Full wwPDB EM Validation Report ⓘ

Feb 24, 2025 – 10:50 AM EST

PDB ID	:	9CZM
EMDB ID	:	EMD-46421
Title	:	Ca2+ bound open-inactivated hSlo1 + beta2N-beta4 channel in nanodisc.
Authors	:	Agarwal, S.; Nimigean, C.
Deposited on	:	2024-08-05
Resolution	:	2.57 Å(reported)
Based on initial model	:	6v22

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:

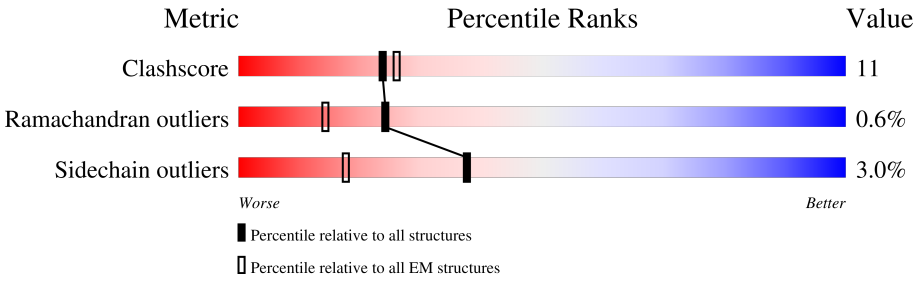
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.57 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	E	239	23% 77% 5% • 16%
1	F	239	22% 76% 7% • 16%
1	G	239	23% 79% 6% • 13%
1	H	239	23% 76% 7% • 16%
2	A	1056	• 76% 7% • 16%
2	B	1056	10% 75% 8% • 16%
2	C	1056	5% 76% 7% • 16%
2	D	1056	11% 75% 9% • 16%

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
3	POV	B	1101	-	-	X	-
3	POV	D	1113	-	-	X	-
6	CLR	B	1108	-	-	X	-
6	CLR	B	1109	-	-	X	-
6	CLR	C	1107	-	-	X	-
6	CLR	D	1109	-	-	X	-
6	CLR	D	1110	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 36052 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.

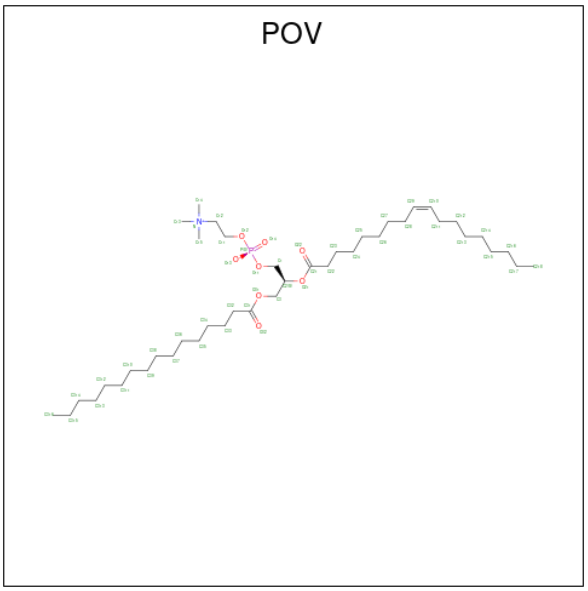
- Molecule 1 is a protein called Large-conductance Ca2+-activated K+ channel beta2 subuni t,Calcium-activated potassium channel subunit beta-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	200	Total	C	N	O	S	0	0
			1579	1010	265	291	13		
1	F	200	Total	C	N	O	S	0	0
			1579	1010	265	291	13		
1	H	200	Total	C	N	O	S	0	0
			1579	1010	265	291	13		
1	G	207	Total	C	N	O	S	0	0
			1640	1051	276	300	13		

- Molecule 2 is a protein called Isoform 5 of Calcium-activated potassium channel subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	890	Total	C	N	O	S	0	0
			7087	4602	1157	1281	47		
2	B	890	Total	C	N	O	S	0	0
			7087	4602	1157	1281	47		
2	C	890	Total	C	N	O	S	0	0
			7087	4602	1157	1281	47		
2	D	890	Total	C	N	O	S	0	0
			7087	4602	1157	1281	47		

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C O 37 33 4	0
3	A	1	Total C O P 31 22 8 1	0
3	A	1	Total C N O P 36 26 1 8 1	0
3	A	1	Total C N O P 24 16 1 6 1	0
3	A	1	Total C N O P 35 25 1 8 1	0
3	A	1	Total C N O P 32 22 1 8 1	0
3	A	1	Total C N O P 40 30 1 8 1	0
3	B	1	Total C O 37 33 4	0
3	B	1	Total C O P 31 22 8 1	0
3	B	1	Total C N O P 36 26 1 8 1	0
3	B	1	Total C N O P 24 16 1 6 1	0
3	B	1	Total C O P 39 30 8 1	0
3	B	1	Total C N O P 35 25 1 8 1	0
3	B	1	Total C N O P 32 22 1 8 1	0

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Mol	Chain	Residues	Atoms	AltConf
3	B	1	Total C N O P 40 30 1 8 1	0
3	B	1	Total C O P 36 27 8 1	0
3	C	1	Total C O P 31 22 8 1	0
3	C	1	Total C N O P 36 26 1 8 1	0
3	C	1	Total C N O P 24 16 1 6 1	0
3	C	1	Total C N O P 35 25 1 8 1	0
3	C	1	Total C N O P 32 22 1 8 1	0
3	C	1	Total C N O P 40 30 1 8 1	0
3	C	1	Total C O P 37 28 8 1	0
3	C	1	Total C O 37 33 4	0
3	D	1	Total C O 37 33 4	0
3	D	1	Total C O P 39 30 8 1	0
3	D	1	Total C O P 31 22 8 1	0
3	D	1	Total C N O P 36 26 1 8 1	0
3	D	1	Total C N O P 24 16 1 6 1	0
3	D	1	Total C N O P 35 25 1 8 1	0
3	D	1	Total C N O P 32 22 1 8 1	0
3	D	1	Total C N O P 36 26 1 8 1	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Mg 1 1	0

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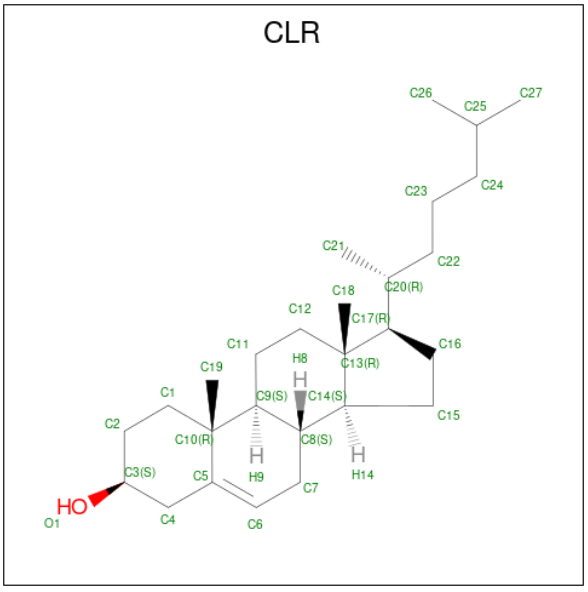
Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Mg 1 1	0
4	C	1	Total Mg 1 1	0
4	D	1	Total Mg 1 1	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



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

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

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

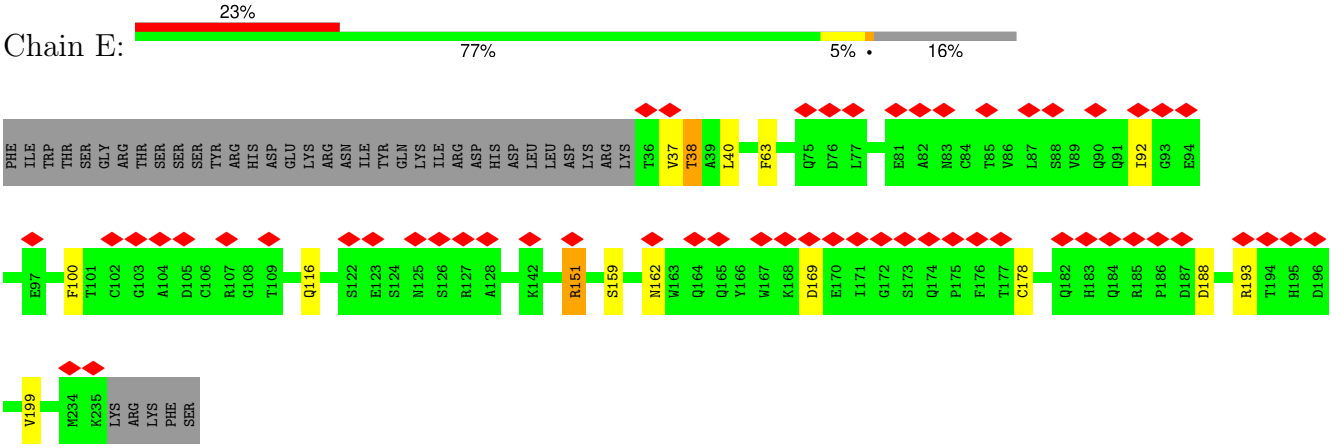
Mol	Chain	Residues	Atoms	AltConf
7	A	4	Total K 4 4	0

3 Residue-property plots (i)

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.

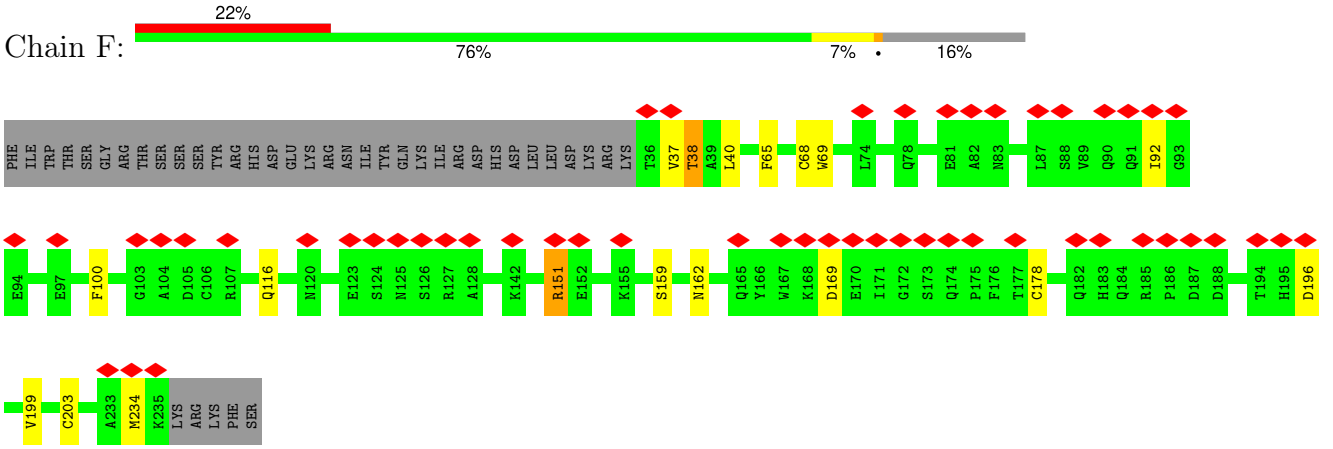
• Molecule 1: Large-conductance Ca2+-activated K+ channel beta2 subunit,Calcium-activated potassium channel subunit beta-4

Chain E:



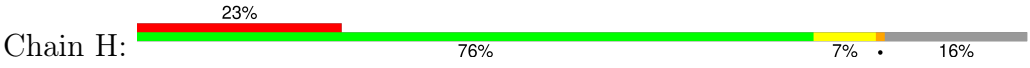
• Molecule 1: Large-conductance Ca2+-activated K+ channel beta2 subunit,Calcium-activated potassium channel subunit beta-4

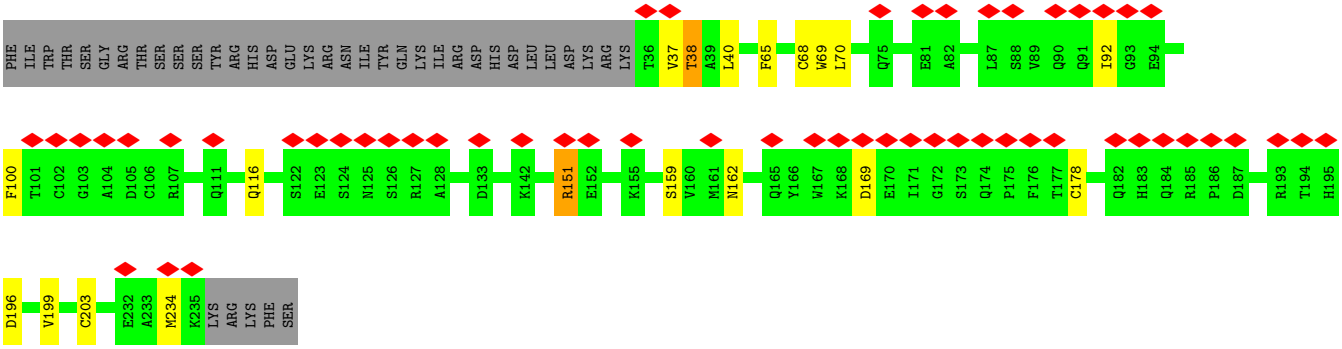
Chain F:



• Molecule 1: Large-conductance Ca2+-activated K+ channel beta2 subunit,Calcium-activated potassium channel subunit beta-4

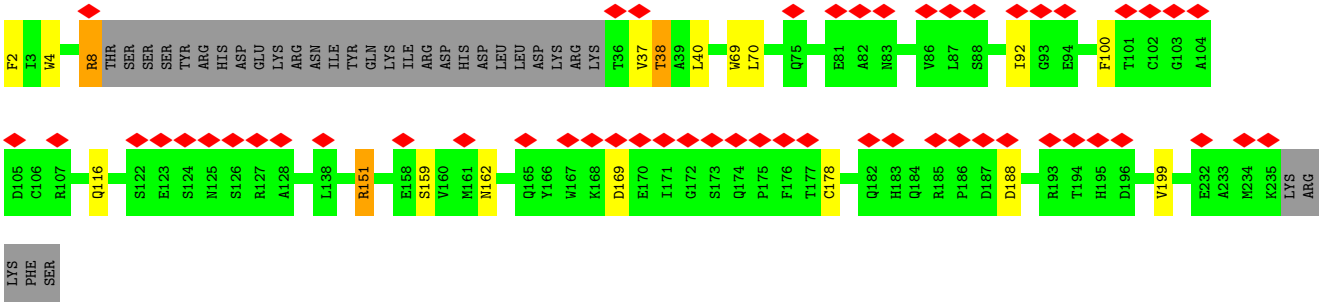
Chain H:





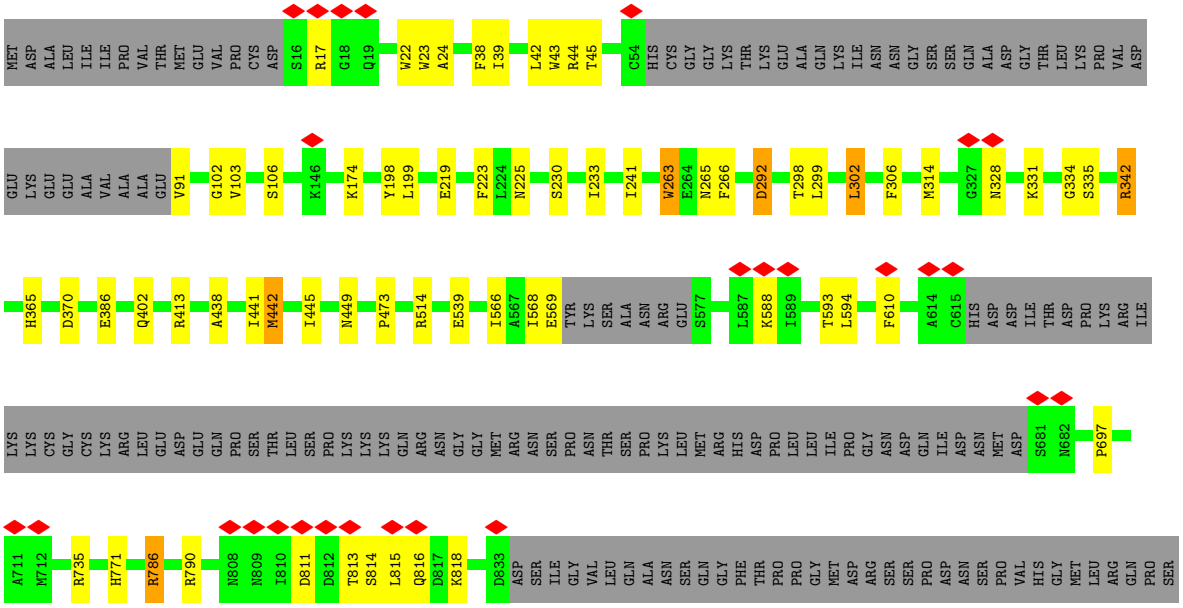
• Molecule 1: Large-conductance Ca2+-activated K+ channel beta2 subunit,Calcium-activated potassium channel subunit beta-4

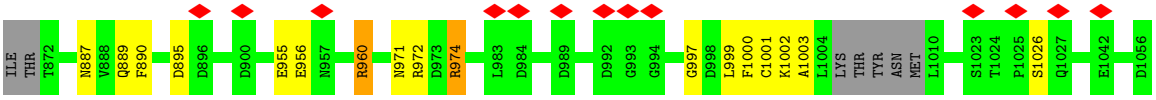
Chain G:



• Molecule 2: Isoform 5 of Calcium-activated potassium channel subunit alpha-1

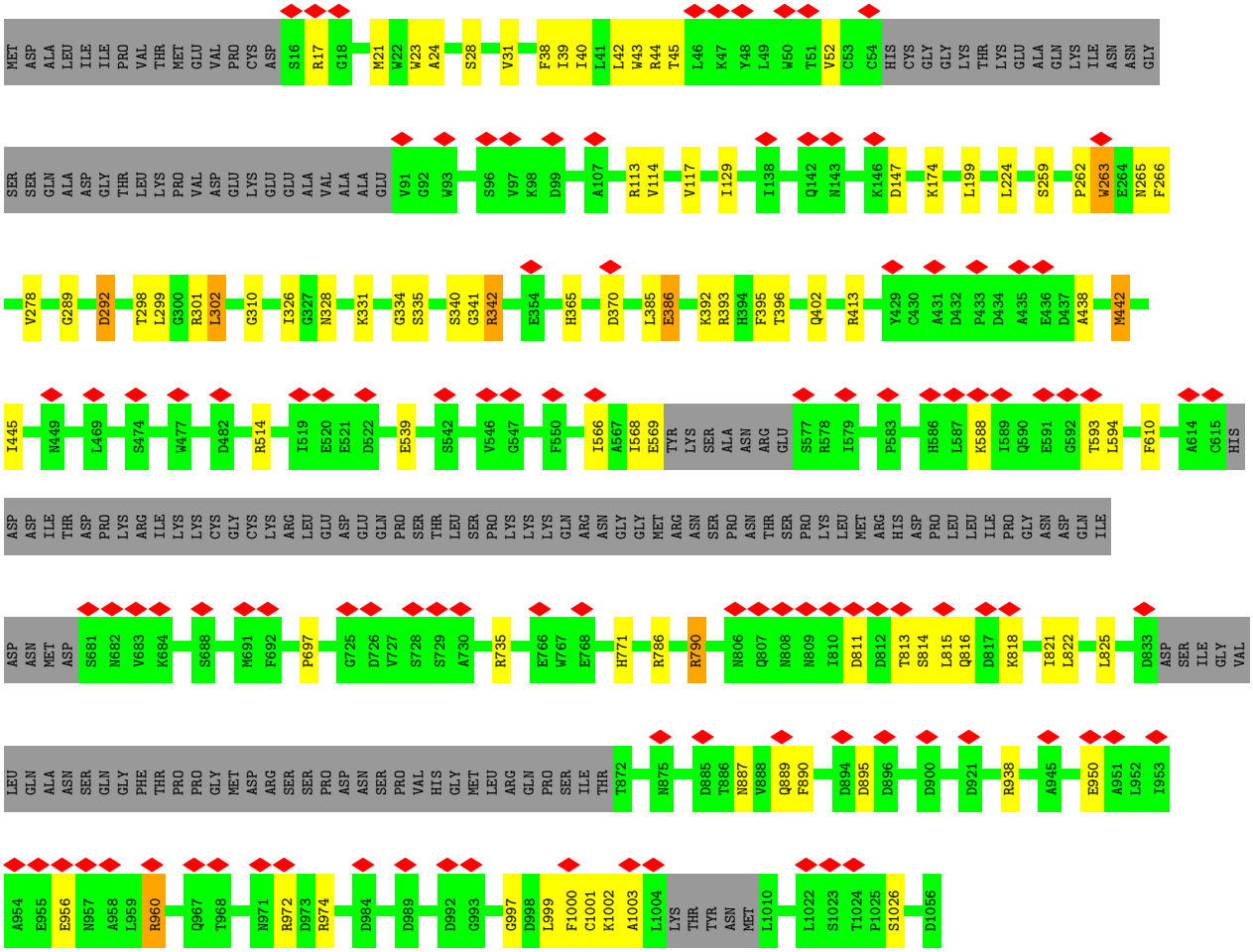
Chain A:





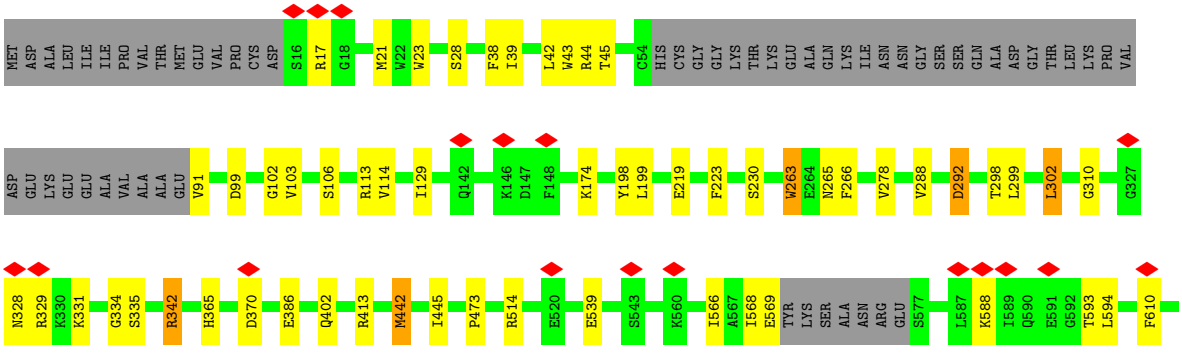
• Molecule 2: Isoform 5 of Calcium-activated potassium channel subunit alpha-1

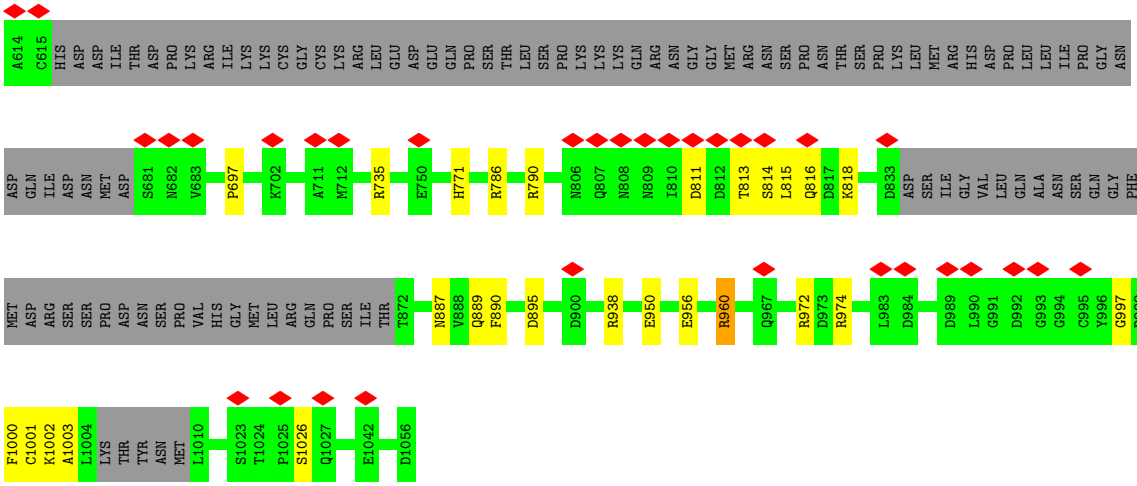
Chain B:



• Molecule 2: Isoform 5 of Calcium-activated potassium channel subunit alpha-1

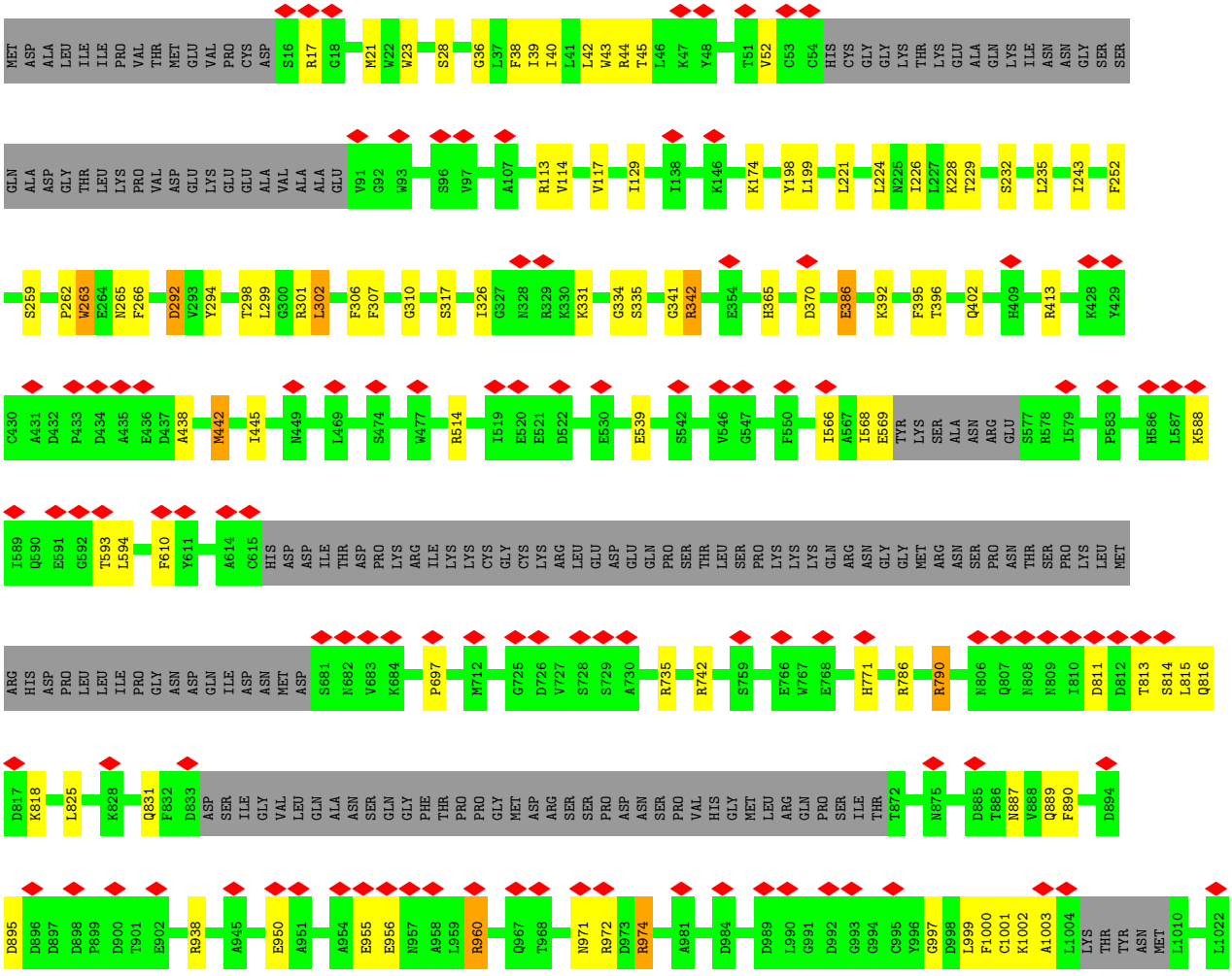
Chain C:





• Molecule 2: Isoform 5 of Calcium-activated potassium channel subunit alpha-1

Chain D:




S1023
S1026
Q1027
Y1039
F1055
D1056

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	175971	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48.45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.061	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0126	Depositor
Map size (Å)	247.5, 247.5, 247.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CA, POV, CLR, K

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	E	0.62	0/1615	0.88	0/2198
1	F	0.62	0/1615	0.88	0/2198
1	G	0.63	0/1678	0.90	0/2282
1	H	0.62	0/1615	0.88	0/2198
2	A	0.61	0/7250	0.89	1/9838 (0.0%)
2	B	0.61	0/7250	0.90	1/9838 (0.0%)
2	C	0.61	0/7250	0.90	1/9838 (0.0%)
2	D	0.61	0/7250	0.90	1/9838 (0.0%)
All	All	0.61	0/35523	0.89	4/48228 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	972	ARG	NE-CZ-NH2	5.45	123.03	120.30
2	C	972	ARG	NE-CZ-NH2	5.40	123.00	120.30
2	A	972	ARG	NE-CZ-NH2	5.33	122.97	120.30
2	B	972	ARG	NE-CZ-NH2	5.30	122.95	120.30

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	E	1579	0	1558	15	0
1	F	1579	0	1558	42	0
1	G	1640	0	1615	20	0
1	H	1579	0	1558	38	0
2	A	7087	0	7080	117	0
2	B	7087	0	7081	205	0
2	C	7087	0	7080	119	0
2	D	7087	0	7081	213	0
3	A	235	0	296	31	0
3	B	310	0	391	65	0
3	C	272	0	341	32	0
3	D	270	0	337	84	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	56	0	92	31	0
6	B	56	0	90	63	0
6	C	56	0	92	45	0
6	D	56	0	92	73	0
7	A	4	0	0	0	0
All	All	36052	0	36342	771	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 11.

