



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:14 am BST

PDB ID : 4N7K
Title : Zinc Substituted Reaction Center of the Rhodobacter sphaeroides
Authors : Hardjasa, A.; Murphy, M.E.P.
Deposited on : 2013-10-15
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

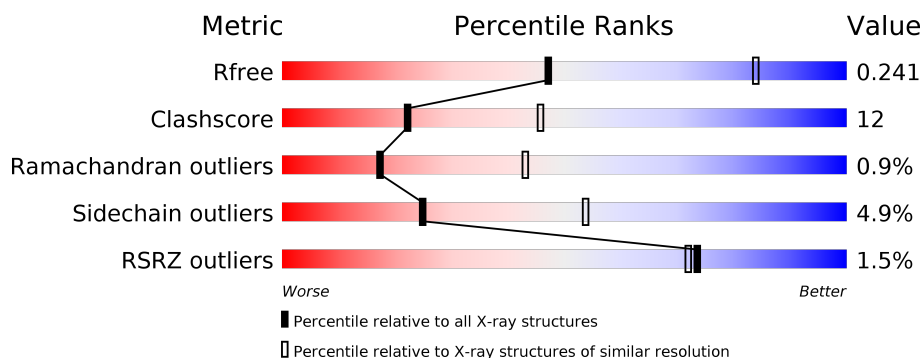
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	241	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>.</div> </div> </div>
2	L	281	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>20%</div> <div>.</div> </div> </div>
3	M	303	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>.</div> </div> </div>

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
10	HTO	L	309	-	-	-	X
10	HTO	L	310	-	-	-	X
14	PC1	M	410	-	-	-	X
5	GGD	H	305	-	-	-	X
7	LDA	L	303	-	-	-	X

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 7634 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Reaction Center H Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	0	5	1
			1849	1183	320	337	9			

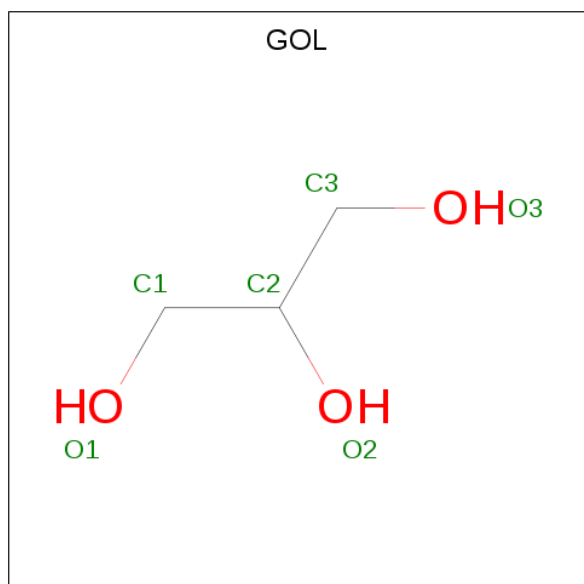
- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	2	0
			2239	1513	355	363	8			

- Molecule 3 is a protein called Reaction center protein M chain.

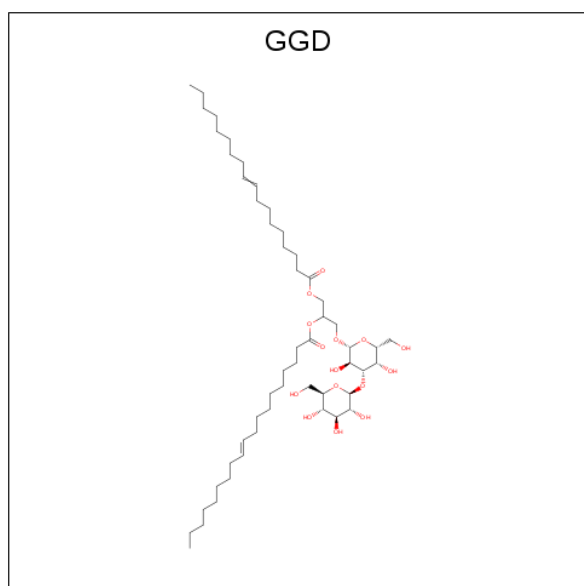
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	1	1
			2411	1607	396	398	10			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



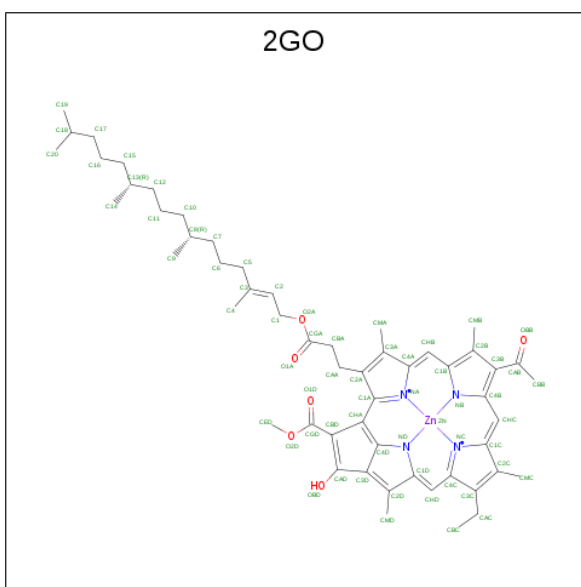
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is NONADEC-10-ENOIC ACID 2-[3,4-DIHYDROXY-6-HYDROXYMETHYL-5-(3,4,5-TRIHYDROXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-2-YLOXY)-TETRAHYDRO-PYRAN-2-YLOXY]-1-OCTADEC-9-ENOYLOXYMETHYL-ETHYL ESTER (three-letter code: GGD) (formula: C₅₂H₉₄O₁₅).



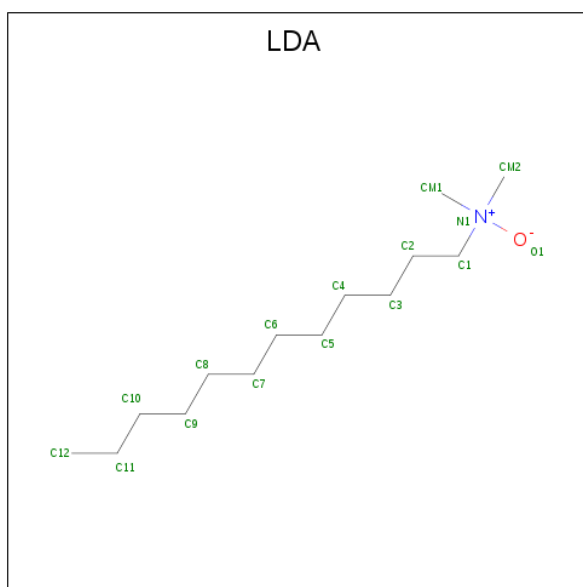
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			57	42	15		

- Molecule 6 is [methyl 9-acetyl-14-ethyl-20-hydroxy-4,8,13,18-tetramethyl-3-{3-oxo-3-[(3,7,11,15-tetramethylhexadec-2-en-1-yl)oxy]propyl}-3,4,20,21-tetradecahydrophorbine-21-carboxylato(2-)-kappa 4 N 23 ,N 24 ,N 25 ,N 26]zinc (three-letter code: 2GO) (formula: C₅₅H₇₀N₄O₆Zn).



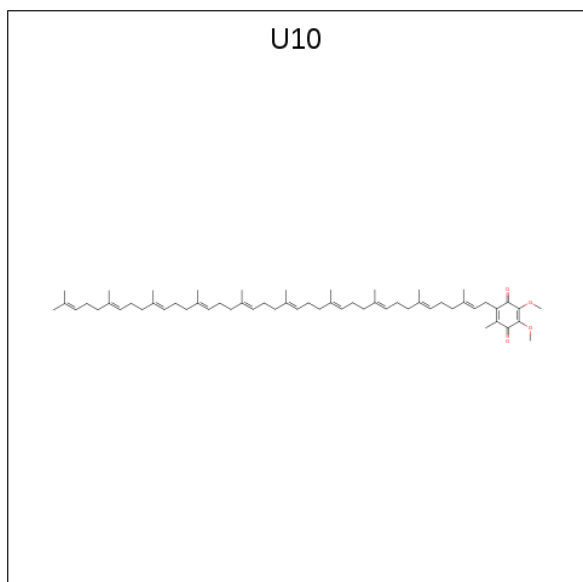
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total 66	C 55	N 4	O 6	Zn 1	0	0
6	L	1	Total 66	C 55	N 4	O 6	Zn 1	0	0
6	L	1	Total 66	C 55	N 4	O 6	Zn 1	0	0
6	M	1	Total 66	C 55	N 4	O 6	Zn 1	0	0
6	M	1	Total 66	C 55	N 4	O 6	Zn 1	0	0
6	M	1	Total 66	C 55	N 4	O 6	Zn 1	0	0

- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $\text{C}_{14}\text{H}_{31}\text{NO}$).



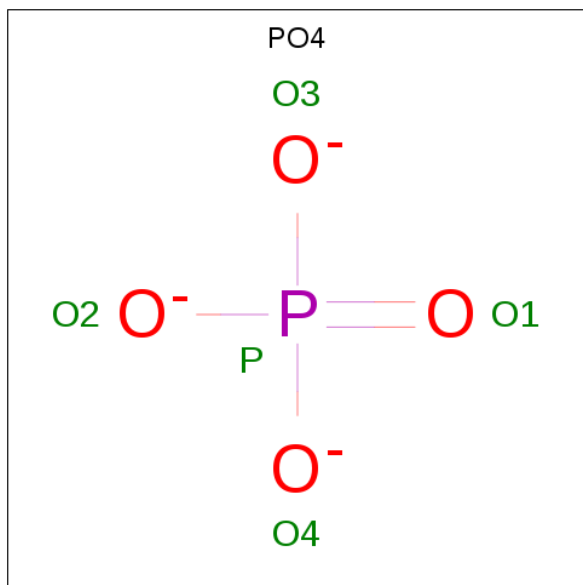
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



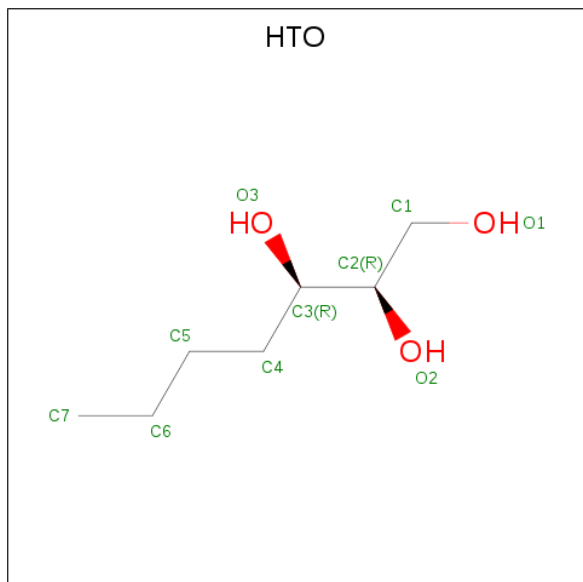
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		
8	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).

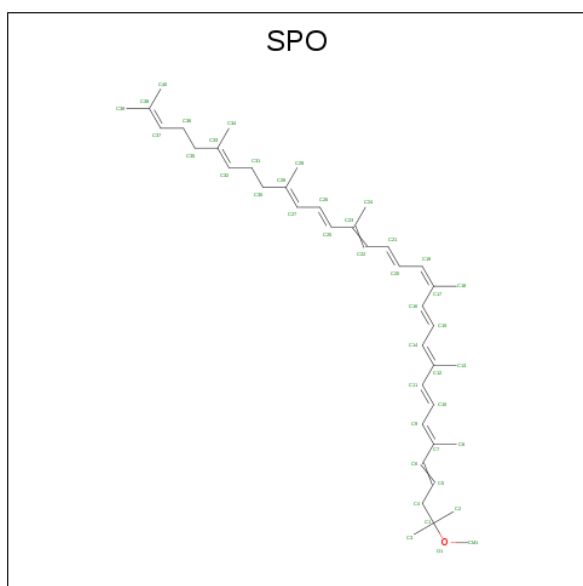


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		
10	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

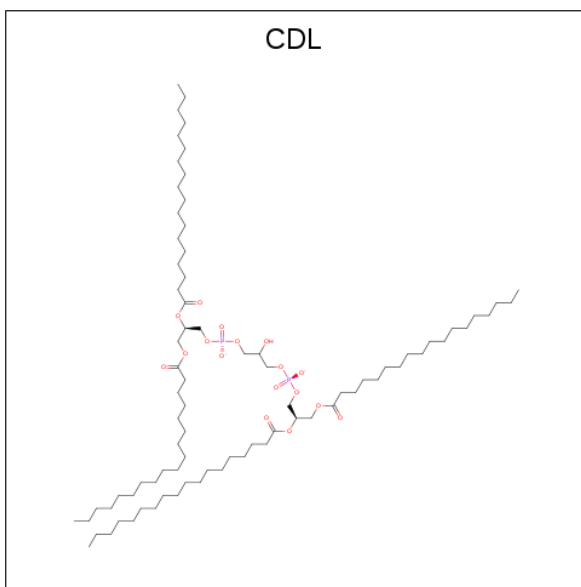
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula: C₄₁H₆₀O).



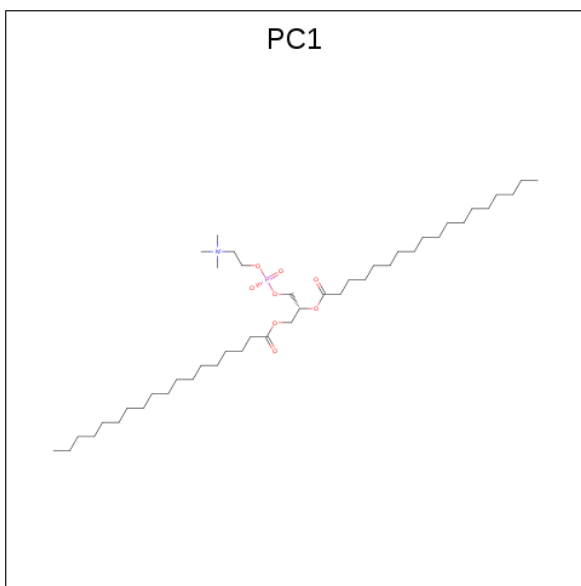
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 14 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	M	1	Total	C	N	O	P	0	0
			43	33	1	8	1		

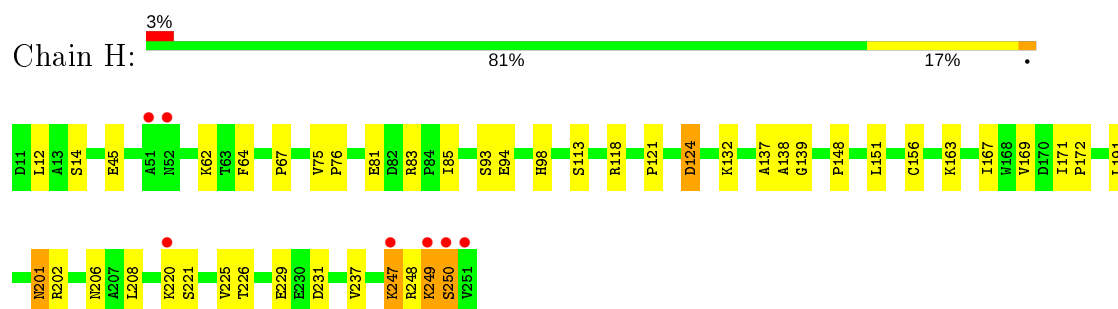
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	109	Total 109	O 109	0	0
15	L	81	Total 81	O 81	0	0
15	M	84	Total 84	O 84	0	0

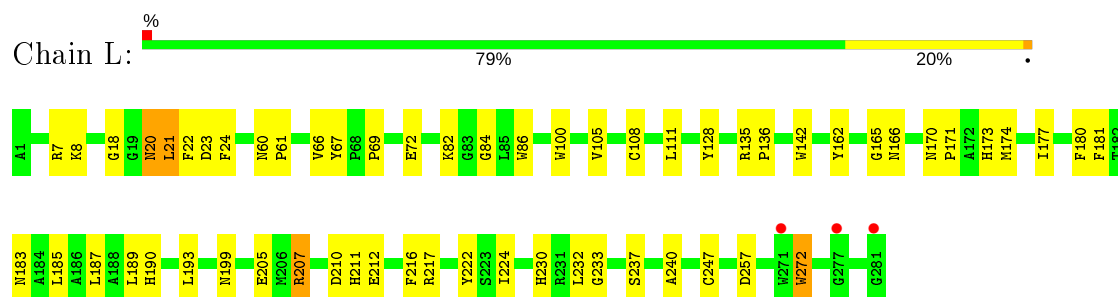
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

