



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:25 PM UTC

PDB ID : 8S3E / pdb_00008s3e
EMDB ID : EMD-19691
Title : Structure of rabbit Slo1 in complex with gamma1/LRRC26
Authors : Redhardt, M.; Raunser, S.; Raisch, T.
Deposited on : 2024-02-20
Resolution : 2.39 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:

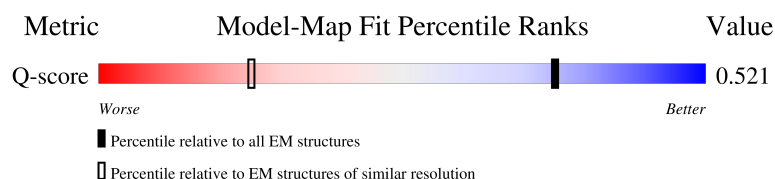
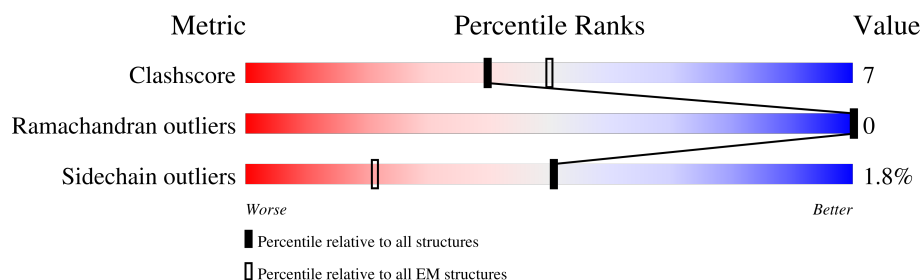
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.39 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	4884 (1.90 - 2.89)

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	1119	
1	B	1119	
1	C	1119	
1	D	1119	

Continued on next page...

Mol	Chain	Length	Quality of chain
2	E	340	 11% 86%
2	F	340	 12% 86%
2	G	340	 11% 86%
2	H	340	 11% 86%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 31585 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 Calcium-activated potassium channel subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	902	Total	C	N	O	S	0	0
			7192	4671	1173	1300	48		
1	B	902	Total	C	N	O	S	0	0
			7192	4671	1173	1300	48		
1	C	902	Total	C	N	O	S	0	0
			7192	4671	1173	1300	48		
1	D	902	Total	C	N	O	S	0	0
			7192	4671	1173	1300	48		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1114	LEU	-	expression tag	UNP Q9BG98
A	1115	GLU	-	expression tag	UNP Q9BG98
A	1116	VAL	-	expression tag	UNP Q9BG98
A	1117	LEU	-	expression tag	UNP Q9BG98
A	1118	PHE	-	expression tag	UNP Q9BG98
A	1119	GLN	-	expression tag	UNP Q9BG98
B	1114	LEU	-	expression tag	UNP Q9BG98
B	1115	GLU	-	expression tag	UNP Q9BG98
B	1116	VAL	-	expression tag	UNP Q9BG98
B	1117	LEU	-	expression tag	UNP Q9BG98
B	1118	PHE	-	expression tag	UNP Q9BG98
B	1119	GLN	-	expression tag	UNP Q9BG98
C	1114	LEU	-	expression tag	UNP Q9BG98
C	1115	GLU	-	expression tag	UNP Q9BG98
C	1116	VAL	-	expression tag	UNP Q9BG98
C	1117	LEU	-	expression tag	UNP Q9BG98
C	1118	PHE	-	expression tag	UNP Q9BG98
C	1119	GLN	-	expression tag	UNP Q9BG98
D	1114	LEU	-	expression tag	UNP Q9BG98
D	1115	GLU	-	expression tag	UNP Q9BG98
D	1116	VAL	-	expression tag	UNP Q9BG98
D	1117	LEU	-	expression tag	UNP Q9BG98

Continued on next page...

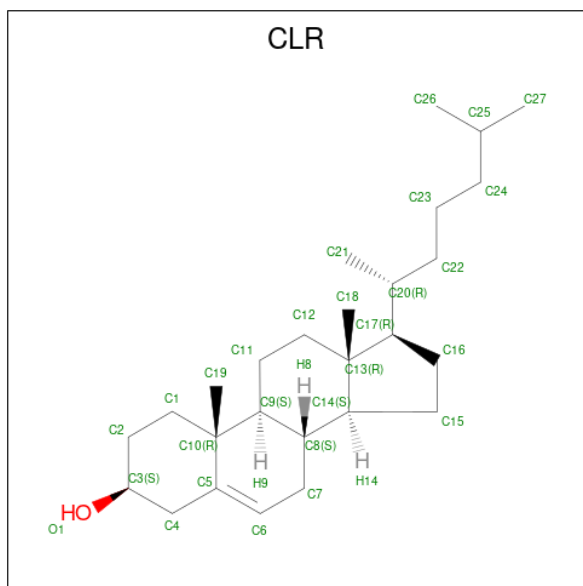
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1118	PHE	-	expression tag	UNP Q9BG98
D	1119	GLN	-	expression tag	UNP Q9BG98

- Molecule 2 is a protein called Leucine-rich repeat-containing protein 26.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	48	Total	C	N	O	S	0	0
			367	228	78	57	4		
2	F	48	Total	C	N	O	S	0	0
			367	228	78	57	4		
2	G	48	Total	C	N	O	S	0	0
			367	228	78	57	4		
2	H	48	Total	C	N	O	S	0	0
			367	228	78	57	4		

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



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

Continued on next page...

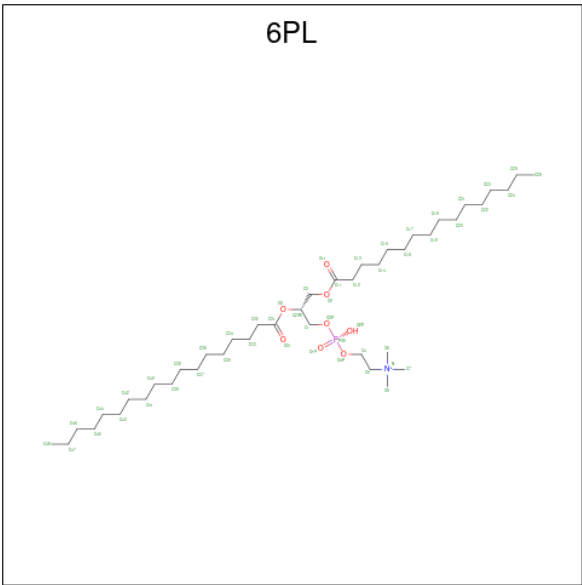
Continued from previous page...

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Ca	0
			2	2	
4	B	2	Total	Ca	0
			2	2	
4	C	2	Total	Ca	0
			2	2	
4	D	2	Total	Ca	0
			2	2	

- Molecule 5 is (4S,7R)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: 6PL) (formula: C₄₂H₈₅NO₈P).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			29	19	1	8	1	
5	A	1	Total	C	O			0
			26	22	4			
5	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
5	A	1	Total	C	O			0
			27	22	5			
5	A	1	Total	C	O			0
			16	12	4			
5	A	1	Total	C	O	P		0
			23	14	8	1		
5	A	1	Total	C	O	P		0
			22	13	8	1		
5	A	1	Total	C	O	P		0
			23	15	7	1		
5	A	1	Total	C	O	P		0
			19	11	7	1		
5	B	1	Total	C	O	P		0
			19	11	7	1		
5	B	1	Total	C	N	O	P	0
			29	19	1	8	1	
5	B	1	Total	C	O			0
			26	22	4			
5	B	1	Total	C	N	O	P	0
			33	23	1	8	1	
5	B	1	Total	C	O			0
			27	22	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total 16	C 12	O 4		0
5	B	1	Total 23	C 14	O 8	P 1	0
5	B	1	Total 22	C 13	O 8	P 1	0
5	B	1	Total 23	C 15	O 7	P 1	0
5	C	1	Total 19	C 11	O 7	P 1	0
5	C	1	Total 29	C 19	N 1	O 8 P 1	0
5	C	1	Total 26	C 22	O 4		0
5	C	1	Total 33	C 23	N 1	O 8 P 1	0
5	C	1	Total 27	C 22	O 5		0
5	C	1	Total 16	C 12	O 4		0
5	C	1	Total 23	C 14	O 8	P 1	0
5	C	1	Total 22	C 13	O 8	P 1	0
5	C	1	Total 23	C 15	O 7	P 1	0
5	D	1	Total 19	C 11	O 7	P 1	0
5	D	1	Total 29	C 19	N 1	O 8 P 1	0
5	D	1	Total 26	C 22	O 4		0
5	D	1	Total 33	C 23	N 1	O 8 P 1	0
5	D	1	Total 27	C 22	O 5		0
5	D	1	Total 16	C 12	O 4		0
5	D	1	Total 23	C 14	O 8	P 1	0
5	D	1	Total 22	C 13	O 8	P 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
5	D	1	Total	C	O	P	0
			23	15	7	1	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	
6	B	1	Total	Mg	0
			1	1	
6	C	1	Total	Mg	0
			1	1	
6	D	1	Total	Mg	0
			1	1	

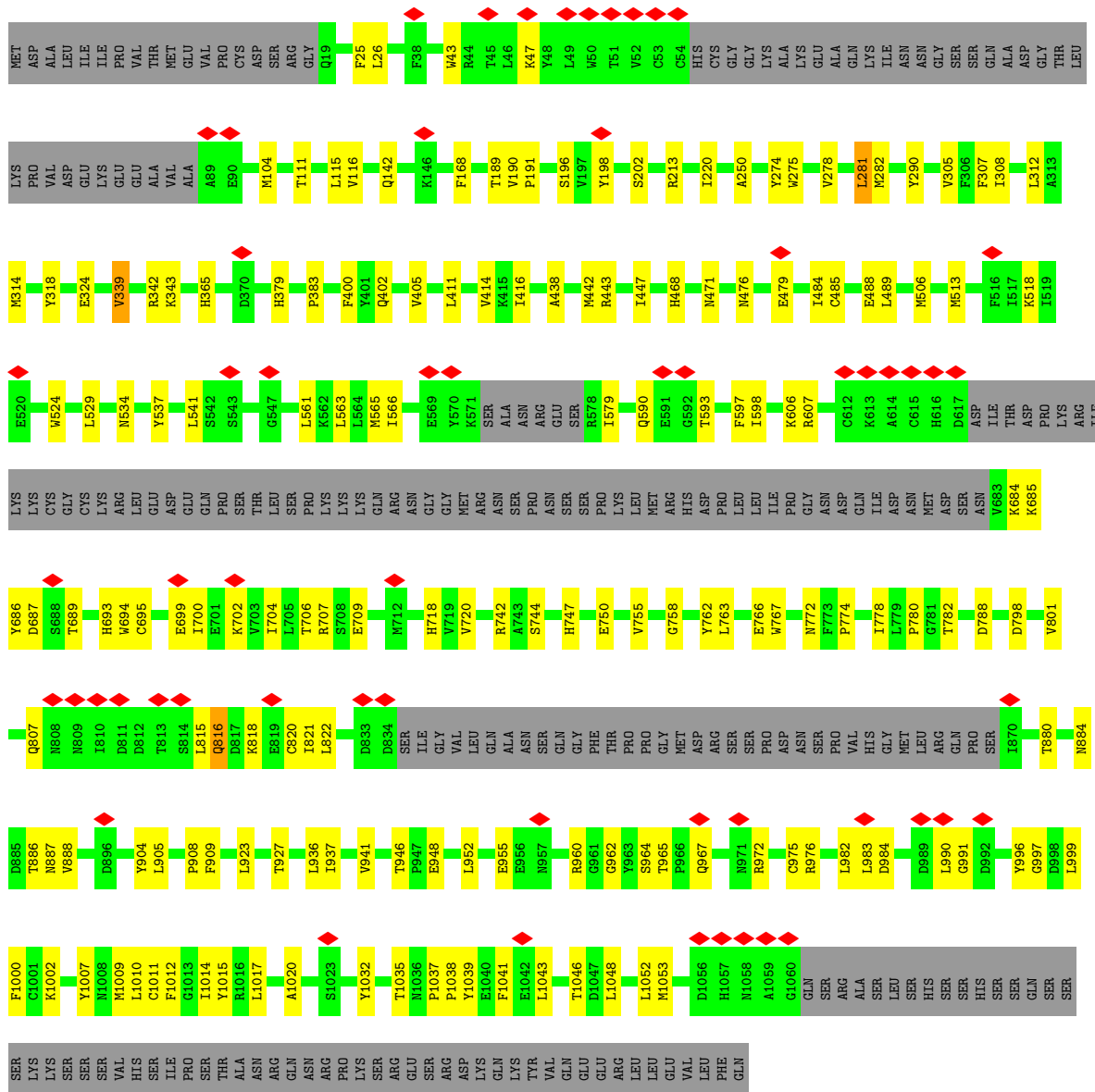
- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	K	0
			2	2	
7	B	1	Total	K	0
			1	1	
7	D	1	Total	K	0
			1	1	

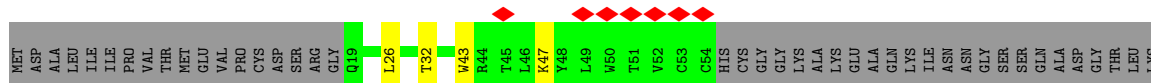
- Molecule 8 is water.

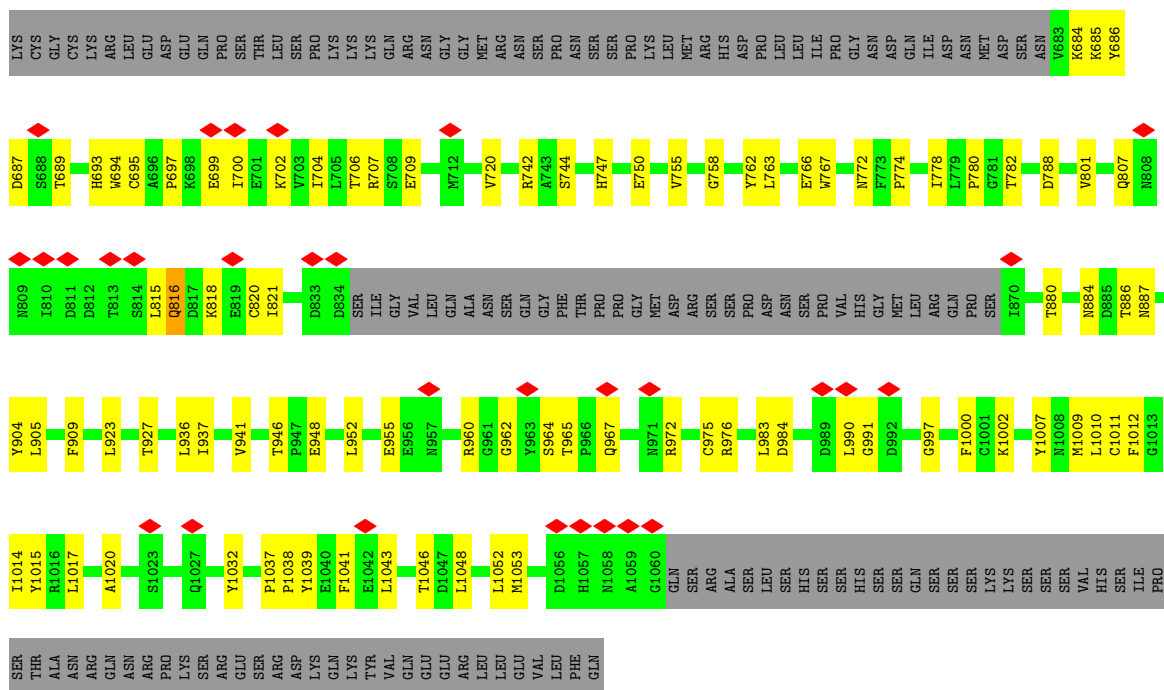
Mol	Chain	Residues	Atoms		AltConf
8	A	3	Total	O	0
			3	3	
8	B	3	Total	O	0
			3	3	
8	C	3	Total	O	0
			3	3	
8	D	4	Total	O	0
			4	4	

Chain B: 5% 65% 15% 19%

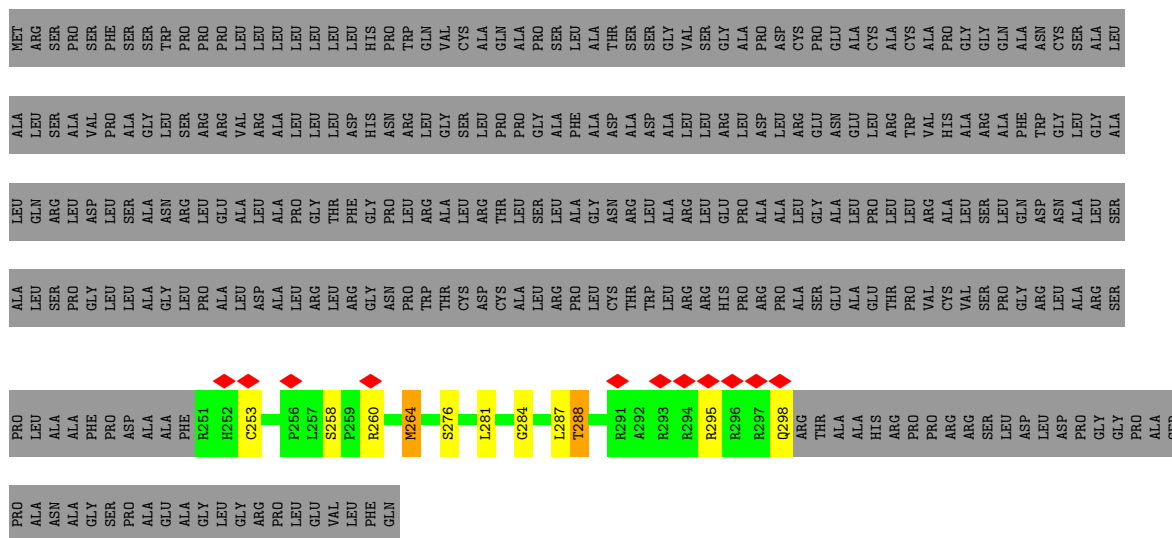


Chain C: 5% 65% 15% 19%

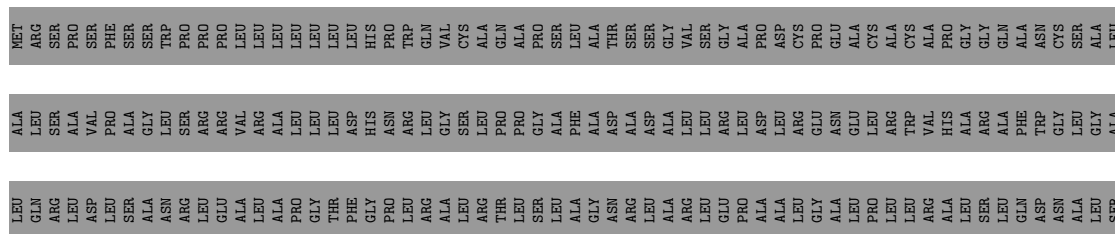


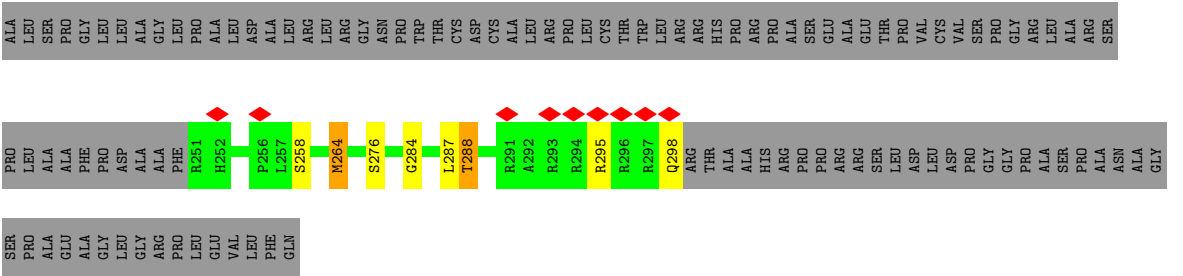


- Molecule 2: Leucine-rich repeat-containing protein 26

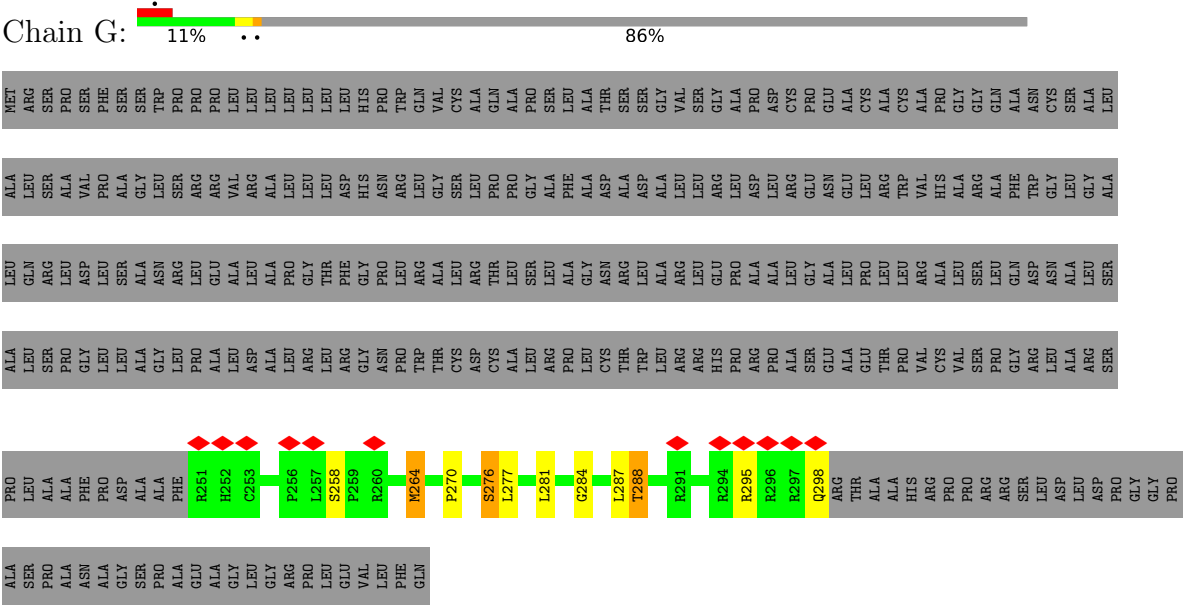


- Molecule 2: Leucine-rich repeat-containing protein 26

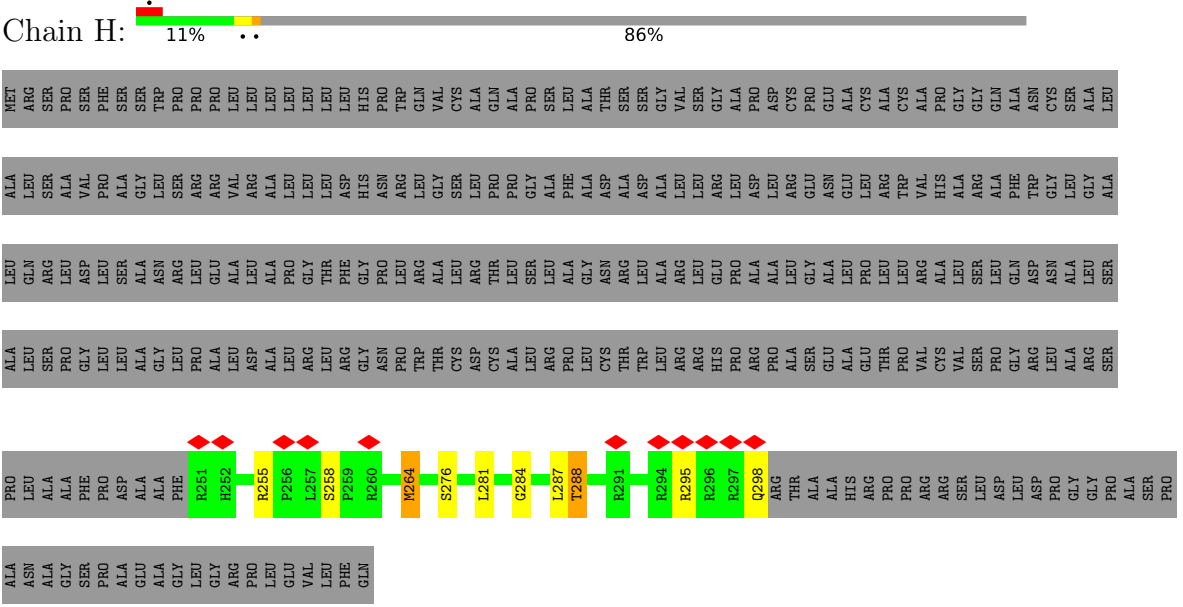




• Molecule 2: Leucine-rich repeat-containing protein 26



• Molecule 2: Leucine-rich repeat-containing protein 26



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	826667	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 ($e^-/\text{\AA}^2$)	52.3	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	72.555	Depositor
Minimum map value	-35.356	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.5	Depositor
Map size ($\text{\AA}$)	348.16, 348.16, 348.16	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.68, 0.68, 0.68	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: 6PL, MG, CA, K, 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	0.11	0/7360	0.28	0/9991
1	B	0.11	0/7360	0.28	0/9991
1	C	0.11	0/7360	0.28	0/9991
1	D	0.11	0/7360	0.28	0/9991
2	E	0.14	0/372	0.39	0/500
2	F	0.13	0/372	0.39	0/500
2	G	0.14	0/372	0.39	0/500
2	H	0.14	0/372	0.39	0/500
All	All	0.11	0/30928	0.29	0/41964

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	7192	0	7176	114	0
1	B	7192	0	7176	119	0
1	C	7192	0	7176	117	0
1	D	7192	0	7176	111	0
2	E	367	0	395	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	367	0	395	3	0
2	G	367	0	395	7	0
2	H	367	0	395	5	0
3	A	112	0	184	5	0
3	B	112	0	184	5	0
3	C	112	0	184	5	0
3	D	112	0	184	6	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	218	0	233	2	0
5	B	218	0	233	1	0
5	C	218	0	233	1	0
5	D	218	0	233	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	A	3	0	0	0	0
8	B	3	0	0	0	0
8	C	3	0	0	0	0
8	D	4	0	0	0	0
All	All	31585	0	31952	450	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 7.