All (771) 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)
2:B:39:ILE:CG2	6:B:1108:CLR:C21	1.78	1.53
1:F:69:TRP:CZ2	2:B:263:TRP:HA	1.46	1.50
2:D:39:ILE:HG22	6:D:1109:CLR:C21	1.40	1.47
2:B:39:ILE:HG22	6:B:1108:CLR:C21	0.94	1.41
2:A:442:MET:SD	2:B:818:LYS:HD3	1.64	1.37
1:H:69:TRP:CZ2	2:D:263:TRP:HA	1.59	1.36
2:B:266:PHE:CZ	3:B:1101:POV:H28A	1.59	1.34
2:D:39:ILE:CG2	6:D:1109:CLR:H211	1.61	1.29
2:D:44:ARG:NE	6:D:1109:CLR:H11	1.50	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:442:MET:SD	2:D:818:LYS:HD3	1.75	1.26
2:B:266:PHE:HZ	3:B:1101:POV:C28	1.50	1.25
1:F:234:MET:SD	2:B:52:VAL:HG13	1.78	1.23
2:D:266:PHE:CZ	3:D:1101:POV:H28A	1.76	1.20
2:B:44:ARG:HH11	6:B:1108:CLR:C19	1.54	1.19
2:B:815:LEU:HA	2:B:818:LYS:HZ1	1.00	1.16
2:B:44:ARG:NE	6:B:1108:CLR:H11	1.60	1.15
2:A:815:LEU:HA	2:A:818:LYS:HZ2	1.06	1.14
2:D:23:TRP:CH2	6:D:1110:CLR:H72	1.81	1.14
2:A:473:PRO:HD3	2:B:825:LEU:HB3	1.29	1.13
2:B:113:ARG:HD3	3:B:1105:POV:O21	1.44	1.13
2:D:113:ARG:HD3	3:D:1106:POV:C21	1.78	1.12
2:A:815:LEU:HA	2:A:818:LYS:NZ	1.64	1.11
2:D:36:GLY:HA2	6:D:1109:CLR:H272	1.29	1.11
2:D:815:LEU:HA	2:D:818:LYS:NZ	1.64	1.11
2:A:442:MET:SD	2:B:818:LYS:CD	2.38	1.10
2:D:44:ARG:HE	6:D:1109:CLR:C1	1.64	1.10
2:B:815:LEU:HA	2:B:818:LYS:NZ	1.64	1.10
2:A:473:PRO:HD2	2:B:825:LEU:HD13	1.27	1.09
2:A:328:ASN:HB2	3:A:1115:POV:C15	1.83	1.08
2:C:815:LEU:HA	2:C:818:LYS:NZ	1.65	1.08
2:D:266:PHE:HZ	3:D:1101:POV:C28	1.65	1.08
2:C:815:LEU:HA	2:C:818:LYS:HZ1	1.05	1.08
3:D:1113:POV:H34	3:D:1113:POV:H25	1.09	1.07
2:B:44:ARG:HH11	6:B:1108:CLR:H192	1.07	1.07
1:F:69:TRP:CE2	2:B:263:TRP:HB3	1.89	1.06
2:D:229:THR:H	3:D:1113:POV:H12A	1.18	1.06
2:D:815:LEU:HA	2:D:818:LYS:HZ2	1.09	1.06
2:B:39:ILE:HG22	6:B:1108:CLR:H212	1.08	1.06
2:C:199:LEU:HD21	6:C:1108:CLR:C19	1.85	1.06
2:D:39:ILE:CG2	6:D:1109:CLR:C21	2.23	1.06
2:D:229:THR:H	3:D:1113:POV:C12	1.69	1.06
2:B:44:ARG:HE	6:B:1108:CLR:C1	1.69	1.05
3:B:1105:POV:H3A	3:B:1105:POV:H23A	1.38	1.05
2:A:442:MET:SD	2:B:818:LYS:HG2	1.98	1.04
1:H:234:MET:SD	2:D:52:VAL:HG13	1.97	1.04
1:F:69:TRP:CZ2	2:B:263:TRP:CA	2.41	1.03
2:B:113:ARG:HD3	3:B:1105:POV:C21	1.87	1.03
6:C:1108:CLR:H211	6:C:1108:CLR:H242	1.38	1.03
2:D:199:LEU:HD21	6:D:1110:CLR:C19	1.88	1.02
2:B:40:ILE:HG13	6:B:1108:CLR:H232	1.42	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1109:CLR:H212	6:B:1109:CLR:H183	1.41	1.01
2:D:226:ILE:HD11	3:D:1106:POV:H32	1.40	1.01
2:D:23:TRP:CZ3	6:D:1110:CLR:H72	1.97	1.00
3:D:1113:POV:H25	3:D:1113:POV:C34	1.92	0.99
2:D:266:PHE:HZ	3:D:1101:POV:H28A	0.83	0.99
6:A:1109:CLR:H183	6:A:1109:CLR:H212	1.43	0.98
2:B:44:ARG:NH1	6:B:1108:CLR:H22	1.79	0.98
2:C:174:LYS:CG	6:C:1107:CLR:H191	1.94	0.98
1:F:69:TRP:CE2	2:B:263:TRP:HA	2.00	0.97
2:A:39:ILE:HG22	6:A:1108:CLR:C21	1.94	0.97
2:A:473:PRO:CD	2:B:825:LEU:HD13	1.95	0.97
2:C:174:LYS:HG2	6:C:1107:CLR:H191	1.44	0.97
2:A:442:MET:SD	2:B:818:LYS:CG	2.54	0.96
2:D:229:THR:H	3:D:1113:POV:C11	1.78	0.96
3:D:1113:POV:H34	3:D:1113:POV:C25	1.96	0.95
2:A:328:ASN:HB2	3:A:1115:POV:H15B	1.45	0.95
1:H:69:TRP:CE2	2:D:263:TRP:HB3	2.01	0.95
2:B:266:PHE:CE1	3:B:1101:POV:H35	2.02	0.95
2:D:44:ARG:NH1	6:D:1109:CLR:H22	1.81	0.95
1:F:203:CYS:SG	2:B:262:PRO:HB2	2.05	0.94
2:A:174:LYS:HG3	6:A:1108:CLR:H182	1.47	0.94
2:B:815:LEU:CA	2:B:818:LYS:HZ1	1.80	0.94
1:F:69:TRP:CD2	2:B:263:TRP:HB3	2.03	0.94
2:B:40:ILE:HG12	6:B:1108:CLR:H183	1.50	0.94
2:C:198:TYR:HE2	6:C:1108:CLR:H11	1.32	0.94
2:B:328:ASN:HB2	3:B:1112:POV:H15	1.50	0.93
2:C:199:LEU:HD21	6:C:1108:CLR:H192	1.48	0.93
2:C:815:LEU:CA	2:C:818:LYS:HZ1	1.82	0.93
1:F:69:TRP:CH2	2:B:263:TRP:HA	2.04	0.92
6:D:1110:CLR:H183	6:D:1110:CLR:H212	1.51	0.92
6:C:1107:CLR:H242	6:C:1107:CLR:H211	1.51	0.92
2:D:235:LEU:HD23	3:D:1113:POV:H23A	1.49	0.92
2:D:228:LYS:HB2	3:D:1113:POV:H11	1.52	0.92
2:B:44:ARG:NH1	6:B:1108:CLR:H192	1.83	0.92
2:C:442:MET:SD	2:D:818:LYS:CD	2.58	0.91
2:D:44:ARG:HE	6:D:1109:CLR:H11	0.76	0.91
3:D:1112:POV:P	3:D:1112:POV:H14B	2.10	0.91
2:A:473:PRO:HD2	2:B:825:LEU:CD1	1.99	0.91
2:A:815:LEU:CA	2:A:818:LYS:HZ2	1.83	0.91
2:B:266:PHE:CZ	3:B:1101:POV:C28	2.33	0.91
2:D:199:LEU:HD21	6:D:1110:CLR:H192	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:266:PHE:CE1	3:D:1101:POV:H35	2.07	0.90
2:D:815:LEU:CA	2:D:818:LYS:HZ2	1.84	0.90
2:B:328:ASN:HB2	3:B:1112:POV:C15	2.01	0.89
3:B:1105:POV:H23A	3:B:1105:POV:C3	2.01	0.89
2:D:226:ILE:CD1	3:D:1106:POV:H32	2.02	0.89
1:H:69:TRP:CH2	2:D:263:TRP:HA	2.08	0.88
2:B:44:ARG:HE	6:B:1108:CLR:H11	0.79	0.88
2:D:23:TRP:CH2	6:D:1110:CLR:C7	2.57	0.88
2:B:299:LEU:CD1	3:B:1101:POV:H31C	2.02	0.88
2:D:229:THR:N	3:D:1113:POV:H12A	1.87	0.88
2:B:44:ARG:NH1	6:B:1108:CLR:C19	2.35	0.88
6:A:1108:CLR:H3	6:A:1108:CLR:H193	1.53	0.88
2:C:473:PRO:HD2	2:D:825:LEU:HD13	1.56	0.88
2:D:44:ARG:HH11	6:D:1109:CLR:C19	1.87	0.88
1:H:69:TRP:CD2	2:D:263:TRP:HB3	2.10	0.87
1:H:69:TRP:CZ2	2:D:263:TRP:CA	2.54	0.86
1:F:92:ILE:HG22	1:F:116:GLN:OE1	1.76	0.86
2:C:334:GLY:O	2:C:413:ARG:NH2	2.09	0.86
2:B:39:ILE:HG21	6:B:1108:CLR:C21	2.04	0.86
2:D:28:SER:HA	6:D:1110:CLR:H232	1.55	0.86
2:A:334:GLY:O	2:A:413:ARG:NH2	2.09	0.85
1:F:68:CYS:HB3	2:B:263:TRP:CE3	2.11	0.85
1:H:69:TRP:CE2	2:D:263:TRP:HA	2.11	0.85
2:C:23:TRP:CH2	6:C:1108:CLR:H72	2.12	0.84
2:D:334:GLY:O	2:D:413:ARG:NH2	2.09	0.84
2:B:334:GLY:O	2:B:413:ARG:NH2	2.09	0.84
6:C:1107:CLR:H181	6:C:1107:CLR:H222	1.57	0.84
2:A:473:PRO:CD	2:B:825:LEU:HB3	2.07	0.84
1:G:92:ILE:HG22	1:G:116:GLN:OE1	1.76	0.84
1:H:92:ILE:HG22	1:H:116:GLN:OE1	1.76	0.84
1:H:203:CYS:SG	2:D:262:PRO:HB2	2.16	0.84
1:E:92:ILE:HG22	1:E:116:GLN:OE1	1.76	0.84
2:D:113:ARG:HD3	3:D:1106:POV:C22	2.07	0.84
2:D:199:LEU:HD21	6:D:1110:CLR:H193	1.60	0.84
2:C:199:LEU:HD21	6:C:1108:CLR:H193	1.59	0.83
2:D:266:PHE:CZ	3:D:1101:POV:C28	2.50	0.83
1:F:69:TRP:CE2	2:B:263:TRP:CB	2.61	0.83
2:D:174:LYS:HG2	6:D:1109:CLR:H191	1.60	0.83
3:B:1112:POV:H33A	3:B:1112:POV:H3A	1.60	0.82
2:D:44:ARG:NE	6:D:1109:CLR:C1	2.32	0.81
2:A:328:ASN:HB2	3:A:1115:POV:H15	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:ARG:NH1	6:D:1109:CLR:C2	2.44	0.81
2:D:815:LEU:CA	2:D:818:LYS:NZ	2.44	0.81
3:A:1114:POV:O13	3:A:1114:POV:H13B	1.81	0.80
3:B:1110:POV:H31F	3:B:1113:POV:H314	1.64	0.80
6:C:1107:CLR:H211	6:C:1107:CLR:C24	2.12	0.80
2:C:473:PRO:CD	2:D:825:LEU:HD13	2.12	0.80
1:H:68:CYS:HB3	2:D:263:TRP:CD2	2.16	0.80
6:A:1108:CLR:H193	6:A:1108:CLR:C3	2.12	0.79
1:F:92:ILE:CG2	1:F:116:GLN:OE1	2.30	0.79
3:A:1116:POV:H314	3:D:1102:POV:H31F	1.64	0.79
2:B:113:ARG:CD	3:B:1105:POV:C21	2.60	0.79
1:F:68:CYS:HB3	2:B:263:TRP:CD2	2.18	0.79
2:B:266:PHE:HZ	3:B:1101:POV:H28A	0.66	0.79
1:E:92:ILE:CG2	1:E:116:GLN:OE1	2.30	0.79
1:G:92:ILE:CG2	1:G:116:GLN:OE1	2.30	0.79
2:D:299:LEU:CD1	3:D:1101:POV:H31C	2.14	0.78
2:C:39:ILE:HG21	6:C:1107:CLR:H211	1.64	0.78
3:B:1105:POV:H3A	3:B:1105:POV:C23	2.13	0.78
2:A:263:TRP:HH2	2:A:298:THR:CB	1.96	0.78
2:C:263:TRP:HH2	2:C:298:THR:CB	1.96	0.78
1:H:68:CYS:HB3	2:D:263:TRP:CE3	2.18	0.78
1:H:92:ILE:CG2	1:H:116:GLN:OE1	2.30	0.78
2:B:263:TRP:HH2	2:B:298:THR:CB	1.96	0.78
2:D:263:TRP:HH2	2:D:298:THR:CB	1.96	0.77
2:A:39:ILE:CG2	6:A:1108:CLR:C21	2.63	0.77
2:D:307:PHE:HA	3:D:1108:POV:H25A	1.65	0.77
2:D:44:ARG:CZ	6:D:1109:CLR:H11	2.15	0.77
2:B:43:TRP:CG	6:B:1108:CLR:H122	2.20	0.76
2:C:263:TRP:HH2	2:C:298:THR:HB	1.50	0.76
1:F:159:SER:O	1:F:162:ASN:OD1	2.04	0.76
1:H:159:SER:O	1:H:162:ASN:OD1	2.04	0.76
2:C:815:LEU:CA	2:C:818:LYS:NZ	2.44	0.76
6:D:1110:CLR:H241	6:D:1110:CLR:C21	2.14	0.76
2:D:263:TRP:HH2	2:D:298:THR:HB	1.51	0.75
1:E:159:SER:O	1:E:162:ASN:OD1	2.04	0.75
2:B:263:TRP:HH2	2:B:298:THR:HB	1.51	0.75
2:B:23:TRP:CH2	6:B:1109:CLR:H6	2.22	0.75
2:A:263:TRP:HH2	2:A:298:THR:HB	1.51	0.75
2:B:815:LEU:CA	2:B:818:LYS:NZ	2.44	0.75
2:A:199:LEU:HD21	6:A:1109:CLR:H22	1.67	0.75
1:G:159:SER:O	1:G:162:ASN:OD1	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:TRP:NE1	2:B:263:TRP:HB3	2.03	0.74
1:F:69:TRP:CE2	2:B:263:TRP:CA	2.67	0.74
2:C:329:ARG:CZ	3:C:1110:POV:H14	2.18	0.74
6:A:1108:CLR:C24	6:A:1108:CLR:H211	2.17	0.74
2:D:229:THR:N	3:D:1113:POV:C11	2.51	0.73
2:D:39:ILE:HG22	6:D:1109:CLR:H211	0.75	0.73
2:A:39:ILE:HG22	6:A:1108:CLR:H211	1.70	0.73
2:A:815:LEU:CA	2:A:818:LYS:NZ	2.44	0.73
2:C:266:PHE:CE1	3:C:1113:POV:H35	2.24	0.73
2:C:23:TRP:CZ3	6:C:1108:CLR:H72	2.24	0.72
2:D:21:MET:CE	6:D:1110:CLR:H42	2.19	0.72
2:A:263:TRP:CH2	2:A:298:THR:HB	2.25	0.72
2:C:113:ARG:HD3	3:C:1104:POV:H22	1.71	0.72
2:D:43:TRP:CG	6:D:1109:CLR:H122	2.25	0.71
1:F:68:CYS:SG	2:B:263:TRP:CH2	2.83	0.71
2:A:514:ARG:HH21	2:A:514:ARG:HG2	1.56	0.71
2:B:263:TRP:CH2	2:B:298:THR:HB	2.25	0.71
2:D:298:THR:HG21	3:D:1102:POV:H22A	1.73	0.71
2:B:299:LEU:HD13	3:B:1101:POV:H31C	1.71	0.71
2:B:514:ARG:HG2	2:B:514:ARG:HH21	1.56	0.71
2:B:44:ARG:HH11	6:B:1108:CLR:H193	1.54	0.71
1:H:69:TRP:CE2	2:D:263:TRP:CB	2.74	0.71
2:A:91:VAL:HG23	2:B:340:SER:O	1.91	0.71
2:D:198:TYR:HE2	6:D:1110:CLR:H11	1.54	0.71
3:A:1116:POV:C27	3:A:1116:POV:H37A	2.21	0.70
2:C:263:TRP:CH2	2:C:298:THR:HB	2.25	0.70
2:D:514:ARG:HG2	2:D:514:ARG:HH21	1.56	0.70
2:C:514:ARG:HG2	2:C:514:ARG:HH21	1.56	0.70
2:D:263:TRP:CH2	2:D:298:THR:HB	2.25	0.70
3:B:1113:POV:C27	3:B:1113:POV:H37A	2.21	0.70
2:C:44:ARG:HE	6:C:1107:CLR:H11	1.56	0.70
2:C:28:SER:HA	6:C:1108:CLR:H222	1.72	0.70
1:F:40:LEU:HD22	2:B:44:ARG:NH2	2.06	0.70
2:D:199:LEU:CD2	6:D:1110:CLR:H192	2.22	0.69
2:D:956:GLU:CD	2:D:960:ARG:HE	1.95	0.69
2:A:438:ALA:O	2:B:818:LYS:HE2	1.92	0.69
2:D:23:TRP:HH2	6:D:1110:CLR:C7	2.03	0.69
1:G:151:ARG:O	1:G:151:ARG:HG3	1.92	0.69
2:A:219:GLU:HG3	2:B:392:LYS:HE3	1.73	0.69
2:D:28:SER:HA	6:D:1110:CLR:C23	2.22	0.69
1:E:151:ARG:O	1:E:151:ARG:HG3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:ARG:HG3	1:F:151:ARG:O	1.92	0.69
2:A:956:GLU:CD	2:A:960:ARG:HE	1.95	0.69
2:B:956:GLU:CD	2:B:960:ARG:HE	1.95	0.69
2:D:301:ARG:HD3	3:D:1102:POV:H33A	1.72	0.69
2:C:956:GLU:CD	2:C:960:ARG:HE	1.95	0.69
6:C:1107:CLR:H242	6:C:1107:CLR:C21	2.21	0.69
2:D:21:MET:HE1	6:D:1110:CLR:H42	1.75	0.69
6:D:1110:CLR:H241	6:D:1110:CLR:H211	1.74	0.68
2:D:229:THR:N	3:D:1113:POV:H11A	2.08	0.68
6:B:1109:CLR:H183	6:B:1109:CLR:C21	2.19	0.68
1:H:151:ARG:O	1:H:151:ARG:HG3	1.92	0.68
2:C:199:LEU:CD2	6:C:1108:CLR:H192	2.22	0.68
3:D:1112:POV:O13	3:D:1112:POV:H13A	1.94	0.68
2:A:39:ILE:HG22	6:A:1108:CLR:H212	1.75	0.68
2:B:44:ARG:HH11	6:B:1108:CLR:H22	1.59	0.68
6:C:1107:CLR:H222	6:C:1107:CLR:C18	2.23	0.68
1:H:68:CYS:SG	2:D:263:TRP:CH2	2.88	0.67
2:D:228:LYS:CB	3:D:1113:POV:H11	2.23	0.67
2:B:301:ARG:HD3	3:B:1114:POV:H33A	1.76	0.67
2:C:198:TYR:CE2	6:C:1108:CLR:H11	2.23	0.67
2:D:113:ARG:CD	3:D:1106:POV:C21	2.66	0.67
2:A:442:MET:HG2	2:B:818:LYS:HE3	1.75	0.67
2:D:36:GLY:HA2	6:D:1109:CLR:C27	2.16	0.66
2:D:228:LYS:HB2	3:D:1113:POV:C11	2.25	0.66
2:D:306:PHE:HB3	3:D:1108:POV:H27	1.75	0.66
2:D:44:ARG:HH11	6:D:1109:CLR:H192	1.60	0.66
2:C:329:ARG:NH1	3:C:1110:POV:C14	2.59	0.66
6:A:1108:CLR:H211	6:A:1108:CLR:H242	1.78	0.66
2:C:219:GLU:HG3	2:D:392:LYS:HE3	1.78	0.66
2:D:39:ILE:CG2	6:D:1109:CLR:H213	2.20	0.66
2:D:174:LYS:CG	6:D:1109:CLR:H191	2.25	0.65
2:D:28:SER:CA	6:D:1110:CLR:H232	2.26	0.65
2:A:960:ARG:HB2	2:A:960:ARG:HH21	1.62	0.65
2:C:102:GLY:C	2:D:396:THR:HG21	2.17	0.65
2:A:539:GLU:O	2:A:594:LEU:HD12	1.97	0.65
2:B:326:ILE:HD13	3:B:1112:POV:H22A	1.79	0.65
2:C:113:ARG:HD3	3:C:1104:POV:C22	2.27	0.65
2:C:473:PRO:HD3	2:D:825:LEU:HB3	1.79	0.65
2:C:539:GLU:O	2:C:594:LEU:HD12	1.97	0.65
3:D:1112:POV:H14B	3:D:1112:POV:O13	1.95	0.65
2:D:117:VAL:HG11	3:D:1106:POV:H27	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:SER:HA	6:B:1109:CLR:H162	1.78	0.64
2:C:43:TRP:CD2	6:C:1107:CLR:H122	2.33	0.64
2:C:44:ARG:HH11	6:C:1107:CLR:H22	1.61	0.64
2:D:44:ARG:HH11	6:D:1109:CLR:H22	1.60	0.64
2:D:229:THR:H	3:D:1113:POV:H11A	1.58	0.64
2:A:314:MET:HG3	3:A:1107:POV:C3	2.27	0.64
2:B:539:GLU:O	2:B:594:LEU:HD12	1.97	0.64
2:C:960:ARG:HH21	2:C:960:ARG:HB2	1.62	0.64
2:B:960:ARG:HH21	2:B:960:ARG:HB2	1.62	0.64
2:C:329:ARG:CZ	3:C:1110:POV:C14	2.75	0.64
2:D:23:TRP:CZ3	6:D:1110:CLR:C7	2.75	0.64
2:D:44:ARG:CZ	6:D:1109:CLR:C2	2.76	0.64
2:D:113:ARG:CD	3:D:1106:POV:H22	2.28	0.64
2:D:960:ARG:HH21	2:D:960:ARG:HB2	1.62	0.64
2:D:44:ARG:HH11	6:D:1109:CLR:C1	2.11	0.64
2:A:198:TYR:HE2	6:A:1109:CLR:H11	1.63	0.63
2:B:40:ILE:CG1	6:B:1108:CLR:H232	2.23	0.63
2:B:266:PHE:CE1	3:B:1101:POV:C35	2.80	0.63
2:A:174:LYS:HG3	6:A:1108:CLR:C18	2.26	0.63
2:B:44:ARG:NE	6:B:1108:CLR:C1	2.43	0.63
2:D:199:LEU:CD2	6:D:1110:CLR:H22	2.29	0.63
2:D:539:GLU:O	2:D:594:LEU:HD12	1.97	0.63
2:A:449:ASN:CG	2:B:890:PHE:HD1	2.02	0.63
3:B:1106:POV:P	3:B:1106:POV:H33A	2.39	0.63
2:D:299:LEU:HD13	3:D:1101:POV:H31C	1.81	0.63
2:D:956:GLU:OE1	2:D:960:ARG:CD	2.47	0.63
2:C:442:MET:SD	2:D:818:LYS:HG2	2.38	0.63
2:D:232:SER:OG	3:D:1113:POV:C12	2.46	0.63
2:A:956:GLU:OE1	2:A:960:ARG:NE	2.32	0.62
2:A:956:GLU:OE1	2:A:960:ARG:CD	2.47	0.62
2:B:278:VAL:HG11	3:B:1110:POV:H39	1.81	0.62
2:B:956:GLU:OE1	2:B:960:ARG:NE	2.32	0.62
2:C:956:GLU:OE1	2:C:960:ARG:CD	2.47	0.62
2:C:956:GLU:OE1	2:C:960:ARG:NE	2.32	0.62
2:C:39:ILE:CG2	6:C:1107:CLR:H211	2.29	0.62
2:B:24:ALA:CB	6:B:1109:CLR:H72	2.30	0.62
2:B:956:GLU:OE1	2:B:960:ARG:CD	2.47	0.62
2:D:301:ARG:CD	3:D:1102:POV:H33A	2.29	0.62
3:C:1104:POV:H23A	3:C:1104:POV:O32	2.00	0.62
2:B:44:ARG:CZ	6:B:1108:CLR:H22	2.29	0.62
2:B:199:LEU:HD21	6:B:1109:CLR:H192	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1105:POV:C211	3:B:1105:POV:H27	2.30	0.62
2:D:956:GLU:OE1	2:D:960:ARG:NE	2.32	0.61
2:C:44:ARG:NH1	6:C:1107:CLR:H22	2.15	0.61
1:G:159:SER:HA	1:G:162:ASN:ND2	2.16	0.61
1:E:159:SER:HA	1:E:162:ASN:ND2	2.16	0.61
1:F:159:SER:HA	1:F:162:ASN:ND2	2.16	0.61
2:D:266:PHE:CE1	3:D:1101:POV:C35	2.82	0.61
1:H:69:TRP:CE2	2:D:263:TRP:CA	2.79	0.61
2:D:113:ARG:CD	3:D:1106:POV:C22	2.77	0.61
2:B:44:ARG:NH1	6:B:1108:CLR:H193	2.14	0.61
2:C:39:ILE:CG2	6:C:1107:CLR:C21	2.79	0.61
1:F:92:ILE:CG2	1:F:116:GLN:CD	2.70	0.61
2:D:815:LEU:HA	2:D:818:LYS:HZ3	1.61	0.61
2:D:235:LEU:CD2	3:D:1113:POV:H23A	2.28	0.60
2:D:514:ARG:HH21	2:D:514:ARG:CG	2.14	0.60
1:H:159:SER:HA	1:H:162:ASN:ND2	2.16	0.60
2:D:23:TRP:HH2	6:D:1110:CLR:C6	2.14	0.60
1:H:92:ILE:CG2	1:H:116:GLN:CD	2.70	0.60
2:A:292:ASP:HB3	2:D:294:TYR:CE1	2.36	0.60
2:A:514:ARG:HH21	2:A:514:ARG:CG	2.14	0.60
1:G:92:ILE:CG2	1:G:116:GLN:CD	2.70	0.60
2:C:514:ARG:HH21	2:C:514:ARG:CG	2.14	0.60
3:D:1111:POV:H3	1:G:70:LEU:HD11	1.83	0.60
1:F:69:TRP:CD1	2:B:263:TRP:HB3	2.36	0.60
2:B:23:TRP:CZ3	6:B:1109:CLR:H6	2.35	0.60
3:C:1105:POV:O14	3:C:1105:POV:H33A	2.02	0.60
2:A:24:ALA:HB1	6:A:1109:CLR:H191	1.83	0.60
1:H:40:LEU:HD22	2:D:44:ARG:NH2	2.17	0.60
2:B:514:ARG:HH21	2:B:514:ARG:CG	2.15	0.60
2:C:43:TRP:CG	6:C:1107:CLR:H122	2.36	0.60
1:E:92:ILE:CG2	1:E:116:GLN:CD	2.70	0.60
2:A:39:ILE:CG2	6:A:1108:CLR:H211	2.31	0.59
3:D:1113:POV:N	3:D:1113:POV:H1	2.17	0.59
3:B:1113:POV:H13B	3:B:1113:POV:O12	2.02	0.59
2:A:815:LEU:HA	2:A:818:LYS:HZ3	1.63	0.59
2:B:174:LYS:HB2	6:B:1108:CLR:H191	1.83	0.59
2:D:36:GLY:CA	6:D:1109:CLR:H272	2.18	0.59
2:C:442:MET:SD	2:D:818:LYS:CG	2.91	0.59
2:B:40:ILE:CG1	6:B:1108:CLR:H183	2.29	0.59
2:B:816:GLN:OE1	2:B:816:GLN:N	2.25	0.59
1:H:68:CYS:SG	2:D:263:TRP:CZ2	2.96	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:263:TRP:HA	1:G:69:TRP:CH2	2.38	0.58
2:A:449:ASN:OD1	2:B:890:PHE:CD1	2.56	0.58
3:A:1116:POV:H13B	3:A:1116:POV:O12	2.02	0.58
2:D:221:LEU:HD13	3:D:1113:POV:H32A	1.85	0.58
2:A:445:ILE:HD12	2:B:821:ILE:HG21	1.84	0.58
2:A:955:GLU:OE2	2:B:790:ARG:HD2	2.02	0.58
2:B:224:LEU:HD22	3:B:1105:POV:H1A	1.85	0.58
2:D:228:LYS:H	3:D:1113:POV:C12	2.15	0.58
3:D:1112:POV:H14B	3:D:1112:POV:O12	2.01	0.58
2:A:449:ASN:CG	2:B:890:PHE:CD1	2.77	0.58
2:B:335:SER:HB2	2:B:413:ARG:O	2.04	0.58
6:C:1108:CLR:H121	6:C:1108:CLR:H212	1.86	0.58
2:D:335:SER:HB2	2:D:413:ARG:O	2.04	0.58
2:B:23:TRP:CZ3	6:B:1109:CLR:C6	2.87	0.58
6:B:1109:CLR:H212	6:B:1109:CLR:C18	2.20	0.58
2:C:266:PHE:CE1	3:C:1113:POV:C35	2.86	0.58
6:C:1108:CLR:H242	6:C:1108:CLR:C21	2.25	0.58
2:C:199:LEU:CD2	6:C:1108:CLR:H22	2.34	0.57
2:A:103:VAL:N	2:B:396:THR:HG21	2.20	0.57
2:C:174:LYS:HG3	6:C:1107:CLR:H8	1.86	0.57
2:A:335:SER:HB2	2:A:413:ARG:O	2.04	0.57
2:C:263:TRP:CH2	2:C:298:THR:CB	2.84	0.57
2:D:232:SER:OG	3:D:1113:POV:H12A	2.05	0.57
1:H:69:TRP:NE1	2:D:263:TRP:HB3	2.18	0.57
2:D:44:ARG:NH1	6:D:1109:CLR:C1	2.66	0.57
2:A:890:PHE:CE2	2:D:442:MET:HE3	2.40	0.57
2:C:335:SER:HB2	2:C:413:ARG:O	2.04	0.57
2:B:114:VAL:HA	3:B:1105:POV:H25	1.87	0.56
2:B:259:SER:OG	3:B:1101:POV:H39	2.05	0.56
2:B:813:THR:HA	2:B:816:GLN:HE22	1.70	0.56
2:B:23:TRP:CH2	6:B:1109:CLR:C6	2.89	0.56
2:B:816:GLN:H	2:B:816:GLN:CD	2.07	0.56
2:C:102:GLY:C	2:D:396:THR:CG2	2.73	0.56
2:C:813:THR:HA	2:C:816:GLN:HE22	1.70	0.56
2:D:224:LEU:HD13	3:D:1106:POV:H32A	1.86	0.56
2:D:229:THR:OG1	3:D:1113:POV:H11A	2.05	0.56
2:B:539:GLU:C	2:B:594:LEU:HD12	2.26	0.56
2:D:39:ILE:HD12	6:D:1109:CLR:H273	1.86	0.56
2:A:473:PRO:CG	2:B:825:LEU:HD13	2.36	0.56
1:F:68:CYS:SG	2:B:263:TRP:CZ2	2.98	0.56
2:A:102:GLY:C	2:B:396:THR:HG21	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:539:GLU:C	2:A:594:LEU:HD12	2.26	0.56
3:C:1109:POV:H13B	3:C:1109:POV:O13	2.06	0.56
2:D:539:GLU:C	2:D:594:LEU:HD12	2.26	0.56
2:C:815:LEU:HA	2:C:818:LYS:HZ2	1.64	0.56
1:F:69:TRP:CG	2:B:263:TRP:HB3	2.40	0.56
2:B:40:ILE:HA	6:B:1108:CLR:H20	1.88	0.56
1:H:100:PHE:CE2	1:H:151:ARG:HA	2.41	0.55
2:C:402:GLN:O	2:C:413:ARG:NH1	2.39	0.55
2:C:887:ASN:O	2:C:890:PHE:HB2	2.07	0.55
2:D:302:LEU:HD13	3:D:1102:POV:H36A	1.86	0.55
2:D:813:THR:HA	2:D:816:GLN:HE22	1.70	0.55
2:A:402:GLN:O	2:A:413:ARG:NH1	2.39	0.55
1:G:100:PHE:CE2	1:G:151:ARG:HA	2.41	0.55
2:A:102:GLY:C	2:B:396:THR:CG2	2.75	0.55
2:B:887:ASN:O	2:B:890:PHE:HB2	2.07	0.55
2:D:44:ARG:HH11	6:D:1109:CLR:C2	2.15	0.55
2:B:402:GLN:O	2:B:413:ARG:NH1	2.39	0.55
2:C:539:GLU:C	2:C:594:LEU:HD12	2.26	0.55
2:A:813:THR:HA	2:A:816:GLN:HE22	1.70	0.55
2:B:263:TRP:CH2	2:B:298:THR:CB	2.84	0.55
2:D:569:GLU:HB3	2:D:594:LEU:O	2.07	0.55
2:A:887:ASN:O	2:A:890:PHE:HB2	2.06	0.55
2:B:114:VAL:HG22	3:B:1105:POV:C25	2.36	0.55
1:E:100:PHE:CE2	1:E:151:ARG:HA	2.41	0.55
1:F:100:PHE:CE2	1:F:151:ARG:HA	2.41	0.55
2:B:31:VAL:HG12	6:B:1109:CLR:H273	1.89	0.54
2:C:473:PRO:HD2	2:D:825:LEU:CD1	2.32	0.54
2:A:569:GLU:HB3	2:A:594:LEU:O	2.07	0.54
2:A:263:TRP:CH2	2:A:298:THR:CB	2.84	0.54
2:C:103:VAL:N	2:D:396:THR:HG21	2.22	0.54
2:B:44:ARG:CZ	6:B:1108:CLR:C2	2.85	0.54
2:B:569:GLU:HB3	2:B:594:LEU:O	2.07	0.54
2:C:266:PHE:HZ	3:C:1113:POV:H28A	1.72	0.54
2:D:887:ASN:O	2:D:890:PHE:HB2	2.06	0.54
2:C:815:LEU:HA	2:C:818:LYS:HG3	1.90	0.54
2:A:960:ARG:HB2	2:A:960:ARG:NH2	2.23	0.54
3:B:1110:POV:H316	3:B:1113:POV:C315	2.38	0.54
2:C:569:GLU:HB3	2:C:594:LEU:O	2.07	0.54
2:C:219:GLU:HG3	2:D:392:LYS:CE	2.38	0.54
2:B:114:VAL:HG22	3:B:1105:POV:H25A	1.89	0.54
2:B:815:LEU:HA	2:B:818:LYS:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:960:ARG:HB2	2:C:960:ARG:NH2	2.23	0.54
2:D:402:GLN:O	2:D:413:ARG:NH1	2.39	0.54
2:A:223:PHE:HD1	2:B:392:LYS:O	1.91	0.53
3:A:1116:POV:C315	3:D:1102:POV:H316	2.38	0.53
2:A:230:SER:HB2	2:B:386:GLU:HG2	1.91	0.53
2:B:289:GLY:HA3	2:C:288:VAL:HG13	1.90	0.53
2:D:263:TRP:CH2	2:D:298:THR:CB	2.84	0.53
2:C:39:ILE:HG21	6:C:1107:CLR:C21	2.33	0.53
2:C:174:LYS:HG2	6:C:1107:CLR:C19	2.26	0.53
2:D:199:LEU:HD11	6:D:1110:CLR:C19	2.39	0.53
1:F:65:PHE:CD1	2:B:263:TRP:NE1	2.76	0.53
1:F:169:ASP:OD1	1:F:169:ASP:O	2.27	0.53
2:D:21:MET:HE2	6:D:1110:CLR:H42	1.88	0.53
2:D:44:ARG:CZ	6:D:1109:CLR:C1	2.82	0.53
2:D:113:ARG:HG3	3:D:1106:POV:H24A	1.91	0.53
2:D:298:THR:CG2	3:D:1102:POV:H22A	2.38	0.53
2:A:815:LEU:HA	2:A:818:LYS:HG3	1.90	0.53
2:B:44:ARG:NH1	6:B:1108:CLR:C2	2.62	0.53
6:D:1110:CLR:H211	6:D:1110:CLR:C24	2.33	0.53
2:D:960:ARG:HB2	2:D:960:ARG:NH2	2.23	0.53
2:B:960:ARG:HB2	2:B:960:ARG:NH2	2.23	0.53
2:D:815:LEU:HA	2:D:818:LYS:HG3	1.90	0.53
3:B:1105:POV:C211	3:B:1105:POV:C27	2.86	0.52
1:H:169:ASP:OD1	1:H:169:ASP:O	2.27	0.52
1:G:169:ASP:OD1	1:G:169:ASP:O	2.27	0.52
1:E:63:PHE:CE1	3:B:1111:POV:C35	2.93	0.52
1:E:199:VAL:HG22	3:A:1101:POV:H26A	1.92	0.52
2:A:442:MET:CE	2:B:818:LYS:HG2	2.38	0.52
1:G:38:THR:HG23	1:G:40:LEU:H	1.75	0.52
1:F:65:PHE:HE1	2:B:263:TRP:HE1	1.52	0.52
1:F:199:VAL:HG22	3:B:1101:POV:H26A	1.92	0.52
1:H:38:THR:HG23	1:H:40:LEU:H	1.74	0.52
1:H:199:VAL:HG22	3:D:1101:POV:H26A	1.92	0.52
6:C:1107:CLR:C18	6:C:1107:CLR:C22	2.86	0.52
2:D:114:VAL:HA	3:D:1106:POV:H27A	1.90	0.52
3:D:1113:POV:N	3:D:1113:POV:C1	2.73	0.52
2:A:815:LEU:CB	2:A:818:LYS:NZ	2.73	0.52
2:C:442:MET:CE	2:C:445:ILE:HD11	2.40	0.52
2:D:44:ARG:NH1	6:D:1109:CLR:H11	2.25	0.52
2:D:44:ARG:HH11	6:D:1109:CLR:H193	1.69	0.52
1:F:38:THR:HG23	1:F:40:LEU:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:THR:HG23	1:E:40:LEU:H	1.75	0.52
2:B:815:LEU:CB	2:B:818:LYS:NZ	2.73	0.52
1:H:68:CYS:SG	3:D:1102:POV:H23	2.50	0.52
2:D:442:MET:CE	2:D:445:ILE:HD11	2.40	0.52
2:D:815:LEU:CB	2:D:818:LYS:NZ	2.73	0.52
2:D:326:ILE:HG12	3:D:1112:POV:H1	1.92	0.51
2:D:816:GLN:OE1	2:D:816:GLN:N	2.25	0.51
2:B:266:PHE:CD1	3:B:1101:POV:H35	2.45	0.51
2:B:292:ASP:OD1	2:B:292:ASP:N	2.43	0.51
2:A:292:ASP:HB3	2:D:294:TYR:CZ	2.46	0.51
2:A:442:MET:CE	2:A:445:ILE:HD11	2.40	0.51
2:C:442:MET:HG2	2:D:818:LYS:HE3	1.92	0.51
2:D:292:ASP:OD1	2:D:292:ASP:N	2.43	0.51
2:B:442:MET:CE	2:B:445:ILE:HD11	2.40	0.51
2:C:129:ILE:HD11	3:C:1109:POV:H25	1.92	0.51
2:C:815:LEU:CB	2:C:818:LYS:NZ	2.73	0.51
2:B:266:PHE:CE2	3:B:1101:POV:C28	2.93	0.51
2:C:816:GLN:OE1	2:C:816:GLN:N	2.25	0.51
1:E:169:ASP:OD1	1:E:169:ASP:O	2.27	0.51
2:A:219:GLU:HG3	2:B:392:LYS:CE	2.38	0.51
3:C:1113:POV:H26A	1:G:199:VAL:HG22	1.92	0.51
2:D:43:TRP:CD1	6:D:1109:CLR:H122	2.45	0.51
2:C:298:THR:HG21	3:C:1112:POV:H22A	1.93	0.51
2:B:43:TRP:HB3	6:B:1108:CLR:C12	2.40	0.51
2:C:263:TRP:HA	1:G:69:TRP:CZ2	2.46	0.51
2:B:39:ILE:CG2	6:B:1108:CLR:H212	1.90	0.51
2:D:514:ARG:CG	2:D:514:ARG:NH2	2.73	0.51
6:D:1110:CLR:H241	6:D:1110:CLR:H213	1.92	0.50
2:D:298:THR:HG23	3:D:1102:POV:H32	1.93	0.50
2:A:514:ARG:CG	2:A:514:ARG:NH2	2.73	0.50
2:D:199:LEU:CD2	6:D:1110:CLR:C19	2.76	0.50
2:A:816:GLN:H	2:A:816:GLN:CD	2.07	0.50
1:F:40:LEU:HD22	2:B:44:ARG:HH22	1.77	0.50
2:A:223:PHE:CD1	2:B:392:LYS:O	2.65	0.50
2:B:147:ASP:OD1	3:B:1111:POV:H11A	2.11	0.50
2:A:266:PHE:CE1	3:A:1101:POV:H35	2.47	0.49
2:B:301:ARG:CD	3:B:1114:POV:H33A	2.40	0.49
3:B:1106:POV:H33A	3:B:1106:POV:O13	2.12	0.49
2:C:514:ARG:CG	2:C:514:ARG:NH2	2.73	0.49
2:B:21:MET:CE	6:B:1109:CLR:H42	2.42	0.49
2:B:40:ILE:HA	6:B:1108:CLR:H121	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:223:PHE:CD1	2:D:392:LYS:O	2.66	0.49
6:C:1108:CLR:H211	6:C:1108:CLR:C24	2.16	0.49
6:A:1109:CLR:H273	6:A:1109:CLR:H211	1.94	0.49
2:B:23:TRP:HH2	6:B:1109:CLR:H6	1.72	0.49
1:H:69:TRP:CG	2:D:263:TRP:HB3	2.48	0.49
2:A:106:SER:HB2	2:B:395:PHE:HB3	1.93	0.49
2:A:292:ASP:OD1	2:A:292:ASP:N	2.43	0.49
2:C:329:ARG:NH2	3:C:1110:POV:H14	2.27	0.49
6:A:1109:CLR:H121	6:A:1109:CLR:C21	2.43	0.49
2:B:44:ARG:NE	6:B:1108:CLR:C2	2.74	0.49
2:C:91:VAL:HA	2:D:341:GLY:HA3	1.94	0.49
2:C:174:LYS:HB2	6:C:1107:CLR:C19	2.43	0.49
2:A:233:ILE:HD13	2:B:385:LEU:O	2.13	0.49
2:A:449:ASN:OD1	2:B:890:PHE:HD1	1.96	0.49
2:C:328:ASN:HB2	3:C:1110:POV:H15A	1.95	0.48
2:A:818:LYS:HE2	2:D:438:ALA:HB1	1.95	0.48
2:D:28:SER:CB	6:D:1110:CLR:H232	2.43	0.48
3:C:1105:POV:N	3:C:1105:POV:O13	2.45	0.48
2:A:241:ILE:HD13	3:A:1106:POV:O14	2.13	0.48
2:A:449:ASN:OD1	2:B:890:PHE:CE1	2.66	0.48
2:B:299:LEU:HD11	3:B:1101:POV:H31C	1.93	0.48
2:B:310:GLY:HA3	3:B:1107:POV:H23A	1.95	0.48
2:C:99:ASP:OD2	2:D:342:ARG:NH1	2.46	0.48
2:A:786:ARG:HD2	2:D:955:GLU:O	2.14	0.48
2:D:39:ILE:HG21	6:D:1109:CLR:H242	1.96	0.48
2:A:328:ASN:CB	3:A:1115:POV:H15B	2.30	0.48
2:D:117:VAL:CG1	3:D:1106:POV:H27	2.44	0.48
1:H:69:TRP:CD1	2:D:263:TRP:HB3	2.48	0.48
6:A:1108:CLR:C21	6:A:1108:CLR:C24	2.90	0.48
2:B:199:LEU:HD21	6:B:1109:CLR:H22	1.96	0.47
2:D:442:MET:HE3	2:D:445:ILE:HD11	1.96	0.47
6:D:1110:CLR:C21	6:D:1110:CLR:C24	2.86	0.47
3:B:1106:POV:P	3:B:1106:POV:C33	3.03	0.47
6:A:1108:CLR:H211	6:A:1108:CLR:H241	1.94	0.47
2:B:442:MET:HE3	2:C:890:PHE:CE2	2.49	0.47
2:C:329:ARG:NH1	3:C:1110:POV:H14A	2.29	0.47
2:A:442:MET:CG	2:B:818:LYS:HD3	2.40	0.47
2:B:40:ILE:HG12	6:B:1108:CLR:C18	2.33	0.47
2:B:266:PHE:CZ	3:B:1101:POV:C27	2.98	0.47
6:D:1110:CLR:H183	6:D:1110:CLR:C21	2.27	0.47
2:C:114:VAL:HG22	3:C:1104:POV:H25	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:292:ASP:OD1	2:C:292:ASP:N	2.43	0.47
2:B:43:TRP:HB3	6:B:1108:CLR:H121	1.97	0.47
3:B:1105:POV:H26	3:B:1105:POV:H23	1.68	0.47
6:C:1108:CLR:H212	6:C:1108:CLR:H183	1.97	0.47
2:D:117:VAL:CG1	3:D:1106:POV:H29	2.44	0.47
3:C:1110:POV:H3A	3:C:1110:POV:H33A	1.97	0.47
3:D:1101:POV:H36A	3:D:1101:POV:H39A	1.50	0.47
2:B:326:ILE:CD1	3:B:1112:POV:H22A	2.45	0.47
2:B:117:VAL:CG1	3:B:1105:POV:H37	2.45	0.46
1:E:188:ASP:OD1	1:F:151:ARG:NH2	2.47	0.46
2:C:328:ASN:C	3:C:1110:POV:C15	2.83	0.46
2:A:23:TRP:HZ3	6:A:1109:CLR:H72	1.81	0.46
6:A:1108:CLR:C21	6:A:1108:CLR:H242	2.43	0.46
2:D:199:LEU:HD21	6:D:1110:CLR:H22	1.97	0.46
2:D:310:GLY:HA3	3:D:1108:POV:H23A	1.96	0.46
6:B:1108:CLR:C21	6:B:1108:CLR:H242	2.45	0.46
2:D:228:LYS:H	3:D:1113:POV:H12	1.79	0.46
2:A:91:VAL:HA	2:B:341:GLY:HA3	1.96	0.46
2:B:514:ARG:CG	2:B:514:ARG:NH2	2.73	0.46
2:C:223:PHE:HD1	2:D:392:LYS:O	1.98	0.46
3:D:1113:POV:O22	3:D:1113:POV:H24A	2.16	0.46
3:A:1101:POV:H36A	3:A:1101:POV:H39A	1.50	0.46
2:B:129:ILE:HD11	3:B:1111:POV:H25	1.96	0.46
2:D:243:ILE:HD12	3:D:1113:POV:H310	1.96	0.46
3:A:1116:POV:H37A	3:A:1116:POV:C26	2.46	0.46
3:B:1110:POV:H31F	3:B:1113:POV:C314	2.42	0.46
3:D:1106:POV:H27A	3:D:1106:POV:H24	1.67	0.46
3:C:1109:POV:H27A	3:C:1109:POV:H24A	1.70	0.46
2:D:816:GLN:H	2:D:816:GLN:CD	2.07	0.46
3:D:1101:POV:H313	3:D:1101:POV:H31A	1.71	0.46
2:C:230:SER:HB2	2:D:386:GLU:HG2	1.97	0.45
1:H:100:PHE:CD2	1:H:151:ARG:HA	2.51	0.45
1:F:69:TRP:CD2	2:B:263:TRP:CB	2.90	0.45
2:B:299:LEU:HD13	3:B:1101:POV:H31F	1.98	0.45
2:D:113:ARG:HD2	3:D:1106:POV:H22	1.98	0.45
1:F:100:PHE:CD2	1:F:151:ARG:HA	2.51	0.45
3:B:1113:POV:H37A	3:B:1113:POV:C26	2.46	0.45
6:B:1108:CLR:H183	6:B:1108:CLR:H20	1.78	0.45
2:A:198:TYR:CE2	6:A:1109:CLR:H11	2.49	0.45
2:B:39:ILE:HB	6:B:1108:CLR:H241	1.98	0.45
2:A:106:SER:CB	2:B:395:PHE:HB3	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:MET:HE1	6:D:1110:CLR:C4	2.46	0.45
1:E:100:PHE:CD2	1:E:151:ARG:HA	2.52	0.45
2:A:441:ILE:HG21	2:B:822:LEU:HD11	1.98	0.45
3:A:1101:POV:H37	3:A:1101:POV:H34	1.79	0.45
2:B:24:ALA:HA	6:B:1109:CLR:H72	1.98	0.45
2:B:28:SER:HB3	6:B:1109:CLR:H181	1.99	0.45
2:D:259:SER:OG	3:D:1101:POV:H39	2.17	0.45
6:D:1110:CLR:C21	6:D:1110:CLR:H121	2.46	0.45
2:B:224:LEU:HD22	3:B:1105:POV:H3	1.99	0.45
2:B:1000:PHE:O	2:B:1000:PHE:CD1	2.70	0.45
2:C:298:THR:HG23	3:C:1112:POV:H32	1.98	0.45
2:D:39:ILE:CG2	6:D:1109:CLR:H242	2.46	0.45
2:D:610:PHE:O	2:D:610:PHE:CD1	2.70	0.45
2:C:43:TRP:O	2:C:43:TRP:CD1	2.70	0.45
2:C:1000:PHE:O	2:C:1000:PHE:CD1	2.70	0.45
2:A:610:PHE:CD1	2:A:610:PHE:O	2.70	0.44
2:D:114:VAL:HG13	3:D:1106:POV:H28	1.99	0.44
1:G:100:PHE:CD2	1:G:151:ARG:HA	2.51	0.44
2:A:43:TRP:CD1	2:A:43:TRP:O	2.70	0.44
2:A:960:ARG:HH21	2:A:960:ARG:CB	2.29	0.44
6:A:1108:CLR:H222	6:A:1108:CLR:H162	1.55	0.44
2:D:1000:PHE:CD1	2:D:1000:PHE:O	2.70	0.44
1:G:8:ARG:H	1:G:8:ARG:HD3	1.82	0.44
1:F:65:PHE:HD1	2:B:263:TRP:NE1	2.13	0.44
2:A:1000:PHE:O	2:A:1000:PHE:CD1	2.70	0.44
3:B:1111:POV:H28A	3:B:1111:POV:H211	1.72	0.44
2:C:610:PHE:O	2:C:610:PHE:CD1	2.70	0.44
3:C:1104:POV:H32A	3:C:1104:POV:H35	1.68	0.44
2:A:816:GLN:OE1	2:A:816:GLN:N	2.25	0.44
2:B:938:ARG:NH1	2:B:950:GLU:OE2	2.46	0.44
3:D:1101:POV:H24	3:D:1101:POV:H27	1.41	0.44
3:D:1101:POV:H37	3:D:1101:POV:H34	1.79	0.44
6:D:1109:CLR:H222	6:D:1109:CLR:H162	1.31	0.44
2:A:91:VAL:HB	2:B:341:GLY:HA3	1.99	0.44
3:B:1112:POV:H33A	3:B:1112:POV:C3	2.38	0.44
2:C:174:LYS:CB	6:C:1107:CLR:H191	2.45	0.44
2:D:28:SER:HB2	6:D:1110:CLR:H232	2.00	0.44
2:D:938:ARG:NH1	2:D:950:GLU:OE2	2.46	0.44
2:B:342:ARG:HE	2:B:342:ARG:HB2	1.45	0.44
2:B:610:PHE:O	2:B:610:PHE:CD1	2.70	0.44
2:A:225:ASN:HA	2:B:393:ARG:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:ILE:C	6:B:1108:CLR:H212	2.38	0.44
2:B:43:TRP:O	2:B:43:TRP:CD1	2.70	0.44
2:B:263:TRP:CD1	2:B:263:TRP:N	2.85	0.44
3:B:1101:POV:H37	3:B:1101:POV:H34	1.79	0.44
2:D:317:SER:CB	3:D:1108:POV:H12A	2.48	0.44
6:A:1108:CLR:H183	6:A:1108:CLR:H20	1.71	0.44
2:D:43:TRP:CD1	2:D:43:TRP:O	2.70	0.44
6:D:1110:CLR:H212	6:D:1110:CLR:H121	1.99	0.44
6:C:1107:CLR:H221	6:C:1107:CLR:H162	1.88	0.43
3:C:1111:POV:H13B	3:C:1111:POV:O12	2.18	0.43
2:A:342:ARG:HE	2:A:342:ARG:HB2	1.45	0.43
2:B:299:LEU:CD1	3:B:1101:POV:H31F	2.48	0.43
2:C:263:TRP:C	2:C:265:ASN:H	2.22	0.43
2:C:938:ARG:NH1	2:C:950:GLU:OE2	2.46	0.43
3:C:1105:POV:H13B	3:C:1105:POV:H11	1.91	0.43
2:A:233:ILE:HG22	2:B:385:LEU:HD22	1.99	0.43
2:B:266:PHE:CD1	3:B:1101:POV:C35	3.01	0.43
3:B:1114:POV:H39	2:C:278:VAL:HG11	1.99	0.43
2:C:310:GLY:HA3	3:C:1106:POV:H23A	2.00	0.43
2:A:895:ASP:OD1	2:A:895:ASP:N	2.51	0.43
2:A:263:TRP:C	2:A:265:ASN:H	2.22	0.43
2:B:28:SER:CA	6:B:1109:CLR:H162	2.46	0.43
6:B:1108:CLR:H182	6:B:1108:CLR:H8	1.77	0.43
2:D:263:TRP:C	2:D:265:ASN:H	2.22	0.43
2:D:342:ARG:HE	2:D:342:ARG:HB2	1.45	0.43
2:D:895:ASP:N	2:D:895:ASP:OD1	2.51	0.43
1:F:203:CYS:SG	2:B:262:PRO:CB	2.93	0.43
3:B:1106:POV:C34	2:C:331:LYS:HE2	2.48	0.43
2:C:960:ARG:HH21	2:C:960:ARG:CB	2.29	0.43
2:D:39:ILE:HD12	6:D:1109:CLR:C27	2.48	0.43
2:D:307:PHE:CA	3:D:1108:POV:H25A	2.41	0.43
6:D:1109:CLR:H183	6:D:1109:CLR:H20	1.68	0.43
1:F:69:TRP:NE1	2:B:263:TRP:CB	2.77	0.43
3:B:1101:POV:H39A	3:B:1101:POV:H36A	1.50	0.43
6:B:1109:CLR:C21	6:B:1109:CLR:H121	2.49	0.43
2:C:816:GLN:H	2:C:816:GLN:CD	2.07	0.43
2:C:895:ASP:OD1	2:C:895:ASP:N	2.51	0.43
6:D:1109:CLR:H211	6:D:1109:CLR:H242	2.00	0.43
2:A:44:ARG:HH11	6:A:1108:CLR:H11	1.84	0.43
2:A:473:PRO:CD	2:B:825:LEU:CD1	2.74	0.43
2:D:331:LYS:HB2	2:D:331:LYS:HE3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:VAL:CG1	2:B:262:PRO:O	2.66	0.43
2:B:263:TRP:C	2:B:265:ASN:H	2.22	0.43
2:B:331:LYS:HB2	2:B:331:LYS:HE3	1.82	0.43
2:D:43:TRP:CE3	6:D:1109:CLR:H17	2.54	0.43
2:B:39:ILE:HG21	6:B:1108:CLR:H242	2.01	0.42
2:B:895:ASP:N	2:B:895:ASP:OD1	2.51	0.42
2:C:23:TRP:HH2	6:C:1108:CLR:H72	1.75	0.42
2:D:235:LEU:HD23	3:D:1113:POV:C23	2.34	0.42
3:A:1101:POV:H31A	3:A:1101:POV:H313	1.71	0.42
3:B:1113:POV:H39A	3:B:1113:POV:H36A	1.57	0.42
2:C:39:ILE:CG2	6:C:1107:CLR:H212	2.49	0.42
3:C:1113:POV:H24	3:C:1113:POV:H27	1.41	0.42
2:D:298:THR:O	2:D:302:LEU:HD22	2.20	0.42
2:A:306:PHE:HB3	3:A:1107:POV:H27	2.00	0.42
2:A:818:LYS:HD2	2:D:438:ALA:HB1	2.02	0.42
2:C:23:TRP:CH2	6:C:1108:CLR:C7	2.95	0.42
2:D:960:ARG:HH21	2:D:960:ARG:CB	2.29	0.42
2:A:298:THR:O	2:A:302:LEU:HD22	2.20	0.42
6:A:1109:CLR:H212	6:A:1109:CLR:H121	2.00	0.42
2:B:43:TRP:CB	6:B:1108:CLR:H122	2.48	0.42
2:B:174:LYS:CB	6:B:1108:CLR:H191	2.48	0.42
2:B:298:THR:O	2:B:302:LEU:HD22	2.20	0.42
2:B:442:MET:HE3	2:B:445:ILE:HD11	2.01	0.42
2:C:199:LEU:HD21	6:C:1108:CLR:H22	2.02	0.42
2:D:117:VAL:HG11	3:D:1106:POV:H29	2.00	0.42
1:H:65:PHE:HE1	2:D:263:TRP:HE1	1.65	0.42
1:H:70:LEU:HD13	3:A:1114:POV:C32	2.49	0.42
2:C:299:LEU:HD23	2:C:299:LEU:HA	1.91	0.42
1:F:196:ASP:OD1	1:F:196:ASP:N	2.53	0.42
3:B:1101:POV:H27	3:B:1101:POV:H24	1.41	0.42
6:B:1109:CLR:H211	6:B:1109:CLR:H231	1.69	0.42
2:A:91:VAL:CA	2:B:341:GLY:HA3	2.50	0.42
2:A:103:VAL:CA	2:B:396:THR:HG21	2.49	0.42
2:D:302:LEU:HD13	2:D:302:LEU:HA	1.73	0.42
2:B:28:SER:HA	6:B:1109:CLR:H20	2.02	0.42
1:F:68:CYS:HB3	2:B:263:TRP:CZ3	2.53	0.42
2:A:38:PHE:O	2:A:42:LEU:HG	2.20	0.42
3:A:1105:POV:C38	3:A:1105:POV:H33A	2.50	0.42
6:A:1109:CLR:H183	6:A:1109:CLR:C21	2.21	0.41
2:B:960:ARG:HH21	2:B:960:ARG:CB	2.29	0.41
6:B:1109:CLR:H182	6:B:1109:CLR:H8	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:SER:HB2	2:D:395:PHE:HB3	2.01	0.41
2:C:302:LEU:HD13	2:C:302:LEU:HA	1.73	0.41
2:A:302:LEU:HD13	2:A:302:LEU:HA	1.73	0.41
3:B:1113:POV:H11A	3:B:1113:POV:H15A	1.71	0.41
2:D:40:ILE:HG12	6:D:1109:CLR:H183	2.02	0.41
1:G:159:SER:HA	1:G:162:ASN:HD21	1.85	0.41
1:H:199:VAL:HG13	3:D:1101:POV:H28	2.03	0.41
3:A:1101:POV:H24	3:A:1101:POV:H27	1.41	0.41
6:A:1108:CLR:H182	6:A:1108:CLR:H8	1.76	0.41
6:A:1109:CLR:H182	6:A:1109:CLR:H8	1.79	0.41
3:A:1116:POV:H36A	3:A:1116:POV:H39A	1.57	0.41
3:C:1111:POV:H32A	3:C:1111:POV:H35	1.75	0.41
3:C:1113:POV:H37	3:C:1113:POV:H34	1.79	0.41
2:D:252:PHE:CG	3:D:1107:POV:H21B	2.56	0.41
2:B:23:TRP:CZ3	6:B:1109:CLR:C7	3.03	0.41
3:B:1106:POV:H29	3:B:1106:POV:H26A	1.88	0.41
2:C:21:MET:CE	6:C:1108:CLR:H42	2.51	0.41
2:C:298:THR:O	2:C:302:LEU:HD22	2.20	0.41
6:C:1108:CLR:H8	6:C:1108:CLR:H182	1.80	0.41
3:A:1106:POV:H211	3:A:1106:POV:H28A	1.79	0.41
3:A:1116:POV:C314	3:D:1102:POV:H31F	2.42	0.41
2:B:174:LYS:HG3	6:B:1108:CLR:H8	2.01	0.41
2:D:232:SER:OG	3:D:1113:POV:N	2.54	0.41
6:D:1109:CLR:H263	6:D:1109:CLR:H231	1.60	0.41
1:E:199:VAL:HG13	3:A:1101:POV:H28	2.03	0.41
1:F:199:VAL:HG13	3:B:1101:POV:H28	2.02	0.41
2:A:263:TRP:CD1	2:A:263:TRP:N	2.85	0.41
3:A:1115:POV:H11A	3:A:1115:POV:H13A	1.67	0.41
2:C:38:PHE:O	2:C:42:LEU:HG	2.20	0.41
2:A:22:TRP:HZ2	3:A:1101:POV:H27A	1.86	0.41
2:A:331:LYS:HB2	2:A:331:LYS:HE3	1.82	0.41
3:A:1116:POV:H26A	3:A:1116:POV:H23A	1.88	0.41
1:H:159:SER:HA	1:H:162:ASN:HD21	1.85	0.41
1:H:196:ASP:OD1	1:H:196:ASP:N	2.53	0.41
2:A:299:LEU:HD23	2:A:299:LEU:HA	1.91	0.41
2:A:890:PHE:CE2	2:D:442:MET:CE	3.03	0.41
3:A:1105:POV:O31	3:A:1105:POV:H34A	2.20	0.41
6:A:1108:CLR:C7	6:A:1108:CLR:H191	2.51	0.41
3:C:1113:POV:H28	1:G:199:VAL:HG13	2.03	0.41
2:D:742:ARG:HA	2:D:742:ARG:HD3	1.93	0.41
6:D:1109:CLR:H182	6:D:1109:CLR:H8	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:8:ARG:H	1:G:8:ARG:CD	2.34	0.41
2:B:38:PHE:O	2:B:42:LEU:HG	2.20	0.41
2:B:438:ALA:HB1	2:C:818:LYS:HE2	2.03	0.41
2:C:956:GLU:OE1	2:C:960:ARG:HD3	2.20	0.41
6:C:1107:CLR:H8	6:C:1107:CLR:H182	1.78	0.41
3:C:1113:POV:H36A	3:C:1113:POV:H39A	1.50	0.41
2:D:129:ILE:HD11	3:D:1111:POV:H25	2.03	0.41
2:D:956:GLU:OE1	2:D:960:ARG:HD3	2.20	0.41
3:D:1111:POV:H3	1:G:70:LEU:CD1	2.49	0.41
1:H:151:ARG:NH2	1:G:188:ASP:OD1	2.47	0.40
2:D:38:PHE:O	2:D:42:LEU:HG	2.20	0.40
1:F:38:THR:HG23	1:F:40:LEU:N	2.37	0.40
2:A:971:ASN:O	2:A:974:ARG:HD3	2.21	0.40
2:B:113:ARG:HG3	3:B:1105:POV:H24A	2.04	0.40
2:D:790:ARG:NH1	2:D:831:GLN:O	2.33	0.40
1:H:70:LEU:HD13	3:A:1114:POV:H32A	2.02	0.40
2:A:199:LEU:HD21	6:A:1109:CLR:C2	2.45	0.40
1:H:38:THR:HG23	1:H:40:LEU:N	2.37	0.40
2:C:174:LYS:HG3	6:C:1107:CLR:H191	1.95	0.40
2:C:342:ARG:HE	2:C:342:ARG:HB2	1.45	0.40
2:D:971:ASN:O	2:D:974:ARG:HD3	2.21	0.40
1:E:193:ARG:HA	1:E:193:ARG:HD2	1.96	0.40
2:A:103:VAL:HA	2:B:396:THR:HG21	2.03	0.40
3:A:1116:POV:H314	3:D:1102:POV:C315	2.43	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	198/239 (83%)	186 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	198/239 (83%)	186 (94%)	12 (6%)	0	100	100
1	G	203/239 (85%)	190 (94%)	13 (6%)	0	100	100
1	H	198/239 (83%)	186 (94%)	12 (6%)	0	100	100
2	A	878/1056 (83%)	843 (96%)	29 (3%)	6 (1%)	19	36
2	B	878/1056 (83%)	843 (96%)	29 (3%)	6 (1%)	19	36
2	C	878/1056 (83%)	843 (96%)	29 (3%)	6 (1%)	19	36
2	D	878/1056 (83%)	843 (96%)	29 (3%)	6 (1%)	19	36
All	All	4309/5180 (83%)	4120 (96%)	165 (4%)	24 (1%)	24	41

