



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 05:19 AM UTC

PDB ID : 7SHF / pdb_00007shf
EMDB ID : EMD-25126
Title : Cryo-EM structure of GPR158 coupled to the RGS7-Gbeta5 complex
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 wwPDB EM Validation Summary 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:

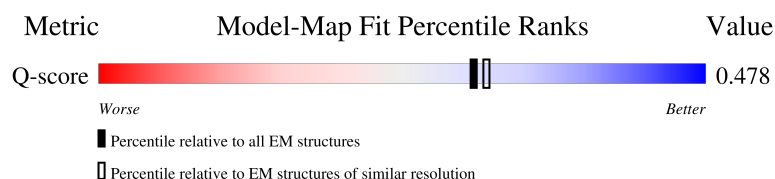
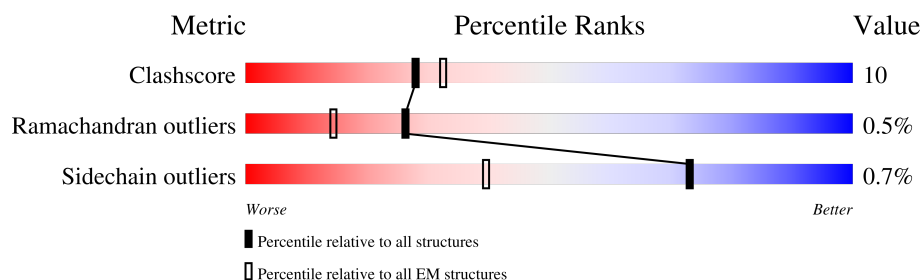
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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	C	469	
2	D	353	
3	A	781	
3	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	A	804	X	-	-	-
4	CLR	A	809	X	-	-	-
4	CLR	B	801	X	-	-	-
5	EIJ	A	813	X	-	-	-
6	PEE	A	814	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11443 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 Isoform 2 of Regulator of G-protein signaling 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	400	Total	C	N	O	S	1	0
			3329	2131	564	622	12		

- Molecule 2 is a protein called Guanine nucleotide-binding protein subunit beta-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	346	Total	C	N	O	S	0	0
			2660	1653	463	521	23		

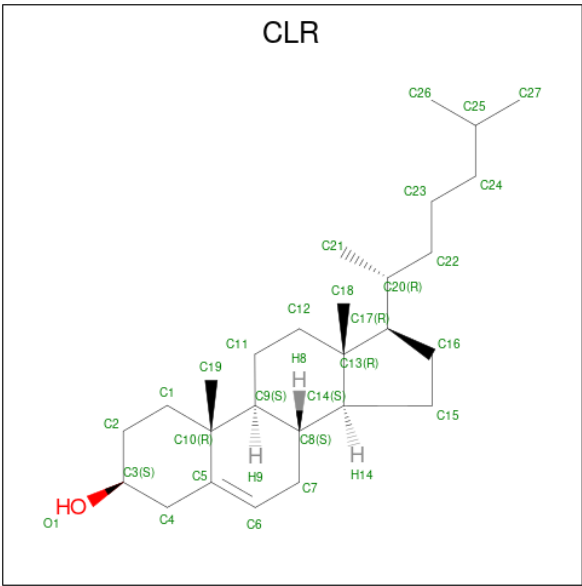
- Molecule 3 is a protein called G-protein coupled receptor 158.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	284	Total	C	N	O	S	0	0
			2322	1547	382	377	16		
3	A	296	Total	C	N	O	S	0	0
			2412	1603	398	395	16		

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 4 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



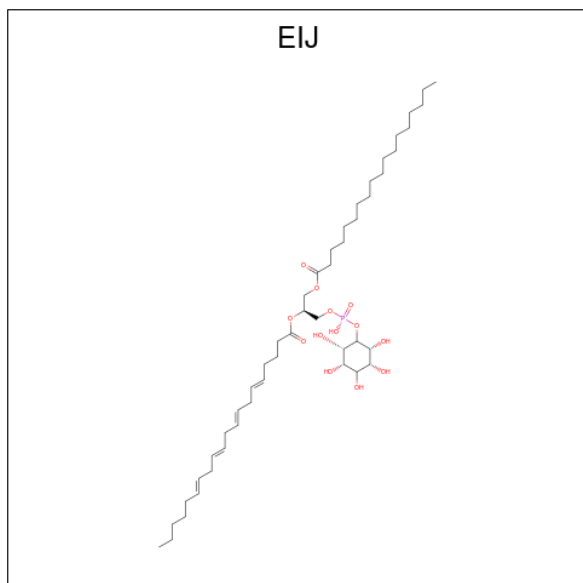
Mol	Chain	Residues	Atoms			AltConf
4	B	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27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

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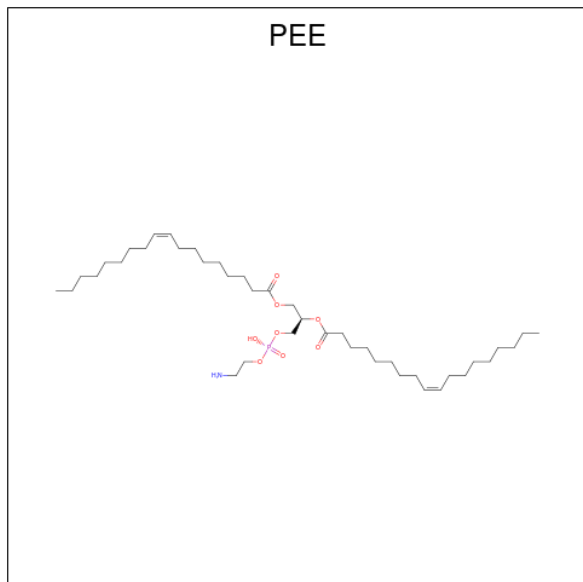
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	
4	A	1	Total	C	O	0
			28	27	1	

- Molecule 5 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).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			55	41	13	1	

- Molecule 6 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).