All (450) 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:975:CYS:HA	1:A:1053:MET:O	1.80	0.82
1:D:975:CYS:HA	1:D:1053:MET:O	1.80	0.82
1:A:284:THR:HG1	1:B:290:TYR:HH	1.26	0.81
1:B:975:CYS:HA	1:B:1053:MET:O	1.80	0.81
1:C:975:CYS:HA	1:C:1053:MET:O	1.80	0.81
1:C:284:THR:HG1	1:D:290:TYR:HH	1.32	0.77
1:A:747:HIS:HB2	1:A:750:GLU:HG3	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:747:HIS:HB2	1:C:750:GLU:HG3	1.67	0.76
1:B:442:MET:HE3	1:C:818:LYS:HD3	1.68	0.75
1:B:747:HIS:HB2	1:B:750:GLU:HG3	1.67	0.75
1:D:747:HIS:HB2	1:D:750:GLU:HG3	1.67	0.74
1:D:308:ILE:O	1:D:312:LEU:HB2	1.89	0.73
1:C:308:ILE:O	1:C:312:LEU:HB2	1.89	0.72
1:A:308:ILE:O	1:A:312:LEU:HB2	1.89	0.72
1:A:442:MET:HE3	1:B:818:LYS:HD3	1.72	0.71
1:B:308:ILE:O	1:B:312:LEU:HB2	1.89	0.71
1:D:807:GLN:O	1:D:816:GLN:NE2	2.27	0.68
1:D:1015:TYR:HB3	1:D:1048:LEU:HB2	1.76	0.68
1:A:807:GLN:O	1:A:816:GLN:NE2	2.27	0.67
1:B:1015:TYR:HB3	1:B:1048:LEU:HB2	1.76	0.67
1:B:807:GLN:O	1:B:816:GLN:NE2	2.27	0.67
1:C:807:GLN:O	1:C:816:GLN:NE2	2.27	0.67
1:A:250:ALA:HA	1:A:281:LEU:HD13	1.78	0.66
1:A:1015:TYR:HB3	1:A:1048:LEU:HB2	1.76	0.66
1:D:250:ALA:HA	1:D:281:LEU:HD13	1.78	0.66
1:C:1015:TYR:HB3	1:C:1048:LEU:HB2	1.76	0.65
1:A:818:LYS:HD3	1:D:442:MET:HE3	1.78	0.65
1:C:250:ALA:HA	1:C:281:LEU:HD13	1.78	0.65
1:B:250:ALA:HA	1:B:281:LEU:HD13	1.78	0.65
1:B:704:ILE:HG12	1:B:778:ILE:HB	1.79	0.65
1:A:704:ILE:HG12	1:A:778:ILE:HB	1.79	0.64
1:C:704:ILE:HG12	1:C:778:ILE:HB	1.79	0.63
1:D:485:CYS:HB3	1:D:488:GLU:HB3	1.81	0.63
1:D:704:ILE:HG12	1:D:778:ILE:HB	1.79	0.62
1:B:485:CYS:HB3	1:B:488:GLU:HB3	1.81	0.62
1:A:485:CYS:HB3	1:A:488:GLU:HB3	1.81	0.61
1:C:485:CYS:HB3	1:C:488:GLU:HB3	1.81	0.61
2:E:295:ARG:O	2:E:298:GLN:NE2	2.24	0.61
1:C:948:GLU:OE2	1:C:948:GLU:N	2.33	0.61
2:G:295:ARG:O	2:G:298:GLN:NE2	2.24	0.61
1:A:579:ILE:HD13	1:A:936:LEU:HD12	1.83	0.61
1:A:948:GLU:OE2	1:A:948:GLU:N	2.33	0.60
1:C:579:ILE:HD13	1:C:936:LEU:HD12	1.83	0.60
1:D:579:ILE:HD13	1:D:936:LEU:HD12	1.83	0.60
1:B:579:ILE:HD13	1:B:936:LEU:HD12	1.83	0.60
1:B:442:MET:HE1	1:C:818:LYS:HA	1.84	0.59
1:C:442:MET:HE3	1:D:818:LYS:HD3	1.86	0.58
2:H:295:ARG:O	2:H:298:GLN:NE2	2.24	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:GLN:HE21	1:D:202:SER:HB3	1.69	0.58
1:B:142:GLN:HE21	1:B:202:SER:HB3	1.69	0.57
1:C:142:GLN:HE21	1:C:202:SER:HB3	1.69	0.57
1:A:142:GLN:HE21	1:A:202:SER:HB3	1.69	0.57
1:D:948:GLU:N	1:D:948:GLU:OE2	2.33	0.57
1:A:305:VAL:HG13	1:B:282:MET:HG2	1.85	0.57
1:A:821:ILE:HD11	1:A:887:ASN:HB3	1.87	0.57
1:A:198:TYR:OH	2:E:260:ARG:NH2	2.38	0.57
1:B:821:ILE:HD11	1:B:887:ASN:HB3	1.87	0.57
1:B:948:GLU:OE2	1:B:948:GLU:N	2.33	0.57
1:D:821:ILE:HD11	1:D:887:ASN:HB3	1.87	0.57
1:C:198:TYR:CD1	2:G:264:MET:HE1	2.40	0.56
2:F:295:ARG:O	2:F:298:GLN:NE2	2.24	0.56
1:C:821:ILE:HD11	1:C:887:ASN:HB3	1.87	0.56
1:C:693:HIS:HB2	1:C:742:ARG:HB3	1.88	0.56
1:A:693:HIS:HB2	1:A:742:ARG:HB3	1.88	0.56
1:D:693:HIS:HB2	1:D:742:ARG:HB3	1.88	0.56
1:B:693:HIS:HB2	1:B:742:ARG:HB3	1.88	0.55
1:A:201:ARG:HB3	2:E:253:CYS:SG	2.46	0.55
1:C:561:LEU:O	1:C:607:ARG:NH2	2.40	0.55
1:B:305:VAL:HG13	1:C:282:MET:HG2	1.89	0.54
1:B:960:ARG:H	1:B:960:ARG:HD3	1.72	0.54
1:C:960:ARG:H	1:C:960:ARG:HD3	1.72	0.54
1:D:965:THR:HG22	1:D:967:GLN:H	1.72	0.54
1:C:32:THR:HA	2:G:270:PRO:HG3	1.89	0.54
1:D:960:ARG:H	1:D:960:ARG:HD3	1.72	0.54
1:A:923:LEU:O	1:A:927:THR:N	2.37	0.54
1:B:965:THR:HG22	1:B:967:GLN:H	1.72	0.54
1:A:960:ARG:H	1:A:960:ARG:HD3	1.72	0.53
1:A:818:LYS:HA	1:D:442:MET:HE1	1.91	0.53
1:A:965:THR:HG22	1:A:967:GLN:H	1.72	0.53
1:C:965:THR:HG22	1:C:967:GLN:H	1.72	0.53
1:D:339:VAL:HG13	1:D:342:ARG:HB3	1.90	0.53
1:A:414:VAL:HG23	1:A:416:ILE:HG13	1.90	0.53
1:B:707:ARG:NE	1:B:788:ASP:OD1	2.40	0.53
1:C:414:VAL:HG23	1:C:416:ILE:HG13	1.90	0.53
1:B:561:LEU:O	1:B:607:ARG:NH2	2.40	0.53
1:A:116:VAL:HG13	1:A:220:ILE:HG12	1.91	0.53
1:A:339:VAL:HG13	1:A:342:ARG:HB3	1.90	0.52
1:A:561:LEU:O	1:A:607:ARG:NH2	2.40	0.52
1:B:116:VAL:HG13	1:B:220:ILE:HG12	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:VAL:HG13	1:B:342:ARG:HB3	1.90	0.52
1:C:339:VAL:HG13	1:C:342:ARG:HB3	1.90	0.52
1:D:116:VAL:HG13	1:D:220:ILE:HG12	1.91	0.52
1:A:707:ARG:NE	1:A:788:ASP:OD1	2.40	0.52
1:C:685:LYS:H	1:C:685:LYS:HD3	1.75	0.52
1:D:414:VAL:HG23	1:D:416:ILE:HG13	1.90	0.52
1:C:116:VAL:HG13	1:C:220:ILE:HG12	1.91	0.52
1:C:524:TRP:HB2	1:C:1032:TYR:CE1	2.45	0.52
1:D:275:TRP:HB2	3:D:1204:CLR:H22	1.92	0.52
1:A:275:TRP:HB2	3:A:1202:CLR:H22	1.92	0.52
1:B:414:VAL:HG23	1:B:416:ILE:HG13	1.90	0.52
1:D:685:LYS:H	1:D:685:LYS:HD3	1.75	0.52
1:B:685:LYS:HD3	1:B:685:LYS:H	1.75	0.51
1:D:513:MET:HE1	1:D:537:TYR:HE2	1.74	0.51
1:D:524:TRP:HB2	1:D:1032:TYR:CE1	2.45	0.51
1:B:923:LEU:O	1:B:927:THR:N	2.37	0.51
1:C:287:THR:HA	1:D:288:VAL:HG22	1.91	0.51
1:A:513:MET:HE1	1:A:537:TYR:HE2	1.74	0.51
1:B:438:ALA:HB1	1:C:818:LYS:HD2	1.93	0.51
1:C:275:TRP:HB2	3:C:1204:CLR:H22	1.92	0.51
1:A:524:TRP:HB2	1:A:1032:TYR:CE1	2.45	0.51
1:B:694:TRP:HZ2	1:B:772:ASN:HB3	1.76	0.51
1:B:275:TRP:HB2	3:B:1204:CLR:H22	1.92	0.51
1:B:513:MET:HE1	1:B:537:TYR:HE2	1.74	0.51
1:A:694:TRP:HZ2	1:A:772:ASN:HB3	1.76	0.51
1:B:524:TRP:HB2	1:B:1032:TYR:CE1	2.45	0.51
1:D:694:TRP:HZ2	1:D:772:ASN:HB3	1.76	0.51
1:A:976:ARG:O	1:A:1052:LEU:HA	2.12	0.50
1:C:923:LEU:O	1:C:927:THR:N	2.37	0.50
1:C:513:MET:HE1	1:C:537:TYR:HE2	1.74	0.50
1:C:694:TRP:HZ2	1:C:772:ASN:HB3	1.76	0.50
1:A:685:LYS:H	1:A:685:LYS:HD3	1.75	0.50
1:D:590:GLN:O	1:D:593:THR:OG1	2.26	0.50
1:D:923:LEU:O	1:D:927:THR:N	2.37	0.50
1:A:442:MET:HE1	1:B:818:LYS:HA	1.93	0.50
1:B:198:TYR:CD1	2:F:264:MET:HE1	2.47	0.50
1:C:707:ARG:NE	1:C:788:ASP:OD1	2.40	0.50
1:D:976:ARG:O	1:D:1052:LEU:HA	2.12	0.50
1:D:991:GLY:HA2	1:D:1043:LEU:HD22	1.93	0.50
1:B:976:ARG:O	1:B:1052:LEU:HA	2.12	0.49
1:C:976:ARG:O	1:C:1052:LEU:HA	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:LYS:HD2	1:D:438:ALA:HB1	1.93	0.49
1:C:590:GLN:O	1:C:593:THR:OG1	2.27	0.49
1:C:991:GLY:HA2	1:C:1043:LEU:HD22	1.93	0.49
1:A:198:TYR:HB3	2:E:264:MET:HE1	1.93	0.49
1:D:707:ARG:NE	1:D:788:ASP:OD1	2.40	0.49
1:B:818:LYS:HE2	1:B:818:LYS:HB2	1.70	0.49
1:B:991:GLY:HA2	1:B:1043:LEU:HD22	1.93	0.49
1:A:991:GLY:HA2	1:A:1043:LEU:HD22	1.93	0.49
1:B:43:TRP:HE1	1:B:47:LYS:HD2	1.78	0.49
1:B:190:VAL:HB	1:B:191:PRO:HD3	1.94	0.48
1:A:43:TRP:HE1	1:A:47:LYS:HD2	1.78	0.48
1:A:190:VAL:HB	1:A:191:PRO:HD3	1.94	0.48
1:C:43:TRP:HE1	1:C:47:LYS:HD2	1.78	0.48
1:D:190:VAL:HB	1:D:191:PRO:HD3	1.94	0.48
1:D:561:LEU:O	1:D:607:ARG:NH2	2.40	0.48
1:C:763:LEU:HA	1:C:766:GLU:OE2	2.14	0.48
1:B:590:GLN:O	1:B:593:THR:OG1	2.27	0.48
1:C:689:THR:HG21	1:C:946:THR:HG21	1.96	0.48
1:D:43:TRP:HE1	1:D:47:LYS:HD2	1.78	0.48
1:D:689:THR:HG21	1:D:946:THR:HG21	1.96	0.48
1:D:763:LEU:HA	1:D:766:GLU:OE2	2.14	0.48
1:C:190:VAL:HB	1:C:191:PRO:HD3	1.94	0.47
1:C:1017:LEU:HB3	1:C:1020:ALA:HB2	1.96	0.47
1:A:314:MET:O	1:A:318:TYR:HB2	2.14	0.47
1:A:1017:LEU:HB3	1:A:1020:ALA:HB2	1.96	0.47
1:D:1017:LEU:HB3	1:D:1020:ALA:HB2	1.96	0.47
1:A:706:THR:H	1:A:709:GLU:HB2	1.79	0.47
1:D:706:THR:H	1:D:709:GLU:HB2	1.79	0.47
1:B:763:LEU:HA	1:B:766:GLU:OE2	2.14	0.47
1:C:706:THR:H	1:C:709:GLU:HB2	1.80	0.47
1:A:590:GLN:O	1:A:593:THR:OG1	2.27	0.47
1:D:314:MET:O	1:D:318:TYR:HB2	2.14	0.47
1:B:693:HIS:N	1:B:742:ARG:O	2.48	0.47
1:B:1017:LEU:HB3	1:B:1020:ALA:HB2	1.96	0.47
1:A:274:TYR:HD2	3:A:1202:CLR:H42	1.80	0.47
1:B:314:MET:O	1:B:318:TYR:HB2	2.14	0.47
1:D:274:TYR:HD2	3:D:1204:CLR:H42	1.80	0.47
1:B:689:THR:HG21	1:B:946:THR:HG21	1.96	0.46
1:B:1038:PRO:HD2	1:B:1041:PHE:HB2	1.98	0.46
1:C:274:TYR:HD2	3:C:1204:CLR:H42	1.80	0.46
1:A:689:THR:HG21	1:A:946:THR:HG21	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:HIS:N	1:A:742:ARG:O	2.48	0.46
1:A:104:MET:HE2	1:A:115:LEU:HD22	1.98	0.46
1:A:763:LEU:HA	1:A:766:GLU:OE2	2.14	0.46
1:C:314:MET:O	1:C:318:TYR:HB2	2.14	0.46
1:D:684:LYS:HB2	1:D:962:GLY:H	1.80	0.46
1:A:684:LYS:HB2	1:A:962:GLY:H	1.80	0.46
1:C:693:HIS:N	1:C:742:ARG:O	2.48	0.46
1:C:984:ASP:OD1	1:C:984:ASP:N	2.49	0.46
1:D:693:HIS:N	1:D:742:ARG:O	2.48	0.46
1:C:169:ILE:HD13	2:G:281:LEU:HD23	1.98	0.46
1:C:379:HIS:O	1:C:402:GLN:HA	2.16	0.46
1:D:104:MET:HE2	1:D:115:LEU:HD22	1.98	0.46
3:A:1204:CLR:H232	3:A:1204:CLR:H17	1.77	0.46
1:A:442:MET:CE	1:B:818:LYS:HD3	2.43	0.46
1:A:984:ASP:N	1:A:984:ASP:OD1	2.49	0.46
1:B:706:THR:H	1:B:709:GLU:HB2	1.79	0.46
1:C:476:ASN:OD1	1:C:479:GLU:N	2.48	0.46
1:A:365:HIS:ND1	1:A:513:MET:HB3	2.31	0.46
1:B:274:TYR:HD2	3:B:1204:CLR:H42	1.80	0.46
1:C:983:LEU:HG	1:C:1046:THR:HA	1.98	0.46
1:A:1038:PRO:HD2	1:A:1041:PHE:HB2	1.98	0.46
1:B:365:HIS:ND1	1:B:513:MET:HB3	2.31	0.46
1:B:948:GLU:H	1:B:948:GLU:CD	2.24	0.46
1:C:684:LYS:HB2	1:C:962:GLY:H	1.80	0.46
1:D:983:LEU:HG	1:D:1046:THR:HA	1.98	0.46
1:D:1038:PRO:HD2	1:D:1041:PHE:HB2	1.98	0.46
1:B:815:LEU:HB3	1:B:818:LYS:NZ	2.31	0.45
1:B:1015:TYR:N	1:B:1048:LEU:O	2.40	0.45
1:C:443:ARG:O	1:C:447:ILE:HG22	2.16	0.45
1:D:443:ARG:O	1:D:447:ILE:HG22	2.16	0.45
1:A:189:THR:HG21	1:A:213:ARG:HH22	1.81	0.45
1:A:826:ASN:HA	1:D:471:ASN:HB3	1.97	0.45
1:B:815:LEU:HB3	1:B:818:LYS:HZ1	1.81	0.45
1:D:695:CYS:HB2	1:D:774:PRO:HG3	1.98	0.45
1:D:815:LEU:HB3	1:D:818:LYS:NZ	2.31	0.45
2:H:284:GLY:O	2:H:288:THR:OG1	2.32	0.45
1:B:442:MET:CE	1:C:818:LYS:HD3	2.42	0.45
1:B:443:ARG:O	1:B:447:ILE:HG22	2.16	0.45
1:B:984:ASP:OD1	1:B:984:ASP:N	2.49	0.45
1:C:541:LEU:HD23	1:C:541:LEU:HA	1.79	0.45
1:C:104:MET:HE2	1:C:115:LEU:HD22	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:HIS:ND1	1:D:513:MET:HB3	2.31	0.45
1:D:379:HIS:O	1:D:402:GLN:HA	2.16	0.45
1:A:443:ARG:O	1:A:447:ILE:HG22	2.16	0.45
1:A:815:LEU:HB3	1:A:818:LYS:NZ	2.31	0.45
1:B:442:MET:CE	1:C:818:LYS:HA	2.45	0.45
1:C:189:THR:HG21	1:C:213:ARG:HH22	1.81	0.45
1:A:379:HIS:O	1:A:402:GLN:HA	2.16	0.45
1:B:695:CYS:HB2	1:B:774:PRO:HG3	1.98	0.45
1:B:983:LEU:HG	1:B:1046:THR:HA	1.98	0.45
1:C:1038:PRO:HD2	1:C:1041:PHE:HB2	1.98	0.45
1:A:718:HIS:O	1:A:798:ASP:N	2.47	0.45
1:D:189:THR:HG21	1:D:213:ARG:HH22	1.81	0.45
1:A:695:CYS:HB2	1:A:774:PRO:HG3	1.98	0.45
1:C:365:HIS:ND1	1:C:513:MET:HB3	2.31	0.45
1:B:684:LYS:HB2	1:B:962:GLY:H	1.80	0.45
1:B:104:MET:HE2	1:B:115:LEU:HD22	1.98	0.44
1:B:379:HIS:O	1:B:402:GLN:HA	2.16	0.44
1:D:198:TYR:CD1	2:H:264:MET:HE1	2.52	0.44
1:A:948:GLU:H	1:A:948:GLU:CD	2.24	0.44
1:B:189:THR:HG21	1:B:213:ARG:HH22	1.81	0.44
1:C:815:LEU:HB3	1:C:818:LYS:NZ	2.31	0.44
1:C:1000:PHE:HD2	1:C:1011:CYS:HB2	1.83	0.44
1:D:476:ASN:OD1	1:D:479:GLU:N	2.48	0.44
1:D:948:GLU:H	1:D:948:GLU:CD	2.24	0.44
1:D:997:GLY:HA3	1:D:1039:TYR:CD1	2.52	0.44
2:F:284:GLY:O	2:F:288:THR:OG1	2.32	0.44
1:A:983:LEU:HG	1:A:1046:THR:HA	1.98	0.44
1:B:997:GLY:HA3	1:B:1039:TYR:CD1	2.52	0.44
1:C:815:LEU:HB3	1:C:818:LYS:HZ1	1.82	0.44
1:C:948:GLU:H	1:C:948:GLU:CD	2.24	0.44
1:C:990:LEU:HD22	1:C:1002:LYS:HD3	2.00	0.44
1:C:997:GLY:HA3	1:C:1039:TYR:CD1	2.53	0.44
1:A:282:MET:HG2	1:D:305:VAL:HG13	1.99	0.44
1:A:476:ASN:OD1	1:A:479:GLU:N	2.48	0.44
1:A:790:ARG:HD2	1:D:955:GLU:OE2	2.18	0.44
1:B:990:LEU:HD22	1:B:1002:LYS:HD3	2.00	0.44
1:B:1000:PHE:HD2	1:B:1011:CYS:HB2	1.83	0.44
1:A:534:ASN:HB3	1:A:598:ILE:HG22	2.00	0.44
1:D:198:TYR:HE1	2:H:255:ARG:HH22	1.66	0.44
2:G:284:GLY:O	2:G:288:THR:OG1	2.32	0.44
1:A:744:SER:OG	1:A:972:ARG:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:GLY:HA3	1:A:1039:TYR:CD1	2.53	0.44
1:A:1014:ILE:HD12	1:A:1037:PRO:HG3	2.00	0.44
1:C:26:LEU:HD21	3:C:1203:CLR:H71	2.00	0.44
1:C:695:CYS:HB2	1:C:774:PRO:HG3	1.98	0.44
1:D:1000:PHE:HD2	1:D:1011:CYS:HB2	1.83	0.44
1:A:198:TYR:CD1	2:E:264:MET:HE1	2.53	0.44
1:B:1014:ILE:HD12	1:B:1037:PRO:HG3	2.00	0.44
1:D:1014:ILE:HD12	1:D:1037:PRO:HG3	2.00	0.44
1:A:26:LEU:HD21	3:A:1201:CLR:H71	2.00	0.44
1:C:1014:ILE:HD12	1:C:1037:PRO:HG3	2.00	0.44
1:D:990:LEU:HD22	1:D:1002:LYS:HD3	2.00	0.44
1:A:541:LEU:HD21	1:A:597:PHE:CZ	2.54	0.43
1:A:563:LEU:HB3	1:A:597:PHE:HD2	1.83	0.43
1:B:308:ILE:HG23	1:B:312:LEU:HD22	2.00	0.43
1:B:744:SER:OG	1:B:972:ARG:HB2	2.18	0.43
1:C:718:HIS:O	1:C:798:ASP:N	2.47	0.43
1:D:534:ASN:HB3	1:D:598:ILE:HG22	2.00	0.43
1:A:990:LEU:HD22	1:A:1002:LYS:HD3	2.00	0.43
1:B:416:ILE:HD13	1:B:447:ILE:HD13	2.00	0.43
1:B:884:ASN:OD1	1:B:886:THR:OG1	2.36	0.43
1:B:1009:MET:HE3	1:B:1009:MET:HB3	1.78	0.43
1:C:744:SER:OG	1:C:972:ARG:HB2	2.18	0.43
3:D:1206:CLR:H232	3:D:1206:CLR:H17	1.77	0.43
1:A:308:ILE:HG23	1:A:312:LEU:HD22	2.00	0.43
1:A:529:LEU:HD21	1:A:905:LEU:HD21	2.00	0.43
1:B:534:ASN:HB3	1:B:598:ILE:HG22	2.00	0.43
1:B:955:GLU:OE2	1:C:790:ARG:HD2	2.18	0.43
1:D:308:ILE:HG23	1:D:312:LEU:HD22	2.00	0.43
2:H:281:LEU:HD23	2:H:281:LEU:HA	1.88	0.43
1:B:541:LEU:HD21	1:B:597:PHE:CZ	2.53	0.43
1:B:685:LYS:HA	1:B:694:TRP:O	2.19	0.43
1:C:762:TYR:O	1:C:766:GLU:HG3	2.19	0.43
1:A:1000:PHE:HD2	1:A:1011:CYS:HB2	1.83	0.43
1:C:529:LEU:HD21	1:C:905:LEU:HD21	2.00	0.43
1:C:534:ASN:HB3	1:C:598:ILE:HG22	2.00	0.43
1:D:541:LEU:HD21	1:D:597:PHE:CZ	2.53	0.43
1:A:904:TYR:HA	1:A:909:PHE:CD2	2.54	0.43
1:B:529:LEU:HD21	1:B:905:LEU:HD21	2.00	0.43
1:D:566:ILE:HA	1:D:1010:LEU:HD21	2.01	0.43
1:D:685:LYS:HA	1:D:694:TRP:O	2.18	0.43
1:D:762:TYR:O	1:D:766:GLU:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:904:TYR:HA	1:D:909:PHE:CD2	2.54	0.43
1:A:685:LYS:HA	1:A:694:TRP:O	2.18	0.43
1:B:563:LEU:HB3	1:B:597:PHE:HD2	1.83	0.43
1:C:362:ASP:O	1:C:368:ARG:NH1	2.44	0.43
1:D:484:ILE:HG23	1:D:489:LEU:HD12	2.01	0.43
2:E:284:GLY:O	2:E:288:THR:OG1	2.32	0.43
1:A:566:ILE:HA	1:A:1010:LEU:HD21	2.01	0.43
1:B:506:MET:HE2	1:B:1012:PHE:HD1	1.84	0.43
1:B:1009:MET:HE3	1:B:1010:LEU:H	1.83	0.43
1:C:108:GLN:HE22	1:D:397:GLN:HE22	1.67	0.43
1:D:529:LEU:HD21	1:D:905:LEU:HD21	2.00	0.43
1:D:563:LEU:HB3	1:D:597:PHE:HD2	1.83	0.43
1:A:168:PHE:HZ	5:A:1208:6PL:H352	1.84	0.43
1:A:281:LEU:HD23	1:A:307:PHE:CE2	2.54	0.43
1:A:416:ILE:HD13	1:A:447:ILE:HD13	2.00	0.43
1:A:438:ALA:O	1:A:442:MET:HG2	2.19	0.43
1:A:1009:MET:HE3	1:A:1010:LEU:H	1.83	0.43
1:B:541:LEU:HD23	1:B:541:LEU:HA	1.79	0.43
1:C:165:GLY:HA2	2:G:277:LEU:HD23	2.00	0.43
1:C:308:ILE:HG23	1:C:312:LEU:HD22	2.00	0.43
1:C:563:LEU:HB3	1:C:597:PHE:HD2	1.84	0.43
1:C:1009:MET:HE3	1:C:1010:LEU:H	1.83	0.43
1:D:281:LEU:HD23	1:D:307:PHE:CE2	2.54	0.43
1:D:438:ALA:O	1:D:442:MET:HG2	2.19	0.43
1:B:904:TYR:HA	1:B:909:PHE:CD2	2.54	0.42
1:C:518:LYS:HA	1:C:518:LYS:HD3	1.86	0.42
1:C:904:TYR:HA	1:C:909:PHE:CD2	2.54	0.42
1:D:26:LEU:HD21	3:D:1203:CLR:H71	2.00	0.42
1:D:744:SER:OG	1:D:972:ARG:HB2	2.18	0.42
1:A:815:LEU:HB3	1:A:818:LYS:HZ1	1.84	0.42
5:A:1212:6PL:H352	5:A:1212:6PL:H321	1.84	0.42
1:A:278:VAL:HG21	3:A:1202:CLR:H191	2.01	0.42
1:A:484:ILE:HG23	1:A:489:LEU:HD12	2.01	0.42
1:A:700:ILE:HA	1:A:767:TRP:CZ2	2.54	0.42
1:A:762:TYR:O	1:A:766:GLU:HG3	2.19	0.42
1:B:26:LEU:HD21	3:B:1203:CLR:H71	2.00	0.42
1:B:168:PHE:HZ	5:B:1210:6PL:H352	1.84	0.42
1:C:168:PHE:HZ	5:C:1210:6PL:H352	1.84	0.42
1:C:541:LEU:HD21	1:C:597:PHE:CZ	2.54	0.42
1:D:168:PHE:HZ	5:D:1210:6PL:H352	1.84	0.42
1:D:362:ASP:O	1:D:368:ARG:NH1	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:699:GLU:HB3	1:D:702:LYS:HB2	2.02	0.42
1:D:984:ASP:OD1	1:D:984:ASP:N	2.49	0.42
1:B:700:ILE:HA	1:B:767:TRP:CZ2	2.54	0.42
1:C:685:LYS:HA	1:C:694:TRP:O	2.18	0.42
1:D:506:MET:HE2	1:D:1012:PHE:HD1	1.84	0.42
1:D:606:LYS:HD3	1:D:606:LYS:HA	1.90	0.42
1:D:686:TYR:OH	1:D:972:ARG:NH1	2.53	0.42
1:D:815:LEU:HB3	1:D:818:LYS:HZ1	1.84	0.42
1:B:484:ILE:HG23	1:B:489:LEU:HD12	2.01	0.42
1:B:762:TYR:O	1:B:766:GLU:HG3	2.19	0.42
1:C:281:LEU:HD23	1:C:307:PHE:CE2	2.54	0.42
1:C:416:ILE:HD13	1:C:447:ILE:HD13	2.00	0.42
1:C:506:MET:HE2	1:C:1012:PHE:HD1	1.84	0.42
1:C:699:GLU:HB3	1:C:702:LYS:HB2	2.02	0.42
1:C:700:ILE:HA	1:C:767:TRP:CZ2	2.54	0.42
1:D:416:ILE:HD13	1:D:447:ILE:HD13	2.00	0.42
1:A:699:GLU:HB3	1:A:702:LYS:HB2	2.02	0.42
1:B:438:ALA:O	1:B:442:MET:HG2	2.19	0.42
1:B:281:LEU:HD23	1:B:307:PHE:CE2	2.54	0.42
1:B:383:PRO:HD3	1:B:400:PHE:CE2	2.55	0.42
1:D:687:ASP:OD1	1:D:687:ASP:N	2.51	0.42
1:D:1009:MET:HE3	1:D:1010:LEU:H	1.83	0.42
1:B:278:VAL:HG21	3:B:1204:CLR:H191	2.01	0.42
1:D:563:LEU:HB3	1:D:597:PHE:CD2	2.55	0.42
1:D:700:ILE:HA	1:D:767:TRP:CZ2	2.54	0.42
1:A:818:LYS:HA	1:D:442:MET:CE	2.50	0.42
1:B:471:ASN:HB3	1:C:826:ASN:HA	2.02	0.42
1:C:108:GLN:NE2	1:D:397:GLN:HE22	2.17	0.42
1:C:566:ILE:HA	1:C:1010:LEU:HD21	2.01	0.42
1:C:686:TYR:OH	1:C:972:ARG:NH1	2.53	0.42
1:C:884:ASN:OD1	1:C:886:THR:OG1	2.36	0.42
1:A:1015:TYR:N	1:A:1048:LEU:O	2.40	0.42
1:B:566:ILE:HA	1:B:1010:LEU:HD21	2.01	0.42
1:B:699:GLU:HB3	1:B:702:LYS:HB2	2.02	0.42
1:D:720:VAL:HA	1:D:755:VAL:HG13	2.02	0.42
2:E:281:LEU:HD23	2:E:281:LEU:HA	1.88	0.42
1:A:468:HIS:HB3	1:B:822:LEU:HD21	2.02	0.41
1:A:506:MET:HE2	1:A:1012:PHE:HD1	1.84	0.41
1:A:720:VAL:HA	1:A:755:VAL:HG13	2.02	0.41
1:B:1007:TYR:N	1:B:1007:TYR:CD1	2.88	0.41
1:C:278:VAL:HG21	3:C:1204:CLR:H191	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1205:CLR:H162	3:D:1205:CLR:H222	1.82	0.41
1:B:1053:MET:HE3	1:B:1053:MET:HB3	1.97	0.41
1:C:484:ILE:HG23	1:C:489:LEU:HD12	2.01	0.41
1:C:438:ALA:O	1:C:442:MET:HG2	2.19	0.41
1:D:818:LYS:HB2	1:D:818:LYS:HE2	1.70	0.41
1:A:383:PRO:HD3	1:A:400:PHE:CE2	2.55	0.41
1:A:686:TYR:OH	1:A:972:ARG:NH1	2.53	0.41
1:C:541:LEU:HD21	1:C:597:PHE:HZ	1.85	0.41
1:C:758:GLY:O	1:C:780:PRO:HA	2.20	0.41
1:C:1007:TYR:N	1:C:1007:TYR:CD1	2.88	0.41
1:D:758:GLY:O	1:D:780:PRO:HA	2.20	0.41
1:B:687:ASP:OD1	1:B:687:ASP:N	2.51	0.41
1:C:161:LEU:HG	2:G:276:SER:CB	2.50	0.41
1:D:685:LYS:NZ	1:D:964:SER:HB2	2.36	0.41
1:A:563:LEU:HB3	1:A:597:PHE:CD2	2.55	0.41
1:B:476:ASN:OD1	1:B:479:GLU:N	2.48	0.41
1:B:563:LEU:HB3	1:B:597:PHE:CD2	2.55	0.41
1:B:718:HIS:O	1:B:798:ASP:N	2.47	0.41
1:C:383:PRO:HD3	1:C:400:PHE:CE2	2.55	0.41
1:C:820:CYS:HB3	1:C:880:THR:HG23	2.03	0.41
1:D:383:PRO:HD3	1:D:400:PHE:CE2	2.55	0.41
1:A:685:LYS:NZ	1:A:964:SER:HB2	2.36	0.41
1:B:518:LYS:HA	1:B:518:LYS:HD3	1.86	0.41
1:B:686:TYR:OH	1:B:972:ARG:NH1	2.53	0.41
3:C:1206:CLR:H232	3:C:1206:CLR:H17	1.78	0.41
1:D:278:VAL:HG21	3:D:1204:CLR:H191	2.01	0.41
1:D:557:CYS:O	1:D:562:LYS:N	2.54	0.41
1:A:557:CYS:O	1:A:562:LYS:N	2.54	0.41
1:B:685:LYS:NZ	1:B:964:SER:HB2	2.36	0.41
1:B:996:TYR:CD2	1:B:1037:PRO:HG2	2.56	0.41
1:D:820:CYS:HB3	1:D:880:THR:HG23	2.03	0.41
1:A:758:GLY:O	1:A:780:PRO:HA	2.20	0.41
1:A:820:CYS:HB3	1:A:880:THR:HG23	2.03	0.41
1:A:884:ASN:OD1	1:A:886:THR:OG1	2.36	0.41
1:B:606:LYS:HD3	1:B:606:LYS:HA	1.90	0.41
1:B:982:LEU:HD22	1:B:999:LEU:HD11	2.03	0.41
1:C:489:LEU:HD23	1:C:489:LEU:HA	1.96	0.41
1:C:563:LEU:HB3	1:C:597:PHE:CD2	2.55	0.41
1:D:541:LEU:HD21	1:D:597:PHE:HZ	1.85	0.41
1:D:937:ILE:O	1:D:941:VAL:HB	2.21	0.41
1:D:1007:TYR:CD1	1:D:1007:TYR:N	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:LYS:HE2	1:A:818:LYS:HB2	1.70	0.41
1:B:26:LEU:HD12	1:B:26:LEU:HA	1.91	0.41
1:B:506:MET:SD	1:B:1035:THR:OG1	2.76	0.41
1:B:758:GLY:O	1:B:780:PRO:HA	2.20	0.41
1:A:822:LEU:HD12	1:A:822:LEU:HA	1.83	0.40
1:A:937:ILE:O	1:A:941:VAL:HB	2.21	0.40
1:B:25:PHE:HE1	1:B:196:SER:HB3	1.87	0.40
1:C:720:VAL:HA	1:C:755:VAL:HG13	2.02	0.40
1:D:697:PRO:HB3	1:D:772:ASN:OD1	2.21	0.40
1:A:1007:TYR:CD1	1:A:1007:TYR:N	2.88	0.40
1:A:1022:LEU:HD23	1:A:1022:LEU:HA	1.95	0.40
1:B:405:VAL:HA	1:B:411:LEU:HD21	2.04	0.40
1:B:720:VAL:HA	1:B:755:VAL:HG13	2.02	0.40
1:B:888:VAL:HG22	1:B:908:PRO:HG2	2.03	0.40
1:C:466:LYS:HD2	1:C:485:CYS:HB2	2.03	0.40
1:C:685:LYS:NZ	1:C:964:SER:HB2	2.36	0.40
1:C:996:TYR:CD2	1:C:1037:PRO:HG2	2.56	0.40
1:C:1053:MET:HE3	1:C:1053:MET:HB3	1.97	0.40
1:D:405:VAL:HA	1:D:411:LEU:HD21	2.04	0.40
1:B:468:HIS:HB3	1:C:822:LEU:HD21	2.04	0.40
1:C:557:CYS:O	1:C:562:LYS:N	2.54	0.40
1:C:933:ILE:HD13	1:C:933:ILE:HA	1.97	0.40
1:A:606:LYS:HD3	1:A:606:LYS:HA	1.90	0.40
1:A:996:TYR:CD2	1:A:1037:PRO:HG2	2.56	0.40
1:B:820:CYS:HB3	1:B:880:THR:HG23	2.03	0.40
1:A:27:ALA:HA	1:A:30:MET:HB3	2.04	0.40
1:A:982:LEU:HD22	1:A:999:LEU:HD11	2.03	0.40
1:B:937:ILE:O	1:B:941:VAL:HB	2.21	0.40
3:B:1203:CLR:H162	3:B:1203:CLR:H222	1.95	0.40
1:C:818:LYS:HB2	1:C:818:LYS:HE2	1.70	0.40
1:D:442:MET:HG2	1:D:442:MET:H	1.75	0.40
1:D:884:ASN:OD1	1:D:886:THR:OG1	2.36	0.40
1:D:1015:TYR:N	1:D:1048:LEU:O	2.41	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	892/1119 (80%)	870 (98%)	22 (2%)	0	100	100
1	B	892/1119 (80%)	870 (98%)	22 (2%)	0	100	100
1	C	892/1119 (80%)	869 (97%)	23 (3%)	0	100	100
1	D	892/1119 (80%)	870 (98%)	22 (2%)	0	100	100
2	E	46/340 (14%)	46 (100%)	0	0	100	100
2	F	46/340 (14%)	46 (100%)	0	0	100	100
2	G	46/340 (14%)	46 (100%)	0	0	100	100
2	H	46/340 (14%)	46 (100%)	0	0	100	100
All	All	3752/5836 (64%)	3663 (98%)	89 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	792/986 (80%)	782 (99%)	10 (1%)	61	80
1	B	792/986 (80%)	782 (99%)	10 (1%)	61	80
1	C	792/986 (80%)	782 (99%)	10 (1%)	61	80
1	D	792/986 (80%)	782 (99%)	10 (1%)	61	80
2	E	37/257 (14%)	32 (86%)	5 (14%)	4	5
2	F	37/257 (14%)	32 (86%)	5 (14%)	4	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	37/257 (14%)	32 (86%)	5 (14%)	4	5
2	H	37/257 (14%)	32 (86%)	5 (14%)	4	5
All	All	3316/4972 (67%)	3256 (98%)	60 (2%)	51	73