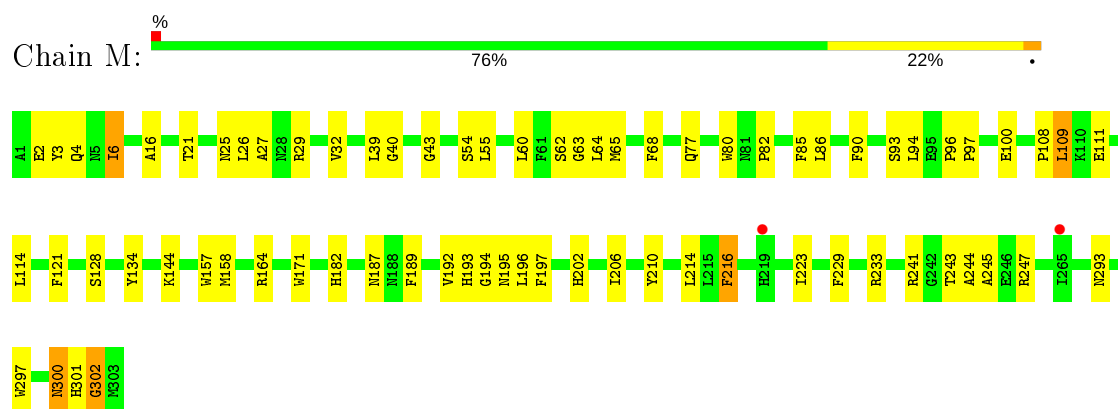
• Molecule 1: Reaction Center H Chain



• Molecule 2: Reaction center protein L chain



• Molecule 3: Reaction center protein M chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.45Å 139.45Å 184.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.91 – 2.85 36.89 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.0 (36.91-2.85) 96.1 (36.89-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.182 , 0.243 0.182 , 0.241	Depositor DCC
R_{free} test set	2368 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7634	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, LDA, GGD, CDL, PO4, PC1, HTO, FE, SPO, U10, 2GO

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	H	0.57	0/1929	0.75	0/2619
2	L	0.57	0/2339	0.66	0/3203
3	M	0.58	0/2508	0.69	0/3424
All	All	0.57	0/6776	0.70	0/9246

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1849	0	1872	35	0
2	L	2239	0	2185	61	0
3	M	2411	0	2319	59	0
4	H	24	0	32	3	0
4	L	18	0	24	3	0
5	H	57	0	68	2	0
6	L	198	0	207	14	0
6	M	198	0	207	27	0
7	L	48	0	93	1	0
7	M	32	0	62	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	46	0	46	14	0
8	M	48	0	63	2	0
9	L	5	0	0	1	0
10	L	20	0	32	0	0
11	M	1	0	0	0	0
12	M	42	0	60	5	0
13	M	81	0	106	2	0
14	M	43	0	60	0	0
15	H	109	0	0	6	0
15	L	81	0	0	3	0
15	M	84	0	0	5	0
All	All	7634	0	7436	173	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (173) 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)
6:L:301:2GO:H9	3:M:206:ILE:HD13	1.48	0.94
3:M:197:PHE:HZ	6:M:402:2GO:H21	1.33	0.93
1:H:118[B]:ARG:HD2	15:M:566:HOH:O	1.72	0.89
3:M:197:PHE:CZ	6:M:402:2GO:H21	2.08	0.88
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.58	0.86
6:M:402:2GO:H19	6:M:402:2GO:CBB	2.05	0.86
6:L:305:2GO:H22	6:L:305:2GO:H19	1.59	0.84
2:L:20:ASN:HD22	2:L:20:ASN:H	1.27	0.81
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.63	0.81
6:L:305:2GO:H21	3:M:210:TYR:HB3	1.62	0.81
2:L:199:ASN:HA	4:L:311:GOL:H31	1.66	0.76
4:L:313:GOL:H12	7:M:403:LDA:O1	1.87	0.75
1:H:248:ARG:HA	1:H:249[B]:LYS:HB3	1.67	0.74
2:L:67:TYR:HB3	15:L:424:HOH:O	1.87	0.74
2:L:181:PHE:CD2	6:M:406:2GO:H20	2.22	0.73
2:L:224:ILE:HG22	8:L:306[A]:U10:H8	1.71	0.73
2:L:230:HIS:CD2	3:M:223:ILE:HG13	2.23	0.73
6:M:402:2GO:H22	6:M:402:2GO:H19	1.70	0.72
3:M:300:ASN:C	3:M:302:GLY:H	1.93	0.72
1:H:98:HIS:CD2	2:L:7:ARG:HE	2.07	0.71
2:L:187:LEU:HD13	3:M:216:PHE:CG	2.26	0.71
1:H:137:ALA:HA	15:H:464:HOH:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:177:ILE:HD13	6:M:401:2GO:H9	1.73	0.69
1:H:81:GLU:HG3	1:H:85[B]:ILE:HD11	1.74	0.69
2:L:224:ILE:HB	8:L:306[A]:U10:C10	2.23	0.68
6:M:406:2GO:H22	6:M:406:2GO:H19	1.76	0.67
2:L:181:PHE:HB3	6:M:406:2GO:H21	1.74	0.67
1:H:248:ARG:HA	1:H:249[A]:LYS:HB3	1.76	0.67
3:M:108:PRO:HG2	3:M:111:GLU:HB2	1.77	0.67
3:M:63:GLY:HA3	6:M:406:2GO:H40	1.75	0.67
1:H:81:GLU:OE1	2:L:8:LYS:NZ	2.27	0.66
6:M:401:2GO:CBB	12:M:408:SPO:H243	2.25	0.66
8:L:306[B]:U10:O3	8:L:306[B]:U10:C4M	2.44	0.65
6:M:402:2GO:H19	6:M:402:2GO:H21	1.79	0.65
3:M:297:TRP:CE2	3:M:302:GLY:HA2	2.32	0.64
2:L:60:ASN:ND2	2:L:61:PRO:HD2	2.12	0.64
2:L:224:ILE:HB	8:L:306[A]:U10:H103	1.79	0.64
2:L:100:TRP:CH2	8:M:407:U10:H251	2.32	0.64
2:L:128:TYR:HD1	6:L:301:2GO:H20	1.63	0.64
6:L:305:2GO:CBB	3:M:210:TYR:HB3	2.26	0.64
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.81	0.63
1:H:121:PRO:HB3	1:H:225:VAL:O	1.99	0.63
8:L:306[B]:U10:H4M2	8:L:306[B]:U10:O3	1.96	0.63
3:M:189:PHE:O	3:M:193:HIS:HD2	1.81	0.63
1:H:132:LYS:HD2	1:H:171:ILE:HD13	1.82	0.62
2:L:189:LEU:HD23	6:M:406:2GO:H8	1.82	0.61
6:L:305:2GO:H20	3:M:210:TYR:CD2	2.34	0.61
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.82	0.61
3:M:300:ASN:O	3:M:302:GLY:N	2.34	0.60
6:M:401:2GO:H21	12:M:408:SPO:H243	1.83	0.60
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.36	0.59
2:L:181:PHE:HB3	6:M:406:2GO:CBB	2.33	0.59
6:L:301:2GO:H19	6:L:301:2GO:H21	1.85	0.59
6:M:401:2GO:H22	6:M:402:2GO:H37	1.84	0.59
1:H:201:ASN:HD22	1:H:201:ASN:H	1.49	0.59
2:L:20:ASN:ND2	2:L:20:ASN:H	1.99	0.58
6:M:402:2GO:CBD	6:M:402:2GO:H31	2.34	0.58
2:L:187:LEU:HD13	3:M:216:PHE:CD2	2.38	0.58
1:H:137:ALA:O	15:H:462:HOH:O	2.17	0.58
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.39	0.58
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.39	0.57
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.87	0.57
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:300:ASN:C	3:M:302:GLY:N	2.56	0.57
6:M:401:2GO:CBB	6:M:401:2GO:H19	2.35	0.57
1:H:156:CYS:HB3	1:H:206:ASN:O	2.05	0.57
2:L:190:HIS:HA	8:L:306[A]:U10:O2	2.05	0.57
15:H:401:HOH:O	13:M:409:CDL:HA32	2.05	0.57
1:H:62:LYS:HE2	1:H:64:PHE:CZ	2.41	0.56
7:L:304:LDA:H121	8:L:306[B]:U10:H1M1	1.87	0.56
3:M:164:ARG:HD3	15:M:551:HOH:O	2.04	0.56
1:H:138:ALA:N	15:H:464:HOH:O	2.32	0.56
5:H:305:GGD:H351	8:M:407:U10:H23	1.89	0.55
4:H:303:GOL:O1	5:H:305:GGD:C44	2.55	0.54
1:H:81:GLU:O	1:H:83:ARG:HG2	2.07	0.54
2:L:22:PHE:HA	2:L:24:PHE:CE2	2.43	0.53
3:M:4:GLN:HA	3:M:4:GLN:NE2	2.24	0.52
2:L:232:LEU:HD21	8:L:306[B]:U10:H1M2	1.91	0.52
3:M:193:HIS:O	3:M:293:ASN:HA	2.09	0.52
2:L:224:ILE:H	8:L:306[A]:U10:H8	1.74	0.51
3:M:189:PHE:O	3:M:193:HIS:CD2	2.62	0.51
3:M:2:GLU:HG3	3:M:3:TYR:N	2.25	0.51
3:M:90:PHE:CD1	3:M:90:PHE:N	2.78	0.51
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.58	0.51
3:M:194:GLY:O	3:M:195:ASN:HB3	2.11	0.51
6:M:401:2GO:H20	12:M:408:SPO:H243	1.92	0.51
3:M:300:ASN:N	3:M:300:ASN:ND2	2.58	0.51
1:H:226:THR:OG1	1:H:229:GLU:HG3	2.11	0.51
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.93	0.51
6:L:301:2GO:H19	6:L:301:2GO:CBB	2.41	0.51
3:M:197:PHE:HZ	6:M:402:2GO:CBB	2.14	0.50
1:H:62:LYS:NZ	4:H:301:GOL:H32	2.27	0.50
2:L:189:LEU:CD2	6:M:406:2GO:H8	2.41	0.50
6:L:305:2GO:H19	6:L:305:2GO:CBB	2.38	0.50
3:M:90:PHE:HD1	3:M:90:PHE:N	2.10	0.50
1:H:75:VAL:HA	1:H:76:PRO:C	2.33	0.49
2:L:183:ASN:ND2	2:L:237[B]:SER:OG	2.45	0.49
3:M:80:TRP:O	3:M:82:PRO:HD3	2.11	0.49
3:M:109:LEU:O	3:M:114:LEU:HB2	2.12	0.49
8:L:306[B]:U10:C3M	8:L:306[B]:U10:O2	2.61	0.49
3:M:157:TRP:CE2	12:M:408:SPO:H293	2.48	0.48
3:M:194:GLY:O	3:M:195:ASN:CB	2.60	0.48
3:M:192:VAL:O	3:M:192:VAL:HG12	2.12	0.48
2:L:174:MET:CE	6:M:401:2GO:H3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:97:PRO:HG2	3:M:171:TRP:HB2	1.95	0.48
2:L:185:LEU:HD13	6:M:406:2GO:ND	2.29	0.48
2:L:224:ILE:HB	8:L:306[A]:U10:H102	1.93	0.48
6:L:305:2GO:H20	3:M:210:TYR:CG	2.49	0.48
13:M:409:CDL:H421	13:M:409:CDL:H381	1.96	0.47
3:M:25:ASN:OD1	3:M:27:ALA:HB3	2.14	0.47
2:L:257:ASP:HB3	15:L:468:HOH:O	2.15	0.47
2:L:187:LEU:HD13	3:M:216:PHE:CB	2.44	0.47
2:L:217:ARG:HD2	15:L:477:HOH:O	2.14	0.47
2:L:233:GLY:HA3	3:M:216:PHE:CE1	2.50	0.46
6:M:401:2GO:H54	6:M:401:2GO:H47	1.96	0.46
3:M:233:ARG:HA	15:M:505:HOH:O	2.14	0.46
6:L:301:2GO:H13	6:L:307:2GO:CGA	2.45	0.46
2:L:82:LYS:HE2	9:L:308:PO4:O1	2.16	0.46
3:M:134:TYR:CE2	3:M:144:LYS:HG3	2.51	0.45
2:L:105:VAL:O	2:L:108:CYS:HB2	2.16	0.45
1:H:167:ILE:HG22	1:H:169:VAL:HG12	1.98	0.45
2:L:216:PHE:CG	8:L:306[A]:U10:H72	2.51	0.45
3:M:85:PHE:HD2	3:M:86:LEU:HD23	1.82	0.45
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.50	0.45
1:H:118[B]:ARG:NH2	15:H:509:HOH:O	2.47	0.45
1:H:98:HIS:HE1	15:H:409:HOH:O	2.00	0.44
3:M:64:LEU:HB3	3:M:68:PHE:CE1	2.52	0.44
1:H:118[B]:ARG:CD	15:M:566:HOH:O	2.47	0.44
2:L:162:TYR:HA	2:L:165:GLY:O	2.17	0.44
2:L:166:ASN:OD1	2:L:166:ASN:C	2.56	0.44
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.52	0.44
3:M:62:SER:OG	3:M:121:PHE:O	2.35	0.44
1:H:124:ASP:CB	1:H:172:PRO:HG3	2.47	0.44
2:L:207:ARG:CG	2:L:211:HIS:CG	3.01	0.44
2:L:66:VAL:HG12	2:L:86:TRP:HB2	1.99	0.43
2:L:18:GLY:O	2:L:21:LEU:HB2	2.18	0.43
2:L:207:ARG:HG2	2:L:211:HIS:CG	2.53	0.43
2:L:222:TYR:HD2	8:L:306[B]:U10:O5	2.02	0.43
2:L:230:HIS:CD2	3:M:223:ILE:CG1	2.98	0.43
3:M:243:THR:O	3:M:247:ARG:HG3	2.18	0.43
6:M:401:2GO:H21	6:M:401:2GO:H19	2.00	0.43
8:L:306[B]:U10:H3M3	8:L:306[B]:U10:O2	2.18	0.43
1:H:138:ALA:HA	1:H:139:GLY:HA2	1.65	0.42
3:M:65:MET:HB3	3:M:121:PHE:CD2	2.55	0.42
1:H:124:ASP:HB2	1:H:172:PRO:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:PRO:HA	2:L:205:GLU:OE1	2.18	0.42
2:L:170:ASN:O	2:L:173:HIS:HB3	2.18	0.42
1:H:247:LYS:HD2	1:H:247:LYS:H	1.84	0.42
1:H:208:LEU:HD21	1:H:237:VAL:HA	2.02	0.42
3:M:77:GLN:HE22	3:M:93:SER:H	1.67	0.42
3:M:6:ILE:HG12	15:M:517:HOH:O	2.19	0.42
2:L:193:LEU:HD21	2:L:212:GLU:HB3	2.02	0.42
3:M:241:ARG:HG3	3:M:245:ALA:HB3	2.01	0.42
1:H:62:LYS:HZ2	4:H:301:GOL:H32	1.85	0.42
3:M:196:LEU:HD12	6:M:402:2GO:C1D	2.50	0.41
2:L:230:HIS:NE2	3:M:223:ILE:HG13	2.34	0.41
1:H:156:CYS:HB2	1:H:248:ARG:HG3	2.03	0.41
3:M:2:GLU:HG3	3:M:3:TYR:H	1.85	0.41
12:M:408:SPO:H10	12:M:408:SPO:H81	1.98	0.41
2:L:111:LEU:HD23	2:L:111:LEU:HA	1.85	0.41
6:L:307:2GO:C1C	6:M:402:2GO:H22	2.51	0.41
3:M:157:TRP:CE3	3:M:158:MET:HG2	2.56	0.41
2:L:171:PRO:O	2:L:174:MET:HB2	2.20	0.41
2:L:187:LEU:HD13	3:M:216:PHE:HB2	2.02	0.41
2:L:66:VAL:O	2:L:86:TRP:HD1	2.03	0.40
1:H:45:GLU:HG3	1:H:94:GLU:CD	2.41	0.40
3:M:40:GLY:HA2	3:M:43:GLY:O	2.21	0.40
6:L:305:2GO:H22	6:L:305:2GO:CHC	2.41	0.40
2:L:84:GLY:HA3	4:L:312:GOL:H11	2.04	0.40
2:L:181:PHE:CG	6:M:406:2GO:H20	2.56	0.40
6:L:305:2GO:H36	6:L:305:2GO:H43	1.62	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 X-ray entries followed by that with respect to entries of similar resolution.

