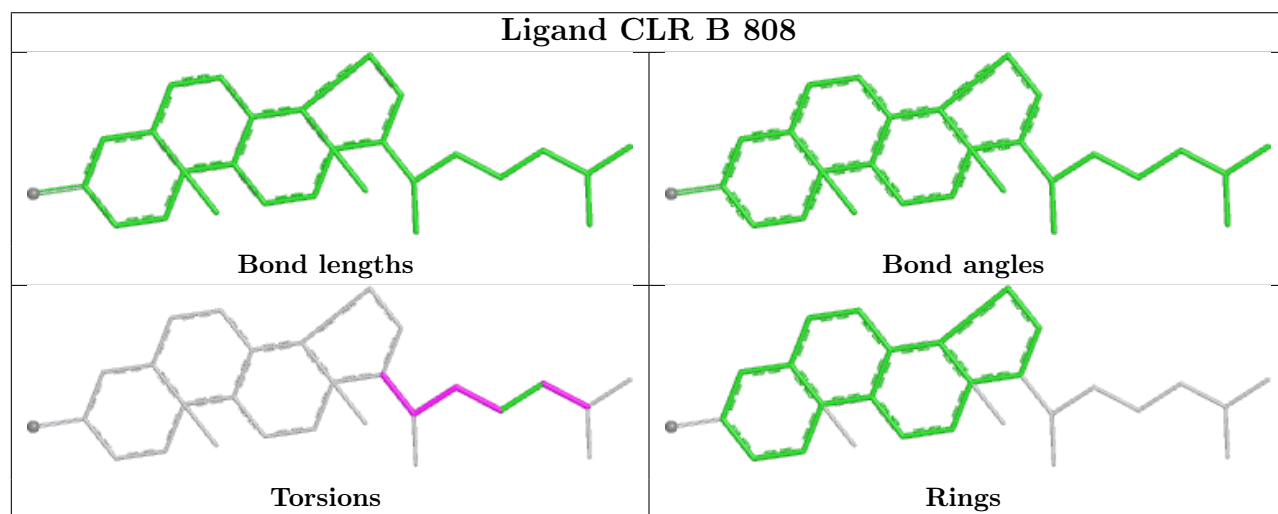
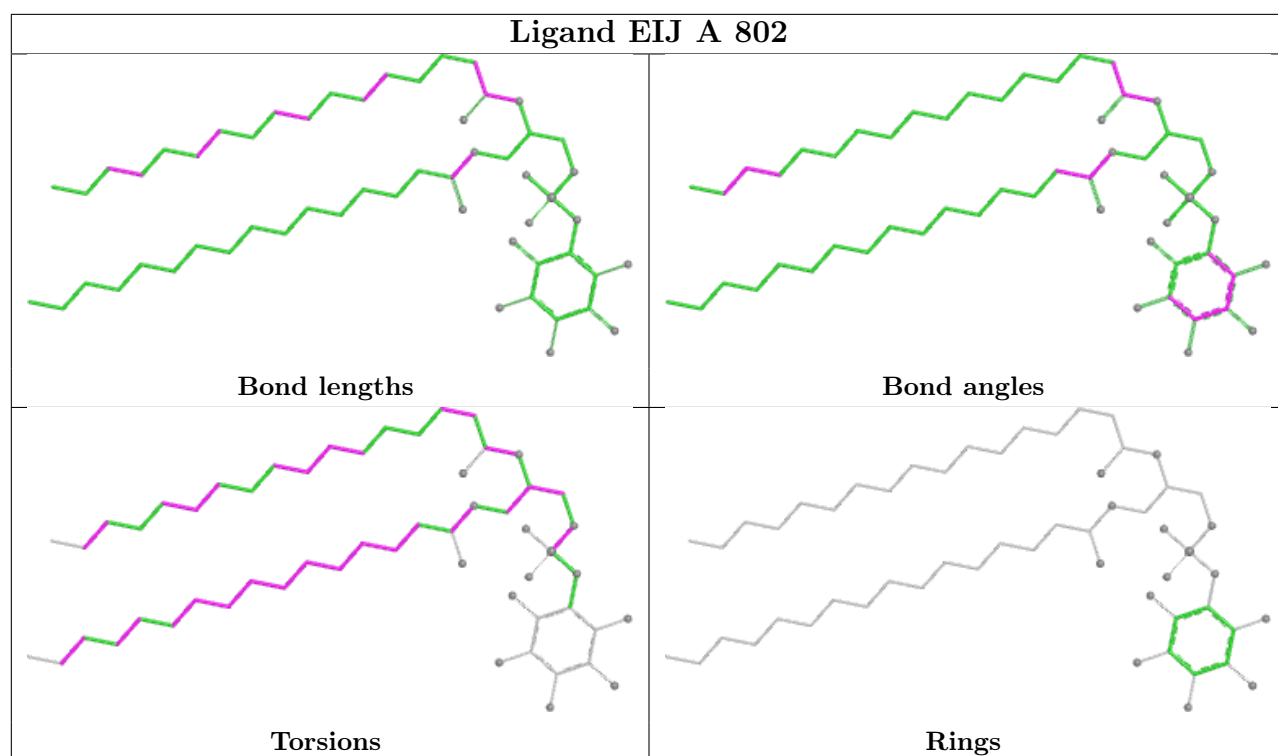