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	THR
1	A	281	LEU
1	A	324	GLU
1	A	339	VAL
1	A	343	LYS
1	A	565	MET
1	A	782	THR
1	A	801	VAL
1	A	816	GLN
1	A	952	LEU
1	B	111	THR
1	B	281	LEU
1	B	324	GLU
1	B	339	VAL
1	B	343	LYS
1	B	565	MET
1	B	782	THR
1	B	801	VAL
1	B	816	GLN
1	B	952	LEU
1	C	111	THR
1	C	281	LEU
1	C	324	GLU
1	C	339	VAL
1	C	343	LYS
1	C	565	MET
1	C	782	THR
1	C	801	VAL
1	C	816	GLN
1	C	952	LEU
1	D	111	THR
1	D	281	LEU
1	D	324	GLU
1	D	339	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	343	LYS
1	D	565	MET
1	D	782	THR
1	D	801	VAL
1	D	816	GLN
1	D	952	LEU
2	E	258	SER
2	E	264	MET
2	E	276	SER
2	E	287	LEU
2	E	288	THR
2	F	258	SER
2	F	264	MET
2	F	276	SER
2	F	287	LEU
2	F	288	THR
2	G	258	SER
2	G	264	MET
2	G	276	SER
2	G	287	LEU
2	G	288	THR
2	H	258	SER
2	H	264	MET
2	H	276	SER
2	H	287	LEU
2	H	288	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	270	GLN
1	A	397	GLN
1	A	616	HIS
1	A	747	HIS
1	A	771	HIS
1	A	793	ASN
1	A	1054	GLN
1	B	142	GLN
1	B	270	GLN
1	B	616	HIS
1	B	747	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	771	HIS
1	B	793	ASN
1	B	826	ASN
1	B	1054	GLN
1	C	142	GLN
1	C	222	GLN
1	C	270	GLN
1	C	397	GLN
1	C	616	HIS
1	C	747	HIS
1	C	771	HIS
1	C	793	ASN
1	C	1054	GLN
1	D	142	GLN
1	D	270	GLN
1	D	397	GLN
1	D	616	HIS
1	D	747	HIS
1	D	771	HIS
1	D	793	ASN
1	D	1054	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 68 ligands modelled in this entry, 16 are monoatomic - leaving 52 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	6PL	C	1210	-	25,25,51	0.53	1 (4%)	27,27,59	0.52	0
3	CLR	A	1201	-	31,31,31	0.37	0	48,48,48	0.52	0
3	CLR	A	1202	-	31,31,31	0.38	0	48,48,48	0.58	0
5	6PL	C	1215	-	21,21,51	0.85	1 (4%)	24,26,59	1.34	2 (8%)
5	6PL	A	1209	-	32,32,51	0.57	0	38,40,59	0.52	0
5	6PL	B	1215	-	21,21,51	0.85	1 (4%)	24,26,59	1.34	2 (8%)
5	6PL	D	1209	-	28,28,51	0.62	0	34,36,59	0.52	0
3	CLR	B	1206	-	31,31,31	0.37	0	48,48,48	4.67	6 (12%)
3	CLR	C	1203	-	31,31,31	0.38	0	48,48,48	0.53	0
5	6PL	D	1214	-	22,22,51	0.84	1 (4%)	25,27,59	1.26	2 (8%)
5	6PL	D	1216	-	21,21,51	0.81	1 (4%)	23,25,59	1.29	2 (8%)
5	6PL	B	1212	-	26,26,51	0.43	0	28,28,59	0.40	0
3	CLR	C	1205	-	31,31,31	0.37	0	48,48,48	0.46	0
5	6PL	A	1214	-	21,21,51	0.81	1 (4%)	23,25,59	1.29	2 (8%)
5	6PL	A	1208	-	25,25,51	0.53	1 (4%)	27,27,59	0.52	0
3	CLR	B	1205	-	31,31,31	0.37	0	48,48,48	0.46	0
5	6PL	A	1207	-	28,28,51	0.61	0	34,36,59	0.52	0
5	6PL	B	1209	-	28,28,51	0.61	0	34,36,59	0.52	0
5	6PL	D	1215	-	21,21,51	0.85	1 (4%)	24,26,59	1.34	2 (8%)
3	CLR	C	1204	-	31,31,31	0.38	0	48,48,48	0.58	0
5	6PL	A	1216	-	17,17,51	1.33	1 (5%)	19,21,59	1.45	2 (10%)
5	6PL	A	1210	-	26,26,51	0.43	0	28,28,59	0.40	0
5	6PL	A	1212	-	22,22,51	0.84	1 (4%)	25,27,59	1.26	2 (8%)
5	6PL	D	1212	-	26,26,51	0.43	0	28,28,59	0.40	0
3	CLR	D	1203	-	31,31,31	0.37	0	48,48,48	0.52	0
3	CLR	D	1205	-	31,31,31	0.37	0	48,48,48	0.46	0
5	6PL	A	1211	-	15,15,51	0.36	0	16,16,59	0.44	0
5	6PL	C	1216	-	21,21,51	0.81	1 (4%)	23,25,59	1.29	2 (8%)
5	6PL	A	1213	-	21,21,51	0.85	1 (4%)	24,26,59	1.34	2 (8%)
3	CLR	A	1204	-	31,31,31	0.38	0	48,48,48	4.66	6 (12%)
5	6PL	B	1214	-	22,22,51	0.85	1 (4%)	25,27,59	1.26	2 (8%)
5	6PL	B	1216	-	21,21,51	0.81	1 (4%)	23,25,59	1.28	2 (8%)
5	6PL	C	1214	-	22,22,51	0.85	1 (4%)	25,27,59	1.26	2 (8%)
5	6PL	C	1202	-	17,17,51	1.33	1 (5%)	19,21,59	1.45	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	6PL	B	1210	-	25,25,51	0.53	1 (4%)	27,27,59	0.53	0
5	6PL	C	1211	-	32,32,51	0.57	0	38,40,59	0.53	0
3	CLR	C	1206	-	31,31,31	0.38	0	48,48,48	4.67	6 (12%)
5	6PL	B	1211	-	32,32,51	0.57	0	38,40,59	0.52	0
5	6PL	C	1212	-	26,26,51	0.44	0	28,28,59	0.40	0
3	CLR	B	1203	-	31,31,31	0.38	0	48,48,48	0.52	0
5	6PL	C	1209	-	28,28,51	0.62	0	34,36,59	0.52	0
5	6PL	C	1213	-	15,15,51	0.36	0	16,16,59	0.45	0
5	6PL	B	1213	-	15,15,51	0.36	0	16,16,59	0.44	0
3	CLR	B	1204	-	31,31,31	0.37	0	48,48,48	0.59	0
5	6PL	D	1211	-	32,32,51	0.57	0	38,40,59	0.52	0
5	6PL	D	1210	-	25,25,51	0.53	1 (4%)	27,27,59	0.52	0
3	CLR	A	1203	-	31,31,31	0.37	0	48,48,48	0.45	0
5	6PL	D	1202	-	17,17,51	1.32	1 (5%)	19,21,59	1.44	2 (10%)
5	6PL	B	1202	-	17,17,51	1.34	1 (5%)	19,21,59	1.44	2 (10%)
5	6PL	D	1213	-	15,15,51	0.36	0	16,16,59	0.44	0
3	CLR	D	1204	-	31,31,31	0.38	0	48,48,48	0.58	0
3	CLR	D	1206	-	31,31,31	0.37	0	48,48,48	4.66	6 (12%)

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	6PL	C	1210	-	-	8/26/26/55	-
3	CLR	A	1201	-	-	1/10/68/68	0/4/4/4
3	CLR	A	1202	-	-	1/10/68/68	0/4/4/4
5	6PL	C	1215	-	-	11/22/22/55	-
5	6PL	A	1209	-	-	11/36/36/55	-
5	6PL	B	1215	-	-	11/22/22/55	-
5	6PL	D	1209	-	-	13/31/31/55	-
3	CLR	B	1206	-	-	5/10/68/68	0/4/4/4
3	CLR	C	1203	-	-	1/10/68/68	0/4/4/4
5	6PL	D	1214	-	-	10/23/23/55	-
5	6PL	D	1216	-	-	8/21/21/55	-
5	6PL	B	1212	-	-	7/28/28/55	-
3	CLR	C	1205	-	-	4/10/68/68	0/4/4/4
5	6PL	A	1214	-	-	8/21/21/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	6PL	A	1208	-	-	8/26/26/55	-
3	CLR	B	1205	-	-	4/10/68/68	0/4/4/4
5	6PL	A	1207	-	-	13/31/31/55	-
5	6PL	B	1209	-	-	13/31/31/55	-
5	6PL	D	1215	-	-	11/22/22/55	-
3	CLR	C	1204	-	-	1/10/68/68	0/4/4/4
5	6PL	A	1216	-	-	6/17/17/55	-
5	6PL	A	1210	-	-	7/28/28/55	-
5	6PL	A	1212	-	-	10/23/23/55	-
5	6PL	D	1212	-	-	7/28/28/55	-
3	CLR	D	1203	-	-	1/10/68/68	0/4/4/4
3	CLR	D	1205	-	-	4/10/68/68	0/4/4/4
5	6PL	A	1211	-	-	1/15/15/55	-
5	6PL	C	1216	-	-	8/21/21/55	-
5	6PL	A	1213	-	-	11/22/22/55	-
3	CLR	A	1204	-	-	5/10/68/68	0/4/4/4
5	6PL	B	1214	-	-	10/23/23/55	-
5	6PL	B	1216	-	-	8/21/21/55	-
5	6PL	C	1214	-	-	10/23/23/55	-
5	6PL	C	1202	-	-	6/17/17/55	-
5	6PL	B	1210	-	-	8/26/26/55	-
5	6PL	C	1211	-	-	11/36/36/55	-
3	CLR	C	1206	-	-	6/10/68/68	0/4/4/4
5	6PL	B	1211	-	-	11/36/36/55	-
5	6PL	C	1212	-	-	7/28/28/55	-
3	CLR	B	1203	-	-	1/10/68/68	0/4/4/4
5	6PL	C	1209	-	-	13/31/31/55	-
5	6PL	C	1213	-	-	1/15/15/55	-
5	6PL	B	1213	-	-	1/15/15/55	-
3	CLR	B	1204	-	-	1/10/68/68	0/4/4/4
5	6PL	D	1211	-	-	11/36/36/55	-
5	6PL	D	1210	-	-	8/26/26/55	-
3	CLR	A	1203	-	-	4/10/68/68	0/4/4/4
5	6PL	D	1202	-	-	6/17/17/55	-
5	6PL	B	1202	-	-	6/17/17/55	-
5	6PL	D	1213	-	-	1/15/15/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLR	D	1204	-	-	1/10/68/68	0/4/4/4
3	CLR	D	1206	-	-	6/10/68/68	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1202	6PL	P-O1P	4.86	1.65	1.50
5	B	1202	6PL	P-O1P	4.86	1.65	1.50
5	A	1216	6PL	P-O1P	4.85	1.65	1.50
5	D	1202	6PL	P-O1P	4.83	1.65	1.50
5	D	1215	6PL	P-O4P	2.90	1.65	1.54
5	D	1214	6PL	P-O4P	2.89	1.65	1.54
5	B	1214	6PL	P-O4P	2.89	1.65	1.54
5	B	1215	6PL	P-O4P	2.89	1.65	1.54
5	C	1214	6PL	P-O4P	2.89	1.65	1.54
5	A	1212	6PL	P-O4P	2.88	1.65	1.54
5	A	1213	6PL	P-O4P	2.88	1.65	1.54
5	A	1214	6PL	P-O4P	2.88	1.65	1.54
5	C	1215	6PL	P-O4P	2.88	1.65	1.54
5	B	1216	6PL	P-O4P	2.88	1.65	1.54
5	D	1216	6PL	P-O4P	2.87	1.65	1.54
5	C	1216	6PL	P-O4P	2.87	1.65	1.54
5	D	1210	6PL	O2-C2	-2.05	1.43	1.47
5	B	1210	6PL	O2-C2	-2.05	1.43	1.47
5	C	1210	6PL	O2-C2	-2.04	1.43	1.47
5	A	1208	6PL	O2-C2	-2.03	1.43	1.47

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1206	CLR	C18-C13-C12	-20.02	81.09	110.61
3	B	1206	CLR	C18-C13-C12	-20.00	81.13	110.61
3	A	1204	CLR	C18-C13-C12	-19.99	81.14	110.61
3	D	1206	CLR	C18-C13-C12	-19.98	81.16	110.61
3	B	1206	CLR	C18-C13-C17	-17.10	80.66	111.68
3	A	1204	CLR	C18-C13-C17	-17.10	80.67	111.68
3	C	1206	CLR	C18-C13-C17	-17.08	80.70	111.68
3	D	1206	CLR	C18-C13-C17	-17.08	80.70	111.68
3	B	1206	CLR	C18-C13-C14	-11.76	90.35	111.68
3	D	1206	CLR	C18-C13-C14	-11.76	90.35	111.68
3	C	1206	CLR	C18-C13-C14	-11.75	90.36	111.68
3	A	1204	CLR	C18-C13-C14	-11.72	90.42	111.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1206	CLR	C12-C13-C17	9.85	131.12	116.60
3	D	1206	CLR	C12-C13-C17	9.85	131.11	116.60
3	B	1206	CLR	C12-C13-C17	9.83	131.08	116.60
3	A	1204	CLR	C12-C13-C17	9.81	131.05	116.60
3	A	1204	CLR	C17-C13-C14	8.24	109.55	100.10
3	D	1206	CLR	C17-C13-C14	8.24	109.55	100.10
3	B	1206	CLR	C17-C13-C14	8.23	109.55	100.10
3	C	1206	CLR	C17-C13-C14	8.22	109.54	100.10
3	A	1204	CLR	C12-C13-C14	5.60	115.62	107.25
3	B	1206	CLR	C12-C13-C14	5.56	115.57	107.25
3	D	1206	CLR	C12-C13-C14	5.56	115.56	107.25
3	C	1206	CLR	C12-C13-C14	5.55	115.54	107.25
5	B	1215	6PL	O4P-P-O3P	-5.01	93.60	106.67
5	D	1215	6PL	O4P-P-O3P	-5.01	93.60	106.67
5	A	1213	6PL	O4P-P-O3P	-5.01	93.61	106.67
5	C	1215	6PL	O4P-P-O3P	-5.00	93.62	106.67
5	B	1214	6PL	O4P-P-O3P	-4.99	93.65	106.67
5	D	1214	6PL	O4P-P-O3P	-4.99	93.66	106.67
5	C	1214	6PL	O4P-P-O3P	-4.99	93.67	106.67
5	A	1212	6PL	O4P-P-O3P	-4.98	93.67	106.67
5	C	1216	6PL	O4P-P-O3P	-4.95	93.75	106.67
5	A	1214	6PL	O4P-P-O3P	-4.95	93.76	106.67
5	D	1216	6PL	O4P-P-O3P	-4.95	93.76	106.67
5	B	1216	6PL	O4P-P-O3P	-4.94	93.80	106.67
5	A	1216	6PL	O3P-P-O1P	-4.72	93.69	106.44
5	C	1202	6PL	O3P-P-O1P	-4.71	93.71	106.44
5	B	1202	6PL	O3P-P-O1P	-4.71	93.72	106.44
5	D	1202	6PL	O3P-P-O1P	-4.70	93.72	106.44
5	C	1202	6PL	O4P-P-O2P	3.19	119.75	107.80
5	D	1202	6PL	O4P-P-O2P	3.18	119.72	107.80
5	A	1216	6PL	O4P-P-O2P	3.18	119.72	107.80
5	B	1202	6PL	O4P-P-O2P	3.17	119.68	107.80
5	C	1216	6PL	O2P-P-O1P	2.29	119.75	110.83
5	A	1214	6PL	O2P-P-O1P	2.29	119.74	110.83
5	D	1216	6PL	O2P-P-O1P	2.28	119.73	110.83
5	C	1214	6PL	O2P-P-O1P	2.28	119.73	110.83
5	C	1215	6PL	O2P-P-O1P	2.28	119.72	110.83
5	A	1213	6PL	O2P-P-O1P	2.28	119.72	110.83
5	B	1216	6PL	O2P-P-O1P	2.28	119.72	110.83
5	D	1214	6PL	O2P-P-O1P	2.28	119.72	110.83
5	B	1215	6PL	O2P-P-O1P	2.28	119.72	110.83
5	A	1212	6PL	O2P-P-O1P	2.28	119.72	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1214	6PL	O2P-P-O1P	2.27	119.69	110.83
5	D	1215	6PL	O2P-P-O1P	2.27	119.68	110.83

There are no chirality outliers.

