



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:07 PM EDT

PDB ID : 4N7L / pdb_00004n7l
Title : Zinc Substituted Reaction Center M(L214H) Variant of 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 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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

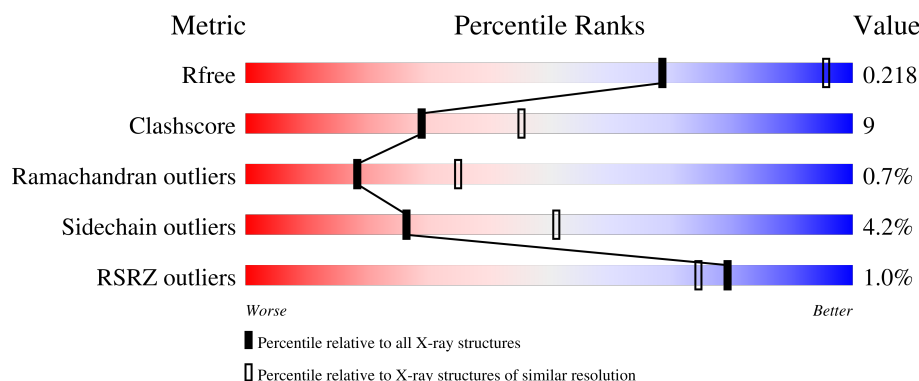
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

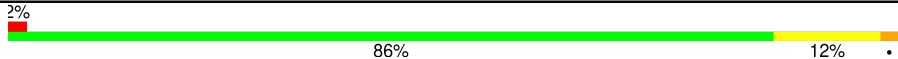
The reported resolution of this entry is 2.85 Å.

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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 of 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	
2	L	281	
3	M	303	

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
14	PC1	M	411	-	-	-	X
8	2GO	L	305	X	-	-	-
8	2GO	L	311	X	-	-	-
8	2GO	M	401	X	-	-	-
8	2GO	M	402	X	-	-	-
8	2GO	M	403	X	-	-	-
8	2GO	M	404	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 7762 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 protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	0	5	1
			1850	1183	321	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
			2413	1607	398	398	10			

There is a discrepancy between the modelled and reference sequences:

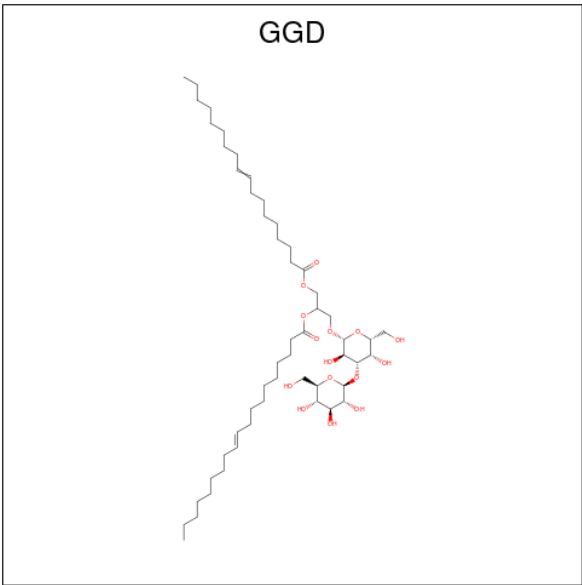
Chain	Residue	Modelled	Actual	Comment	Reference
M	214	HIS	LEU	engineered mutation	UNP P0C0Y9

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



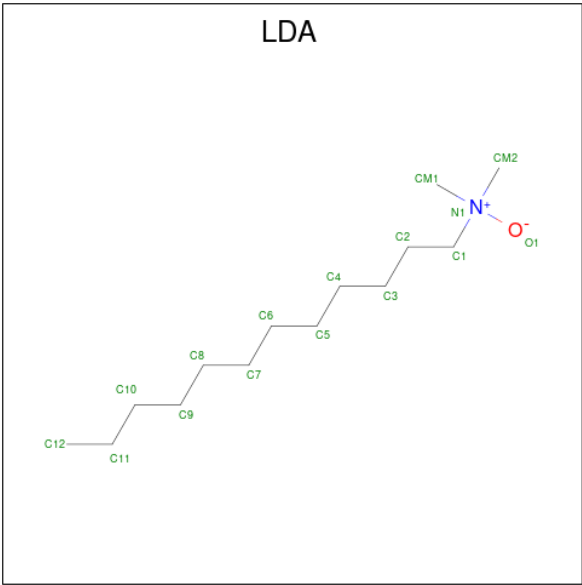
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- 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 (CCD ID: GGD) (formula: C₅₂H₉₄O₁₅).



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

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



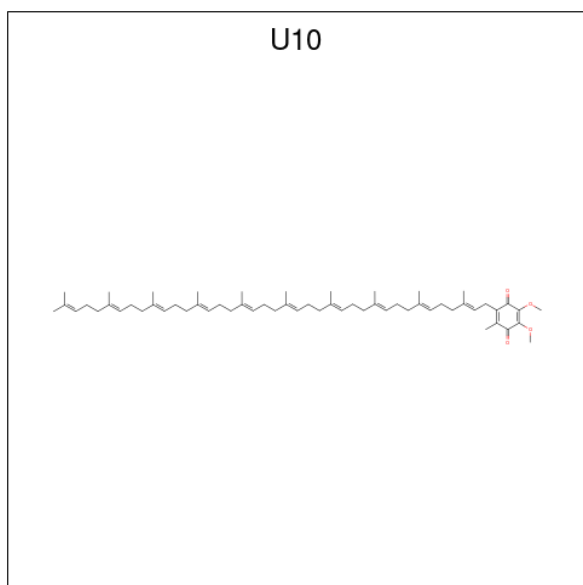
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 7 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).

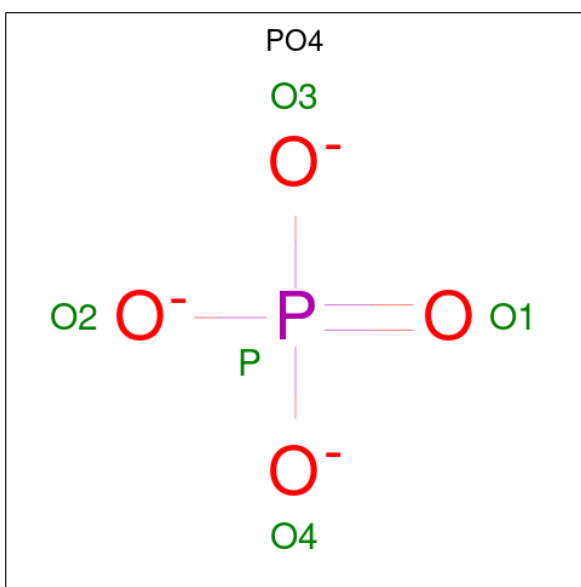


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	1
			46	38	8		
7	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is (T-4-S)-[(3S,4S,13R,14R,21R,23R,25R)-9-acetyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-(3-oxo-3-[(2E,7R,11R)-3,7,11,15-tetramethylhexadec-2-en-1-yl]oxy}propyl)-23,25-didehydro-13,14-dihydrophorbine-23,25-diido-kappa 4 N 23 ,N 24 , N 25 ,N 26]zinc (CCD ID: 2GO) (formula: C₅₅H₇₄N₄O₆Zn).

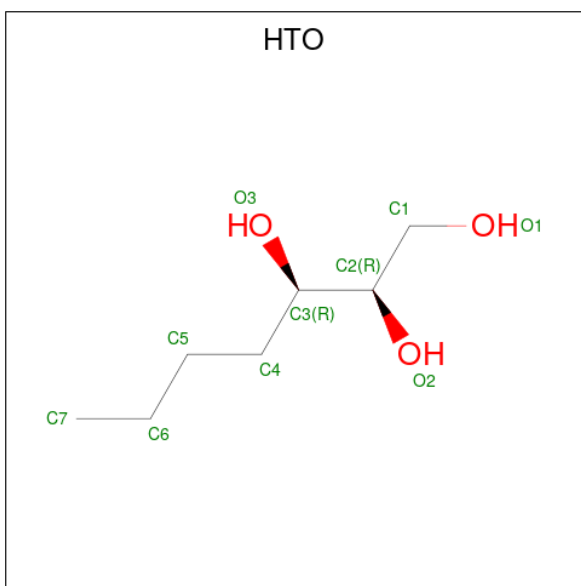


- Molecule 9 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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 (CCD ID: HTO) (formula: $C_7H_{16}O_3$).

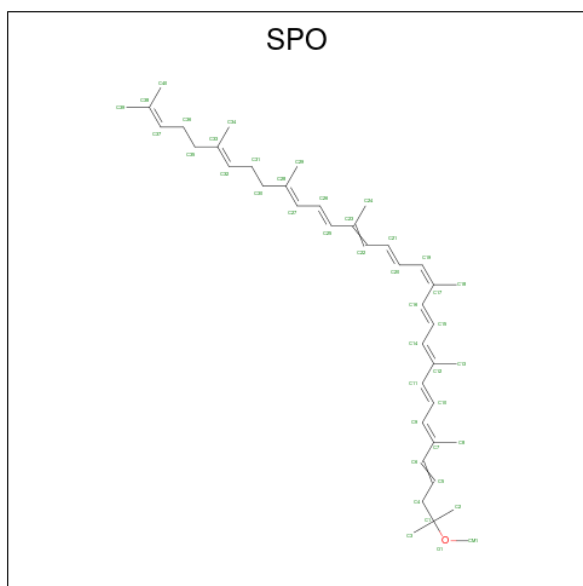


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		
10	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 11 is FE (III) ION (CCD ID: FE) (formula: Fe).

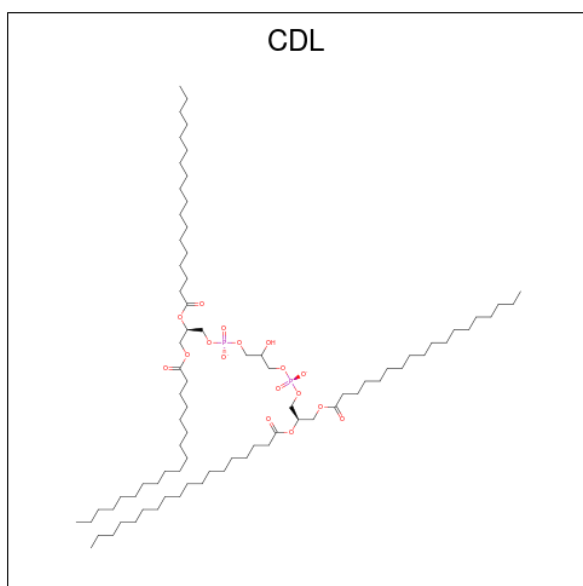
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is SPHEROIDENE (CCD ID: SPO) (formula: $C_{41}H_{60}O$).



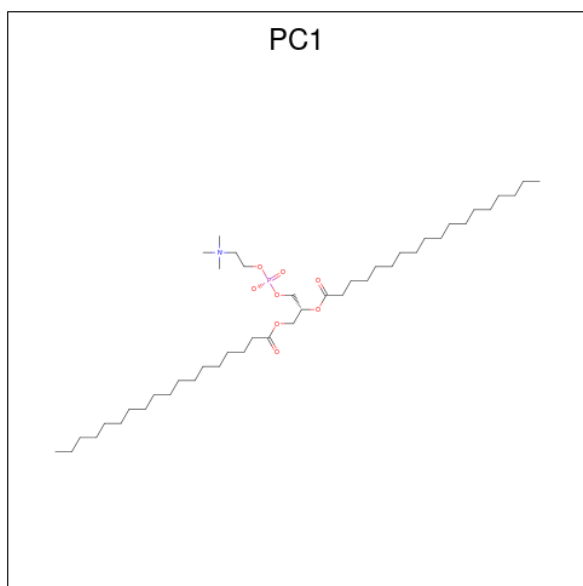
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 13 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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 (CCD ID: 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		

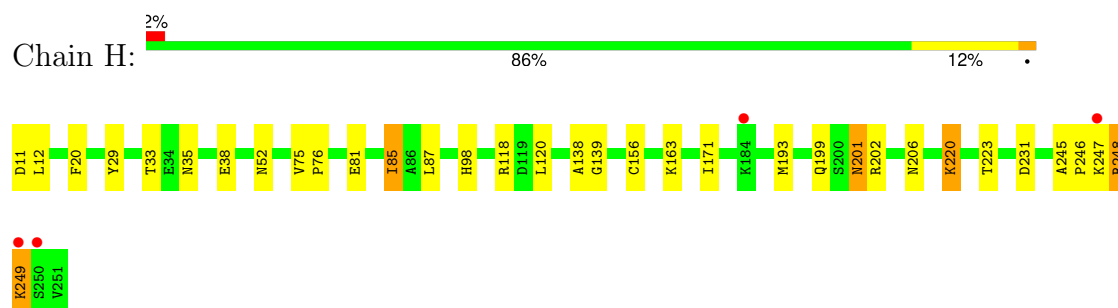
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	156	Total	O	0	0
			156	156		
15	L	114	Total	O	0	0
			114	114		
15	M	129	Total	O	0	0
			129	129		

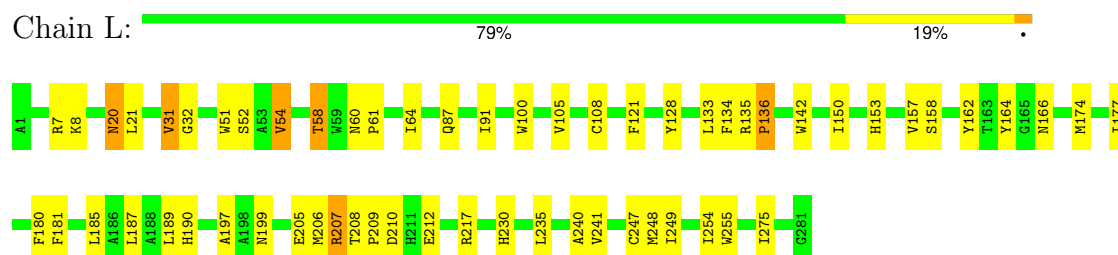
3 Residue-property plots [i](#)

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 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.