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	370	ASP
2	B	370	ASP
2	C	370	ASP
2	D	370	ASP
2	A	566	ILE
2	B	566	ILE
2	C	566	ILE
2	D	566	ILE
2	A	1003	ALA
2	B	1003	ALA
2	C	1003	ALA
2	D	1003	ALA
2	A	814	SER
2	B	814	SER
2	C	814	SER
2	D	814	SER
2	A	997	GLY
2	B	997	GLY
2	C	997	GLY
2	D	997	GLY
2	A	697	PRO
2	B	697	PRO
2	C	697	PRO
2	D	697	PRO

5.3.2 Protein sidechains (i)

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	E	180/218 (83%)	176 (98%)	4 (2%)	47	70
1	F	180/218 (83%)	176 (98%)	4 (2%)	47	70
1	G	186/218 (85%)	179 (96%)	7 (4%)	28	52
1	H	180/218 (83%)	176 (98%)	4 (2%)	47	70
2	A	782/928 (84%)	758 (97%)	24 (3%)	35	59
2	B	782/928 (84%)	758 (97%)	24 (3%)	35	59
2	C	782/928 (84%)	758 (97%)	24 (3%)	35	59
2	D	782/928 (84%)	758 (97%)	24 (3%)	35	59
All	All	3854/4584 (84%)	3739 (97%)	115 (3%)	37	60

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	37	VAL
1	E	38	THR
1	E	151	ARG
1	E	178	CYS
1	F	37	VAL
1	F	38	THR
1	F	151	ARG
1	F	178	CYS
1	H	37	VAL
1	H	38	THR
1	H	151	ARG
1	H	178	CYS
2	A	17	ARG
2	A	45	THR
2	A	263	TRP
2	A	292	ASP
2	A	302	LEU
2	A	342	ARG
2	A	365	HIS

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Mol	Chain	Res	Type
2	A	386	GLU
2	A	442	MET
2	A	568	ILE
2	A	588	LYS
2	A	593	THR
2	A	735	ARG
2	A	771	HIS
2	A	786	ARG
2	A	790	ARG
2	A	811	ASP
2	A	889	GLN
2	A	960	ARG
2	A	974	ARG
2	A	999	LEU
2	A	1001	CYS
2	A	1002	LYS
2	A	1026	SER
2	B	17	ARG
2	B	45	THR
2	B	263	TRP
2	B	292	ASP
2	B	302	LEU
2	B	342	ARG
2	B	365	HIS
2	B	386	GLU
2	B	442	MET
2	B	568	ILE
2	B	588	LYS
2	B	593	THR
2	B	735	ARG
2	B	771	HIS
2	B	786	ARG
2	B	790	ARG
2	B	811	ASP
2	B	889	GLN
2	B	960	ARG
2	B	974	ARG
2	B	999	LEU
2	B	1001	CYS
2	B	1002	LYS
2	B	1026	SER
2	C	17	ARG

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Mol	Chain	Res	Type
2	C	45	THR
2	C	263	TRP
2	C	292	ASP
2	C	302	LEU
2	C	342	ARG
2	C	365	HIS
2	C	386	GLU
2	C	442	MET
2	C	568	ILE
2	C	588	LYS
2	C	593	THR
2	C	735	ARG
2	C	771	HIS
2	C	786	ARG
2	C	790	ARG
2	C	811	ASP
2	C	889	GLN
2	C	960	ARG
2	C	974	ARG
2	C	999	LEU
2	C	1001	CYS
2	C	1002	LYS
2	C	1026	SER
2	D	17	ARG
2	D	45	THR
2	D	263	TRP
2	D	292	ASP
2	D	302	LEU
2	D	342	ARG
2	D	365	HIS
2	D	386	GLU
2	D	442	MET
2	D	568	ILE
2	D	588	LYS
2	D	593	THR
2	D	735	ARG
2	D	771	HIS
2	D	786	ARG
2	D	790	ARG
2	D	811	ASP
2	D	889	GLN
2	D	960	ARG

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Mol	Chain	Res	Type
2	D	974	ARG
2	D	999	LEU
2	D	1001	CYS
2	D	1002	LYS
2	D	1026	SER
1	G	2	PHE
1	G	4	TRP
1	G	8	ARG
1	G	37	VAL
1	G	38	THR
1	G	151	ARG
1	G	178	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	116	GLN
2	A	108	GLN
2	A	157	ASN
2	A	409	HIS
2	A	718	HIS
2	A	771	HIS
2	B	157	ASN
2	B	718	HIS
2	B	771	HIS
2	C	157	ASN
2	C	771	HIS
2	C	893	GLN
2	D	157	ASN
2	D	771	HIS

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 56 ligands modelled in this entry, 16 are monoatomic - leaving 40 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	$\#\|Z\| > 2$
3	POV	A	1101	-	36,36,51	1.05	2 (5%)	37,37,59	1.02	2 (5%)
3	POV	C	1112	-	36,36,51	1.12	2 (5%)	39,41,59	1.26	4 (10%)
3	POV	D	1107	-	35,35,51	0.59	0	41,43,59	0.52	0
3	POV	A	1107	-	23,23,51	1.12	2 (8%)	28,30,59	3.06	8 (28%)
3	POV	D	1101	-	36,36,51	1.06	2 (5%)	37,37,59	1.01	2 (5%)
3	POV	C	1111	-	39,39,51	1.09	2 (5%)	45,47,59	1.11	4 (8%)
3	POV	D	1106	-	30,30,51	1.22	2 (6%)	33,35,59	1.33	4 (12%)
3	POV	A	1116	-	39,39,51	1.08	2 (5%)	45,47,59	1.12	4 (8%)
3	POV	B	1105	-	30,30,51	1.22	2 (6%)	33,35,59	1.32	4 (12%)
6	CLR	A	1108	-	31,31,31	0.76	1 (3%)	48,48,48	5.18	13 (27%)
3	POV	C	1106	-	23,23,51	1.12	2 (8%)	28,30,59	3.06	8 (28%)
3	POV	B	1110	-	38,38,51	0.69	1 (2%)	41,43,59	0.84	2 (4%)
3	POV	B	1107	-	23,23,51	0.79	1 (4%)	28,30,59	0.79	1 (3%)
3	POV	B	1113	-	39,39,51	1.09	2 (5%)	45,47,59	1.12	4 (8%)
3	POV	C	1109	-	34,34,51	1.15	2 (5%)	40,42,59	2.57	9 (22%)
6	CLR	D	1109	-	31,31,31	0.84	2 (6%)	48,48,48	1.58	7 (14%)
3	POV	A	1105	-	30,30,51	1.22	2 (6%)	33,35,59	1.33	4 (12%)
3	POV	D	1102	-	38,38,51	0.69	1 (2%)	41,43,59	0.84	2 (4%)
3	POV	C	1105	-	35,35,51	1.13	2 (5%)	41,43,59	2.54	9 (21%)
3	POV	B	1111	-	34,34,51	1.15	2 (5%)	40,42,59	2.58	9 (22%)
3	POV	A	1114	-	34,34,51	1.15	2 (5%)	40,42,59	2.57	9 (22%)
6	CLR	B	1109	-	31,31,31	0.82	2 (6%)	48,48,48	1.55	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CLR	D	1110	-	31,31,31	0.83	2 (6%)	48,48,48	1.50	8 (16%)
6	CLR	C	1108	-	31,31,31	0.84	2 (6%)	48,48,48	1.51	8 (16%)
3	POV	C	1104	-	30,30,51	1.23	2 (6%)	33,35,59	1.29	4 (12%)
3	POV	B	1101	-	36,36,51	1.06	2 (5%)	37,37,59	1.02	2 (5%)
3	POV	D	1108	-	23,23,51	1.12	2 (8%)	28,30,59	3.04	8 (28%)
3	POV	D	1112	-	31,31,51	1.22	2 (6%)	37,39,59	1.19	4 (10%)
3	POV	C	1113	-	36,36,51	1.06	2 (5%)	37,37,59	1.01	2 (5%)
3	POV	B	1114	-	35,35,51	0.72	1 (2%)	38,40,59	0.87	2 (5%)
3	POV	A	1106	-	35,35,51	1.13	2 (5%)	41,43,59	2.54	9 (21%)
6	CLR	A	1109	-	31,31,31	0.83	2 (6%)	48,48,48	1.54	8 (16%)
3	POV	B	1112	-	31,31,51	1.22	2 (6%)	37,39,59	1.15	3 (8%)
3	POV	C	1110	-	31,31,51	1.22	2 (6%)	37,39,59	1.19	4 (10%)
6	CLR	C	1107	-	31,31,31	0.83	2 (6%)	48,48,48	1.55	8 (16%)
3	POV	D	1111	-	34,34,51	1.15	2 (5%)	40,42,59	2.58	10 (25%)
6	CLR	B	1108	-	31,31,31	0.85	2 (6%)	48,48,48	1.56	8 (16%)
3	POV	D	1113	-	35,35,51	1.10	2 (5%)	38,40,59	1.15	3 (7%)
3	POV	A	1115	-	31,31,51	1.22	2 (6%)	37,39,59	1.19	3 (8%)
3	POV	B	1106	-	35,35,51	1.13	2 (5%)	41,43,59	2.54	9 (21%)

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
3	POV	A	1101	-	-	15/36/36/55	-
3	POV	C	1112	-	-	17/38/38/55	-
3	POV	D	1107	-	-	12/39/39/55	-
3	POV	A	1107	-	-	11/25/25/55	-
3	POV	D	1101	-	-	15/36/36/55	-
3	POV	C	1111	-	-	16/43/43/55	-
3	POV	D	1106	-	-	14/32/32/55	-
3	POV	A	1116	-	-	17/43/43/55	-
3	POV	B	1105	-	-	22/32/32/55	-
6	CLR	A	1108	-	-	6/10/68/68	0/4/4/4
3	POV	C	1106	-	-	8/25/25/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	B	1110	-	-	7/40/40/55	-
3	POV	B	1107	-	-	5/25/25/55	-
3	POV	B	1113	-	-	17/43/43/55	-
3	POV	C	1109	-	-	23/38/38/55	-
6	CLR	D	1109	-	-	8/10/68/68	0/4/4/4
3	POV	A	1105	-	-	17/32/32/55	-
3	POV	D	1102	-	-	7/40/40/55	-
3	POV	C	1105	-	-	16/39/39/55	-
3	POV	B	1111	-	-	18/38/38/55	-
3	POV	A	1114	-	-	18/38/38/55	-
6	CLR	B	1109	-	-	3/10/68/68	0/4/4/4
6	CLR	D	1110	-	-	3/10/68/68	0/4/4/4
6	CLR	C	1108	-	-	4/10/68/68	0/4/4/4
3	POV	C	1104	-	-	13/32/32/55	-
3	POV	B	1101	-	-	15/36/36/55	-
3	POV	D	1108	-	-	11/25/25/55	-
3	POV	D	1112	-	-	12/35/35/55	-
3	POV	C	1113	-	-	15/36/36/55	-
3	POV	B	1114	-	-	6/37/37/55	-
3	POV	A	1106	-	-	22/39/39/55	-
6	CLR	A	1109	-	-	4/10/68/68	0/4/4/4
3	POV	B	1112	-	-	11/35/35/55	-
3	POV	C	1110	-	-	18/35/35/55	-
6	CLR	C	1107	-	-	5/10/68/68	0/4/4/4
3	POV	D	1111	-	-	19/38/38/55	-
6	CLR	B	1108	-	-	6/10/68/68	0/4/4/4
3	POV	D	1113	-	-	22/39/39/55	-
3	POV	A	1115	-	-	14/35/35/55	-
3	POV	B	1106	-	-	18/39/39/55	-