All (346) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1204	CLR	C13-C17-C20-C22
3	A	1204	CLR	C16-C17-C20-C22
3	B	1206	CLR	C13-C17-C20-C22
3	B	1206	CLR	C16-C17-C20-C22
3	C	1206	CLR	C13-C17-C20-C22
3	C	1206	CLR	C16-C17-C20-C22
3	D	1206	CLR	C13-C17-C20-C22
3	D	1206	CLR	C16-C17-C20-C22
5	A	1207	6PL	C1-O3P-P-O1P
5	A	1207	6PL	C1-O3P-P-O2P
5	A	1207	6PL	C1-O3P-P-O4P
5	A	1207	6PL	C4-O4P-P-O3P
5	A	1207	6PL	C5-C4-O4P-P
5	A	1207	6PL	C32-C31-O2-C2
5	A	1209	6PL	C1-O3P-P-O1P
5	A	1209	6PL	C4-O4P-P-O3P
5	A	1209	6PL	C4-O4P-P-O2P
5	A	1210	6PL	C32-C31-O2-C2
5	A	1212	6PL	C1-O3P-P-O2P
5	A	1212	6PL	C1-O3P-P-O4P
5	A	1213	6PL	C1-C2-O2-C31
5	A	1213	6PL	C1-O3P-P-O2P
5	A	1213	6PL	C1-O3P-P-O4P
5	A	1213	6PL	C32-C31-O2-C2
5	A	1214	6PL	O2-C2-C3-O3
5	A	1214	6PL	C1-O3P-P-O4P
5	A	1216	6PL	C1-C2-C3-O3
5	A	1216	6PL	O2-C2-C3-O3
5	A	1216	6PL	C1-O3P-P-O2P
5	B	1202	6PL	C1-C2-C3-O3
5	B	1202	6PL	O2-C2-C3-O3
5	B	1202	6PL	C1-O3P-P-O2P
5	B	1209	6PL	C1-O3P-P-O1P
5	B	1209	6PL	C1-O3P-P-O2P
5	B	1209	6PL	C1-O3P-P-O4P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	1209	6PL	C4-O4P-P-O3P
5	B	1209	6PL	C5-C4-O4P-P
5	B	1209	6PL	C32-C31-O2-C2
5	B	1211	6PL	C1-O3P-P-O1P
5	B	1211	6PL	C4-O4P-P-O3P
5	B	1211	6PL	C4-O4P-P-O2P
5	B	1212	6PL	C32-C31-O2-C2
5	B	1214	6PL	C1-O3P-P-O2P
5	B	1214	6PL	C1-O3P-P-O4P
5	B	1215	6PL	C1-C2-O2-C31
5	B	1215	6PL	C1-O3P-P-O2P
5	B	1215	6PL	C1-O3P-P-O4P
5	B	1215	6PL	C32-C31-O2-C2
5	B	1216	6PL	O2-C2-C3-O3
5	B	1216	6PL	C1-O3P-P-O4P
5	C	1202	6PL	C1-C2-C3-O3
5	C	1202	6PL	O2-C2-C3-O3
5	C	1202	6PL	C1-O3P-P-O2P
5	C	1209	6PL	C1-O3P-P-O1P
5	C	1209	6PL	C1-O3P-P-O2P
5	C	1209	6PL	C1-O3P-P-O4P
5	C	1209	6PL	C4-O4P-P-O3P
5	C	1209	6PL	C5-C4-O4P-P
5	C	1209	6PL	C32-C31-O2-C2
5	C	1211	6PL	C1-O3P-P-O1P
5	C	1211	6PL	C4-O4P-P-O3P
5	C	1211	6PL	C4-O4P-P-O2P
5	C	1212	6PL	C32-C31-O2-C2
5	C	1214	6PL	C1-O3P-P-O2P
5	C	1214	6PL	C1-O3P-P-O4P
5	C	1215	6PL	C1-C2-O2-C31
5	C	1215	6PL	C1-O3P-P-O2P
5	C	1215	6PL	C1-O3P-P-O4P
5	C	1215	6PL	C32-C31-O2-C2
5	C	1216	6PL	O2-C2-C3-O3
5	C	1216	6PL	C1-O3P-P-O4P
5	D	1202	6PL	C1-C2-C3-O3
5	D	1202	6PL	O2-C2-C3-O3
5	D	1202	6PL	C1-O3P-P-O2P
5	D	1209	6PL	C1-O3P-P-O1P
5	D	1209	6PL	C1-O3P-P-O2P
5	D	1209	6PL	C1-O3P-P-O4P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	1209	6PL	C4-O4P-P-O3P
5	D	1209	6PL	C5-C4-O4P-P
5	D	1209	6PL	C32-C31-O2-C2
5	D	1211	6PL	C1-O3P-P-O1P
5	D	1211	6PL	C4-O4P-P-O3P
5	D	1211	6PL	C4-O4P-P-O2P
5	D	1212	6PL	C32-C31-O2-C2
5	D	1214	6PL	C1-O3P-P-O2P
5	D	1214	6PL	C1-O3P-P-O4P
5	D	1215	6PL	C1-C2-O2-C31
5	D	1215	6PL	C1-O3P-P-O2P
5	D	1215	6PL	C1-O3P-P-O4P
5	D	1215	6PL	C32-C31-O2-C2
5	D	1216	6PL	O2-C2-C3-O3
5	D	1216	6PL	C1-O3P-P-O4P
5	A	1208	6PL	O11-C11-O3-C3
5	A	1209	6PL	O11-C11-O3-C3
5	B	1210	6PL	O11-C11-O3-C3
5	B	1211	6PL	O11-C11-O3-C3
5	C	1210	6PL	O11-C11-O3-C3
5	C	1211	6PL	O11-C11-O3-C3
5	D	1210	6PL	O11-C11-O3-C3
5	D	1211	6PL	O11-C11-O3-C3
5	A	1209	6PL	C12-C11-O3-C3
5	B	1211	6PL	C12-C11-O3-C3
5	C	1211	6PL	C12-C11-O3-C3
5	D	1211	6PL	C12-C11-O3-C3
5	A	1214	6PL	O11-C11-O3-C3
5	B	1216	6PL	O11-C11-O3-C3
5	C	1216	6PL	O11-C11-O3-C3
5	D	1216	6PL	O11-C11-O3-C3
3	A	1204	CLR	C13-C17-C20-C21
3	B	1206	CLR	C13-C17-C20-C21
3	C	1206	CLR	C13-C17-C20-C21
3	D	1206	CLR	C13-C17-C20-C21
5	A	1207	6PL	O31-C31-O2-C2
5	B	1209	6PL	O31-C31-O2-C2
5	C	1209	6PL	O31-C31-O2-C2
5	D	1209	6PL	O31-C31-O2-C2
5	A	1208	6PL	C12-C11-O3-C3
5	B	1210	6PL	C12-C11-O3-C3
5	C	1210	6PL	C12-C11-O3-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	1210	6PL	C12-C11-O3-C3
3	A	1204	CLR	C16-C17-C20-C21
3	B	1206	CLR	C16-C17-C20-C21
3	C	1206	CLR	C16-C17-C20-C21
3	D	1206	CLR	C16-C17-C20-C21
5	A	1212	6PL	O11-C11-O3-C3
5	A	1213	6PL	O11-C11-O3-C3
5	B	1214	6PL	O11-C11-O3-C3
5	B	1215	6PL	O11-C11-O3-C3
5	C	1214	6PL	O11-C11-O3-C3
5	C	1215	6PL	O11-C11-O3-C3
5	D	1214	6PL	O11-C11-O3-C3
5	D	1215	6PL	O11-C11-O3-C3
5	A	1214	6PL	C12-C11-O3-C3
5	B	1216	6PL	C12-C11-O3-C3
5	C	1216	6PL	C12-C11-O3-C3
5	D	1216	6PL	C12-C11-O3-C3
5	A	1207	6PL	C12-C11-O3-C3
5	A	1213	6PL	C12-C11-O3-C3
5	B	1209	6PL	C12-C11-O3-C3
5	B	1215	6PL	C12-C11-O3-C3
5	C	1209	6PL	C12-C11-O3-C3
5	C	1215	6PL	C12-C11-O3-C3
5	D	1209	6PL	C12-C11-O3-C3
5	D	1215	6PL	C12-C11-O3-C3
5	A	1210	6PL	O31-C31-O2-C2
5	A	1213	6PL	O31-C31-O2-C2
5	B	1212	6PL	O31-C31-O2-C2
5	B	1215	6PL	O31-C31-O2-C2
5	C	1212	6PL	O31-C31-O2-C2
5	C	1215	6PL	O31-C31-O2-C2
5	D	1212	6PL	O31-C31-O2-C2
5	D	1215	6PL	O31-C31-O2-C2
5	A	1212	6PL	C12-C11-O3-C3
5	B	1214	6PL	C12-C11-O3-C3
5	C	1214	6PL	C12-C11-O3-C3
5	D	1214	6PL	C12-C11-O3-C3
5	A	1209	6PL	C2-C1-O3P-P
5	B	1211	6PL	C2-C1-O3P-P
5	C	1211	6PL	C2-C1-O3P-P
5	D	1211	6PL	C2-C1-O3P-P
5	A	1207	6PL	O11-C11-O3-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	1209	6PL	O11-C11-O3-C3
5	C	1209	6PL	O11-C11-O3-C3
5	D	1209	6PL	O11-C11-O3-C3
3	D	1203	CLR	C20-C22-C23-C24
3	A	1201	CLR	C20-C22-C23-C24
3	B	1203	CLR	C20-C22-C23-C24
3	C	1203	CLR	C20-C22-C23-C24
5	B	1214	6PL	C31-C32-C33-C34
5	C	1214	6PL	C31-C32-C33-C34
5	D	1214	6PL	C31-C32-C33-C34
5	A	1212	6PL	C31-C32-C33-C34
5	B	1212	6PL	C34-C35-C36-C37
5	D	1212	6PL	C34-C35-C36-C37
5	C	1212	6PL	C34-C35-C36-C37
5	A	1210	6PL	C34-C35-C36-C37
3	A	1202	CLR	C20-C22-C23-C24
3	B	1204	CLR	C20-C22-C23-C24
3	C	1204	CLR	C20-C22-C23-C24
3	D	1204	CLR	C20-C22-C23-C24
5	B	1214	6PL	C34-C35-C36-C37
5	C	1214	6PL	C34-C35-C36-C37
5	D	1214	6PL	C34-C35-C36-C37
5	A	1212	6PL	C34-C35-C36-C37
5	A	1212	6PL	C1-O3P-P-O1P
5	A	1213	6PL	C1-O3P-P-O1P
5	A	1214	6PL	C1-O3P-P-O1P
5	A	1216	6PL	C1-O3P-P-O1P
5	B	1202	6PL	C1-O3P-P-O1P
5	B	1214	6PL	C1-O3P-P-O1P
5	B	1215	6PL	C1-O3P-P-O1P
5	B	1216	6PL	C1-O3P-P-O1P
5	C	1202	6PL	C1-O3P-P-O1P
5	C	1214	6PL	C1-O3P-P-O1P
5	C	1215	6PL	C1-O3P-P-O1P
5	C	1216	6PL	C1-O3P-P-O1P
5	D	1202	6PL	C1-O3P-P-O1P
5	D	1214	6PL	C1-O3P-P-O1P
5	D	1215	6PL	C1-O3P-P-O1P
5	D	1216	6PL	C1-O3P-P-O1P
3	A	1203	CLR	C16-C17-C20-C21
3	B	1205	CLR	C16-C17-C20-C21
3	C	1205	CLR	C16-C17-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	1205	CLR	C16-C17-C20-C21
5	A	1213	6PL	O2-C2-C3-O3
5	B	1215	6PL	O2-C2-C3-O3
5	C	1215	6PL	O2-C2-C3-O3
5	D	1215	6PL	O2-C2-C3-O3
3	A	1203	CLR	C13-C17-C20-C21
3	B	1205	CLR	C13-C17-C20-C21
3	C	1205	CLR	C13-C17-C20-C21
3	D	1205	CLR	C13-C17-C20-C21
3	A	1203	CLR	C13-C17-C20-C22
3	B	1205	CLR	C13-C17-C20-C22
3	C	1205	CLR	C13-C17-C20-C22
3	D	1205	CLR	C13-C17-C20-C22
5	A	1208	6PL	C1-C2-C3-O3
5	B	1210	6PL	C1-C2-C3-O3
5	C	1210	6PL	C1-C2-C3-O3
5	D	1210	6PL	C1-C2-C3-O3
5	A	1208	6PL	O2-C2-C3-O3
5	B	1210	6PL	O2-C2-C3-O3
5	C	1210	6PL	O2-C2-C3-O3
5	D	1210	6PL	O2-C2-C3-O3
5	A	1210	6PL	O2-C2-C3-O3
5	B	1212	6PL	O2-C2-C3-O3
5	C	1212	6PL	O2-C2-C3-O3
5	D	1212	6PL	O2-C2-C3-O3
5	A	1214	6PL	C1-C2-C3-O3
5	B	1216	6PL	C1-C2-C3-O3
5	C	1216	6PL	C1-C2-C3-O3
5	D	1216	6PL	C1-C2-C3-O3
3	A	1203	CLR	C16-C17-C20-C22
3	B	1205	CLR	C16-C17-C20-C22
3	C	1205	CLR	C16-C17-C20-C22
3	D	1205	CLR	C16-C17-C20-C22
5	A	1212	6PL	O3P-C1-C2-C3
5	B	1214	6PL	O3P-C1-C2-C3
5	C	1214	6PL	O3P-C1-C2-C3
5	D	1214	6PL	O3P-C1-C2-C3
5	A	1216	6PL	C1-O3P-P-O4P
5	B	1202	6PL	C1-O3P-P-O4P
5	C	1202	6PL	C1-O3P-P-O4P
5	D	1202	6PL	C1-O3P-P-O4P
5	A	1208	6PL	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	1210	6PL	C11-C12-C13-C14
5	D	1210	6PL	C11-C12-C13-C14
5	B	1210	6PL	C11-C12-C13-C14
5	A	1216	6PL	C2-C1-O3P-P
5	B	1202	6PL	C2-C1-O3P-P
5	C	1202	6PL	C2-C1-O3P-P
5	D	1202	6PL	C2-C1-O3P-P
5	A	1210	6PL	C1-C2-C3-O3
5	A	1213	6PL	C1-C2-C3-O3
5	B	1212	6PL	C1-C2-C3-O3
5	B	1215	6PL	C1-C2-C3-O3
5	C	1212	6PL	C1-C2-C3-O3
5	C	1215	6PL	C1-C2-C3-O3
5	D	1212	6PL	C1-C2-C3-O3
5	D	1215	6PL	C1-C2-C3-O3
5	A	1207	6PL	C4-O4P-P-O1P
5	B	1209	6PL	C4-O4P-P-O1P
5	C	1209	6PL	C4-O4P-P-O1P
5	D	1209	6PL	C4-O4P-P-O1P
5	C	1215	6PL	C32-C33-C34-C35
5	A	1213	6PL	C32-C33-C34-C35
5	B	1215	6PL	C32-C33-C34-C35
5	D	1215	6PL	C32-C33-C34-C35
5	A	1210	6PL	C11-C12-C13-C14
5	B	1212	6PL	C11-C12-C13-C14
5	C	1212	6PL	C11-C12-C13-C14
5	D	1212	6PL	C11-C12-C13-C14
5	A	1212	6PL	O3P-C1-C2-O2
5	B	1214	6PL	O3P-C1-C2-O2
5	C	1214	6PL	O3P-C1-C2-O2
5	D	1214	6PL	O3P-C1-C2-O2
3	A	1204	CLR	C21-C20-C22-C23
3	B	1206	CLR	C21-C20-C22-C23
3	C	1206	CLR	C21-C20-C22-C23
3	D	1206	CLR	C21-C20-C22-C23
5	A	1214	6PL	O3P-C1-C2-O2
5	B	1216	6PL	O3P-C1-C2-O2
5	C	1216	6PL	O3P-C1-C2-O2
5	D	1216	6PL	O3P-C1-C2-O2
5	A	1207	6PL	C2-C1-O3P-P
5	B	1209	6PL	C2-C1-O3P-P
5	C	1209	6PL	C2-C1-O3P-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	1209	6PL	C2-C1-O3P-P
5	C	1214	6PL	C32-C33-C34-C35
5	B	1214	6PL	C32-C33-C34-C35
5	A	1212	6PL	C32-C33-C34-C35
5	D	1214	6PL	C32-C33-C34-C35
5	A	1207	6PL	O2-C2-C3-O3
5	B	1209	6PL	O2-C2-C3-O3
5	C	1209	6PL	O2-C2-C3-O3
5	D	1209	6PL	O2-C2-C3-O3
5	B	1212	6PL	C33-C34-C35-C36
5	C	1212	6PL	C33-C34-C35-C36
5	D	1212	6PL	C33-C34-C35-C36
5	A	1210	6PL	C33-C34-C35-C36
5	A	1211	6PL	O3P-C1-C2-O2
5	B	1213	6PL	O3P-C1-C2-O2
5	C	1213	6PL	O3P-C1-C2-O2
5	D	1213	6PL	O3P-C1-C2-O2
5	A	1214	6PL	C1-O3P-P-O2P
5	B	1216	6PL	C1-O3P-P-O2P
5	C	1216	6PL	C1-O3P-P-O2P
5	D	1216	6PL	C1-O3P-P-O2P
5	A	1207	6PL	C1-C2-C3-O3
5	B	1209	6PL	C1-C2-C3-O3
5	C	1209	6PL	C1-C2-C3-O3
5	D	1209	6PL	C1-C2-C3-O3
5	A	1209	6PL	O31-C31-O2-C2
5	C	1211	6PL	O31-C31-O2-C2
5	B	1211	6PL	O31-C31-O2-C2
5	D	1211	6PL	O31-C31-O2-C2
5	A	1209	6PL	C32-C31-O2-C2
5	B	1211	6PL	C32-C31-O2-C2
5	C	1211	6PL	C32-C31-O2-C2
5	D	1211	6PL	C32-C31-O2-C2
5	D	1210	6PL	O2-C31-C32-C33
5	A	1208	6PL	O2-C31-C32-C33
5	B	1210	6PL	O2-C31-C32-C33
5	C	1210	6PL	O2-C31-C32-C33
5	A	1209	6PL	C4-C5-N-C6
5	B	1211	6PL	C4-C5-N-C6
5	C	1211	6PL	C4-C5-N-C6
5	D	1211	6PL	C4-C5-N-C6
5	A	1209	6PL	C4-C5-N-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1209	6PL	C4-C5-N-C8
5	B	1211	6PL	C4-C5-N-C7
5	B	1211	6PL	C4-C5-N-C8
5	C	1211	6PL	C4-C5-N-C7
5	C	1211	6PL	C4-C5-N-C8
5	D	1211	6PL	C4-C5-N-C7
5	D	1211	6PL	C4-C5-N-C8
5	B	1210	6PL	O31-C31-C32-C33
5	C	1210	6PL	O31-C31-C32-C33
5	D	1210	6PL	O31-C31-C32-C33
5	A	1208	6PL	O31-C31-C32-C33
3	C	1206	CLR	C17-C20-C22-C23
5	B	1210	6PL	C33-C34-C35-C36
5	D	1210	6PL	C33-C34-C35-C36
5	A	1208	6PL	C33-C34-C35-C36
5	C	1210	6PL	C33-C34-C35-C36
3	D	1206	CLR	C17-C20-C22-C23

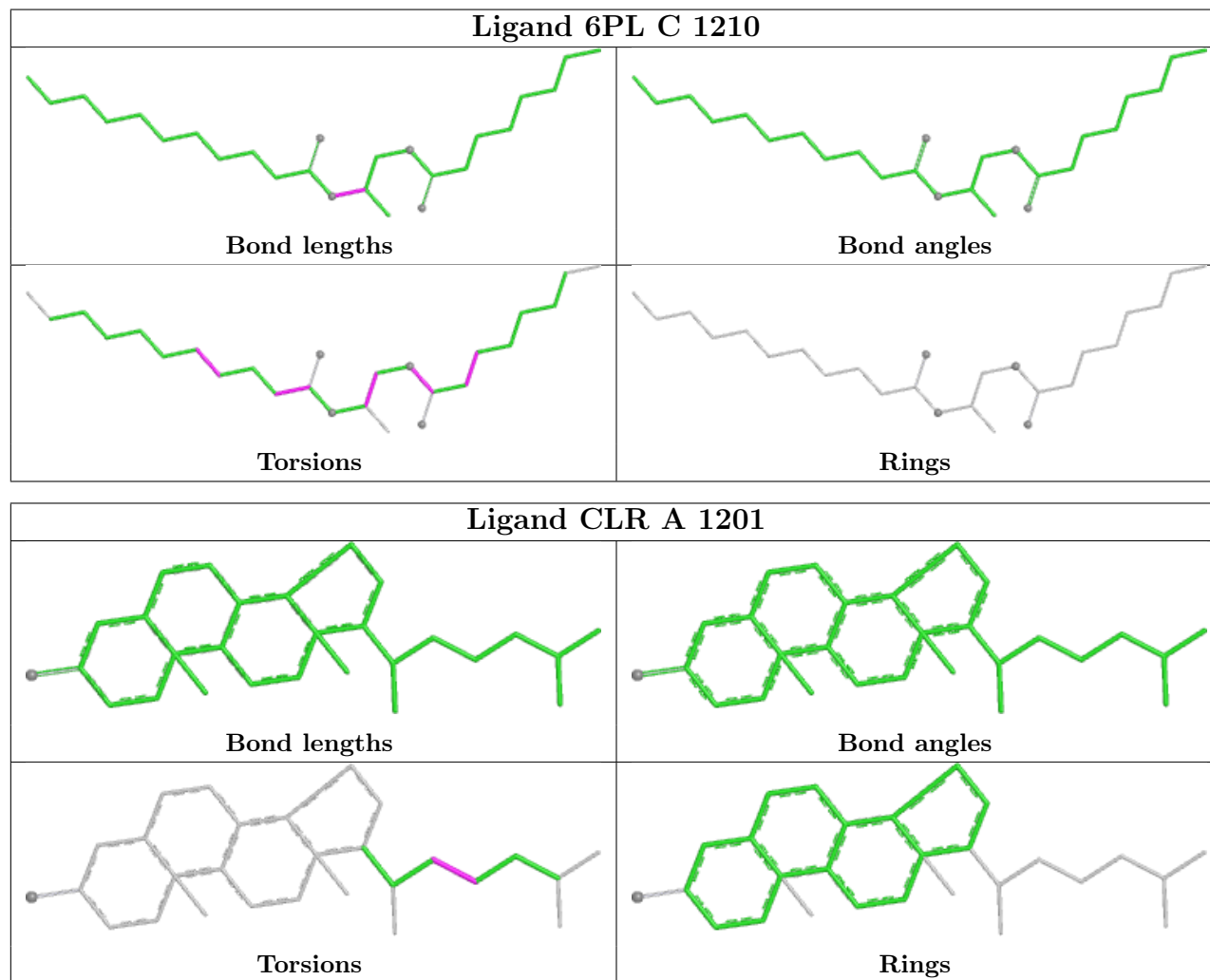
There are no ring outliers.

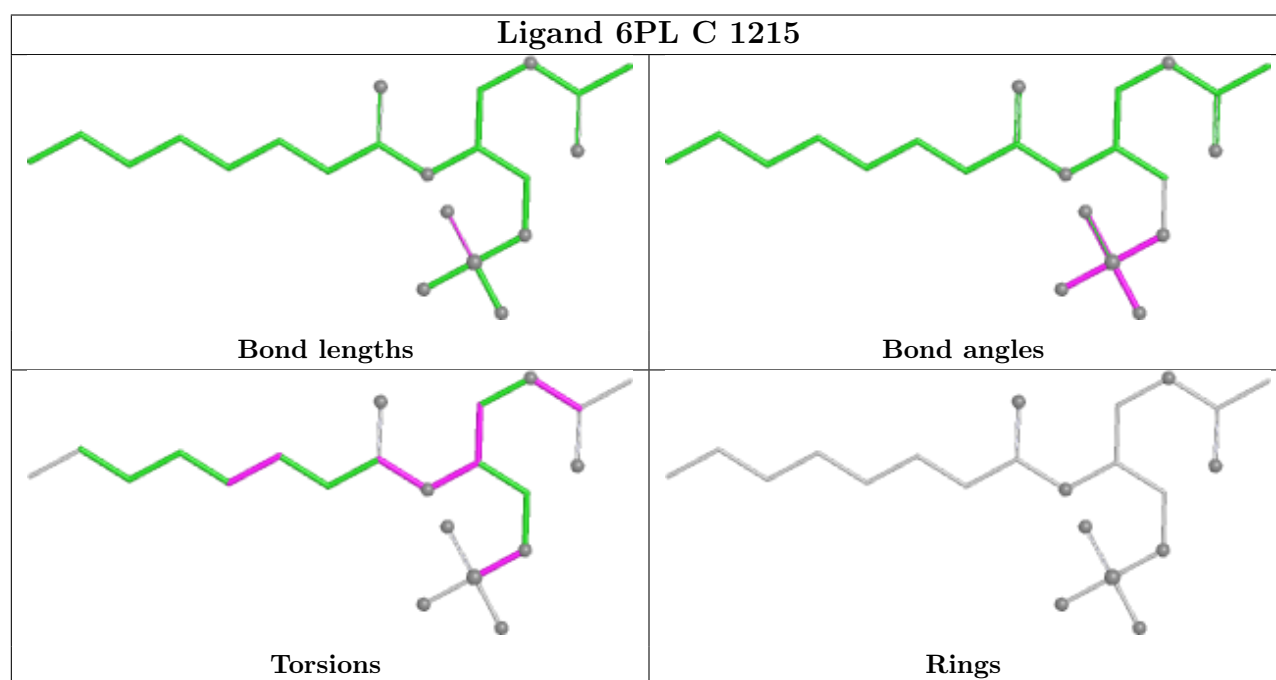
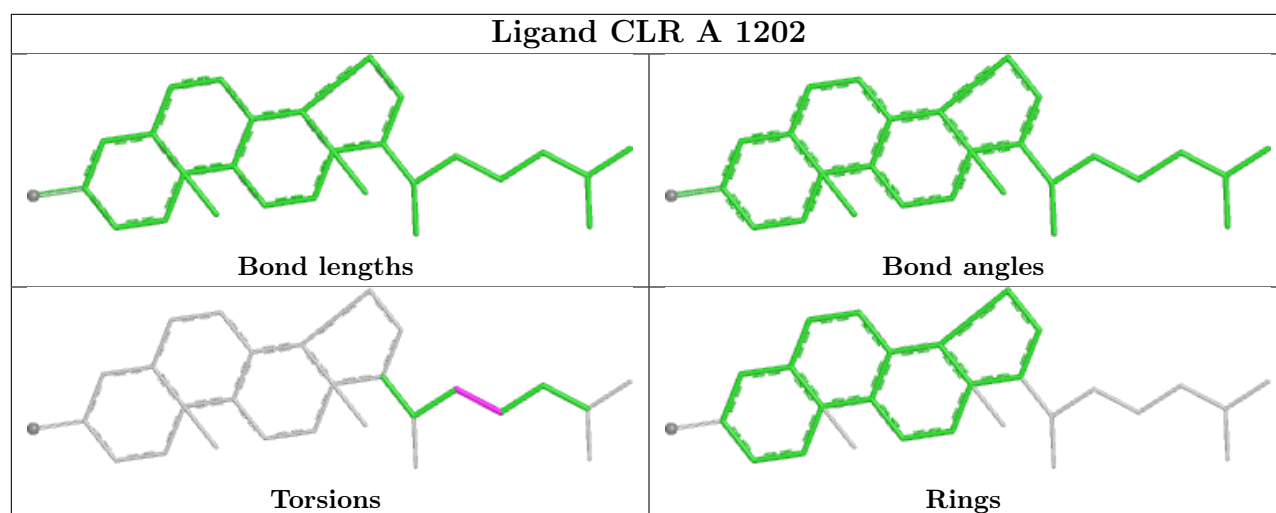
17 monomers are involved in 26 short contacts:

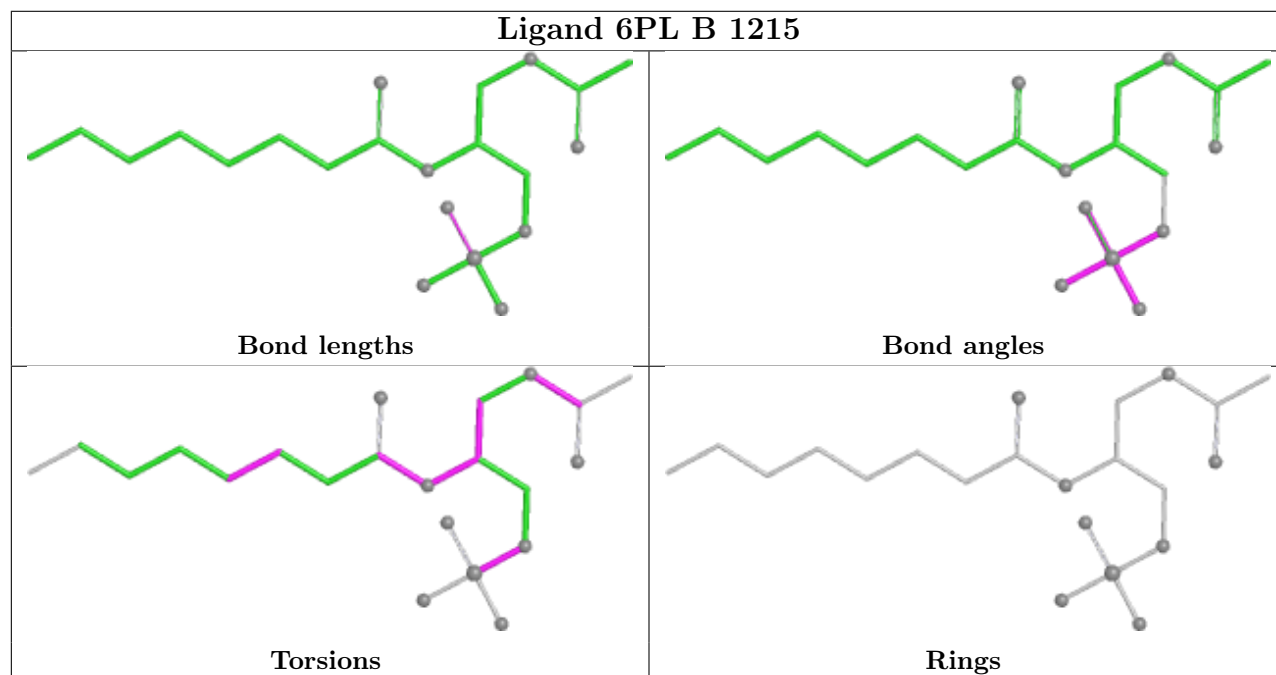
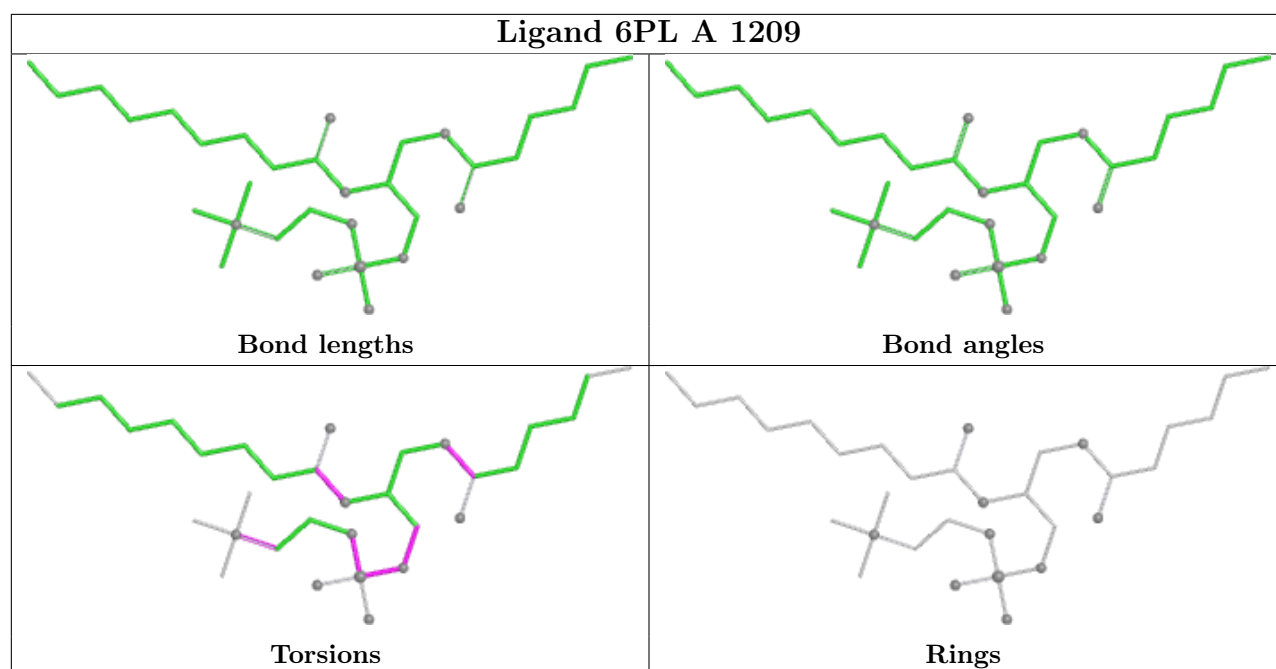
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1210	6PL	1	0
3	A	1201	CLR	1	0
3	A	1202	CLR	3	0
3	C	1203	CLR	1	0
5	A	1208	6PL	1	0
3	C	1204	CLR	3	0
5	A	1212	6PL	1	0
3	D	1203	CLR	1	0
3	D	1205	CLR	1	0
3	A	1204	CLR	1	0
5	B	1210	6PL	1	0
3	C	1206	CLR	1	0
3	B	1203	CLR	2	0
3	B	1204	CLR	3	0
5	D	1210	6PL	1	0
3	D	1204	CLR	3	0
3	D	1206	CLR	1	0

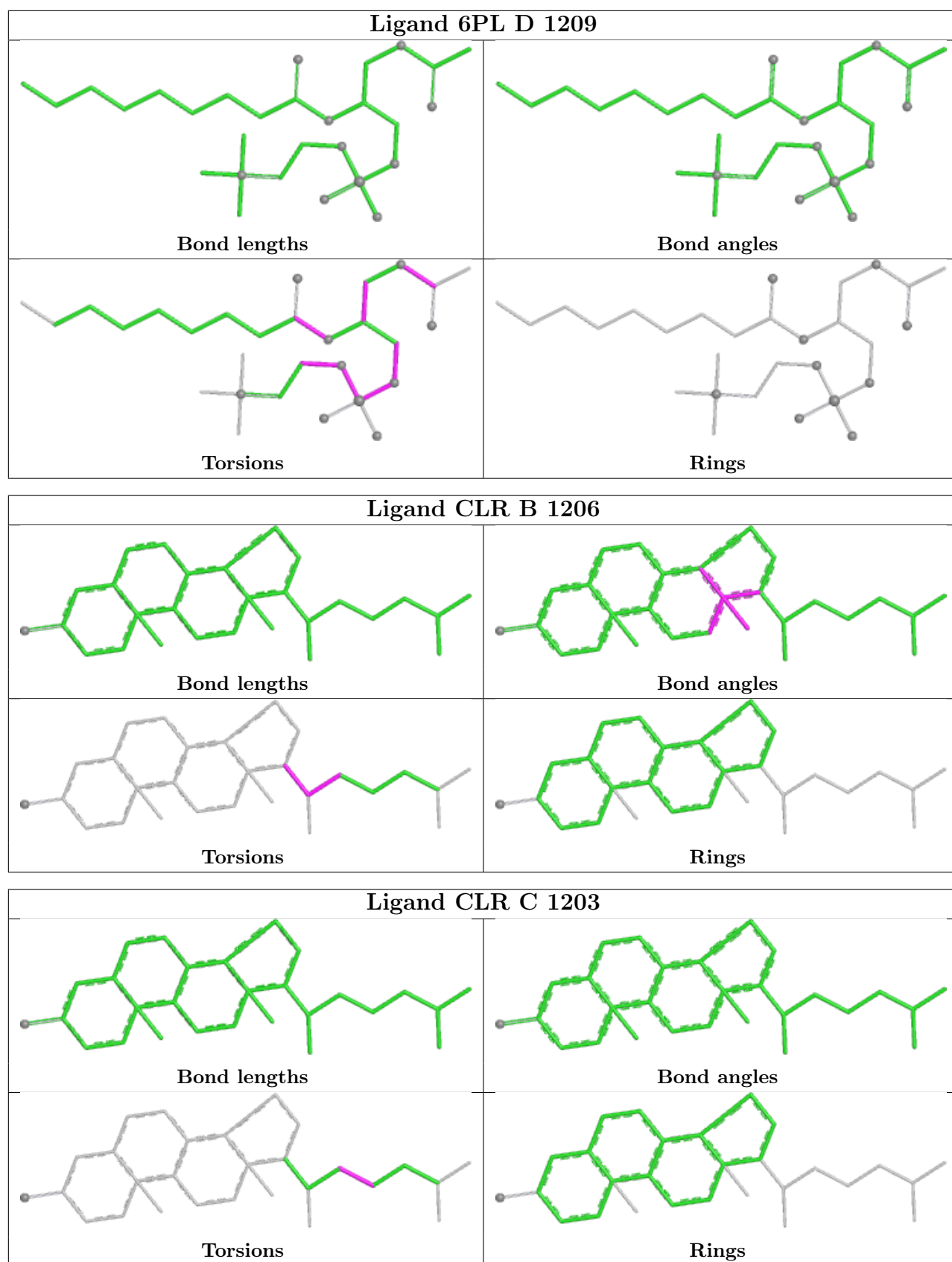
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