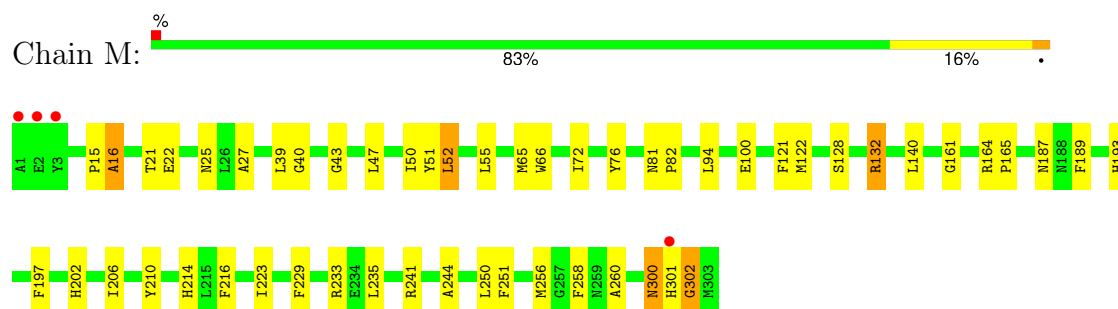
- Molecule 1: Reaction center protein H chain



- 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	139.59Å 139.59Å 184.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.57 – 2.85 50.57 – 2.85	Depositor EDS
% Data completeness (in resolution range)	87.2 (50.57-2.85) 87.2 (50.57-2.85)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.86Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.165 , 0.216 0.171 , 0.218	Depositor DCC
R_{free} test set	2153 reflections (4.40%)	wwPDB-VP
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7762	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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

5.1 Standard geometry

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

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	0.90	2/1930 (0.1%)	1.07	4/2621 (0.2%)
2	L	0.86	0/2339	0.96	4/3203 (0.1%)
3	M	0.85	1/2511 (0.0%)	0.99	0/3428
All	All	0.87	3/6780 (0.0%)	1.00	8/9252 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	M	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	85[A]	ILE	C-O	-6.30	1.17	1.24
1	H	85[B]	ILE	C-O	-6.30	1.17	1.24
3	M	233	ARG	CA-C	-6.27	1.46	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	171	ILE	CA-C-N	-5.77	113.73	119.56
1	H	171	ILE	C-N-CA	-5.77	113.73	119.56
2	L	121	PHE	N-CA-C	-5.37	105.54	111.71
2	L	58	THR	N-CA-C	5.36	117.23	108.76
1	H	248	ARG	CA-C-N	5.13	130.94	121.70
1	H	248	ARG	C-N-CA	5.13	130.94	121.70
2	L	275	ILE	CA-C-N	-5.12	115.30	120.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	L	275	ILE	C-N-CA	-5.12	115.30	120.21

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	300	ASN	Peptide

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	1850	0	1873	22	0
2	L	2239	0	2185	48	0
3	M	2413	0	2315	48	0
4	H	30	0	40	1	0
4	L	12	0	16	0	0
5	H	57	0	68	1	0
6	L	48	0	93	0	0
6	M	32	0	62	0	0
7	L	46	0	46	10	0
7	M	48	0	63	3	0
8	L	132	0	138	13	0
8	M	264	0	276	30	0
9	L	5	0	0	0	0
10	L	20	0	32	1	0
11	M	1	0	0	0	0
12	M	42	0	60	5	0
13	M	81	0	106	1	0
14	M	43	0	60	1	0
15	H	156	0	0	1	1
15	L	114	0	0	2	0
15	M	129	0	0	5	0
All	All	7762	0	7433	129	1

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 9.

All (129) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:210:TYR:HB3	8:M:402:2GO:H21	1.64	0.79
8:M:404:2GO:H19	8:M:404:2GO:H22	1.72	0.70
3:M:55:LEU:HB3	15:M:559:HOH:O	1.91	0.70
3:M:210:TYR:HB3	8:M:402:2GO:CBB	2.21	0.70
2:L:58:THR:HA	15:L:424:HOH:O	1.95	0.65
8:M:402:2GO:H19	8:M:402:2GO:H22	1.79	0.65
2:L:181:PHE:HB3	8:L:311:2GO:CBB	2.27	0.64
2:L:181:PHE:CD2	8:L:311:2GO:H20	2.33	0.64
7:L:304[B]:U10:O3	7:L:304[B]:U10:H4M3	1.98	0.63
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.80	0.63
3:M:65:MET:HB3	3:M:121:PHE:CD2	2.35	0.60
3:M:210:TYR:CD2	8:M:402:2GO:H20	2.36	0.60
1:H:81:GLU:HG3	1:H:85[B]:ILE:HD11	1.85	0.59
8:M:403:2GO:H21	12:M:409:SPO:H243	1.86	0.58
2:L:189:LEU:HD23	8:L:311:2GO:H7	1.86	0.57
8:L:311:2GO:H25	8:M:403:2GO:H43	1.86	0.57
2:L:164:TYR:O	15:L:469:HOH:O	2.17	0.57
7:L:304[A]:U10:H3M1	15:M:606:HOH:O	2.04	0.57
1:H:75:VAL:HA	1:H:76:PRO:C	2.30	0.57
3:M:197:PHE:CZ	8:M:404:2GO:H21	2.40	0.56
8:M:401:2GO:H19	8:M:401:2GO:H21	1.87	0.56
3:M:256:MET:HE3	3:M:258:PHE:CE1	2.41	0.55
7:L:304[A]:U10:H152	8:L:311:2GO:H1	1.89	0.55
1:H:248:ARG:HA	1:H:249[A]:LYS:HB3	1.89	0.55
3:M:300:ASN:O	3:M:302:GLY:N	2.40	0.55
1:H:248:ARG:HA	1:H:249[B]:LYS:HB3	1.89	0.55
2:L:230:HIS:CD2	3:M:223:ILE:HG13	2.42	0.54
1:H:199:GLN:OE1	1:H:202:ARG:NH1	2.39	0.54
1:H:201:ASN:H	1:H:201:ASN:HD22	1.56	0.53
3:M:300:ASN:C	3:M:302:GLY:N	2.66	0.53
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.43	0.53
3:M:15:PRO:O	3:M:16:ALA:C	2.50	0.53
2:L:51:TRP:O	2:L:54:VAL:N	2.41	0.52
3:M:197:PHE:HZ	8:M:404:2GO:CBB	2.23	0.52
3:M:189:PHE:O	3:M:193:HIS:HD2	1.92	0.52
2:L:20:ASN:HD22	2:L:20:ASN:H	1.59	0.51
3:M:52:LEU:HB2	15:M:556:HOH:O	2.10	0.51
8:L:311:2GO:H21	8:M:403:2GO:H35	1.92	0.51
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.92	0.51
2:L:189:LEU:CD2	8:L:311:2GO:H7	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:65:MET:HB3	3:M:121:PHE:CE2	2.47	0.50
2:L:187:LEU:HD13	3:M:216:PHE:CG	2.46	0.49
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.45	0.49
7:L:304[B]:U10:O3	7:L:304[B]:U10:C4M	2.60	0.49
2:L:212:GLU:OE2	7:L:304[A]:U10:H3M2	2.13	0.49
7:L:304[B]:U10:H152	14:M:411:PC1:H281	1.95	0.49
3:M:206:ILE:HD13	8:M:401:2GO:H8	1.93	0.48
1:H:156:CYS:HB3	1:H:206:ASN:O	2.14	0.48
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.49	0.48
2:L:217:ARG:O	3:M:50:ILE:HA	2.14	0.48
1:H:118[A]:ARG:HG3	1:H:120:LEU:HD12	1.95	0.47
2:L:100:TRP:CH2	7:M:408:U10:H251	2.50	0.47
2:L:61:PRO:O	2:L:150:ILE:HD12	2.14	0.47
1:H:87:LEU:HD11	2:L:8:LYS:HA	1.96	0.47
7:L:304[B]:U10:H153	3:M:47:LEU:HD11	1.96	0.47
2:L:133:LEU:HD23	2:L:134:PHE:CE1	2.49	0.47
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.50	0.47
1:H:206:ASN:HD21	1:H:248:ARG:HD3	1.79	0.47
3:M:260:ALA:HB2	7:M:408:U10:H103	1.96	0.47
2:L:207:ARG:NH1	3:M:140:LEU:O	2.48	0.47
3:M:197:PHE:CE1	8:M:404:2GO:H16	2.50	0.47
2:L:31:VAL:HG12	2:L:32:GLY:N	2.30	0.46
2:L:157:VAL:HG11	8:M:404:2GO:H20	1.97	0.46
3:M:21:THR:O	3:M:22:GLU:C	2.56	0.46
2:L:87:GLN:HE21	2:L:142:TRP:CD1	2.34	0.46
2:L:135:ARG:HD2	2:L:248:MET:O	2.15	0.46
3:M:197:PHE:CZ	8:M:404:2GO:CBB	2.99	0.46
1:H:29:TYR:O	1:H:33:THR:HG23	2.16	0.46
2:L:185:LEU:HD13	8:L:311:2GO:ND	2.31	0.45
3:M:161:GLY:HA3	12:M:409:SPO:H292	1.98	0.45
7:L:304[B]:U10:H121	7:L:304[B]:U10:H101	1.62	0.45
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.34	0.45
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.98	0.45
1:H:52:ASN:ND2	5:H:306:GGD:HA41	2.31	0.45
3:M:25:ASN:OD1	3:M:27:ALA:HB3	2.17	0.44
3:M:206:ILE:HD13	8:M:401:2GO:CMD	2.47	0.44
7:L:304[B]:U10:O2	7:L:304[B]:U10:H3M3	2.17	0.44
2:L:187:LEU:HD13	3:M:216:PHE:HB2	1.99	0.44
8:M:403:2GO:CBB	12:M:409:SPO:H243	2.46	0.44
2:L:187:LEU:HD13	3:M:216:PHE:CB	2.48	0.44
2:L:128:TYR:HD1	8:M:401:2GO:H20	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:40:GLY:HA2	3:M:43:GLY:O	2.18	0.44
3:M:76:TYR:CD2	3:M:76:TYR:C	2.95	0.44
2:L:91:ILE:HD11	10:L:307:HTO:H2	1.99	0.43
8:L:311:2GO:H15	8:L:311:2GO:H10	2.00	0.43
2:L:174:MET:HB3	8:M:403:2GO:O1D	2.18	0.43
3:M:210:TYR:CG	8:M:402:2GO:H20	2.53	0.43
1:H:138:ALA:HA	1:H:139:GLY:HA2	1.76	0.43
2:L:208:THR:HB	2:L:209:PRO:HD2	2.01	0.42
2:L:60:ASN:O	2:L:64:ILE:HD12	2.19	0.42
8:L:305:2GO:CBB	8:L:305:2GO:H25	2.49	0.42
3:M:50:ILE:CG1	3:M:51:TYR:N	2.82	0.42
3:M:251:PHE:CD1	3:M:251:PHE:C	2.97	0.42
8:M:402:2GO:CHD	8:M:402:2GO:H14	2.50	0.42
2:L:255:TRP:CD1	2:L:255:TRP:C	2.98	0.42
2:L:105:VAL:O	2:L:108:CYS:HB2	2.20	0.42
1:H:38:GLU:OE1	3:M:241:ARG:NH2	2.49	0.42
2:L:205:GLU:O	2:L:206:MET:C	2.63	0.42
3:M:66:TRP:CZ2	3:M:122:MET:HE3	2.55	0.42
1:H:98:HIS:CD2	2:L:7:ARG:HE	2.38	0.42
8:L:311:2GO:H21	8:M:403:2GO:C1	2.49	0.42
1:H:20:PHE:CD2	1:H:20:PHE:C	2.98	0.42
2:L:166:ASN:OD1	2:L:166:ASN:C	2.63	0.42
12:M:409:SPO:H20	12:M:409:SPO:H181	1.85	0.42
1:H:206:ASN:HB2	15:M:515:HOH:O	2.19	0.41
2:L:177:ILE:HD11	8:L:305:2GO:C1B	2.50	0.41
8:M:401:2GO:C2B	8:M:402:2GO:H68	2.51	0.41
13:M:410:CDL:C75	13:M:410:CDL:C74	2.98	0.41
4:H:305:GOL:H31	2:L:199:ASN:HA	2.02	0.41
2:L:150:ILE:O	2:L:153:HIS:ND1	2.52	0.41
3:M:250:LEU:HD23	3:M:250:LEU:HA	1.94	0.41
8:M:403:2GO:H21	8:M:403:2GO:H19	2.02	0.41
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.68	0.41
3:M:214:HIS:CE1	8:M:402:2GO:NA	2.88	0.41
7:M:408:U10:H353	7:M:408:U10:C30	2.51	0.41
12:M:409:SPO:H15	12:M:409:SPO:H131	1.84	0.41
1:H:35:ASN:OD1	3:M:260:ALA:HB1	2.21	0.41
8:L:305:2GO:CGA	8:M:401:2GO:H13	2.50	0.41
3:M:81:ASN:HA	3:M:82:PRO:HD2	1.96	0.41
3:M:210:TYR:CB	8:M:402:2GO:H21	2.44	0.41
2:L:177:ILE:HD13	8:M:403:2GO:H8	2.02	0.41
3:M:132:ARG:HB2	15:M:559:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:190:HIS:ND1	7:L:304[A]:U10:O2	2.30	0.41
2:L:197:ALA:HB1	3:M:235:LEU:HD11	2.02	0.41
2:L:230:HIS:NE2	3:M:223:ILE:HG13	2.36	0.41
8:M:401:2GO:H34	8:M:402:2GO:H21	2.01	0.41
1:H:220[B]:LYS:HD3	15:H:533:HOH:O	2.21	0.41
2:L:241:VAL:HG21	8:M:402:2GO:H11	2.02	0.40
1:H:245:ALA:N	1:H:246:PRO:HD2	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:433:HOH:O	15:H:433:HOH:O[4_555]	1.98	0.22