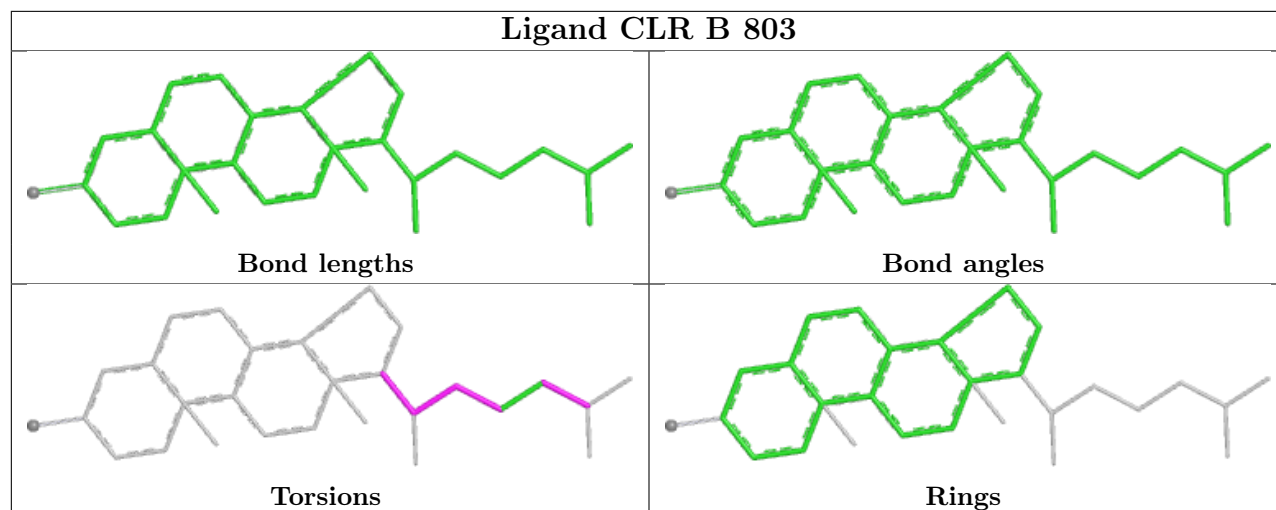












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

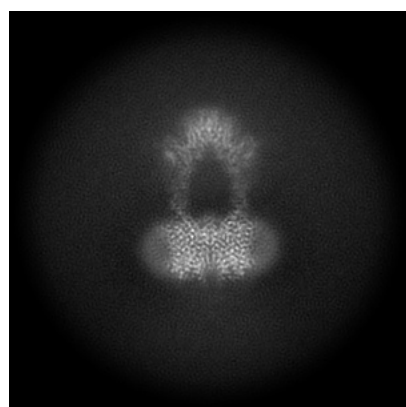
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25125. These allow visual inspection of the internal detail of the map and identification of artifacts.

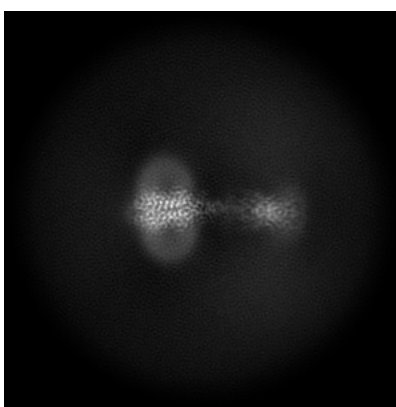
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