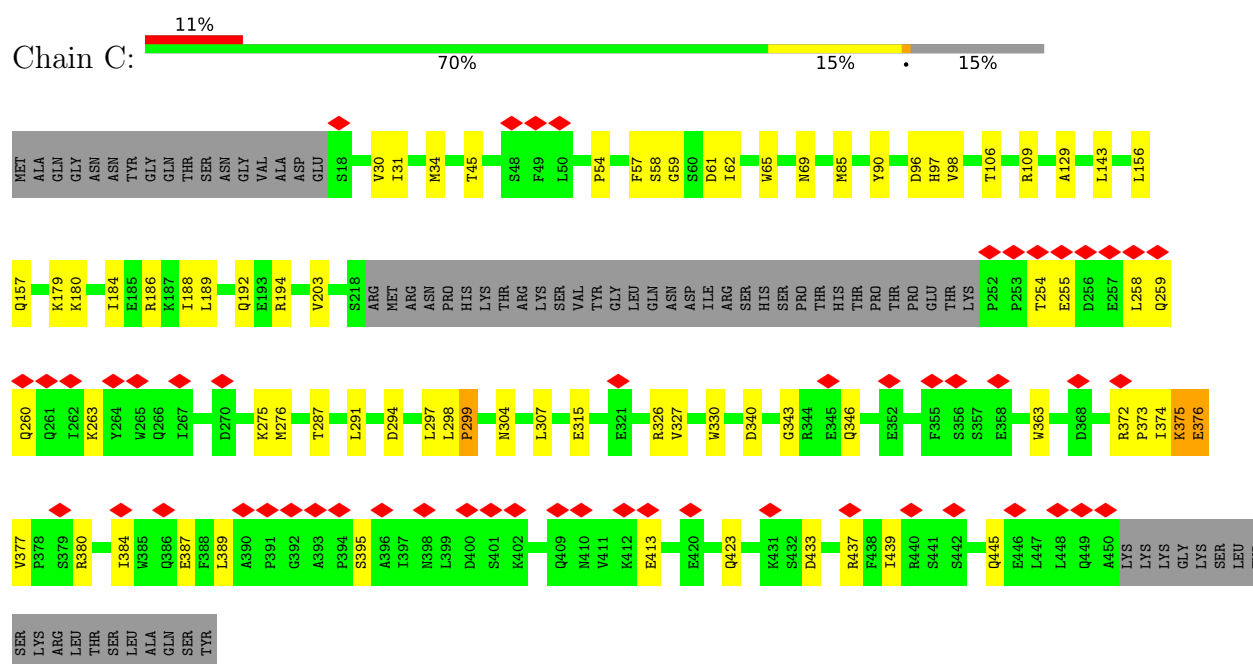


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	49	39	1	8	1	0

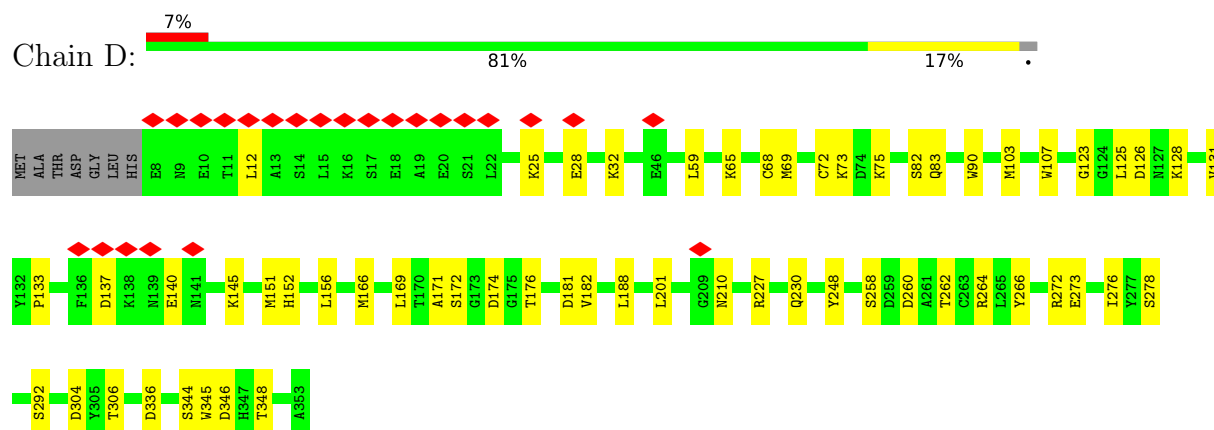
3 Residue-property plots

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

- Molecule 1: Isoform 2 of Regulator of G-protein signaling 7



- Molecule 2: Guanine nucleotide-binding protein subunit beta-5



- Molecule 3: G-protein coupled receptor 158

Frequency	Percentage
Daily	30%
Weekly	6%
Not at all	64%

- Molecule 3: G-protein coupled receptor 158

Frequency	Percentage
Often	29%
Sometimes	9%
Never	62%

GLN	ASP	SER	TRP	MET
PRO	SER	LEU	SER	GLY
GLY	LEU	HIS	ARG	ALA
LEU	SER	ARG	THR	ALA
GLY	ALA	ALA	ASP	TVR
HIS	PRO	LEU	GLY	PRO
LEU	PRO	THR	THR	LEU
GLN	GLN	LEU	ILE	LEU
TRP	VAL	THR	LEU	LEU
ARG	PHE	HIS	ALA	CYS
ARG	LEU	ALA	GLN	LEU
ARG	GLN	THR	LYS	LEU
LYS	LEU	ASN	LEU	LEU
ASP	ALA	ASN	ALA	ALA
GLY	THR	PHE	ALA	ALA
GLY	ARG	LEU	GLU	GLN
GLY	GLU	ASN	GLU	LEU
ASP	GLU	VAL	VAL	GLY
SER	SER	MET	PRO	LEU
LYS	ARG	LEU	MET	GLY
SER	ILE	GLN	ASP	ALA
HIS	LEU	SER	VAL	VAL
PHE	HIS	LEU	ALA	GLY
LYS	GLN	ASN	SER	ALA
TRP	ASP	SER	SER	ALA
LYS	LEU	ARG	TYR	SER
PRO	SER	GLU	LEU	ARG
PRO	SER	GLN	THR	ASP
TVR	SER	ASN	GLY	GLN
LEU	ALA	LEU	ASP	GLY
GLU	PRO	GLN	SER	ARG
CYS	HIS	ASP	HIS	PRO
GLU	LEU	ASP	GLN	ASP
ASN	ALA	LEU	LEU	SER
GLY	ASN	ASP	LYS	PRO
SER	ALA	TRP	ARG	ARG
TYR	THR	TYR	ALA	GLU
LEU	LEU	GLN	ASN	GLU
PRO	GLU	GLN	ARG	THR
GLY	THR	LEU	SER	THR
TRP	GLU	VAL	GLY	LYS
LEU	TRP	TRP	ARG	GLY
VAL	PHE	SER	TYR	LYS
THR	HIS	LEU	GLU	PRO
LEU	GLY	LEU	LEU	HIS
SER	LEU	GLU	ALA	ALA
SER	ARG	GLY	GLY	GLN
ALA	ARG	GLU	LEU	GLN
SER	LYS	PRO	PRO	GLN
ILE	TRP	SER	GLY	PRO
GLY	ARG	ILE	LYS	GLY
LEU	PRO	SER	TRP	ARG
GLN	HIS	ARG	PRO	ALA
PRO	LEU	ALA	PRO	SER
ASN	HIS	ALA	ALA	ALA
LEU	ARG	ILE	LEU	SER
VAL	ARG	THR	SER	ASP
PRO	GLY	PHE	ALA	SER
GLU	PRO	SER	HIS	ALA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	151954	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	3.320	Depositor
Minimum map value	-2.164	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.359	Depositor
Map size (Å)	349.2, 349.2, 349.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: CLR, PEE, 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	C	0.21	0/3417	0.40	1/4623 (0.0%)
2	D	0.18	0/2713	0.32	0/3666
3	A	0.29	0/2471	0.57	5/3350 (0.1%)
3	B	0.22	0/2380	0.49	2/3227 (0.1%)
All	All	0.23	0/10981	0.45	8/14866 (0.1%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	299	PRO	N-CA-C	9.77	122.62	110.70
3	A	407	PRO	N-CA-CB	7.68	111.32	103.25
3	A	499	VAL	N-CA-C	-6.53	106.16	112.29
3	A	526	VAL	N-CA-C	-6.30	107.36	113.53
3	B	714	ILE	N-CA-C	-6.18	104.32	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3329	0	3260	50	0
2	D	2660	0	2562	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2412	0	2507	62	0
3	B	2322	0	2417	49	0
4	A	336	0	552	52	0
4	B	280	0	459	28	0
5	A	55	0	0	1	0
6	A	49	0	71	2	0
All	All	11443	0	11828	223	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 10.

The worst 5 of 223 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)
3:B:460:PHE:CE2	4:B:803:CLR:H231	1.43	1.50
4:A:811:CLR:C18	4:A:812:CLR:C21	1.92	1.46
4:A:811:CLR:C18	4:A:812:CLR:H212	1.48	1.42
3:B:460:PHE:HE2	4:B:803:CLR:C23	1.56	1.18
3:B:460:PHE:CE2	4:B:803:CLR:C23	2.26	1.18

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	C	397/469 (85%)	376 (95%)	20 (5%)	1 (0%)	36	65
2	D	344/353 (98%)	326 (95%)	18 (5%)	0	100	100
3	A	292/781 (37%)	262 (90%)	27 (9%)	3 (1%)	12	40
3	B	280/781 (36%)	249 (89%)	28 (10%)	3 (1%)	11	38
All	All	1313/2384 (55%)	1213 (92%)	93 (7%)	7 (0%)	26	54

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	638	LEU
3	A	407	PRO
3	A	566	ASP
3	A	638	LEU
3	B	414	LYS

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	C	365/425 (86%)	360 (99%)	5 (1%)	59	70
2	D	290/295 (98%)	290 (100%)	0	100	100
3	A	263/677 (39%)	262 (100%)	1 (0%)	84	83
3	B	253/677 (37%)	251 (99%)	2 (1%)	73	77
All	All	1171/2074 (56%)	1163 (99%)	8 (1%)	73	78

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	611	ARG
3	B	713	ASP
1	C	376	GLU
1	C	375	LYS
3	B	712	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	618	HIS
3	A	736	ASN
2	D	64	ASN
3	B	516	GLN
3	B	669	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	807	-	31,31,31	0.32	0	48,48,48	0.60	0
4	CLR	B	806	-	31,31,31	0.28	0	48,48,48	0.48	0
6	PEE	A	814	-	48,48,50	1.77	11 (22%)	51,53,55	1.59	5 (9%)
4	CLR	A	805	-	31,31,31	0.34	0	48,48,48	0.61	0
4	CLR	A	802	-	31,31,31	0.30	0	48,48,48	0.45	0
4	CLR	B	807	-	31,31,31	0.29	0	48,48,48	0.73	1 (2%)
4	CLR	B	809	-	31,31,31	0.29	0	48,48,48	0.43	0
4	CLR	A	810	-	31,31,31	0.34	0	48,48,48	0.81	0
4	CLR	A	804	-	31,31,31	0.33	0	48,48,48	0.62	0
4	CLR	A	811	-	31,31,31	0.28	0	48,48,48	0.71	2 (4%)
4	CLR	A	801	-	31,31,31	0.34	0	48,48,48	0.48	0
4	CLR	A	809	-	31,31,31	0.33	0	48,48,48	0.51	0
4	CLR	B	805	-	31,31,31	0.29	0	48,48,48	0.43	0
4	CLR	B	803	-	31,31,31	0.27	0	48,48,48	0.71	1 (2%)
4	CLR	A	803	-	31,31,31	0.35	0	48,48,48	1.29	5 (10%)
4	CLR	B	810	-	31,31,31	0.30	0	48,48,48	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CLR	A	808	-	31,31,31	0.29	0	48,48,48	0.87	1 (2%)
4	CLR	A	812	-	31,31,31	0.29	0	48,48,48	0.37	0
5	EIJ	A	813	-	55,55,61	1.60	11 (20%)	64,67,73	1.48	3 (4%)
4	CLR	B	801	-	31,31,31	0.45	0	48,48,48	1.96	11 (22%)
4	CLR	B	802	-	31,31,31	0.30	0	48,48,48	0.46	0
4	CLR	B	808	-	31,31,31	0.29	0	48,48,48	0.49	0
4	CLR	A	806	-	31,31,31	0.32	0	48,48,48	0.91	3 (6%)
4	CLR	B	804	-	31,31,31	0.30	0	48,48,48	0.47	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	A	807	-	-	5/10/68/68	0/4/4/4
4	CLR	B	806	-	-	6/10/68/68	0/4/4/4
6	PEE	A	814	-	1/1/4/8	27/52/52/54	-
4	CLR	A	805	-	-	9/10/68/68	0/4/4/4
4	CLR	A	802	-	-	10/10/68/68	0/4/4/4
4	CLR	B	807	-	-	8/10/68/68	0/4/4/4
4	CLR	B	809	-	-	7/10/68/68	0/4/4/4
4	CLR	A	810	-	-	4/10/68/68	0/4/4/4
4	CLR	A	804	-	1/1/10/11	8/10/68/68	0/4/4/4
4	CLR	A	811	-	-	9/10/68/68	0/4/4/4
4	CLR	A	809	-	1/1/10/11	7/10/68/68	0/4/4/4
4	CLR	A	801	-	-	7/10/68/68	0/4/4/4
4	CLR	B	805	-	-	7/10/68/68	0/4/4/4
4	CLR	B	803	-	-	8/10/68/68	0/4/4/4
4	CLR	A	803	-	1/1/10/11	7/10/68/68	0/4/4/4
4	CLR	B	810	-	-	10/10/68/68	0/4/4/4
4	CLR	A	808	-	-	10/10/68/68	0/4/4/4
5	EIJ	A	813	-	2/2/10/18	19/50/74/80	0/1/1/1
4	CLR	A	812	-	-	9/10/68/68	0/4/4/4
4	CLR	B	801	-	2/2/10/11	6/10/68/68	0/4/4/4
4	CLR	B	802	-	-	9/10/68/68	0/4/4/4
4	CLR	B	808	-	-	9/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CLR	A	806	-	-	2/10/68/68	0/4/4/4
4	CLR	B	804	-	-	8/10/68/68	0/4/4/4

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	814	PEE	O3-C30	4.45	1.46	1.33
5	A	813	EIJ	C10-C09	4.12	1.55	1.31
5	A	813	EIJ	C13-C12	4.02	1.54	1.31
5	A	813	EIJ	C07-C06	3.98	1.54	1.31
6	A	814	PEE	C24-C25	-3.91	1.32	1.51

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	813	EIJ	C09-C08-C07	8.47	153.73	112.02
6	A	814	PEE	C21-C22-C23	7.59	152.74	114.37
4	B	801	CLR	C7-C8-C9	6.50	117.23	109.72
4	B	801	CLR	C10-C9-C8	4.75	119.66	112.71
4	B	801	CLR	C13-C17-C20	4.62	126.63	119.50

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	801	CLR	C8
4	B	801	CLR	C17
4	A	803	CLR	C8
4	A	804	CLR	C17
4	A	809	CLR	C17

5 of 211 torsion outliers are listed below:

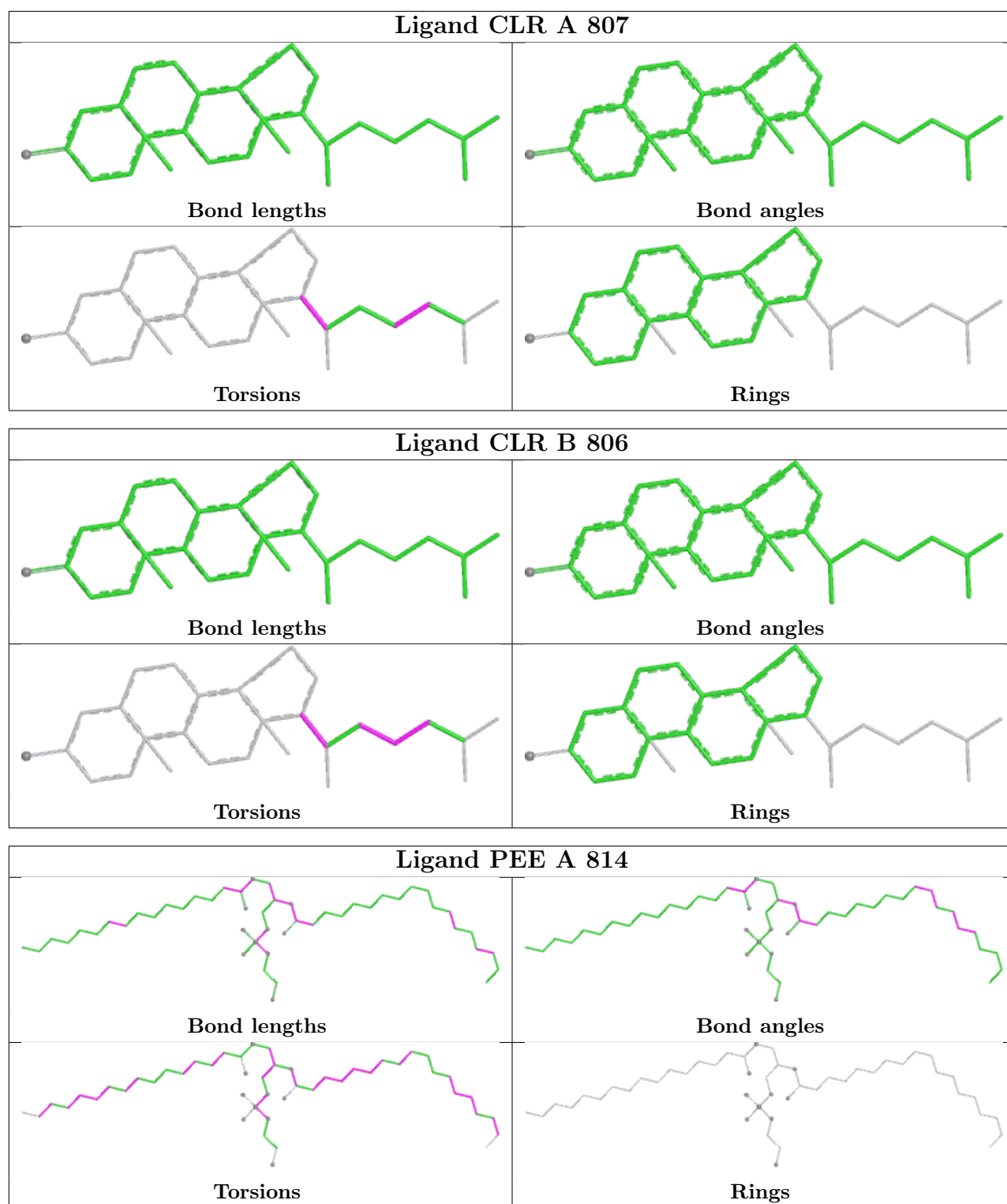
Mol	Chain	Res	Type	Atoms
4	B	804	CLR	C13-C17-C20-C21
4	B	804	CLR	C13-C17-C20-C22
4	B	804	CLR	C16-C17-C20-C22
4	B	808	CLR	C13-C17-C20-C21
4	B	808	CLR	C16-C17-C20-C21

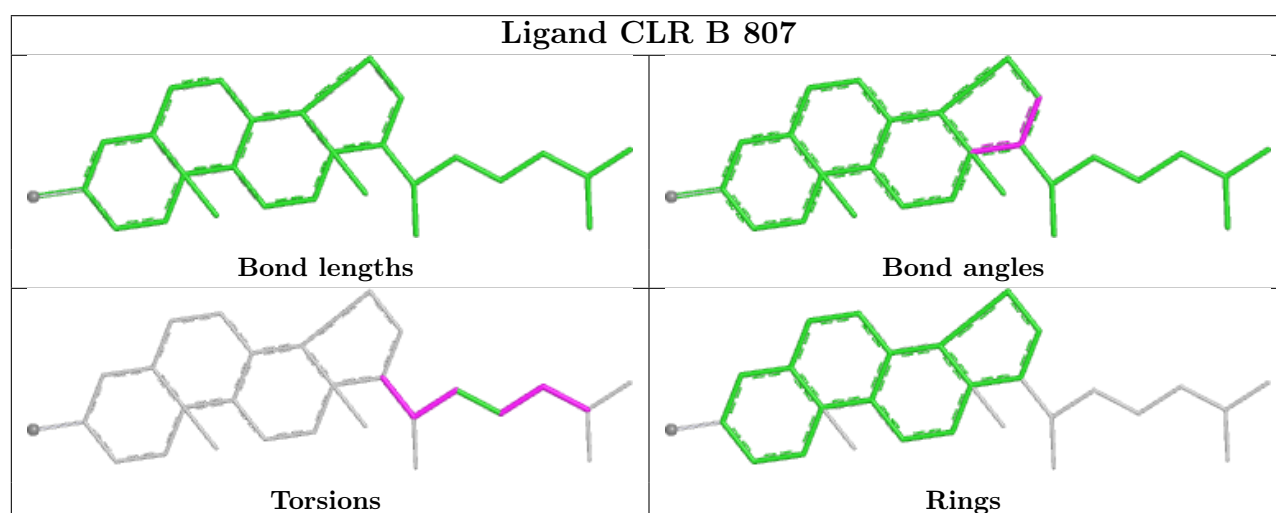
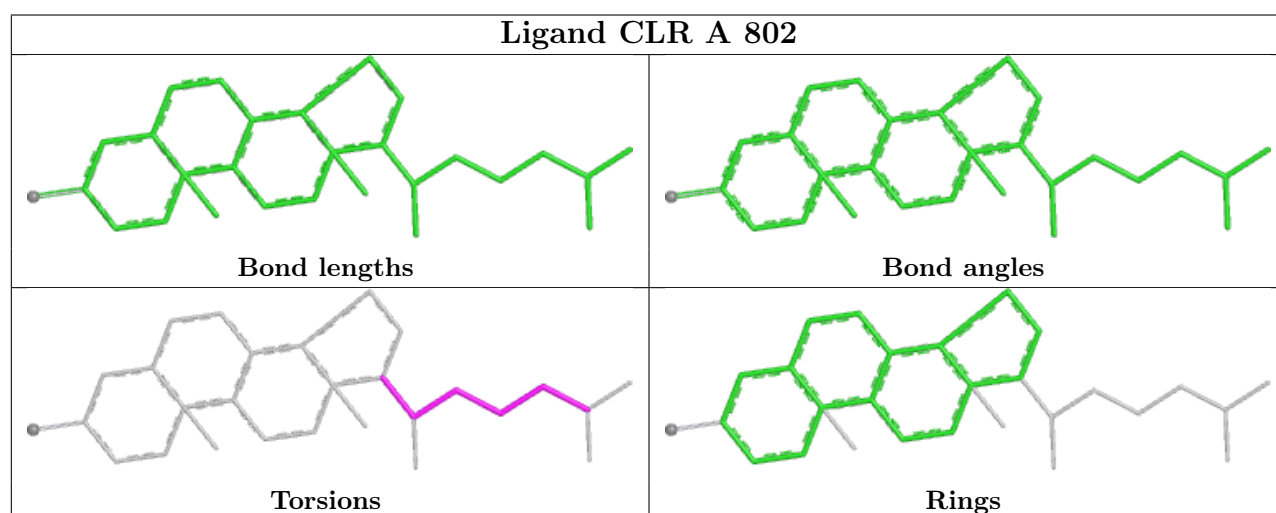
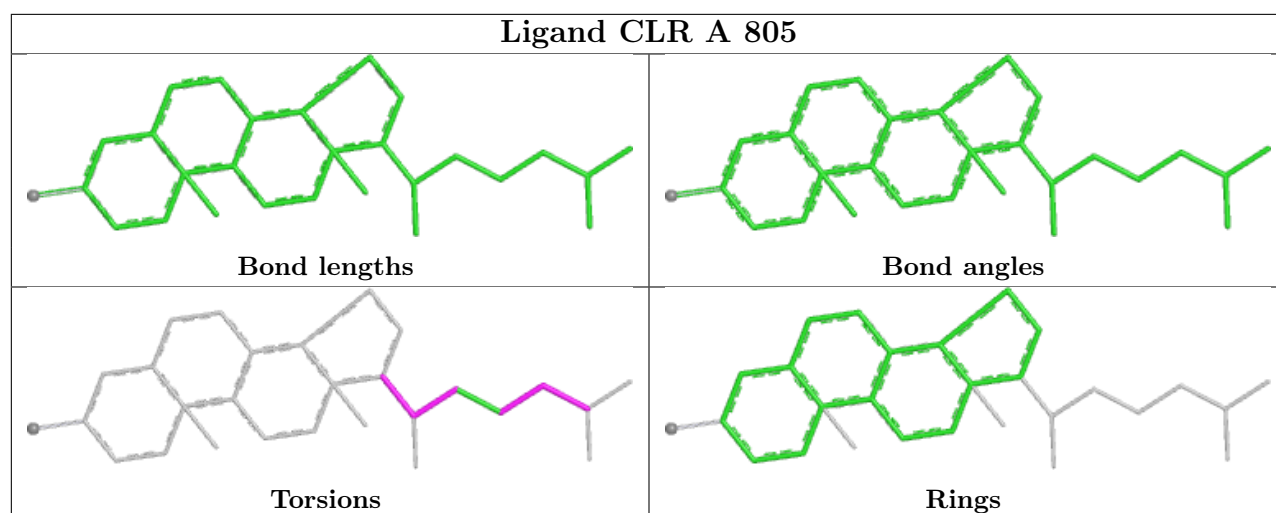
There are no ring outliers.