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	235 (96%)	8 (3%)	2 (1%)	16	31
2	L	281/281 (100%)	259 (92%)	20 (7%)	2 (1%)	18	35
3	M	302/303 (100%)	280 (93%)	19 (6%)	3 (1%)	12	25
All	All	828/825 (100%)	774 (94%)	47 (6%)	7 (1%)	18	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	301	HIS
3	M	16	ALA
3	M	302	GLY
1	H	249[A]	LYS
1	H	249[B]	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	52	SER
2	L	31	VAL

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	200/196 (102%)	188 (94%)	12 (6%)	17	36
2	L	221/220 (100%)	210 (95%)	11 (5%)	22	44
3	M	237/237 (100%)	230 (97%)	7 (3%)	36	61
All	All	658/653 (101%)	628 (95%)	30 (5%)	26	48

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	11	ASP
1	H	12	LEU
1	H	163[A]	LYS
1	H	163[B]	LYS
1	H	193	MET
1	H	201	ASN
1	H	220[A]	LYS
1	H	220[B]	LYS
1	H	220[C]	LYS
1	H	223	THR
1	H	231	ASP
1	H	247	LYS
2	L	20	ASN
2	L	21	LEU
2	L	54	VAL
2	L	136	PRO
2	L	158	SER
2	L	207	ARG
2	L	210	ASP
2	L	235	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	247	CYS
2	L	249	ILE
2	L	254	ILE
3	M	39	LEU
3	M	52	LEU
3	M	72	ILE
3	M	94	LEU
3	M	100	GLU
3	M	128	SER
3	M	132	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	44	ASN
1	H	98	HIS
1	H	201	ASN
1	H	206	ASN
2	L	20	ASN
2	L	258	GLN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
8	2GO	M	402	3	72,74,74	1.55	15 (20%)	78,115,115	1.91	20 (25%)
4	GOL	H	304	-	5,5,5	0.45	0	5,5,5	0.37	0
6	LDA	L	303	-	13,15,15	1.99	2 (15%)	14,17,17	0.51	0
10	HTO	L	308	-	9,9,9	0.83	0	10,10,10	0.90	0
10	HTO	L	307	-	9,9,9	0.84	0	10,10,10	0.75	0
7	U10	L	304[A]	-	23,23,63	2.02	2 (8%)	30,31,79	2.67	7 (23%)
12	SPO	M	409	-	41,41,41	0.74	0	47,50,50	1.84	14 (29%)
6	LDA	L	302	-	13,15,15	1.93	1 (7%)	14,17,17	0.48	0
8	2GO	L	311	-	72,74,74	1.87	14 (19%)	78,115,115	2.17	22 (28%)
4	GOL	H	303	-	5,5,5	0.39	0	5,5,5	0.26	0
8	2GO	L	305	2	72,74,74	1.59	15 (20%)	78,115,115	1.84	20 (25%)
14	PC1	M	411	-	42,42,53	1.41	3 (7%)	48,50,61	2.30	10 (20%)
8	2GO	M	404	3	72,74,74	1.65	14 (19%)	78,115,115	1.96	22 (28%)
5	GGD	H	306	-	58,58,68	1.01	3 (5%)	72,72,82	1.39	10 (13%)
4	GOL	L	309	-	5,5,5	0.57	0	5,5,5	0.67	0
6	LDA	M	405	-	13,15,15	1.87	1 (7%)	14,17,17	0.68	1 (7%)
4	GOL	H	305	-	5,5,5	0.73	0	5,5,5	0.97	0
9	PO4	L	306	-	4,4,4	0.93	0	6,6,6	0.54	0
7	U10	M	408	-	48,48,63	1.76	3 (6%)	60,61,79	1.80	11 (18%)
13	CDL	M	410	-	80,80,99	3.54	5 (6%)	86,92,111	1.34	8 (9%)
8	2GO	M	401	2	72,74,74	1.59	14 (19%)	78,115,115	2.09	22 (28%)
8	2GO	M	403	3	72,74,74	1.69	12 (16%)	78,115,115	1.92	21 (26%)
7	U10	L	304[B]	-	23,23,63	2.09	2 (8%)	30,31,79	1.46	4 (13%)
4	GOL	H	302	-	5,5,5	0.72	0	5,5,5	1.14	0
6	LDA	L	301	-	13,15,15	1.95	1 (7%)	14,17,17	0.50	0
4	GOL	L	310	-	5,5,5	0.65	0	5,5,5	0.58	0
4	GOL	H	301	-	5,5,5	0.72	0	5,5,5	0.62	0
6	LDA	M	406	-	13,15,15	2.04	2 (15%)	14,17,17	0.73	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
8	2GO	M	402	3	1/1/21/25	9/41/137/137	-
4	GOL	H	304	-	-	1/4/4/4	-
6	LDA	L	303	-	-	5/13/13/13	-
10	HTO	L	308	-	-	2/10/10/10	-
10	HTO	L	307	-	-	5/10/10/10	-
7	U10	L	304[A]	-	-	6/15/39/87	0/1/1/1
12	SPO	M	409	-	-	7/47/47/47	-
6	LDA	L	302	-	-	3/13/13/13	-
8	2GO	L	311	-	1/1/21/25	14/41/137/137	-
4	GOL	H	303	-	-	0/4/4/4	-
8	2GO	L	305	2	1/1/21/25	2/41/137/137	-
14	PC1	M	411	-	-	26/46/46/57	-
8	2GO	M	404	3	1/1/21/25	8/41/137/137	-
5	GGD	H	306	-	-	14/47/87/97	0/2/2/2
4	GOL	L	309	-	-	2/4/4/4	-
6	LDA	M	405	-	-	9/13/13/13	-
4	GOL	H	305	-	-	2/4/4/4	-
7	U10	M	408	-	-	9/45/69/87	0/1/1/1
13	CDL	M	410	-	-	42/91/91/110	-
8	2GO	M	401	2	1/1/21/25	10/41/137/137	-
8	2GO	M	403	3	1/1/21/25	17/41/137/137	-
7	U10	L	304[B]	-	-	6/15/39/87	0/1/1/1
4	GOL	H	302	-	-	2/4/4/4	-
6	LDA	L	301	-	-	6/13/13/13	-
4	GOL	L	310	-	-	1/4/4/4	-
4	GOL	H	301	-	-	2/4/4/4	-
6	LDA	M	406	-	-	7/13/13/13	-

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	410	CDL	C75-C74	29.52	2.98	1.51
7	L	304[B]	U10	C6-C1	8.90	1.51	1.35
7	M	408	U10	C6-C1	8.82	1.51	1.35
7	L	304[A]	U10	C6-C1	8.09	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	406	LDA	O1-N1	-6.90	1.25	1.42
6	L	303	LDA	O1-N1	-6.73	1.25	1.42
6	L	301	LDA	O1-N1	-6.70	1.25	1.42
6	L	302	LDA	O1-N1	-6.67	1.25	1.42
6	M	405	LDA	O1-N1	-6.13	1.27	1.42
14	M	411	PC1	O31-C31	5.84	1.50	1.33
8	L	311	2GO	O2D-CGD	5.60	1.47	1.33
8	M	404	2GO	C3D-C4D	-5.19	1.32	1.44
8	L	311	2GO	CHD-C1D	5.11	1.48	1.38
8	M	402	2GO	O2D-CGD	5.08	1.45	1.33
13	M	410	CDL	OA8-CA7	5.07	1.48	1.33
8	M	401	2GO	O2D-CGD	5.00	1.45	1.33
8	M	403	2GO	O2A-CGA	4.95	1.47	1.33
13	M	410	CDL	OB8-CB7	4.91	1.47	1.33
8	M	401	2GO	O2A-CGA	4.89	1.47	1.33
8	L	311	2GO	O2A-CGA	4.86	1.47	1.33
14	M	411	PC1	O21-C21	4.85	1.48	1.34
13	M	410	CDL	OA6-CA5	4.84	1.48	1.34
13	M	410	CDL	OB6-CB5	4.76	1.47	1.34
8	M	403	2GO	C3D-C4D	-4.58	1.33	1.44
8	L	311	2GO	C3B-C4B	4.57	1.50	1.41
8	M	404	2GO	O2D-CGD	4.55	1.44	1.33
8	M	403	2GO	OBD-CAD	4.45	1.30	1.22
8	L	305	2GO	O2D-CGD	4.42	1.44	1.33
5	H	306	GGD	OC8-CC7	4.24	1.45	1.33
8	M	403	2GO	O2D-CGD	4.23	1.43	1.33
8	L	311	2GO	CHC-C4B	4.18	1.48	1.39
8	M	403	2GO	CHB-C1B	4.09	1.48	1.39
8	L	311	2GO	C3D-C2D	4.04	1.50	1.39
5	H	306	GGD	OC6-CC5	4.01	1.45	1.34
8	L	311	2GO	CHB-C1B	4.00	1.48	1.39
8	L	305	2GO	C3D-C4D	-3.96	1.35	1.44
8	L	305	2GO	CHB-C1B	3.95	1.48	1.39
8	M	404	2GO	O2A-CGA	3.85	1.44	1.33
7	L	304[B]	U10	C4-C3	3.83	1.50	1.36
8	L	311	2GO	CHD-C4C	3.83	1.50	1.39
8	L	305	2GO	O2A-CGA	3.81	1.44	1.33
8	M	401	2GO	C3D-C4D	-3.81	1.35	1.44
8	M	403	2GO	C3D-C2D	3.73	1.49	1.39
8	M	402	2GO	O2A-CGA	3.73	1.44	1.33
7	M	408	U10	C4-C3	3.71	1.49	1.36
8	M	404	2GO	CHB-C1B	3.60	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	304[A]	U10	C4-C3	3.56	1.49	1.36
8	M	401	2GO	C3B-C4B	3.54	1.48	1.41
8	M	404	2GO	C3B-C4B	3.54	1.48	1.41
8	L	311	2GO	C3D-C4D	-3.54	1.36	1.44
8	L	305	2GO	OBD-CAD	3.53	1.28	1.22
8	M	402	2GO	C3D-C4D	-3.50	1.36	1.44
8	M	402	2GO	CHB-C1B	3.41	1.47	1.39
8	M	404	2GO	CHD-C1D	3.40	1.45	1.38
8	L	305	2GO	C3B-C4B	3.37	1.47	1.41
8	L	311	2GO	C1B-C2B	3.35	1.51	1.43
8	M	402	2GO	C3D-C2D	3.33	1.48	1.39
8	M	401	2GO	OBD-CAD	3.23	1.28	1.22
8	M	404	2GO	OBD-CAD	3.21	1.28	1.22
8	L	305	2GO	CHD-C1D	3.16	1.44	1.38
8	M	404	2GO	C1D-ND	-3.07	1.31	1.38
8	M	401	2GO	CHD-C1D	3.03	1.44	1.38
8	L	305	2GO	C3D-C2D	2.96	1.47	1.39
8	M	403	2GO	C3B-C4B	2.95	1.46	1.41
8	M	402	2GO	CHD-C1D	2.93	1.44	1.38
8	M	404	2GO	C3C-C4C	-2.90	1.47	1.51
8	M	403	2GO	CHD-C1D	2.87	1.44	1.38
8	M	404	2GO	CHC-C4B	2.86	1.45	1.39
8	L	311	2GO	C4D-CHA	2.78	1.47	1.38
8	L	311	2GO	C1D-C2D	2.74	1.50	1.45
8	M	402	2GO	OBD-CAD	2.70	1.27	1.22
8	M	402	2GO	C3B-C4B	2.68	1.46	1.41
7	M	408	U10	C33-C34	2.63	1.39	1.33
8	M	402	2GO	CHD-C4C	2.63	1.46	1.39
8	M	402	2GO	CHC-C4B	2.63	1.45	1.39
8	M	403	2GO	CHD-C4C	2.57	1.46	1.39
8	M	401	2GO	C3C-C4C	-2.55	1.48	1.51
8	L	311	2GO	OBD-CAD	2.55	1.26	1.22
8	M	401	2GO	C1D-ND	-2.52	1.32	1.38
8	M	402	2GO	CHB-C4A	-2.49	1.31	1.37
8	M	403	2GO	C4B-NB	-2.48	1.32	1.38
8	M	401	2GO	C3D-C2D	2.38	1.45	1.39
8	M	404	2GO	C3D-C2D	2.34	1.45	1.39
8	M	401	2GO	C1B-C2B	2.33	1.48	1.43
8	L	311	2GO	C4C-NC	2.31	1.33	1.28
8	L	305	2GO	CHD-C4C	2.30	1.45	1.39
8	M	404	2GO	CHD-C4C	2.30	1.45	1.39
14	M	411	PC1	C3-C2	2.29	1.58	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	401	2GO	CHB-C1B	2.27	1.44	1.39
8	M	402	2GO	C1B-C2B	2.24	1.48	1.43
8	M	401	2GO	CHC-C4B	2.22	1.44	1.39
8	L	305	2GO	C4B-NB	-2.22	1.33	1.38
8	M	401	2GO	CHD-C4C	2.19	1.45	1.39
8	L	305	2GO	CHB-C4A	-2.19	1.32	1.37
8	L	305	2GO	C1D-ND	-2.18	1.33	1.38
8	L	305	2GO	CHC-C1C	-2.15	1.32	1.37
8	M	402	2GO	C1D-ND	-2.15	1.33	1.38
8	M	401	2GO	CHB-C4A	-2.14	1.32	1.37
8	M	402	2GO	C4C-NC	2.12	1.33	1.28
6	M	406	LDA	C1-N1	-2.10	1.49	1.51
8	M	403	2GO	C3C-C4C	-2.09	1.49	1.51
8	L	305	2GO	C1B-C2B	2.09	1.48	1.43
6	L	303	LDA	C1-N1	-2.09	1.49	1.51
8	M	404	2GO	C1B-NB	-2.07	1.33	1.38
5	H	306	GGD	OA1-CA1	2.07	1.43	1.40
8	M	402	2GO	C1B-NB	-2.06	1.33	1.38
8	L	305	2GO	C3C-C4C	-2.06	1.49	1.51
8	M	403	2GO	CBD-CGD	-2.04	1.46	1.52
8	M	404	2GO	C1B-C2B	2.03	1.47	1.43