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	H	245/241 (102%)	230 (94%)	11 (4%)	4 (2%)	9	28
2	L	281/281 (100%)	262 (93%)	17 (6%)	2 (1%)	22	50
3	M	302/303 (100%)	277 (92%)	23 (8%)	2 (1%)	22	50
All	All	828/825 (100%)	769 (93%)	51 (6%)	8 (1%)	17	40

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	250	SER
3	M	301	HIS
1	H	249[A]	LYS
1	H	249[B]	LYS
3	M	302	GLY
1	H	124	ASP
2	L	23	ASP
2	L	272	TRP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	H	199/196 (102%)	184 (92%)	15 (8%)	13	34
2	L	221/220 (100%)	214 (97%)	7 (3%)	39	69
3	M	237/237 (100%)	224 (94%)	13 (6%)	21	49
All	All	657/653 (101%)	622 (95%)	35 (5%)	25	50

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	LEU
1	H	14	SER
1	H	93	SER
1	H	113	SER
1	H	163[A]	LYS

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Mol	Chain	Res	Type
1	H	163[B]	LYS
1	H	191	LEU
1	H	201	ASN
1	H	202	ARG
1	H	220[A]	LYS
1	H	220[B]	LYS
1	H	220[C]	LYS
1	H	221	SER
1	H	231	ASP
1	H	247	LYS
2	L	20	ASN
2	L	21	LEU
2	L	72	GLU
2	L	207	ARG
2	L	210	ASP
2	L	247	CYS
2	L	272	TRP
3	M	6	ILE
3	M	29	ARG
3	M	39	LEU
3	M	54	SER
3	M	60	LEU
3	M	94	LEU
3	M	96	PRO
3	M	100	GLU
3	M	109	LEU
3	M	182	HIS
3	M	214	LEU
3	M	216	PHE
3	M	300	ASN

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

Mol	Chain	Res	Type
1	H	98	HIS
1	H	201	ASN
2	L	20	ASN
2	L	159	ASN
2	L	183	ASN
3	M	4	GLN
3	M	77	GLN
3	M	187	ASN

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Mol	Chain	Res	Type
3	M	193	HIS
3	M	300	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 1 is monoatomic - leaving 28 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
10	HTO	L	310	-	9,9,9	0.70	0	10,10,10	0.63	0
4	GOL	L	311	-	5,5,5	0.44	0	5,5,5	0.41	0
7	LDA	M	403	-	12,15,15	2.20	1 (8%)	14,17,17	0.70	0
10	HTO	L	309	-	9,9,9	0.75	0	10,10,10	0.79	0
7	LDA	L	304	-	12,15,15	2.14	1 (8%)	14,17,17	0.64	0
6	2GO	L	305	-	59,74,74	2.09	16 (27%)	52,115,115	2.63	15 (28%)
7	LDA	L	303	-	12,15,15	2.11	1 (8%)	14,17,17	0.46	0
13	CDL	M	409	-	80,80,99	3.56	5 (6%)	86,92,111	1.25	8 (9%)
6	2GO	M	401	3	59,74,74	2.05	14 (23%)	52,115,115	2.63	14 (26%)
14	PC1	M	410	-	42,42,53	1.17	2 (4%)	48,50,61	2.49	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	2GO	M	402	3	59,74,74	2.03	15 (25%)	52,115,115	2.81	13 (25%)
6	2GO	M	406	-	59,74,74	2.10	17 (28%)	52,115,115	2.69	14 (26%)
4	GOL	H	303	-	5,5,5	0.51	0	5,5,5	0.44	0
6	2GO	L	301	2	59,74,74	2.17	15 (25%)	52,115,115	2.50	15 (28%)
4	GOL	L	312	-	5,5,5	0.33	0	5,5,5	0.42	0
4	GOL	H	301	-	5,5,5	0.42	0	5,5,5	0.54	0
8	U10	M	407	-	48,48,63	1.47	4 (8%)	58,61,79	1.59	12 (20%)
5	GGD	H	305	-	58,58,68	1.04	3 (5%)	72,72,82	1.52	12 (16%)
8	U10	L	306[A]	-	23,23,63	2.07	2 (8%)	28,31,79	1.36	4 (14%)
4	GOL	H	304	-	5,5,5	0.44	0	5,5,5	0.58	0
8	U10	L	306[B]	-	23,23,63	1.94	2 (8%)	28,31,79	1.35	4 (14%)
12	SPO	M	408	-	40,41,41	0.79	0	47,50,50	1.51	11 (23%)
6	2GO	L	307	2	59,74,74	1.99	13 (22%)	52,115,115	2.32	13 (25%)
9	PO4	L	308	-	4,4,4	0.98	0	6,6,6	0.38	0
4	GOL	H	302	-	5,5,5	0.78	0	5,5,5	1.06	0
4	GOL	L	313	-	5,5,5	0.35	0	5,5,5	0.54	0
7	LDA	M	404	-	12,15,15	2.11	1 (8%)	14,17,17	0.61	0
7	LDA	L	302	-	12,15,15	2.11	1 (8%)	14,17,17	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HTO	L	310	-	-	3/10/10/10	-
4	GOL	L	311	-	-	2/4/4/4	-
7	LDA	M	403	-	-	5/13/13/13	-
10	HTO	L	309	-	-	6/10/10/10	-
7	LDA	L	304	-	-	8/13/13/13	-
6	2GO	L	305	-	-	15/37/97/97	-
7	LDA	L	303	-	-	5/13/13/13	-
13	CDL	M	409	-	-	50/91/91/110	-
6	2GO	M	401	3	-	15/37/97/97	-
14	PC1	M	410	-	-	23/46/46/57	-
6	2GO	M	402	3	-	13/37/97/97	-
6	2GO	M	406	-	-	15/37/97/97	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	H	303	-	-	4/4/4/4	-
6	2GO	L	301	2	-	11/37/97/97	-
4	GOL	L	312	-	-	4/4/4/4	-
4	GOL	H	301	-	-	4/4/4/4	-
8	U10	M	407	-	-	9/45/69/87	0/1/1/1
5	GGD	H	305	-	-	13/47/87/97	0/2/2/2
8	U10	L	306[A]	-	-	3/15/39/87	0/1/1/1
4	GOL	H	304	-	-	2/4/4/4	-
8	U10	L	306[B]	-	-	5/15/39/87	0/1/1/1
12	SPO	M	408	-	-	9/47/47/47	-
6	2GO	L	307	2	-	6/37/97/97	-
4	GOL	H	302	-	-	2/4/4/4	-
4	GOL	L	313	-	-	2/4/4/4	-
7	LDA	M	404	-	-	6/13/13/13	-
7	LDA	L	302	-	-	6/13/13/13	-

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	409	CDL	C35-C34	29.93	3.19	1.51
8	L	306[A]	U10	C6-C1	8.53	1.50	1.35
8	L	306[B]	U10	C6-C1	8.14	1.50	1.35
7	M	403	LDA	O1-N1	-7.32	1.25	1.42
7	L	304	LDA	O1-N1	-7.30	1.25	1.42
7	M	404	LDA	O1-N1	-7.21	1.25	1.42
7	L	302	LDA	O1-N1	-7.15	1.25	1.42
8	M	407	U10	C6-C1	7.14	1.48	1.35
7	L	303	LDA	O1-N1	-7.11	1.25	1.42
6	L	301	2GO	O2D-CGD	6.63	1.48	1.33
6	L	305	2GO	O2D-CGD	6.13	1.46	1.33
6	L	305	2GO	C3D-C2D	5.52	1.49	1.39
6	M	401	2GO	O2D-CGD	5.36	1.45	1.33
6	L	307	2GO	O2D-CGD	5.28	1.45	1.33
6	M	406	2GO	C3D-C2D	5.17	1.48	1.39
6	M	402	2GO	O2D-CGD	5.10	1.44	1.33
6	L	301	2GO	O2A-CGA	5.06	1.48	1.33
6	M	406	2GO	O2D-CGD	5.01	1.44	1.33
13	M	409	CDL	OB6-CB5	4.99	1.48	1.34
6	M	401	2GO	O2A-CGA	4.94	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	401	2GO	C3D-C2D	4.89	1.48	1.39
13	M	409	CDL	OB8-CB7	4.88	1.47	1.33
6	M	401	2GO	C3B-C2B	4.78	1.48	1.39
6	L	305	2GO	C2A-C3A	4.76	1.51	1.37
6	L	301	2GO	C3B-C2B	4.76	1.48	1.39
6	L	307	2GO	C3C-C2C	4.76	1.51	1.37
14	M	410	PC1	O31-C31	4.74	1.47	1.33
6	L	305	2GO	C3C-C2C	4.73	1.51	1.37
13	M	409	CDL	OA6-CA5	4.72	1.47	1.34
6	M	406	2GO	O2A-CGA	4.70	1.47	1.33
14	M	410	PC1	O21-C21	4.66	1.47	1.34
6	M	402	2GO	C3B-C2B	4.65	1.47	1.39
13	M	409	CDL	OA8-CA7	4.64	1.46	1.33
6	L	307	2GO	C3D-C2D	4.63	1.47	1.39
6	L	305	2GO	O2A-CGA	4.58	1.46	1.33
6	L	301	2GO	C3C-C2C	4.57	1.51	1.37
6	M	406	2GO	C2A-C3A	4.56	1.51	1.37
6	M	402	2GO	C3D-C2D	4.54	1.47	1.39
6	M	406	2GO	C1A-C2A	4.53	1.52	1.40
6	M	402	2GO	O2A-CGA	4.52	1.46	1.33
6	L	301	2GO	C2A-C3A	4.52	1.51	1.37
6	L	305	2GO	C1A-C2A	4.44	1.52	1.40
6	M	406	2GO	C3B-C2B	4.43	1.47	1.39
6	L	307	2GO	C3B-C2B	4.41	1.47	1.39
5	H	305	GGD	OC8-CC7	4.40	1.46	1.33
6	L	307	2GO	C2A-C3A	4.40	1.50	1.37
6	L	307	2GO	O2A-CGA	4.33	1.46	1.33
6	M	401	2GO	C3C-C2C	4.29	1.50	1.37
6	L	301	2GO	C1A-C2A	4.26	1.52	1.40
6	M	406	2GO	C1A-CHA	4.22	1.50	1.43
5	H	305	GGD	OC6-CC5	4.17	1.46	1.34
6	L	301	2GO	C3D-C2D	4.15	1.46	1.39
6	M	402	2GO	C1A-C2A	4.14	1.51	1.40
6	M	402	2GO	C2A-C3A	4.11	1.49	1.37
6	L	307	2GO	C1A-C2A	4.08	1.51	1.40
6	M	401	2GO	C1A-C2A	4.05	1.51	1.40
6	L	301	2GO	C1C-C2C	4.00	1.51	1.42
6	L	305	2GO	C4A-C3A	3.99	1.51	1.42
6	M	402	2GO	C1C-NC	-3.98	1.32	1.37
6	M	402	2GO	C3C-C2C	3.97	1.49	1.37
6	M	406	2GO	C1C-C2C	3.88	1.51	1.42
6	L	307	2GO	C4C-NC	-3.87	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	301	2GO	C4C-NC	-3.83	1.30	1.35
6	M	401	2GO	C2A-C3A	3.80	1.48	1.37
6	M	406	2GO	C3C-C2C	3.79	1.48	1.37
6	L	305	2GO	C1C-C2C	3.74	1.51	1.42
6	L	307	2GO	C1C-C2C	3.73	1.51	1.42
6	M	406	2GO	C4A-C3A	3.68	1.50	1.42
6	M	401	2GO	C1C-C2C	3.66	1.50	1.42
6	L	301	2GO	C4A-C3A	3.60	1.50	1.42
6	L	307	2GO	C4A-C3A	3.55	1.50	1.42
6	M	401	2GO	C4A-C3A	3.51	1.50	1.42
8	M	407	U10	C4-C3	3.49	1.50	1.36
6	M	402	2GO	C4A-C3A	3.49	1.50	1.42
6	L	305	2GO	C3B-C2B	3.47	1.45	1.39
6	L	301	2GO	C1D-ND	-3.43	1.32	1.37
6	M	401	2GO	C4C-NC	-3.38	1.30	1.35
6	M	401	2GO	C1D-C2D	3.32	1.50	1.42
6	M	402	2GO	C1C-C2C	3.30	1.50	1.42
6	M	406	2GO	C4C-NC	-3.29	1.30	1.35
8	L	306[A]	U10	C4-C3	3.28	1.49	1.36
6	M	402	2GO	C1A-CHA	3.21	1.48	1.43
6	M	406	2GO	C1D-C2D	3.11	1.49	1.42
6	M	402	2GO	C4C-NC	-3.11	1.31	1.35
6	L	305	2GO	C1D-C2D	3.09	1.49	1.42
6	M	402	2GO	C1D-ND	-3.06	1.33	1.37
8	L	306[B]	U10	C4-C3	3.05	1.48	1.36
6	M	402	2GO	C1D-C2D	2.86	1.49	1.42
6	L	301	2GO	C1D-C2D	2.84	1.49	1.42
6	L	301	2GO	C1A-CHA	2.70	1.47	1.43
6	L	305	2GO	C4C-NC	-2.63	1.31	1.35
6	M	401	2GO	C1B-CHB	2.52	1.48	1.41
6	L	301	2GO	C1B-CHB	2.50	1.47	1.41
6	L	305	2GO	C1A-CHA	2.49	1.47	1.43
6	L	307	2GO	C1D-C2D	2.47	1.48	1.42
6	M	401	2GO	C4C-CHD	2.45	1.47	1.41
6	M	406	2GO	C4C-CHD	2.43	1.47	1.41
6	L	305	2GO	C4C-CHD	2.41	1.47	1.41
6	L	305	2GO	C1B-CHB	2.38	1.47	1.41
6	M	406	2GO	C4B-CHC	2.34	1.47	1.41
6	M	406	2GO	C1B-CHB	2.33	1.47	1.41
8	M	407	U10	C33-C34	2.33	1.38	1.33
6	M	406	2GO	OBD-CAD	-2.33	1.26	1.33
6	M	402	2GO	C4C-CHD	2.31	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	305	2GO	C1D-ND	-2.29	1.34	1.37
8	M	407	U10	C31-C29	2.28	1.56	1.51
6	L	307	2GO	C1B-CHB	2.26	1.47	1.41
5	H	305	GGD	OA1-CA1	2.18	1.43	1.40
6	M	401	2GO	C1D-ND	-2.15	1.34	1.37
6	L	301	2GO	C4A-NA	-2.15	1.34	1.37
6	M	406	2GO	C1D-ND	-2.11	1.34	1.37
6	L	305	2GO	C4B-CHC	2.04	1.46	1.41
6	L	307	2GO	C1A-CHA	2.00	1.46	1.43