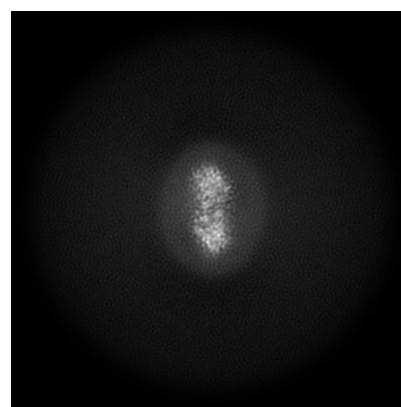
6.1.1 Primary map



X



Y

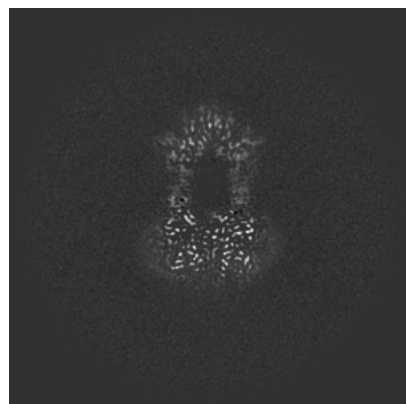


Z

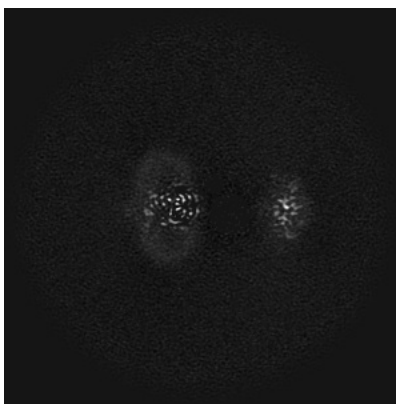
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

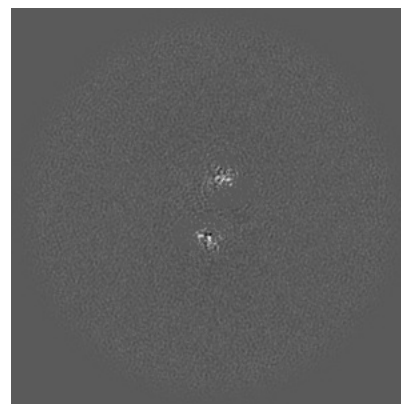
6.2.1 Primary map



X Index: 200



Y Index: 200

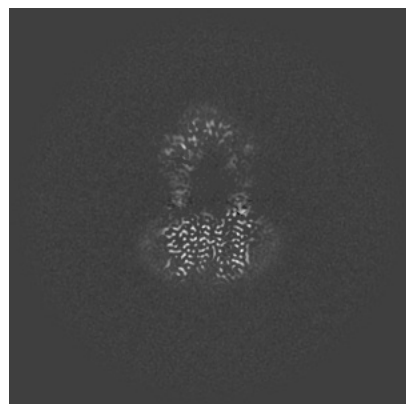


Z Index: 200

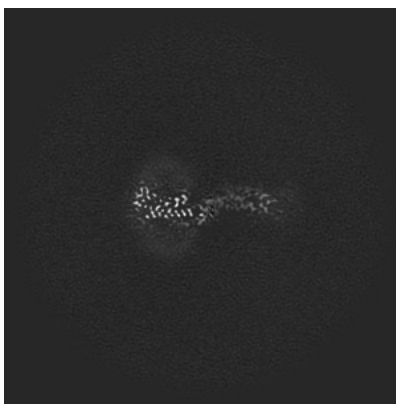
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

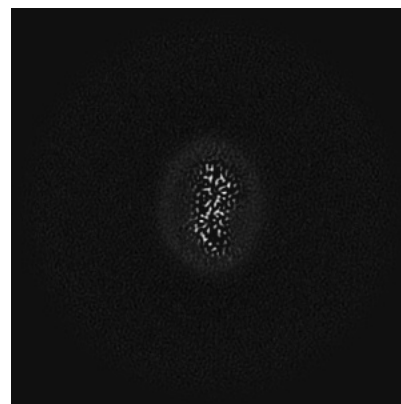
6.3.1 Primary map



X Index: 207



Y Index: 171

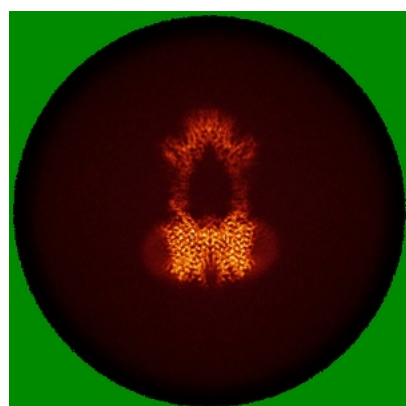


Z Index: 175

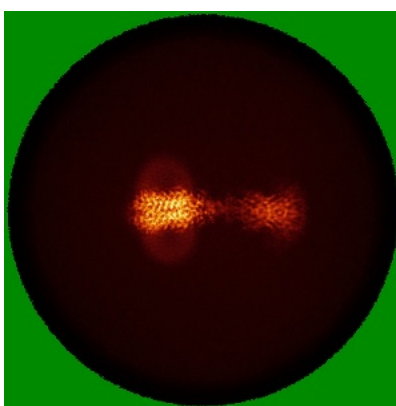
The images above show the largest variance slices of the map in three orthogonal directions.