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	304[A]	U10	C7-C6-C5	8.73	128.66	118.52
14	M	411	PC1	C15-N-C13	-7.79	88.51	108.98
8	M	403	2GO	CMD-C2D-C1D	7.12	137.27	124.73
7	L	304[A]	U10	C7-C6-C1	-6.81	113.21	124.89
14	M	411	PC1	C14-N-C13	-6.63	91.55	108.98
8	L	311	2GO	O2D-CGD-CBD	6.46	122.53	111.23
8	L	305	2GO	CMD-C2D-C1D	6.33	135.87	124.73
8	L	311	2GO	C2B-C1B-NB	6.19	116.79	109.02
7	M	408	U10	C30-C29-C31	6.00	125.65	115.23
8	M	402	2GO	CMD-C2D-C1D	5.98	135.25	124.73
8	M	401	2GO	CMD-C2D-C1D	5.88	135.08	124.73
14	M	411	PC1	O21-C21-C22	5.78	124.00	111.48
8	L	311	2GO	CMD-C2D-C1D	5.74	134.84	124.73
8	L	311	2GO	CMB-C2B-C1B	5.52	133.83	125.42
8	M	402	2GO	C2B-C1B-NB	5.47	115.88	109.02
8	M	404	2GO	C2B-C1B-NB	5.41	115.82	109.02
12	M	409	SPO	C4-C5-C6	-5.33	117.43	124.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	401	2GO	O2D-CGD-CBD	5.25	120.40	111.23
13	M	410	CDL	OA6-CA5-C11	5.25	122.83	111.48
8	M	404	2GO	CMD-C2D-C1D	5.21	133.90	124.73
8	M	401	2GO	C3C-C4C-CHD	-5.04	112.77	123.39
13	M	410	CDL	OB6-CB5-C51	5.00	122.31	111.48
14	M	411	PC1	C15-N-C14	4.99	122.08	108.98
7	L	304[A]	U10	C8-C7-C6	4.97	124.32	112.08
8	M	402	2GO	O2D-CGD-CBD	4.87	119.75	111.23
8	L	305	2GO	C3C-C4C-NC	4.86	116.77	111.10
8	M	401	2GO	C2B-C1B-NB	4.84	115.10	109.02
8	M	403	2GO	C2B-C1B-NB	4.64	114.85	109.02
5	H	306	GGD	OB1-CA3-CA2	4.61	118.95	107.23
13	M	410	CDL	C76-C75-C74	4.53	137.25	114.37
8	M	404	2GO	C3C-C4C-CHD	-4.52	113.86	123.39
5	H	306	GGD	OC6-CC5-C14	4.41	121.03	111.48
8	L	305	2GO	C3C-C4C-CHD	-4.27	114.40	123.39
14	M	411	PC1	C3-O31-C31	4.22	132.53	117.12
13	M	410	CDL	C75-C74-C73	-4.22	93.06	114.37
14	M	411	PC1	C13-N-C12	-4.21	93.16	109.91
8	M	403	2GO	C3C-C4C-CHD	-4.17	114.61	123.39
8	L	305	2GO	C2B-C1B-NB	4.16	114.24	109.02
8	M	404	2GO	O2D-CGD-O1D	-4.09	115.89	123.85
8	M	401	2GO	C3C-C4C-NC	4.09	115.86	111.10
8	L	311	2GO	CED-O2D-CGD	4.09	125.19	115.92
8	L	311	2GO	C3C-C4C-NC	4.06	115.83	111.10
8	M	401	2GO	C3D-C2D-C1D	-4.04	100.32	105.83
8	M	402	2GO	CMB-C2B-C1B	4.01	131.52	125.42
8	M	404	2GO	C3C-C4C-NC	3.96	115.71	111.10
7	L	304[B]	U10	C7-C8-C9	-3.94	120.04	126.83
8	M	403	2GO	O2D-CGD-CBD	3.92	118.08	111.23
8	L	305	2GO	O2A-CGA-O1A	-3.91	113.84	123.63
8	M	401	2GO	C1-O2A-CGA	3.90	126.08	116.65
7	M	408	U10	C25-C24-C26	3.89	121.98	115.23
8	M	401	2GO	O1D-CGD-CBD	-3.88	116.86	124.52
8	M	404	2GO	C2A-C1A-NA	3.87	115.49	110.99
7	M	408	U10	C20-C19-C21	3.83	121.88	115.23
7	L	304[B]	U10	C10-C9-C11	3.74	121.72	115.23
8	M	401	2GO	CMB-C2B-C1B	3.73	131.10	125.42
8	L	305	2GO	O2A-CGA-CBA	3.71	123.15	111.83
8	M	403	2GO	C3C-C4C-NC	3.70	115.42	111.10
7	L	304[A]	U10	C1M-C1-C6	-3.70	118.37	124.45
8	L	311	2GO	CHD-C1D-ND	-3.70	118.70	124.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	401	2GO	C2A-C1A-NA	3.65	115.24	110.99
8	M	404	2GO	C3D-C2D-C1D	-3.58	100.94	105.83
12	M	409	SPO	C21-C22-C23	-3.56	122.29	127.28
8	L	305	2GO	C2A-C1A-NA	3.47	115.03	110.99
12	M	409	SPO	C20-C19-C17	-3.46	122.43	127.28
7	M	408	U10	C4M-O4-C4	3.45	128.61	116.47
8	M	401	2GO	CHD-C1D-ND	-3.44	119.13	124.82
8	M	402	2GO	CHD-C1D-ND	-3.41	119.18	124.82
8	M	404	2GO	O2A-CGA-CBA	3.41	122.23	111.83
7	M	408	U10	C15-C14-C16	3.37	121.08	115.23
8	M	403	2GO	C3D-C2D-C1D	-3.37	101.23	105.83
8	M	402	2GO	CAC-C3C-C4C	3.36	120.04	112.58
8	M	404	2GO	O2D-CGD-CBD	3.34	117.06	111.23
8	L	305	2GO	C3D-C2D-C1D	-3.31	101.31	105.83
8	L	305	2GO	O2D-CGD-CBD	3.29	116.98	111.23
8	L	311	2GO	CBB-CAB-C3B	-3.27	113.51	120.40
12	M	409	SPO	C6-C7-C9	-3.24	113.91	119.01
8	L	311	2GO	C1-O2A-CGA	3.22	124.45	116.65
5	H	306	GGD	OC8-CC7-C31	3.22	121.65	111.83
8	M	401	2GO	C1D-CHD-C4C	-3.17	118.98	126.62
8	L	311	2GO	C2A-C1A-NA	3.16	114.67	110.99
8	M	403	2GO	CAB-C3B-C2B	-3.16	121.17	127.74
8	M	403	2GO	C2A-C1A-NA	3.15	114.66	110.99
8	M	402	2GO	C3C-C4C-CHD	-3.14	116.78	123.39
8	M	403	2GO	C1D-CHD-C4C	-3.11	119.11	126.62
8	M	404	2GO	O2A-CGA-O1A	-3.09	115.89	123.63
8	M	404	2GO	CHD-C1D-ND	-3.07	119.74	124.82
5	H	306	GGD	OC8-CC7-OC9	-3.05	115.99	123.63
8	L	311	2GO	CAC-C3C-C4C	3.05	119.34	112.58
8	M	402	2GO	C1-C2-C3	-3.05	121.21	126.20
8	M	402	2GO	C3D-C2D-C1D	-3.04	101.68	105.83
8	M	404	2GO	OBB-CAB-C3B	3.03	125.78	120.43
12	M	409	SPO	C8-C7-C6	3.01	122.69	118.09
12	M	409	SPO	C15-C14-C12	-3.01	123.06	127.28
8	M	404	2GO	CED-O2D-CGD	3.01	122.74	115.92
8	M	402	2GO	C3D-C4D-ND	3.01	116.11	110.51
8	M	402	2GO	CAB-C3B-C2B	-2.98	121.55	127.74
8	M	403	2GO	CMB-C2B-C1B	2.98	129.96	125.42
12	M	409	SPO	C34-C33-C35	2.97	120.38	115.23
8	M	402	2GO	C3C-C4C-NC	2.97	114.56	111.10
5	H	306	GGD	OC8-CC6-CC4	2.96	116.92	108.40
7	M	408	U10	C31-C29-C28	-2.93	114.59	121.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	311	2GO	C3C-C4C-CHD	-2.93	117.22	123.39
8	L	311	2GO	C3D-C2D-C1D	-2.89	101.89	105.83
14	M	411	PC1	C15-N-C12	2.89	121.40	109.91
8	L	311	2GO	C3D-C4D-ND	2.88	115.88	110.51
8	M	403	2GO	CHD-C1D-ND	-2.88	120.05	124.82
8	M	401	2GO	CED-O2D-CGD	2.87	122.42	115.92
8	L	311	2GO	O2D-CGD-O1D	-2.85	118.31	123.85
8	M	401	2GO	O2A-CGA-CBA	2.83	120.48	111.83
8	M	404	2GO	CMB-C2B-C1B	2.82	129.72	125.42
8	M	401	2GO	C6-C5-C3	-2.80	106.65	113.47
14	M	411	PC1	O21-C21-O22	-2.77	117.23	123.70
13	M	410	CDL	OA6-CA5-OA7	-2.75	117.27	123.70
13	M	410	CDL	OB8-CB7-C71	2.74	120.18	111.83
8	M	402	2GO	O2A-CGA-CBA	2.73	120.17	111.83
8	L	311	2GO	O1D-CGD-CBD	-2.73	119.14	124.52
8	M	403	2GO	CAA-C2A-C1A	2.72	120.90	111.97
8	M	403	2GO	C3D-C4D-ND	2.70	115.54	110.51
8	M	403	2GO	CMD-C2D-C3D	-2.70	121.50	127.69
8	M	404	2GO	C3D-C4D-ND	2.70	115.54	110.51
8	L	305	2GO	CHD-C1D-ND	-2.67	120.40	124.82
8	M	402	2GO	O2A-CGA-O1A	-2.66	116.97	123.63
8	L	305	2GO	C2A-C1A-CHA	-2.66	119.25	123.87
8	M	403	2GO	C4-C3-C2	-2.64	116.85	123.63
14	M	411	PC1	C3-C2-C1	2.64	117.93	111.78
7	L	304[A]	U10	C7-C8-C9	-2.63	122.30	126.83
8	M	402	2GO	C2A-C1A-NA	2.63	114.05	110.99
7	M	408	U10	C17-C18-C19	-2.62	121.62	127.62
8	M	403	2GO	C1-O2A-CGA	2.60	122.94	116.65
8	M	404	2GO	C2A-C1A-CHA	-2.58	119.38	123.87
8	M	401	2GO	O2A-CGA-O1A	-2.57	117.19	123.63
12	M	409	SPO	C27-C26-C25	-2.56	115.79	123.20
8	M	401	2GO	CAA-CBA-CGA	2.56	120.47	113.21
8	M	401	2GO	C3D-C4D-ND	2.56	115.27	110.51
8	M	404	2GO	OBD-CAD-C3D	-2.56	122.44	128.42
8	L	311	2GO	C4D-C3D-CAD	-2.54	105.34	108.11
8	L	311	2GO	CAA-C2A-C1A	2.52	120.23	111.97
12	M	409	SPO	C18-C17-C16	2.52	121.93	118.09
8	M	401	2GO	C2A-C1A-CHA	-2.51	119.51	123.87
8	L	305	2GO	C1D-CHD-C4C	-2.50	120.58	126.62
8	L	305	2GO	C3D-C4D-ND	2.48	115.13	110.51
13	M	410	CDL	OB6-CB5-OB7	-2.48	117.91	123.70
8	M	404	2GO	C1D-CHD-C4C	-2.48	120.65	126.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	401	2GO	C2D-C1D-ND	2.45	114.09	110.35
8	L	311	2GO	O2A-CGA-CBA	2.42	119.22	111.83
8	M	403	2GO	O2A-CGA-CBA	2.42	119.21	111.83
5	H	306	GGD	CB1-OB1-CA3	2.42	123.70	117.98
7	L	304[B]	U10	C16-C14-C15	2.40	120.10	114.59
14	M	411	PC1	O31-C31-C32	2.39	119.12	111.83
8	M	401	2GO	C4-C3-C5	2.38	119.36	115.23
8	M	402	2GO	CHB-C1B-C2B	-2.37	120.55	127.43
5	H	306	GGD	CC6-CC4-CC3	-2.37	106.27	111.78
5	H	306	GGD	OC6-CC5-OC7	-2.36	118.19	123.70
8	M	403	2GO	CHB-C1B-C2B	-2.35	120.59	127.43
13	M	410	CDL	OB8-CB7-OB9	-2.34	117.77	123.63
8	M	402	2GO	O2D-CGD-O1D	-2.34	119.30	123.85
12	M	409	SPO	C13-C12-C11	2.31	121.62	118.09
8	M	402	2GO	C1D-CHD-C4C	-2.30	121.07	126.62
8	M	403	2GO	O1D-CGD-CBD	-2.29	120.00	124.52
8	L	305	2GO	O2D-CGD-O1D	-2.29	119.39	123.85
7	L	304[A]	U10	O2-C2-C3	-2.28	116.21	121.03
7	M	408	U10	C17-C16-C14	-2.27	105.66	113.19
8	M	402	2GO	CBB-CAB-C3B	-2.22	115.73	120.40
8	L	305	2GO	C1-O2A-CGA	2.21	122.00	116.65
7	M	408	U10	C41-C39-C40	2.19	119.63	114.59
8	L	311	2GO	C3B-C2B-C1B	-2.19	99.41	106.40
5	H	306	GGD	CA1-OA5-CA5	2.18	117.98	113.72
8	L	305	2GO	C4C-NC-C1C	-2.18	104.42	106.91
8	M	404	2GO	CAA-C2A-C1A	2.18	119.11	111.97
7	L	304[B]	U10	C12-C13-C14	-2.17	120.39	127.64
8	M	404	2GO	CBB-CAB-C3B	-2.17	115.82	120.40
8	M	403	2GO	CHC-C4B-NB	-2.17	120.49	124.24
8	L	311	2GO	CAB-C3B-C2B	-2.17	123.24	127.74
12	M	409	SPO	C29-C28-C30	2.15	118.97	115.23
8	M	404	2GO	CHB-C1B-C2B	-2.15	121.19	127.43
7	M	408	U10	C21-C19-C18	-2.13	116.38	121.17
8	L	305	2GO	CMD-C2D-C3D	-2.13	122.80	127.69
7	M	408	U10	C32-C31-C29	2.13	120.23	113.19
8	M	401	2GO	CHC-C4B-C3B	-2.12	123.29	131.72
12	M	409	SPO	C31-C32-C33	-2.10	122.81	127.62
8	M	403	2GO	O2A-CGA-O1A	-2.09	118.41	123.63
8	L	305	2GO	CHC-C4B-C3B	-2.08	123.46	131.72
12	M	409	SPO	C14-C15-C16	-2.07	117.20	123.20
8	L	305	2GO	OBD-CAD-C3D	-2.06	123.59	128.42
7	L	304[A]	U10	C3M-O3-C3	2.05	123.68	116.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	405	LDA	O1-N1-C1	2.03	114.26	109.27
8	L	305	2GO	CHB-C1B-C2B	-2.03	121.53	127.43
8	M	404	2GO	C2D-C1D-ND	2.03	113.44	110.35
8	L	311	2GO	OBB-CAB-CBB	2.02	124.30	119.77
8	M	402	2GO	CMD-C2D-C3D	-2.02	123.07	127.69
5	H	306	GGD	C15-C14-CC5	-2.01	106.33	113.69
12	M	409	SPO	C13-C12-C14	-2.00	119.57	122.82