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	401	2GO	CMA-C3A-C2A	-10.45	105.24	124.94
6	M	406	2GO	CMC-C2C-C3C	-9.35	107.32	124.94
14	M	410	PC1	C15-N-C13	-9.16	85.42	108.97
14	M	410	PC1	C15-N-C14	-8.94	85.98	108.97
6	M	402	2GO	CMA-C3A-C2A	-8.26	109.36	124.94
6	M	402	2GO	CMC-C2C-C3C	-8.17	109.53	124.94
6	L	307	2GO	CMA-C3A-C2A	-7.81	110.22	124.94
6	L	301	2GO	CMA-C3A-C2A	-7.69	110.44	124.94
6	M	402	2GO	CAA-C2A-C3A	-7.59	105.43	127.25
6	M	402	2GO	CHA-CBD-CGD	-7.37	101.44	125.12
6	M	401	2GO	CMC-C2C-C3C	-7.35	111.08	124.94
6	L	305	2GO	CHA-CBD-CAD	-7.21	100.04	107.17
6	M	406	2GO	CMA-C3A-C2A	-6.89	111.96	124.94
6	L	301	2GO	CAD-CBD-CGD	-6.88	106.06	126.70
6	L	305	2GO	CMA-C3A-C2A	-6.85	112.03	124.94
6	L	301	2GO	CMC-C2C-C3C	-6.83	112.07	124.94
6	M	402	2GO	CAD-CBD-CGD	-6.73	106.52	126.70
6	L	307	2GO	CMC-C2C-C3C	-6.67	112.36	124.94
6	L	305	2GO	CAD-CBD-CGD	-6.67	106.71	126.70
6	L	305	2GO	CMC-C2C-C3C	-6.40	112.88	124.94
6	M	406	2GO	CAD-CBD-CGD	-6.35	107.66	126.70
6	M	406	2GO	CHA-CBD-CAD	-6.34	100.90	107.17
8	M	407	U10	C30-C29-C31	5.97	125.31	115.27
13	M	409	CDL	C36-C35-C34	5.94	144.58	114.42
6	M	406	2GO	CAA-C2A-C3A	-5.73	110.79	127.25
6	L	307	2GO	CAA-C2A-C3A	-5.57	111.23	127.25
14	M	410	PC1	O21-C21-C22	5.56	123.49	111.50
6	M	402	2GO	CHA-CBD-CAD	-5.53	101.70	107.17
6	L	307	2GO	CHA-CBD-CAD	-5.43	101.80	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	410	PC1	C15-N-C12	-5.37	87.94	109.92
6	M	401	2GO	CAA-C2A-C3A	-5.35	111.87	127.25
6	M	401	2GO	CHA-CBD-CAD	-5.29	101.94	107.17
6	L	305	2GO	O2D-CGD-CBD	5.27	121.36	111.80
6	M	401	2GO	CAD-CBD-CGD	-5.15	111.26	126.70
13	M	409	CDL	OA6-CA5-C11	5.08	122.44	111.50
6	L	301	2GO	CHA-CBD-CAD	-4.94	102.28	107.17
6	L	301	2GO	CAA-C2A-C3A	-4.90	113.17	127.25
6	M	406	2GO	O2D-CGD-CBD	4.82	120.55	111.80
6	L	305	2GO	CAA-C2A-C3A	-4.71	113.71	127.25
6	L	305	2GO	CHA-CBD-CGD	-4.66	110.17	125.12
6	M	406	2GO	C4D-C3D-CAD	-4.54	105.94	108.47
14	M	410	PC1	C14-N-C13	4.47	120.48	108.97
6	M	401	2GO	O2D-CGD-CBD	4.45	119.89	111.80
13	M	409	CDL	OB6-CB5-C51	4.36	120.90	111.50
6	L	307	2GO	CAD-CBD-CGD	-4.33	113.71	126.70
5	H	305	GGD	CA4-CA3-CA2	4.30	117.05	110.85
5	H	305	GGD	CA1-CA2-CA3	4.28	117.59	110.07
6	L	301	2GO	CED-O2D-CGD	4.26	123.91	115.86
6	M	406	2GO	CHA-CBD-CGD	-4.11	111.93	125.12
6	L	307	2GO	C4-C3-C5	3.92	121.87	115.27
6	L	305	2GO	C4D-C3D-CAD	-3.82	106.34	108.47
5	H	305	GGD	CA3-CA4-CA5	3.75	117.65	109.66
6	M	401	2GO	C1-O2A-CGA	3.73	126.23	116.44
5	H	305	GGD	OC6-CC5-C14	3.67	119.40	111.50
6	M	406	2GO	C1-O2A-CGA	3.65	126.02	116.44
6	M	402	2GO	O2A-CGA-CBA	3.54	123.02	111.91
6	L	301	2GO	C1-O2A-CGA	3.48	125.58	116.44
6	M	402	2GO	O2D-CGD-O1D	-3.33	117.11	123.53
5	H	305	GGD	OA5-CA1-CA2	3.33	117.39	110.35
12	M	408	SPO	C20-C19-C17	-3.33	122.56	127.31
6	M	401	2GO	CHA-CBD-CGD	-3.29	114.54	125.12
6	L	301	2GO	O1D-CGD-CBD	-3.27	118.58	124.62
6	L	305	2GO	O2A-CGA-CBA	3.15	121.80	111.91
8	M	407	U10	C1M-C1-C6	-3.14	119.28	124.40
6	L	307	2GO	O2A-CGA-CBA	3.12	121.71	111.91
6	M	406	2GO	CMB-C2B-C3B	3.12	130.52	124.68
6	L	301	2GO	O2D-CGD-CBD	3.12	117.46	111.80
6	L	307	2GO	CMB-C2B-C3B	3.11	130.50	124.68
5	H	305	GGD	CA1-OA5-CA5	3.08	119.73	113.69
5	H	305	GGD	OB5-CB5-CB4	3.01	115.16	109.69
12	M	408	SPO	C21-C22-C23	-3.01	123.01	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	305	2GO	O2A-CGA-O1A	-3.01	116.00	123.59
5	H	305	GGD	CB3-CB4-CB5	2.98	115.55	110.24
6	L	305	2GO	O2D-CGD-O1D	-2.97	117.81	123.53
6	L	301	2GO	C4-C3-C5	2.96	120.26	115.27
6	L	301	2GO	CHA-CBD-CGD	-2.96	115.61	125.12
6	M	402	2GO	CMB-C2B-C3B	2.96	130.21	124.68
6	L	307	2GO	O2A-CGA-O1A	-2.94	116.18	123.59
6	L	301	2GO	C5-C3-C2	-2.89	115.27	121.12
8	L	306[A]	U10	C10-C9-C8	-2.88	116.29	123.68
14	M	410	PC1	O31-C31-C32	2.86	120.89	111.91
6	L	305	2GO	CED-O2D-CGD	2.85	121.25	115.86
8	M	407	U10	C4M-O4-C4	2.82	126.47	116.47
8	L	306[B]	U10	C10-C9-C11	2.78	119.95	115.27
8	M	407	U10	C25-C24-C26	2.78	119.95	115.27
14	M	410	PC1	O21-C21-O22	-2.75	117.05	123.70
12	M	408	SPO	C40-C38-C39	2.74	120.65	114.60
8	M	407	U10	C26-C27-C28	-2.73	102.91	111.88
6	M	402	2GO	O2A-CGA-O1A	-2.72	116.73	123.59
6	L	307	2GO	O2D-CGD-CBD	2.66	116.62	111.80
8	L	306[B]	U10	C1M-C1-C6	-2.66	120.07	124.40
6	M	402	2GO	C4D-C3D-CAD	-2.64	107.00	108.47
8	M	407	U10	C32-C31-C29	2.63	121.61	112.98
13	M	409	CDL	OA6-CA5-OA7	-2.62	117.37	123.70
12	M	408	SPO	C13-C12-C11	2.61	122.19	118.08
6	M	402	2GO	CED-O2D-CGD	2.61	120.79	115.86
6	L	307	2GO	O2D-CGD-O1D	-2.61	118.51	123.53
6	M	401	2GO	O1D-CGD-CBD	-2.57	119.88	124.62
6	L	301	2GO	C11-C12-C13	-2.54	107.69	115.92
8	L	306[A]	U10	C1M-C1-C6	-2.53	120.27	124.40
8	M	407	U10	C20-C19-C21	2.52	119.50	115.27
13	M	409	CDL	OA8-CA7-C31	2.49	119.71	111.91
12	M	408	SPO	C29-C28-C30	2.48	119.45	115.27
6	M	406	2GO	O2D-CGD-O1D	-2.44	118.84	123.53
6	M	401	2GO	CMB-C2B-C3B	2.43	129.22	124.68
6	M	402	2GO	O2D-CGD-CBD	2.41	116.18	111.80
14	M	410	PC1	O21-C2-C3	2.39	117.05	108.40
6	M	406	2GO	O2A-CGA-CBA	2.39	119.40	111.91
8	M	407	U10	C15-C14-C16	2.38	119.28	115.27
6	M	401	2GO	O2A-C1-C2	2.38	114.88	108.64
14	M	410	PC1	O31-C31-O32	-2.37	117.61	123.59
8	L	306[A]	U10	C3M-O3-C3	2.36	124.84	116.47
14	M	410	PC1	C13-N-C12	2.36	119.56	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	305	2GO	C1-C2-C3	-2.34	122.00	126.04
6	M	401	2GO	C1-C2-C3	2.33	130.07	126.04
13	M	409	CDL	OB8-CB7-C71	2.33	119.20	111.91
6	L	305	2GO	CMB-C2B-C3B	2.28	128.94	124.68
8	M	407	U10	C31-C29-C28	-2.27	116.52	121.12
8	L	306[A]	U10	C10-C9-C11	2.26	119.08	115.27
12	M	408	SPO	C2-C1-C4	-2.26	107.38	110.86
6	L	307	2GO	C1-O2A-CGA	2.24	122.31	116.44
5	H	305	GGD	OC8-CC6-CC4	2.22	114.89	108.43
12	M	408	SPO	C40-C38-C37	-2.22	116.23	122.65
12	M	408	SPO	C14-C15-C16	-2.22	116.30	123.22
6	M	401	2GO	C4-C3-C2	-2.21	118.01	123.68
8	M	407	U10	C6-C1-C2	2.21	120.93	119.18
13	M	409	CDL	OA8-CA7-OA9	-2.20	118.04	123.59
8	L	306[B]	U10	C16-C14-C15	2.19	119.44	114.60
6	L	301	2GO	O2A-CGA-CBA	2.18	118.73	111.91
14	M	410	PC1	C14-N-C12	2.17	118.81	109.92
12	M	408	SPO	C34-C33-C35	2.17	118.93	115.27
6	M	406	2GO	O1D-CGD-CBD	-2.17	120.61	124.62
5	H	305	GGD	OC6-CC5-OC7	-2.17	118.47	123.70
5	H	305	GGD	OC8-CC7-C31	2.16	118.70	111.91
8	M	407	U10	C30-C29-C28	-2.15	118.16	123.68
8	L	306[B]	U10	C7-C8-C9	-2.15	123.21	126.79
12	M	408	SPO	C8-C7-C6	2.13	121.44	118.08
6	M	401	2GO	CMD-C2D-C3D	-2.13	120.69	124.68
6	M	406	2GO	CED-O2D-CGD	2.10	119.84	115.86
8	M	407	U10	C17-C18-C19	-2.10	122.60	127.66
6	L	301	2GO	C16-C17-C18	-2.09	106.14	115.98
12	M	408	SPO	C24-C23-C25	2.09	121.36	118.08
5	H	305	GGD	OA5-CA5-CA6	2.08	111.61	106.44
6	L	305	2GO	O1D-CGD-CBD	-2.06	120.81	124.62
13	M	409	CDL	OB8-CB7-OB9	-2.05	118.42	123.59
6	L	307	2GO	C11-C10-C8	-2.05	109.29	115.92

There are no chirality outliers.

All (246) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	L	310	HTO	O1-C1-C2-O2
10	L	310	HTO	O1-C1-C2-C3
4	L	311	GOL	C1-C2-C3-O3
7	M	403	LDA	C2-C1-N1-CM1

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Mol	Chain	Res	Type	Atoms
10	L	309	HTO	C1-C2-C3-O3
10	L	309	HTO	C1-C2-C3-C4
10	L	309	HTO	O2-C2-C3-O3
10	L	309	HTO	O2-C2-C3-C4
7	L	304	LDA	C2-C1-N1-O1
7	L	304	LDA	C2-C1-N1-CM1
7	L	304	LDA	C2-C1-N1-CM2
6	L	305	2GO	C4C-C3C-CAC-CBC
6	L	305	2GO	C1A-C2A-CAA-CBA
6	L	305	2GO	O2A-C1-C2-C3
13	M	409	CDL	CA3-OA5-PA1-OA2
13	M	409	CDL	CA3-OA5-PA1-OA3
13	M	409	CDL	CB2-OB2-PB2-OB3
13	M	409	CDL	CB3-OB5-PB2-OB2
13	M	409	CDL	CB3-OB5-PB2-OB3
13	M	409	CDL	CB3-OB5-PB2-OB4
13	M	409	CDL	OB9-CB7-OB8-CB6
6	M	401	2GO	C3A-C2A-CAA-CBA
14	M	410	PC1	C1-O11-P-O14
14	M	410	PC1	C1-O11-P-O13
14	M	410	PC1	O13-C11-C12-N
14	M	410	PC1	O22-C21-O21-C2
14	M	410	PC1	C22-C21-O21-C2
6	M	402	2GO	C4C-C3C-CAC-CBC
6	M	402	2GO	C1A-C2A-CAA-CBA
6	M	406	2GO	C1A-C2A-CAA-CBA
6	M	406	2GO	O2A-C1-C2-C3
4	H	303	GOL	C1-C2-C3-O3
6	L	301	2GO	C2C-C3C-CAC-CBC
6	L	301	2GO	C1A-C2A-CAA-CBA
4	L	312	GOL	O1-C1-C2-C3
4	L	312	GOL	C1-C2-C3-O3
4	H	301	GOL	O1-C1-C2-O2
4	H	301	GOL	O1-C1-C2-C3
5	H	305	GGD	OC7-CC5-OC6-CC4
5	H	305	GGD	C14-CC5-OC6-CC4
8	L	306[A]	U10	C12-C11-C9-C8
8	L	306[A]	U10	C12-C11-C9-C10
4	H	304	GOL	O1-C1-C2-C3
12	M	408	SPO	C2-C1-C4-C5
12	M	408	SPO	C3-C1-C4-C5
12	M	408	SPO	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
12	M	408	SPO	C5-C6-C7-C9
6	L	307	2GO	C4C-C3C-CAC-CBC
6	L	307	2GO	C2C-C3C-CAC-CBC
6	L	307	2GO	C1A-C2A-CAA-CBA
4	H	302	GOL	C1-C2-C3-O3
4	L	313	GOL	O1-C1-C2-C3
13	M	409	CDL	C71-CB7-OB8-CB6
14	M	410	PC1	O32-C31-O31-C3
6	L	307	2GO	CBD-CGD-O2D-CED
13	M	409	CDL	C11-CA5-OA6-CA4
14	M	410	PC1	C32-C31-O31-C3
6	M	406	2GO	C10-C11-C12-C13
13	M	409	CDL	C31-CA7-OA8-CA6
13	M	409	CDL	OA9-CA7-OA8-CA6
14	M	410	PC1	C31-C32-C33-C34
6	M	401	2GO	C11-C12-C13-C14
13	M	409	CDL	OA7-CA5-OA6-CA4
6	M	401	2GO	C15-C16-C17-C18
13	M	409	CDL	CB5-C51-C52-C53
4	L	311	GOL	O2-C2-C3-O3
4	L	312	GOL	O1-C1-C2-O2
4	L	313	GOL	O1-C1-C2-O2
13	M	409	CDL	CA5-C11-C12-C13
5	H	305	GGD	CC7-C31-C32-C33
6	L	307	2GO	O1D-CGD-O2D-CED
6	M	406	2GO	C5-C6-C7-C8
6	M	401	2GO	C11-C10-C8-C7
8	L	306[B]	U10	C4-C3-O3-C3M
8	M	407	U10	C14-C16-C17-C18
8	M	407	U10	C24-C26-C27-C28
8	M	407	U10	C29-C31-C32-C33
8	L	306[B]	U10	C9-C11-C12-C13
6	M	401	2GO	C10-C11-C12-C13
14	M	410	PC1	C11-O13-P-O11
8	M	407	U10	C30-C29-C31-C32
6	L	301	2GO	O1D-CGD-O2D-CED
6	M	402	2GO	C3-C5-C6-C7
7	L	303	LDA	C6-C7-C8-C9
13	M	409	CDL	C71-C72-C73-C74
14	M	410	PC1	C3-C2-O21-C21
7	L	304	LDA	C4-C5-C6-C7
13	M	409	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
7	L	302	LDA	C5-C6-C7-C8
5	H	305	GGD	CA2-CA1-OA1-CC3
7	L	304	LDA	C7-C8-C9-C10
5	H	305	GGD	C40-C41-C42-C43
13	M	409	CDL	C16-C17-C18-C19
14	M	410	PC1	C29-C2A-C2B-C2C
7	L	303	LDA	C5-C6-C7-C8
13	M	409	CDL	C17-C18-C19-C20
13	M	409	CDL	C35-C36-C37-C38
14	M	410	PC1	C22-C23-C24-C25
14	M	410	PC1	C27-C28-C29-C2A
13	M	409	CDL	C53-C54-C55-C56
14	M	410	PC1	C11-C12-N-C13
6	M	401	2GO	C16-C17-C18-C20
13	M	409	CDL	C54-C55-C56-C57
5	H	305	GGD	C34-C35-C36-C37
7	L	302	LDA	C6-C7-C8-C9
7	L	302	LDA	C7-C8-C9-C10
7	M	403	LDA	C4-C5-C6-C7
6	M	401	2GO	C16-C17-C18-C19
8	M	407	U10	C28-C29-C31-C32
13	M	409	CDL	C20-C21-C22-C23
4	H	303	GOL	O2-C2-C3-O3
4	L	312	GOL	O2-C2-C3-O3
13	M	409	CDL	O1-C1-CA2-OA2
6	M	406	2GO	C8-C10-C11-C12
7	L	302	LDA	C3-C4-C5-C6
6	L	305	2GO	C11-C10-C8-C7
13	M	409	CDL	C11-C12-C13-C14
13	M	409	CDL	C12-C13-C14-C15
6	L	305	2GO	C11-C10-C8-C9
6	L	301	2GO	C11-C12-C13-C14
5	H	305	GGD	OB5-CB5-CB6-OB6
7	M	403	LDA	C2-C3-C4-C5
7	L	304	LDA	C5-C6-C7-C8
13	M	409	CDL	C33-C34-C35-C36
7	L	302	LDA	C2-C3-C4-C5
7	L	303	LDA	C11-C10-C9-C8
13	M	409	CDL	C18-C19-C20-C21
6	L	301	2GO	CBD-CGD-O2D-CED
7	M	403	LDA	C11-C10-C9-C8
12	M	408	SPO	C4-C1-O1-CM1