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1115	POV	O31-C31	4.32	1.45	1.33
3	D	1101	POV	O21-C21	4.31	1.45	1.33
3	D	1112	POV	O31-C31	4.31	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1106	POV	O31-C31	4.31	1.45	1.33
3	B	1101	POV	O21-C21	4.31	1.45	1.33
3	B	1105	POV	O31-C31	4.31	1.45	1.33
3	C	1109	POV	O31-C31	4.30	1.45	1.33
3	A	1114	POV	O31-C31	4.30	1.45	1.33
3	C	1110	POV	O31-C31	4.29	1.45	1.33
3	A	1105	POV	O31-C31	4.29	1.45	1.33
3	C	1105	POV	O31-C31	4.29	1.45	1.33
3	A	1101	POV	O21-C21	4.29	1.45	1.33
3	C	1113	POV	O31-C31	4.29	1.45	1.33
3	C	1113	POV	O21-C21	4.28	1.45	1.33
3	B	1112	POV	O31-C31	4.28	1.45	1.33
3	B	1106	POV	O31-C31	4.27	1.45	1.33
3	B	1113	POV	O31-C31	4.27	1.45	1.33
3	B	1111	POV	O31-C31	4.27	1.45	1.33
3	D	1106	POV	O31-C31	4.27	1.45	1.33
3	D	1111	POV	O31-C31	4.27	1.45	1.33
3	C	1104	POV	O31-C31	4.27	1.45	1.33
3	D	1113	POV	O31-C31	4.27	1.45	1.33
3	A	1101	POV	O31-C31	4.27	1.45	1.33
3	D	1101	POV	O31-C31	4.26	1.45	1.33
3	A	1116	POV	O31-C31	4.26	1.45	1.33
3	C	1111	POV	O31-C31	4.25	1.45	1.33
3	B	1101	POV	O31-C31	4.25	1.45	1.33
3	C	1112	POV	O31-C31	4.25	1.45	1.33
3	C	1104	POV	O21-C21	4.16	1.46	1.34
3	B	1112	POV	O21-C21	4.16	1.46	1.34
3	D	1106	POV	O21-C21	4.12	1.45	1.34
3	D	1111	POV	O21-C21	4.12	1.45	1.34
3	D	1108	POV	O21-C21	4.10	1.45	1.34
3	D	1112	POV	O21-C21	4.10	1.45	1.34
3	A	1105	POV	O21-C21	4.10	1.45	1.34
3	C	1112	POV	O21-C21	4.09	1.45	1.34
3	B	1105	POV	O21-C21	4.09	1.45	1.34
3	A	1107	POV	O21-C21	4.09	1.45	1.34
3	B	1111	POV	O21-C21	4.09	1.45	1.34
3	C	1110	POV	O21-C21	4.09	1.45	1.34
3	A	1115	POV	O21-C21	4.09	1.45	1.34
3	A	1114	POV	O21-C21	4.08	1.45	1.34
3	C	1106	POV	O21-C21	4.08	1.45	1.34
3	D	1113	POV	O21-C21	4.08	1.45	1.34
3	B	1106	POV	O21-C21	4.08	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1109	POV	O21-C21	4.08	1.45	1.34
3	A	1106	POV	O21-C21	4.06	1.45	1.34
3	B	1113	POV	O21-C21	4.06	1.45	1.34
3	C	1105	POV	O21-C21	4.06	1.45	1.34
3	C	1111	POV	O21-C21	4.05	1.45	1.34
3	A	1116	POV	O21-C21	4.04	1.45	1.34
3	B	1114	POV	P-O12	3.05	1.66	1.54
3	B	1110	POV	P-O12	3.05	1.66	1.54
3	D	1102	POV	P-O12	3.04	1.66	1.54
3	C	1106	POV	O21-C2	-2.37	1.43	1.47
3	A	1107	POV	O21-C2	-2.37	1.43	1.47
3	D	1108	POV	O21-C2	-2.35	1.43	1.47
3	B	1107	POV	O21-C2	-2.21	1.43	1.47
6	C	1108	CLR	C10-C9	-2.21	1.52	1.56
6	A	1109	CLR	C10-C9	-2.19	1.52	1.56
6	D	1109	CLR	C10-C9	-2.17	1.52	1.56
6	D	1110	CLR	C10-C9	-2.15	1.52	1.56
6	C	1107	CLR	C10-C9	-2.15	1.52	1.56
6	B	1108	CLR	C10-C9	-2.14	1.52	1.56
6	B	1109	CLR	C10-C9	-2.13	1.52	1.56
6	B	1108	CLR	C13-C14	-2.09	1.51	1.55
6	C	1107	CLR	C13-C14	-2.06	1.51	1.55
6	B	1109	CLR	C13-C14	-2.04	1.51	1.55
6	C	1108	CLR	C13-C14	-2.04	1.51	1.55
6	D	1109	CLR	C13-C14	-2.04	1.51	1.55
6	A	1109	CLR	C13-C14	-2.02	1.51	1.55
6	A	1108	CLR	C13-C14	-2.01	1.51	1.55
6	D	1110	CLR	C13-C14	-2.01	1.51	1.55

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1108	CLR	C19-C10-C9	-23.26	85.56	111.66
6	A	1108	CLR	C19-C10-C1	-15.66	85.61	109.43
6	A	1108	CLR	C19-C10-C5	-15.50	84.70	108.38
6	A	1108	CLR	C1-C10-C9	8.74	120.31	108.74
3	D	1108	POV	C15-N-C14	-8.62	86.33	108.98
3	A	1107	POV	C15-N-C14	-8.61	86.36	108.98
3	B	1111	POV	C15-N-C14	-8.60	86.39	108.98
3	C	1106	POV	C15-N-C14	-8.60	86.40	108.98
3	C	1105	POV	C15-N-C13	-8.59	86.40	108.98
3	A	1114	POV	C15-N-C13	-8.59	86.40	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1106	POV	C15-N-C14	-8.58	86.44	108.98
3	D	1111	POV	C15-N-C13	-8.57	86.45	108.98
3	C	1105	POV	C15-N-C14	-8.57	86.46	108.98
3	B	1111	POV	C15-N-C13	-8.57	86.47	108.98
3	C	1109	POV	C15-N-C13	-8.56	86.48	108.98
3	A	1114	POV	C15-N-C14	-8.56	86.48	108.98
3	D	1111	POV	C15-N-C14	-8.56	86.48	108.98
3	B	1106	POV	C15-N-C13	-8.56	86.50	108.98
3	B	1106	POV	C15-N-C14	-8.55	86.51	108.98
3	A	1107	POV	C15-N-C13	-8.55	86.52	108.98
3	C	1109	POV	C15-N-C14	-8.55	86.53	108.98
3	A	1106	POV	C15-N-C13	-8.54	86.55	108.98
3	C	1106	POV	C15-N-C13	-8.54	86.55	108.98
3	D	1108	POV	C15-N-C13	-8.52	86.59	108.98
6	A	1108	CLR	C1-C10-C5	6.46	119.88	108.74
3	B	1106	POV	C15-N-C12	-5.91	86.43	109.91
3	D	1111	POV	C15-N-C12	-5.90	86.48	109.91
3	A	1106	POV	C15-N-C12	-5.89	86.49	109.91
3	A	1114	POV	C15-N-C12	-5.89	86.49	109.91
3	C	1109	POV	C15-N-C12	-5.89	86.50	109.91
3	C	1105	POV	C15-N-C12	-5.87	86.57	109.91
3	C	1106	POV	C15-N-C12	-5.87	86.57	109.91
3	B	1111	POV	C15-N-C12	-5.87	86.59	109.91
3	D	1108	POV	C15-N-C12	-5.86	86.60	109.91
3	A	1107	POV	C15-N-C12	-5.86	86.61	109.91
6	A	1108	CLR	C9-C10-C5	5.57	117.81	109.65
6	A	1108	CLR	C13-C17-C20	-4.93	111.89	119.50
6	D	1109	CLR	C13-C17-C20	-4.90	111.92	119.50
6	B	1108	CLR	C13-C17-C20	-4.87	111.97	119.50
6	A	1109	CLR	C13-C17-C20	-4.71	112.23	119.50
6	B	1109	CLR	C13-C17-C20	-4.68	112.27	119.50
6	C	1107	CLR	C13-C17-C20	-4.67	112.28	119.50
6	C	1108	CLR	C13-C17-C20	-4.65	112.32	119.50
6	D	1110	CLR	C13-C17-C20	-4.57	112.44	119.50
6	A	1108	CLR	C13-C14-C8	-4.40	108.16	114.41
6	D	1109	CLR	C13-C14-C8	-4.32	108.28	114.41
6	B	1108	CLR	C13-C14-C8	-4.22	108.42	114.41
3	C	1106	POV	C2-O21-C21	-4.14	111.81	117.78
3	D	1112	POV	O21-C21-C22	4.13	120.41	111.48
6	C	1107	CLR	C13-C14-C8	-4.11	108.57	114.41
3	D	1111	POV	O21-C21-C22	4.11	120.38	111.48
6	B	1109	CLR	C13-C14-C8	-4.10	108.59	114.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1112	POV	O21-C21-C22	4.10	120.35	111.48
3	A	1107	POV	C14-N-C13	4.10	119.74	108.98
3	B	1111	POV	O21-C21-C22	4.10	120.34	111.48
3	A	1107	POV	C2-O21-C21	-4.08	111.89	117.78
3	A	1107	POV	O21-C21-C22	4.08	120.31	111.48
3	B	1111	POV	C14-N-C13	4.08	119.69	108.98
3	D	1108	POV	C14-N-C13	4.08	119.69	108.98
3	A	1115	POV	O21-C21-C22	4.07	120.30	111.48
3	B	1106	POV	O21-C21-C22	4.07	120.29	111.48
3	C	1105	POV	O21-C21-C22	4.07	120.28	111.48
3	C	1106	POV	C14-N-C13	4.07	119.66	108.98
3	C	1106	POV	O21-C21-C22	4.06	120.27	111.48
3	C	1105	POV	C14-N-C13	4.06	119.64	108.98
3	C	1109	POV	C14-N-C13	4.06	119.64	108.98
3	D	1111	POV	C14-N-C13	4.06	119.63	108.98
3	A	1106	POV	C14-N-C13	4.05	119.63	108.98
3	A	1106	POV	O21-C21-C22	4.05	120.24	111.48
3	C	1109	POV	O21-C21-C22	4.05	120.24	111.48
3	A	1116	POV	O21-C21-C22	4.04	120.21	111.48
3	B	1106	POV	C14-N-C13	4.03	119.57	108.98
3	D	1106	POV	O21-C21-C22	4.03	120.20	111.48
3	C	1110	POV	O21-C21-C22	4.03	120.20	111.48
3	A	1114	POV	C14-N-C13	4.03	119.56	108.98
6	A	1109	CLR	C13-C14-C8	-4.03	108.70	114.41
3	D	1113	POV	O21-C21-C22	4.02	120.18	111.48
3	D	1108	POV	O21-C21-C22	4.02	120.18	111.48
3	B	1113	POV	O21-C21-C22	4.02	120.18	111.48
3	C	1111	POV	O21-C21-C22	4.01	120.17	111.48
3	A	1114	POV	O21-C21-C22	4.01	120.16	111.48
3	A	1105	POV	O21-C21-C22	3.98	120.10	111.48
3	D	1108	POV	C2-O21-C21	-3.95	112.08	117.78
3	B	1105	POV	O21-C21-C22	3.93	119.99	111.48
3	B	1112	POV	O21-C21-C22	3.93	119.98	111.48
3	C	1104	POV	O21-C21-C22	3.90	119.91	111.48
6	C	1108	CLR	C13-C14-C8	-3.84	108.96	114.41
6	D	1110	CLR	C13-C14-C8	-3.81	109.00	114.41
6	B	1108	CLR	C17-C13-C14	3.59	104.22	100.10
6	D	1109	CLR	C17-C13-C14	3.42	104.02	100.10
6	C	1107	CLR	C17-C13-C14	3.39	103.99	100.10
6	A	1108	CLR	C17-C13-C14	3.38	103.98	100.10
6	B	1109	CLR	C17-C13-C14	3.37	103.97	100.10
3	B	1110	POV	O12-P-O11	-3.32	98.02	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1102	POV	O12-P-O11	-3.32	98.02	106.67
3	B	1114	POV	O12-P-O11	-3.31	98.03	106.67
6	A	1108	CLR	C4-C5-C10	3.18	120.49	116.42
6	A	1109	CLR	C4-C5-C10	3.01	120.28	116.42
6	A	1109	CLR	C17-C13-C14	3.00	103.54	100.10
6	C	1108	CLR	C17-C13-C14	2.98	103.52	100.10
6	D	1110	CLR	C17-C13-C14	2.93	103.46	100.10
6	C	1107	CLR	C11-C12-C13	-2.89	107.87	112.74
6	B	1108	CLR	C11-C12-C13	-2.85	107.92	112.74
6	C	1108	CLR	C4-C5-C10	2.84	120.06	116.42
6	D	1109	CLR	C11-C12-C13	-2.84	107.95	112.74
6	B	1109	CLR	C4-C5-C10	2.82	120.03	116.42
3	B	1113	POV	O31-C31-C32	2.79	120.33	111.83
3	A	1116	POV	O31-C31-C32	2.78	120.32	111.83
3	A	1106	POV	O31-C31-C32	2.78	120.32	111.83
3	C	1112	POV	O31-C31-C32	2.78	120.31	111.83
3	B	1112	POV	O31-C31-C32	2.77	120.29	111.83
3	D	1113	POV	O31-C31-C32	2.77	120.27	111.83
3	B	1105	POV	O31-C31-C32	2.76	120.26	111.83
3	A	1105	POV	O31-C31-C32	2.76	120.24	111.83
3	A	1115	POV	O31-C31-C32	2.75	120.23	111.83
3	B	1111	POV	O31-C31-C32	2.75	120.22	111.83
3	A	1114	POV	O31-C31-C32	2.75	120.21	111.83
6	A	1108	CLR	C11-C12-C13	-2.74	108.11	112.74
3	D	1111	POV	O31-C31-C32	2.74	120.20	111.83
3	D	1106	POV	O31-C31-C32	2.74	120.19	111.83
3	C	1105	POV	O31-C31-C32	2.74	120.18	111.83
6	D	1110	CLR	C4-C5-C10	2.73	119.92	116.42
3	C	1104	POV	O31-C31-C32	2.73	120.16	111.83
3	C	1110	POV	O31-C31-C32	2.73	120.16	111.83
3	B	1106	POV	O31-C31-C32	2.73	120.15	111.83
3	C	1111	POV	O31-C31-C32	2.73	120.15	111.83
3	D	1101	POV	O21-C21-C22	2.72	120.13	111.83
3	A	1101	POV	O21-C21-C22	2.72	120.12	111.83
3	C	1113	POV	O21-C21-C22	2.72	120.12	111.83
3	B	1101	POV	O21-C21-C22	2.72	120.12	111.83
3	C	1109	POV	O31-C31-C32	2.71	120.10	111.83
3	B	1101	POV	O31-C31-C32	2.71	120.09	111.83
3	D	1112	POV	O31-C31-C32	2.71	120.09	111.83
3	A	1101	POV	O31-C31-C32	2.70	120.07	111.83
3	D	1101	POV	O31-C31-C32	2.69	120.05	111.83
3	C	1113	POV	O31-C31-C32	2.69	120.02	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1109	CLR	C11-C12-C13	-2.68	108.22	112.74
6	D	1109	CLR	C4-C5-C10	2.65	119.82	116.42
6	C	1108	CLR	C11-C12-C13	-2.65	108.27	112.74
3	B	1110	POV	O13-P-O14	2.63	121.07	110.83
3	D	1102	POV	O13-P-O14	2.62	121.05	110.83
3	B	1114	POV	O13-P-O14	2.62	121.05	110.83
3	B	1107	POV	O21-C2-C1	2.59	112.17	106.21
6	A	1109	CLR	C11-C12-C13	-2.59	108.37	112.74
6	C	1107	CLR	C4-C5-C10	2.55	119.69	116.42
3	C	1111	POV	C2-O21-C21	-2.55	111.70	117.80
3	B	1111	POV	C2-O21-C21	-2.53	111.75	117.80
3	C	1105	POV	C2-O21-C21	-2.52	111.76	117.80
3	C	1110	POV	C2-O21-C21	-2.52	111.76	117.80
3	A	1105	POV	C2-O21-C21	-2.51	111.78	117.80
3	A	1106	POV	C2-O21-C21	-2.50	111.82	117.80
6	D	1110	CLR	C11-C12-C13	-2.49	108.53	112.74
3	D	1106	POV	C2-O21-C21	-2.49	111.85	117.80
3	A	1115	POV	C2-O21-C21	-2.48	111.87	117.80
3	C	1109	POV	C13-N-C12	2.47	119.75	109.91
3	A	1116	POV	C2-O21-C21	-2.47	111.89	117.80
3	D	1111	POV	C2-O21-C21	-2.46	111.90	117.80
3	B	1106	POV	C2-O21-C21	-2.46	111.90	117.80
3	B	1113	POV	C2-O21-C21	-2.46	111.91	117.80
3	D	1111	POV	C13-N-C12	2.46	119.68	109.91
3	B	1105	POV	C2-O21-C21	-2.46	111.91	117.80
3	D	1112	POV	C2-O21-C21	-2.46	111.91	117.80
3	A	1106	POV	C14-N-C12	2.46	119.68	109.91
3	D	1108	POV	C14-N-C12	2.46	119.67	109.91
3	A	1114	POV	C13-N-C12	2.46	119.67	109.91
3	B	1106	POV	C14-N-C12	2.45	119.67	109.91
3	C	1106	POV	C14-N-C12	2.45	119.66	109.91
3	C	1112	POV	C2-O21-C21	-2.45	111.93	117.80
3	B	1106	POV	C13-N-C12	2.45	119.64	109.91
3	A	1114	POV	C14-N-C12	2.45	119.64	109.91
3	C	1105	POV	C13-N-C12	2.44	119.63	109.91
3	C	1105	POV	C14-N-C12	2.44	119.61	109.91
3	B	1111	POV	C13-N-C12	2.44	119.61	109.91
3	C	1109	POV	C2-O21-C21	-2.44	111.97	117.80
3	A	1107	POV	C13-N-C12	2.44	119.59	109.91
3	B	1111	POV	C14-N-C12	2.43	119.59	109.91
3	A	1106	POV	C13-N-C12	2.43	119.58	109.91
3	C	1106	POV	C13-N-C12	2.43	119.57	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1107	POV	C14-N-C12	2.43	119.56	109.91
3	D	1111	POV	C14-N-C12	2.43	119.56	109.91
6	D	1110	CLR	C7-C6-C5	-2.42	120.93	125.02
3	D	1108	POV	C13-N-C12	2.42	119.54	109.91
3	A	1114	POV	C2-O21-C21	-2.42	112.01	117.80
3	C	1109	POV	C14-N-C12	2.41	119.51	109.91
6	C	1108	CLR	C7-C6-C5	-2.38	121.00	125.02
6	A	1109	CLR	C10-C5-C6	-2.37	119.47	122.93
6	A	1109	CLR	C7-C6-C5	-2.36	121.03	125.02
3	C	1112	POV	O13-P-O14	2.35	119.97	110.83
3	A	1105	POV	O13-P-O14	2.34	119.97	110.83
3	C	1104	POV	O13-P-O14	2.34	119.95	110.83
3	D	1106	POV	O13-P-O14	2.33	119.92	110.83
3	B	1105	POV	O13-P-O14	2.33	119.91	110.83
6	D	1110	CLR	C7-C8-C9	2.32	112.40	109.72
6	A	1109	CLR	C7-C8-C9	2.31	112.39	109.72
3	D	1113	POV	C2-O21-C21	-2.30	112.28	117.80
6	A	1108	CLR	C10-C9-C8	-2.29	109.36	112.71
6	C	1108	CLR	C10-C5-C6	-2.28	119.60	122.93
6	A	1108	CLR	C8-C7-C6	-2.27	109.62	112.76
6	C	1108	CLR	C7-C8-C9	2.24	112.31	109.72
6	B	1109	CLR	C7-C6-C5	-2.22	121.27	125.02
6	D	1110	CLR	C10-C5-C6	-2.22	119.69	122.93
6	B	1109	CLR	C10-C5-C6	-2.21	119.70	122.93
6	B	1109	CLR	C7-C8-C9	2.16	112.22	109.72
6	C	1107	CLR	C7-C6-C5	-2.13	121.42	125.02
3	B	1112	POV	C2-O21-C21	-2.11	112.74	117.80
6	B	1108	CLR	C4-C5-C10	2.08	119.09	116.42
6	D	1109	CLR	C7-C6-C5	-2.08	121.50	125.02
3	C	1104	POV	C2-O21-C21	-2.07	112.83	117.80
3	C	1111	POV	C11-C12-N	-2.06	109.20	115.82
3	A	1116	POV	C11-C12-N	-2.03	109.30	115.82
6	C	1107	CLR	C7-C8-C9	2.03	112.07	109.72
6	B	1108	CLR	C7-C8-C9	2.03	112.06	109.72
3	D	1111	POV	O21-C21-O22	-2.03	118.97	123.70
6	B	1108	CLR	C3-C4-C5	-2.02	108.83	112.05
3	D	1112	POV	O21-C21-O22	-2.02	118.98	123.70
6	B	1109	CLR	C3-C4-C5	-2.02	108.84	112.05
3	B	1113	POV	C11-C12-N	-2.01	109.36	115.82
6	D	1109	CLR	C7-C8-C9	2.01	112.04	109.72
6	C	1107	CLR	C10-C5-C6	-2.01	120.00	122.93
3	C	1110	POV	C11-C12-N	-2.00	109.39	115.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1108	CLR	C1-C10-C9	2.00	111.38	108.74

There are no chirality outliers.

All (510) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1105	POV	C1-O11-P-O12
3	A	1105	POV	C22-C21-O21-C2
3	A	1106	POV	C1-O11-P-O12
3	A	1106	POV	C1-O11-P-O13
3	A	1106	POV	C1-O11-P-O14
3	A	1106	POV	C11-O12-P-O11
3	A	1106	POV	C11-O12-P-O13
3	A	1107	POV	C11-O12-P-O11
3	A	1107	POV	C11-O12-P-O14
3	A	1114	POV	C1-O11-P-O12
3	A	1114	POV	C1-O11-P-O14
3	A	1114	POV	C11-O12-P-O11
3	A	1115	POV	C1-O11-P-O12
3	A	1115	POV	C1-O11-P-O13
3	A	1115	POV	O12-C11-C12-N
3	A	1116	POV	C1-O11-P-O13
3	B	1105	POV	C1-O11-P-O12
3	B	1105	POV	C1-O11-P-O13
3	B	1105	POV	C1-O11-P-O14
3	B	1105	POV	C22-C21-O21-C2
3	B	1105	POV	C32-C31-O31-C3
3	B	1106	POV	C11-O12-P-O11
3	B	1106	POV	C11-O12-P-O13
3	B	1107	POV	O11-C1-C2-C3
3	B	1107	POV	O11-C1-C2-O21
3	B	1107	POV	C1-C2-O21-C21
3	B	1107	POV	O12-C11-C12-N
3	B	1111	POV	C1-O11-P-O12
3	B	1111	POV	C1-O11-P-O13
3	B	1111	POV	C1-O11-P-O14
3	B	1111	POV	C11-O12-P-O11
3	B	1111	POV	C11-O12-P-O13
3	B	1112	POV	O12-C11-C12-N
3	B	1113	POV	C1-O11-P-O13
3	C	1104	POV	C1-O11-P-O12
3	C	1104	POV	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
3	C	1104	POV	C1-O11-P-O14
3	C	1105	POV	C11-O12-P-O14
3	C	1106	POV	C1-O11-P-O12
3	C	1106	POV	C1-O11-P-O13
3	C	1106	POV	C11-O12-P-O14
3	C	1109	POV	C1-O11-P-O12
3	C	1109	POV	C1-O11-P-O13
3	C	1109	POV	C11-O12-P-O11
3	C	1110	POV	C1-O11-P-O12
3	C	1110	POV	C1-O11-P-O13
3	C	1110	POV	C1-O11-P-O14
3	C	1110	POV	C11-O12-P-O14
3	C	1110	POV	O12-C11-C12-N
3	C	1111	POV	C11-O12-P-O11
3	C	1111	POV	C11-O12-P-O14
3	C	1112	POV	C22-C21-O21-C2
3	D	1107	POV	C11-O12-P-O11
3	D	1107	POV	C11-O12-P-O13
3	D	1108	POV	C1-O11-P-O12
3	D	1108	POV	C1-O11-P-O13
3	D	1108	POV	C11-O12-P-O11
3	D	1111	POV	C1-O11-P-O12
3	D	1111	POV	C1-O11-P-O13
3	D	1111	POV	C11-O12-P-O11
3	D	1112	POV	C1-O11-P-O12
3	D	1112	POV	C1-O11-P-O13
3	D	1113	POV	C1-O11-P-O14
6	A	1108	CLR	C16-C17-C20-C21
6	A	1108	CLR	C16-C17-C20-C22
6	D	1109	CLR	C13-C17-C20-C21
6	D	1109	CLR	C16-C17-C20-C22
3	B	1105	POV	O32-C31-O31-C3
3	D	1106	POV	O32-C31-O31-C3
3	D	1106	POV	C32-C31-O31-C3
3	B	1112	POV	O32-C31-O31-C3
6	D	1109	CLR	C16-C17-C20-C21
6	A	1108	CLR	C13-C17-C20-C21
6	D	1109	CLR	C13-C17-C20-C22
3	A	1105	POV	O22-C21-O21-C2
3	B	1105	POV	O22-C21-O21-C2
3	C	1112	POV	O22-C21-O21-C2
6	B	1109	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
6	C	1108	CLR	C21-C20-C22-C23
6	B	1108	CLR	C16-C17-C20-C21
6	A	1108	CLR	C13-C17-C20-C22
3	B	1112	POV	C32-C31-O31-C3
3	C	1110	POV	C32-C31-O31-C3
3	D	1111	POV	C32-C31-O31-C3
3	C	1110	POV	O32-C31-O31-C3
6	C	1108	CLR	C17-C20-C22-C23
3	C	1112	POV	C32-C31-O31-C3
6	B	1108	CLR	C16-C17-C20-C22
3	D	1111	POV	O32-C31-O31-C3
3	C	1105	POV	C24-C25-C26-C27
3	A	1105	POV	C32-C31-O31-C3
3	C	1104	POV	C32-C31-O31-C3
3	C	1112	POV	O32-C31-O31-C3
3	A	1105	POV	C33-C34-C35-C36
3	A	1116	POV	C36-C37-C38-C39
3	B	1113	POV	C36-C37-C38-C39
3	C	1109	POV	C24-C25-C26-C27
3	A	1105	POV	O32-C31-O31-C3
3	B	1111	POV	C32-C31-O31-C3
3	C	1109	POV	C32-C31-O31-C3
3	A	1101	POV	C312-C313-C314-C315
3	B	1101	POV	C312-C313-C314-C315
3	C	1113	POV	C312-C313-C314-C315
3	D	1101	POV	C312-C313-C314-C315
3	A	1101	POV	C36-C37-C38-C39
3	B	1101	POV	C36-C37-C38-C39
3	B	1105	POV	C25-C26-C27-C28
3	B	1106	POV	C24-C25-C26-C27
3	C	1111	POV	C36-C37-C38-C39
3	C	1113	POV	C36-C37-C38-C39
3	D	1101	POV	C36-C37-C38-C39
6	B	1108	CLR	C13-C17-C20-C21
3	C	1113	POV	C310-C311-C312-C313
3	D	1101	POV	C310-C311-C312-C313
3	A	1101	POV	C310-C311-C312-C313
3	B	1101	POV	C310-C311-C312-C313
3	A	1101	POV	C34-C35-C36-C37
3	A	1116	POV	C23-C24-C25-C26
3	B	1101	POV	C34-C35-C36-C37
3	B	1113	POV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
3	C	1113	POV	C34-C35-C36-C37
3	D	1101	POV	C34-C35-C36-C37
3	C	1109	POV	O32-C31-O31-C3
3	B	1105	POV	C23-C24-C25-C26
3	C	1110	POV	C31-C32-C33-C34
6	B	1108	CLR	C13-C17-C20-C22
3	C	1111	POV	C32-C33-C34-C35
3	A	1101	POV	C24-C25-C26-C27
3	A	1106	POV	C24-C25-C26-C27
3	B	1101	POV	C24-C25-C26-C27
3	C	1113	POV	C24-C25-C26-C27
3	D	1101	POV	C24-C25-C26-C27
3	D	1113	POV	C31-C32-C33-C34
3	A	1101	POV	C21-C22-C23-C24
3	A	1107	POV	C21-C22-C23-C24
3	B	1101	POV	C21-C22-C23-C24
3	C	1104	POV	C21-C22-C23-C24
3	D	1101	POV	C21-C22-C23-C24
3	B	1111	POV	O32-C31-O31-C3
6	A	1109	CLR	C22-C23-C24-C25
6	B	1108	CLR	C22-C23-C24-C25
3	A	1115	POV	C31-C32-C33-C34
3	B	1112	POV	C21-C22-C23-C24
3	C	1109	POV	C31-C32-C33-C34
3	C	1113	POV	C21-C22-C23-C24
6	B	1109	CLR	C22-C23-C24-C25
6	C	1107	CLR	C22-C23-C24-C25
3	C	1104	POV	O32-C31-O31-C3
3	B	1105	POV	C31-C32-C33-C34
3	B	1106	POV	C21-C22-C23-C24
3	A	1106	POV	C26-C27-C28-C29
6	C	1107	CLR	C13-C17-C20-C22
3	B	1111	POV	C31-C32-C33-C34
3	C	1105	POV	C21-C22-C23-C24
6	C	1107	CLR	C13-C17-C20-C21
6	B	1109	CLR	C17-C20-C22-C23
3	A	1106	POV	C11-C12-N-C13
3	A	1107	POV	C11-C12-N-C14
3	A	1114	POV	C11-C12-N-C13
3	B	1106	POV	C11-C12-N-C14
3	B	1111	POV	C11-C12-N-C14
3	C	1105	POV	C11-C12-N-C15

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Mol	Chain	Res	Type	Atoms
3	C	1109	POV	C11-C12-N-C13
3	D	1108	POV	C11-C12-N-C14
3	D	1111	POV	C11-C12-N-C13
3	B	1110	POV	C22-C21-O21-C2
3	B	1114	POV	C22-C21-O21-C2
3	D	1102	POV	C22-C21-O21-C2
3	D	1106	POV	C22-C21-O21-C2
3	D	1112	POV	C22-C21-O21-C2
6	C	1107	CLR	C16-C17-C20-C21
3	B	1110	POV	O22-C21-O21-C2
3	B	1114	POV	O22-C21-O21-C2
3	D	1102	POV	O22-C21-O21-C2
3	D	1106	POV	O22-C21-O21-C2
3	A	1115	POV	C32-C31-O31-C3
6	C	1108	CLR	C23-C24-C25-C27
6	D	1110	CLR	C23-C24-C25-C27
3	A	1106	POV	C22-C21-O21-C2
6	D	1110	CLR	C23-C24-C25-C26
3	A	1101	POV	C311-C310-C39-C38
3	A	1105	POV	C34-C35-C36-C37
3	B	1101	POV	C311-C310-C39-C38
3	B	1105	POV	C22-C23-C24-C25
3	C	1104	POV	C22-C23-C24-C25
3	C	1111	POV	C311-C312-C313-C314
3	C	1113	POV	C311-C310-C39-C38
3	D	1101	POV	C311-C310-C39-C38
3	A	1114	POV	C31-C32-C33-C34
3	A	1101	POV	C23-C24-C25-C26
3	A	1105	POV	C23-C24-C25-C26
3	B	1101	POV	C23-C24-C25-C26
3	C	1112	POV	C33-C34-C35-C36
3	C	1113	POV	C23-C24-C25-C26
3	D	1101	POV	C23-C24-C25-C26
3	D	1112	POV	O22-C21-O21-C2
3	B	1105	POV	C21-C22-C23-C24
6	A	1109	CLR	C23-C24-C25-C26
3	D	1113	POV	C310-C311-C312-C313
3	D	1107	POV	C22-C21-O21-C2
3	A	1106	POV	C31-C32-C33-C34
3	B	1112	POV	C32-C33-C34-C35
3	D	1113	POV	C35-C36-C37-C38
3	A	1106	POV	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
3	C	1111	POV	C22-C23-C24-C25
3	D	1106	POV	C33-C34-C35-C36
3	A	1106	POV	C11-C12-N-C15
3	B	1106	POV	C11-C12-N-C15
3	C	1106	POV	C11-C12-N-C14
3	A	1115	POV	C32-C33-C34-C35
3	B	1105	POV	C34-C35-C36-C37
3	D	1106	POV	C25-C26-C27-C28
3	A	1115	POV	O32-C31-O31-C3
3	A	1107	POV	C22-C21-O21-C2
3	B	1111	POV	C22-C21-O21-C2
3	C	1106	POV	C22-C21-O21-C2
3	A	1101	POV	C22-C21-O21-C2
3	B	1101	POV	C22-C21-O21-C2
3	C	1113	POV	C22-C21-O21-C2
3	D	1101	POV	C22-C21-O21-C2
3	C	1111	POV	C311-C310-C39-C38
3	C	1104	POV	C33-C34-C35-C36
3	A	1106	POV	O22-C21-O21-C2
3	D	1107	POV	O22-C21-O21-C2
3	D	1106	POV	C32-C33-C34-C35
6	C	1108	CLR	C23-C24-C25-C26
3	A	1116	POV	C22-C23-C24-C25
3	B	1113	POV	C22-C23-C24-C25
3	C	1110	POV	C33-C34-C35-C36
3	D	1113	POV	C33-C34-C35-C36
3	A	1114	POV	C29-C210-C211-C212
3	A	1105	POV	C24-C25-C26-C27
3	C	1105	POV	C22-C21-O21-C2
3	C	1109	POV	C22-C21-O21-C2
3	C	1111	POV	C22-C21-O21-C2
3	D	1113	POV	C22-C21-O21-C2
3	D	1112	POV	C34-C35-C36-C37
3	C	1109	POV	O22-C21-O21-C2
6	A	1108	CLR	C22-C23-C24-C25
3	D	1108	POV	C21-C22-C23-C24
3	B	1111	POV	C22-C23-C24-C25
3	A	1107	POV	C11-C12-N-C15
3	B	1111	POV	C11-C12-N-C15
3	C	1105	POV	C11-C12-N-C14
3	C	1110	POV	C22-C21-O21-C2
3	A	1106	POV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
3	A	1106	POV	O32-C31-O31-C3
3	B	1106	POV	C23-C24-C25-C26
3	B	1106	POV	C210-C211-C212-C213
3	C	1105	POV	C210-C211-C212-C213
3	C	1109	POV	C26-C27-C28-C29
3	A	1101	POV	O22-C21-O21-C2
3	B	1101	POV	O22-C21-O21-C2
3	C	1113	POV	O22-C21-O21-C2
3	C	1105	POV	C25-C26-C27-C28
6	D	1109	CLR	C22-C23-C24-C25
3	C	1113	POV	C31-C32-C33-C34
3	B	1106	POV	C25-C26-C27-C28
3	C	1105	POV	C23-C24-C25-C26
3	D	1108	POV	C22-C23-C24-C25
3	A	1105	POV	C25-C26-C27-C28
3	D	1113	POV	C39-C310-C311-C312
3	D	1101	POV	O22-C21-O21-C2
3	A	1101	POV	C31-C32-C33-C34
3	B	1101	POV	C31-C32-C33-C34
3	D	1101	POV	C31-C32-C33-C34
3	C	1106	POV	O22-C21-O21-C2
3	D	1113	POV	O22-C21-O21-C2
3	C	1110	POV	C32-C33-C34-C35
3	C	1111	POV	C310-C311-C312-C313
3	D	1113	POV	C311-C310-C39-C38
3	D	1113	POV	C22-C23-C24-C25
3	B	1106	POV	C211-C212-C213-C214
3	C	1105	POV	C211-C212-C213-C214
3	A	1106	POV	C210-C211-C212-C213
3	A	1114	POV	C26-C27-C28-C29
3	D	1111	POV	O11-C1-C2-C3
3	A	1107	POV	O22-C21-O21-C2
3	B	1111	POV	O22-C21-O21-C2
3	D	1113	POV	C32-C33-C34-C35
3	A	1106	POV	C211-C212-C213-C214
3	A	1106	POV	C23-C24-C25-C26
3	C	1105	POV	O22-C21-O21-C2
3	B	1112	POV	C1-C2-C3-O31
3	C	1112	POV	C1-C2-C3-O31
3	D	1113	POV	C1-C2-C3-O31
3	A	1105	POV	C26-C27-C28-C29
3	B	1110	POV	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
3	B	1114	POV	C32-C31-O31-C3
3	D	1102	POV	C32-C31-O31-C3
3	C	1106	POV	C22-C23-C24-C25
3	A	1105	POV	C1-O11-P-O14
3	C	1112	POV	C35-C36-C37-C38
3	D	1106	POV	C26-C27-C28-C29
3	A	1116	POV	C22-C21-O21-C2
3	B	1113	POV	C22-C21-O21-C2
3	A	1105	POV	C35-C36-C37-C38
3	A	1115	POV	C33-C34-C35-C36
3	A	1107	POV	C23-C24-C25-C26
3	A	1101	POV	C37-C38-C39-C310
3	B	1101	POV	C37-C38-C39-C310
3	C	1113	POV	C37-C38-C39-C310
3	D	1101	POV	C37-C38-C39-C310
3	C	1112	POV	C24-C25-C26-C27
3	D	1113	POV	C36-C37-C38-C39
3	B	1111	POV	C21-C22-C23-C24
3	C	1111	POV	O22-C21-O21-C2
3	D	1112	POV	C22-C23-C24-C25
6	A	1109	CLR	C23-C24-C25-C27
3	B	1111	POV	C32-C33-C34-C35
3	D	1107	POV	C211-C212-C213-C214
3	B	1105	POV	C33-C34-C35-C36
3	A	1101	POV	C212-C213-C214-C215
3	B	1101	POV	C212-C213-C214-C215
3	C	1113	POV	C212-C213-C214-C215
3	D	1101	POV	C212-C213-C214-C215
3	B	1111	POV	O11-C1-C2-C3
3	C	1109	POV	O11-C1-C2-C3
3	C	1104	POV	C35-C36-C37-C38
3	B	1110	POV	O32-C31-O31-C3
3	B	1114	POV	O32-C31-O31-C3
3	D	1102	POV	O32-C31-O31-C3
3	B	1106	POV	C26-C27-C28-C29
3	B	1111	POV	O11-C1-C2-O21
3	C	1109	POV	C22-C23-C24-C25
3	C	1111	POV	C39-C310-C311-C312
3	D	1113	POV	C34-C35-C36-C37
3	A	1116	POV	C32-C33-C34-C35
3	D	1113	POV	O21-C2-C3-O31
3	B	1113	POV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
3	C	1110	POV	O22-C21-O21-C2
3	A	1107	POV	C24-C25-C26-C27
3	B	1105	POV	C27-C28-C29-C210
3	D	1111	POV	C29-C210-C211-C212
3	B	1105	POV	O21-C21-C22-C23
3	D	1112	POV	C21-C22-C23-C24
3	A	1116	POV	O22-C21-O21-C2
3	B	1113	POV	O22-C21-O21-C2
3	D	1108	POV	C11-C12-N-C15
3	B	1110	POV	O11-C1-C2-O21
3	B	1114	POV	O11-C1-C2-O21
3	C	1109	POV	O11-C1-C2-O21
3	D	1102	POV	O11-C1-C2-O21
3	B	1106	POV	C22-C21-O21-C2
3	C	1105	POV	C12-C11-O12-P
3	D	1111	POV	C12-C11-O12-P
3	D	1113	POV	C12-C11-O12-P
3	C	1112	POV	O21-C2-C3-O31
3	A	1116	POV	C310-C311-C312-C313
3	B	1113	POV	C310-C311-C312-C313
3	D	1106	POV	C23-C24-C25-C26
3	C	1109	POV	O12-C11-C12-N
3	D	1111	POV	O12-C11-C12-N
6	D	1109	CLR	C23-C24-C25-C26
3	C	1112	POV	C22-C23-C24-C25
3	A	1114	POV	C24-C25-C26-C27
3	D	1112	POV	C32-C31-O31-C3
3	D	1113	POV	C32-C31-O31-C3
3	D	1106	POV	O21-C21-C22-C23
3	B	1110	POV	O11-C1-C2-C3
3	B	1114	POV	O11-C1-C2-C3
3	C	1112	POV	O11-C1-C2-C3
3	D	1102	POV	O11-C1-C2-C3
3	D	1106	POV	C34-C35-C36-C37
3	C	1105	POV	C29-C210-C211-C212
3	A	1115	POV	C2-C1-O11-P
3	C	1111	POV	C24-C25-C26-C27
3	B	1106	POV	O22-C21-O21-C2
6	C	1107	CLR	C16-C17-C20-C22
3	B	1105	POV	O11-C1-C2-O21
3	C	1112	POV	O11-C1-C2-O21
3	D	1111	POV	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
3	A	1105	POV	C32-C33-C34-C35
3	C	1109	POV	C23-C24-C25-C26
3	D	1112	POV	O32-C31-O31-C3
3	D	1113	POV	O32-C31-O31-C3
3	B	1112	POV	O21-C2-C3-O31
3	B	1112	POV	C31-C32-C33-C34
3	C	1112	POV	C311-C310-C39-C38
3	A	1115	POV	C21-C22-C23-C24
3	C	1109	POV	C32-C33-C34-C35
3	C	1111	POV	C312-C313-C314-C315
3	D	1113	POV	C23-C24-C25-C26
3	C	1109	POV	C27-C28-C29-C210
3	D	1111	POV	C32-C33-C34-C35
3	A	1114	POV	C1-O11-P-O13
3	A	1114	POV	C11-O12-P-O14
3	A	1116	POV	C1-O11-P-O12
3	A	1116	POV	C1-O11-P-O14
3	A	1116	POV	C11-O12-P-O14
3	B	1106	POV	C1-O11-P-O12
3	B	1106	POV	C1-O11-P-O13
3	B	1106	POV	C1-O11-P-O14
3	B	1107	POV	C11-O12-P-O14
3	B	1112	POV	C11-O12-P-O14
3	B	1113	POV	C1-O11-P-O12
3	B	1113	POV	C1-O11-P-O14
3	B	1113	POV	C11-O12-P-O14
3	C	1105	POV	C1-O11-P-O14
3	C	1109	POV	C11-O12-P-O14
3	D	1108	POV	C11-O12-P-O14
3	D	1108	POV	C1-C2-O21-C21
3	D	1111	POV	C11-O12-P-O14
3	D	1113	POV	O12-C11-C12-N
3	A	1106	POV	C2-C1-O11-P
3	B	1105	POV	C35-C36-C37-C38
3	C	1109	POV	C21-C22-C23-C24
3	A	1114	POV	C22-C21-O21-C2
3	D	1107	POV	C1-C2-O21-C21
3	A	1114	POV	C23-C24-C25-C26
3	D	1107	POV	C21-C22-C23-C24
3	A	1114	POV	O22-C21-O21-C2
3	C	1105	POV	O31-C31-C32-C33
3	C	1109	POV	C29-C210-C211-C212