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	L	305	2GO	ND
8	L	311	2GO	ND
8	M	401	2GO	ND
8	M	402	2GO	ND
8	M	403	2GO	ND
8	M	404	2GO	ND

All (217) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	301	GOL	O1-C1-C2-C3
4	H	302	GOL	C1-C2-C3-O3
4	H	305	GOL	C1-C2-C3-O3
5	H	306	GGD	OC7-CC5-OC6-CC4
5	H	306	GGD	C14-CC5-OC6-CC4
6	M	405	LDA	C2-C1-N1-O1
6	M	405	LDA	C2-C1-N1-CM1
7	L	304[A]	U10	C1-C6-C7-C8
7	L	304[A]	U10	C5-C6-C7-C8
7	M	408	U10	C14-C16-C17-C18
7	M	408	U10	C31-C32-C33-C34
8	L	311	2GO	C2B-C3B-CAB-CBB
8	L	311	2GO	C2B-C3B-CAB-OBB
8	M	401	2GO	CHA-CBD-CGD-O1D
8	M	401	2GO	CHA-CBD-CGD-O2D
8	M	402	2GO	C2B-C3B-CAB-CBB
10	L	307	HTO	O3-C3-C4-C5
12	M	409	SPO	O1-C1-C4-C5
12	M	409	SPO	C2-C1-C4-C5
12	M	409	SPO	C3-C1-C4-C5
13	M	410	CDL	CA2-OA2-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	M	410	CDL	CA3-OA5-PA1-OA2
13	M	410	CDL	CA3-OA5-PA1-OA4
13	M	410	CDL	CB3-OB5-PB2-OB2
13	M	410	CDL	CB3-OB5-PB2-OB3
14	M	411	PC1	C11-O13-P-O11
14	M	411	PC1	C1-O11-P-O12
14	M	411	PC1	C1-O11-P-O14
14	M	411	PC1	C1-O11-P-O13
14	M	411	PC1	C22-C21-O21-C2
13	M	410	CDL	OA9-CA7-OA8-CA6
13	M	410	CDL	OB7-CB5-OB6-CB4
13	M	410	CDL	C31-CA7-OA8-CA6
13	M	410	CDL	C71-CB7-OB8-CB6
5	H	306	GGD	CA2-CA3-OB1-CB1
8	L	311	2GO	CBD-CGD-O2D-CED
13	M	410	CDL	C51-CB5-OB6-CB4
7	M	408	U10	C30-C29-C31-C32
8	M	403	2GO	CBA-CGA-O2A-C1
8	M	403	2GO	O1A-CGA-O2A-C1
13	M	410	CDL	OB9-CB7-OB8-CB6
14	M	411	PC1	O22-C21-O21-C2
7	M	408	U10	C28-C29-C31-C32
7	L	304[B]	U10	C9-C11-C12-C13
7	M	408	U10	C34-C36-C37-C38
8	M	403	2GO	CBD-CGD-O2D-CED
5	H	306	GGD	OB5-CB5-CB6-OB6
8	L	311	2GO	O1D-CGD-O2D-CED
7	L	304[B]	U10	C12-C11-C9-C10
7	L	304[B]	U10	C12-C11-C9-C8
8	M	403	2GO	C6-C7-C8-C9
8	M	403	2GO	C11-C12-C13-C14
5	H	306	GGD	CB4-CB5-CB6-OB6
13	M	410	CDL	C57-C58-C59-C60
4	H	302	GOL	O2-C2-C3-O3
7	L	304[A]	U10	C9-C11-C12-C13
7	M	408	U10	C19-C21-C22-C23
13	M	410	CDL	CA5-C11-C12-C13
13	M	410	CDL	CB5-C51-C52-C53
8	M	401	2GO	C13-C15-C16-C17
14	M	411	PC1	C31-C32-C33-C34
8	L	311	2GO	C4B-C3B-CAB-CBB
8	L	311	2GO	C4B-C3B-CAB-OB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	L	310	GOL	C1-C2-C3-O3
8	L	311	2GO	O2A-C1-C2-C3
5	H	306	GGD	OA5-CA5-CA6-OA6
6	L	301	LDA	C2-C3-C4-C5
6	M	405	LDA	C2-C3-C4-C5
13	M	410	CDL	C52-C53-C54-C55
14	M	411	PC1	C28-C29-C2A-C2B
5	H	306	GGD	C33-C34-C35-C36
5	H	306	GGD	C31-CC7-OC8-CC6
6	M	405	LDA	C4-C5-C6-C7
13	M	410	CDL	C31-C32-C33-C34
4	H	301	GOL	O1-C1-C2-O2
4	H	305	GOL	O2-C2-C3-O3
8	M	403	2GO	C11-C12-C13-C15
8	M	403	2GO	O1D-CGD-O2D-CED
7	M	408	U10	C29-C31-C32-C33
14	M	411	PC1	C27-C28-C29-C2A
13	M	410	CDL	C11-C12-C13-C14
14	M	411	PC1	C11-C12-N-C15
6	M	405	LDA	C11-C10-C9-C8
6	M	406	LDA	C3-C4-C5-C6
6	M	406	LDA	C11-C10-C9-C8
10	L	307	HTO	O1-C1-C2-O2
13	M	410	CDL	C71-C72-C73-C74
6	L	303	LDA	C7-C8-C9-C10
5	H	306	GGD	OC9-CC7-OC8-CC6
13	M	410	CDL	C58-C59-C60-C61
6	L	303	LDA	C1-C2-C3-C4
14	M	411	PC1	C29-C2A-C2B-C2C
13	M	410	CDL	C38-C39-C40-C41
8	L	311	2GO	C5-C6-C7-C8
8	M	403	2GO	C6-C7-C8-C10
6	M	405	LDA	C6-C7-C8-C9
5	H	306	GGD	C35-C36-C37-C38
8	M	403	2GO	C10-C11-C12-C13
6	M	405	LDA	C7-C8-C9-C10
13	M	410	CDL	C59-C60-C61-C62
7	L	304[B]	U10	C4-C3-O3-C3M
6	L	303	LDA	C4-C5-C6-C7
8	M	402	2GO	O2A-C1-C2-C3
14	M	411	PC1	C3-C2-O21-C21
13	M	410	CDL	OA5-CA3-CA4-OA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	L	301	LDA	C5-C6-C7-C8
5	H	306	GGD	CA4-CA3-OB1-CB1
14	M	411	PC1	C25-C26-C27-C28
6	L	301	LDA	C9-C10-C11-C12
6	M	406	LDA	C9-C10-C11-C12
8	M	403	2GO	C15-C16-C17-C18
14	M	411	PC1	C2B-C2C-C2D-C2E
4	L	309	GOL	O2-C2-C3-O3
8	L	305	2GO	C14-C13-C15-C16
14	M	411	PC1	C2-C1-O11-P
8	L	311	2GO	C6-C7-C8-C10
13	M	410	CDL	C15-C16-C17-C18
14	M	411	PC1	C22-C23-C24-C25
6	L	301	LDA	C4-C5-C6-C7
14	M	411	PC1	C33-C34-C35-C36
13	M	410	CDL	C41-C42-C43-C44
10	L	307	HTO	C4-C5-C6-C7
14	M	411	PC1	C21-C22-C23-C24
14	M	411	PC1	C35-C36-C37-C38
8	M	402	2GO	C13-C15-C16-C17
13	M	410	CDL	OB6-CB4-CB6-OB8
13	M	410	CDL	C51-C52-C53-C54
8	M	402	2GO	C4B-C3B-CAB-CBB
8	M	402	2GO	C4C-C3C-CAC-CBC
4	H	304	GOL	O1-C1-C2-O2
13	M	410	CDL	C13-C14-C15-C16
8	M	403	2GO	C5-C6-C7-C8
13	M	410	CDL	C80-C81-C82-C83
8	M	402	2GO	C2B-C3B-CAB-OB
8	M	404	2GO	C2B-C3B-CAB-OB
14	M	411	PC1	O11-C1-C2-O21
7	M	408	U10	C5-C6-C7-C8
8	M	401	2GO	C11-C10-C8-C9
13	M	410	CDL	C14-C15-C16-C17
6	M	406	LDA	C1-C2-C3-C4
6	L	301	LDA	C2-C1-N1-CM2
6	M	405	LDA	C2-C1-N1-CM2
10	L	307	HTO	C1-C2-C3-O3
14	M	411	PC1	O13-C11-C12-N
13	M	410	CDL	C61-C62-C63-C64
13	M	410	CDL	OA5-CA3-CA4-CA6
14	M	411	PC1	O11-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	M	401	2GO	C12-C13-C15-C16
8	L	311	2GO	C6-C7-C8-C9
14	M	411	PC1	C11-C12-N-C13
13	M	410	CDL	C72-C73-C74-C75
6	L	302	LDA	C4-C5-C6-C7
13	M	410	CDL	CB3-CB4-CB6-OB8
12	M	409	SPO	C4-C1-O1-CM1
6	L	302	LDA	C7-C8-C9-C10
8	M	402	2GO	CHA-CBD-CGD-O1D
8	M	402	2GO	CHA-CBD-CGD-O2D
8	M	403	2GO	CHA-CBD-CGD-O1D
8	M	403	2GO	CHA-CBD-CGD-O2D
13	M	410	CDL	CA3-OA5-PA1-OA3
14	M	411	PC1	C11-O13-P-O14
5	H	306	GGD	CC7-C31-C32-C33
14	M	411	PC1	C37-C38-C39-C3A
8	M	401	2GO	C2B-C3B-CAB-CBB
8	L	311	2GO	C11-C12-C13-C14
5	H	306	GGD	C31-C32-C33-C34
7	L	304[A]	U10	C5-C4-O4-C4M
6	M	406	LDA	N1-C1-C2-C3
8	M	403	2GO	C8-C10-C11-C12
10	L	308	HTO	C3-C4-C5-C6
13	M	410	CDL	C77-C78-C79-C80
12	M	409	SPO	C2-C1-O1-CM1
12	M	409	SPO	C3-C1-O1-CM1
8	M	402	2GO	C8-C10-C11-C12
8	M	404	2GO	C4B-C3B-CAB-OB
8	M	401	2GO	C14-C13-C15-C16
8	L	311	2GO	C4-C3-C5-C6
4	L	309	GOL	C1-C2-C3-O3
6	M	405	LDA	C9-C10-C11-C12
8	M	401	2GO	C2B-C3B-CAB-OB
8	M	404	2GO	C2B-C3B-CAB-CBB
8	M	404	2GO	CAA-CBA-CGA-O2A
8	L	311	2GO	C11-C12-C13-C15
8	M	403	2GO	C4-C3-C5-C6
8	L	311	2GO	C2-C3-C5-C6
8	M	401	2GO	C4B-C3B-CAB-CBB
8	M	404	2GO	C4B-C3B-CAB-CBB
6	L	303	LDA	C5-C6-C7-C8
6	L	303	LDA	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	M	401	2GO	CBD-CGD-O2D-CED
8	M	403	2GO	C3-C5-C6-C7
7	L	304[A]	U10	C12-C11-C9-C10
8	M	404	2GO	C6-C7-C8-C9
6	M	406	LDA	C5-C6-C7-C8
13	M	410	CDL	C11-CA5-OA6-CA4
6	L	302	LDA	C11-C10-C9-C8
8	M	403	2GO	C13-C15-C16-C17
10	L	308	HTO	C1-C2-C3-O3
13	M	410	CDL	C52-C51-CB5-OB6
13	M	410	CDL	C12-C11-CA5-OA6
13	M	410	CDL	OA7-CA5-OA6-CA4
14	M	411	PC1	C34-C35-C36-C37
8	M	404	2GO	C6-C7-C8-C10
7	L	304[A]	U10	C3-C4-O4-C4M
7	L	304[B]	U10	C3-C4-O4-C4M
10	L	307	HTO	C2-C3-C4-C5
13	M	410	CDL	C52-C51-CB5-OB7
7	L	304[B]	U10	C5-C4-O4-C4M
6	L	301	LDA	C2-C1-N1-O1
6	M	406	LDA	C2-C1-N1-O1
12	M	409	SPO	C1-C4-C5-C6
5	H	306	GGD	C17-C18-C19-C20
13	M	410	CDL	C79-C80-C81-C82
8	L	305	2GO	CAD-CBD-CGD-O2D
8	M	404	2GO	CAD-CBD-CGD-O2D
13	M	410	CDL	C12-C11-CA5-OA7
7	M	408	U10	C5-C4-O4-C4M

There are no ring outliers.