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Mol	Chain	Res	Type	Atoms
10	L	309	HTO	C4-C5-C6-C7
4	H	304	GOL	O1-C1-C2-O2
4	H	302	GOL	O2-C2-C3-O3
13	M	409	CDL	C51-CB5-OB6-CB4
14	M	410	PC1	C21-C22-C23-C24
7	M	404	LDA	C1-C2-C3-C4
13	M	409	CDL	C36-C37-C38-C39
7	L	302	LDA	C4-C5-C6-C7
5	H	305	GGD	CC5-C14-C15-C16
14	M	410	PC1	C35-C36-C37-C38
12	M	408	SPO	C2-C1-O1-CM1
12	M	408	SPO	C3-C1-O1-CM1
6	M	406	2GO	C11-C12-C13-C15
6	L	301	2GO	C11-C12-C13-C15
6	M	402	2GO	C6-C7-C8-C9
6	M	402	2GO	C11-C10-C8-C9
13	M	409	CDL	C81-C82-C83-C84
7	L	304	LDA	N1-C1-C2-C3
6	M	406	2GO	C16-C17-C18-C20
13	M	409	CDL	CA3-CA4-CA6-OA8
14	M	410	PC1	C2B-C2C-C2D-C2E
13	M	409	CDL	CB7-C71-C72-C73
6	L	305	2GO	C3-C5-C6-C7
13	M	409	CDL	OB5-CB3-CB4-OB6
13	M	409	CDL	OB7-CB5-OB6-CB4
6	L	305	2GO	C16-C17-C18-C20
13	M	409	CDL	C39-C40-C41-C42
6	M	401	2GO	C11-C10-C8-C9
6	M	406	2GO	C11-C12-C13-C14
6	L	305	2GO	C16-C17-C18-C19
6	L	301	2GO	C8-C10-C11-C12
7	M	404	LDA	C9-C10-C11-C12
6	L	305	2GO	C6-C7-C8-C10
6	M	402	2GO	C6-C7-C8-C10
6	M	402	2GO	C11-C10-C8-C7
13	M	409	CDL	C55-C56-C57-C58
7	M	404	LDA	C3-C4-C5-C6
8	L	306[B]	U10	C2-C3-O3-C3M
6	M	402	2GO	C16-C17-C18-C19
13	M	409	CDL	C73-C74-C75-C76
13	M	409	CDL	OA6-CA4-CA6-OA8
14	M	410	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
4	H	301	GOL	O2-C2-C3-O3
14	M	410	PC1	C28-C29-C2A-C2B
13	M	409	CDL	CB2-OB2-PB2-OB5
7	L	304	LDA	C1-C2-C3-C4
13	M	409	CDL	CB2-OB2-PB2-OB4
14	M	410	PC1	C11-O13-P-O14
13	M	409	CDL	OB5-CB3-CB4-CB6
5	H	305	GGD	C32-C33-C34-C35
6	L	305	2GO	O1D-CGD-O2D-CED
14	M	410	PC1	C33-C34-C35-C36
6	M	402	2GO	C5-C6-C7-C8
5	H	305	GGD	C39-C40-C41-C42
12	M	408	SPO	C1-C4-C5-C6
6	M	406	2GO	C6-C7-C8-C10
6	L	301	2GO	C11-C10-C8-C7
7	L	303	LDA	C3-C4-C5-C6
7	L	303	LDA	C9-C10-C11-C12
6	L	301	2GO	C3-C5-C6-C7
13	M	409	CDL	C72-C73-C74-C75
5	H	305	GGD	CC4-CC3-OA1-CA1
6	L	305	2GO	C6-C7-C8-C9
6	M	406	2GO	C6-C7-C8-C9
8	L	306[A]	U10	C9-C11-C12-C13
6	M	406	2GO	C16-C17-C18-C19
6	L	305	2GO	C8-C10-C11-C12
6	L	305	2GO	CAD-CBD-CGD-O1D
6	M	401	2GO	CAD-CBD-CGD-O1D
6	M	402	2GO	CAD-CBD-CGD-O1D
6	M	406	2GO	CAD-CBD-CGD-O1D
6	L	307	2GO	CAD-CBD-CGD-O1D
6	L	305	2GO	CAD-CBD-CGD-O2D
6	M	402	2GO	CAD-CBD-CGD-O2D
13	M	409	CDL	CB3-CB4-CB6-OB8
7	M	403	LDA	N1-C1-C2-C3
13	M	409	CDL	CB2-C1-CA2-OA2
5	H	305	GGD	OA5-CA1-OA1-CC3
8	L	306[B]	U10	C12-C11-C9-C10
6	M	406	2GO	C2-C1-O2A-CGA
8	M	407	U10	C34-C36-C37-C38
8	M	407	U10	C25-C24-C26-C27
6	M	402	2GO	C11-C12-C13-C15
6	L	305	2GO	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
7	M	404	LDA	C2-C3-C4-C5
8	M	407	U10	C31-C32-C33-C34
10	L	309	HTO	C3-C4-C5-C6
4	H	303	GOL	O1-C1-C2-C3
13	M	409	CDL	C75-C76-C77-C78
14	M	410	PC1	C25-C26-C27-C28
4	H	303	GOL	O1-C1-C2-O2
6	M	406	2GO	CAD-CBD-CGD-O2D
6	M	401	2GO	C4C-C3C-CAC-CBC
6	L	301	2GO	C11-C10-C8-C9
13	M	409	CDL	C78-C79-C80-C81
10	L	310	HTO	C3-C4-C5-C6
7	M	404	LDA	C6-C7-C8-C9
13	M	409	CDL	C52-C51-CB5-OB6
8	M	407	U10	C23-C24-C26-C27
6	M	401	2GO	C2C-C3C-CAC-CBC
14	M	410	PC1	C1-C2-C3-O31
6	M	406	2GO	C2C-C3C-CAC-CBC
6	M	401	2GO	O2A-C1-C2-C3
13	M	409	CDL	C12-C11-CA5-OA6
6	L	301	2GO	CAD-CBD-CGD-O1D
12	M	408	SPO	C15-C16-C17-C18
4	H	301	GOL	C1-C2-C3-O3
6	M	401	2GO	CAD-CBD-CGD-O2D
13	M	409	CDL	C52-C51-CB5-OB7
5	H	305	GGD	C32-C31-CC7-OC8
6	M	401	2GO	C8-C10-C11-C12
6	M	402	2GO	C11-C12-C13-C14
13	M	409	CDL	C12-C11-CA5-OA7
6	M	401	2GO	C11-C12-C13-C15
8	L	306[B]	U10	C12-C11-C9-C8
7	M	404	LDA	C7-C8-C9-C10

There are no ring outliers.

20 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	311	GOL	1	0
7	M	403	LDA	1	0
7	L	304	LDA	1	0
6	L	305	2GO	8	0
13	M	409	CDL	2	0

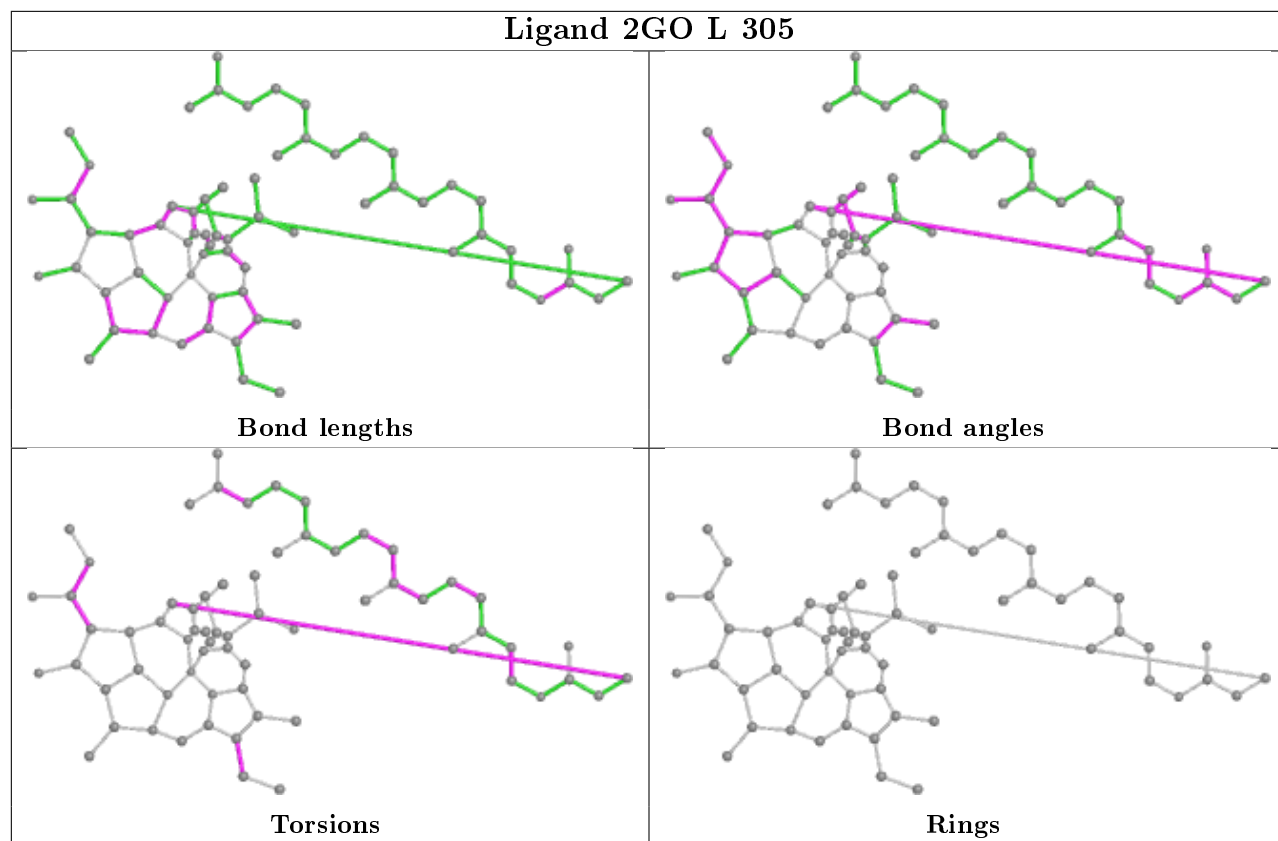
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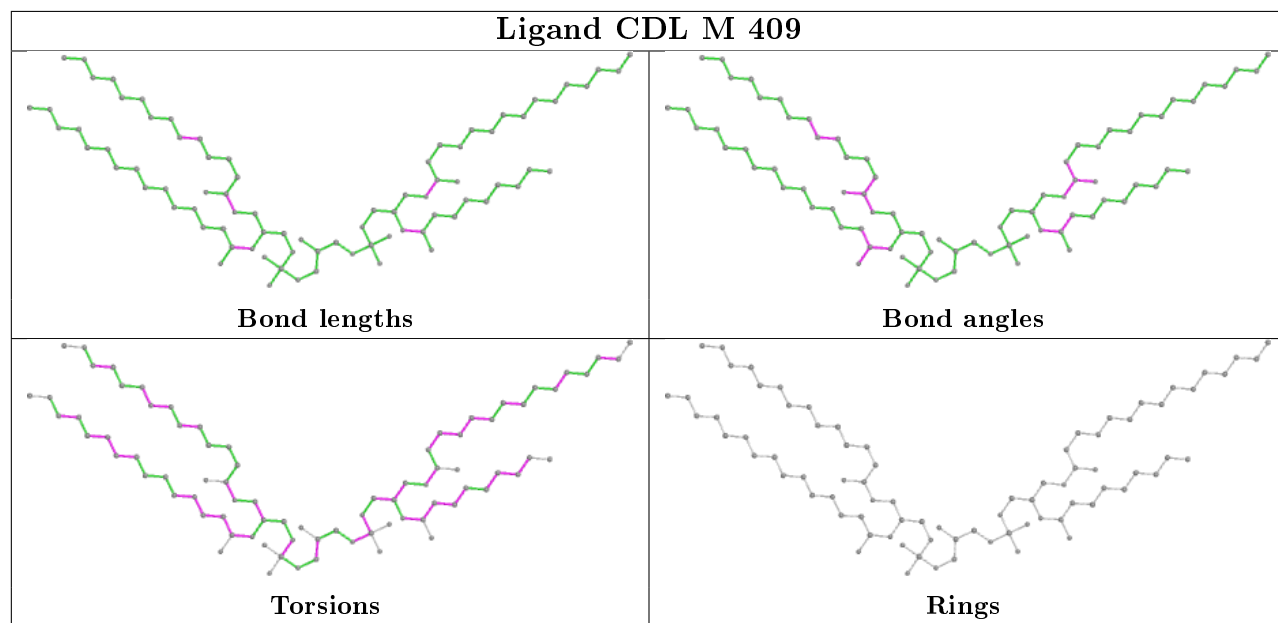
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	401	2GO	9	0
6	M	402	2GO	10	0
6	M	406	2GO	9	0
4	H	303	GOL	1	0
6	L	301	2GO	5	0
4	L	312	GOL	1	0
4	H	301	GOL	2	0
8	M	407	U10	2	0
5	H	305	GGD	2	0
8	L	306[A]	U10	7	0
8	L	306[B]	U10	7	0
12	M	408	SPO	5	0
6	L	307	2GO	2	0
9	L	308	PO4	1	0
4	L	313	GOL	1	0

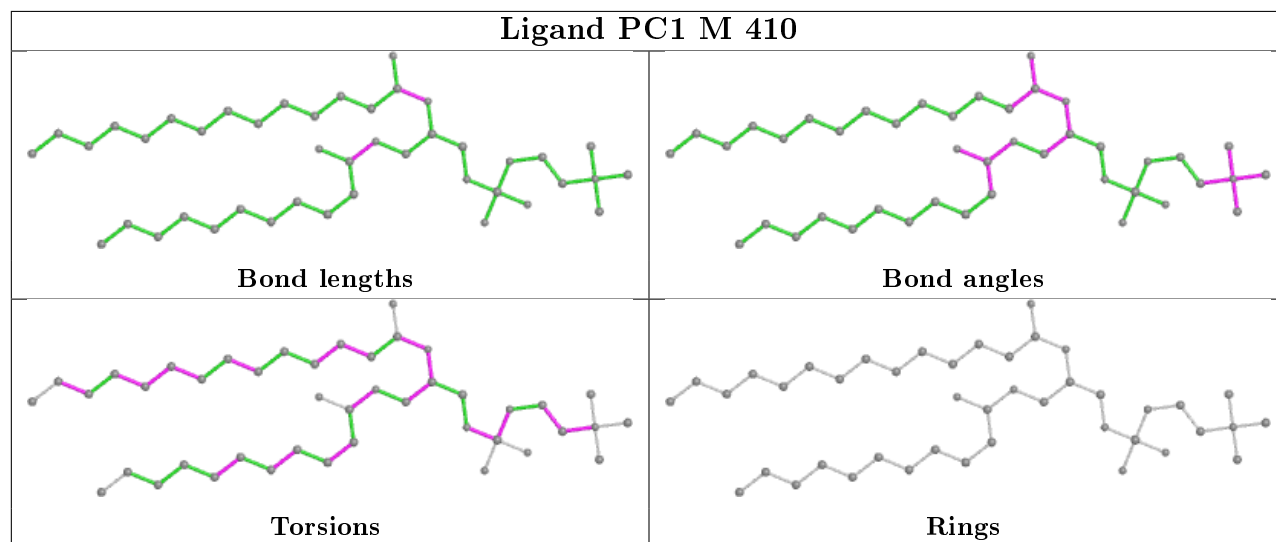
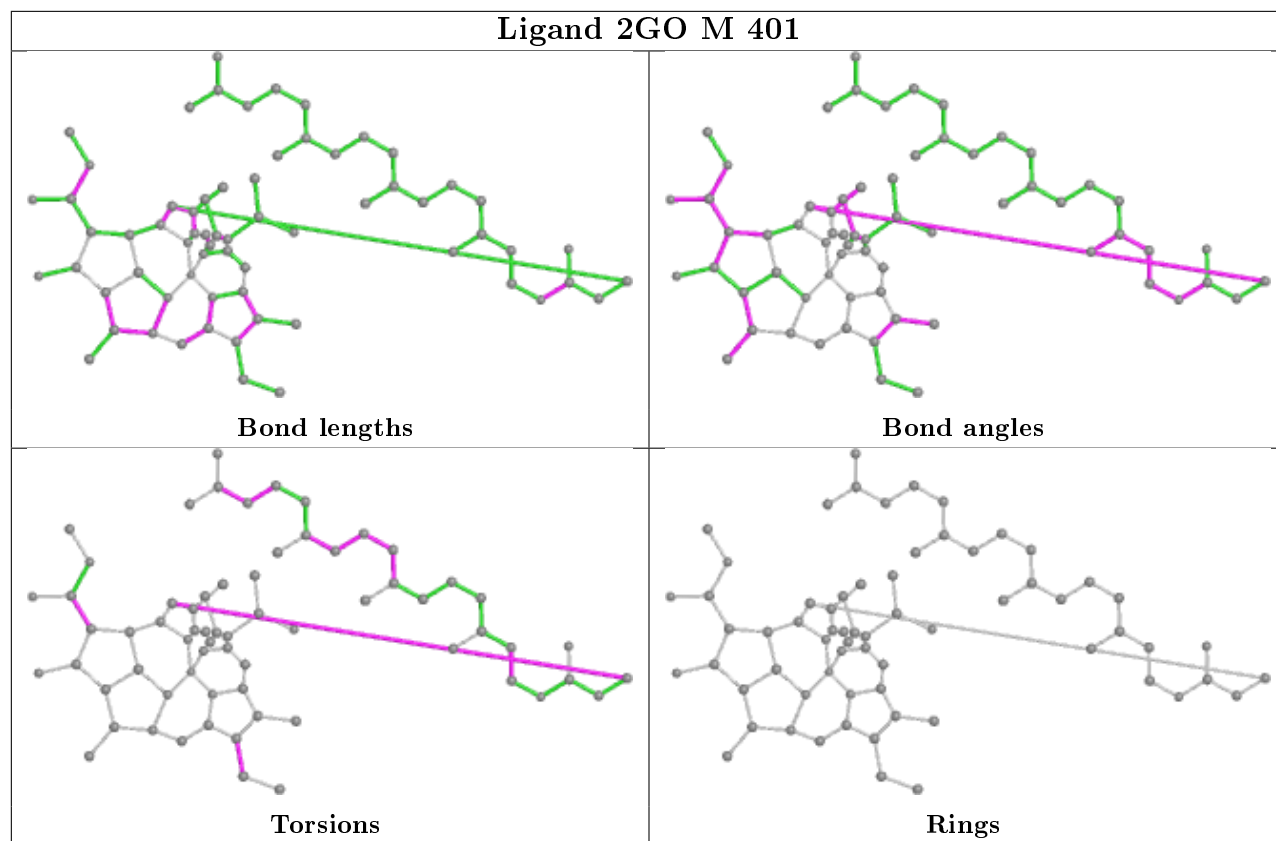
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