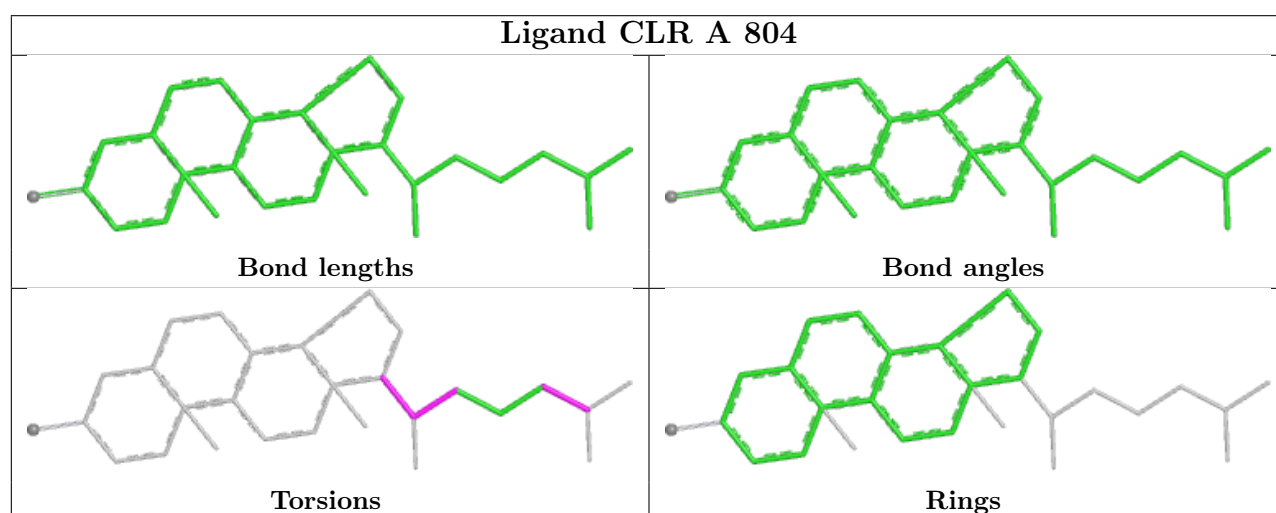
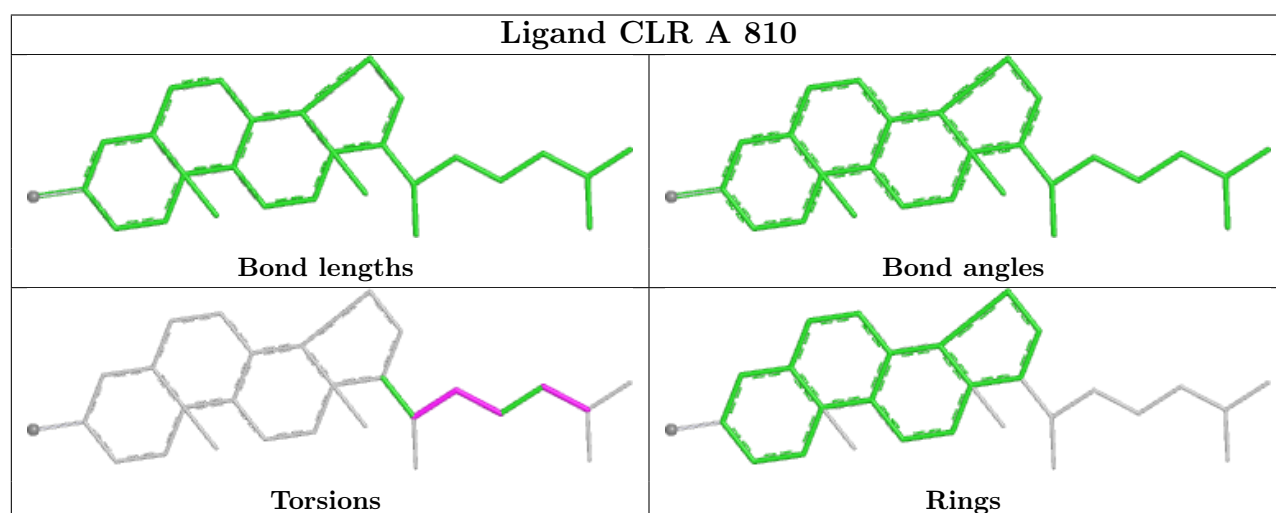
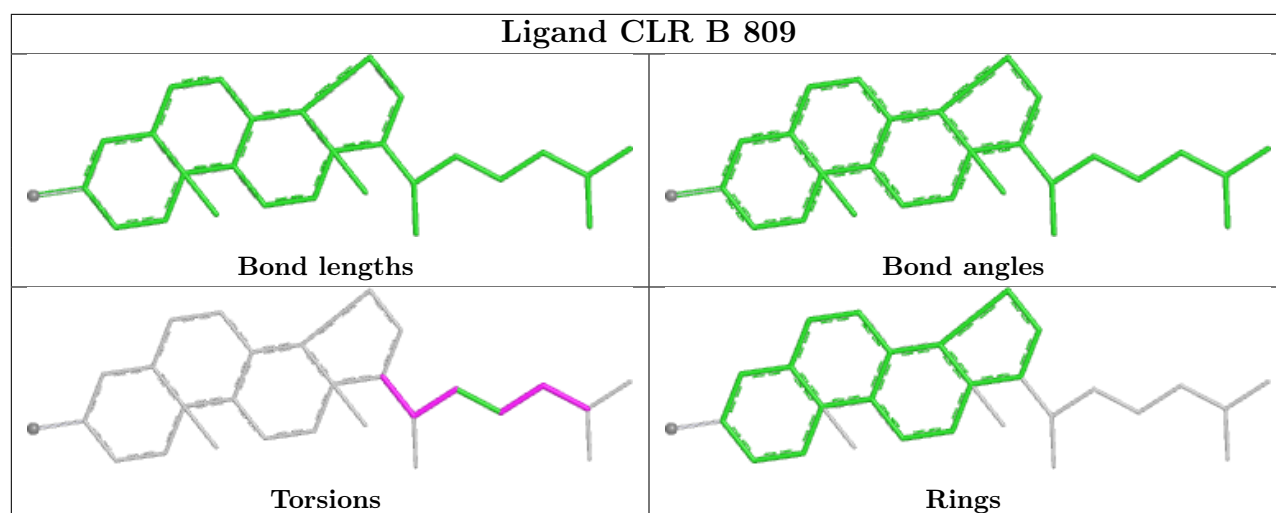
23 monomers are involved in 78 short contacts:

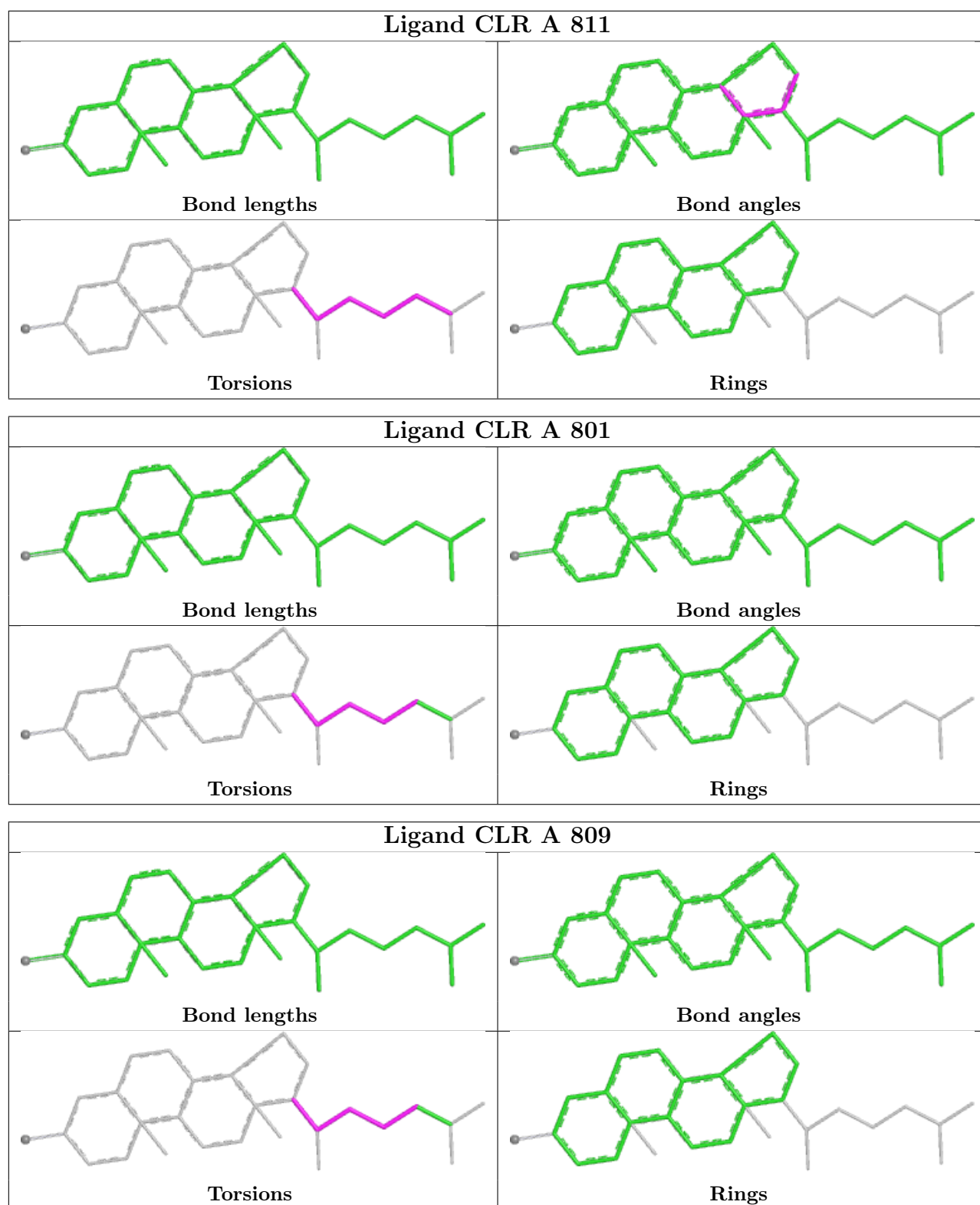
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	807	CLR	2	0
4	B	806	CLR	1	0
6	A	814	PEE	2	0
4	A	805	CLR	2	0
4	A	802	CLR	5	0
4	B	807	CLR	1	0
4	B	809	CLR	2	0
4	A	810	CLR	3	0
4	A	804	CLR	4	0
4	A	811	CLR	14	0
4	A	801	CLR	1	0
4	A	809	CLR	3	0
4	B	805	CLR	1	0
4	B	803	CLR	11	0
4	A	803	CLR	5	0
4	B	810	CLR	3	0
4	A	808	CLR	5	0
4	A	812	CLR	20	0
5	A	813	EIJ	1	0
4	B	801	CLR	4	0
4	B	808	CLR	4	0
4	A	806	CLR	3	0
4	B	804	CLR	2	0

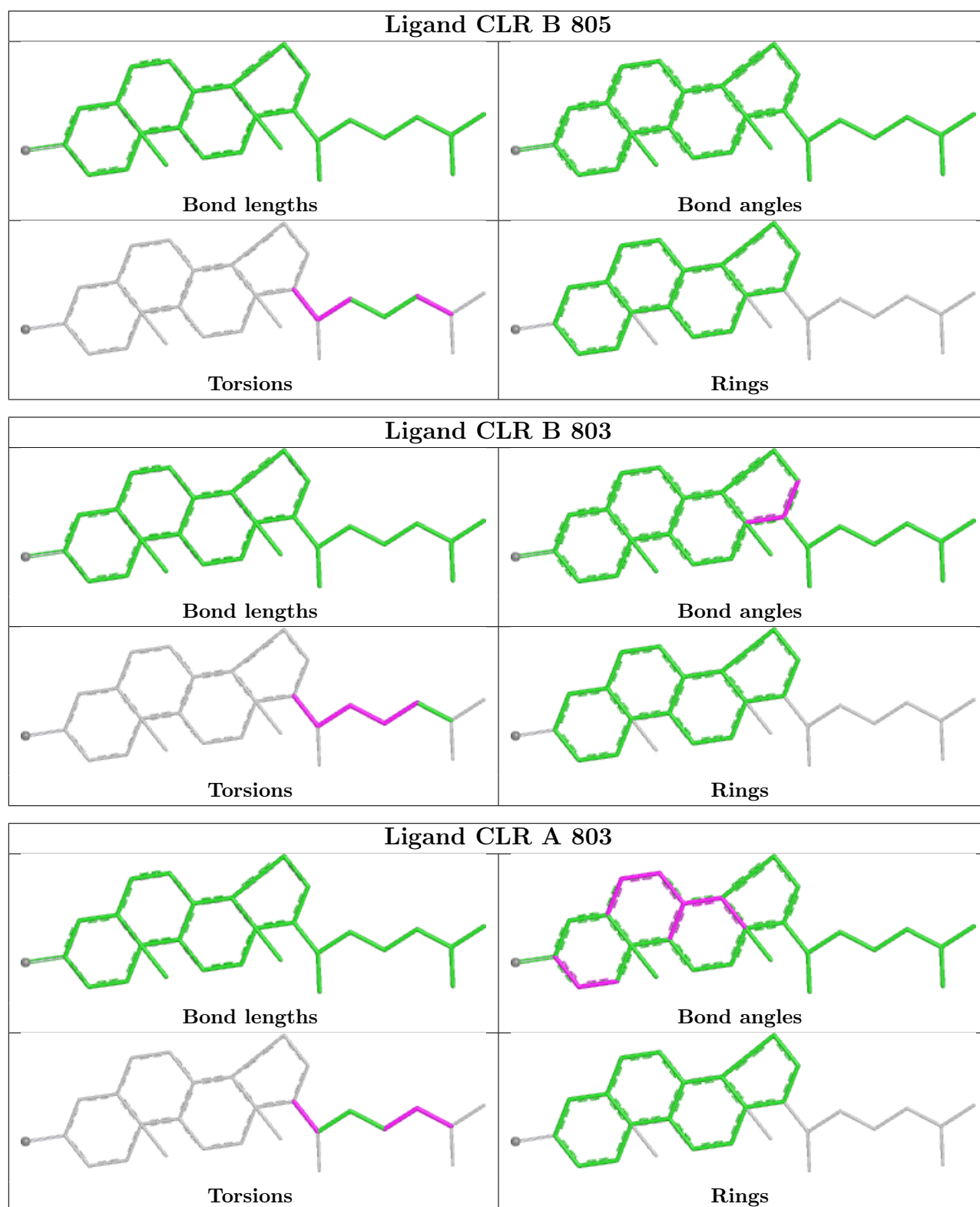
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