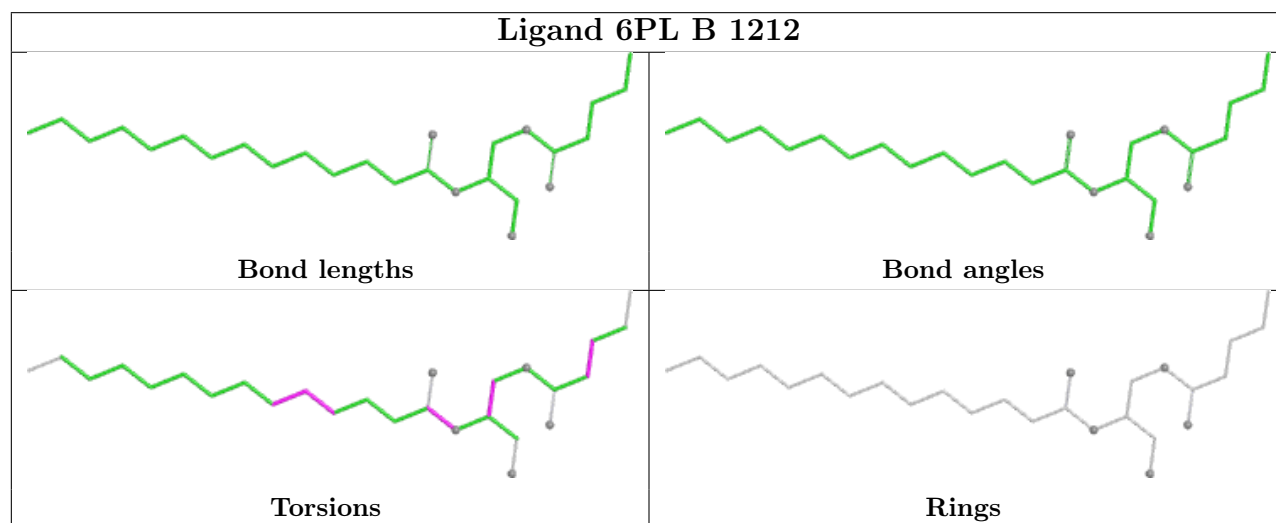
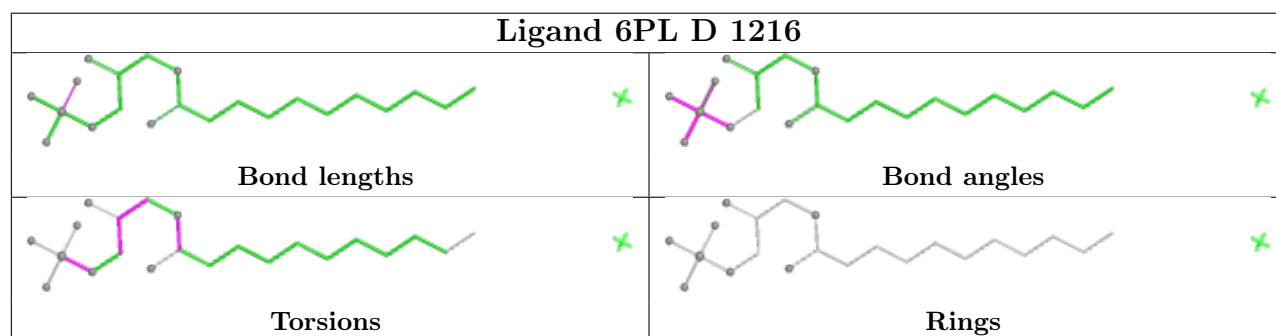
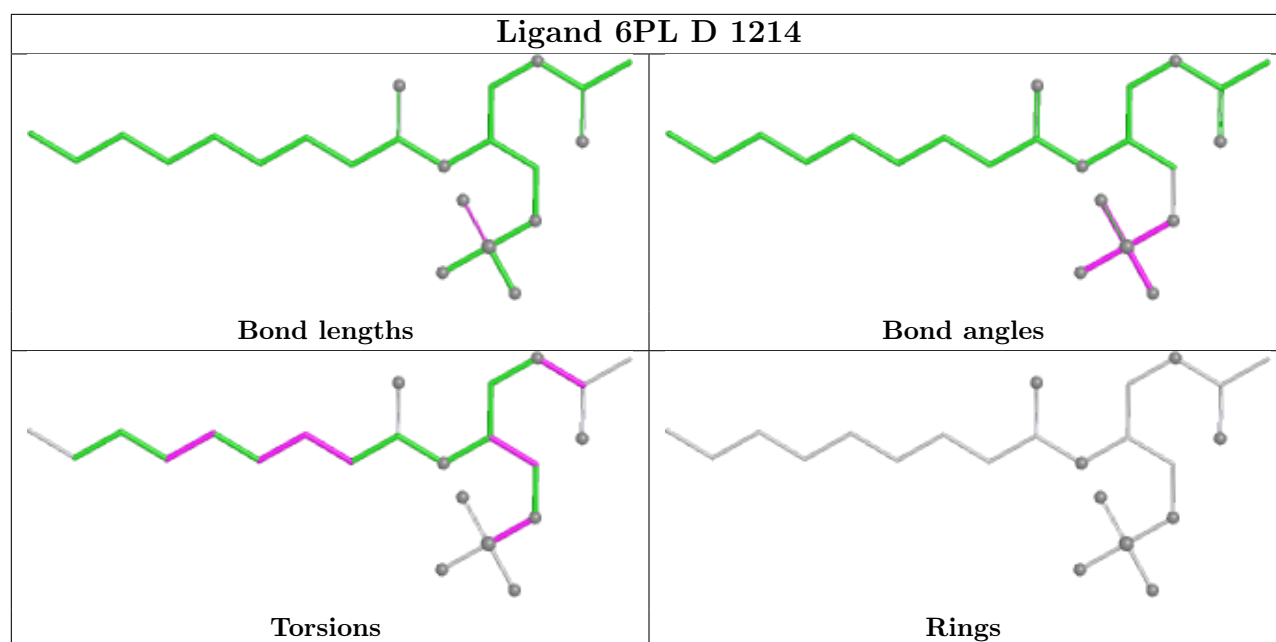
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

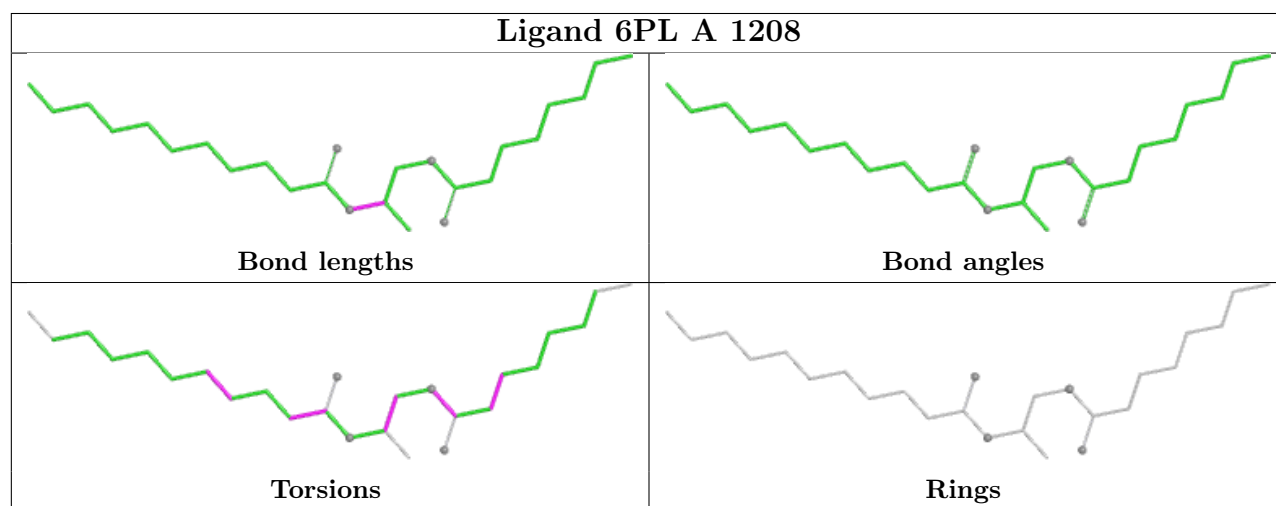
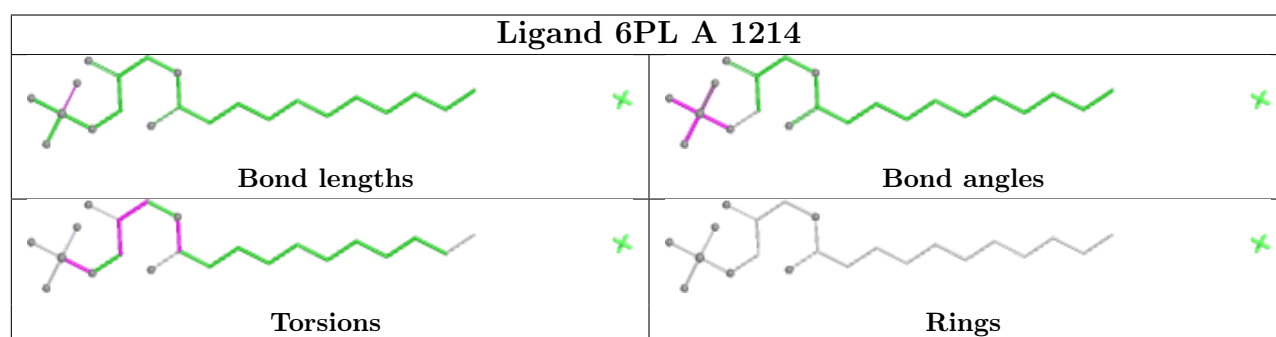
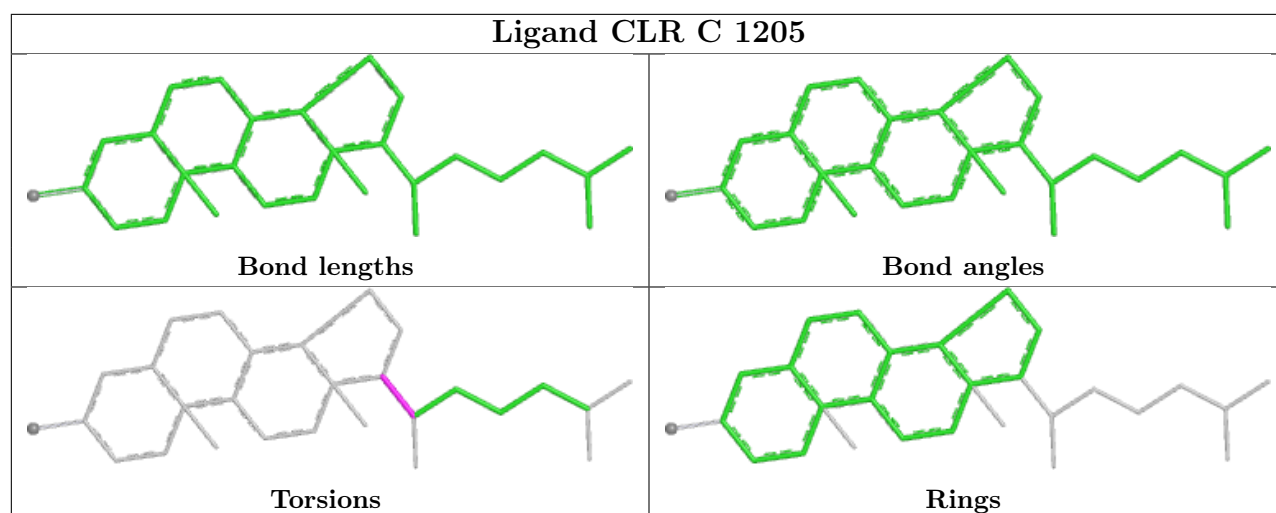


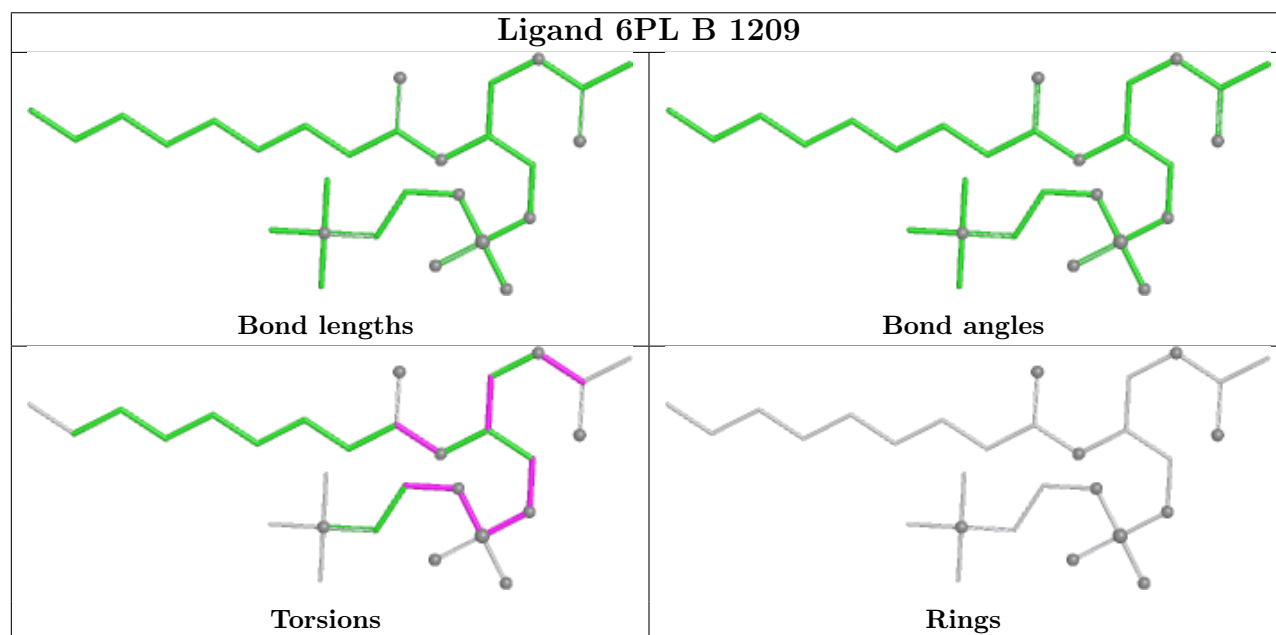
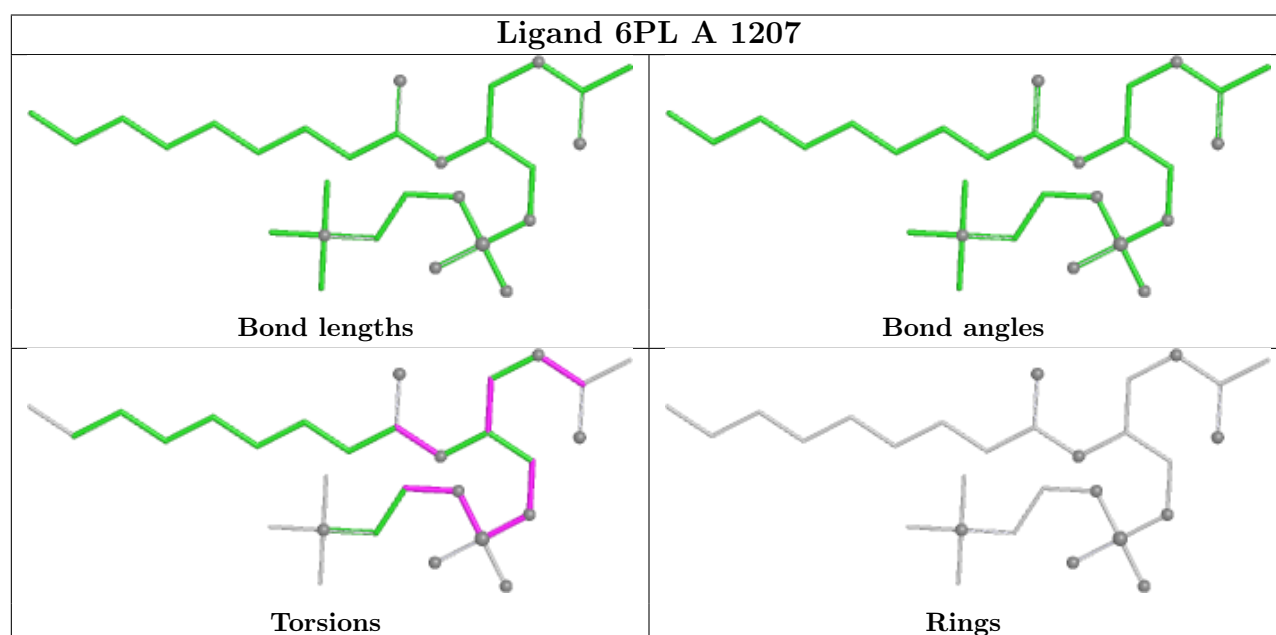
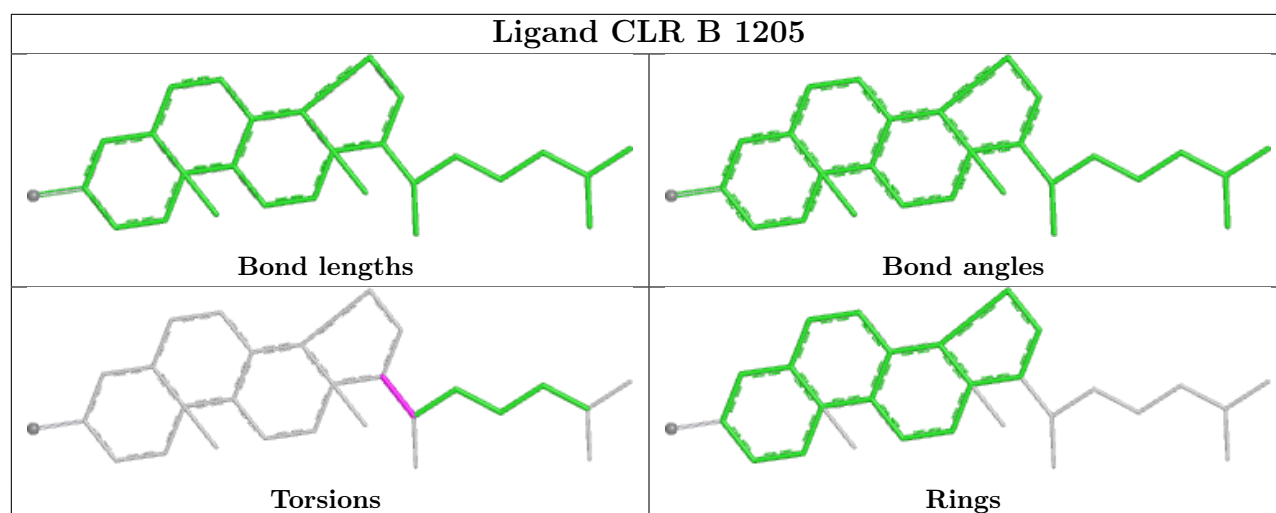


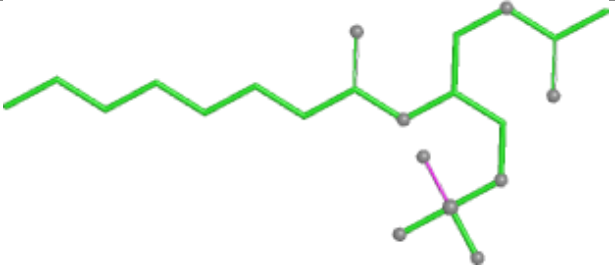
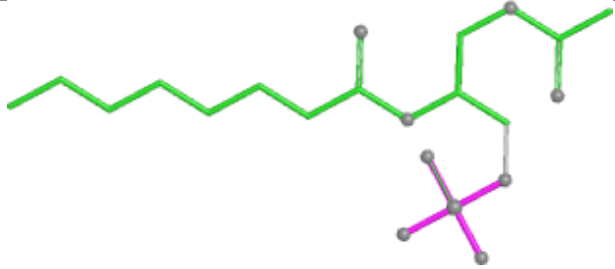
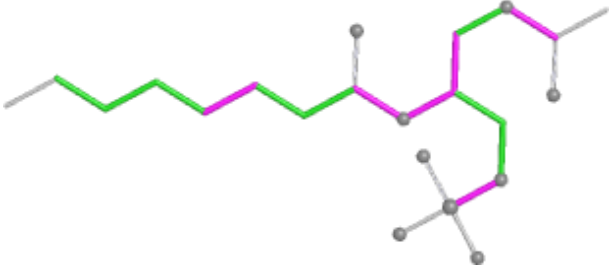
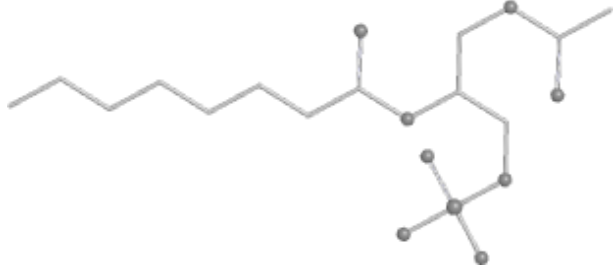
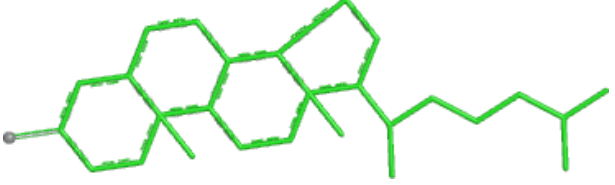
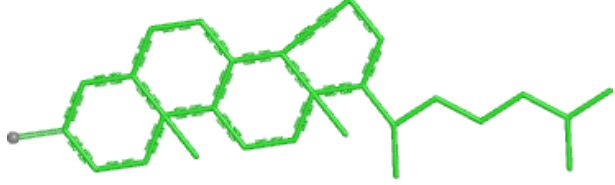
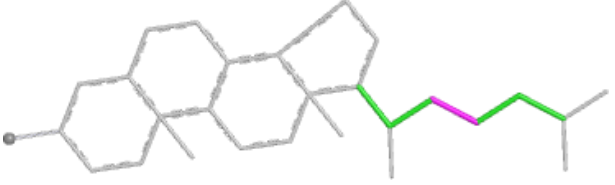
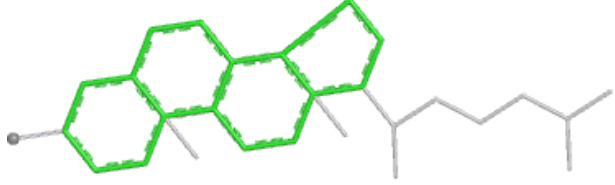
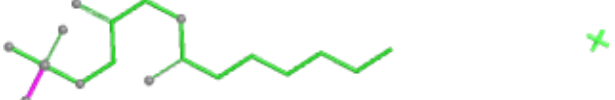
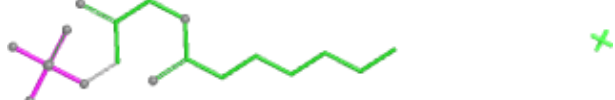
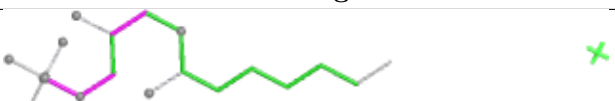
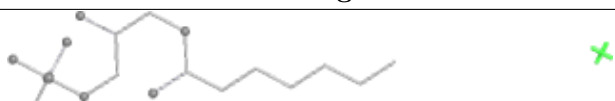


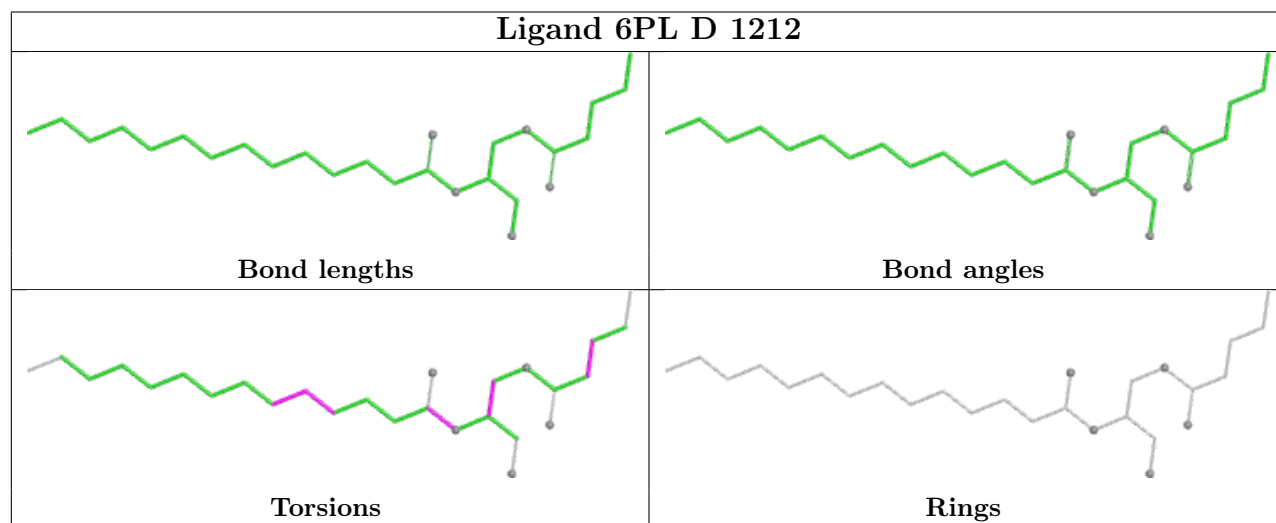
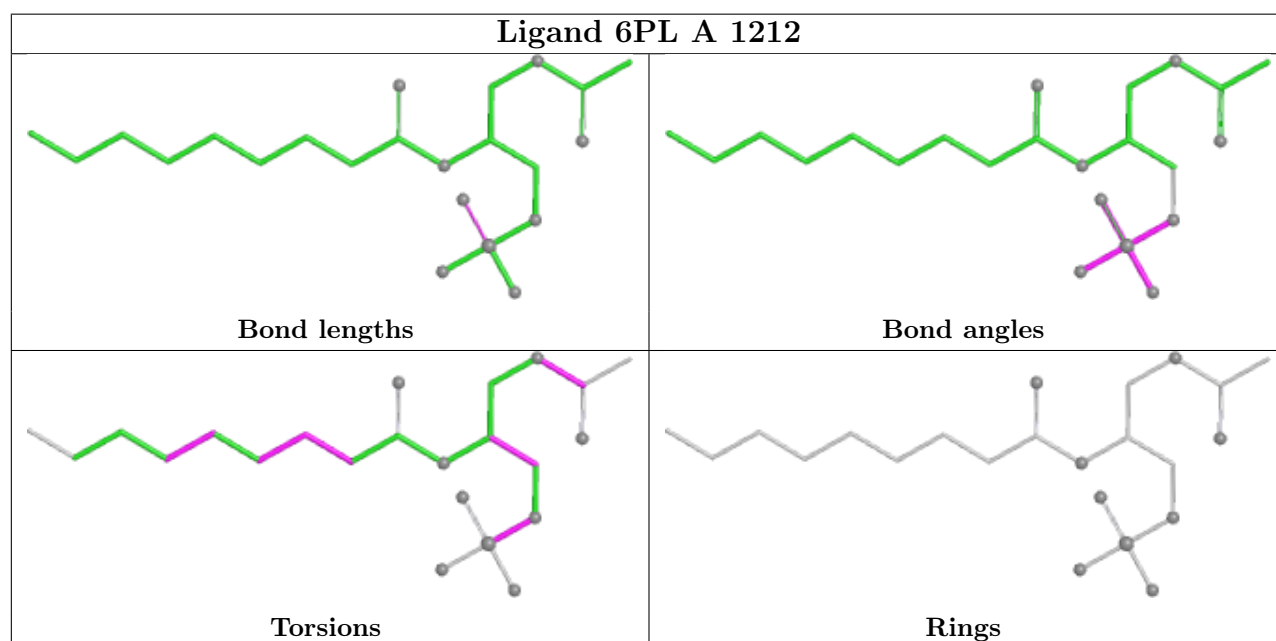
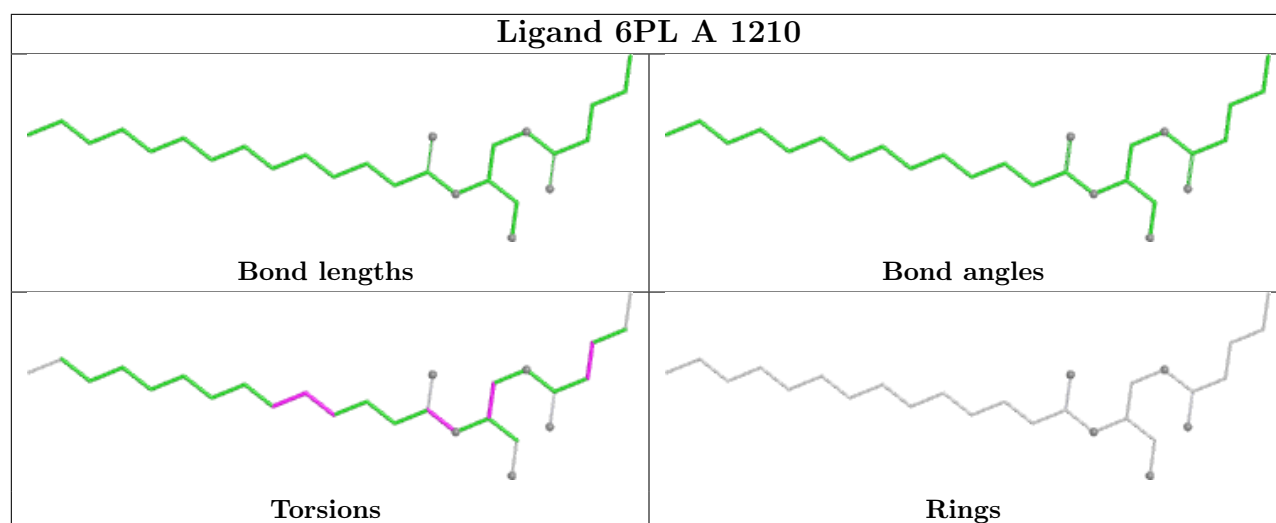