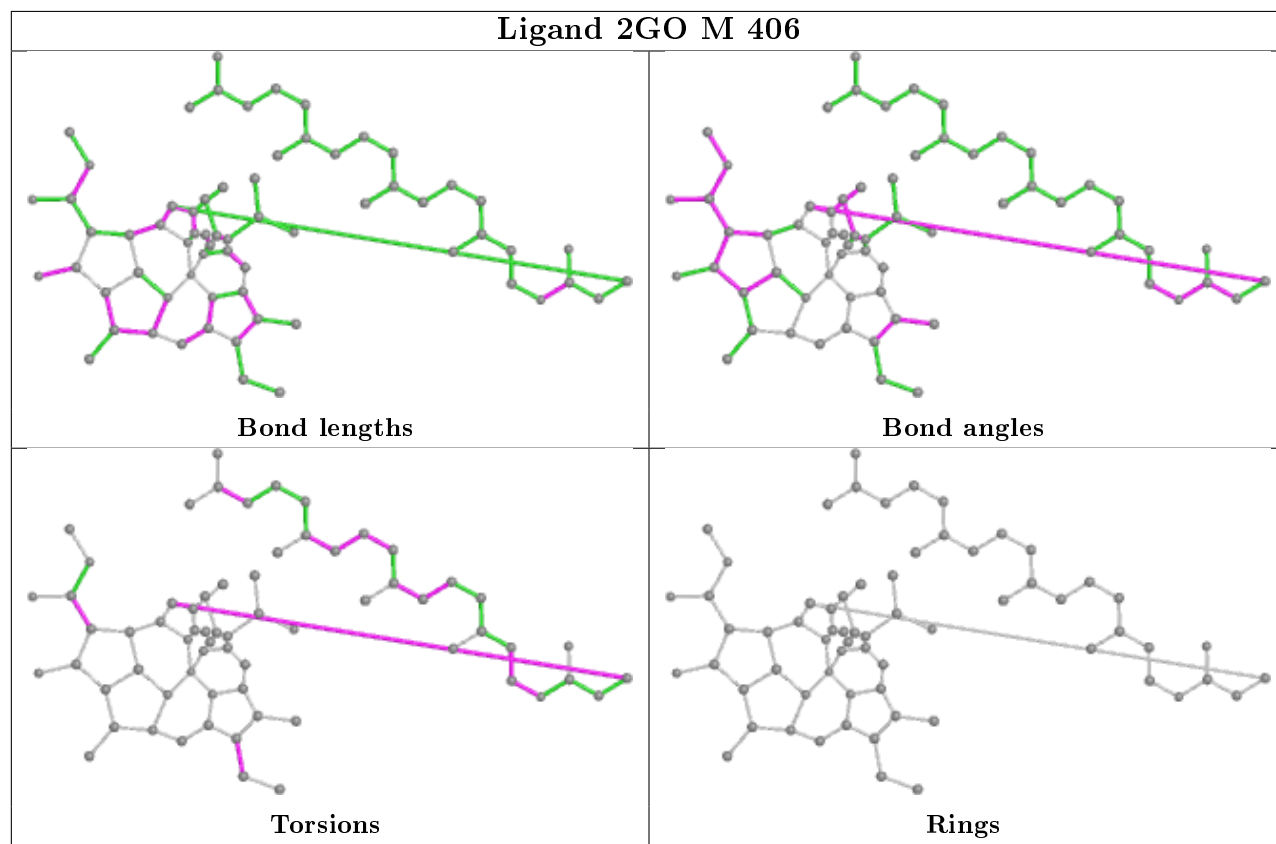
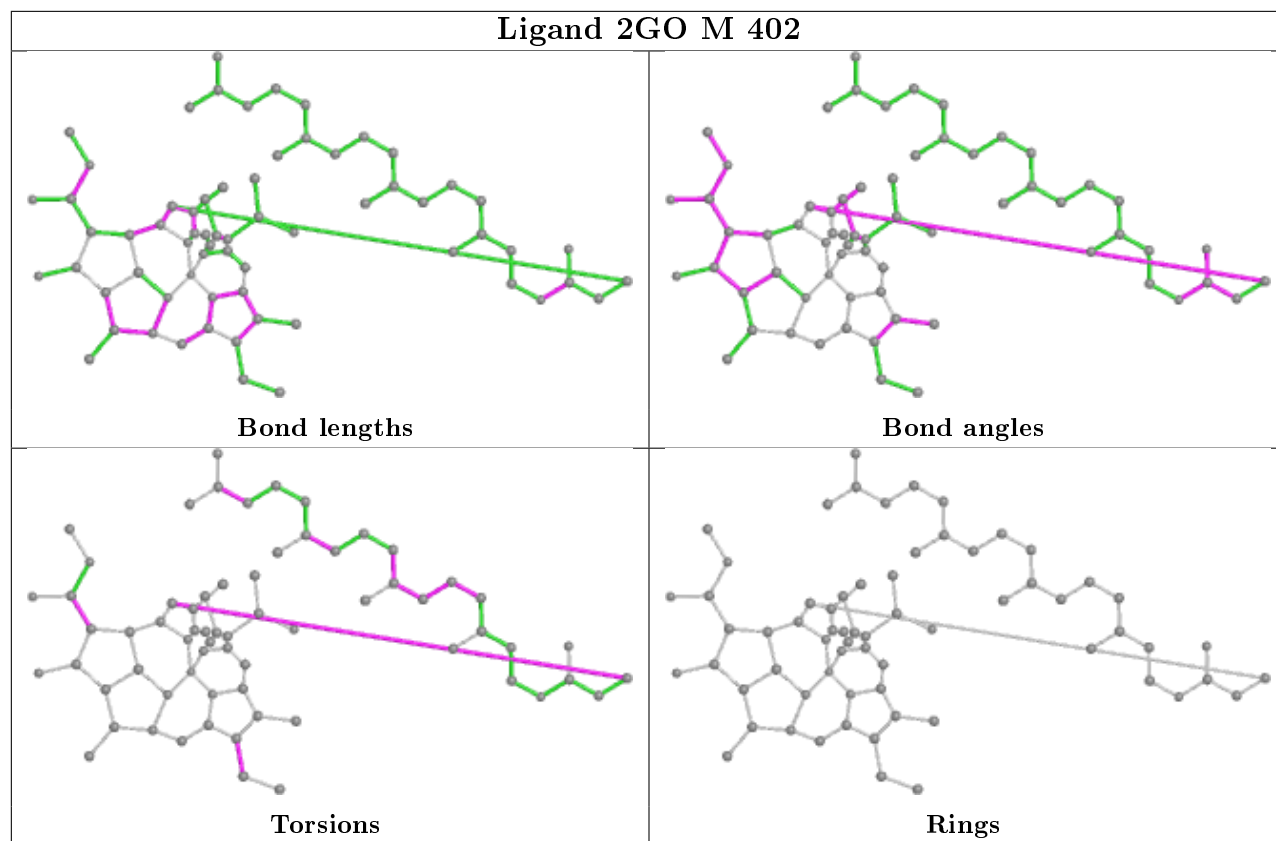
Ligand 2GO L 305