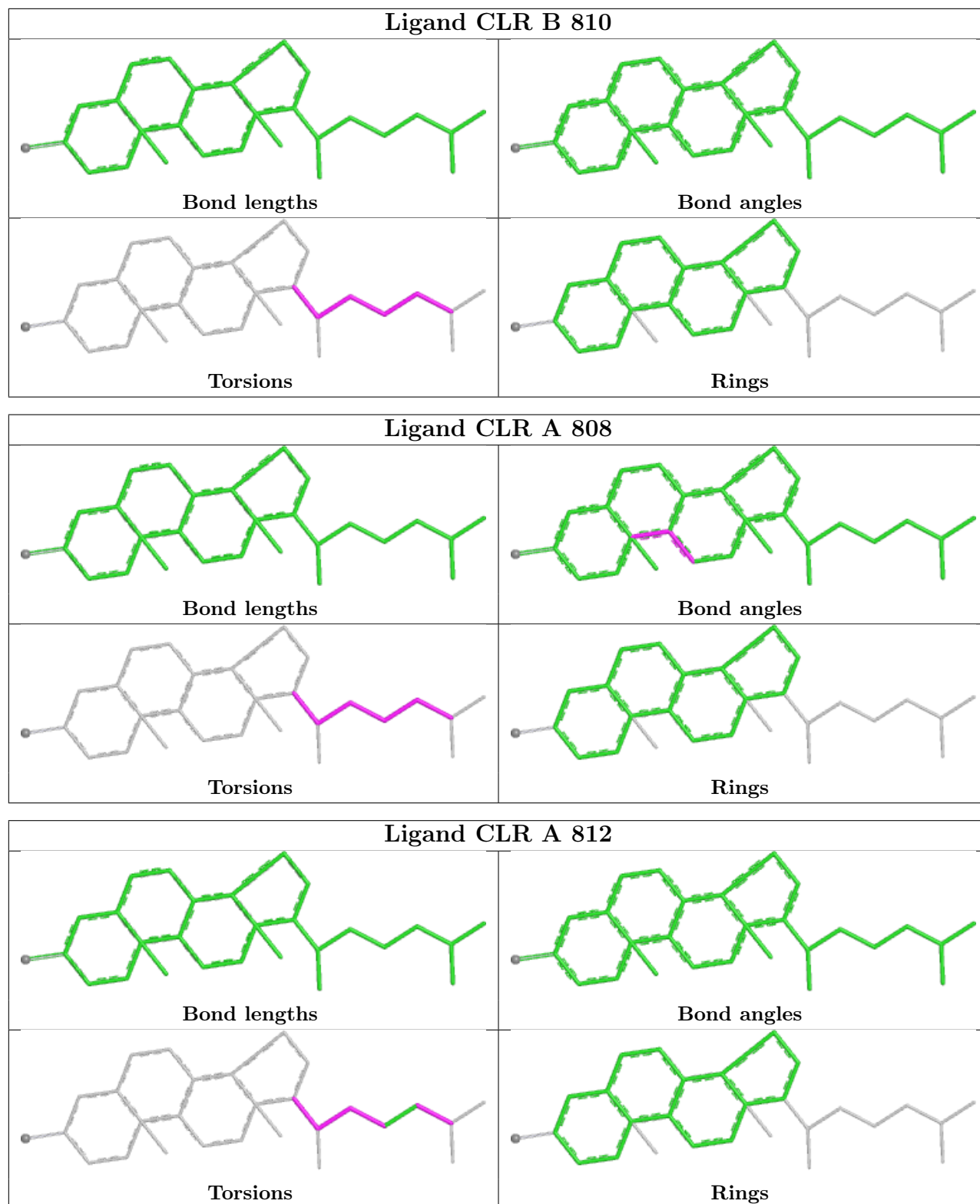


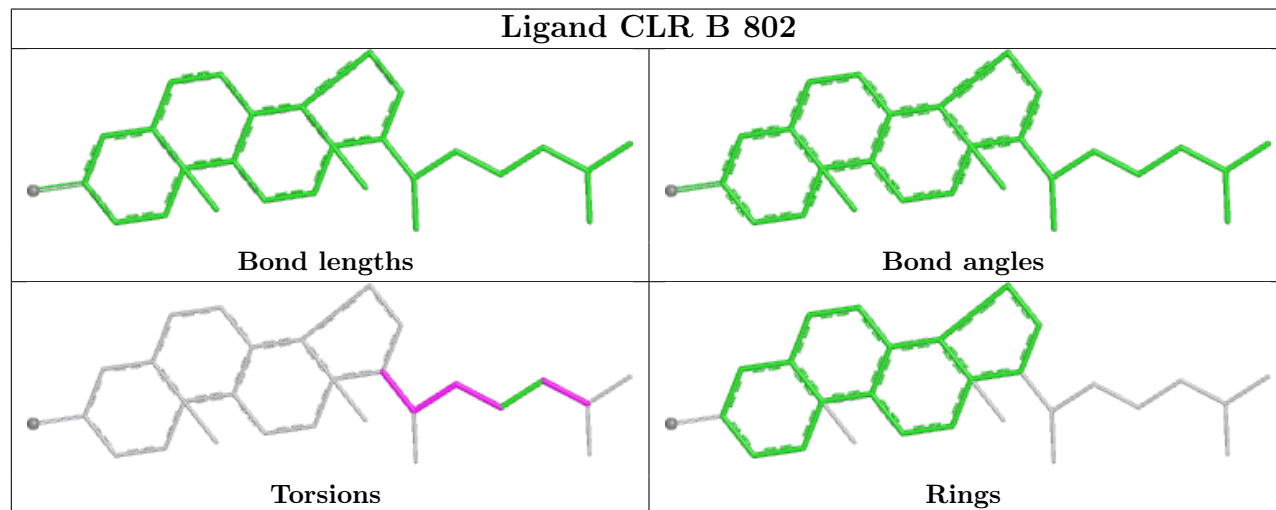
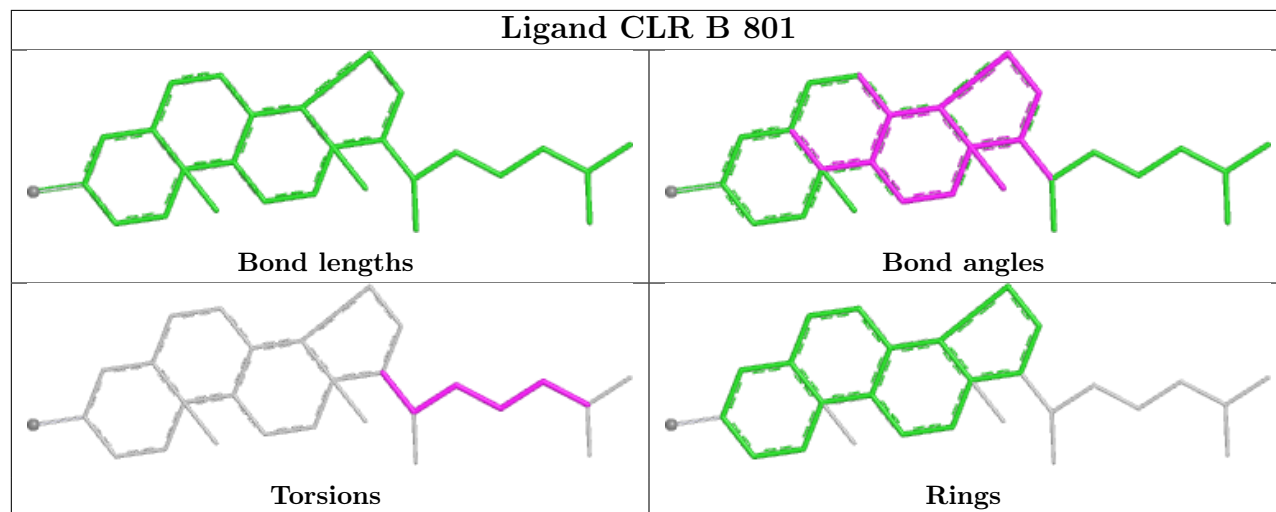
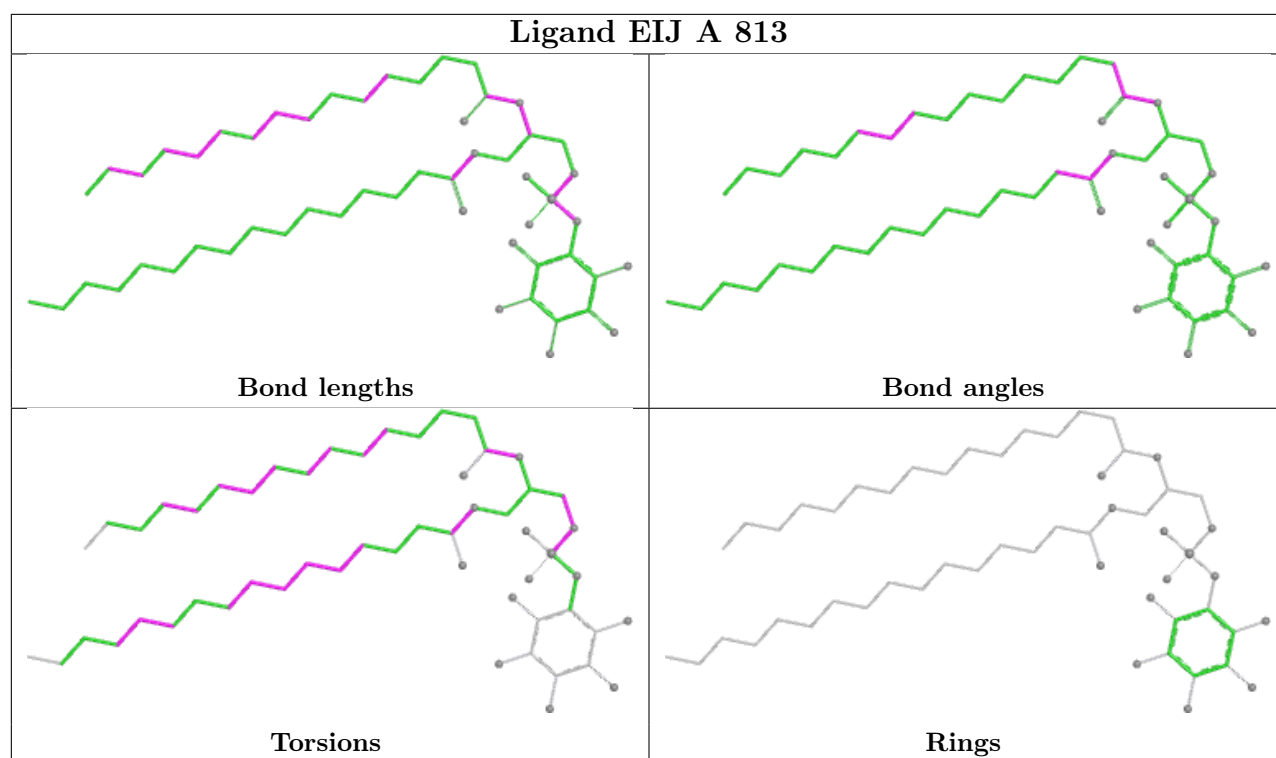