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Mol	Chain	Res	Type	Atoms
3	A	1115	POV	C22-C21-O21-C2
6	B	1108	CLR	C20-C22-C23-C24
3	A	1115	POV	O22-C21-O21-C2
3	C	1113	POV	C39-C310-C311-C312
3	D	1101	POV	C39-C310-C311-C312
3	A	1101	POV	C39-C310-C311-C312
3	A	1116	POV	C311-C312-C313-C314
3	B	1101	POV	C39-C310-C311-C312
3	B	1113	POV	C311-C312-C313-C314
3	A	1101	POV	O31-C31-C32-C33
3	B	1101	POV	O31-C31-C32-C33
3	C	1113	POV	O31-C31-C32-C33
3	D	1101	POV	O31-C31-C32-C33
3	D	1107	POV	O11-C1-C2-O21
3	B	1105	POV	O11-C1-C2-C3
3	D	1107	POV	C11-C12-N-C13
3	A	1107	POV	O11-C1-C2-C3
6	A	1109	CLR	C20-C22-C23-C24
3	B	1105	POV	C2-C1-O11-P
3	D	1111	POV	C11-C12-N-C15
6	D	1110	CLR	C20-C22-C23-C24
3	A	1116	POV	C311-C310-C39-C38
3	C	1110	POV	C1-C2-O21-C21
3	C	1110	POV	C3-C2-O21-C21
3	D	1107	POV	C3-C2-O21-C21
3	B	1113	POV	C311-C310-C39-C38
3	C	1104	POV	C32-C33-C34-C35
3	D	1106	POV	C24-C25-C26-C27
3	C	1111	POV	C35-C36-C37-C38
3	A	1107	POV	O11-C1-C2-O21
3	C	1109	POV	C11-C12-N-C15
3	B	1110	POV	C311-C312-C313-C314
3	D	1102	POV	C311-C312-C313-C314
3	A	1116	POV	O21-C2-C3-O31
3	B	1113	POV	O21-C2-C3-O31
3	C	1104	POV	C34-C35-C36-C37
3	C	1104	POV	C25-C26-C27-C28
6	D	1109	CLR	C21-C20-C22-C23
3	D	1106	POV	C27-C28-C29-C210
3	C	1110	POV	C2-C1-O11-P
3	D	1111	POV	O22-C21-O21-C2
3	A	1114	POV	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	C	1112	POV	C23-C24-C25-C26
3	C	1110	POV	C1-C2-C3-O31
3	C	1112	POV	C36-C37-C38-C39
3	D	1111	POV	C27-C28-C29-C210
3	A	1105	POV	O31-C31-C32-C33
6	D	1109	CLR	C17-C20-C22-C23
3	D	1107	POV	O11-C1-C2-C3
3	D	1113	POV	O11-C1-C2-C3
3	A	1114	POV	C27-C28-C29-C210
3	D	1112	POV	C35-C36-C37-C38
3	B	1105	POV	C32-C33-C34-C35
3	B	1113	POV	C35-C36-C37-C38
3	B	1112	POV	C33-C34-C35-C36
3	A	1116	POV	C35-C36-C37-C38
3	D	1111	POV	C22-C23-C24-C25
3	A	1105	POV	C1-O11-P-O13
3	A	1114	POV	O32-C31-O31-C3
3	C	1110	POV	C21-C22-C23-C24
3	D	1111	POV	C26-C27-C28-C29
3	C	1112	POV	C37-C38-C39-C310
3	A	1114	POV	C32-C31-O31-C3
3	D	1113	POV	O11-C1-C2-O21
3	A	1106	POV	C12-C11-O12-P
3	D	1112	POV	O31-C31-C32-C33
3	C	1109	POV	O21-C2-C3-O31
3	B	1105	POV	O22-C21-C22-C23
3	A	1115	POV	O11-C1-C2-C3
3	A	1106	POV	O12-C11-C12-N
3	A	1114	POV	O12-C11-C12-N
3	D	1111	POV	C22-C21-O21-C2
3	C	1111	POV	O31-C31-C32-C33
3	D	1107	POV	C24-C25-C26-C27
6	A	1108	CLR	C23-C24-C25-C26
3	B	1106	POV	C29-C210-C211-C212
3	A	1116	POV	O31-C31-C32-C33
3	B	1113	POV	O31-C31-C32-C33
3	D	1108	POV	C24-C25-C26-C27
3	C	1112	POV	C25-C26-C27-C28
3	B	1106	POV	C3-C2-O21-C21
3	D	1108	POV	C23-C24-C25-C26
3	A	1115	POV	O11-C1-C2-O21
3	B	1111	POV	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
3	C	1106	POV	C11-C12-N-C15
3	A	1116	POV	O32-C31-C32-C33
3	B	1113	POV	O32-C31-C32-C33
3	C	1111	POV	O32-C31-C32-C33
3	D	1112	POV	O32-C31-C32-C33
3	A	1106	POV	C1-C2-C3-O31
3	C	1110	POV	O31-C31-C32-C33
3	D	1106	POV	C22-C23-C24-C25
3	C	1105	POV	O11-C1-C2-C3
3	A	1105	POV	O21-C21-C22-C23
3	C	1104	POV	C23-C24-C25-C26
3	B	1112	POV	C35-C36-C37-C38

There are no ring outliers.

40 monomers are involved in 420 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	POV	8	0
3	C	1112	POV	2	0
3	D	1107	POV	1	0
3	A	1107	POV	2	0
3	D	1101	POV	15	0
3	C	1111	POV	2	0
3	D	1106	POV	17	0
3	A	1116	POV	9	0
3	B	1105	POV	16	0
6	A	1108	CLR	19	0
3	C	1106	POV	1	0
3	B	1110	POV	4	0
3	B	1107	POV	1	0
3	B	1113	POV	8	0
3	C	1109	POV	3	0
6	D	1109	CLR	40	0
3	A	1105	POV	2	0
3	D	1102	POV	11	0
3	C	1105	POV	3	0
3	B	1111	POV	4	0
3	A	1114	POV	3	0
6	B	1109	CLR	22	0
6	D	1110	CLR	33	0
6	C	1108	CLR	20	0
3	C	1104	POV	5	0

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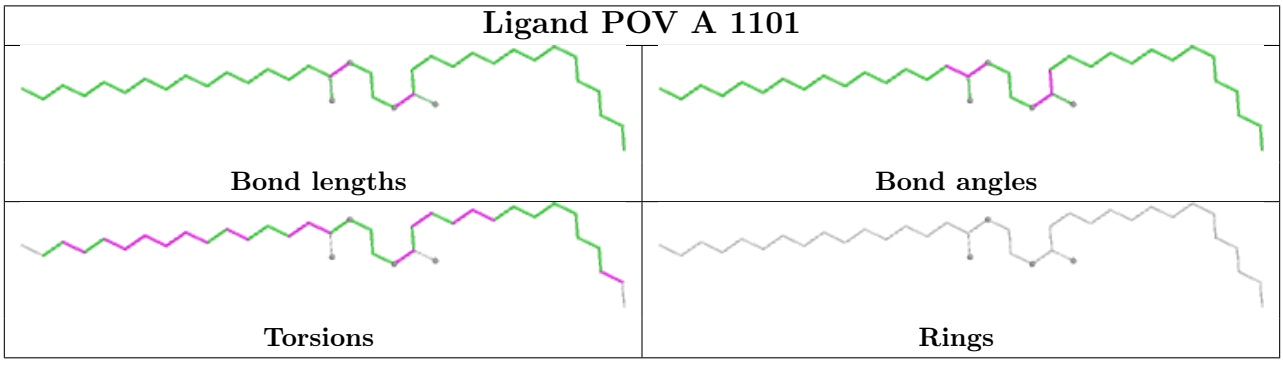
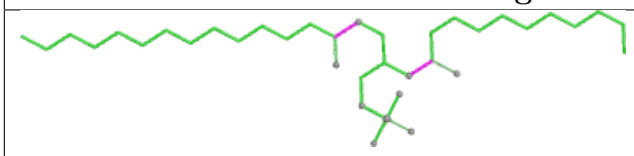
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1101	POV	21	0
3	D	1108	POV	5	0
3	D	1112	POV	5	0
3	C	1113	POV	8	0
3	B	1114	POV	3	0
3	A	1106	POV	2	0
6	A	1109	CLR	12	0
3	B	1112	POV	6	0
3	C	1110	POV	8	0
6	C	1107	CLR	25	0
3	D	1111	POV	3	0
6	B	1108	CLR	41	0
3	D	1113	POV	27	0
3	A	1115	POV	5	0
3	B	1106	POV	5	0

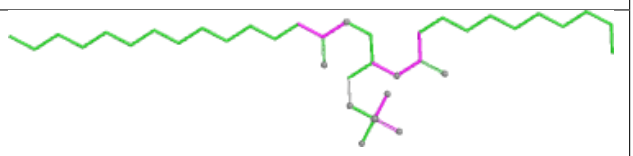
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



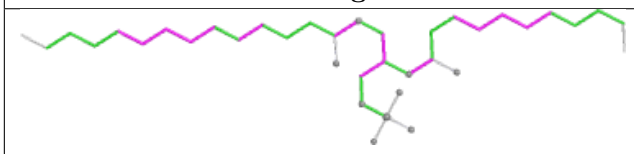
Ligand POV C 1112



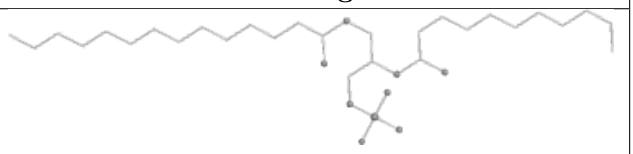
Bond lengths



Bond angles

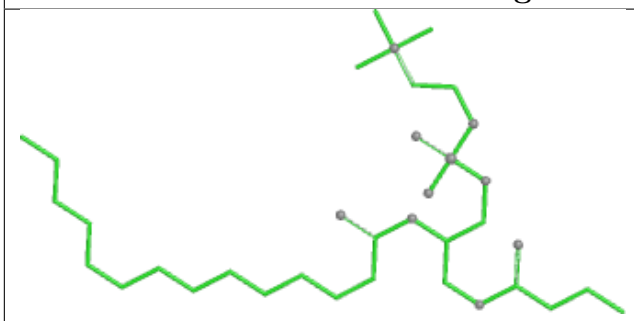


Torsions

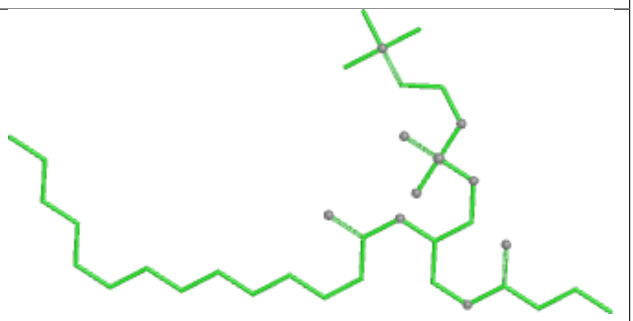


Rings

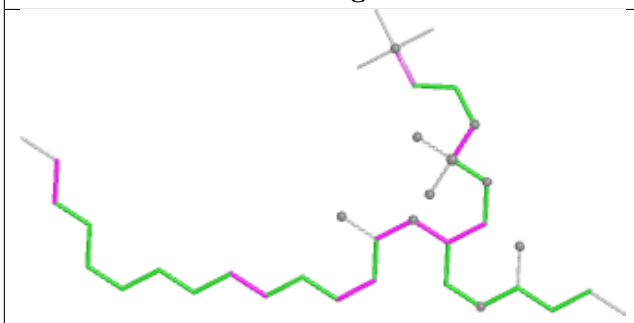
Ligand POV D 1107



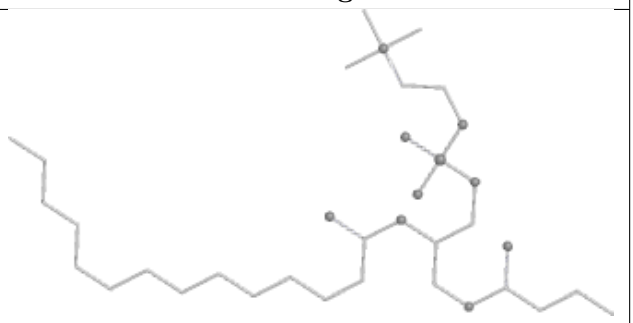
Bond lengths



Bond angles

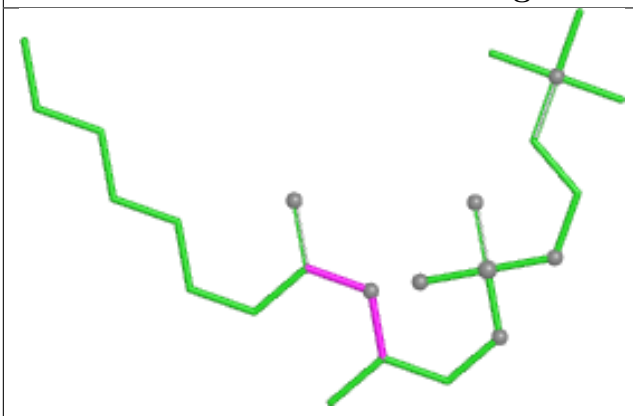


Torsions

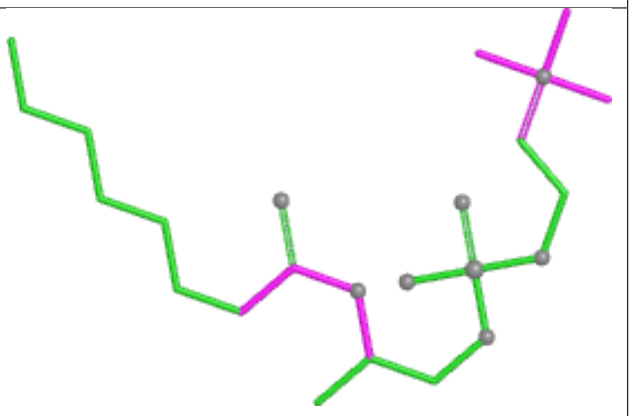


Rings

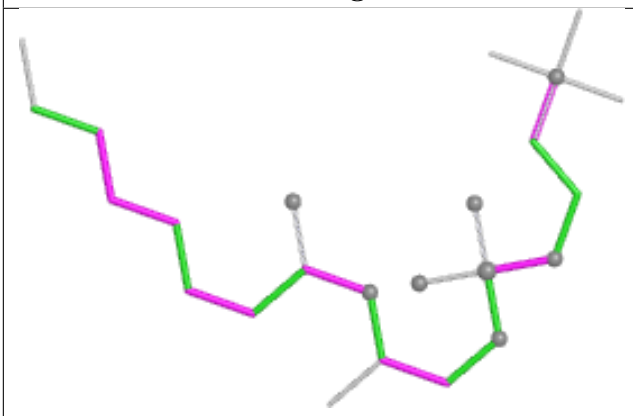
Ligand POV A 1107



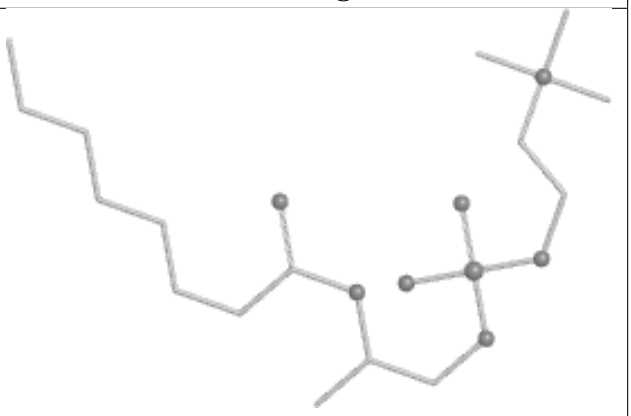
Bond lengths



Bond angles

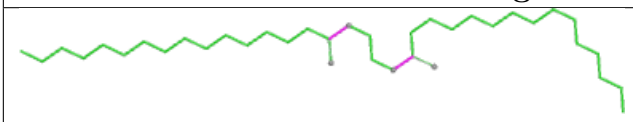


Torsions

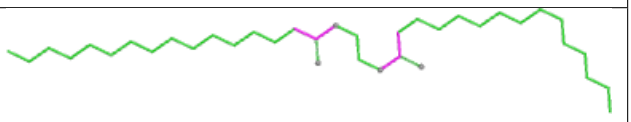


Rings

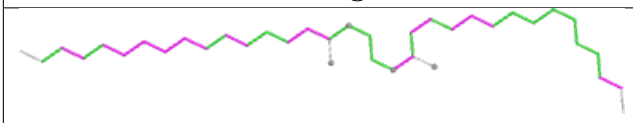
Ligand POV D 1101



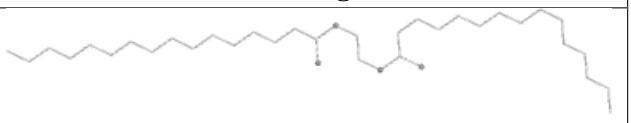
Bond lengths



Bond angles

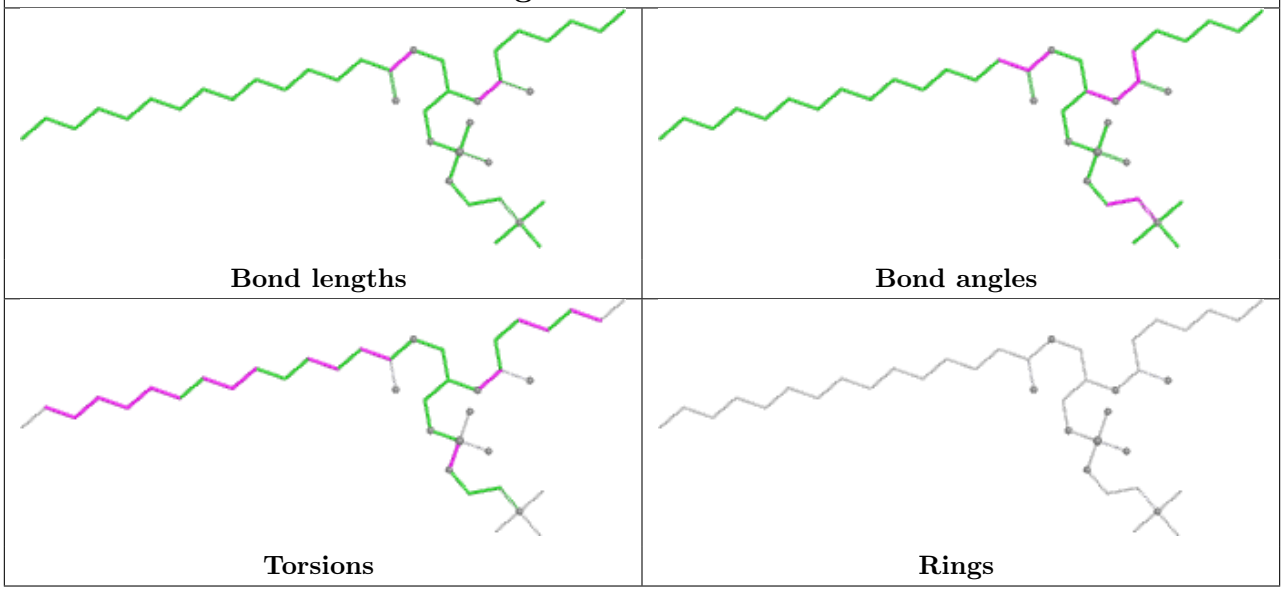


Torsions

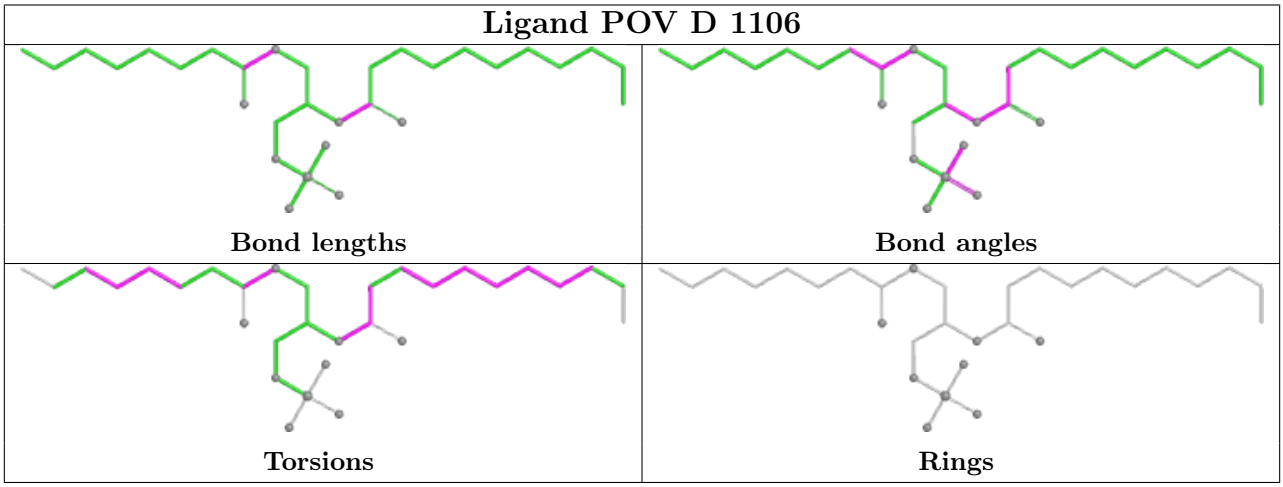


Rings

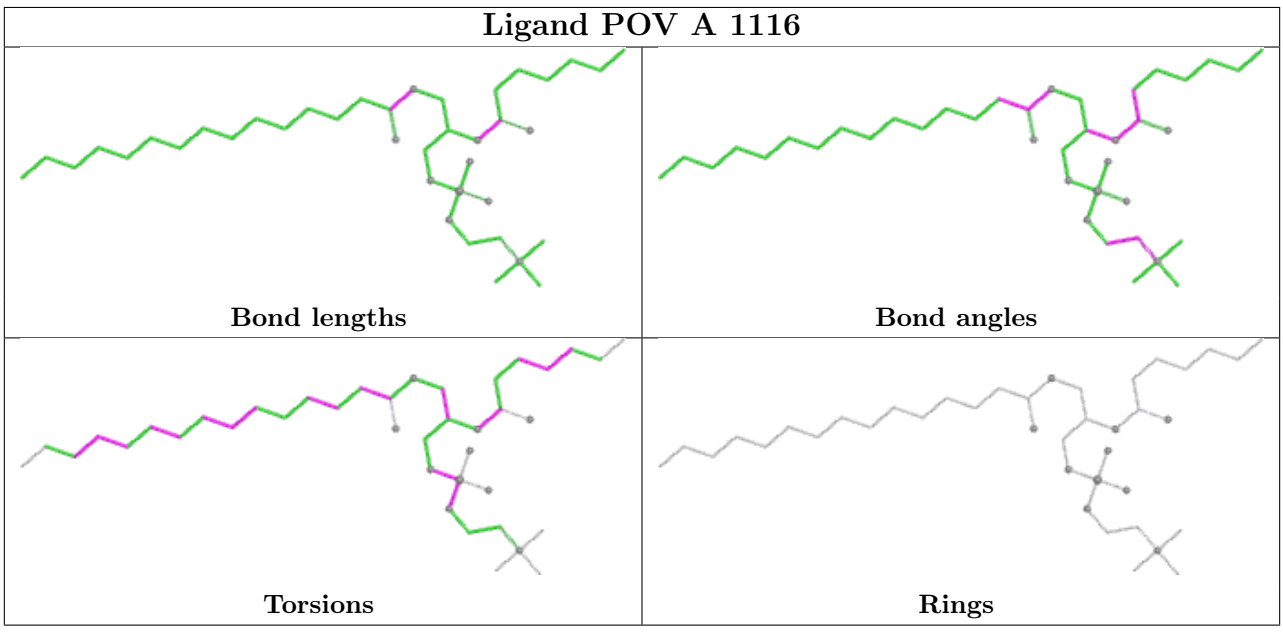
Ligand POV C 1111



Ligand POV D 1106

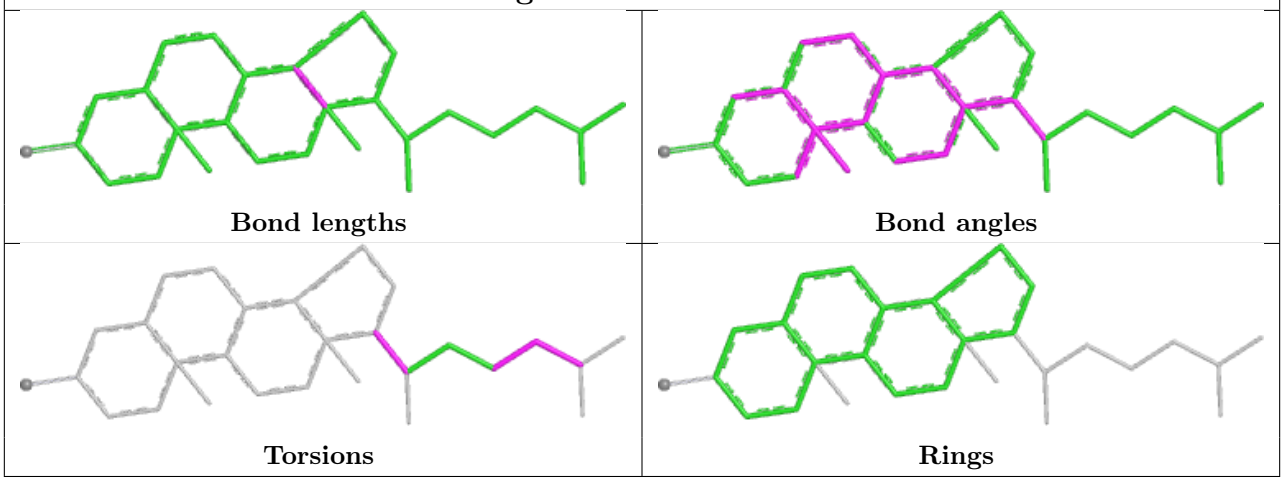


Ligand POV A 1116



Ligand POV B 1105

Ligand CLR A 1108



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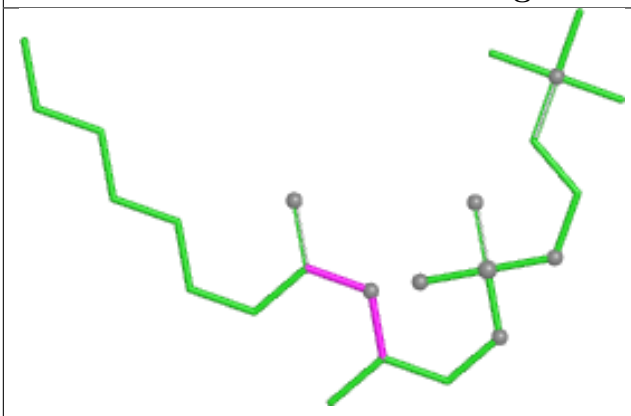
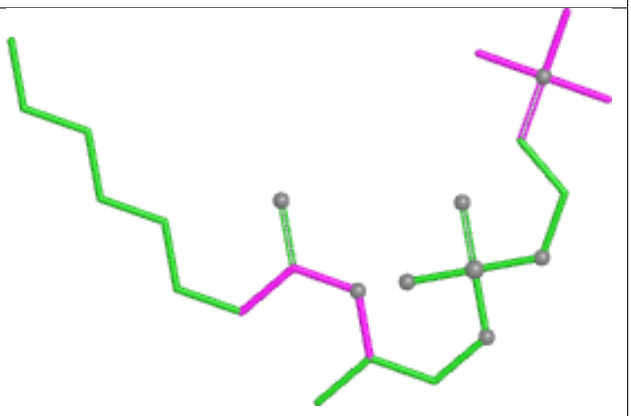
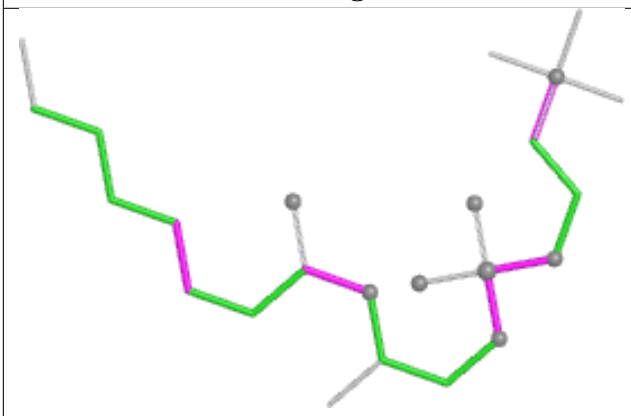