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

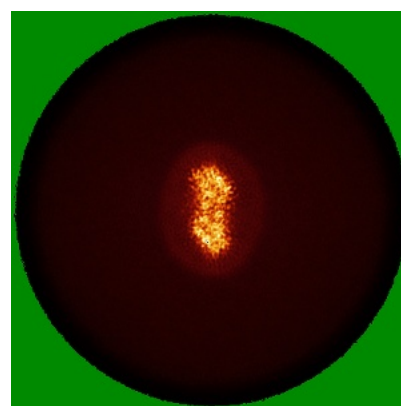
6.4.1 Primary map



X



Y

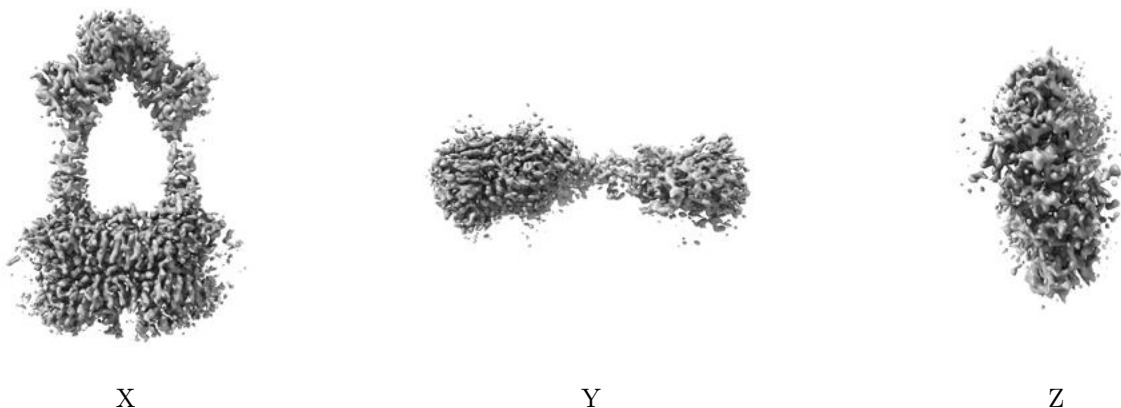


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.593. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

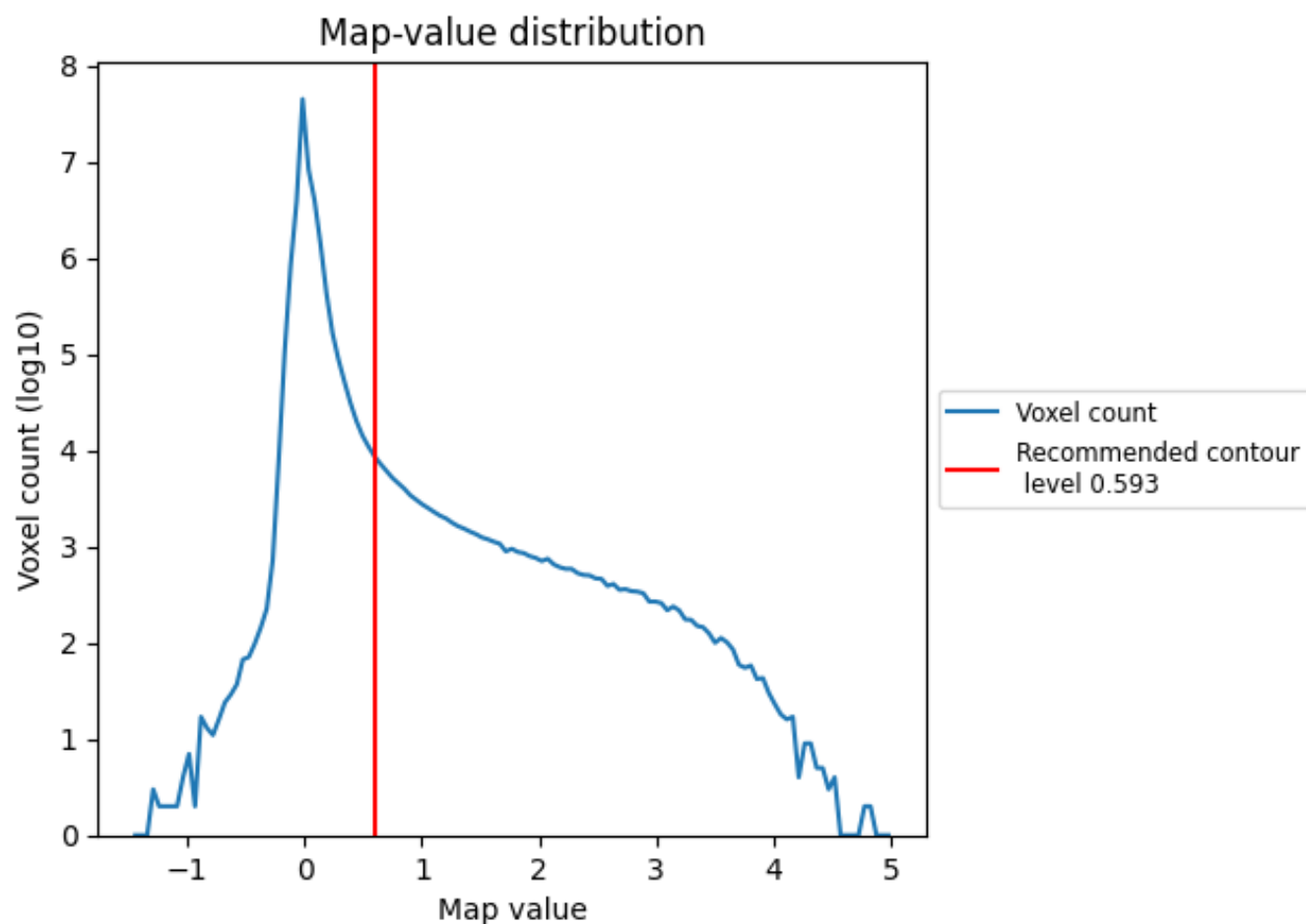
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