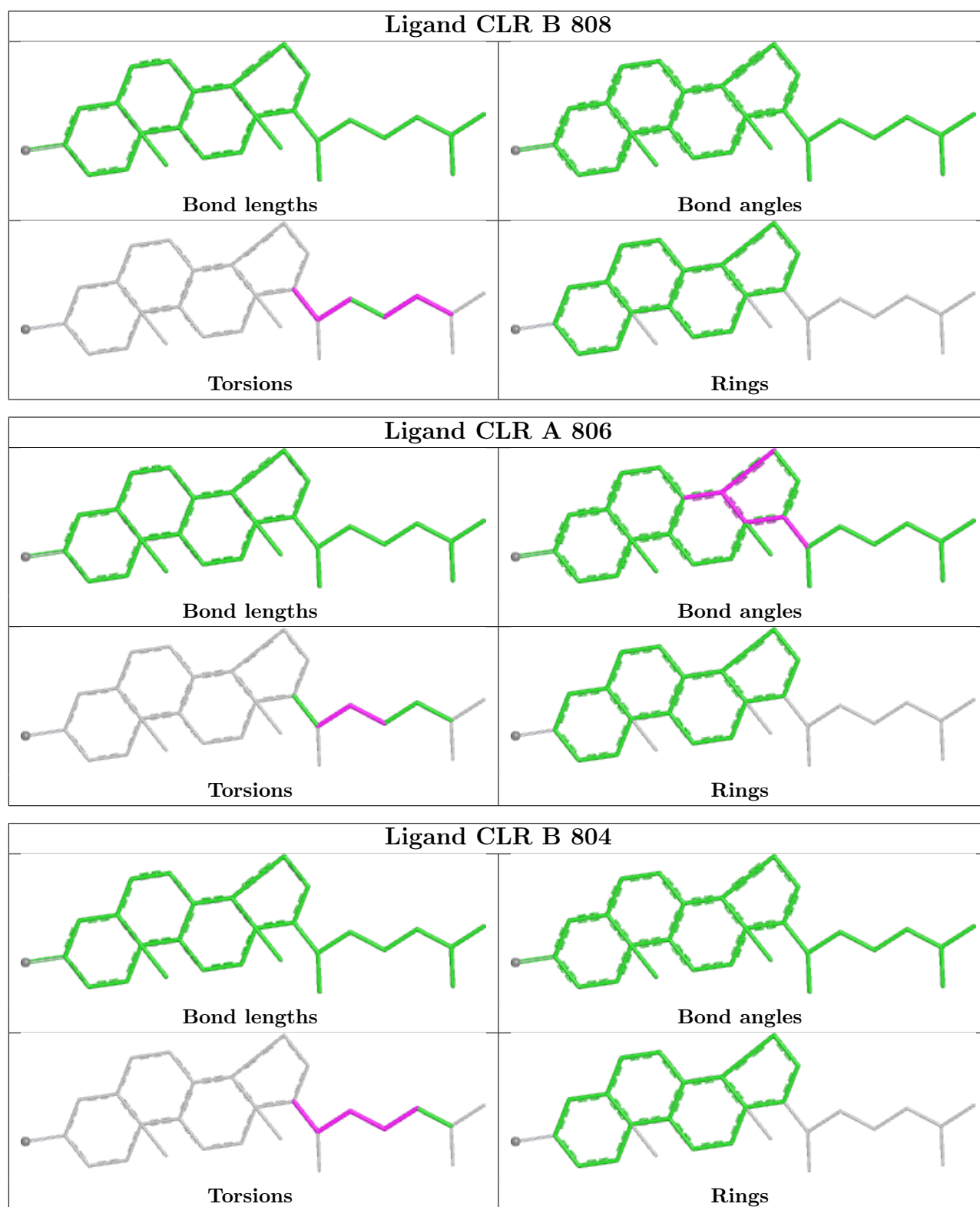












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

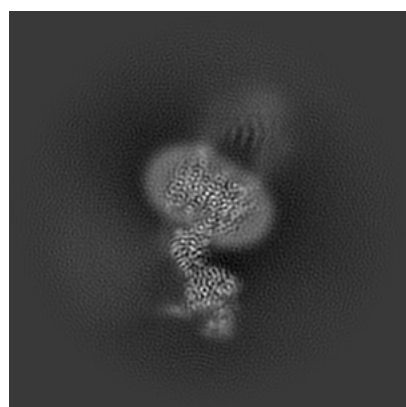
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25126. These allow visual inspection of the internal detail of the map and identification of artifacts.

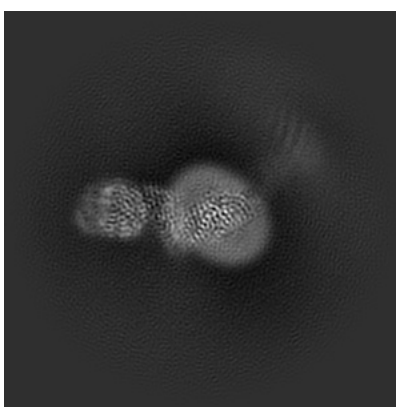
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

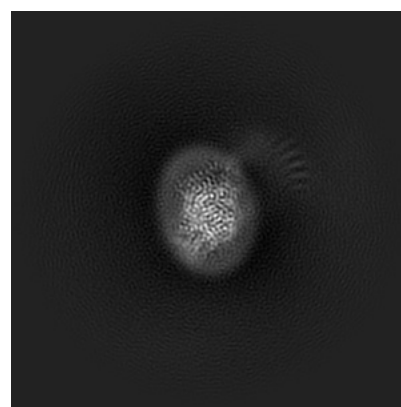
6.1.1 Primary map



X



Y

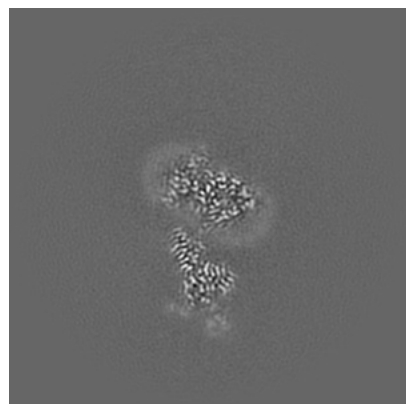


Z

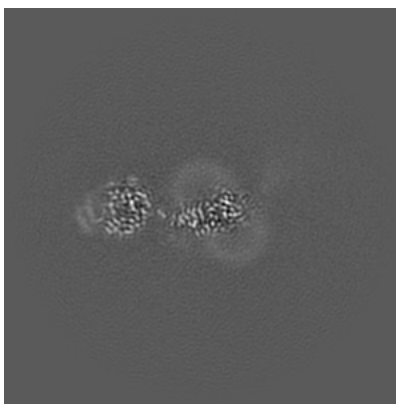
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

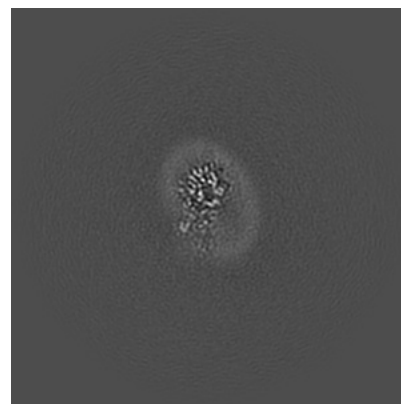
6.2.1 Primary map



X Index: 200



Y Index: 200

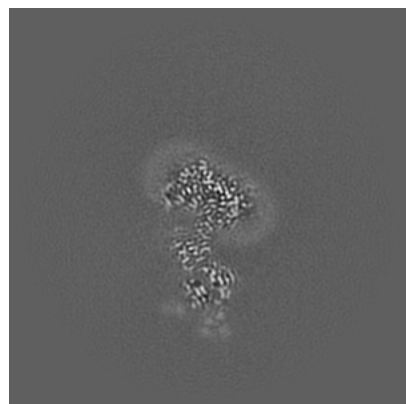


Z Index: 200

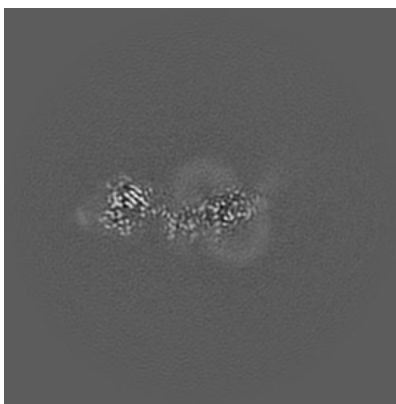
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

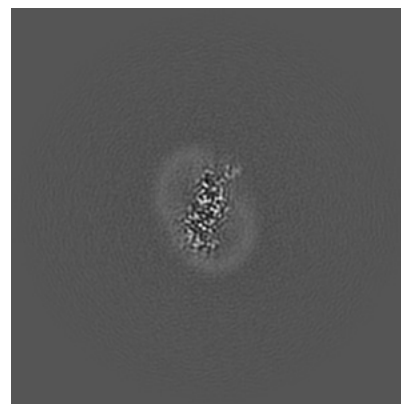
6.3.1 Primary map



X Index: 193



Y Index: 195

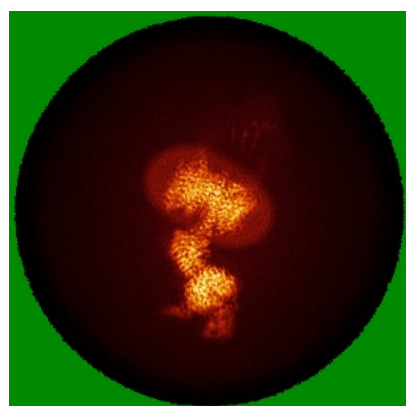


Z Index: 218

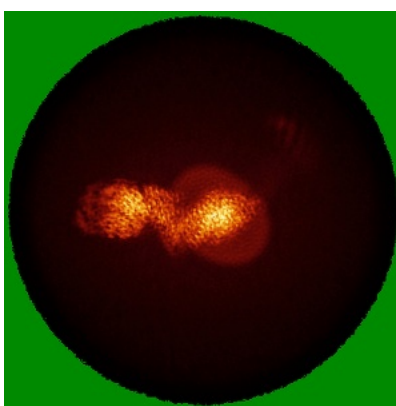
The images above show the largest variance slices of the map in three orthogonal directions.