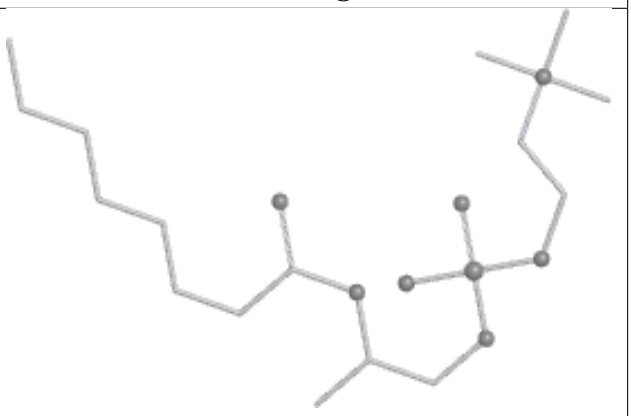
Bond lengths



Bond angles

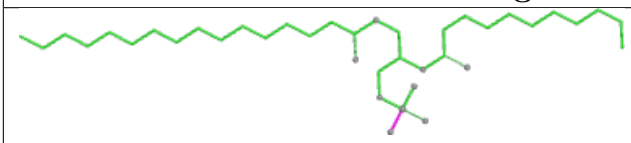


Torsions

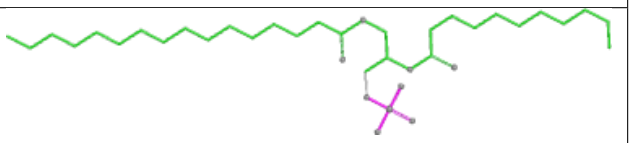


Rings

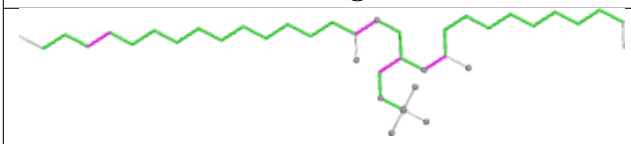
Ligand POV B 1110



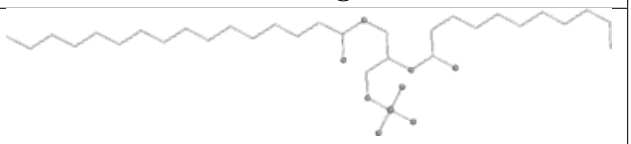
Bond lengths



Bond angles

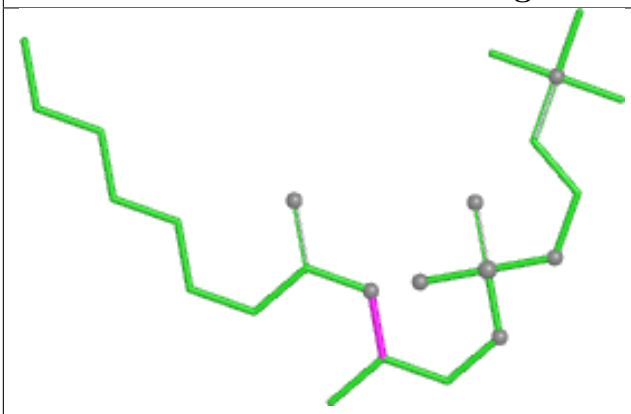


Torsions

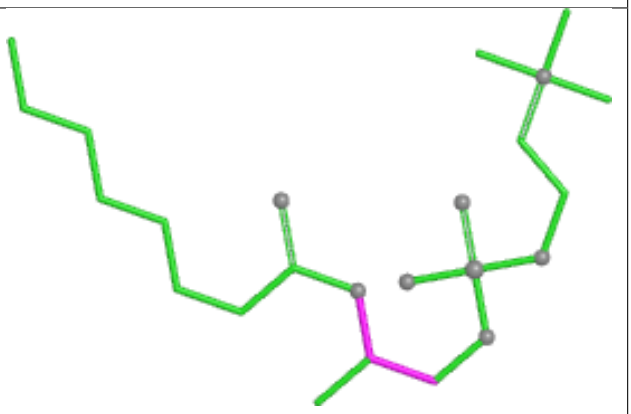


Rings

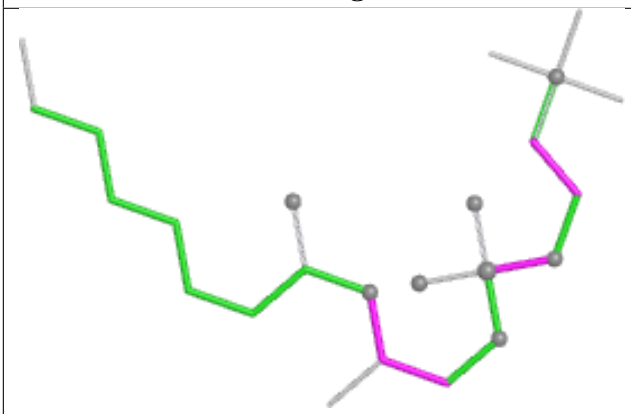
Ligand POV B 1107



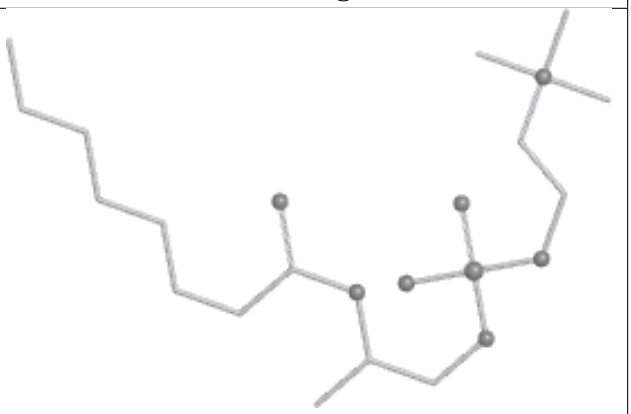
Bond lengths



Bond angles

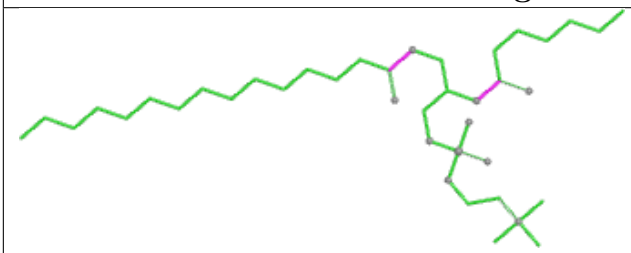


Torsions

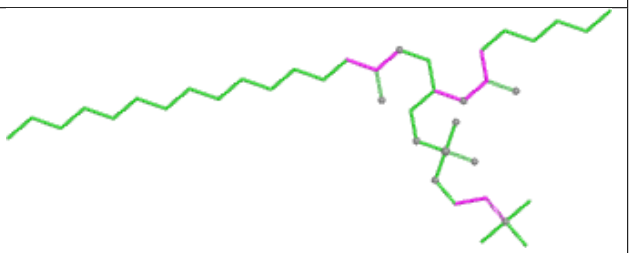


Rings

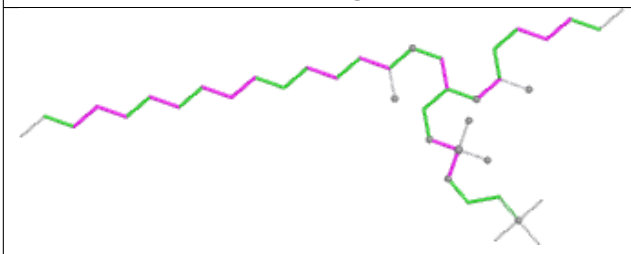
Ligand POV B 1113



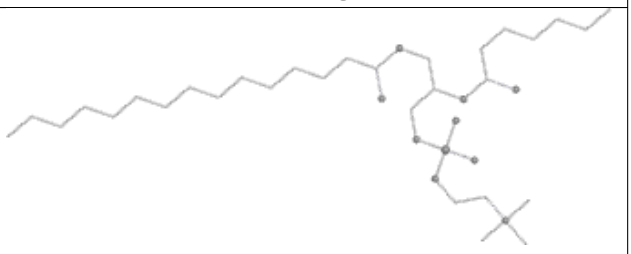
Bond lengths



Bond angles

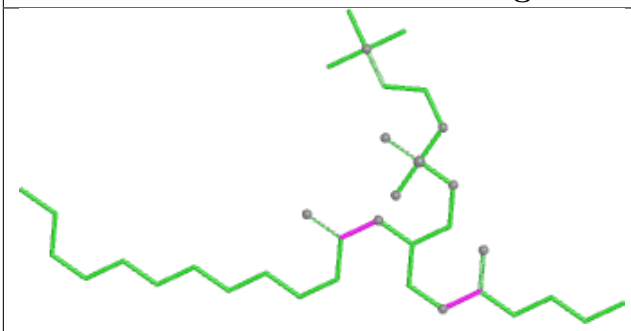


Torsions

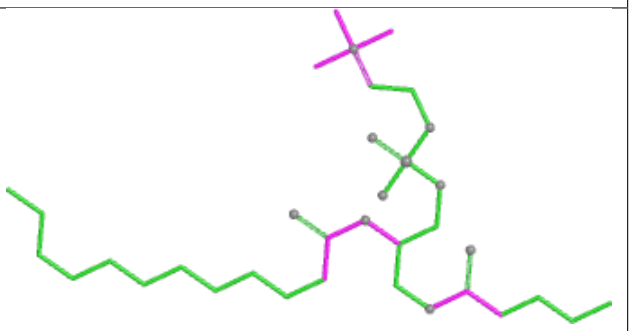


Rings

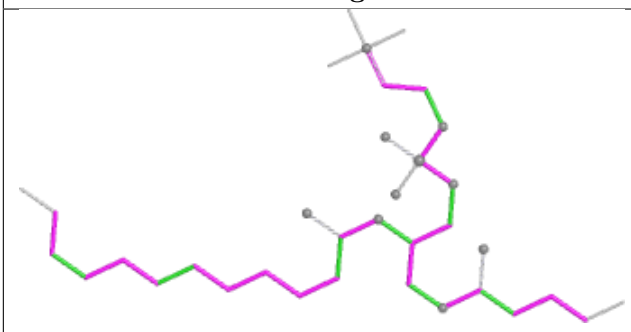
Ligand POV C 1109



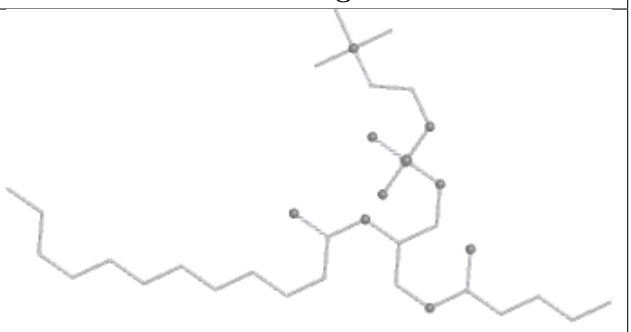
Bond lengths



Bond angles

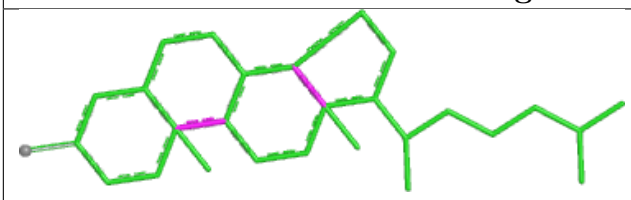


Torsions

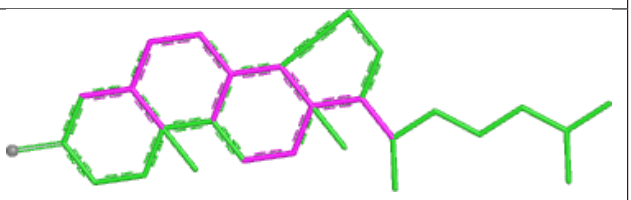


Rings

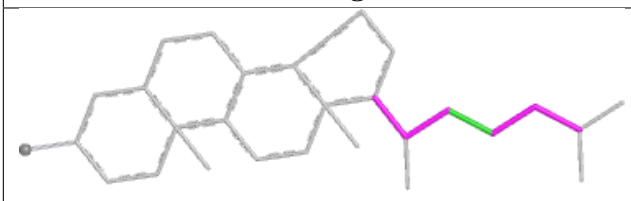
Ligand CLR D 1109



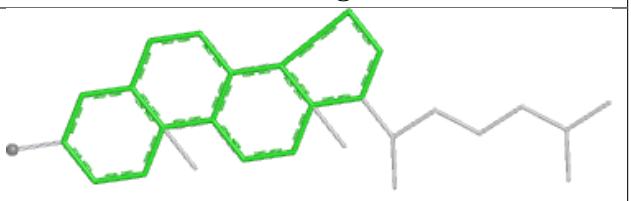
Bond lengths



Bond angles

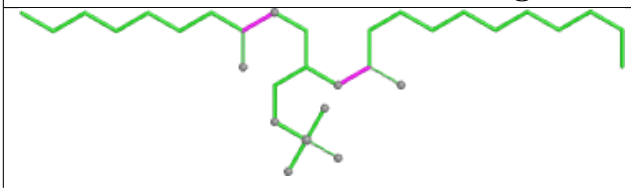


Torsions

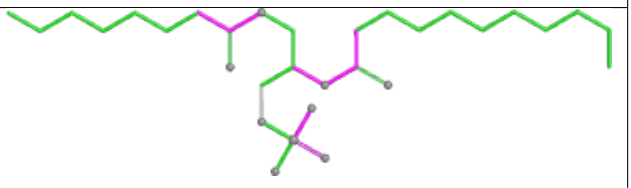


Rings

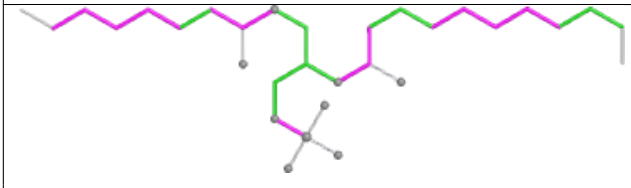
Ligand POV A 1105



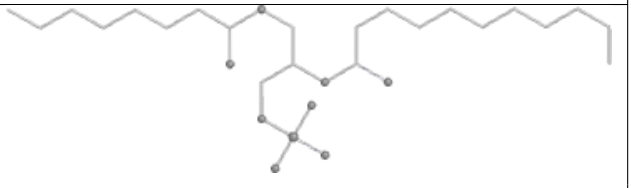
Bond lengths



Bond angles

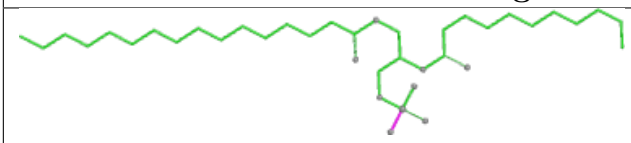


Torsions

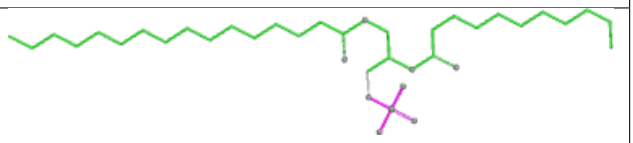


Rings

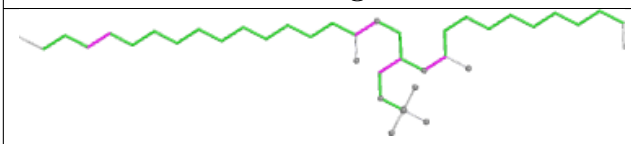
Ligand POV D 1102



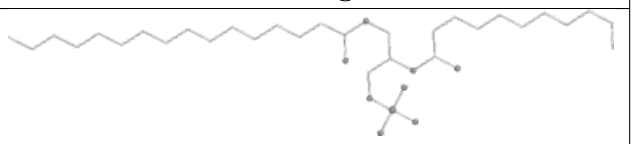
Bond lengths



Bond angles

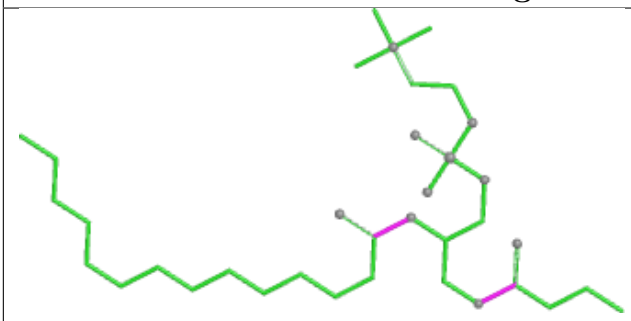


Torsions

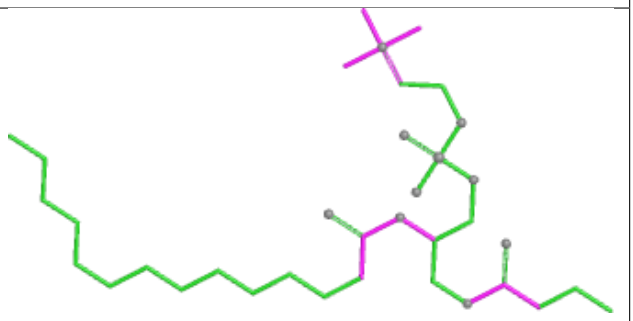


Rings

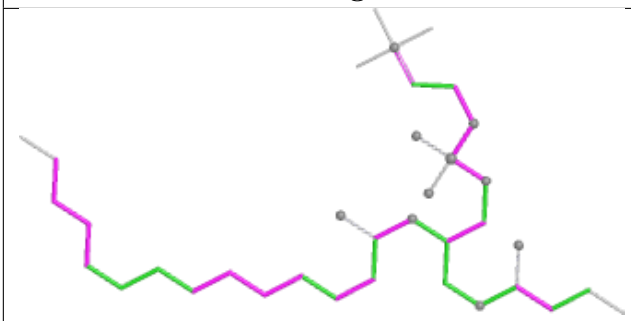
Ligand POV C 1105



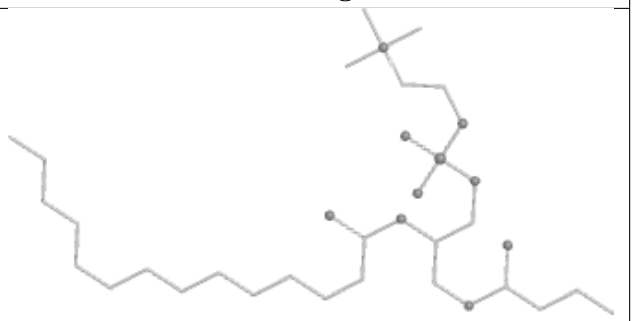
Bond lengths



Bond angles

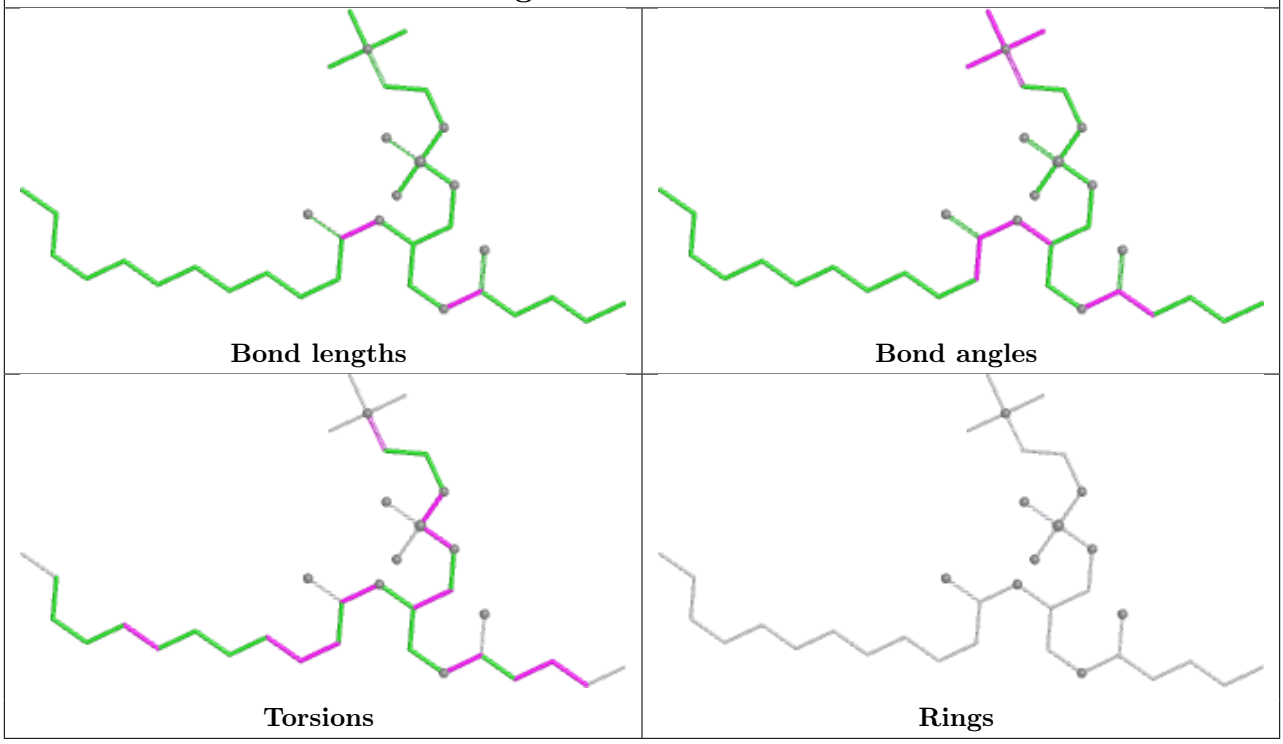


Torsions

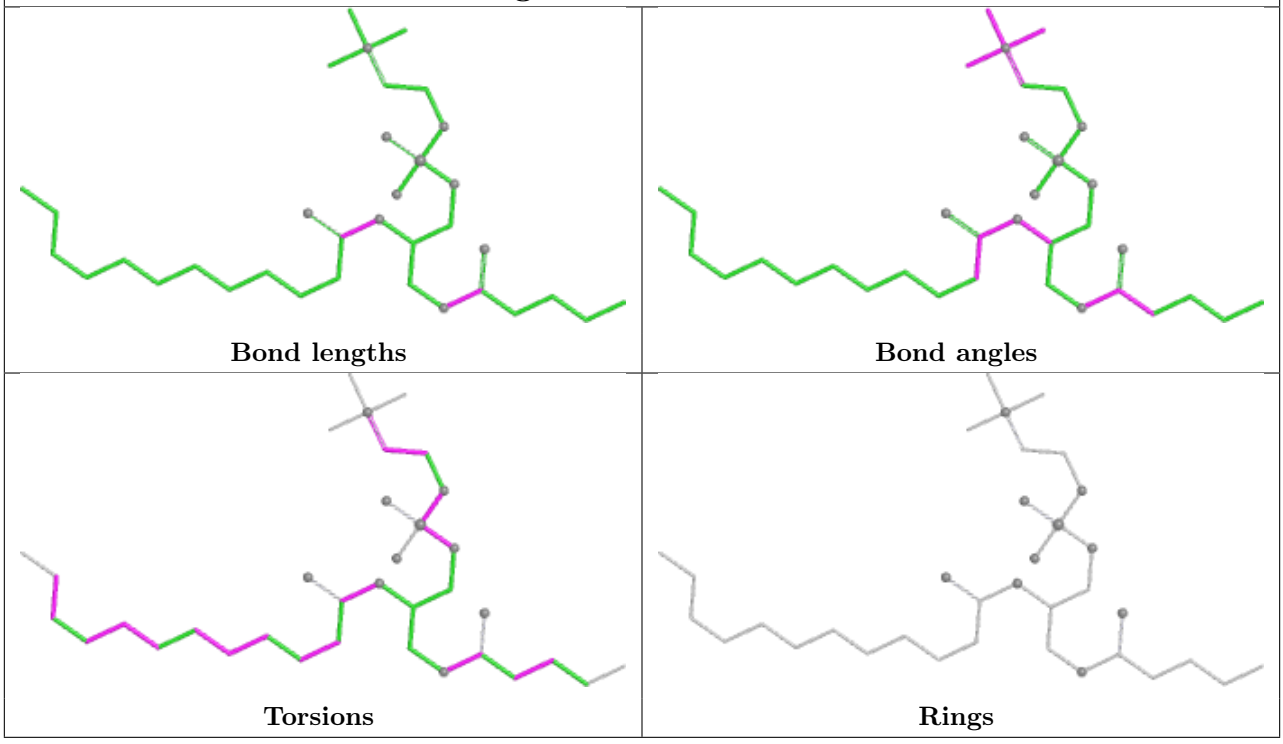


Rings

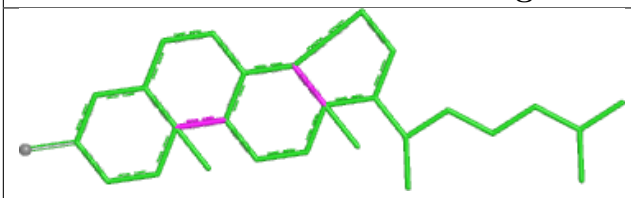
Ligand POV B 1111



Ligand POV A 1114



Ligand CLR B 1109



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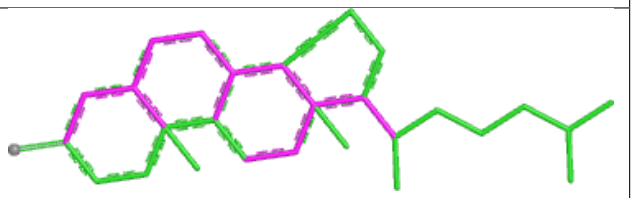
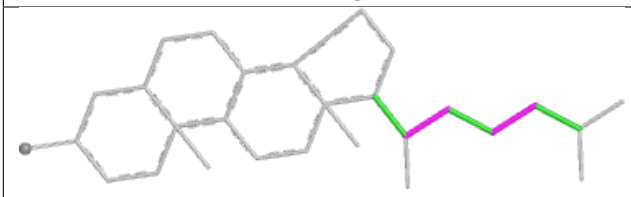
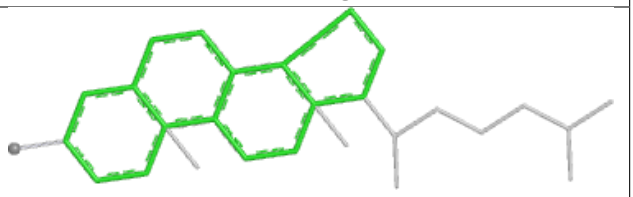


Bond angles

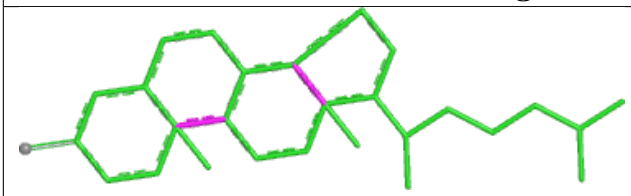


Torsions

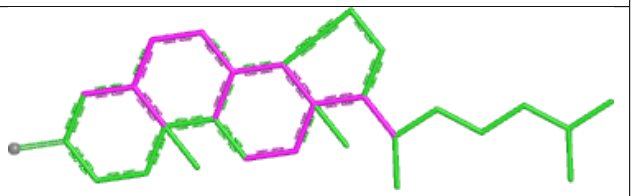


Rings

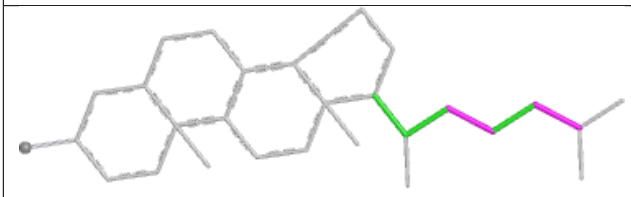
Ligand CLR D 1110



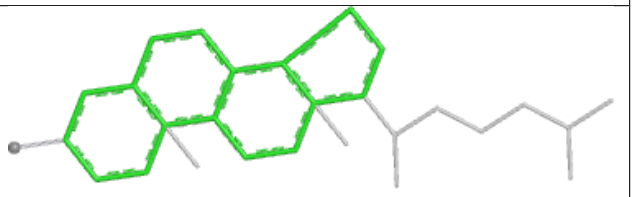
Bond lengths



Bond angles

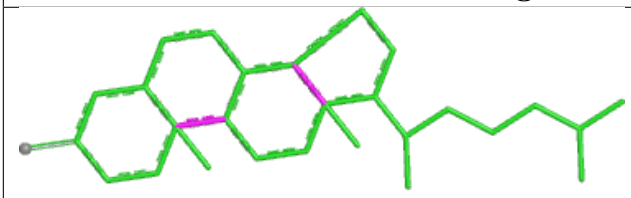


Torsions



Rings

Ligand CLR C 1108



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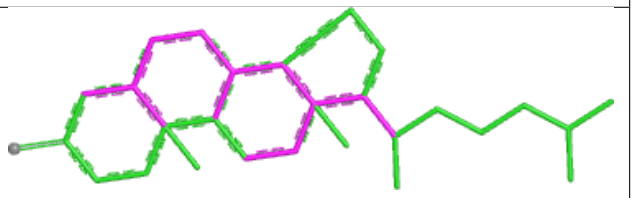
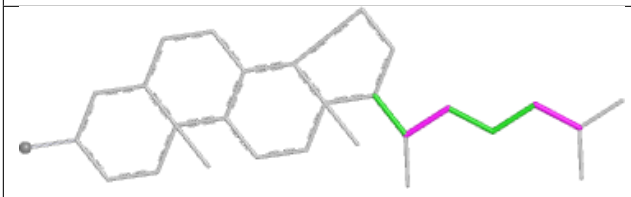
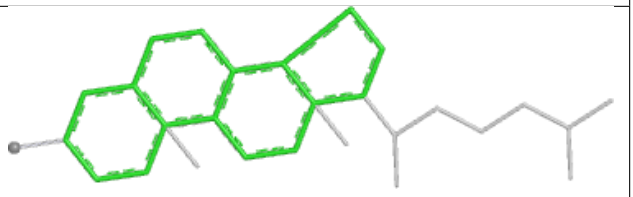