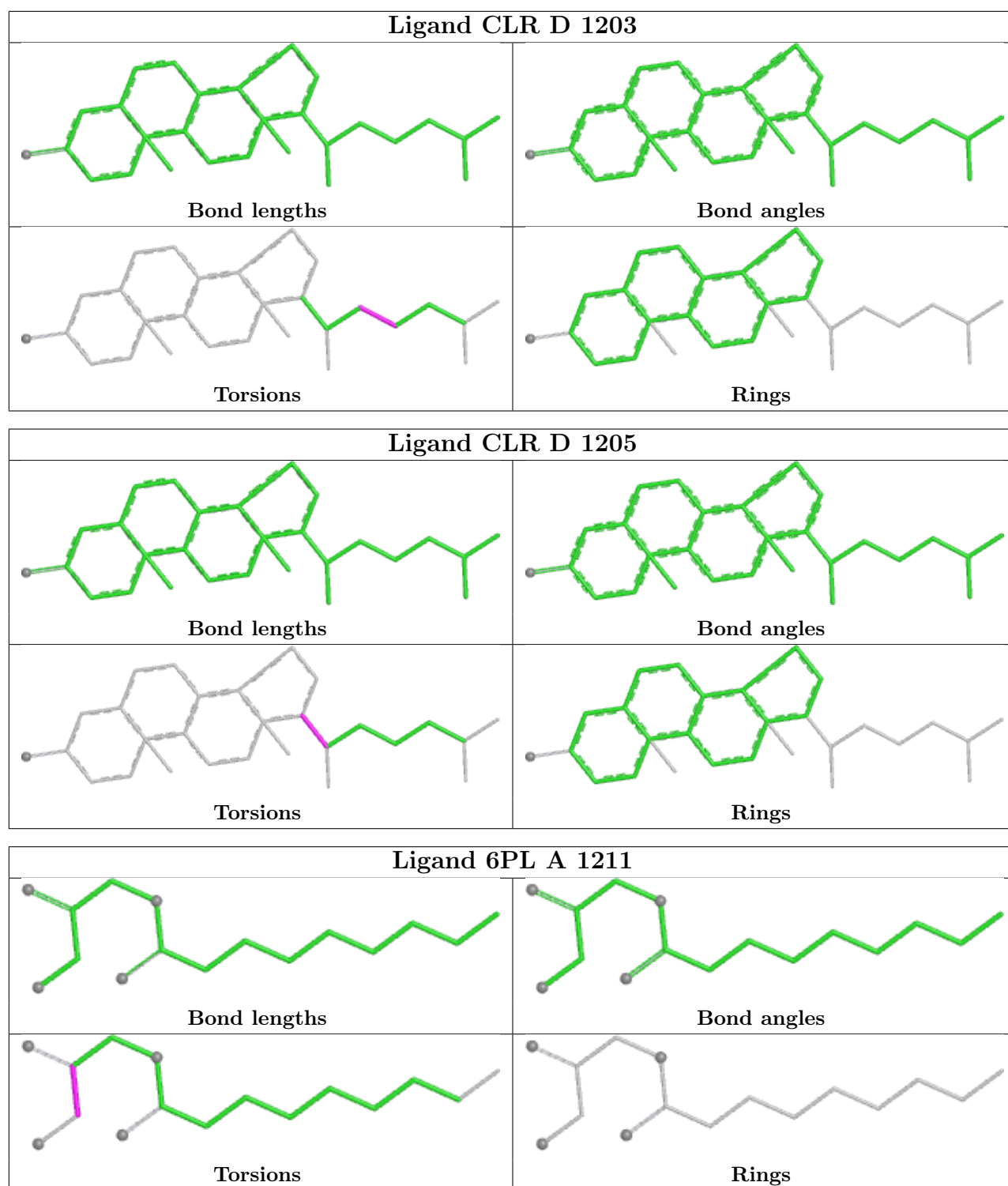


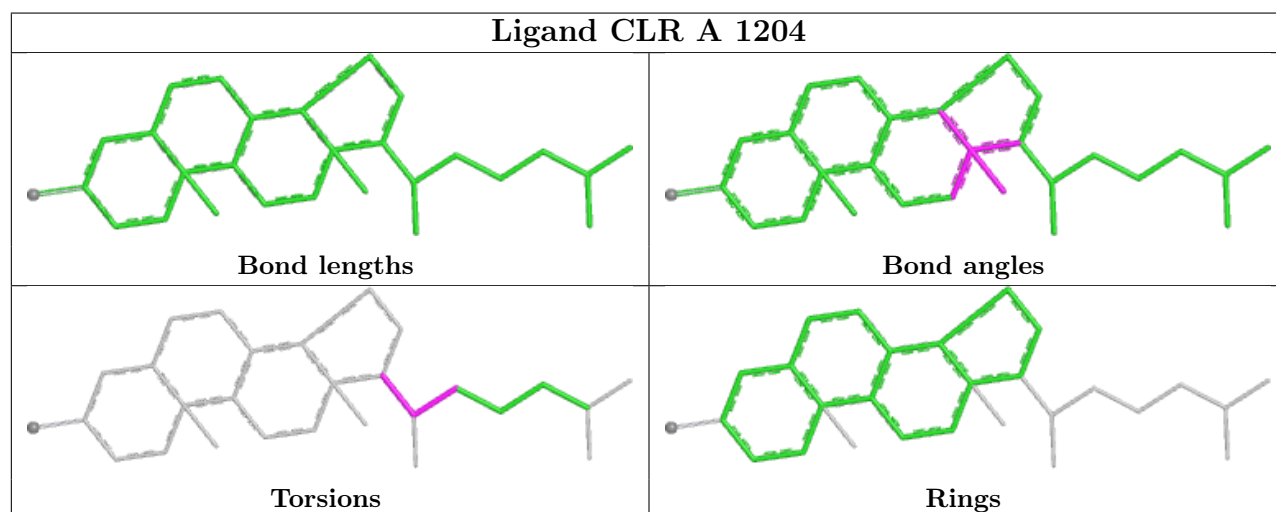
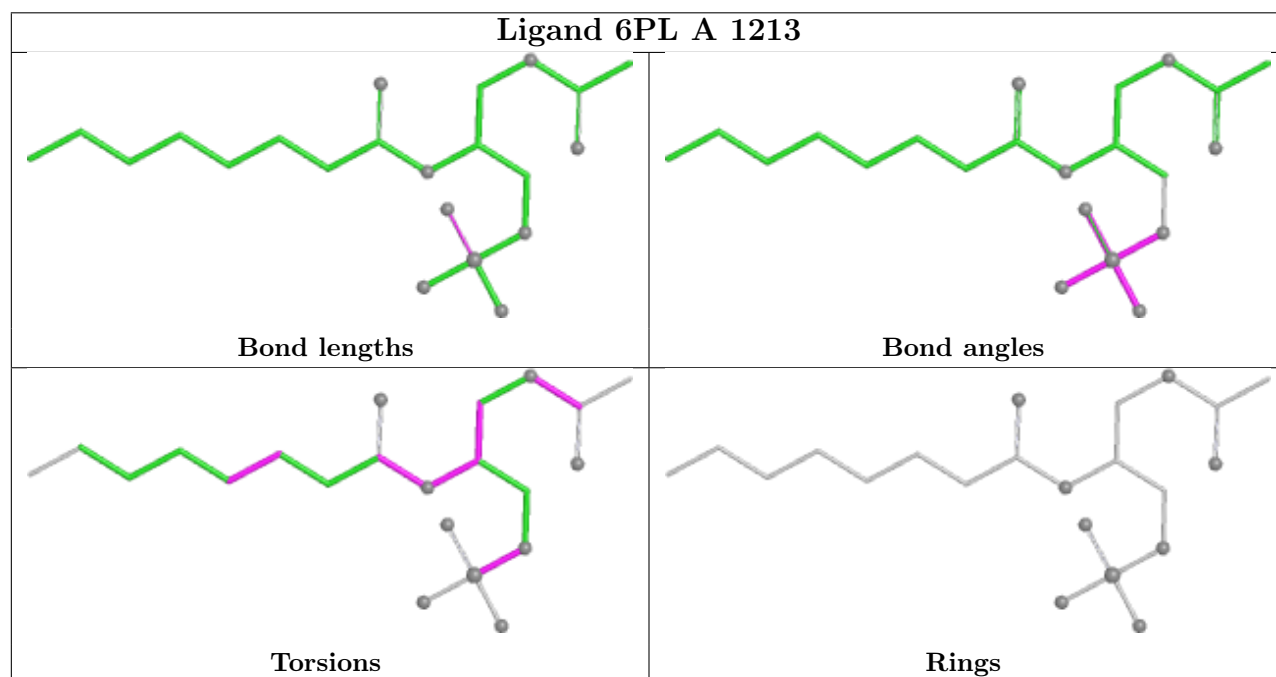
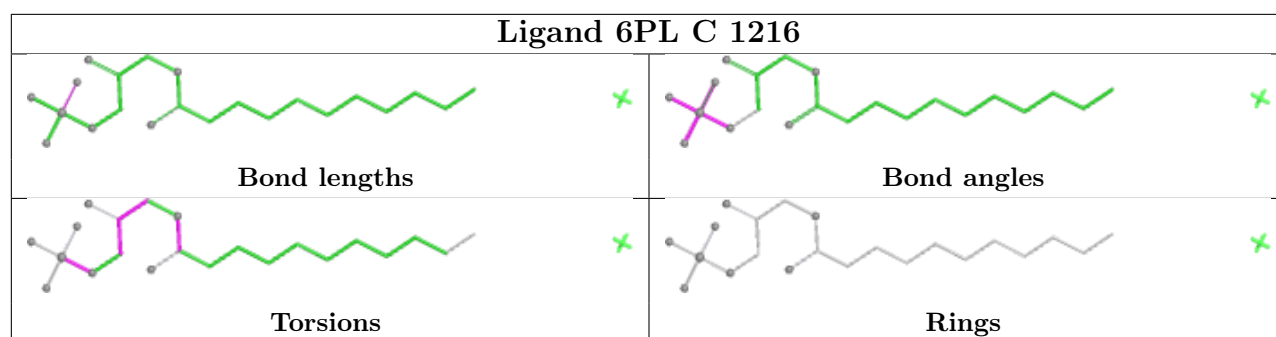


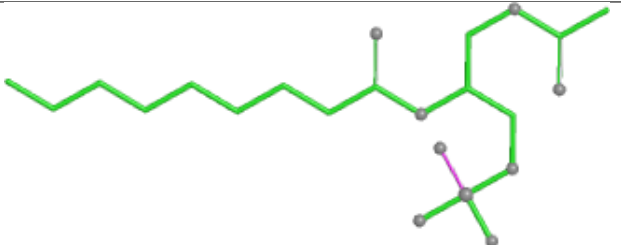
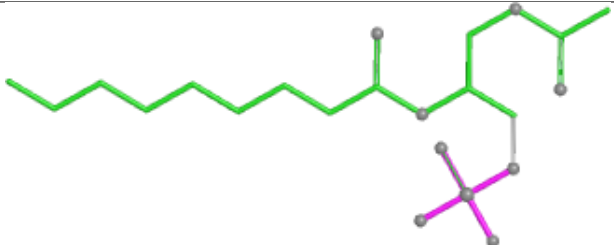
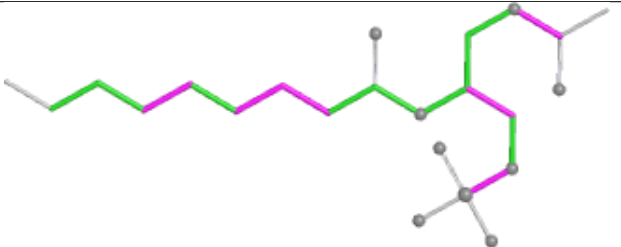
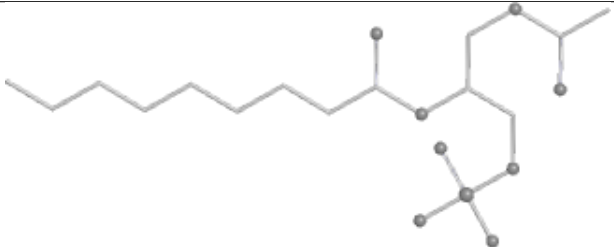
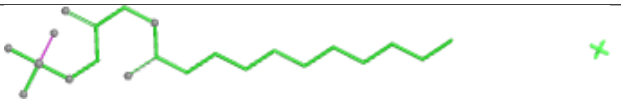
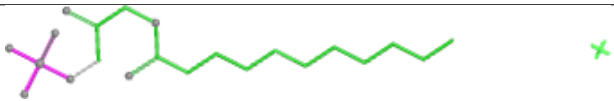
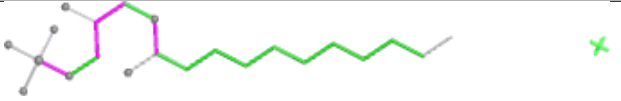
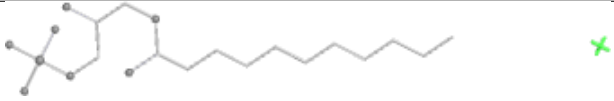
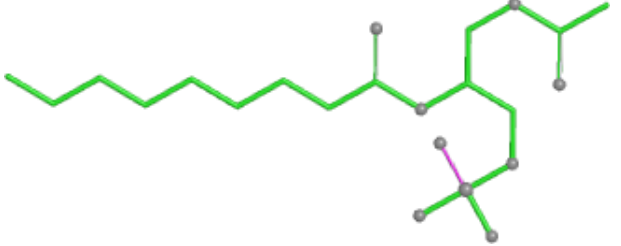
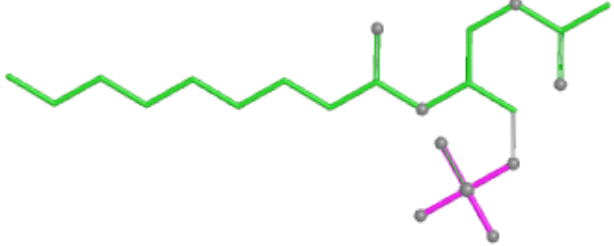
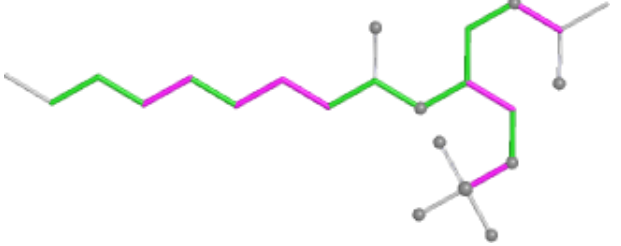
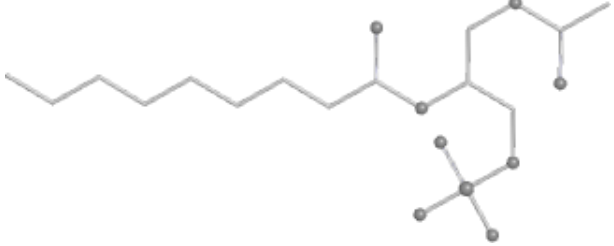


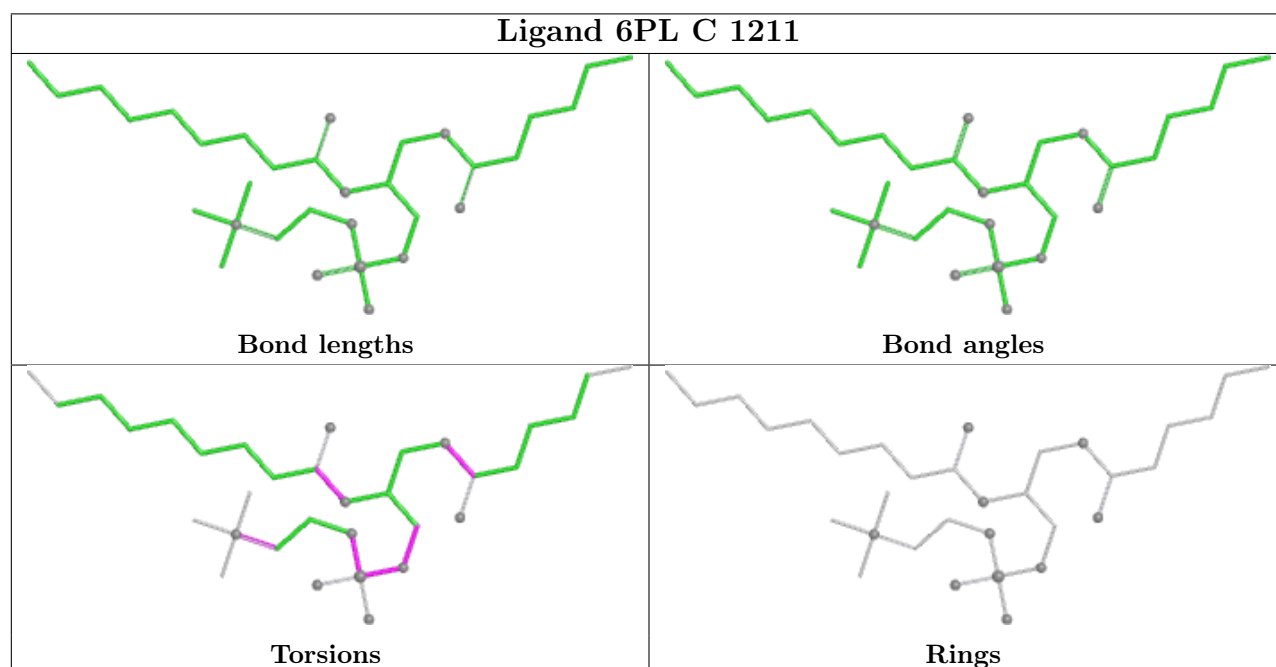
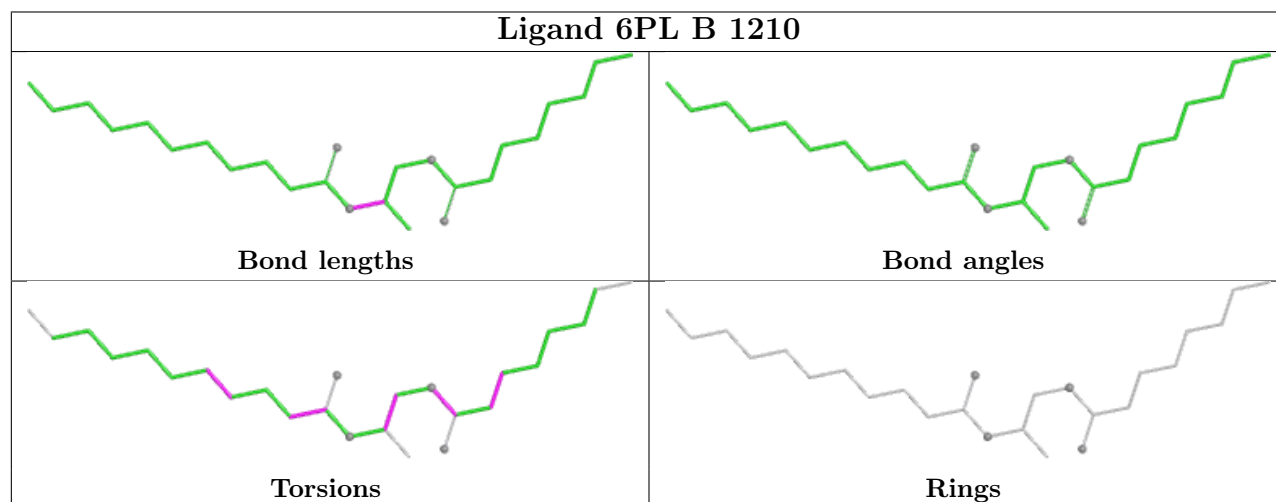
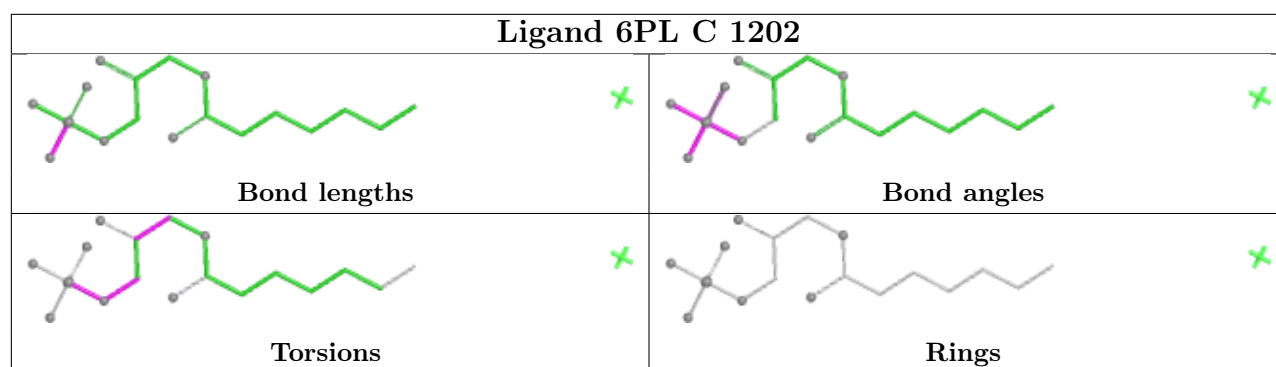
Ligand 6PL D 1215			
			
Bond lengths		Bond angles	
			
Torsions		Rings	
Ligand CLR C 1204			
			
Bond lengths		Bond angles	
			
Torsions		Rings	
Ligand 6PL A 1216			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

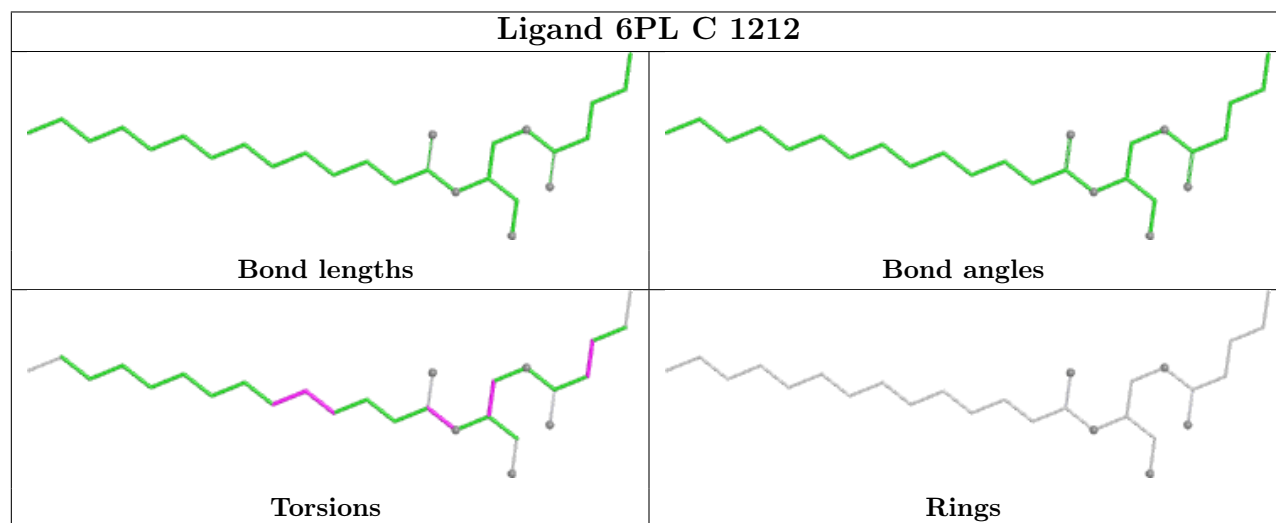
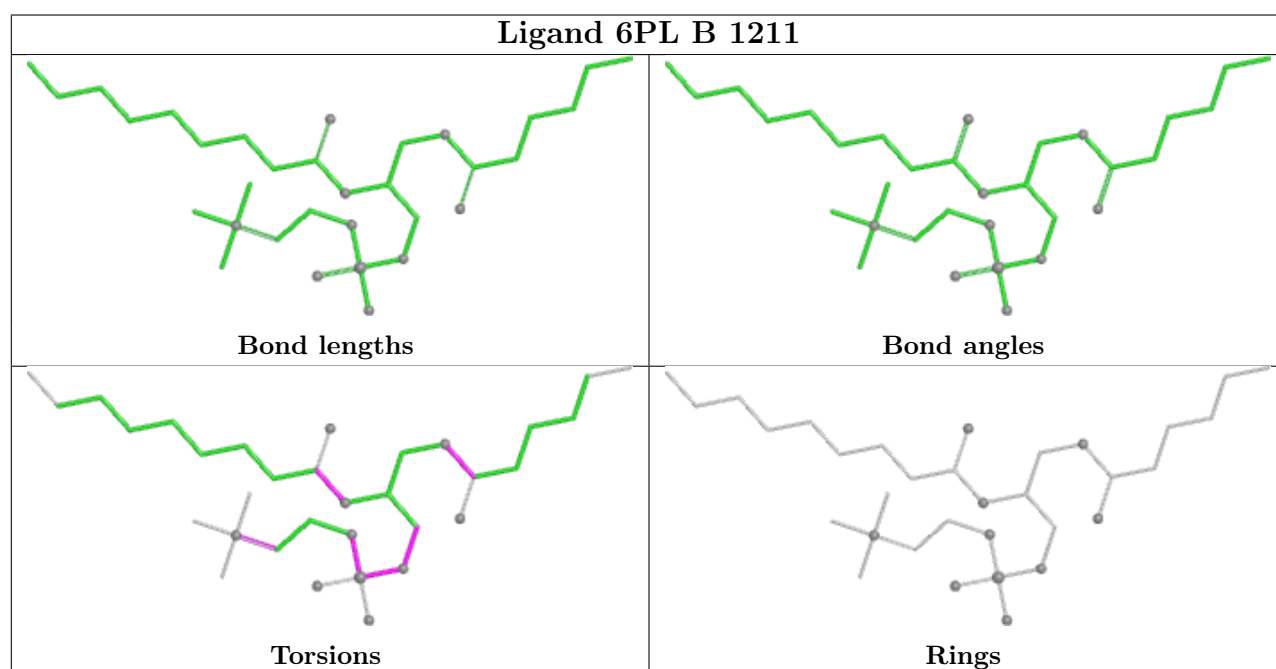
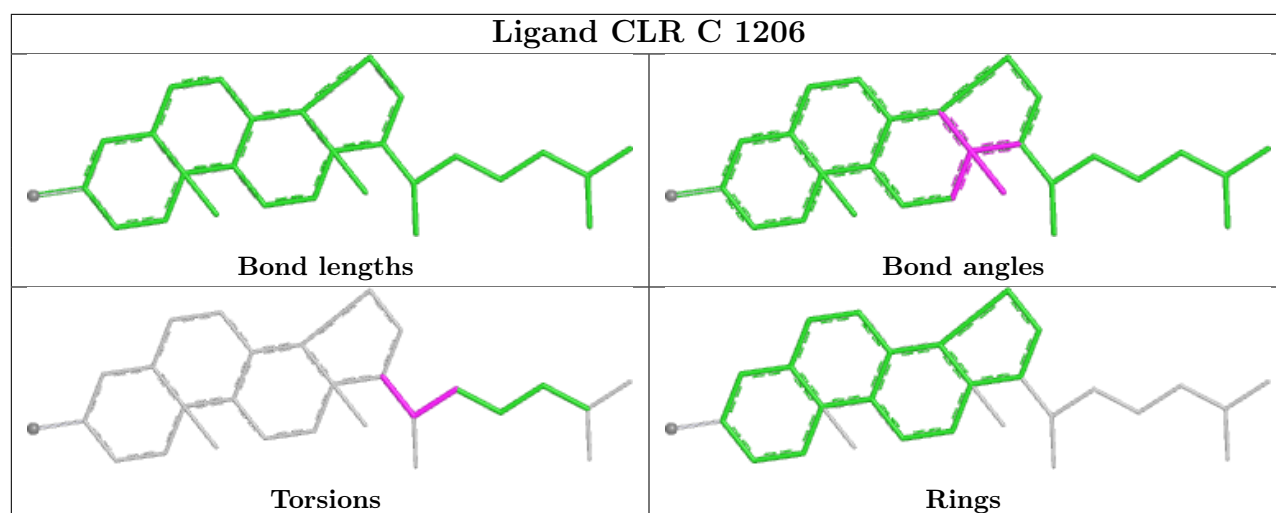