15 monomers are involved in 58 short contacts:

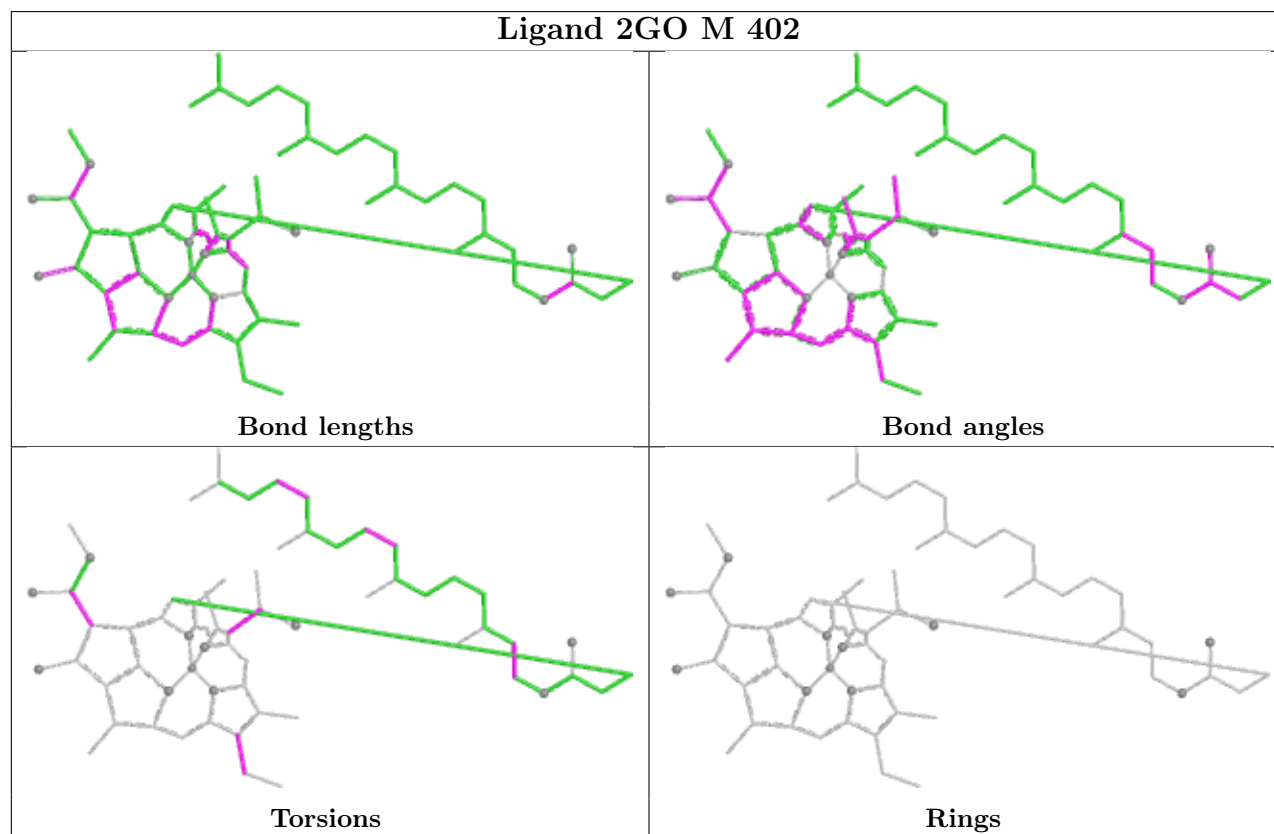
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	402	2GO	11	0
10	L	307	HTO	1	0
7	L	304[A]	U10	4	0
12	M	409	SPO	5	0
8	L	311	2GO	10	0
8	L	305	2GO	3	0
14	M	411	PC1	1	0
8	M	404	2GO	6	0
5	H	306	GGD	1	0

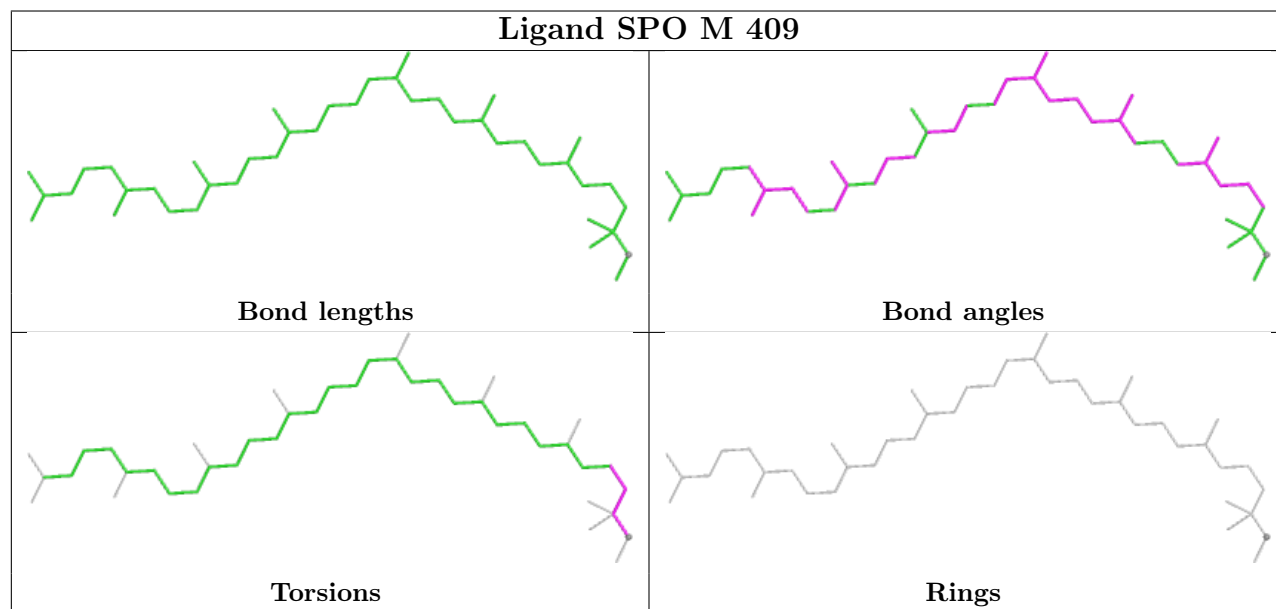
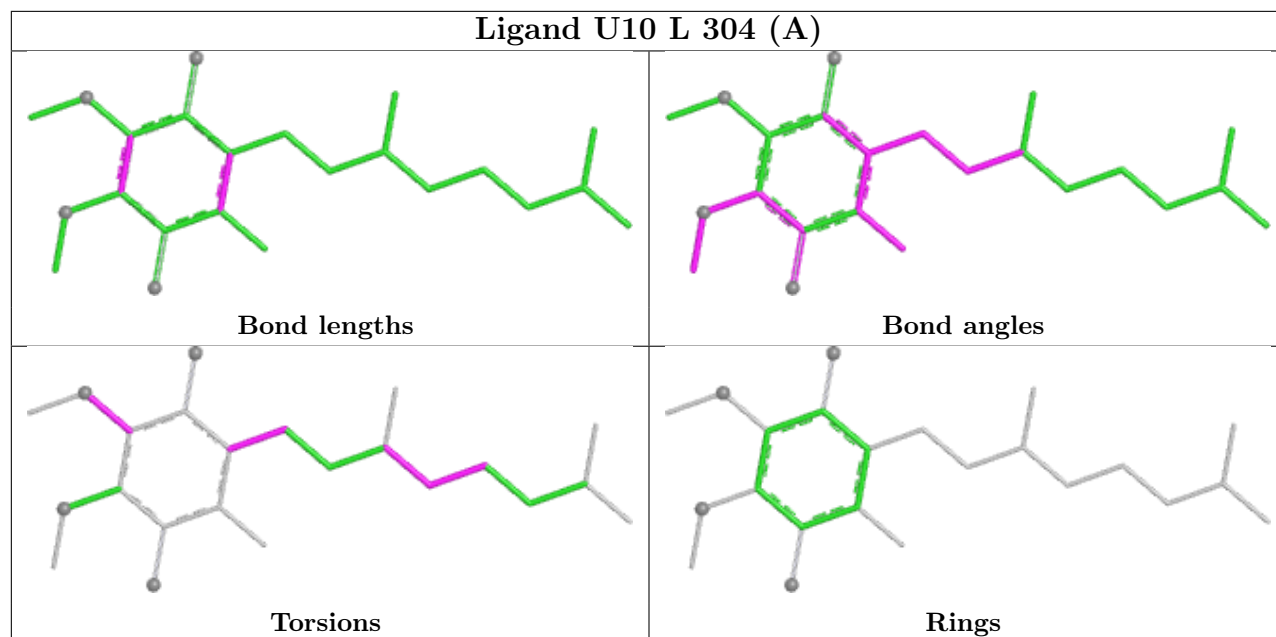
Continued on next page...

Continued from previous page...

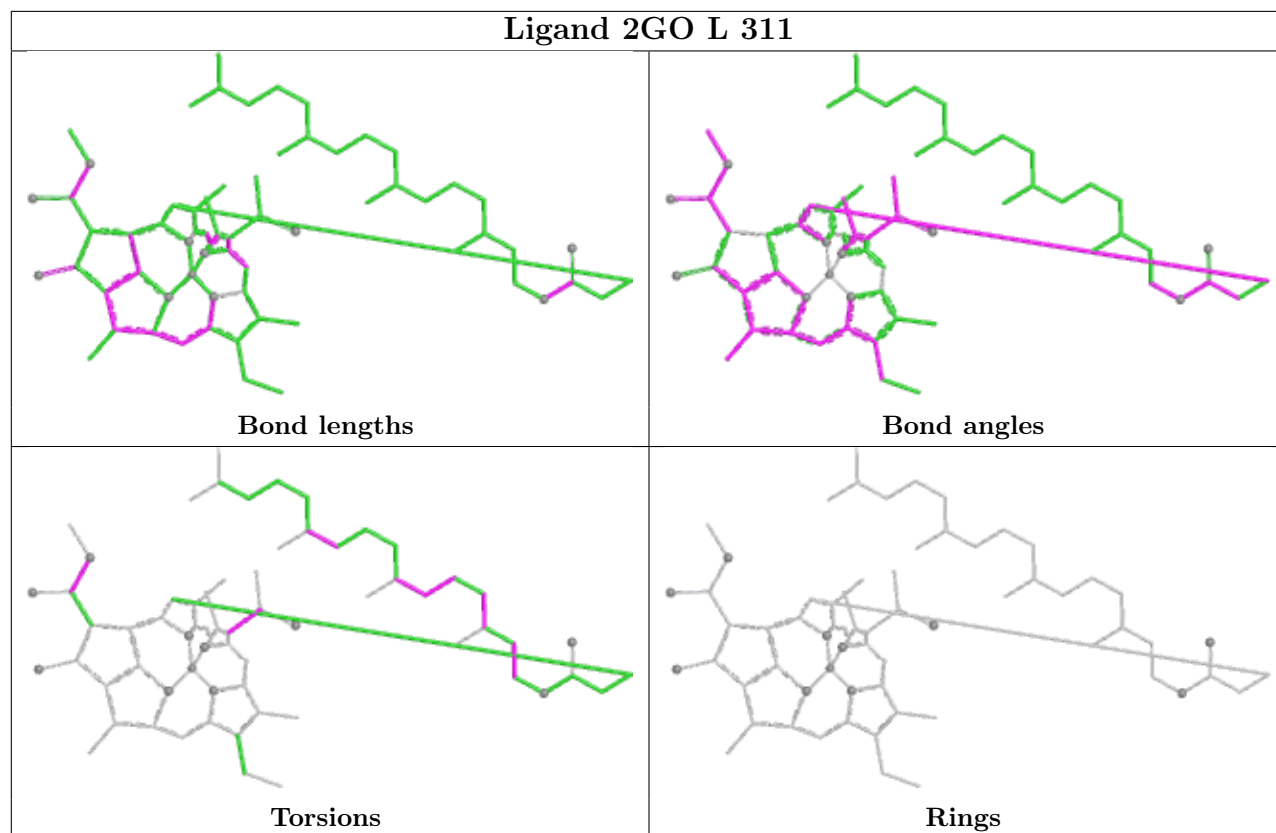
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	305	GOL	1	0
7	M	408	U10	3	0
13	M	410	CDL	1	0
8	M	401	2GO	7	0
8	M	403	2GO	8	0
7	L	304[B]	U10	6	0