Bond angles



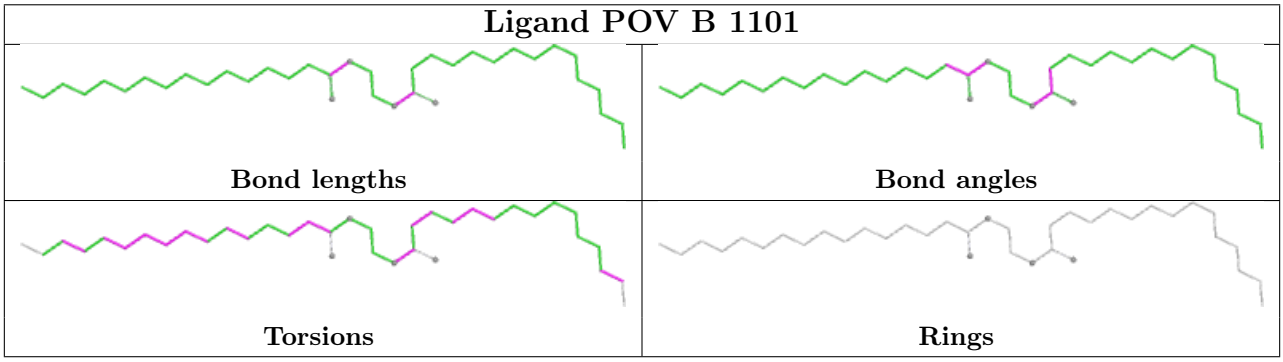
Torsions



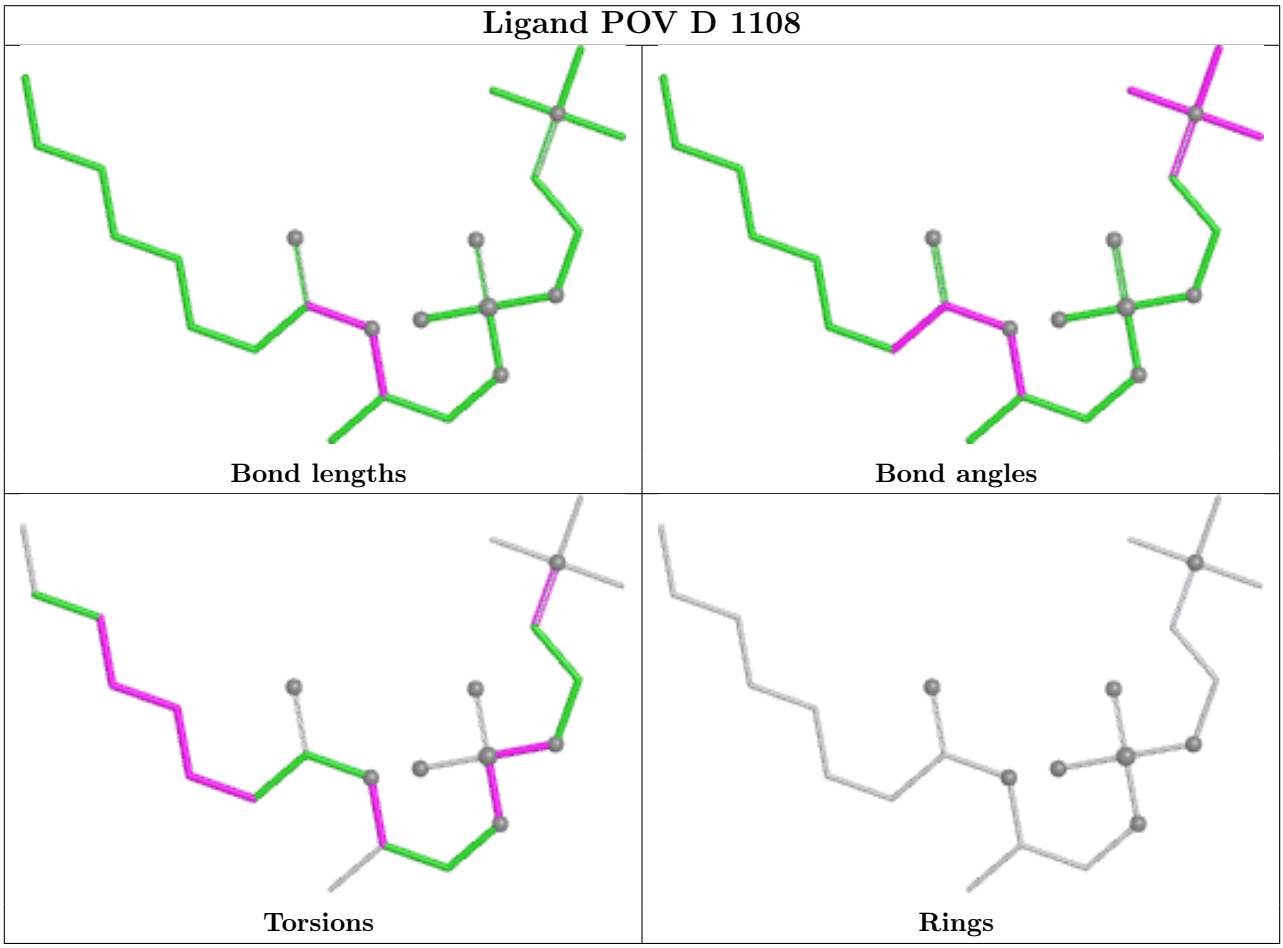
Rings

Ligand POV C 1104

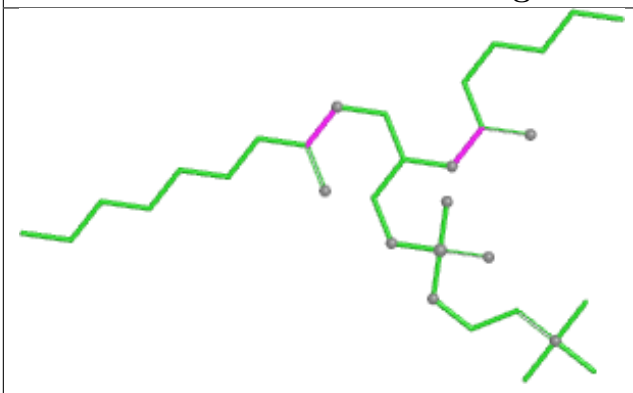
Ligand POV B 1101



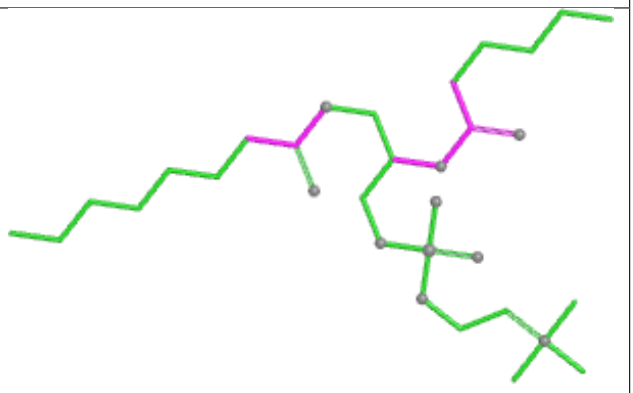
Ligand POV D 1108



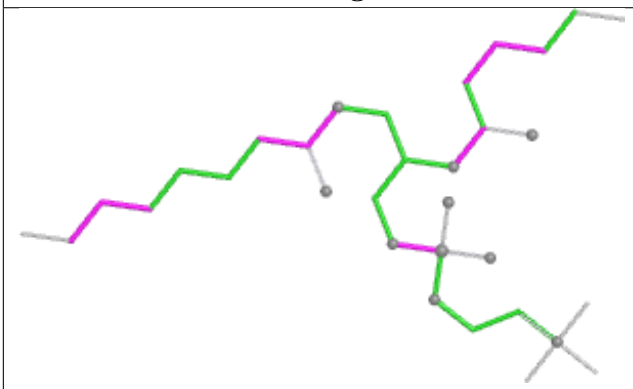
Ligand POV D 1112



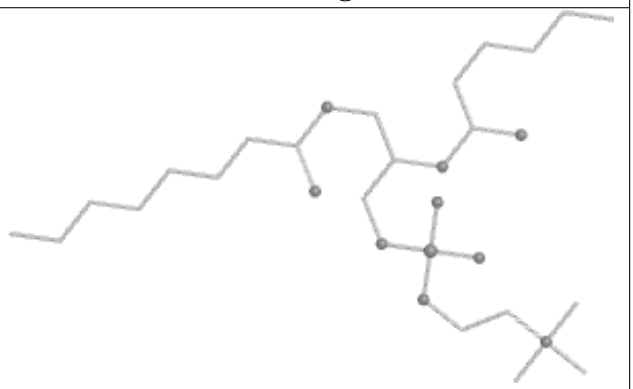
Bond lengths



Bond angles

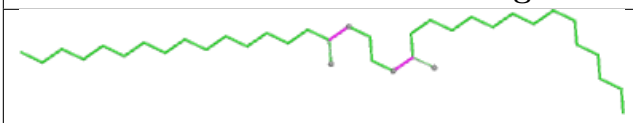


Torsions

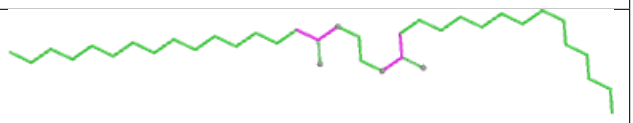


Rings

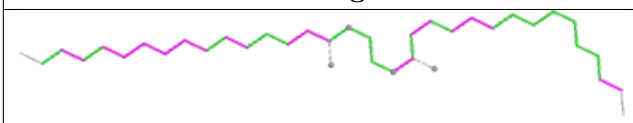
Ligand POV C 1113



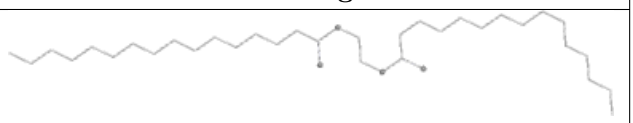
Bond lengths



Bond angles

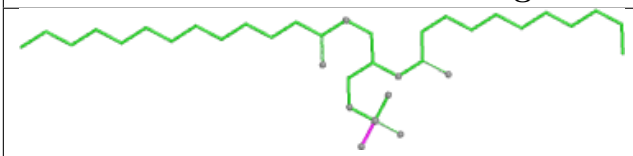


Torsions

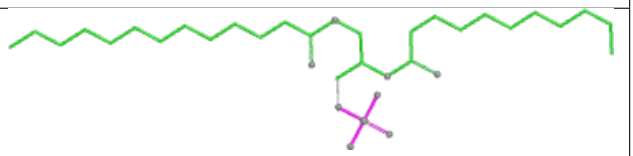


Rings

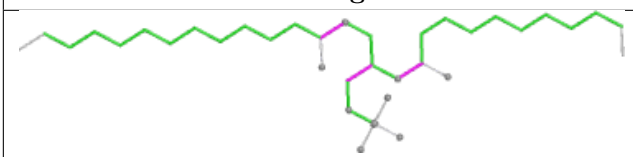
Ligand POV B 1114



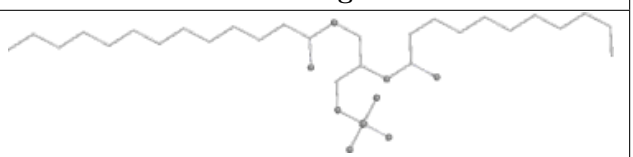
Bond lengths



Bond angles

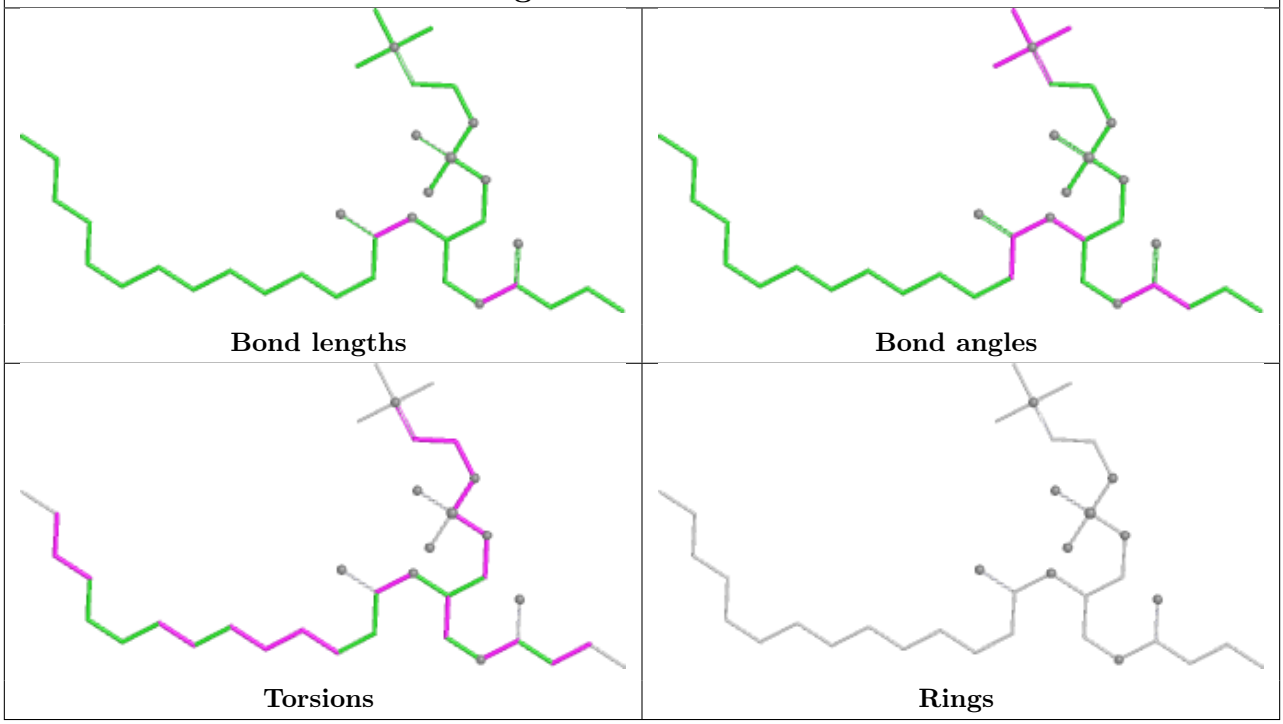


Torsions

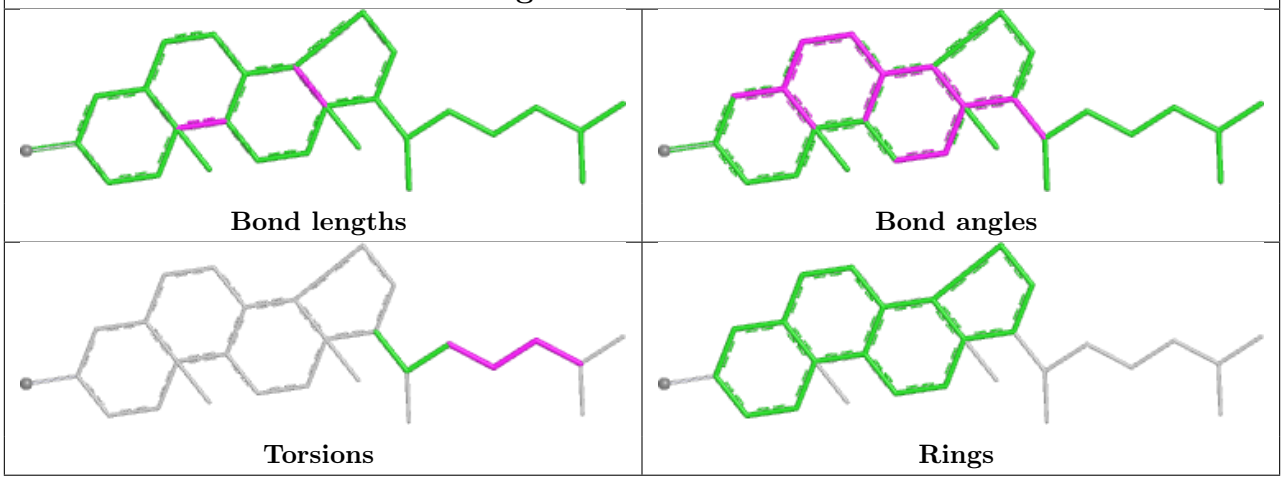


Rings

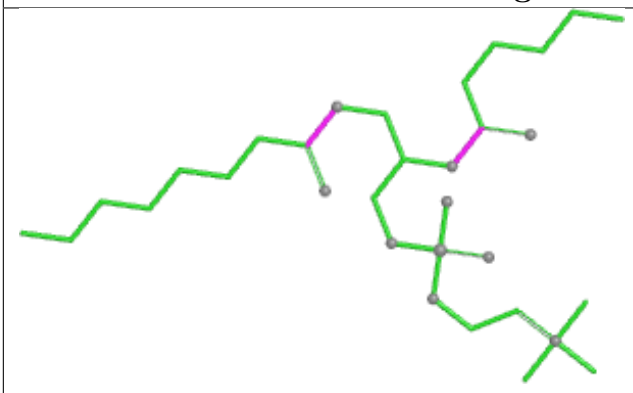
Ligand POV A 1106



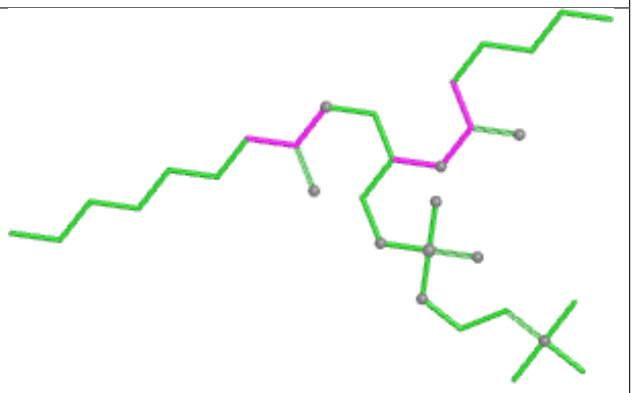
Ligand CLR A 1109



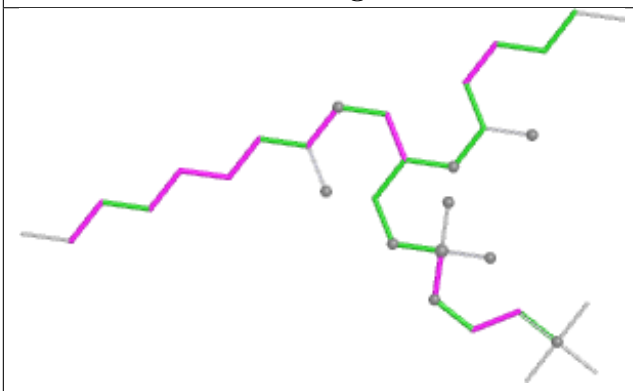
Ligand POV B 1112



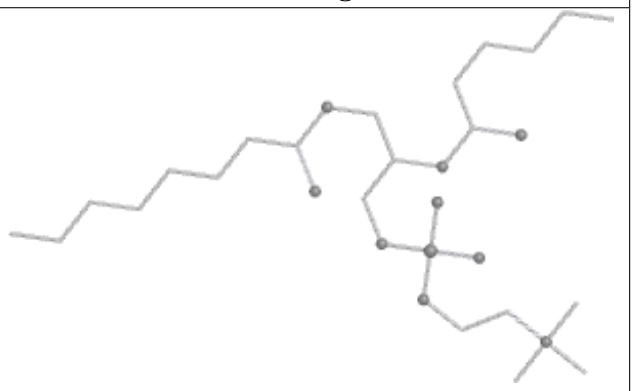
Bond lengths



Bond angles

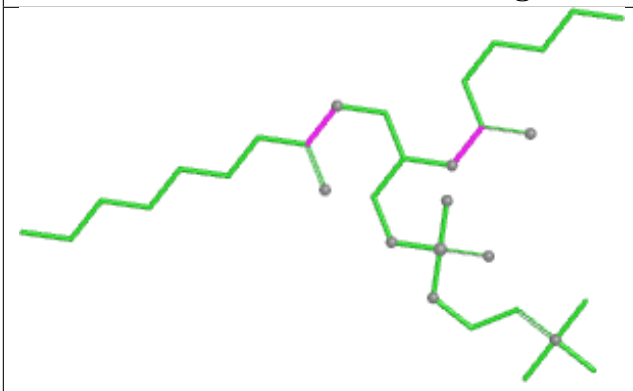


Torsions

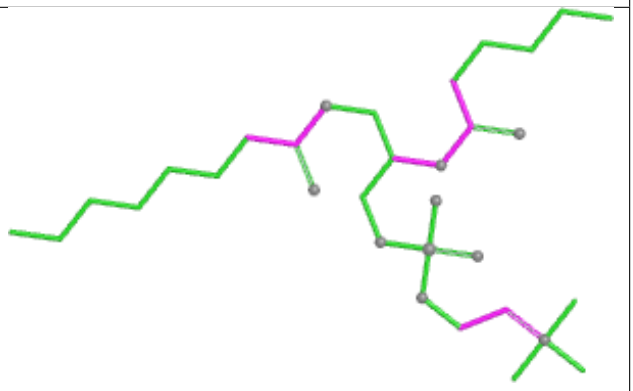


Rings

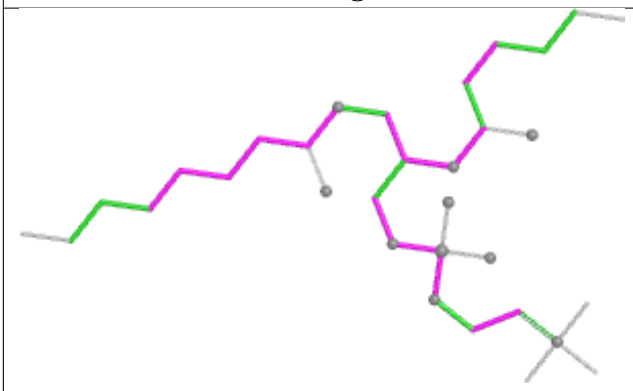
Ligand POV C 1110



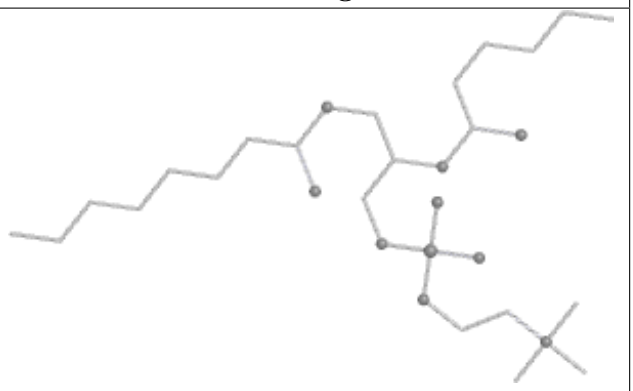
Bond lengths



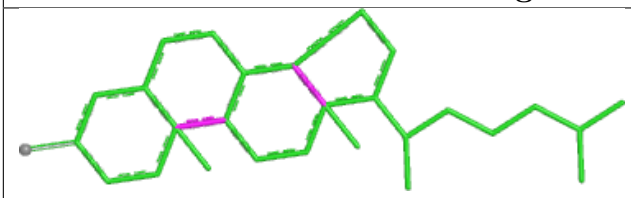
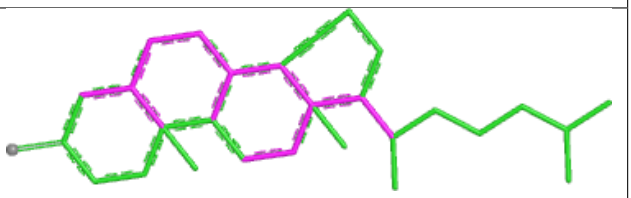
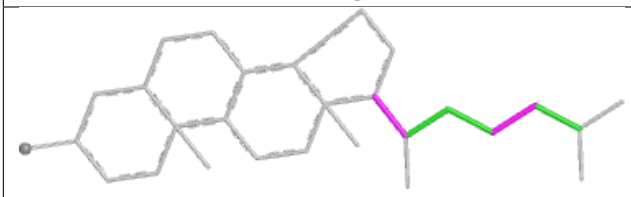
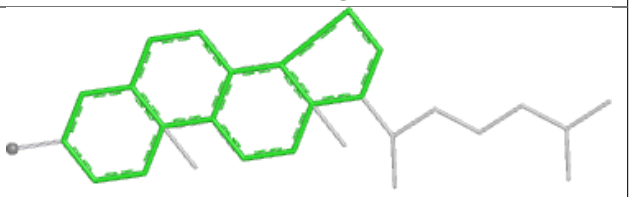
Bond angles

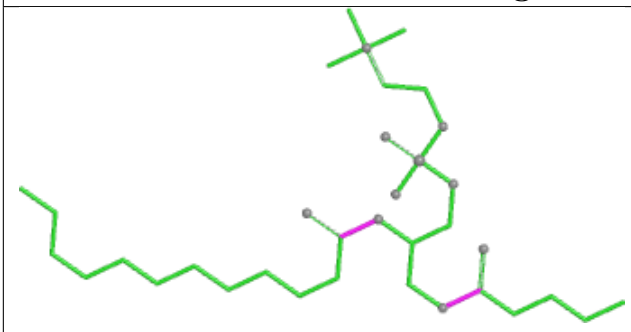
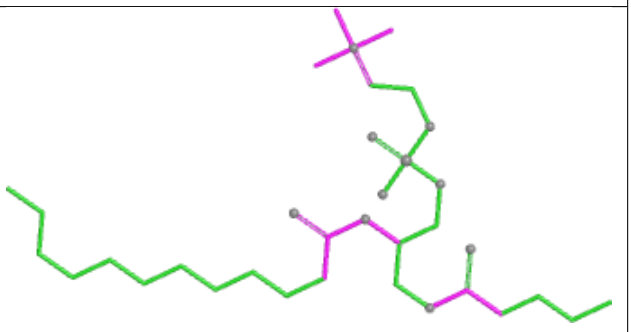
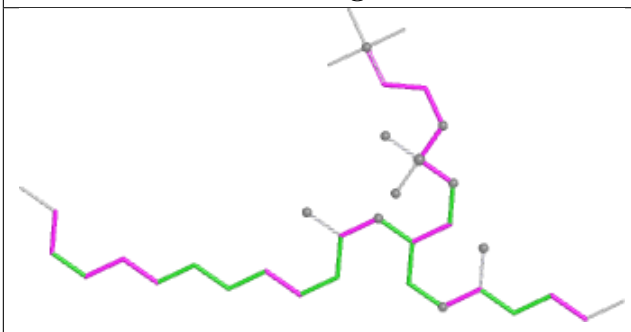
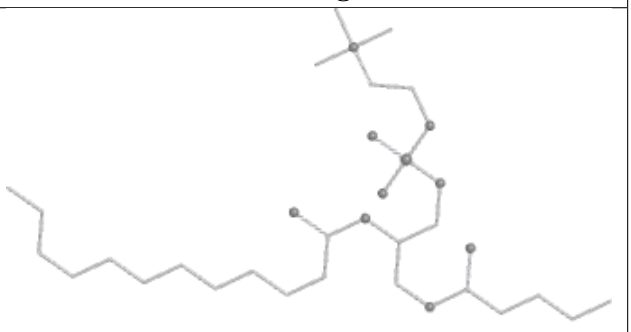


Torsions

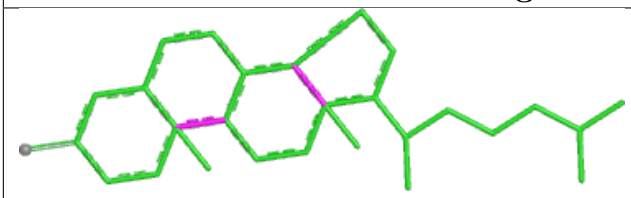


Rings

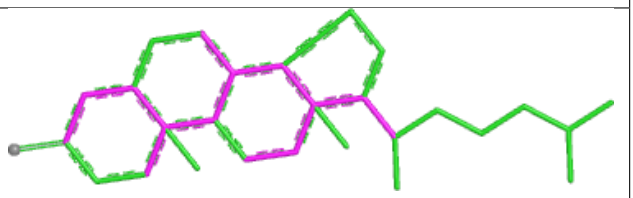
Ligand CLR C 1107	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV D 1111	
 Bond lengths	 Bond angles
 Torsions	 Rings

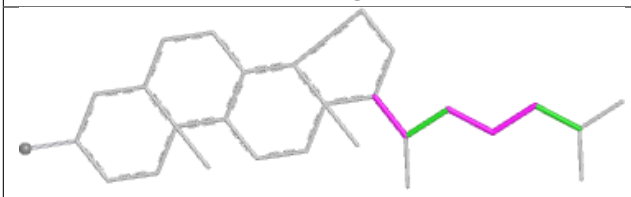
Ligand CLR B 1108



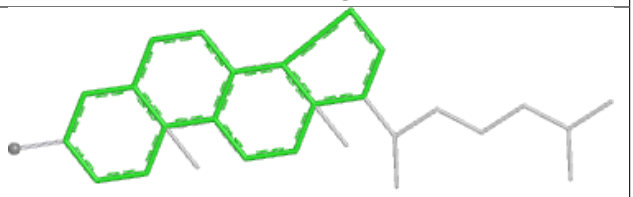
Bond lengths



Bond angles

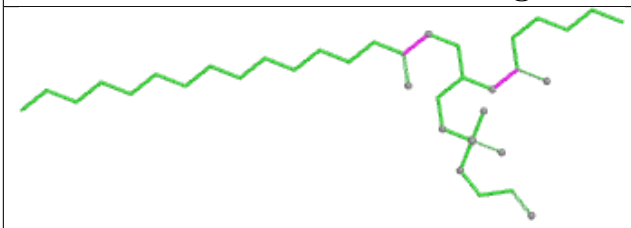


Torsions

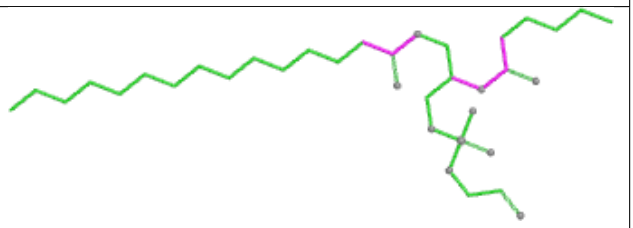


Rings

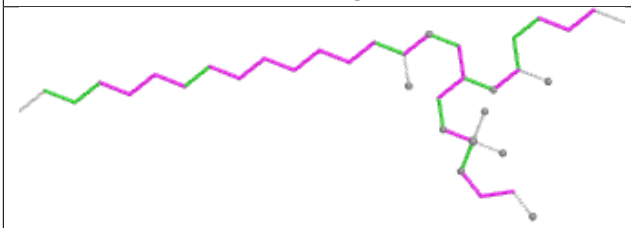
Ligand POV D 1113



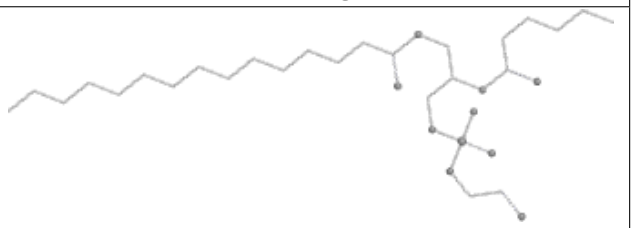
Bond lengths



Bond angles

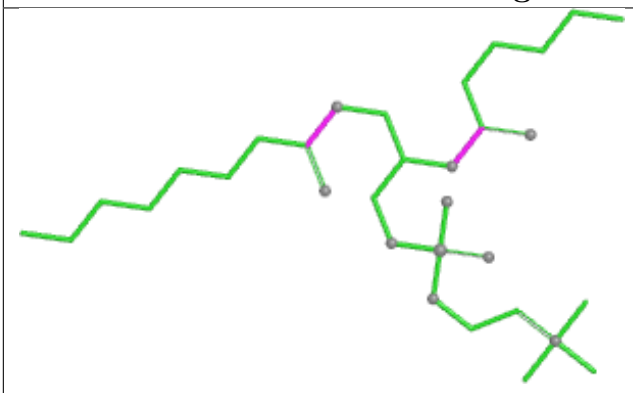


Torsions

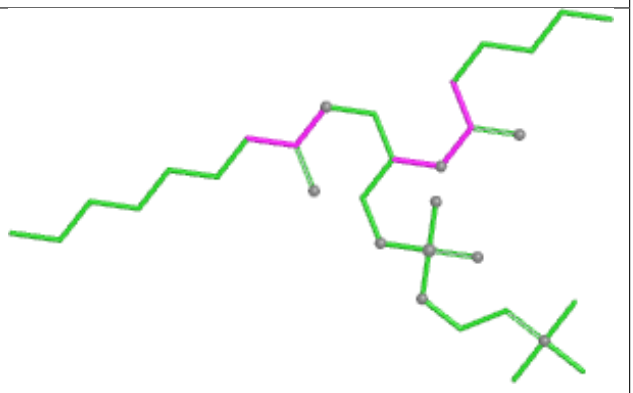


Rings

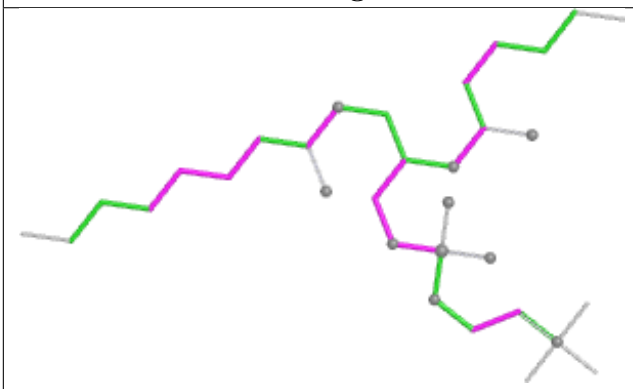
Ligand POV A 1115



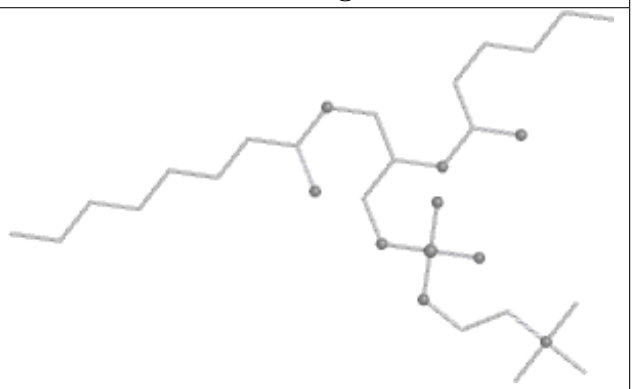
Bond lengths



Bond angles

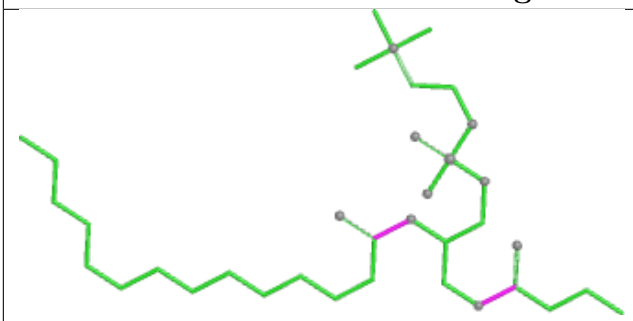


Torsions

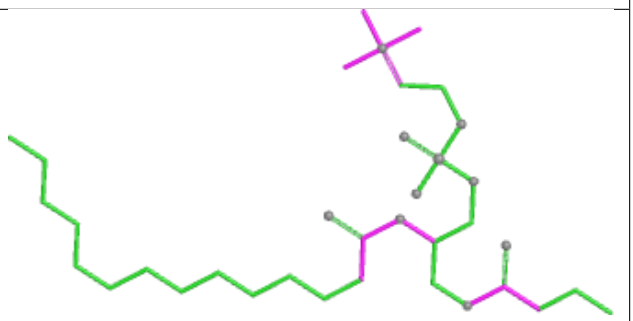


Rings

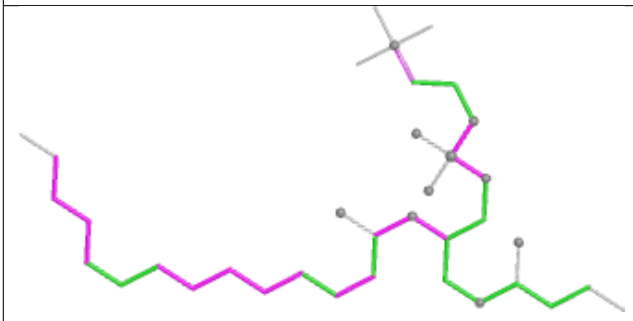
Ligand POV B 1106



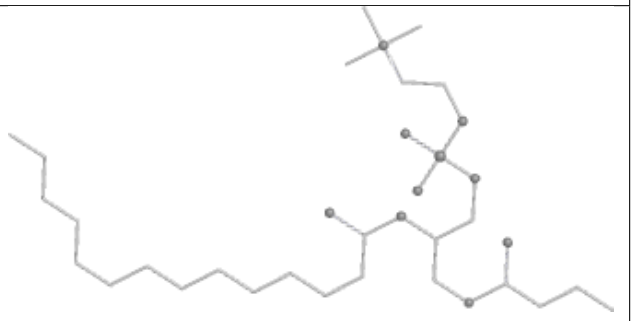
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

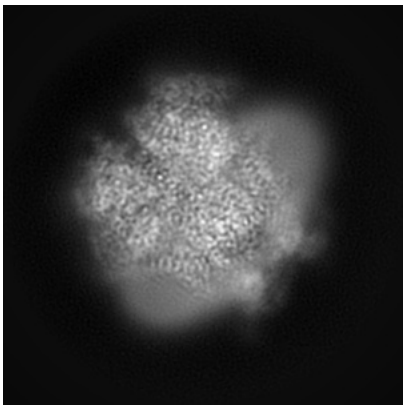
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-46421. These allow visual inspection of the internal detail of the map and identification of artifacts.