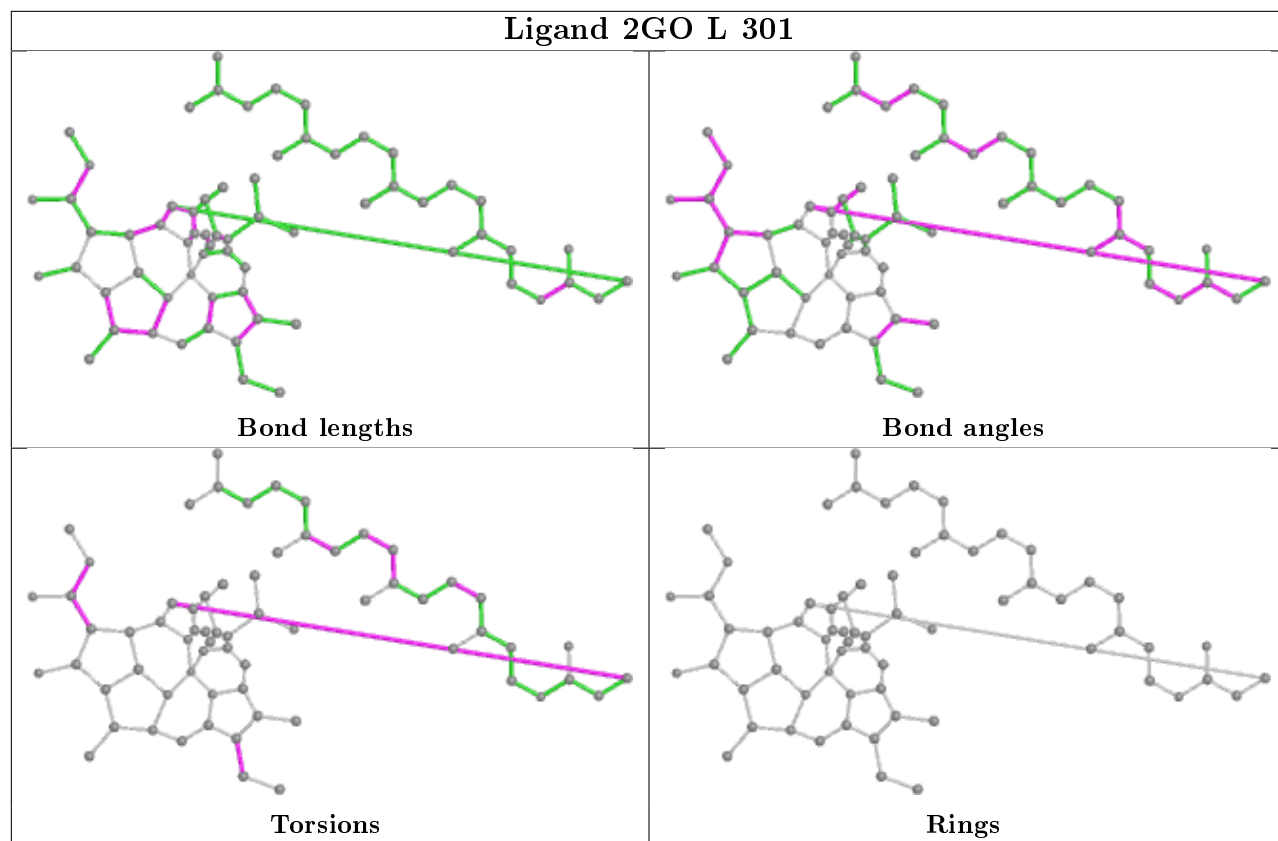
Ligand CDL M 409



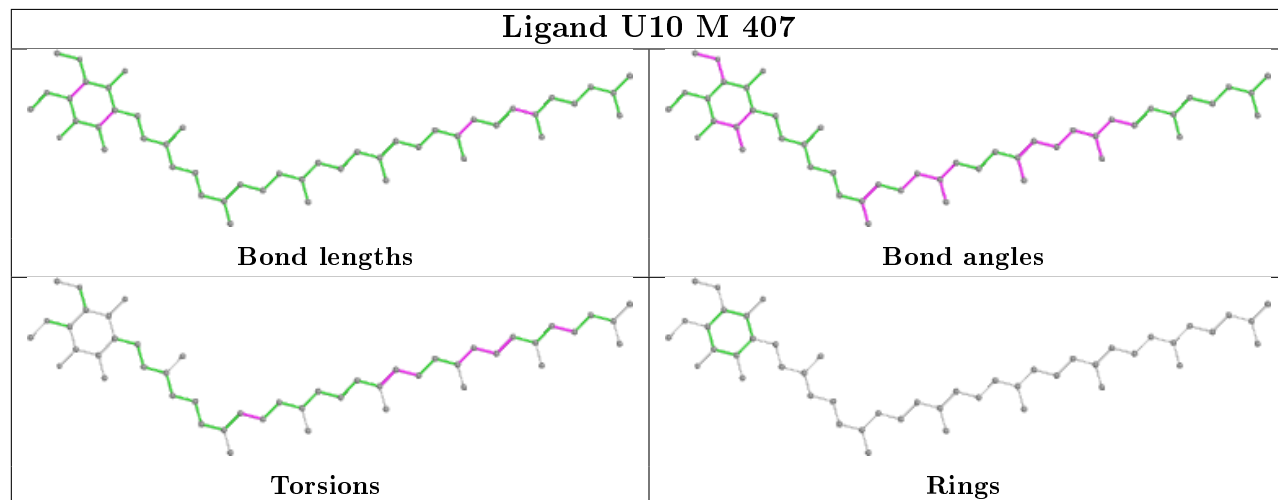


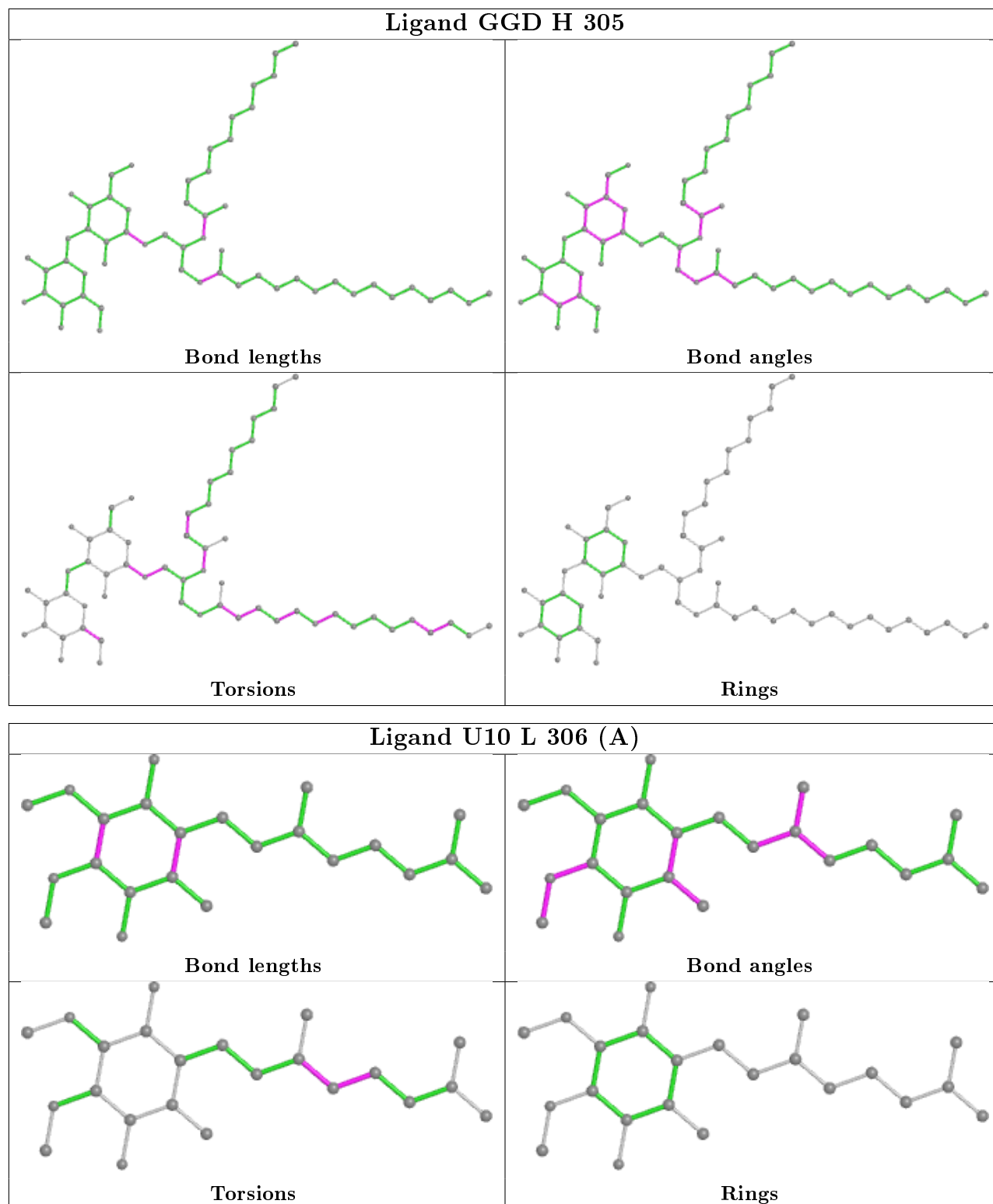


Ligand 2GO L 301

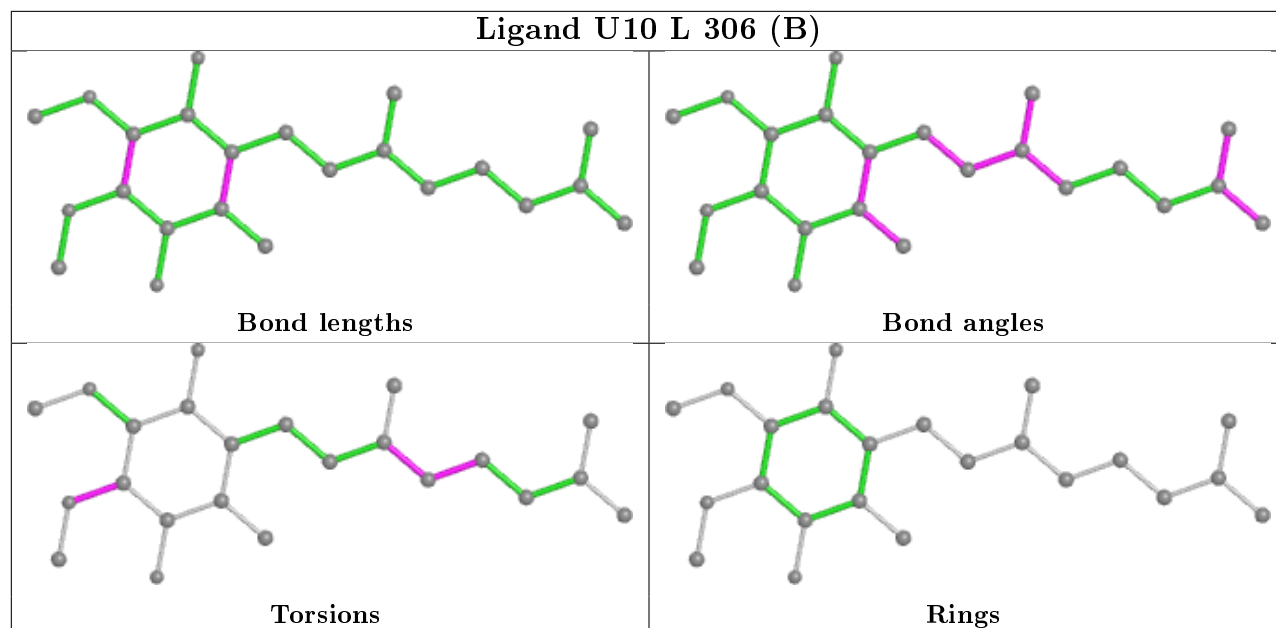


Ligand U10 M 407

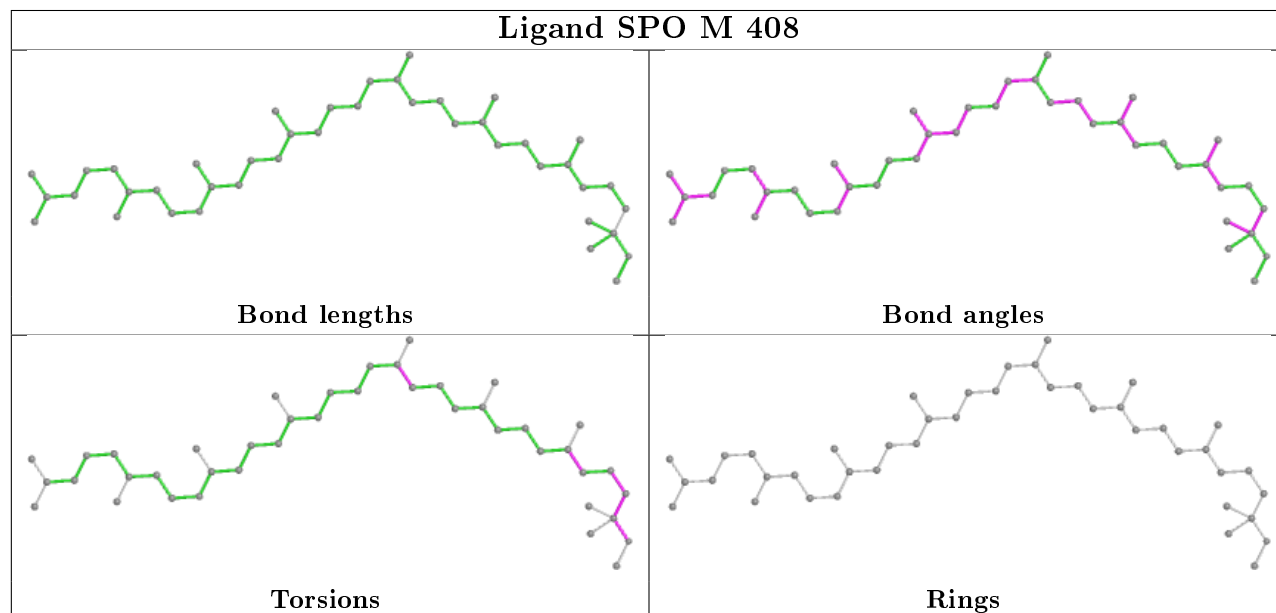


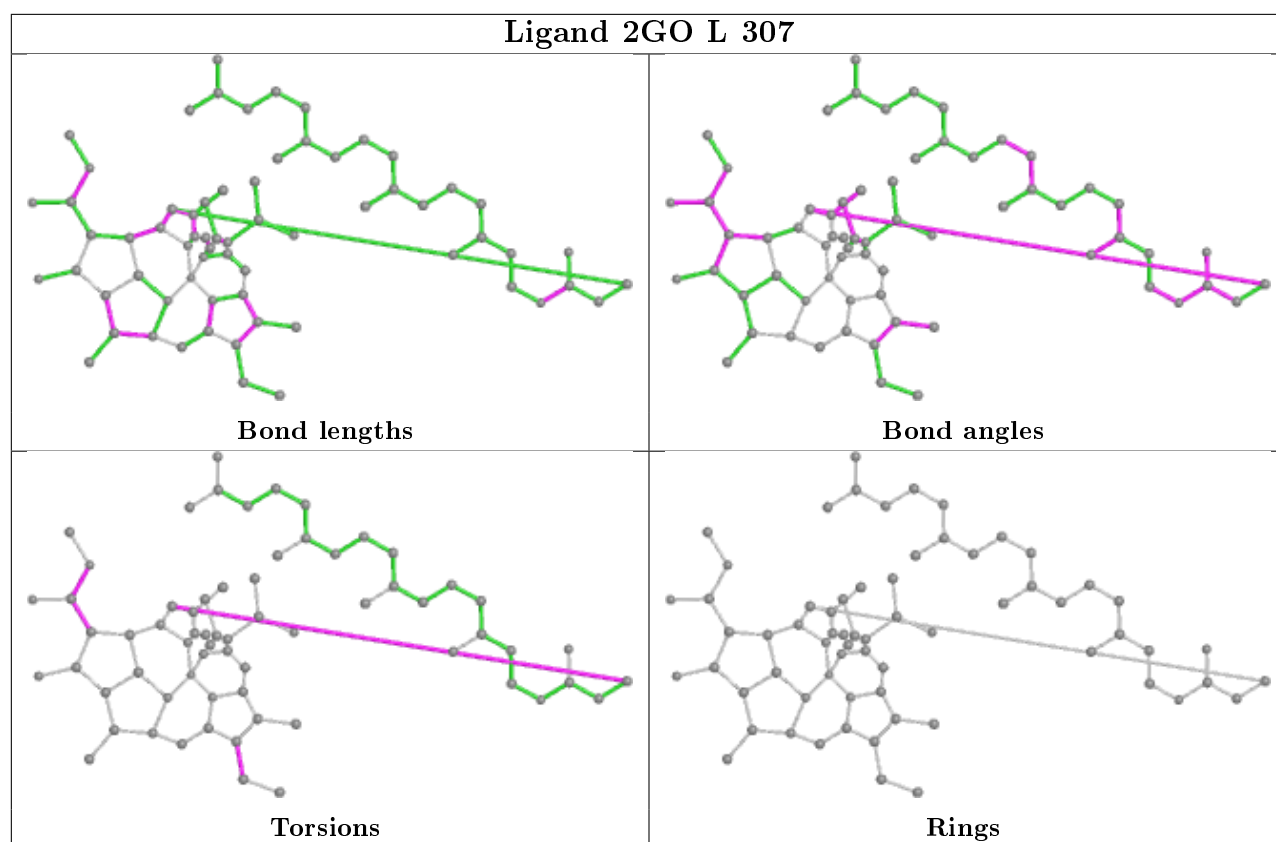


Ligand U10 L 306 (B)



Ligand SPO M 408





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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	H	241/241 (100%)	-0.34	7 (2%)	51	47	41, 54, 77, 161	3 (1%)
2	L	281/281 (100%)	-0.56	3 (1%)	80	80	37, 53, 79, 101	0
3	M	303/303 (100%)	-0.23	2 (0%)	87	87	37, 55, 81, 123	6 (1%)
All	All	825/825 (100%)	-0.37	12 (1%)	73	72	37, 54, 80, 161	9 (1%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	5.2
1	H	249[A]	LYS	3.7
2	L	281	GLY	3.4
1	H	220[A]	LYS	3.1
1	H	251	VAL	3.1
1	H	51	ALA	2.7
1	H	247	LYS	2.6
1	H	52	ASN	2.6
2	L	277	GLY	2.3
3	M	219	HIS	2.2
2	L	271[A]	TRP	2.1
3	M	265	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

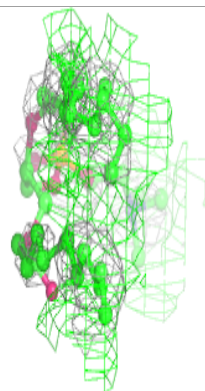
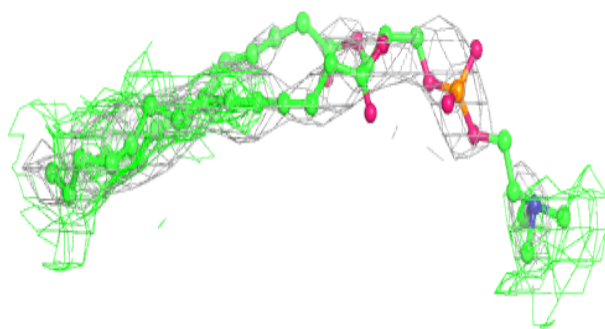
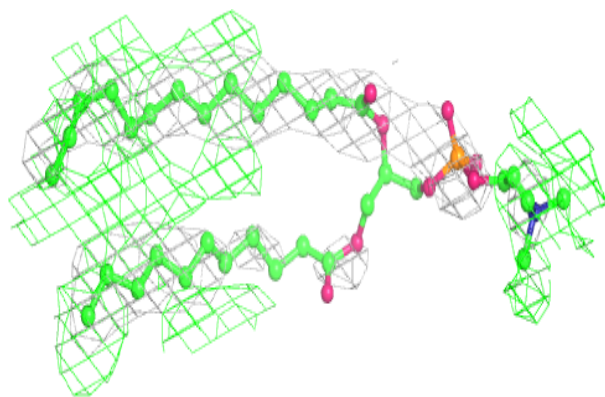
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	PC1	M	410	43/54	0.39	0.49	78,117,175,190	0
7	LDA	L	303	16/16	0.44	0.56	76,95,143,148	0
7	LDA	L	304	16/16	0.57	0.39	68,96,124,125	0
5	GGD	H	305	57/67	0.62	0.54	49,107,216,221	0
10	HTO	L	309	10/10	0.64	0.87	88,103,117,127	0
4	GOL	H	303	6/6	0.71	0.31	73,85,90,96	0
4	GOL	L	312	6/6	0.73	0.35	87,88,92,95	0
10	HTO	L	310	10/10	0.75	0.82	86,114,140,156	0
7	LDA	L	302	16/16	0.80	0.40	42,105,140,143	0
4	GOL	H	304	6/6	0.81	0.24	74,85,89,94	0
13	CDL	M	409	81/100	0.83	0.37	70,101,156,164	0
4	GOL	H	301	6/6	0.85	0.43	94,109,111,112	0
8	U10	L	306[B]	23/63	0.85	0.29	43,68,73,75	23
8	U10	L	306[A]	23/63	0.85	0.29	50,71,86,91	23
7	LDA	M	404	16/16	0.87	0.39	67,87,102,106	0
4	GOL	H	302	6/6	0.89	0.45	56,65,69,81	0
4	GOL	L	313	6/6	0.89	0.14	84,89,93,93	0
4	GOL	L	311	6/6	0.90	0.36	60,73,85,104	0
8	U10	M	407	48/63	0.92	0.31	43,54,99,111	0
7	LDA	M	403	16/16	0.94	0.22	42,60,67,68	0
6	2GO	M	406	66/66	0.94	0.20	60,76,135,142	0
12	SPO	M	408	42/42	0.94	0.23	46,64,98,112	0
9	PO4	L	308	5/5	0.94	0.13	97,97,98,98	0
6	2GO	L	307	66/66	0.97	0.15	35,48,59,63	0
6	2GO	L	301	66/66	0.98	0.14	29,39,59,68	0
6	2GO	M	401	66/66	0.98	0.18	35,47,88,92	0
6	2GO	L	305	66/66	0.98	0.15	31,47,56,58	0
6	2GO	M	402	66/66	0.99	0.17	39,50,75,86	0
11	FE	M	405	1/1	1.00	0.16	46,46,46,46	0

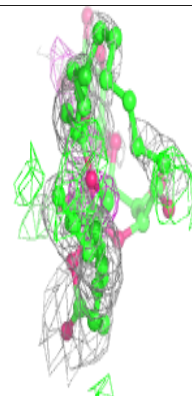
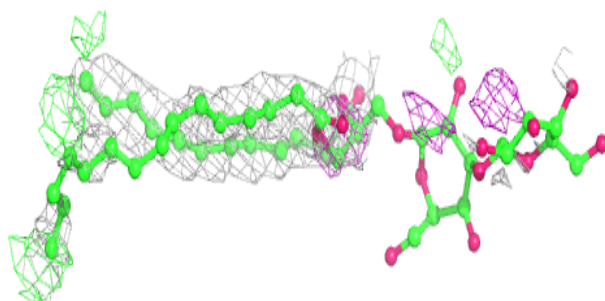
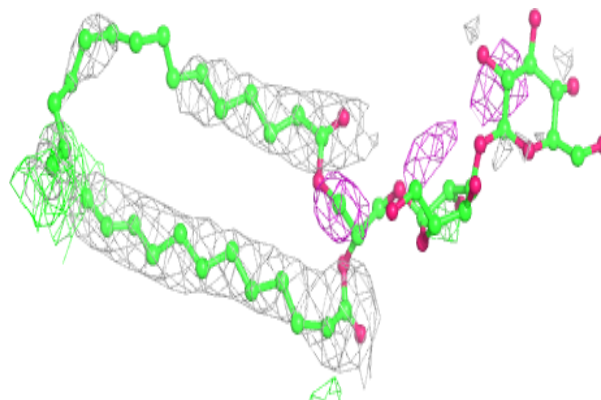
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PC1 M 410:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

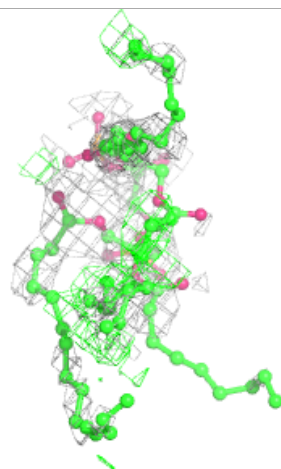
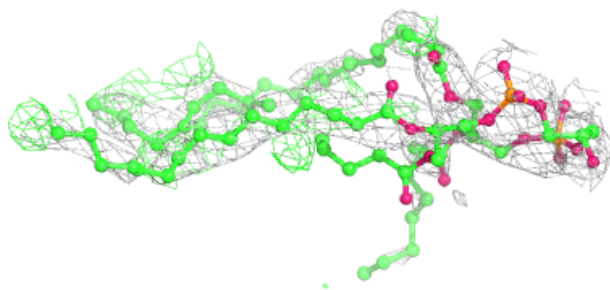
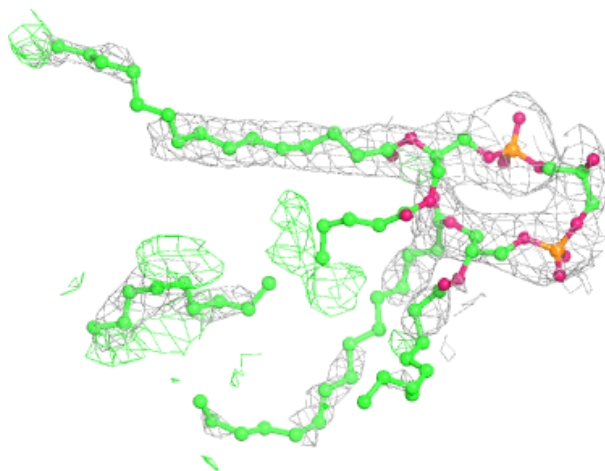
**Electron density around GGD H 305:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



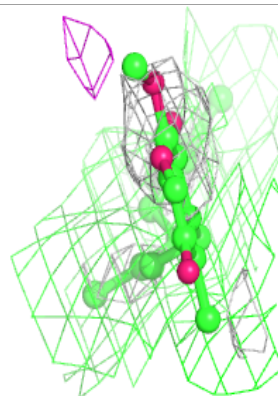
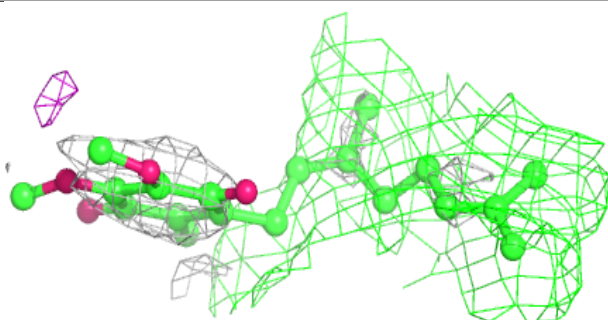
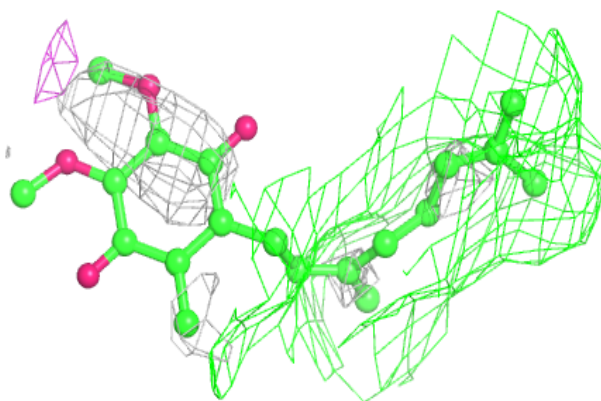
Electron density around CDL M 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

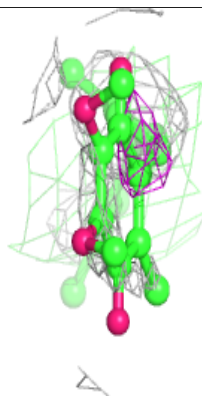
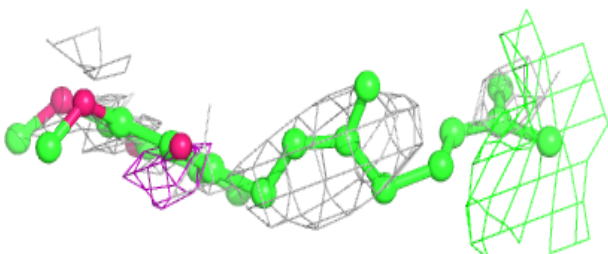
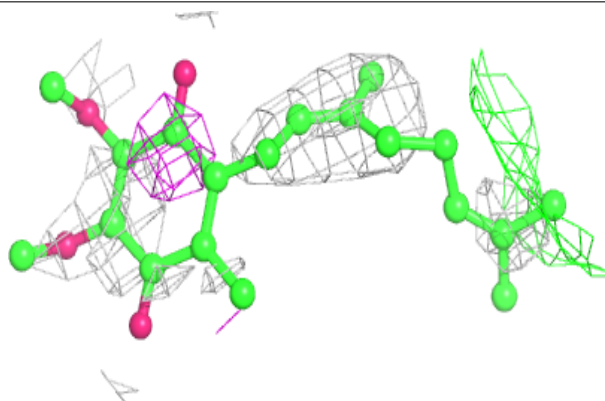