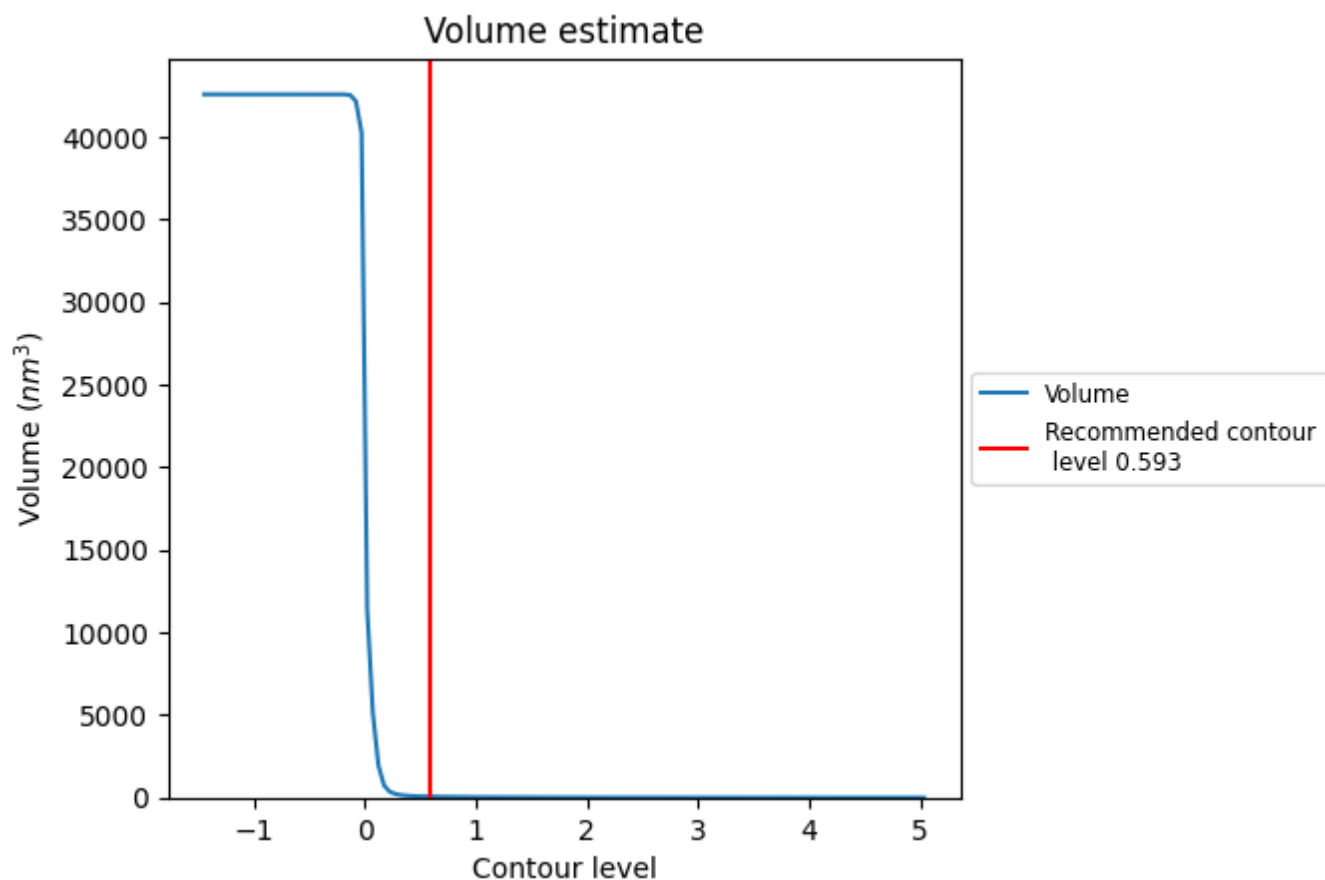
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