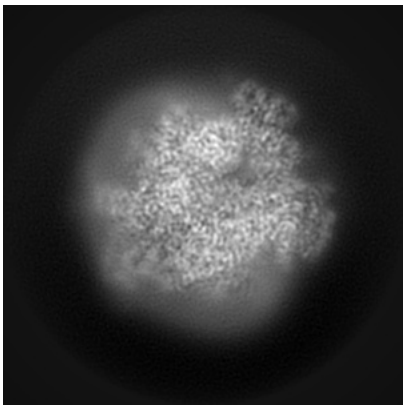
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

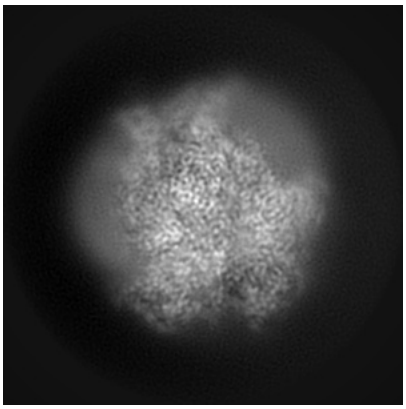
6.1.1 Primary map



X

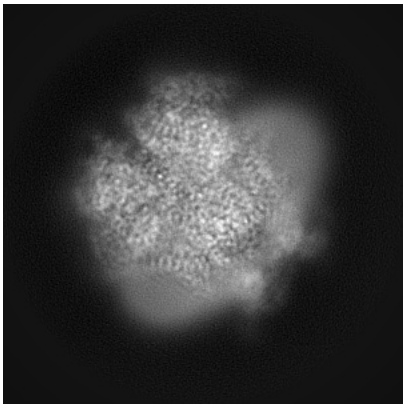


Y

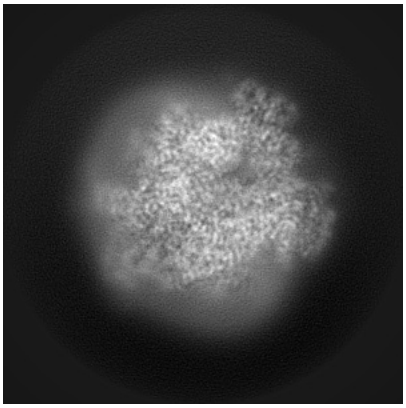


Z

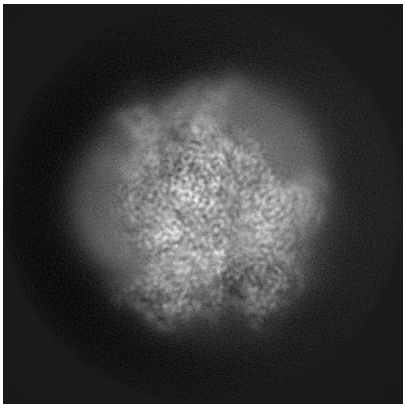
6.1.2 Raw map



X



Y

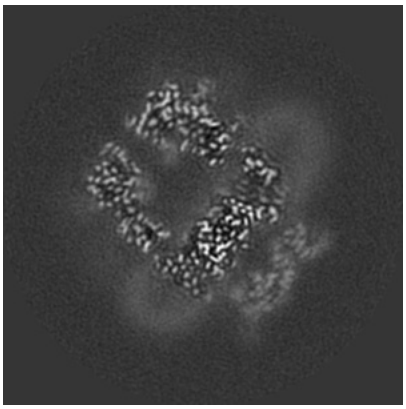


Z

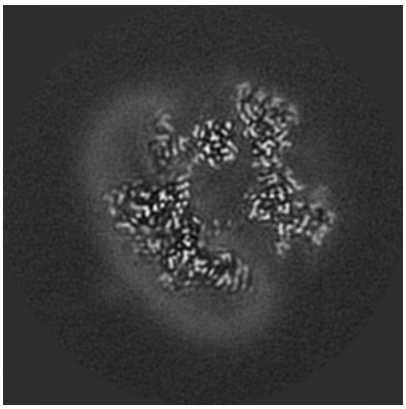
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

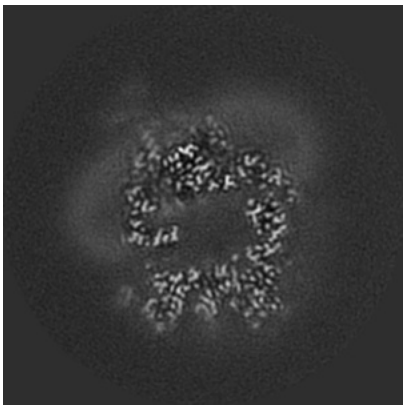
6.2.1 Primary map



X Index: 150

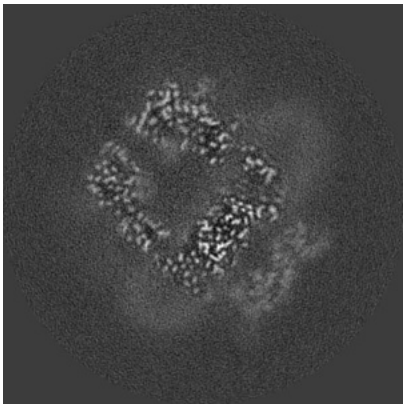


Y Index: 150

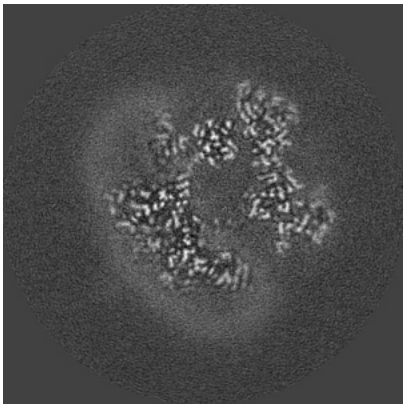


Z Index: 150

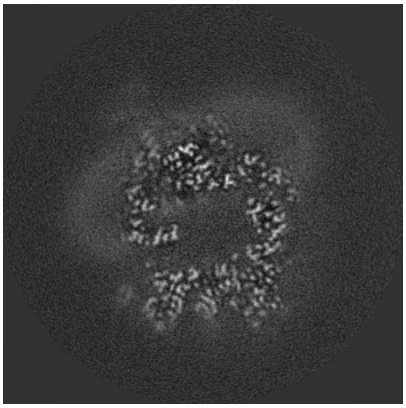
6.2.2 Raw map



X Index: 150



Y Index: 150

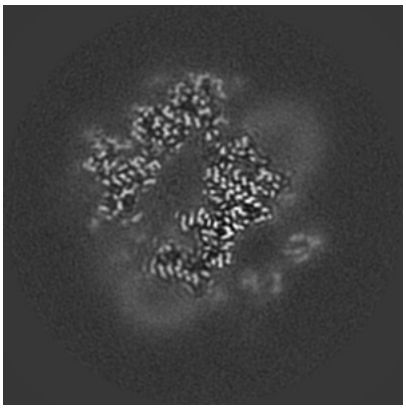


Z Index: 150

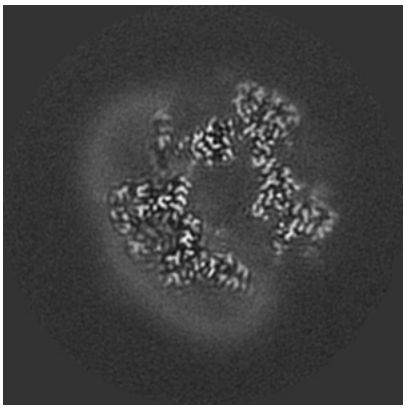
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

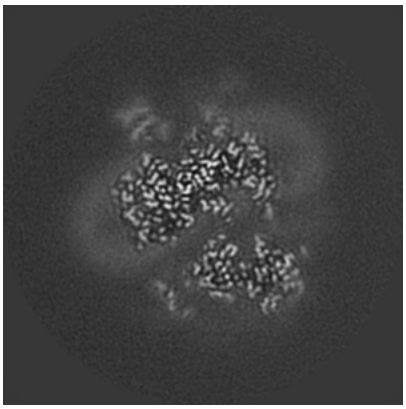
6.3.1 Primary map



X Index: 137

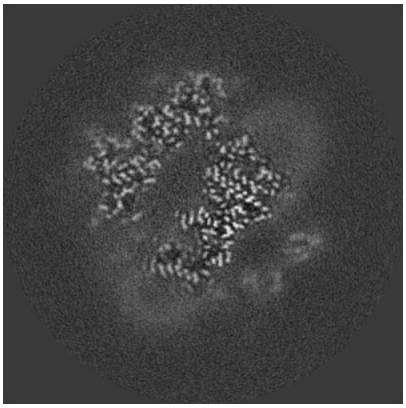


Y Index: 148

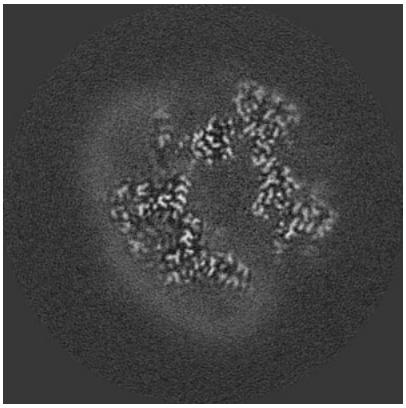


Z Index: 136

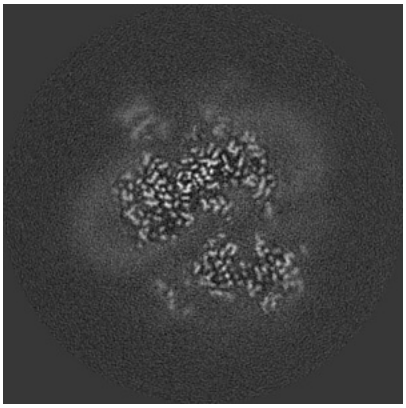
6.3.2 Raw map



X Index: 137



Y Index: 148

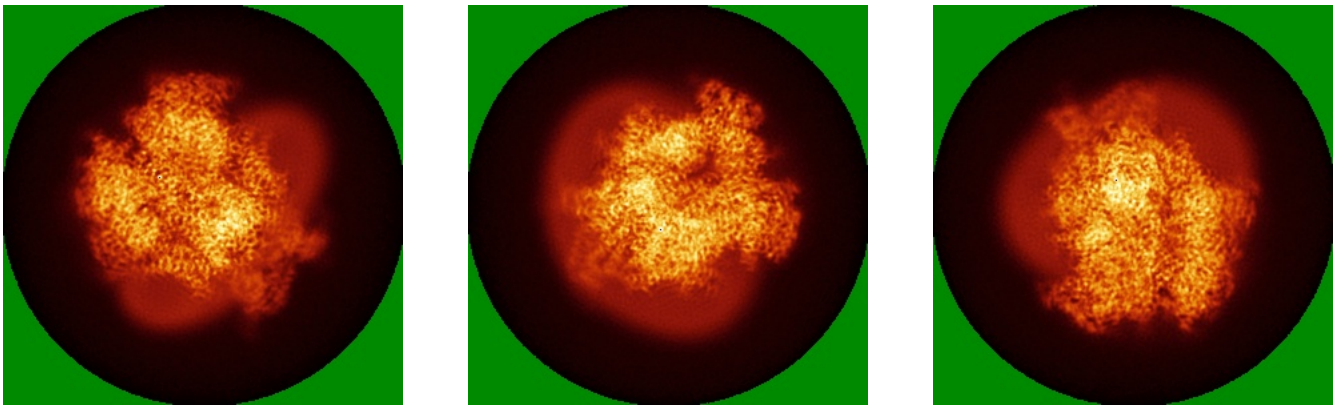


Z Index: 136

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

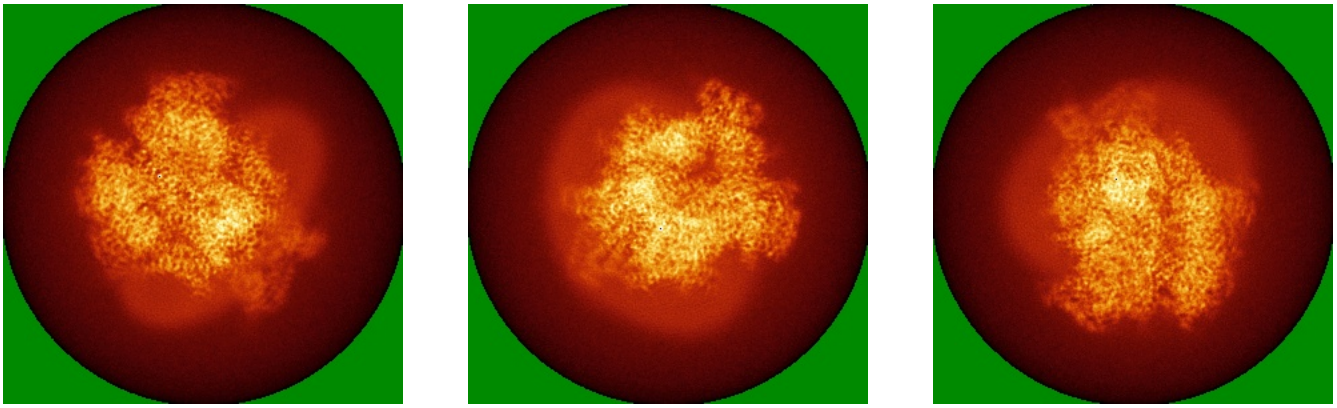
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

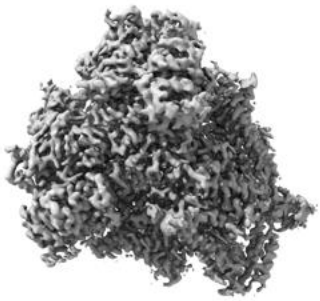


X Y Z

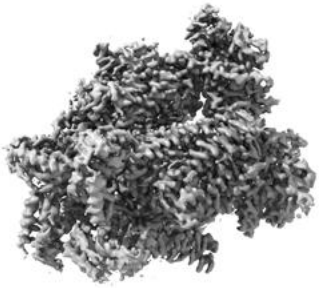
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X

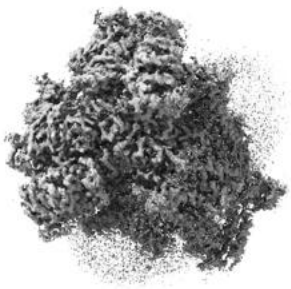


Y

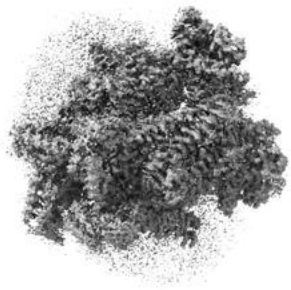
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0126. 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



X



Y

Z

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.

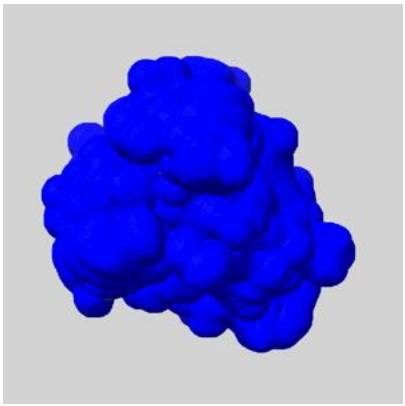
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

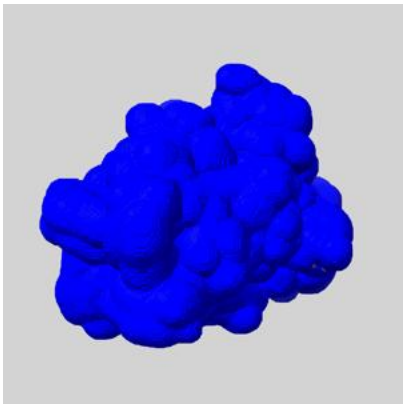
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

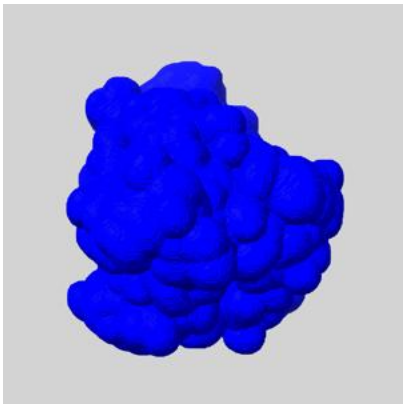
6.6.1 emd_46421_msk_1.map



X



Y

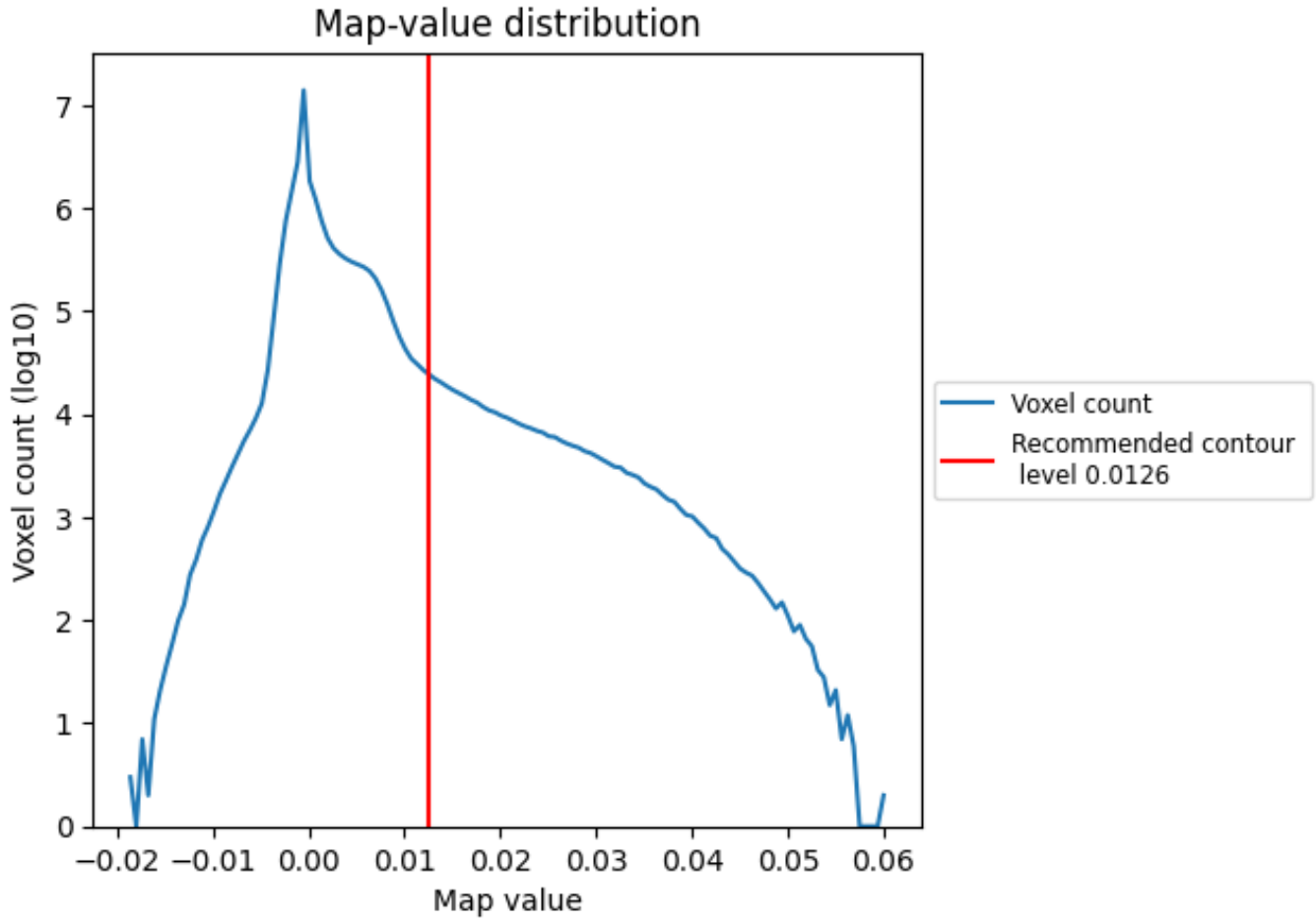


Z

7 Map analysis

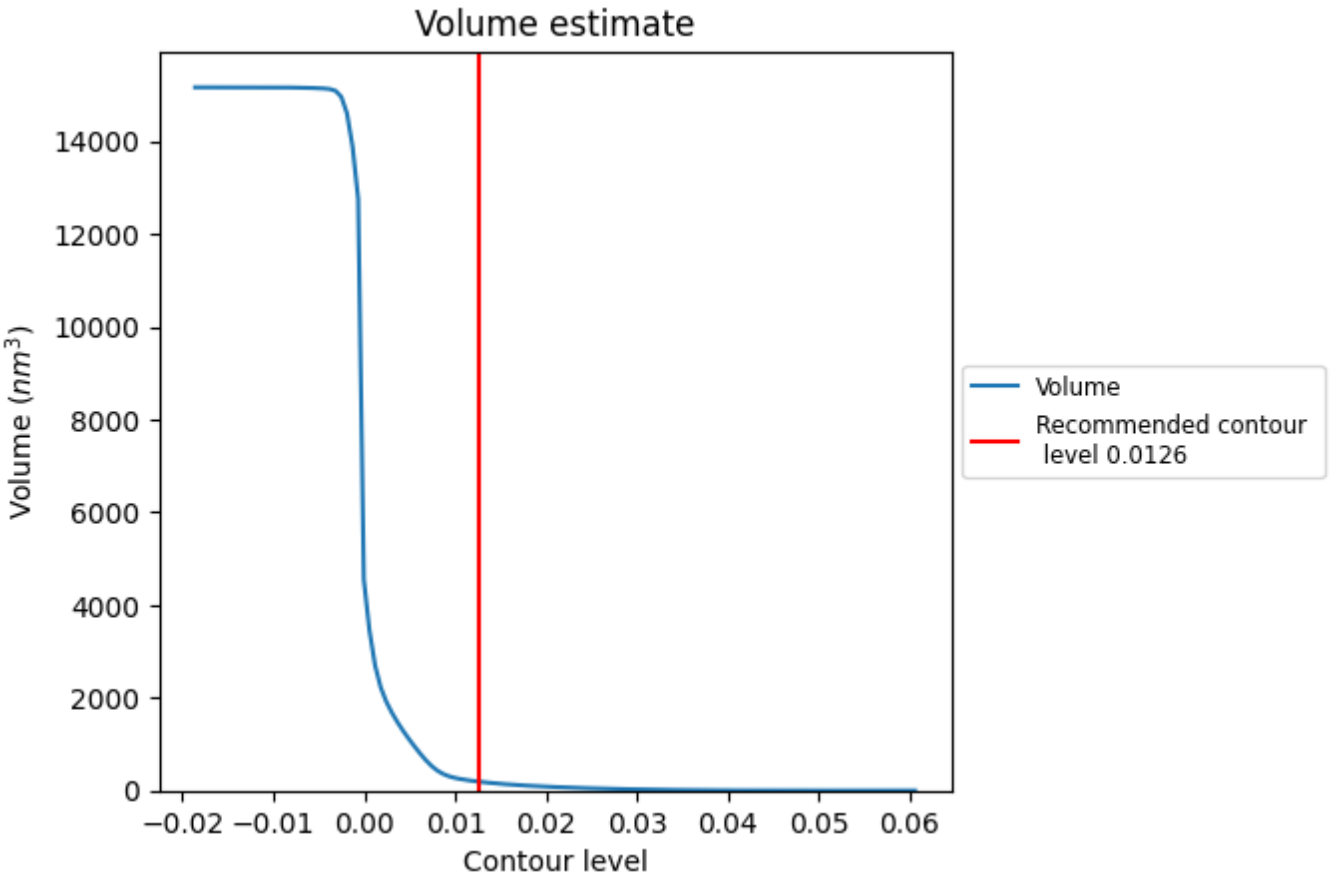
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

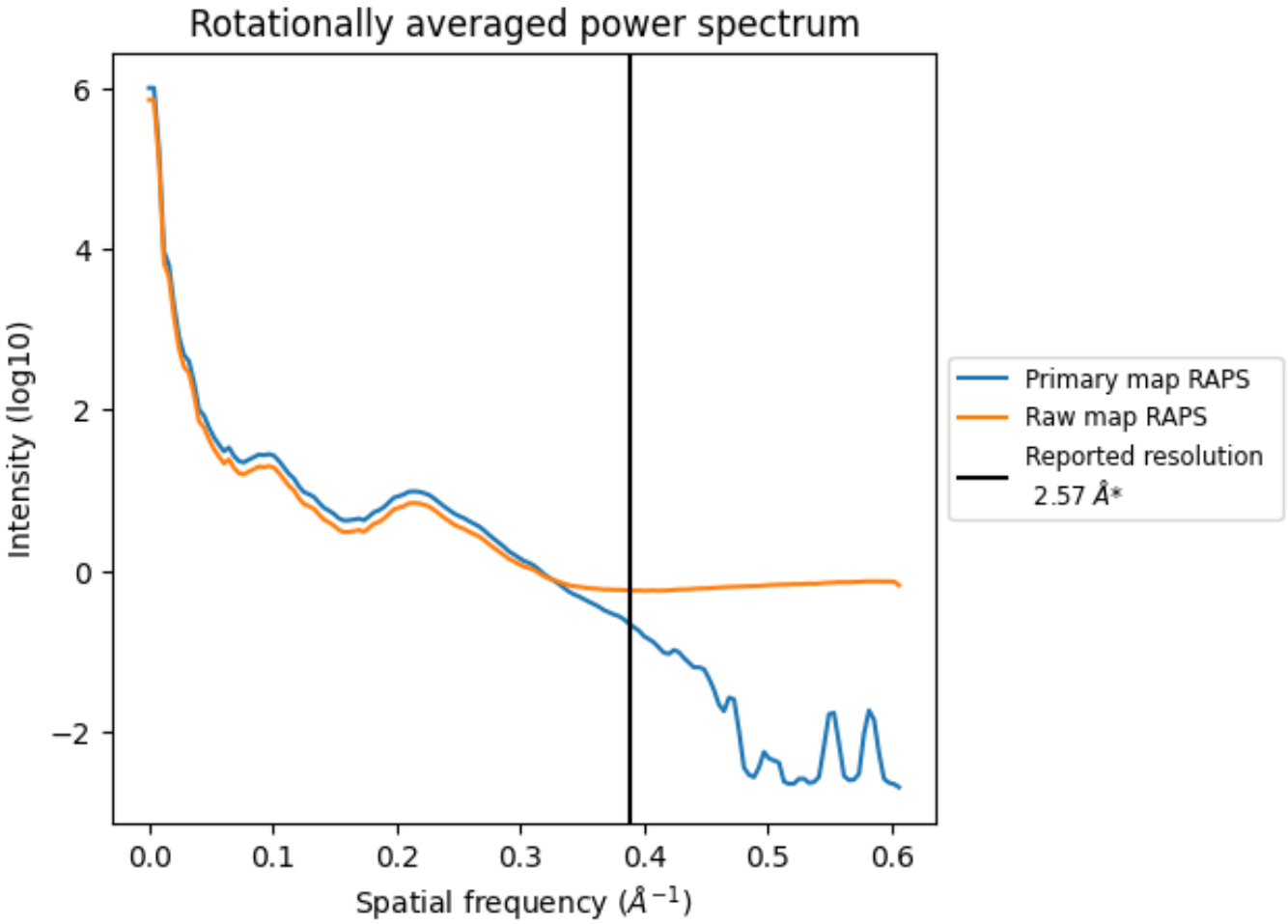
7.2 Volume estimate (i)



The volume at the recommended contour level is 192 nm^3; this corresponds to an approximate mass of 174 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 (i)

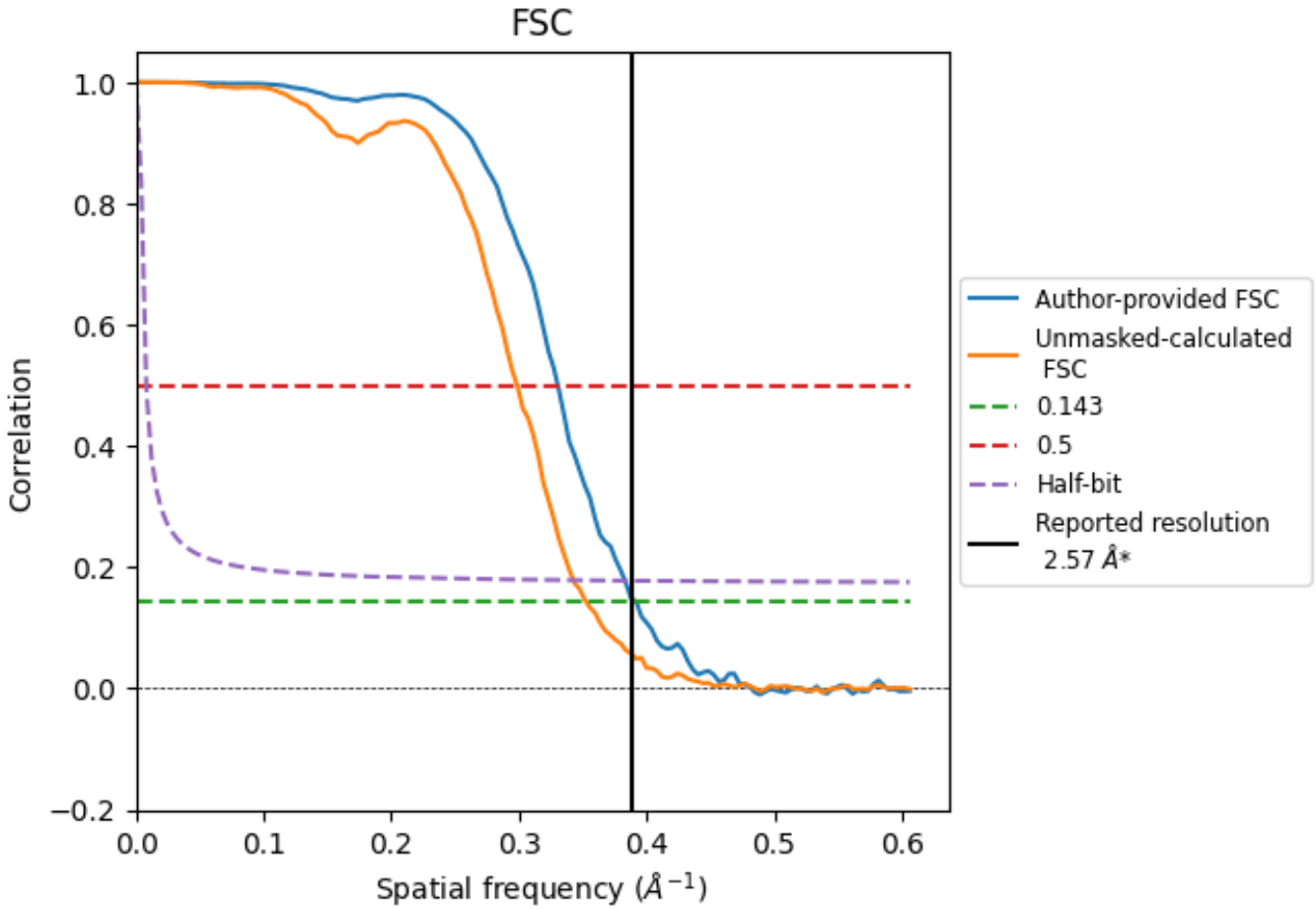


*Reported resolution corresponds to spatial frequency of 0.389 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.389 Å^{-1}

8.2 Resolution estimates (i)

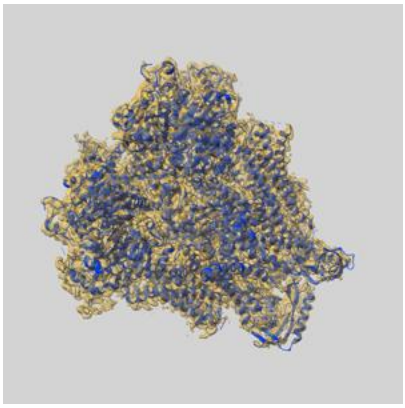
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.57	-	-
Author-provided FSC curve	2.55	3.03	2.61
Unmasked-calculated*	2.84	3.35	2.92

*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 2.84 differs from the reported value 2.57 by more than 10 %

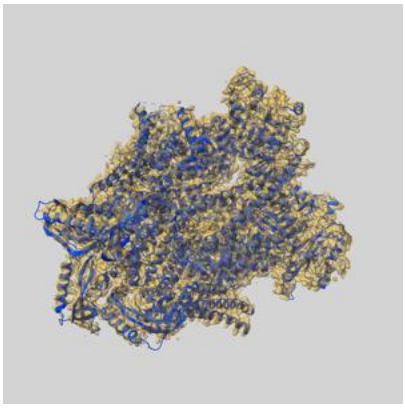
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-46421 and PDB model 9CZM. Per-residue inclusion information can be found in section 3 on page 9.

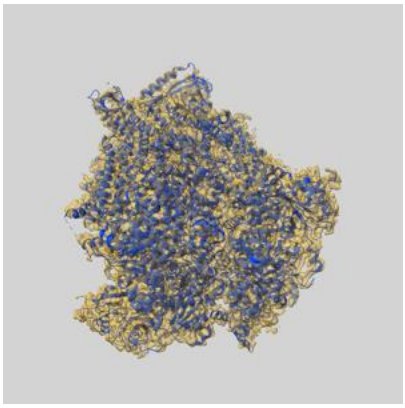
9.1 Map-model overlay



X



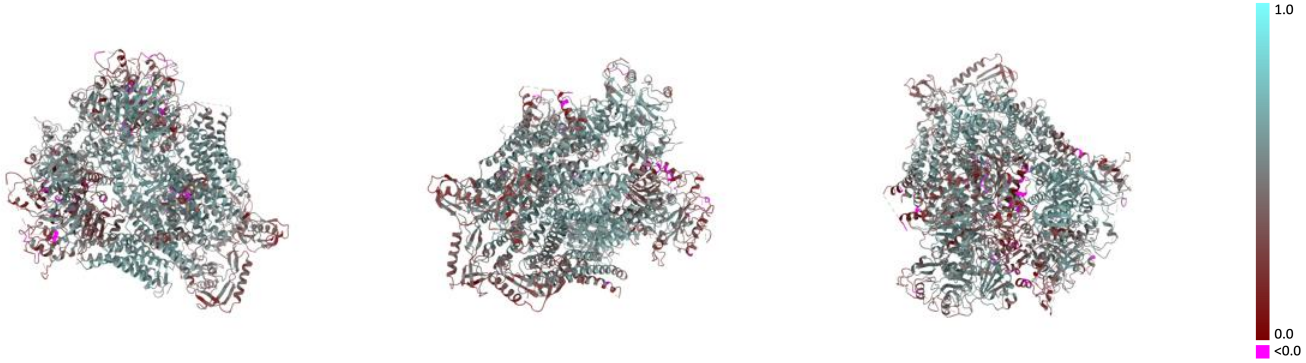
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0126 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.

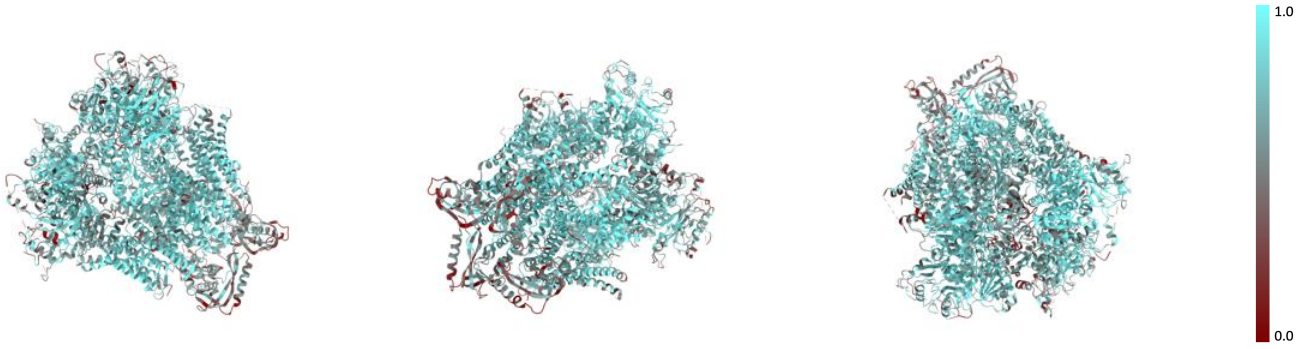
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

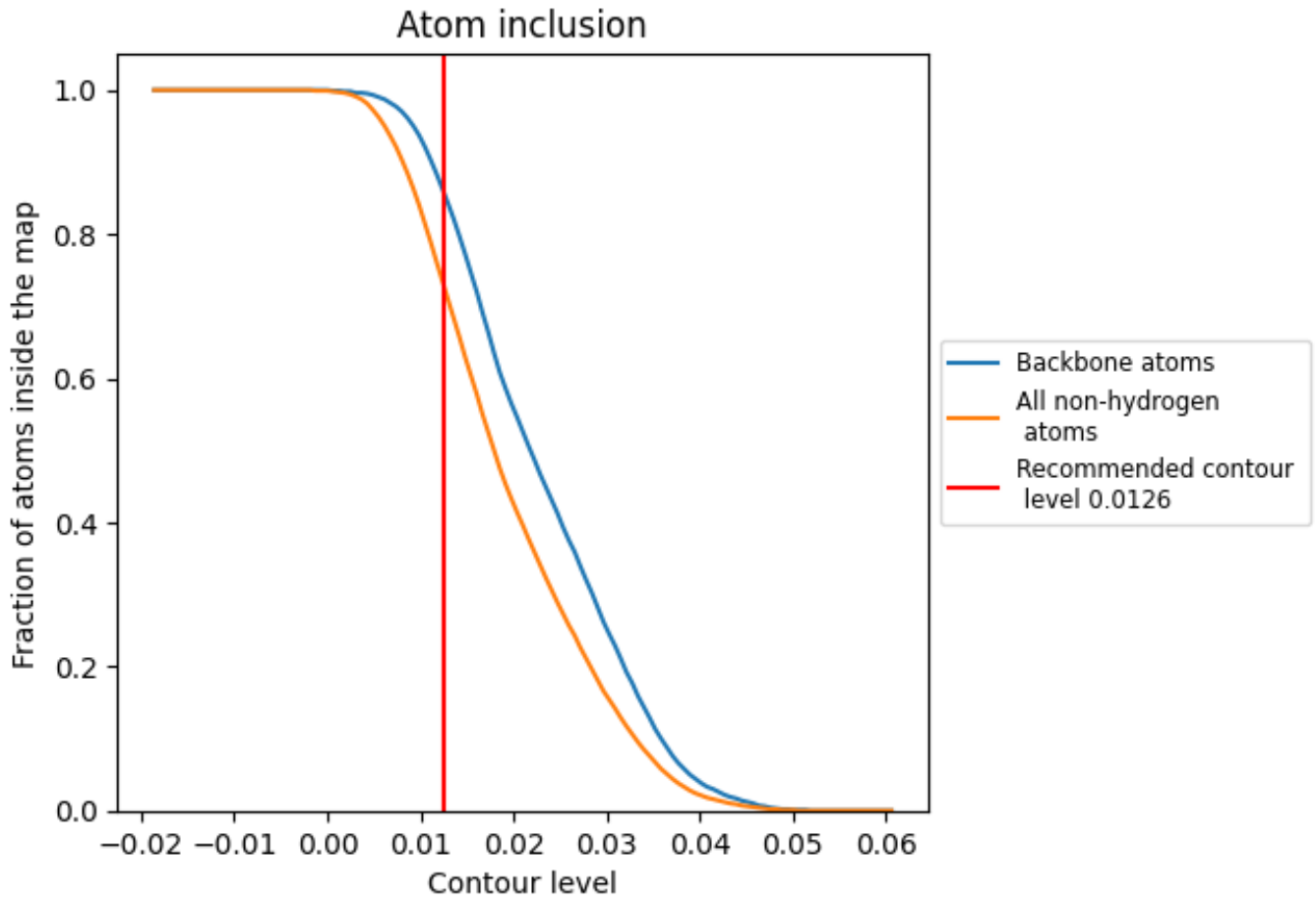
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0126).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 72% 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 (0.0126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7250	0.4730
A	0.8390	0.5770
B	0.6860	0.3990
C	0.8140	0.5470
D	0.6900	0.3990
E	0.5760	0.4510
F	0.5710	0.4270
G	0.5810	0.4320
H	0.5820	0.4320