Electron density around U10 L 306 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

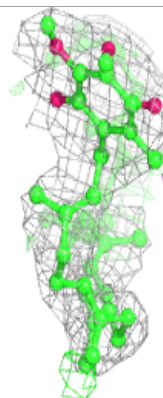
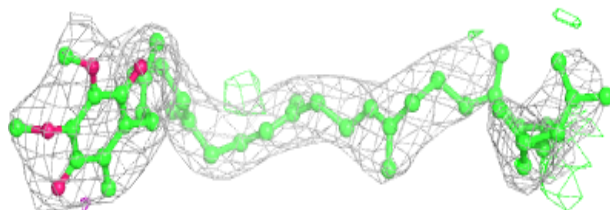
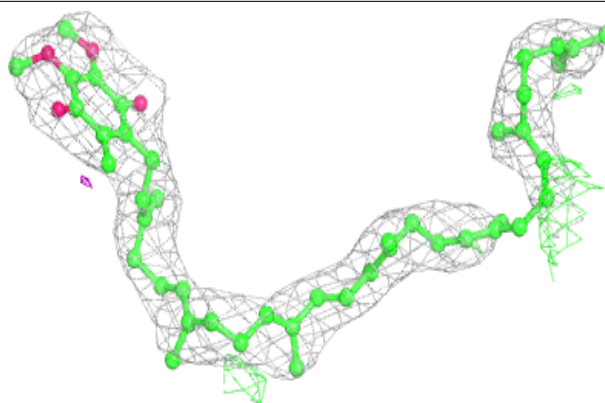
**Electron density around U10 L 306 (A):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

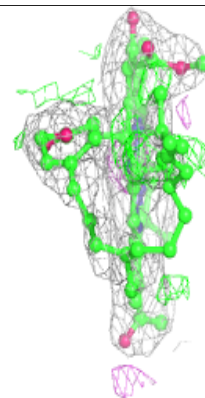
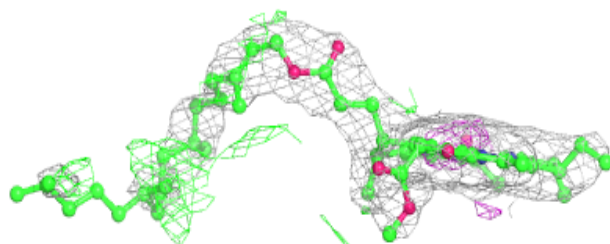
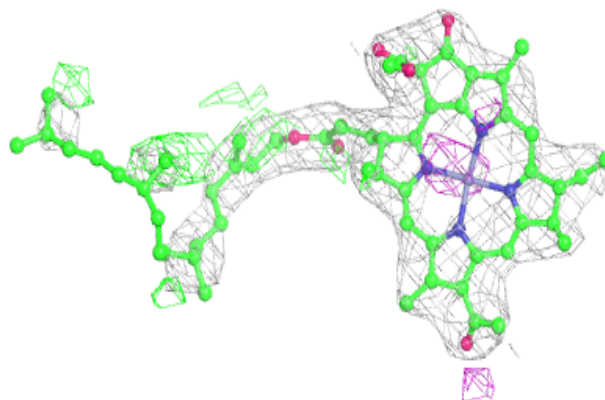


Electron density around U10 M 407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

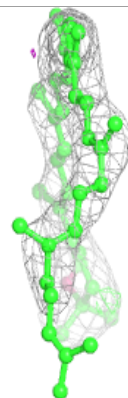
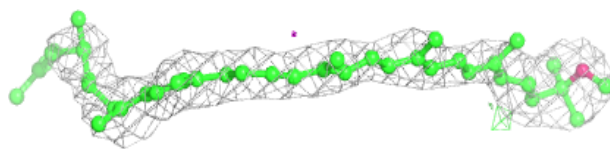
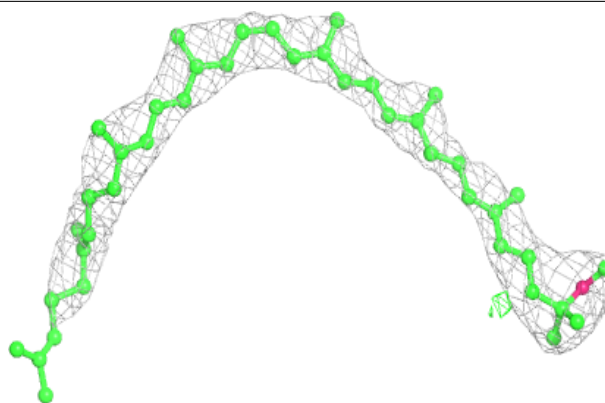
**Electron density around 2GO M 406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

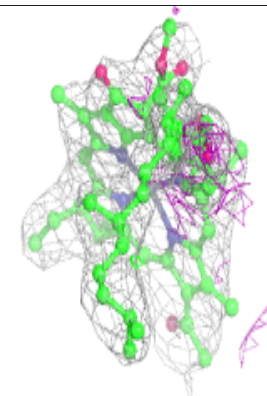
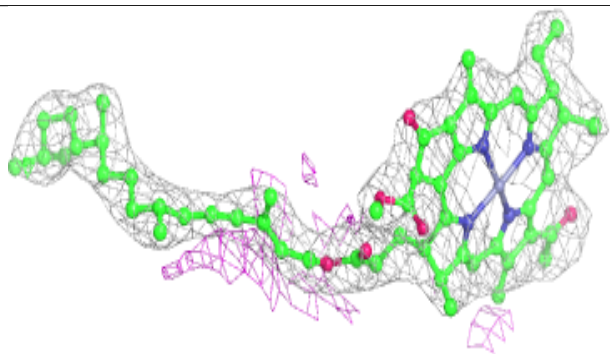
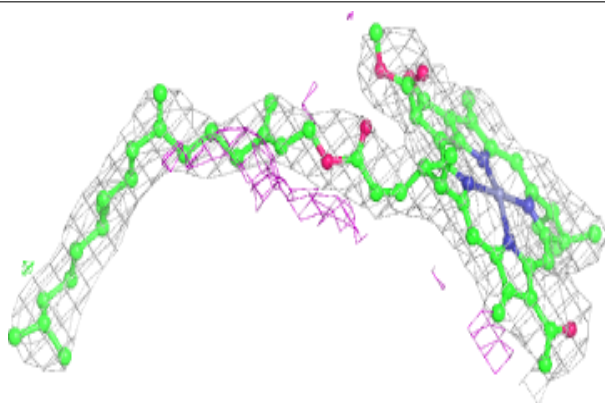


Electron density around SPO M 408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

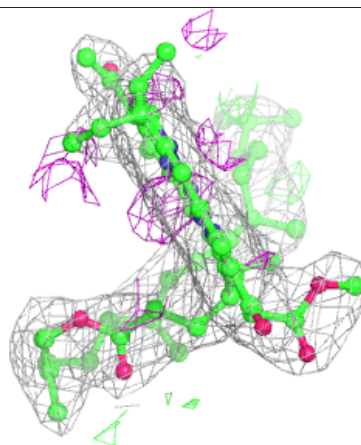
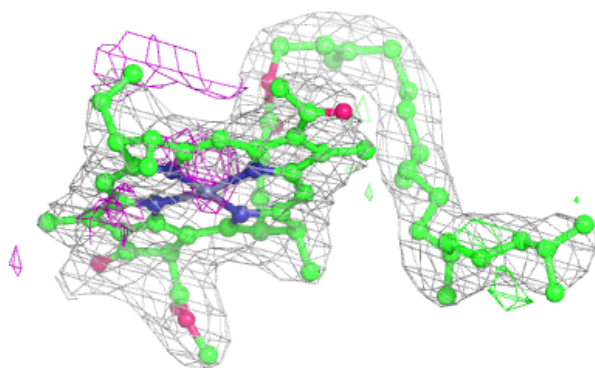
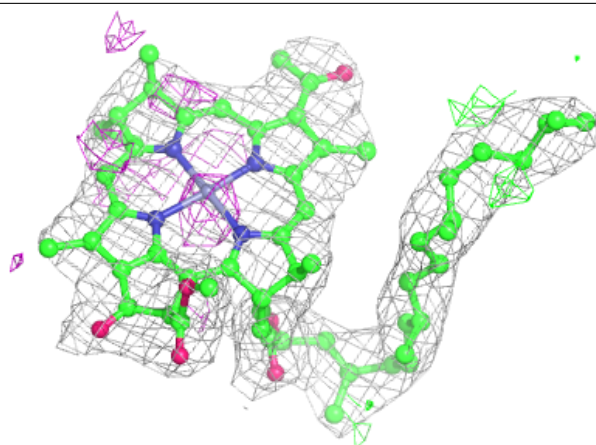
**Electron density around 2GO L 307:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



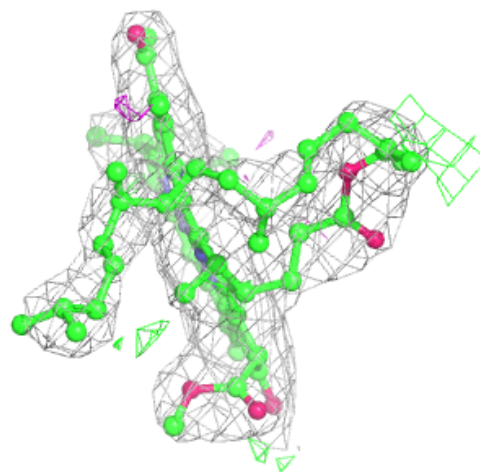
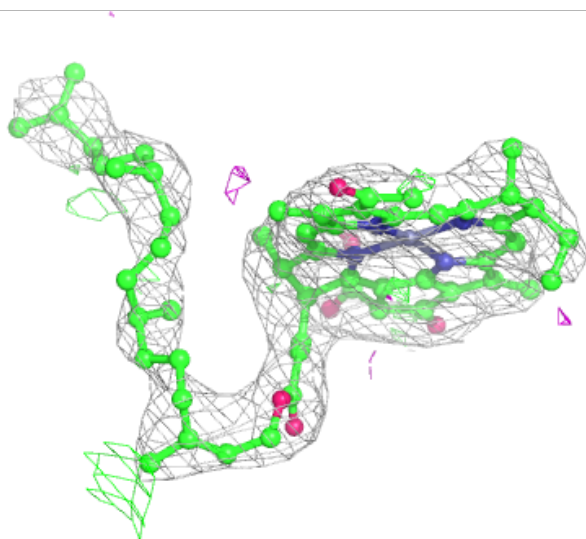
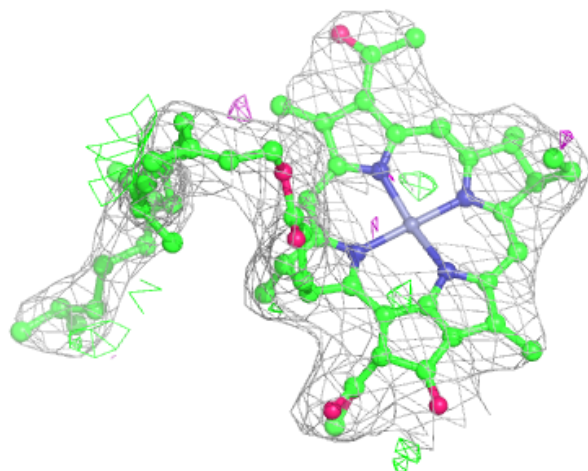
Electron density around 2GO L 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



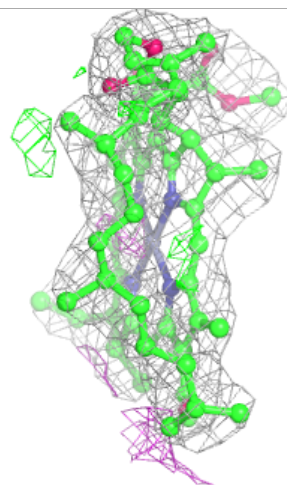
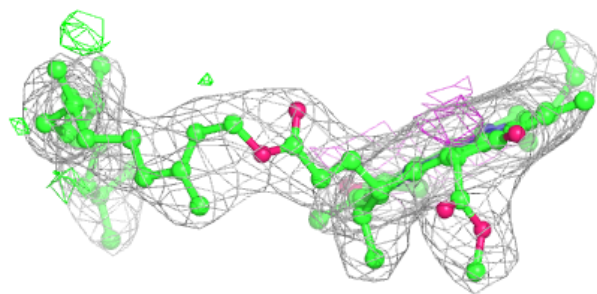
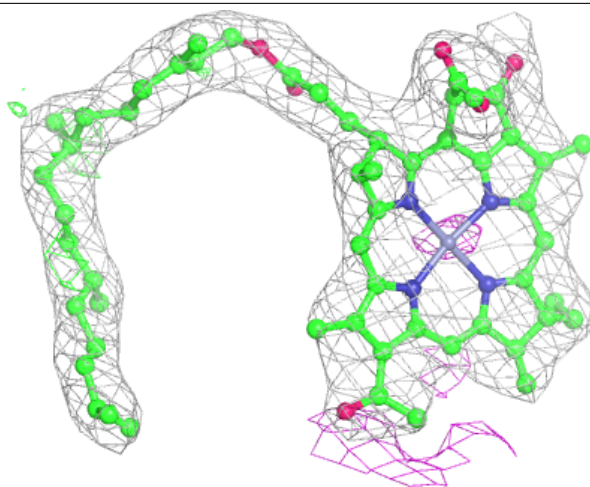
Electron density around 2GO M 401:

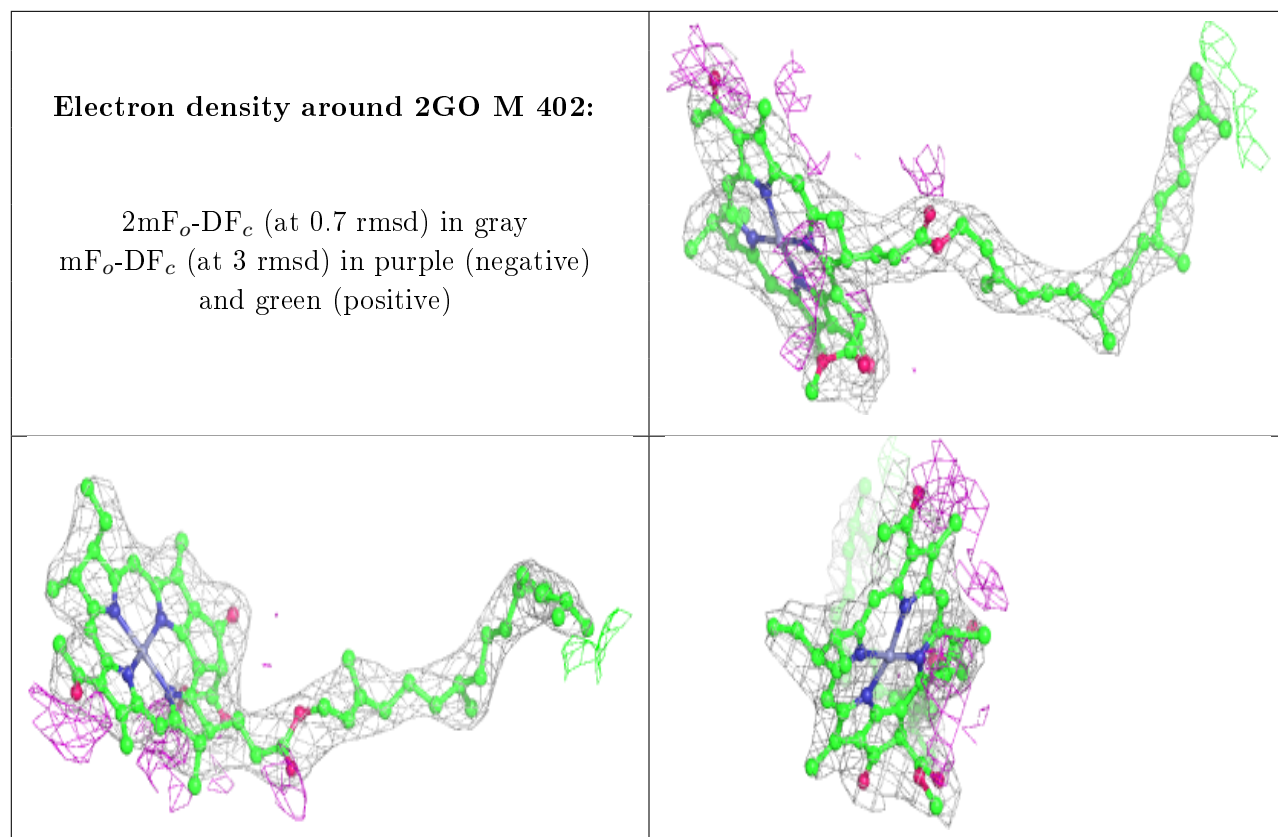
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 2GO L 305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.