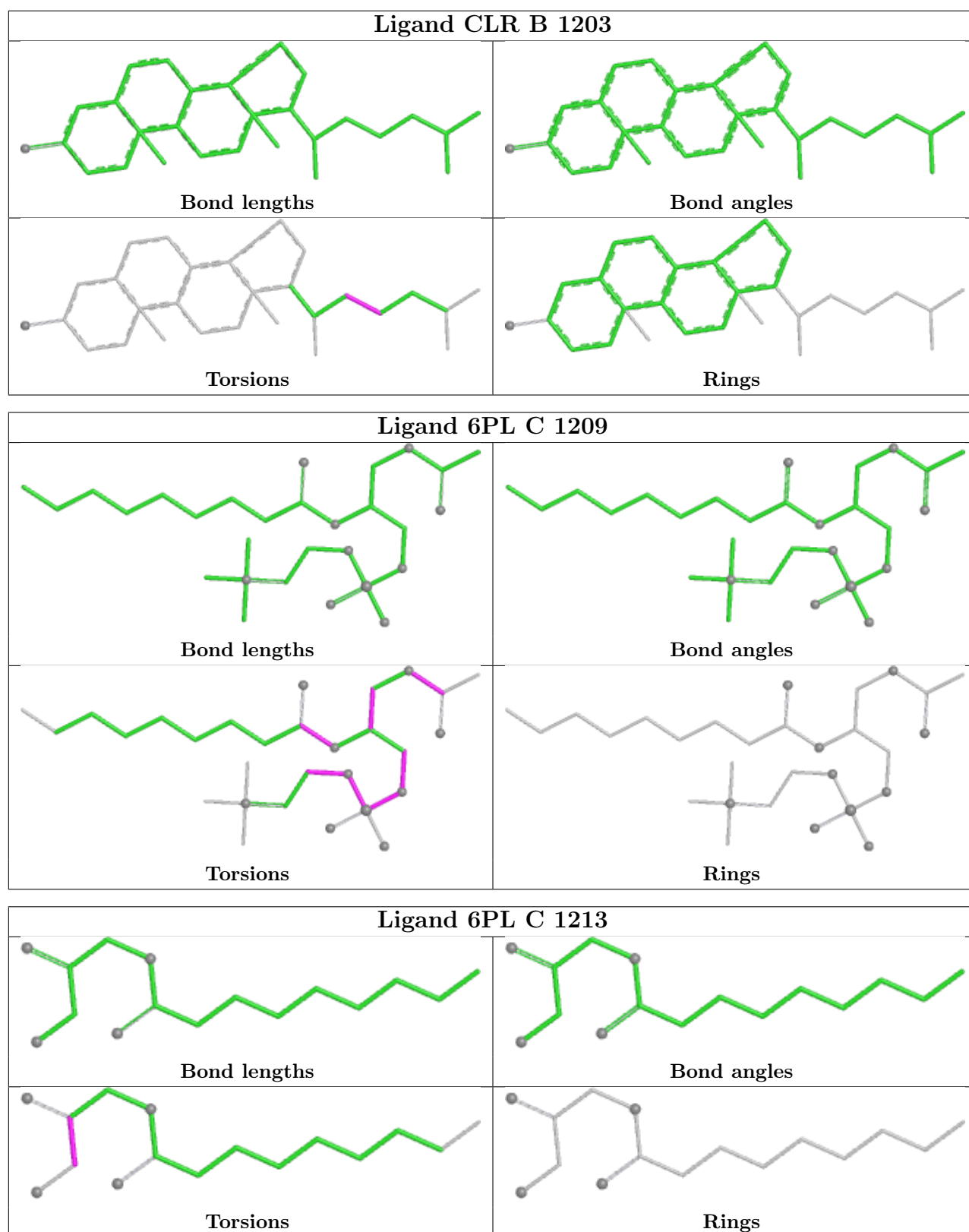


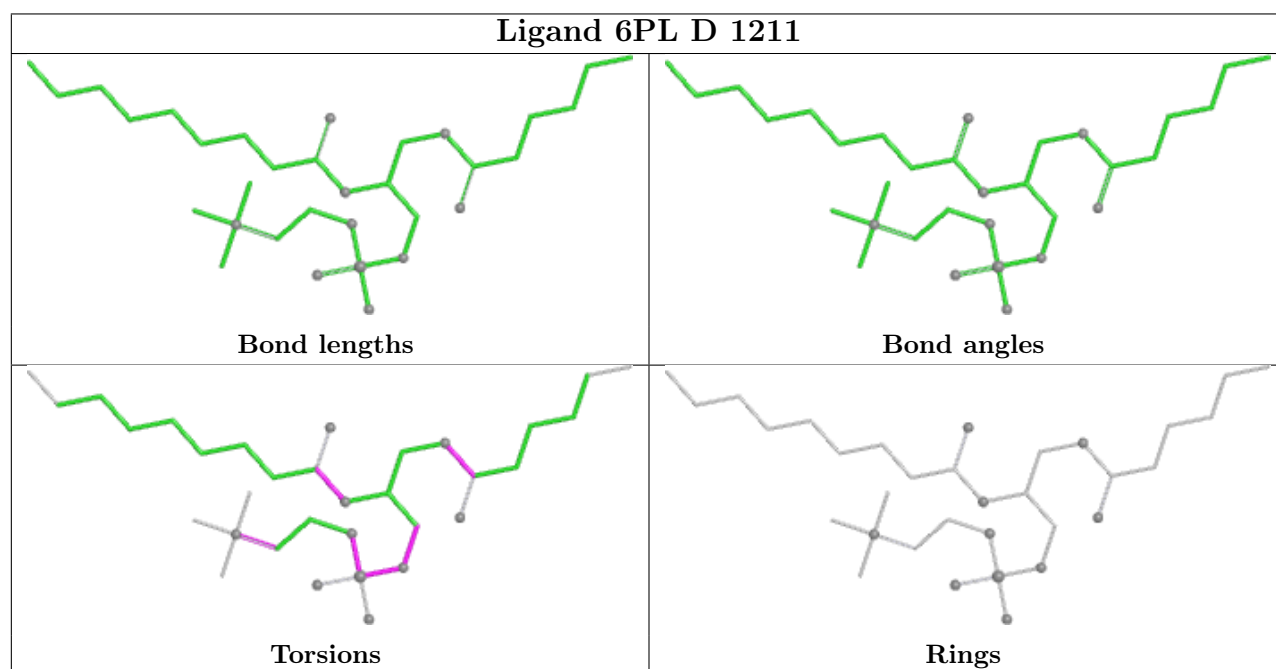
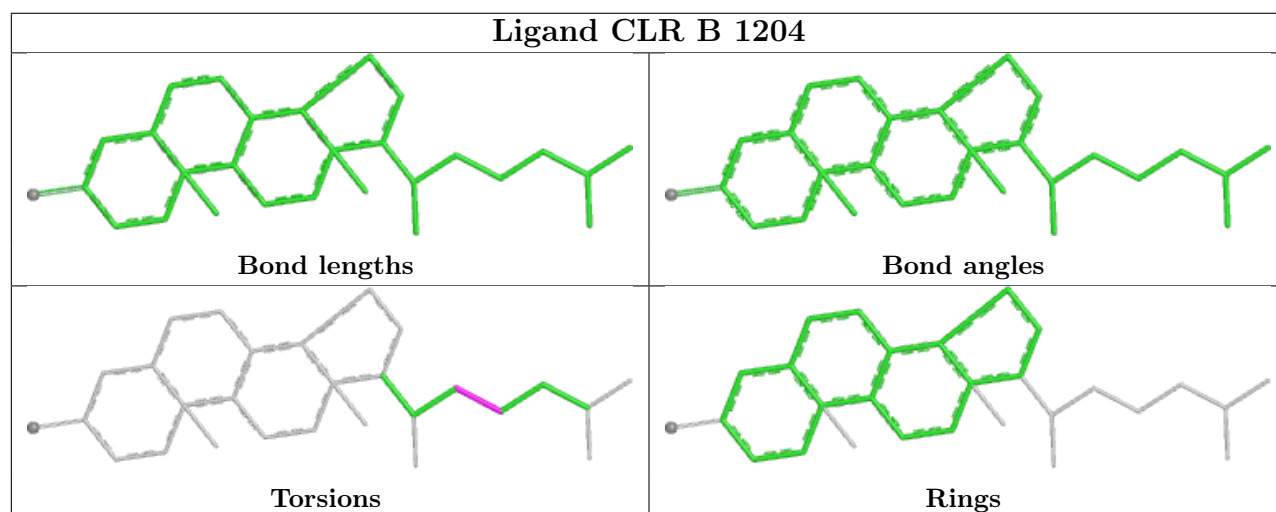
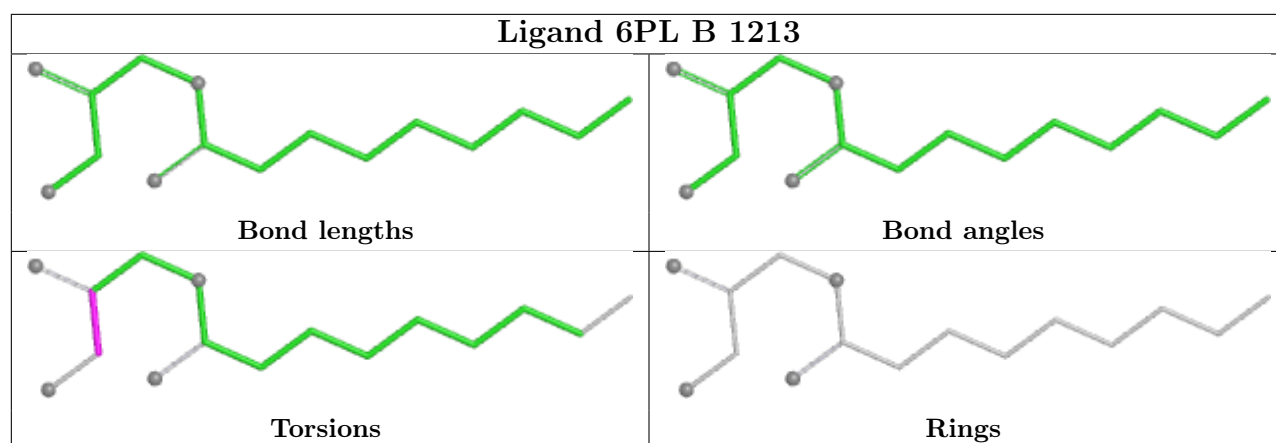


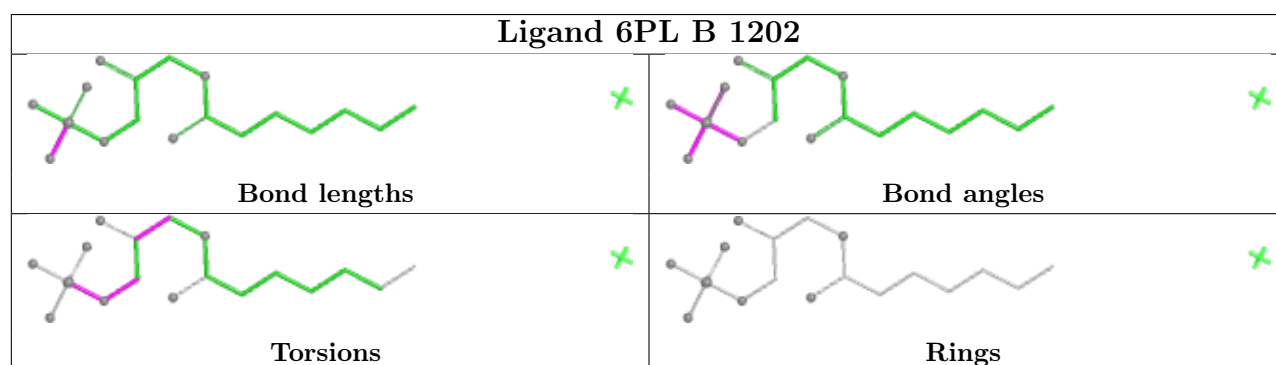
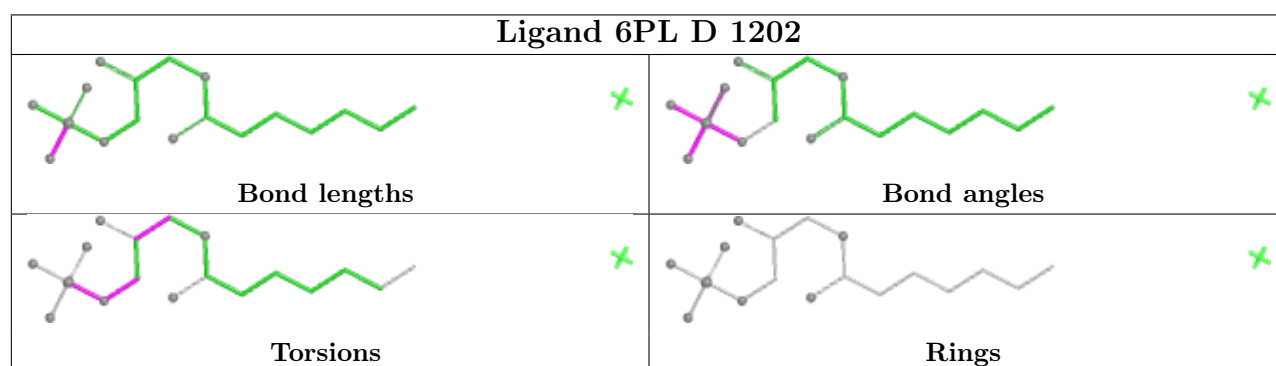
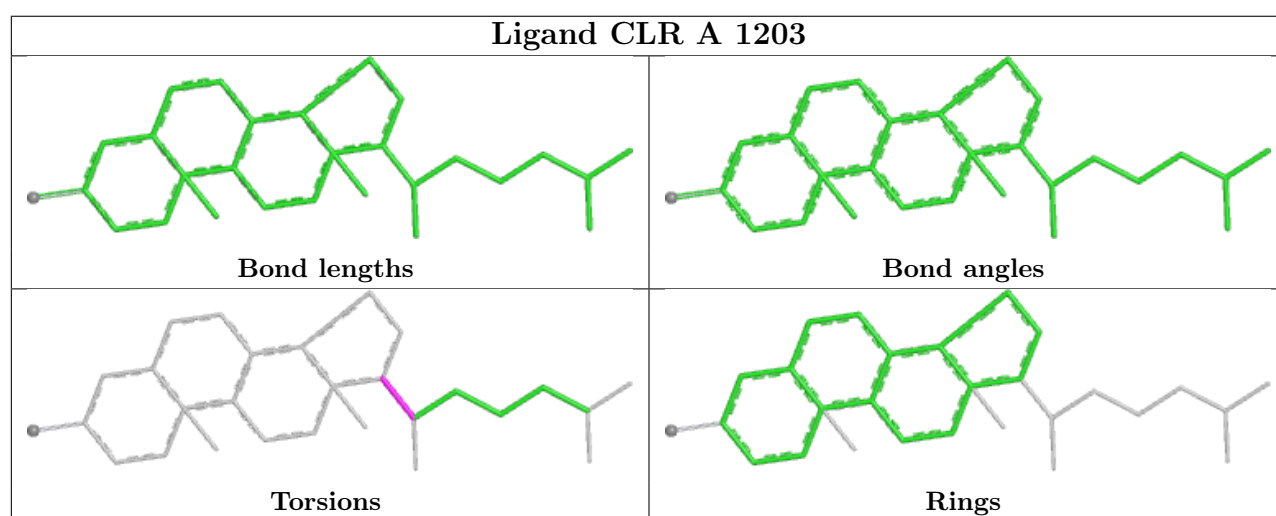
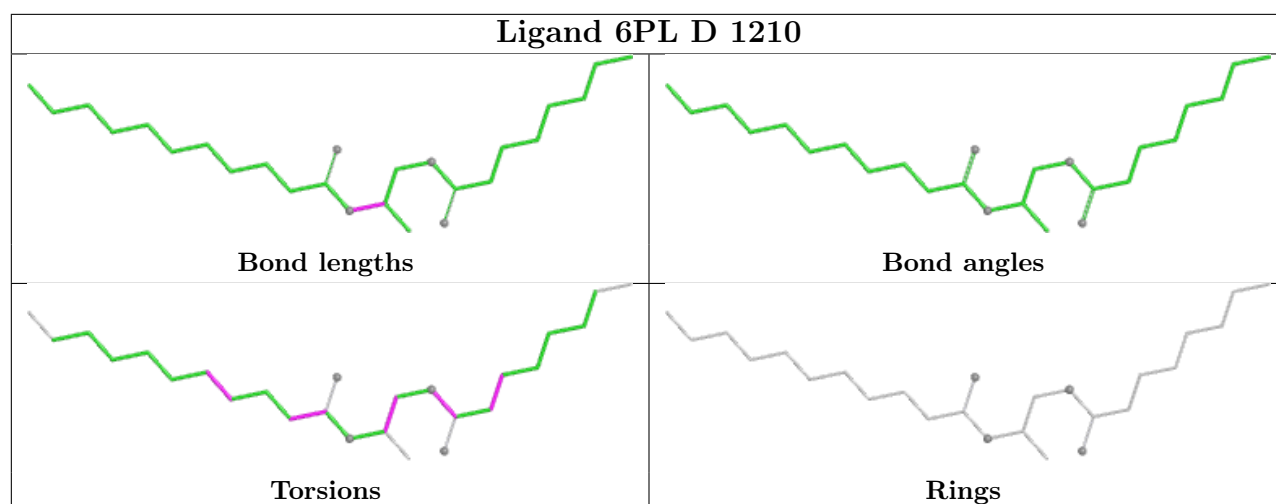
Ligand 6PL B 1214			
			
Bond lengths		Bond angles	
			
Torsions		Rings	
Ligand 6PL B 1216			
			
Bond lengths		Bond angles	
			
Torsions		Rings	
Ligand 6PL C 1214			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

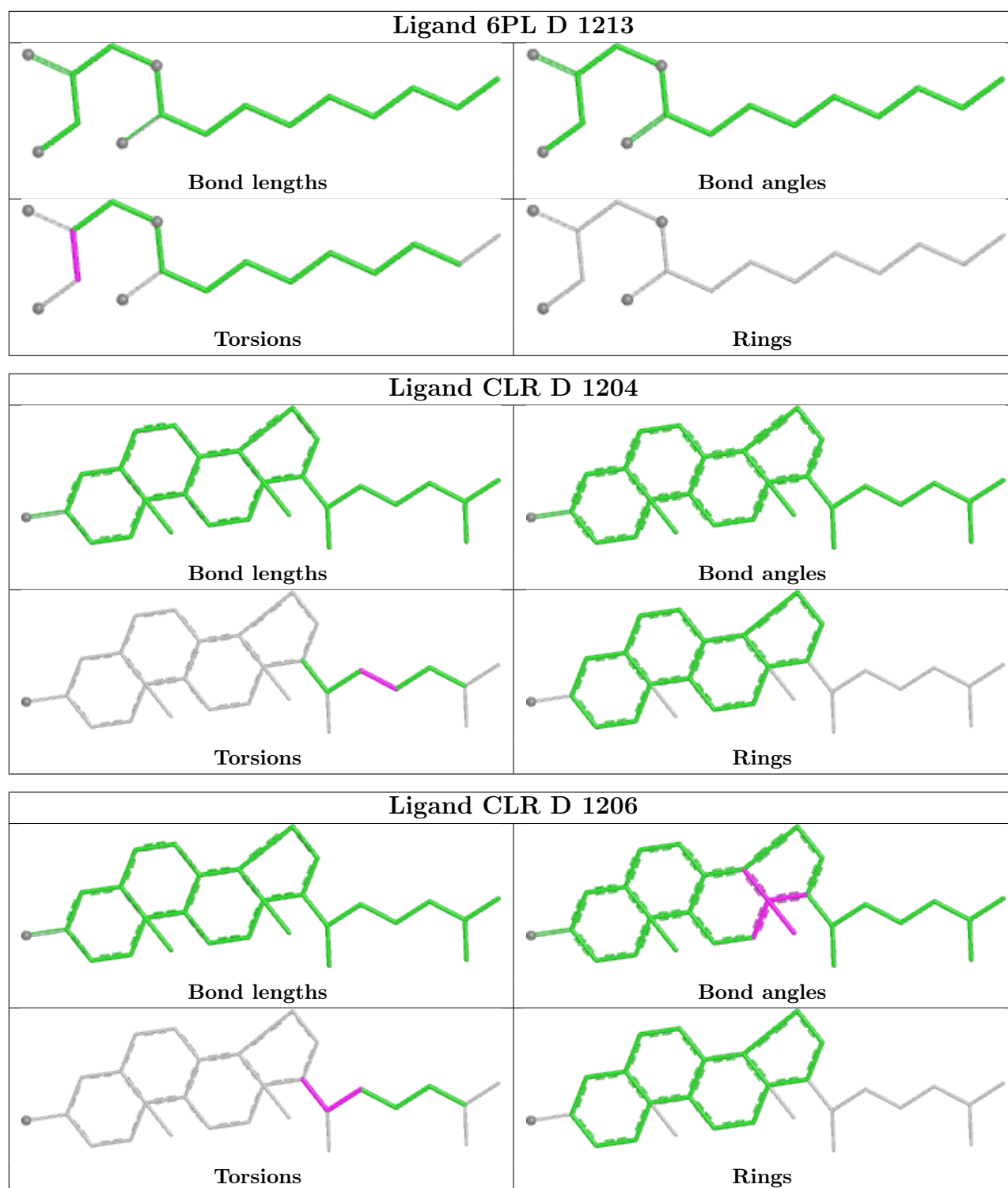












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

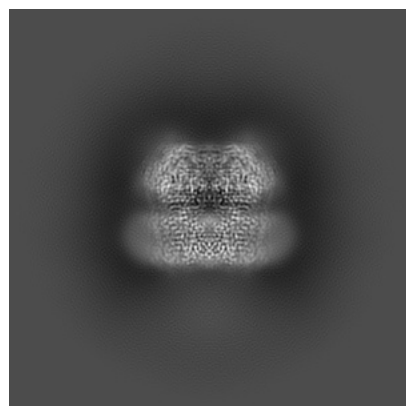
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19691. These allow visual inspection of the internal detail of the map and identification of artifacts.

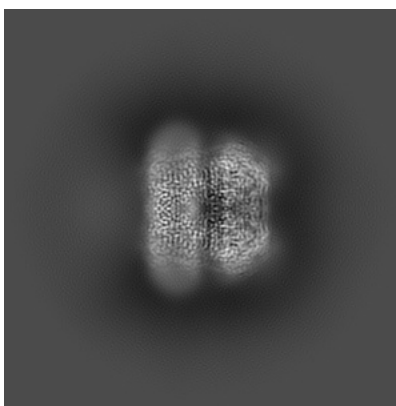
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

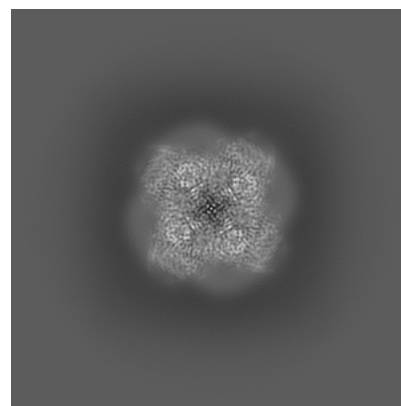
6.1.1 Primary map



X

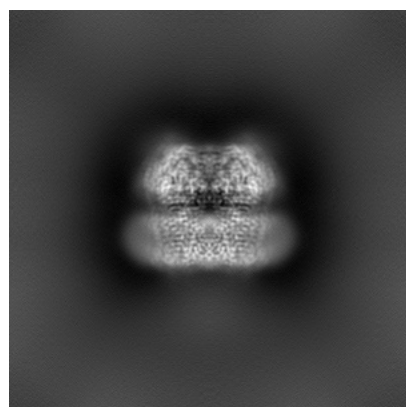


Y

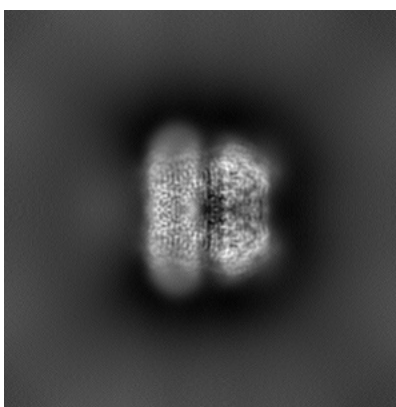


Z

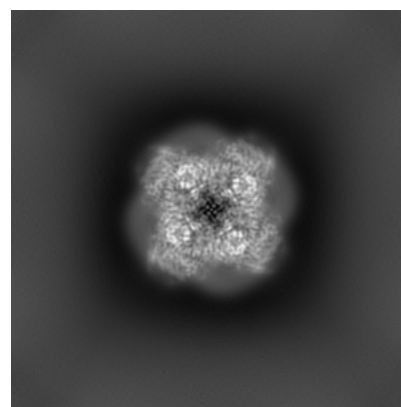
6.1.2 Raw map



X



Y



Z

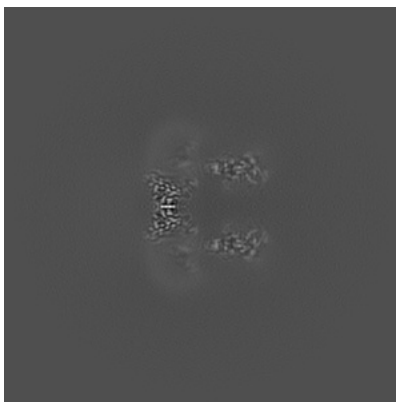
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

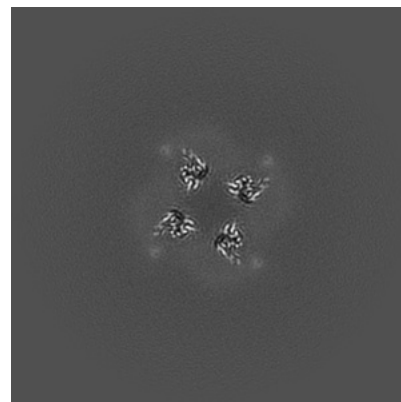
6.2.1 Primary map



X Index: 256

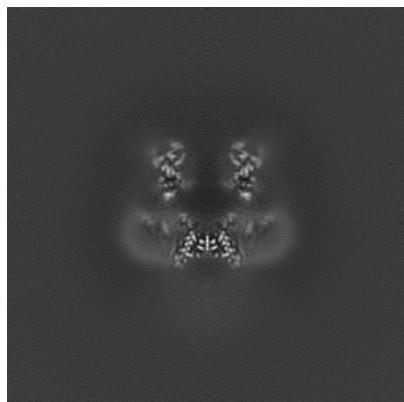


Y Index: 256

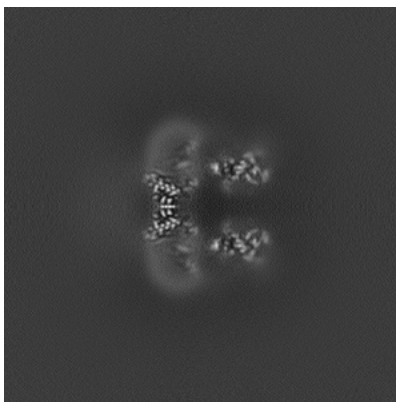


Z Index: 256

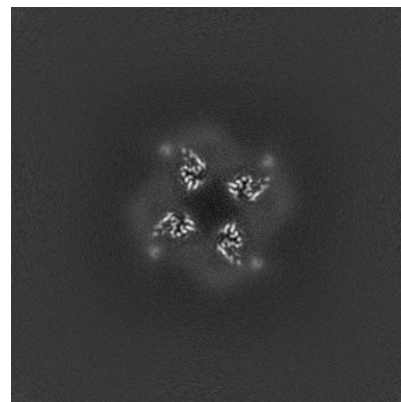
6.2.2 Raw map



X Index: 256



Y Index: 256

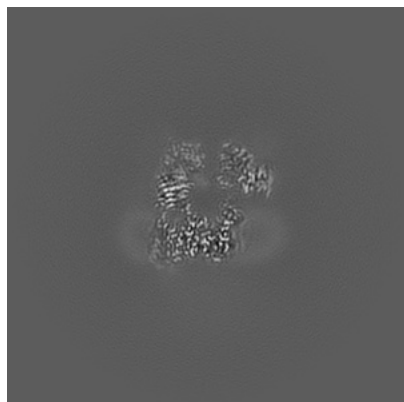


Z Index: 256

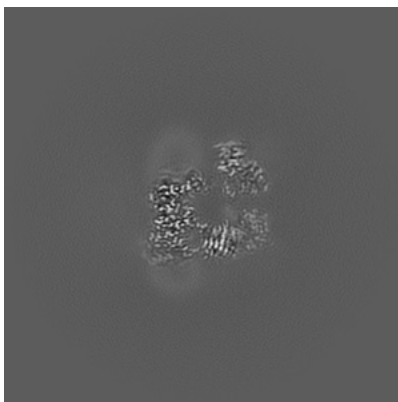
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

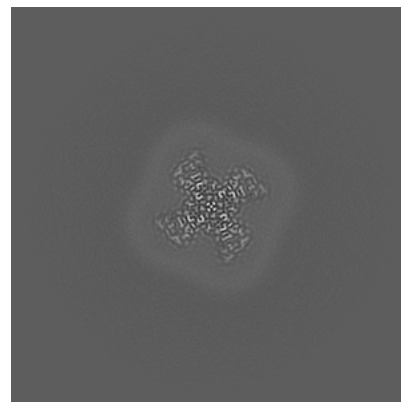
6.3.1 Primary map



X Index: 278

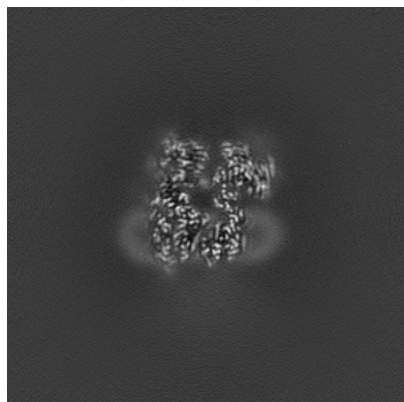


Y Index: 234

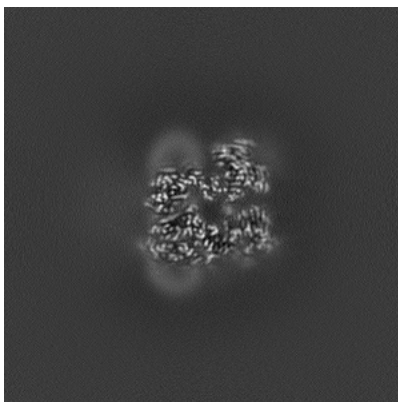


Z Index: 206

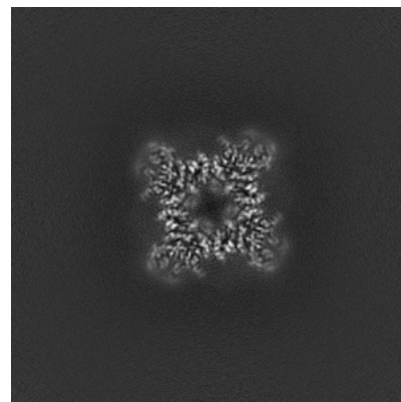
6.3.2 Raw map



X Index: 286



Y Index: 226

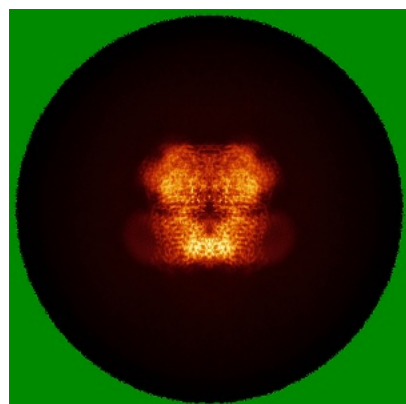


Z Index: 285

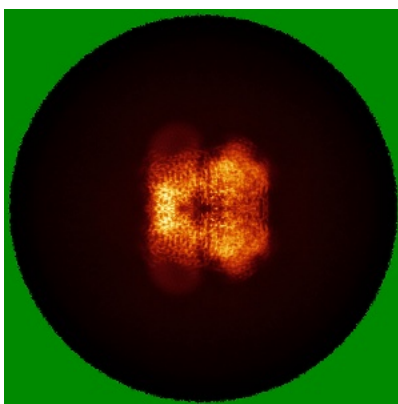
The images above show the largest variance slices of the map in three orthogonal directions.