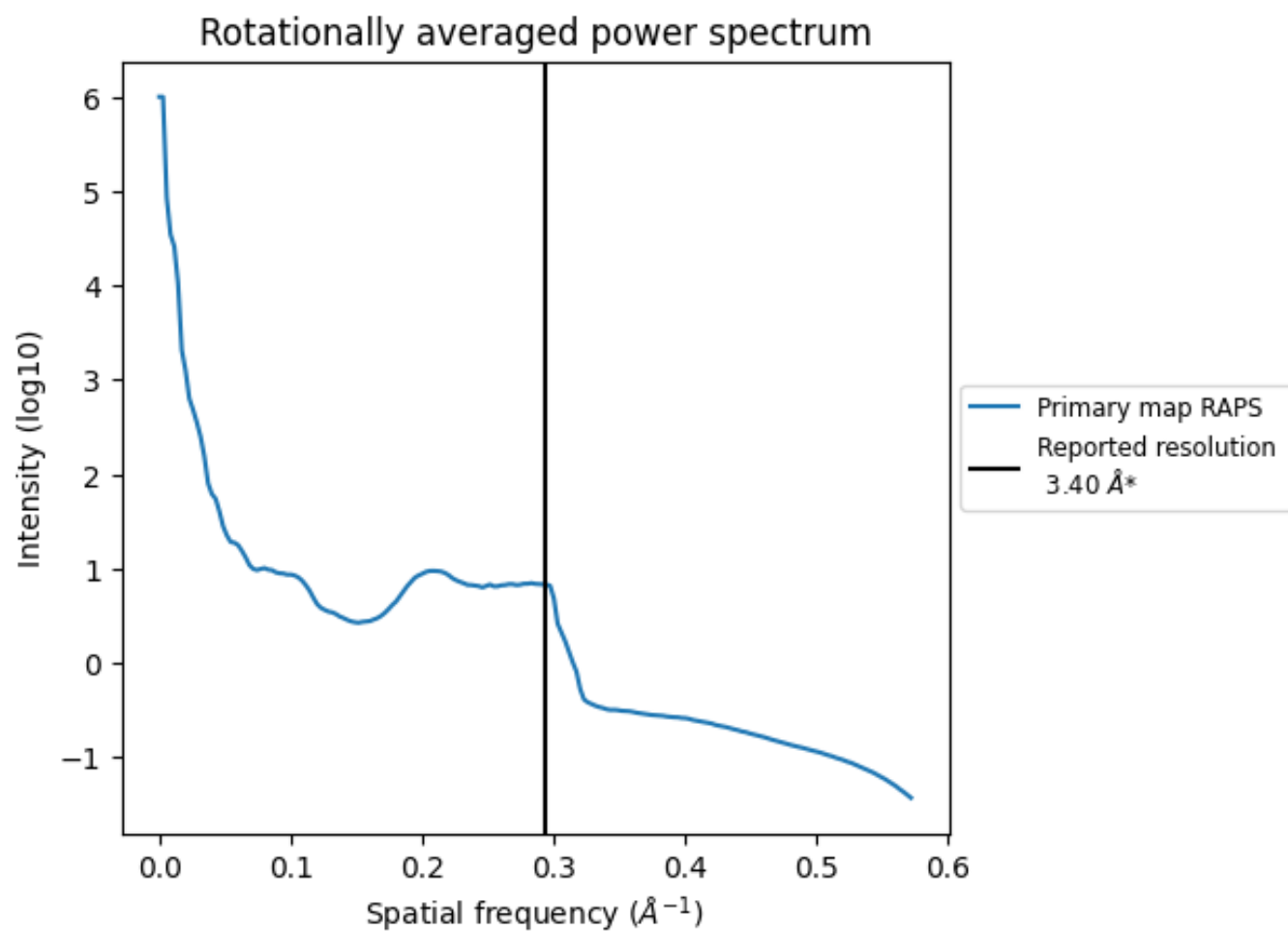
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 56 nm^3 ; this corresponds to an approximate mass of 50 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 0.294 Å⁻¹