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

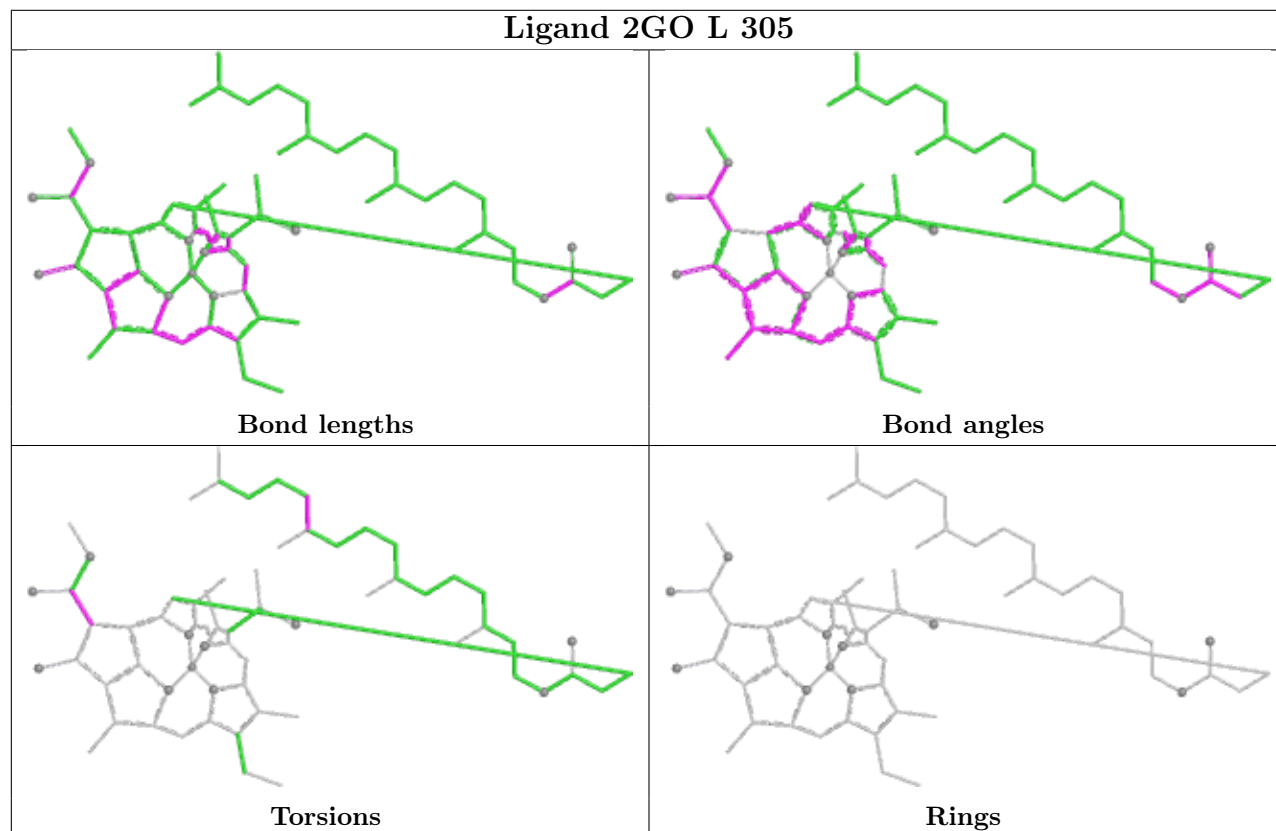


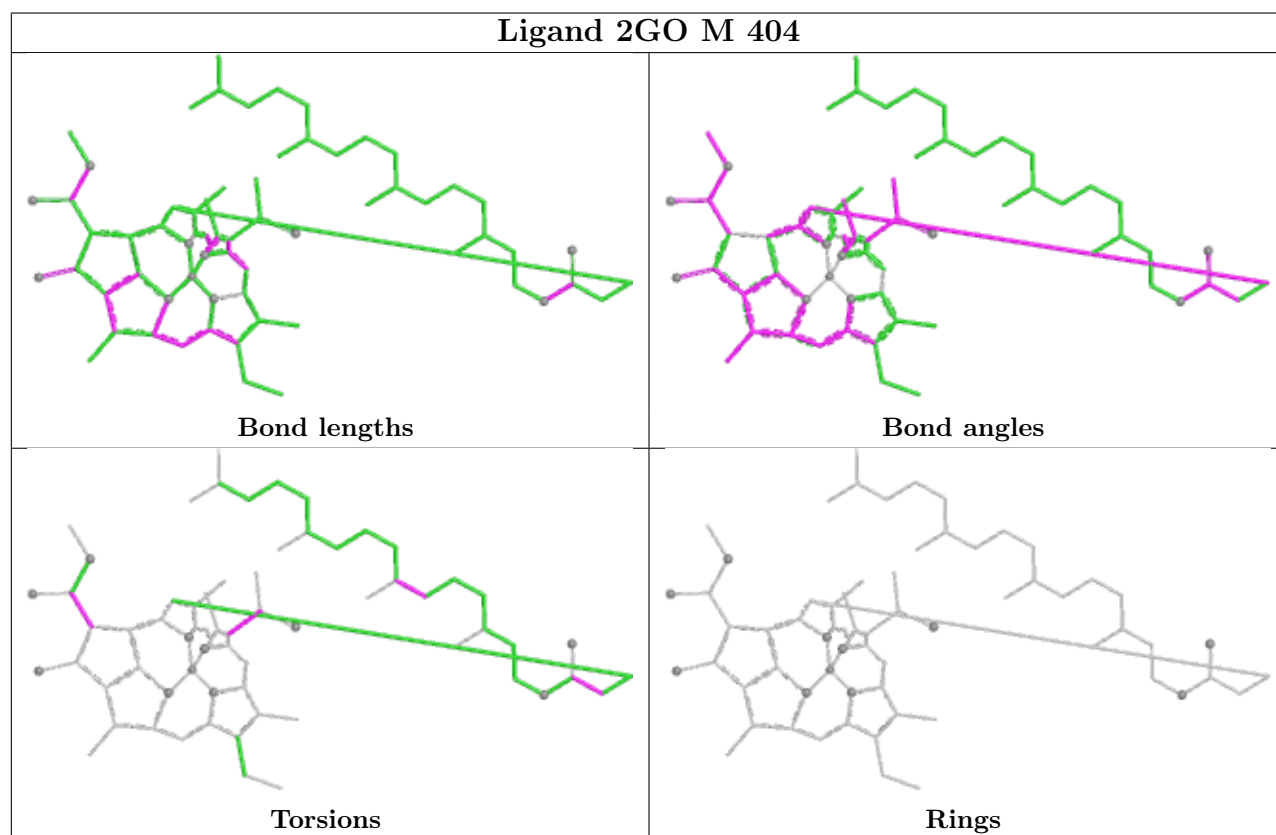
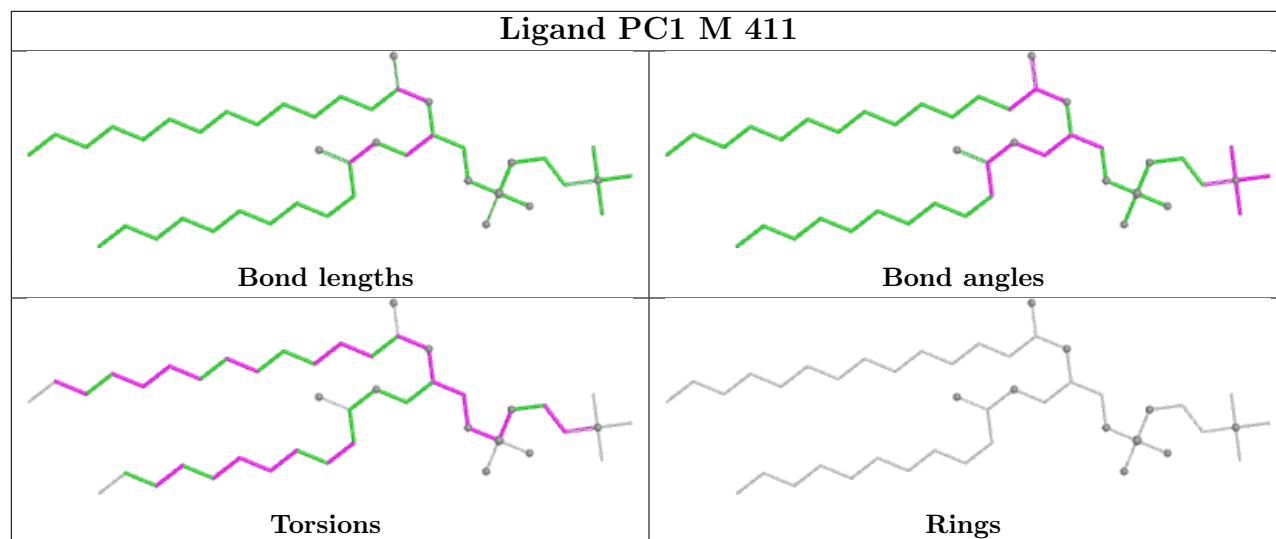


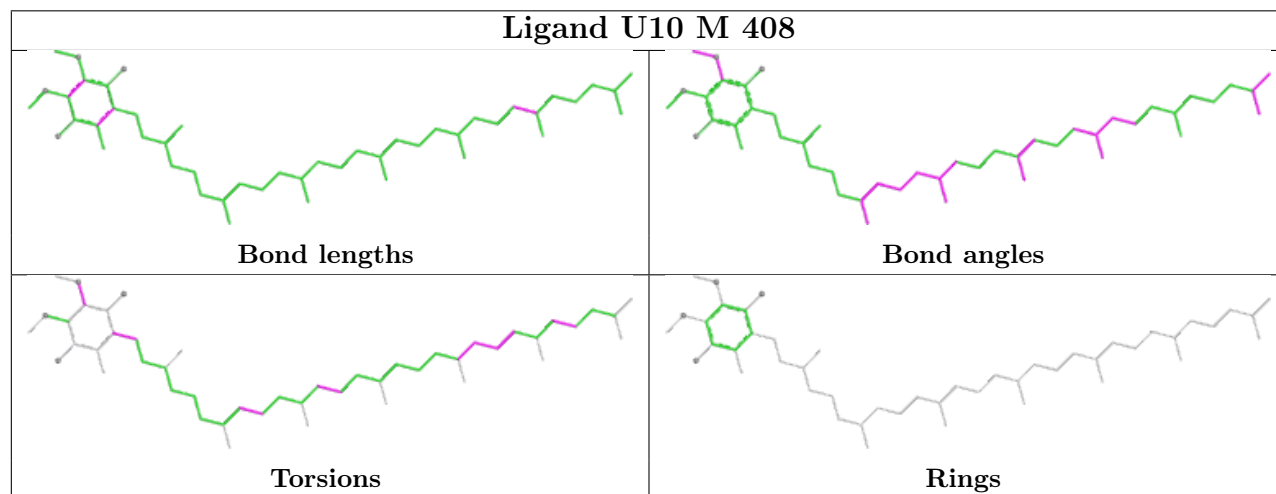
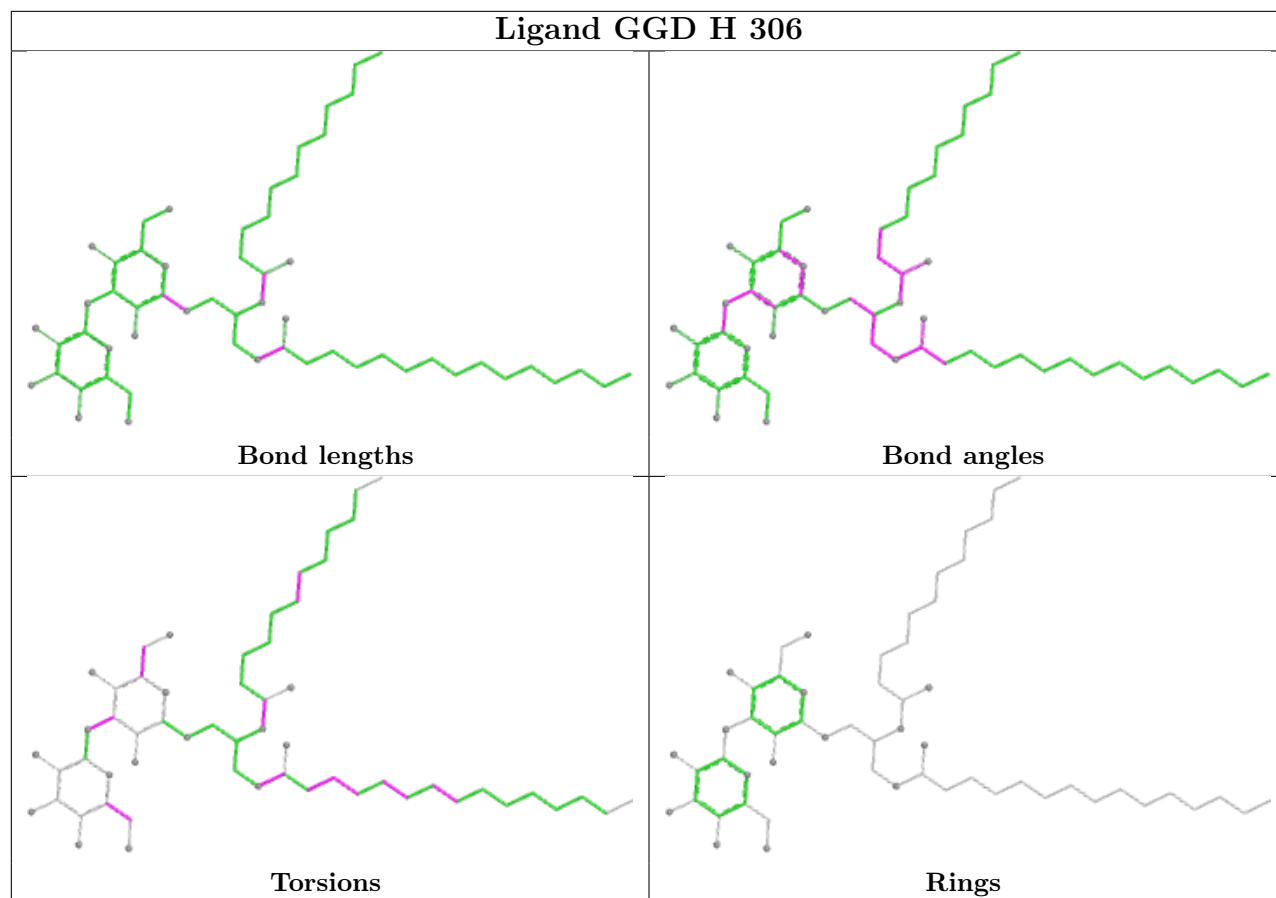
Ligand 2GO L 311