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

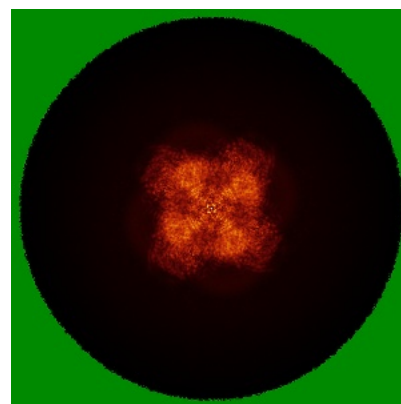
6.4.1 Primary map



X

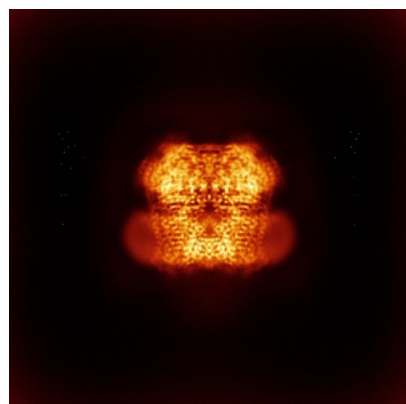


Y

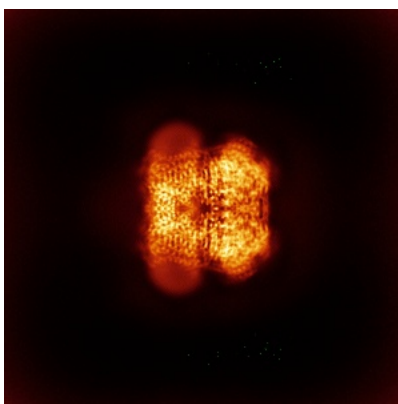


Z

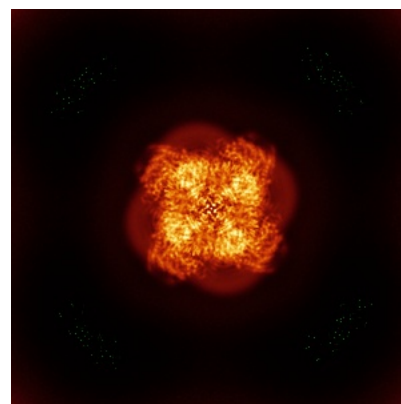
6.4.2 Raw map



X



Y

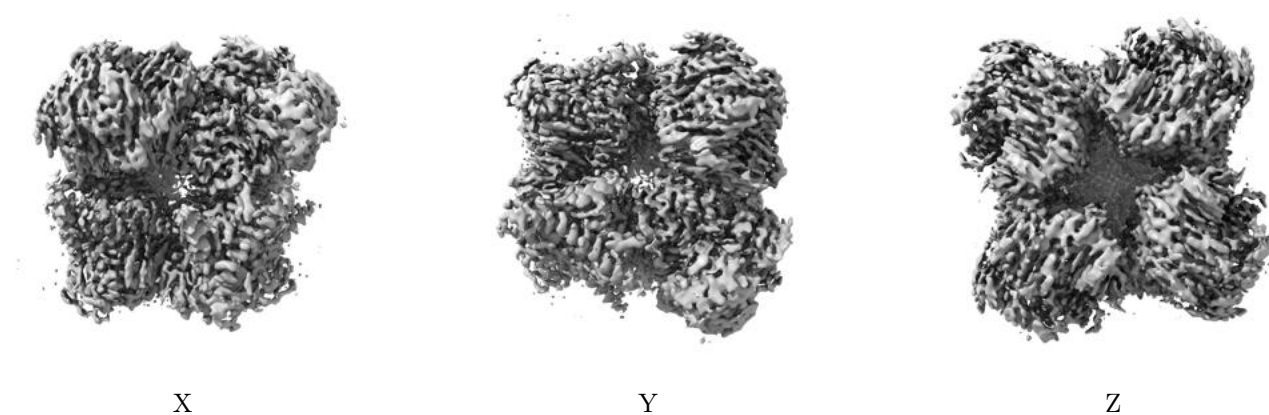


Z

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.

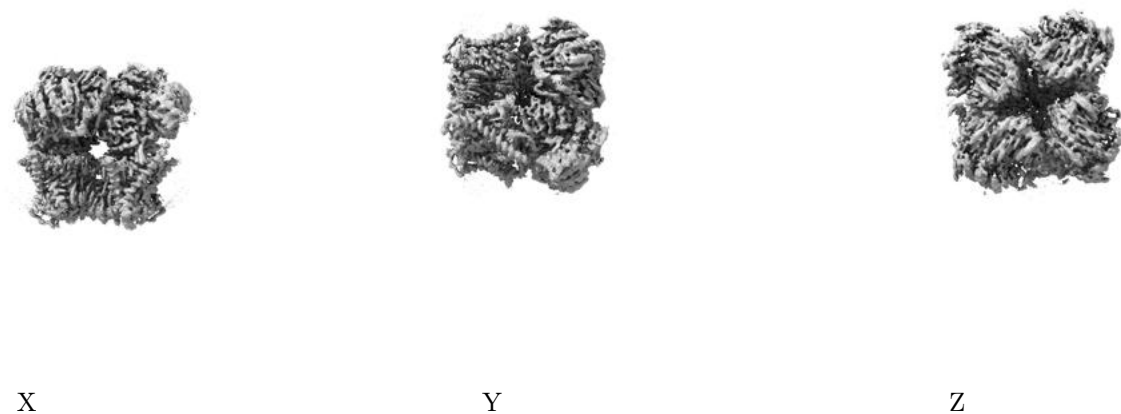
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.5. 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.

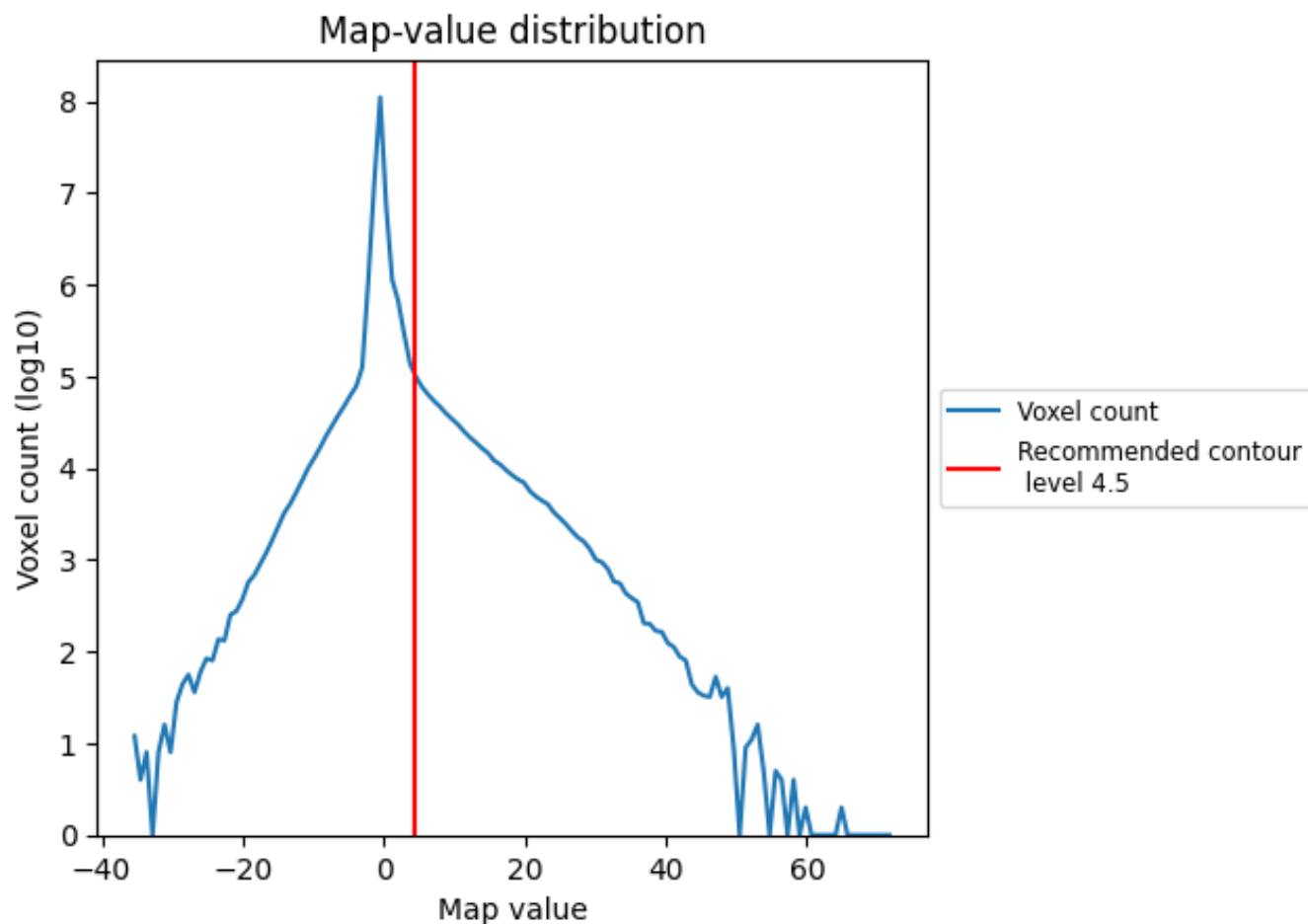
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

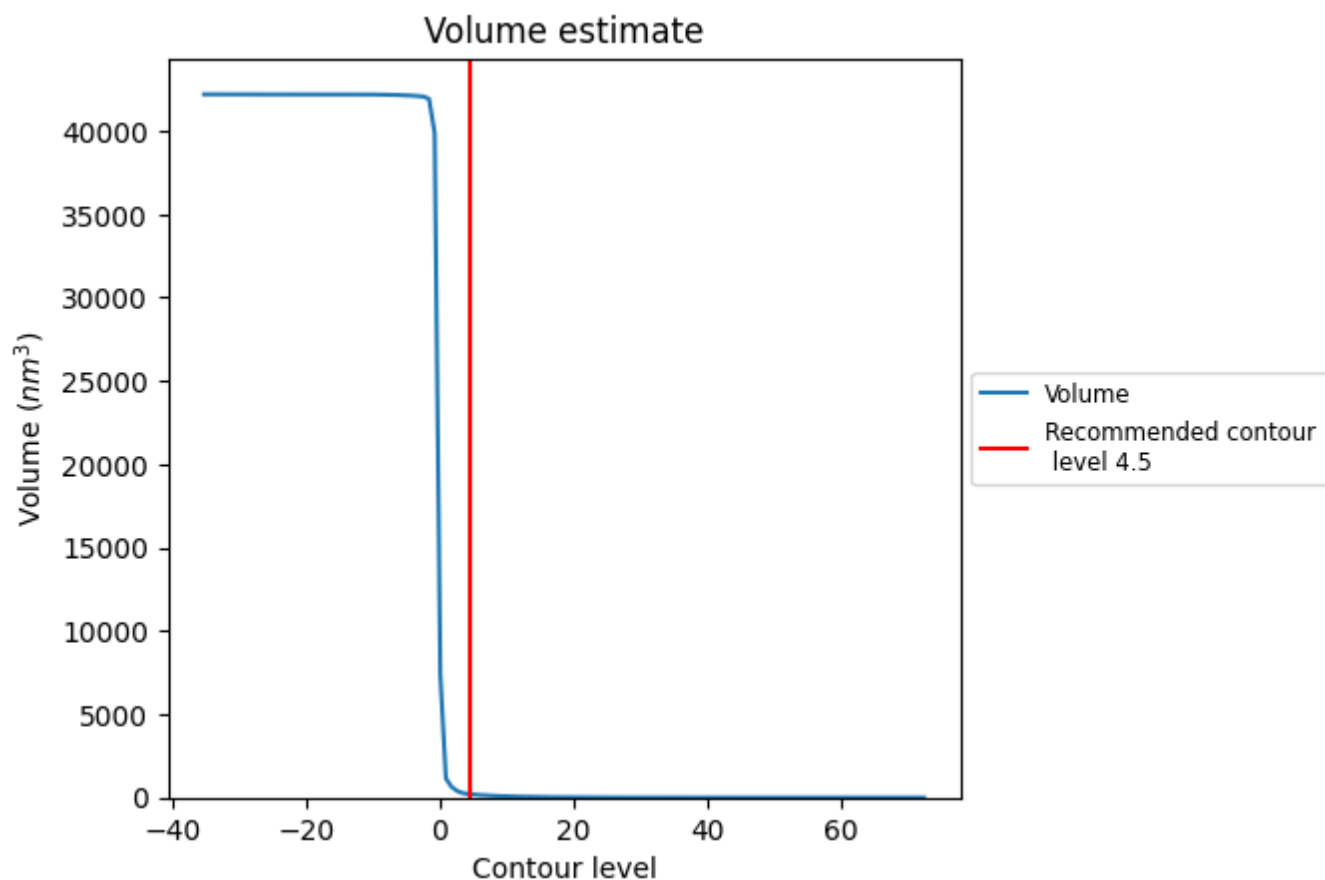
This section contains the results of statistical analysis of the map.

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.

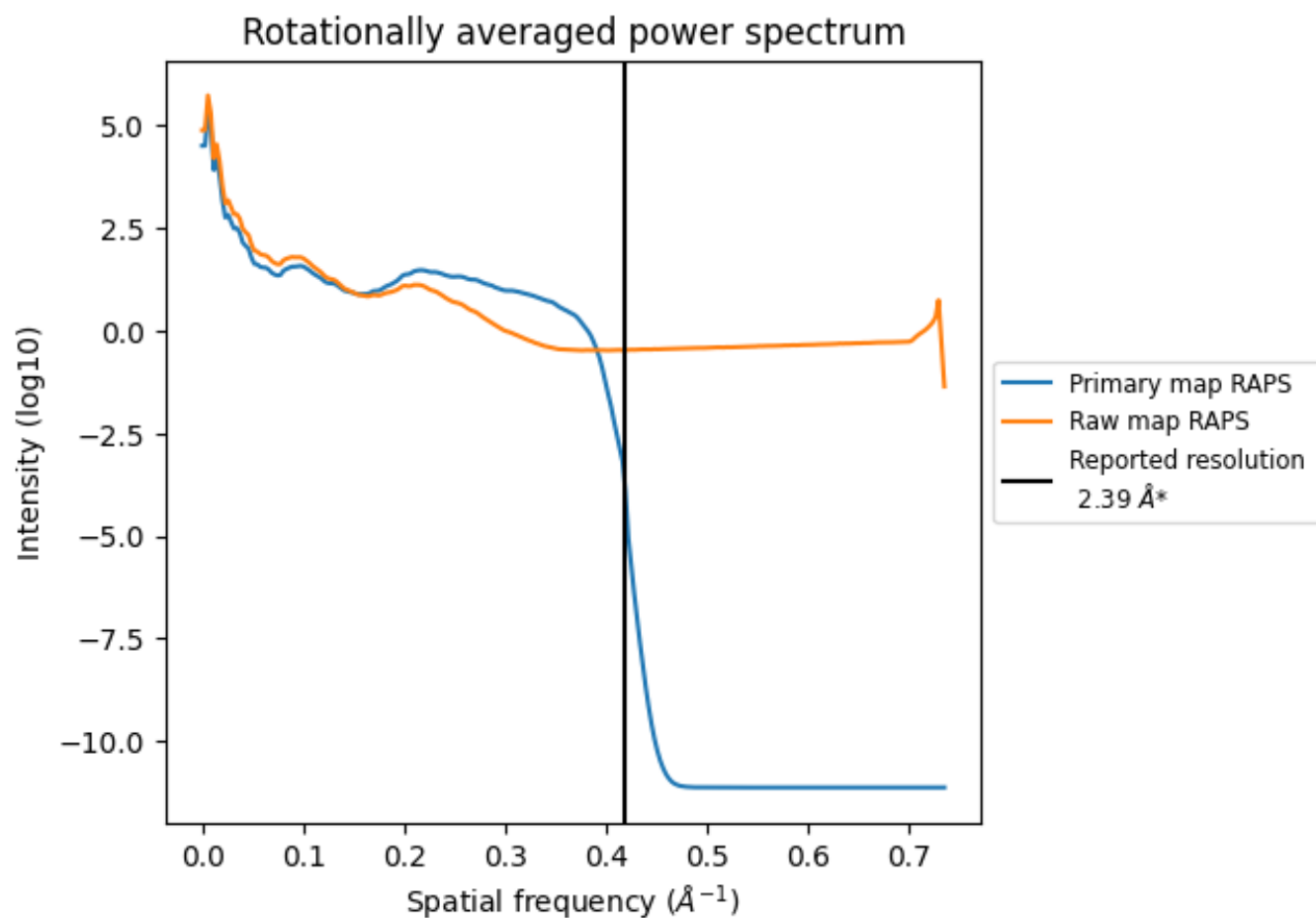
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 204 nm^3 ; this corresponds to an approximate mass of 184 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 ⓘ

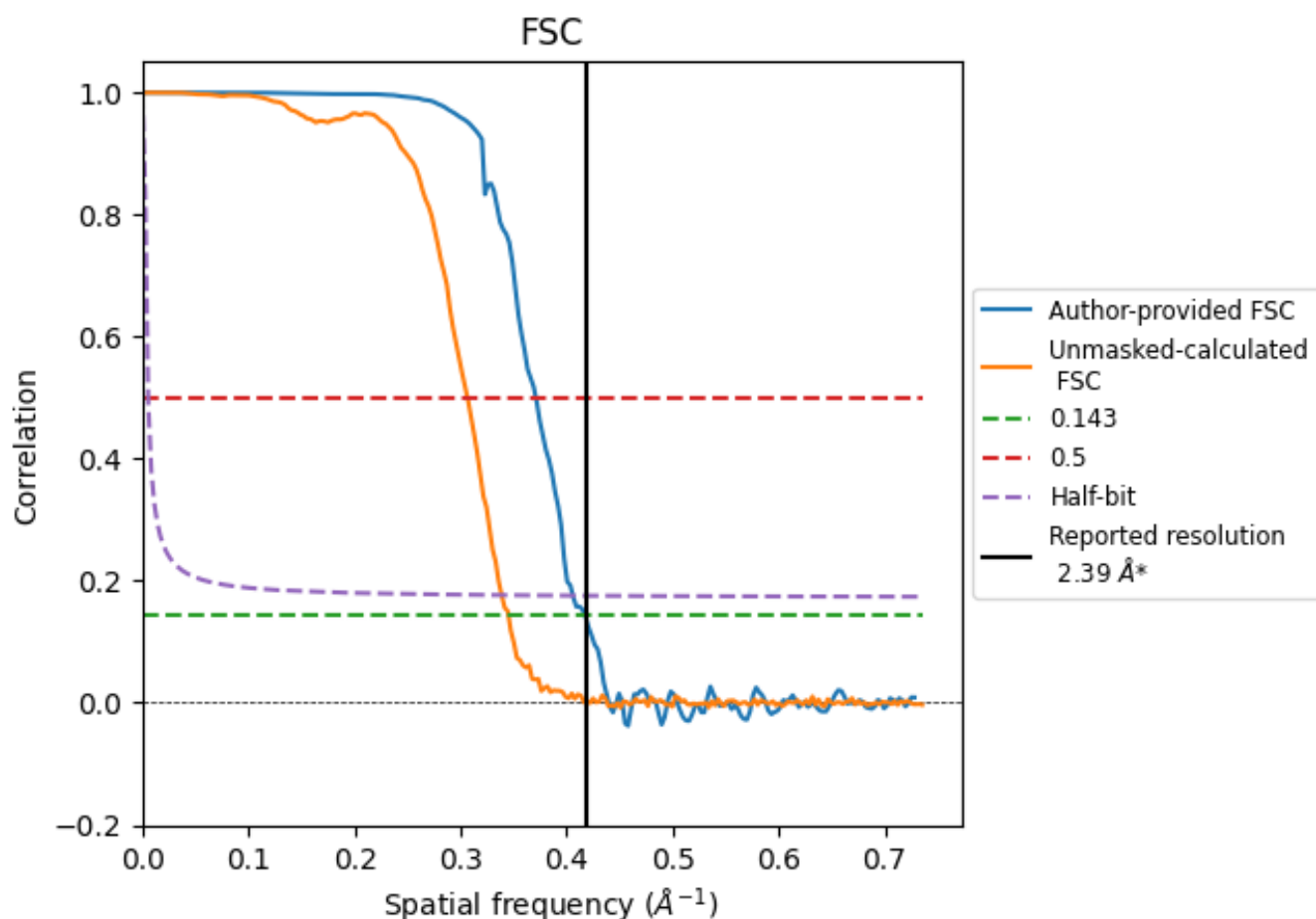


*Reported resolution corresponds to spatial frequency of 0.418 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.418 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

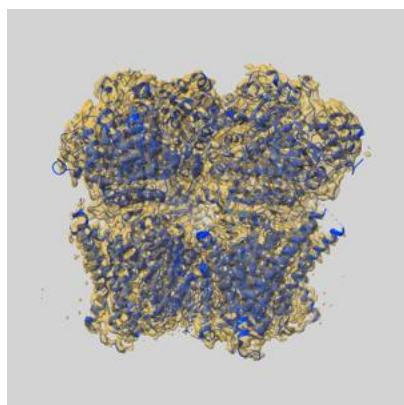
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.39	-	-
Author-provided FSC curve	2.39	2.69	2.46
Unmasked-calculated*	2.90	3.26	2.95

*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 2.90 differs from the reported value 2.39 by more than 10 %

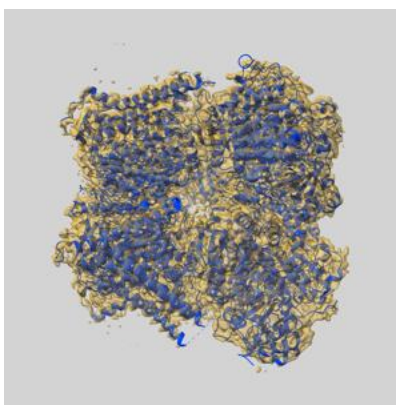
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19691 and PDB model 8S3E. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

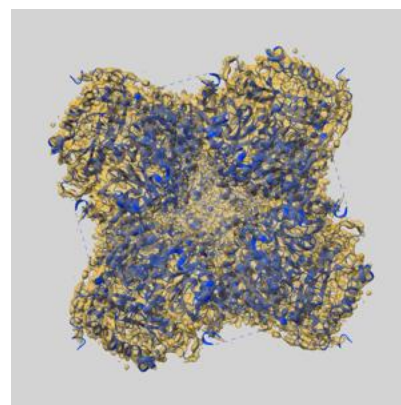
9.1 Map-model overlay [i](#)



X



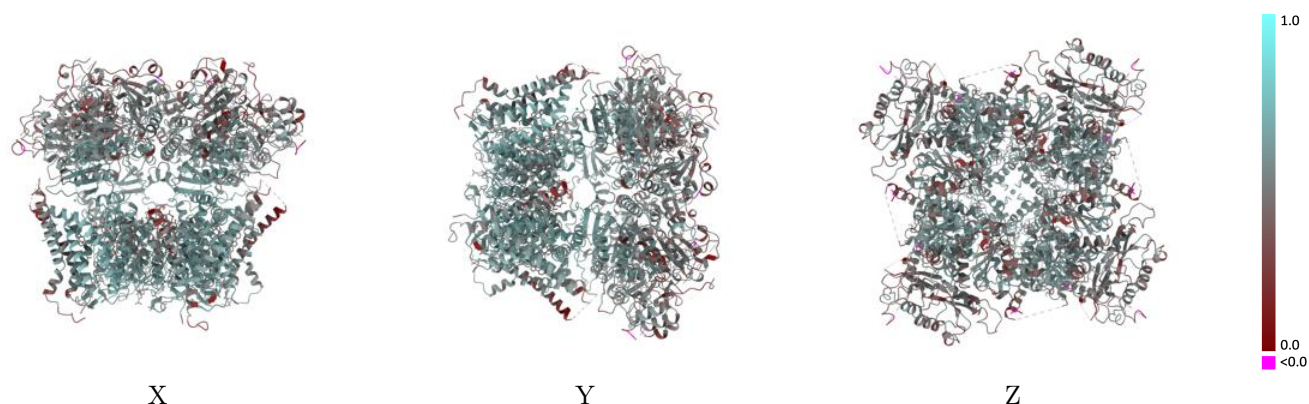
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5 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](#)

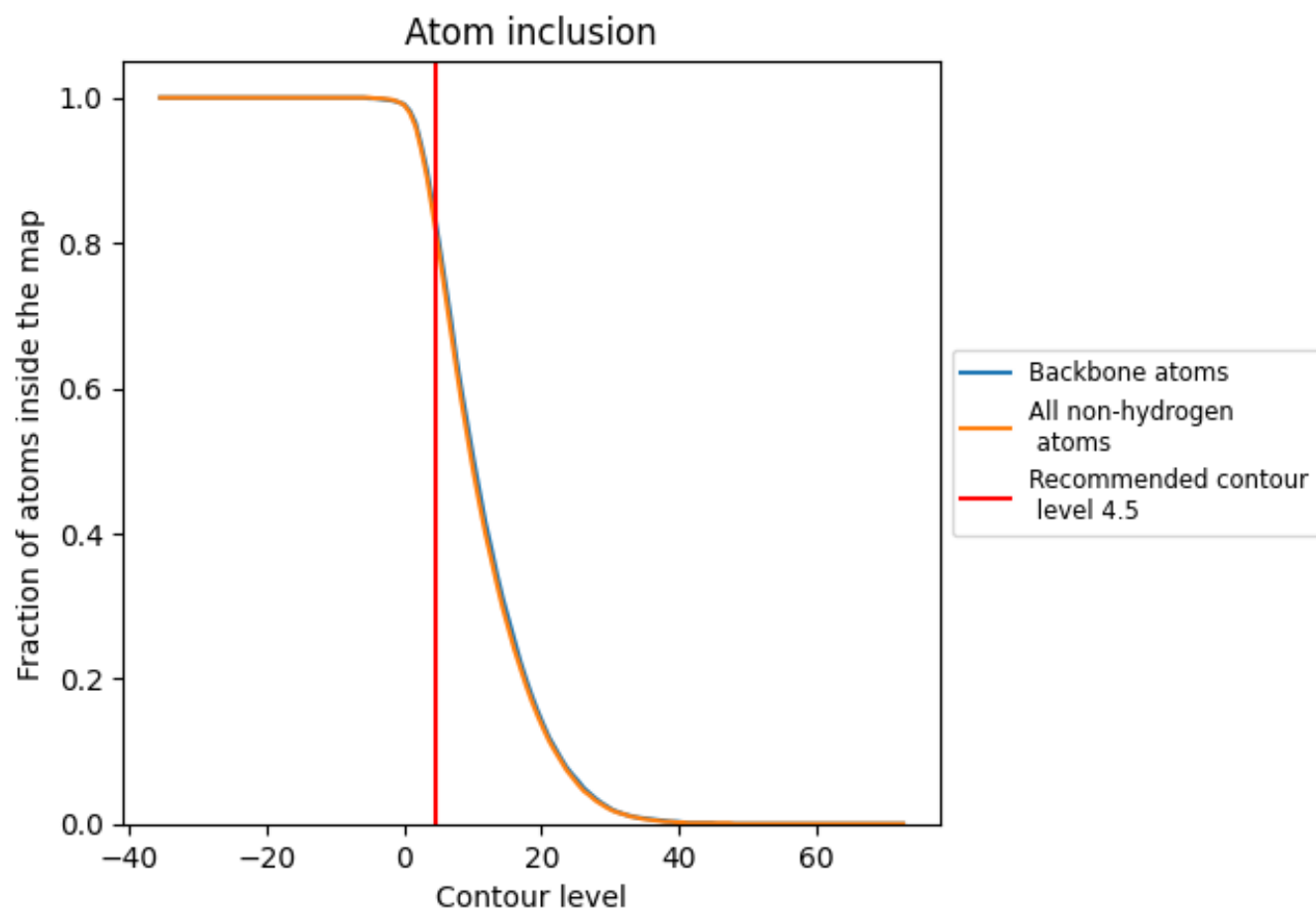


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 82% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8250	0.5210
A	0.8370	0.5250
B	0.8380	0.5220
C	0.8360	0.5220
D	0.8350	0.5230
E	0.6610	0.5040
F	0.6810	0.5060
G	0.6240	0.4500
H	0.6260	0.4590

1.0

0.0

<0.0