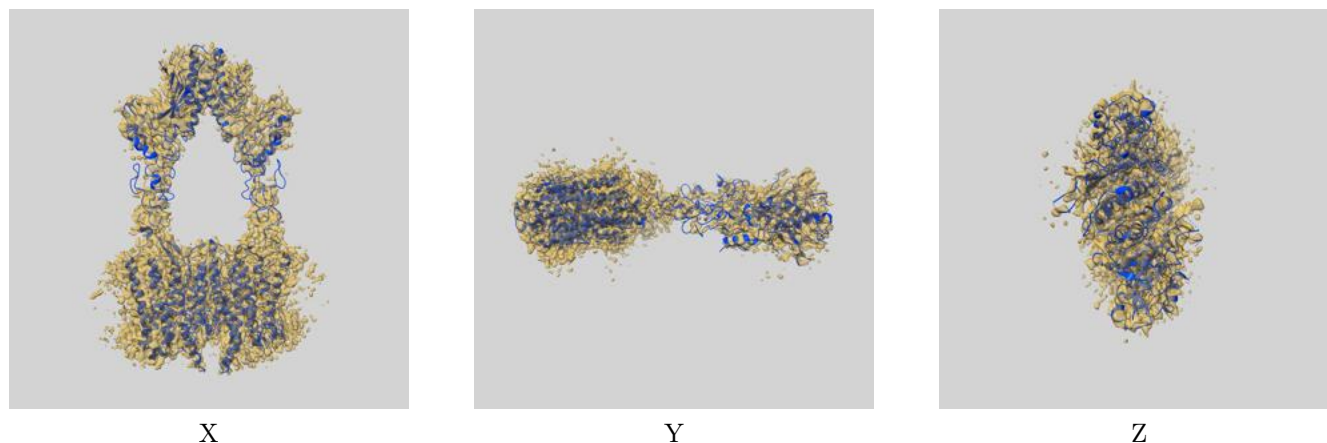
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

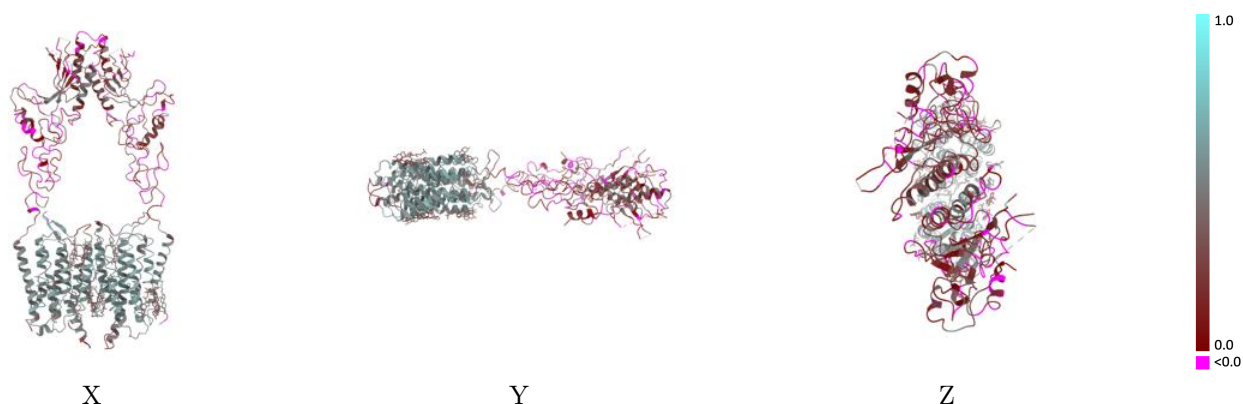
This section contains information regarding the fit between EMDB map EMD-25125 and PDB model 7SHE. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



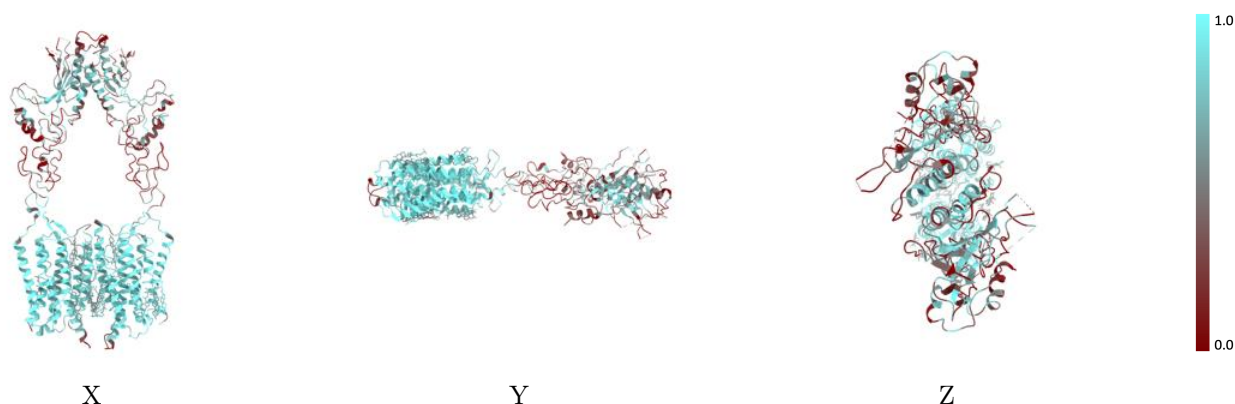
The images above show the 3D surface view of the map at the recommended contour level 0.593 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