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

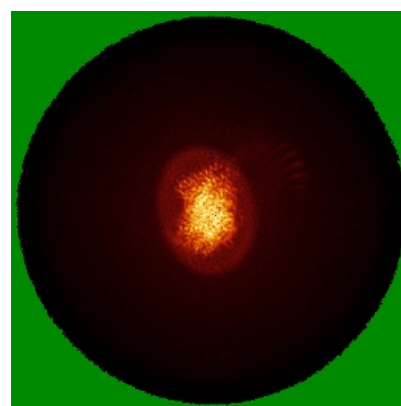
6.4.1 Primary map



X



Y

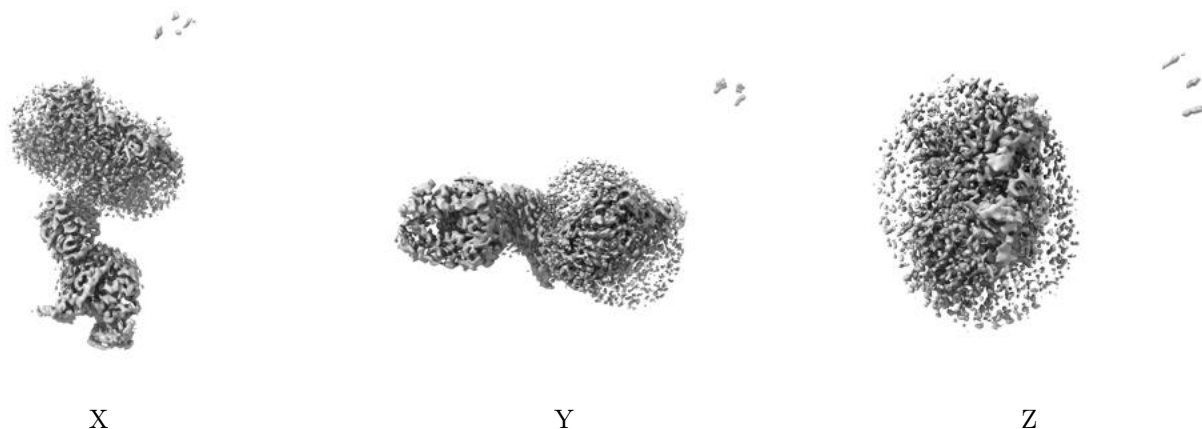


Z

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 0.359. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

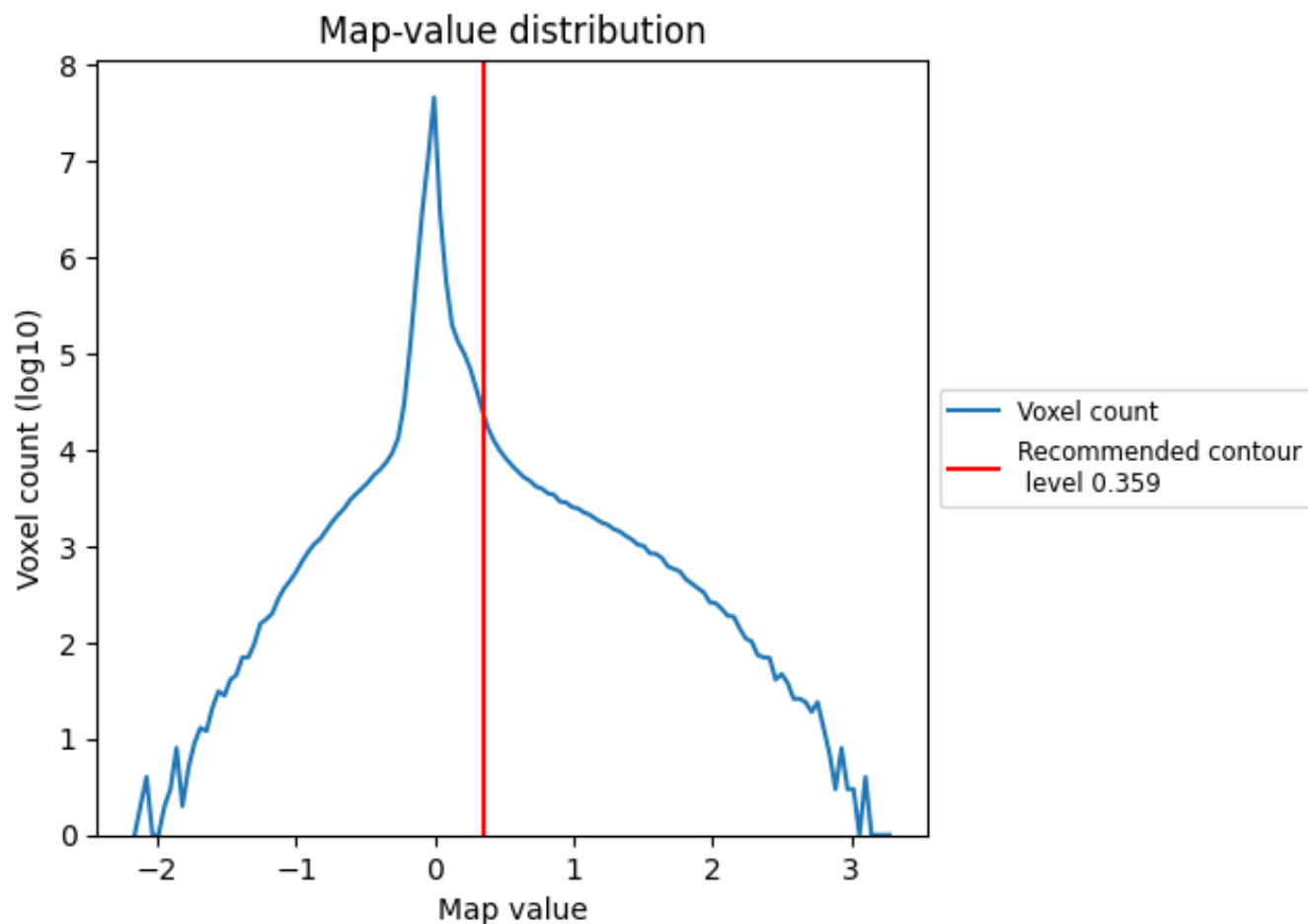
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

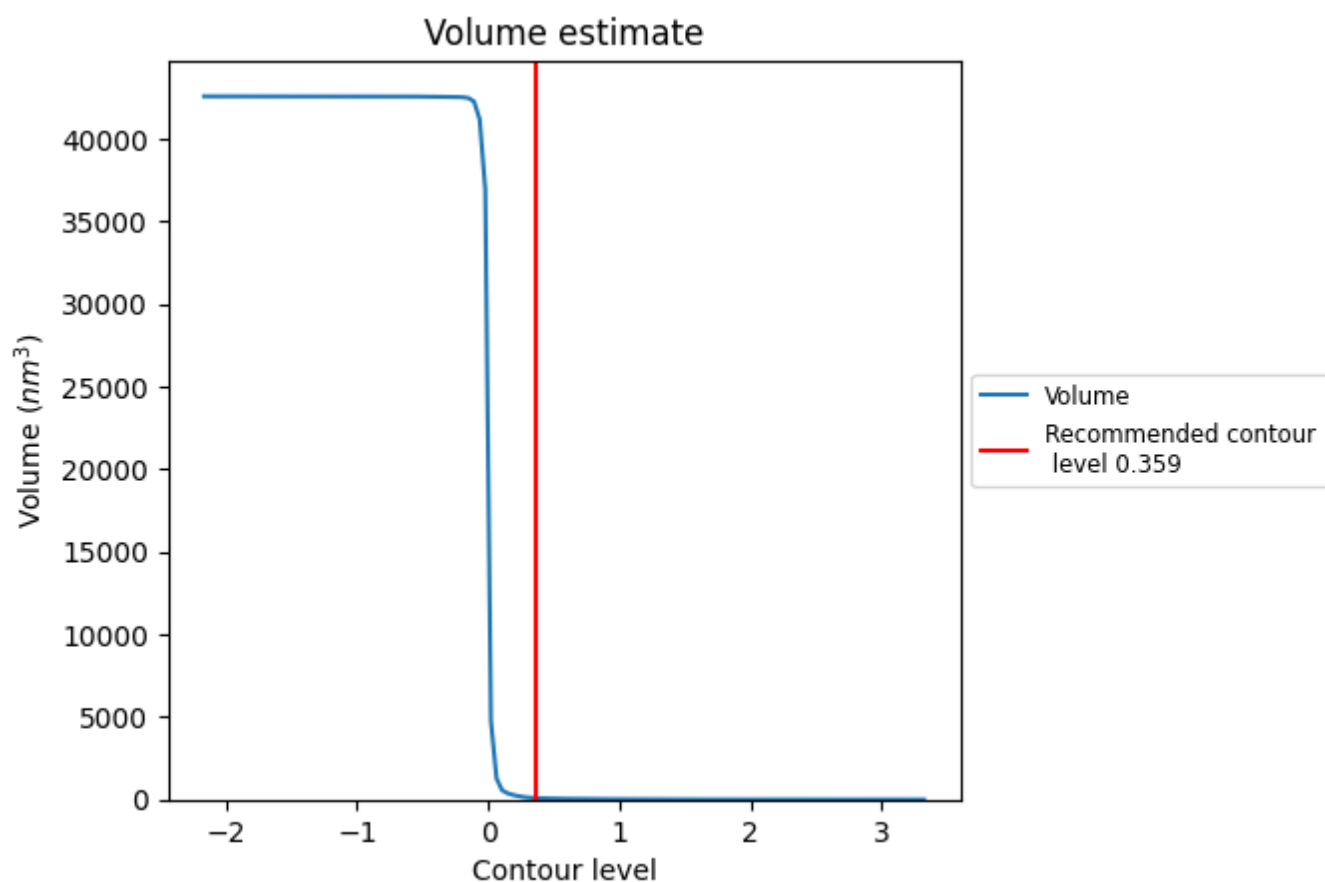
This section contains the results of statistical analysis of the map.

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.