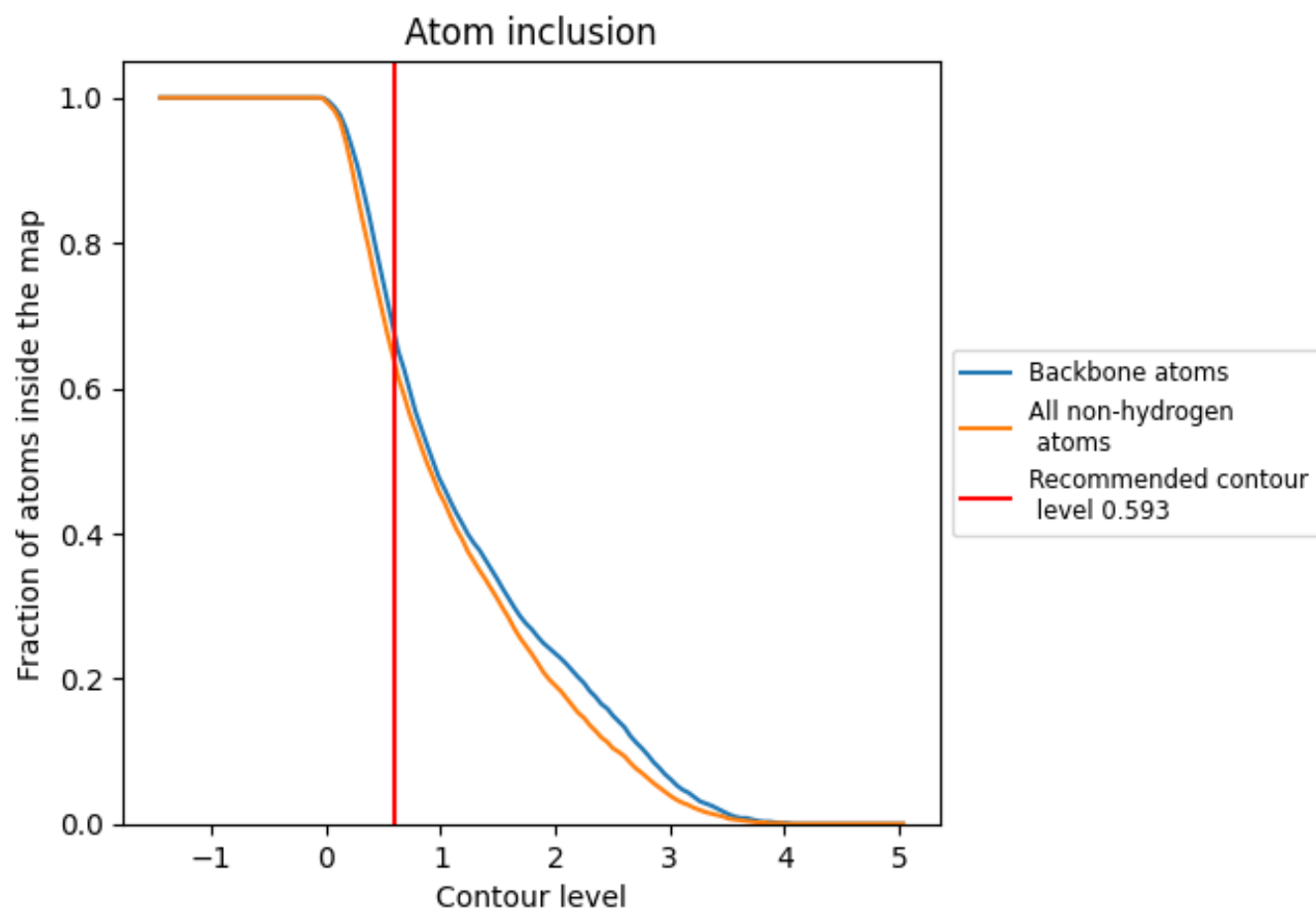
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.593).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 64% 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 (0.593) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6380	0.3520
A	0.6490	0.3520
B	0.6260	0.3510