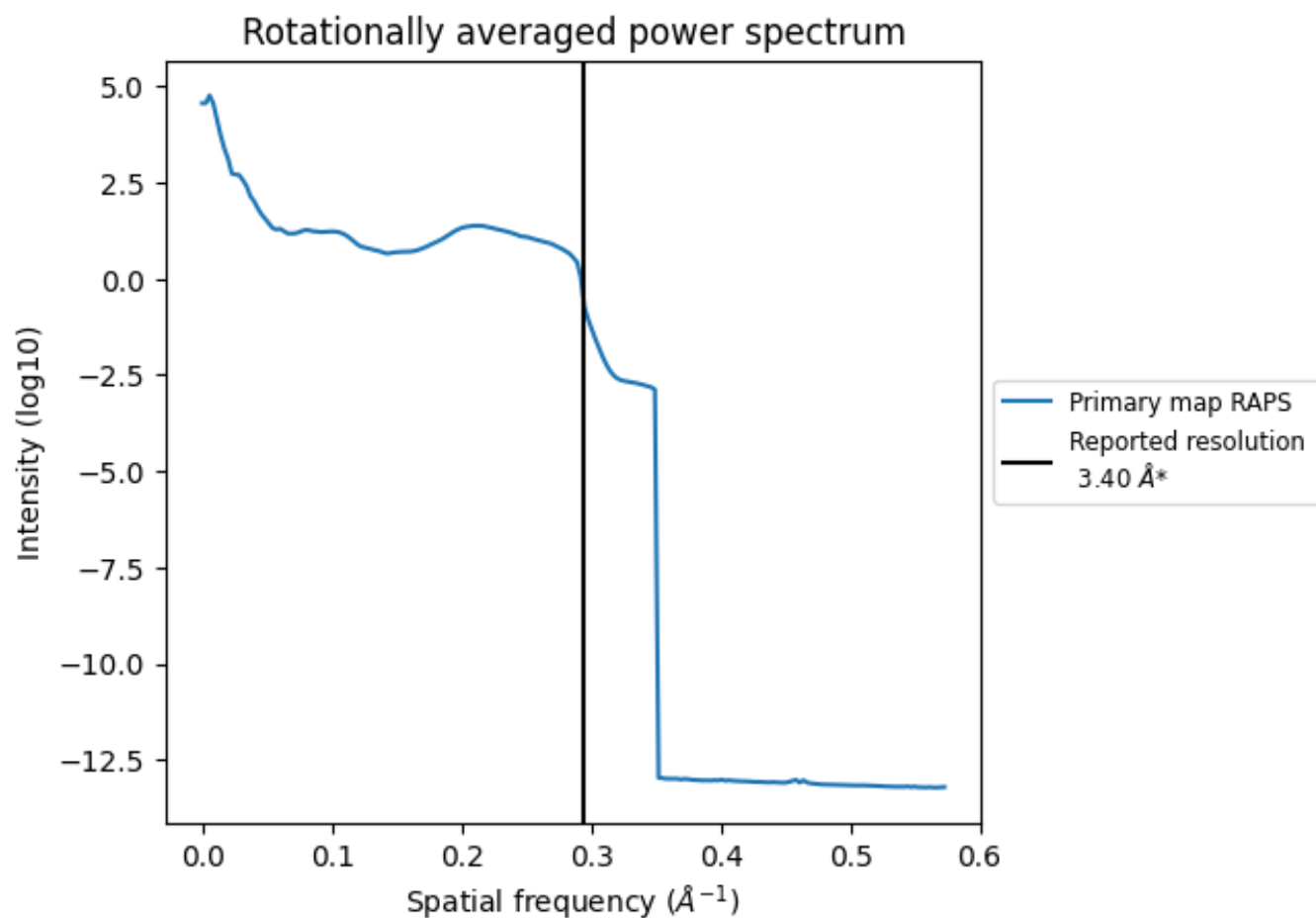
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 90 nm³; this corresponds to an approximate mass of 81 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

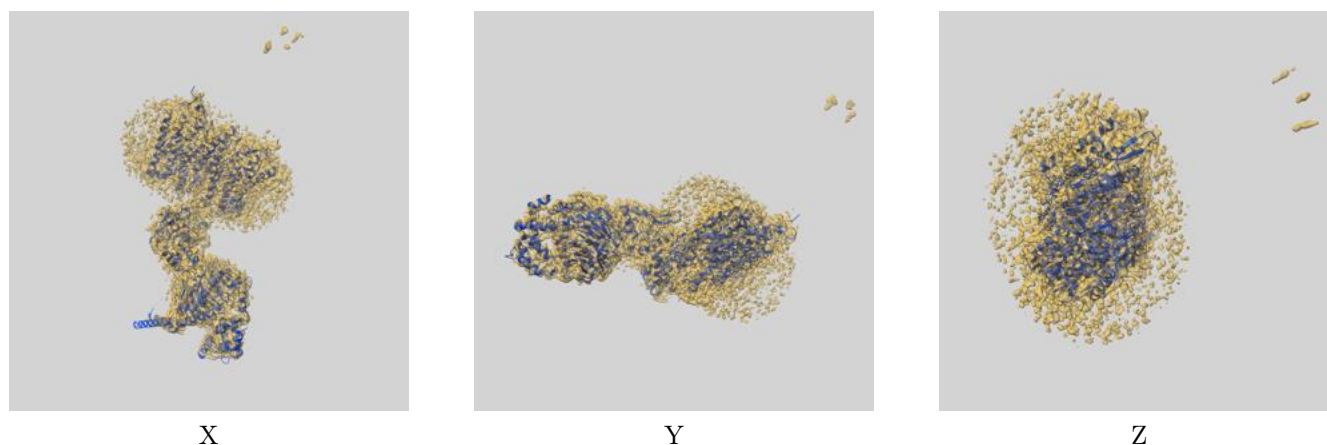
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

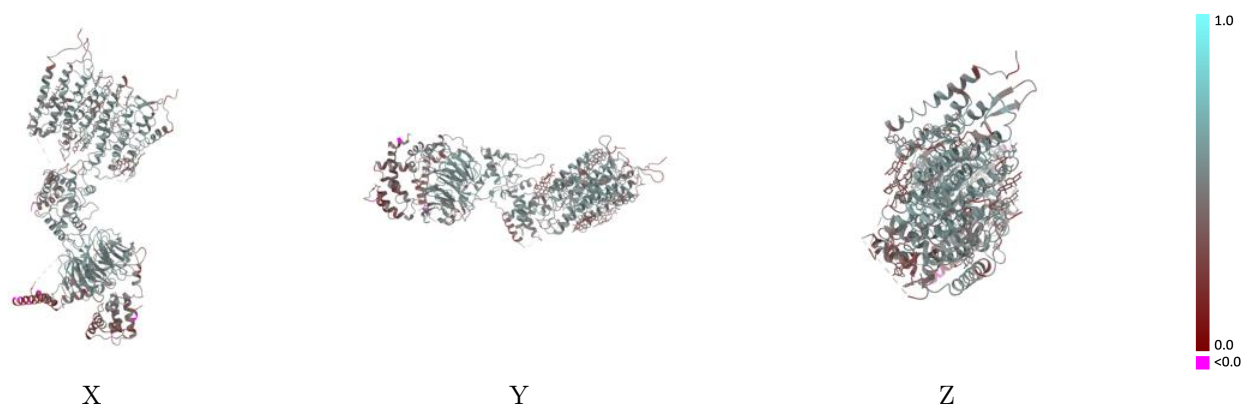
This section contains information regarding the fit between EMDB map EMD-25126 and PDB model 7SHF. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



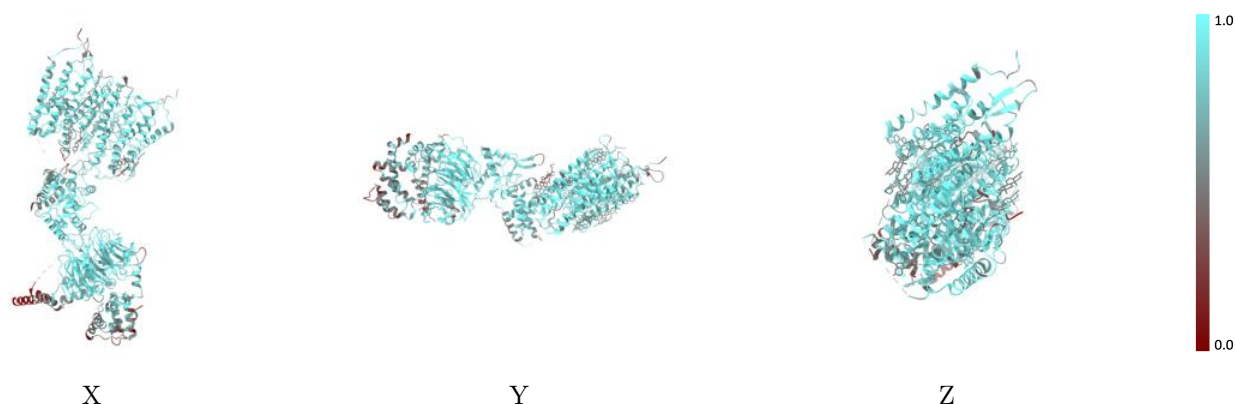
The images above show the 3D surface view of the map at the recommended contour level 0.359 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



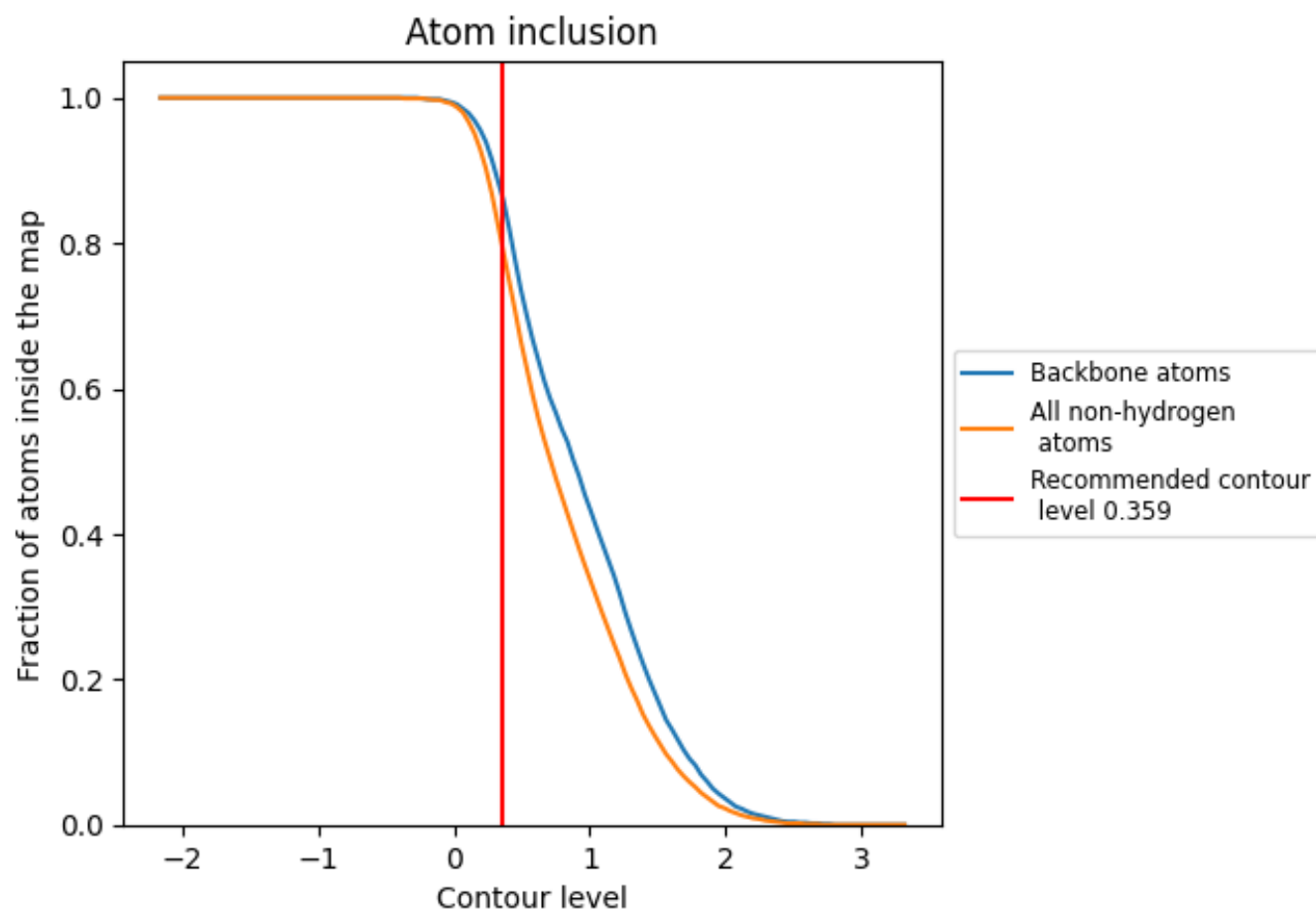
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.359).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 79% 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 (0.359) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7930	0.4780
A	0.8410	0.4970
B	0.7840	0.4680
C	0.7260	0.4540
D	0.8330	0.4980