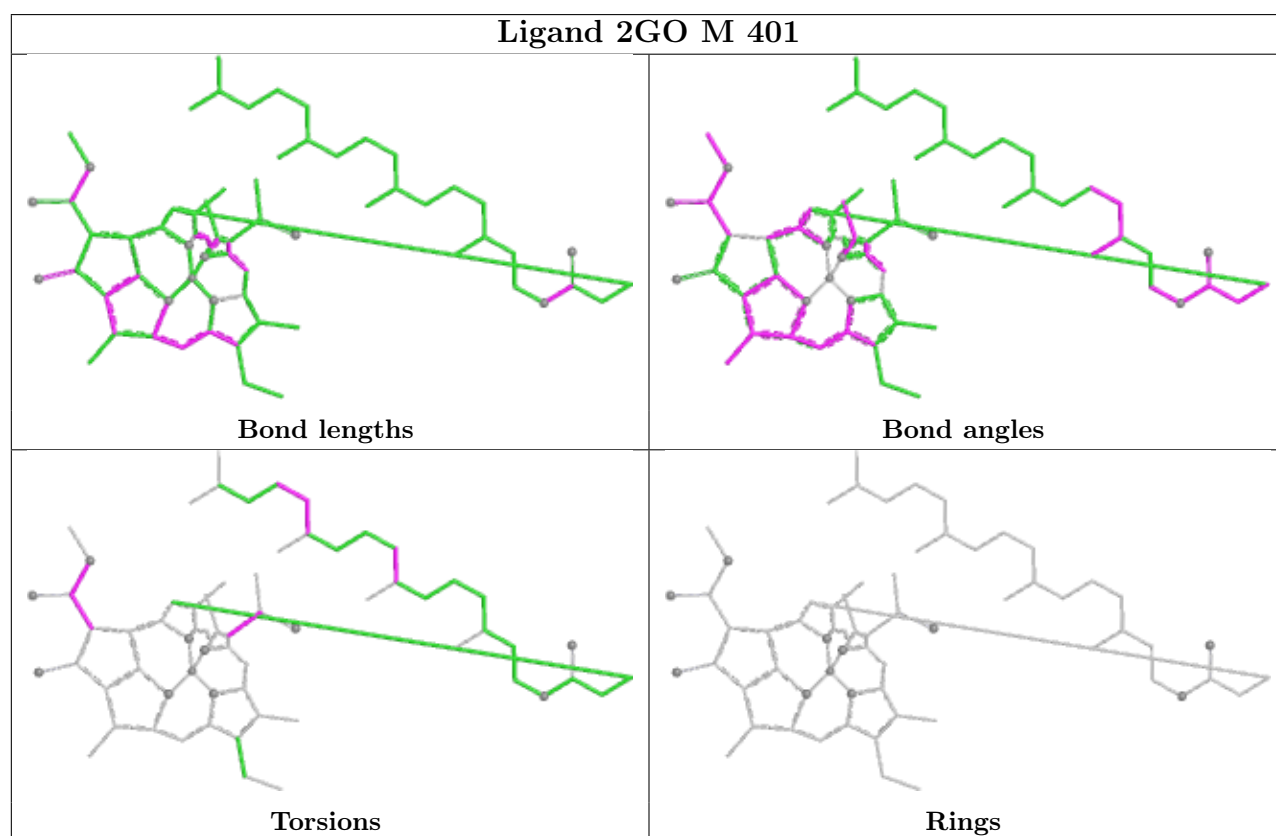
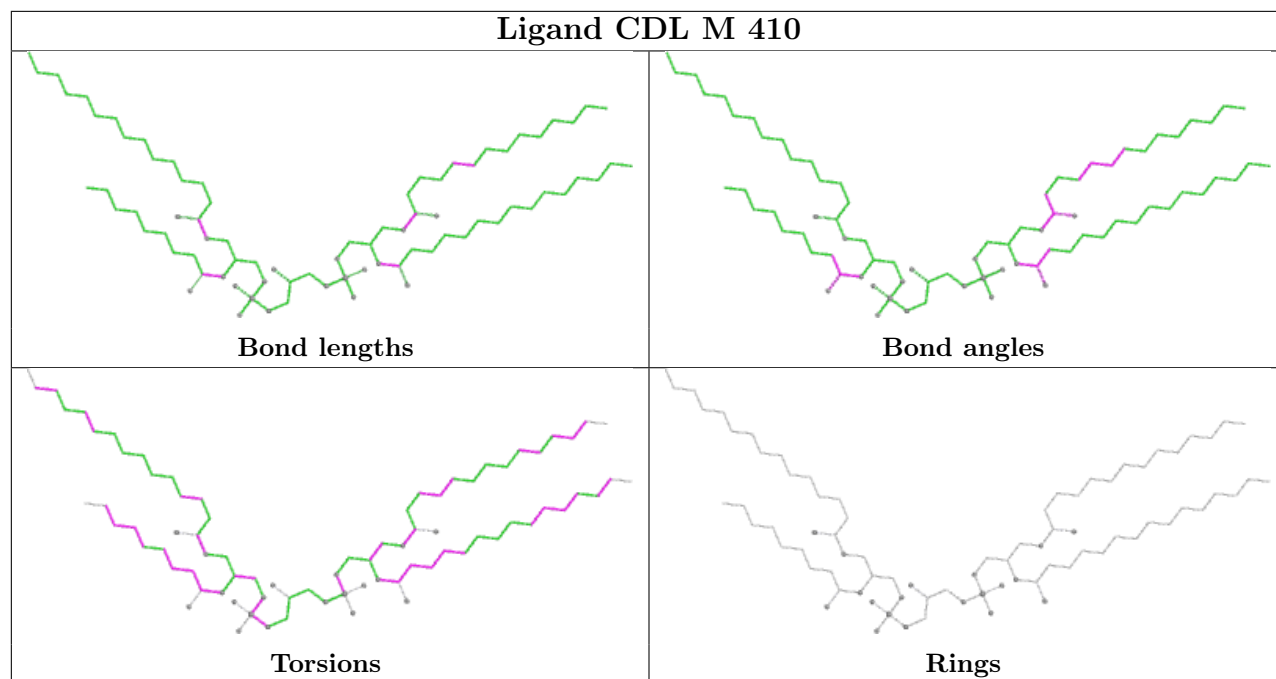


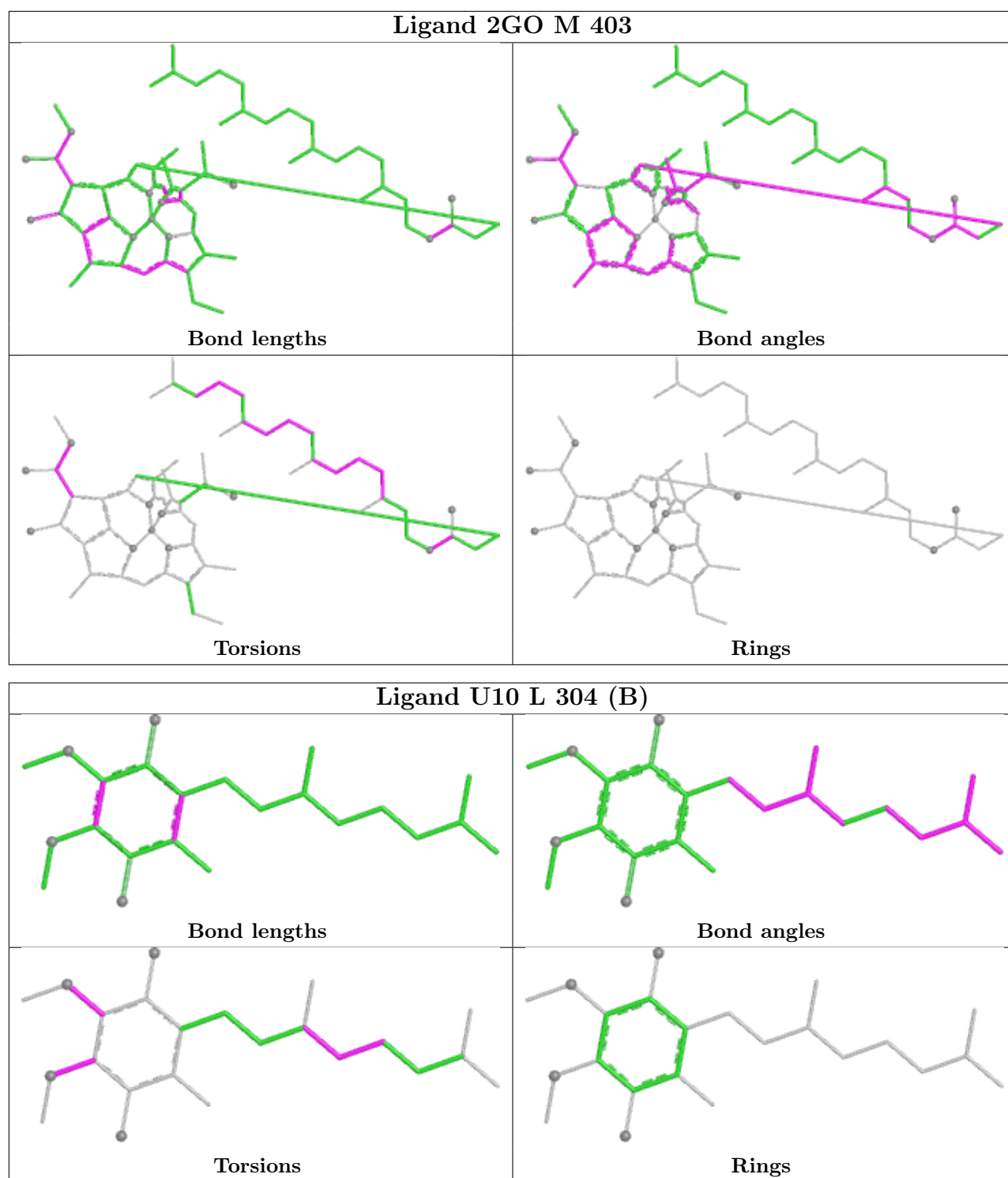
Ligand 2GO L 305











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.46	4 (1%) 69 63	27, 47, 67, 141	8 (3%)
2	L	281/281 (100%)	-0.35	0 100 100	34, 48, 81, 109	2 (0%)
3	M	303/303 (100%)	-0.38	4 (1%) 75 68	31, 50, 77, 92	7 (2%)
All	All	825/825 (100%)	-0.39	8 (0%) 79 74	27, 48, 78, 141	17 (2%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	11.7
3	M	2	GLU	6.7
3	M	301	HIS	3.6
1	H	250	SER	3.0
1	H	249[A]	LYS	2.7
3	M	3	TYR	2.7
1	H	184	LYS	2.6
1	H	247	LYS	2.4

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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,

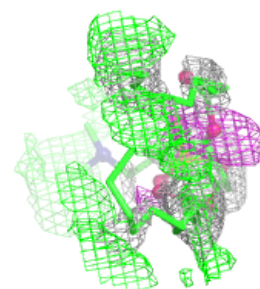
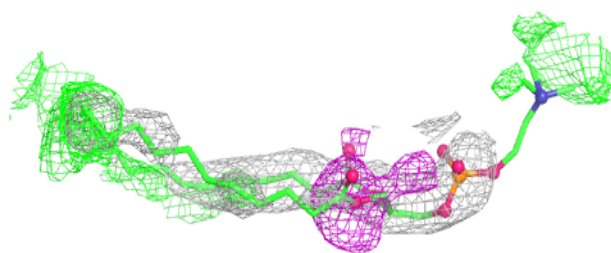
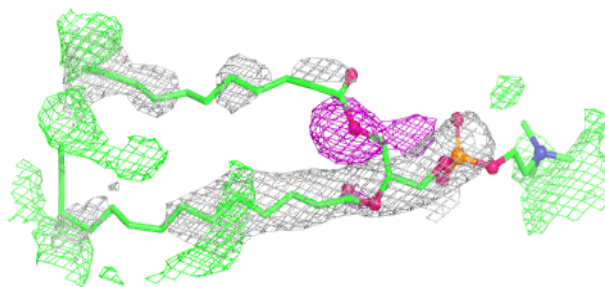
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	HTO	L	308	10/10	0.73	0.27	89,100,116,127	0
14	PC1	M	411	43/54	0.75	0.40	79,115,160,164	0
6	LDA	L	302	16/16	0.80	0.39	74,96,139,142	0
4	GOL	H	301	6/6	0.82	0.25	90,106,116,120	0
5	GGD	H	306	57/67	0.83	0.26	67,132,184,197	0
6	LDA	L	303	16/16	0.85	0.27	70,118,144,144	0
8	2GO	L	311	66/66	0.86	0.27	75,108,133,143	0
4	GOL	H	303	6/6	0.86	0.17	97,113,117,118	0
6	LDA	L	301	16/16	0.86	0.26	63,114,151,153	0
4	GOL	H	304	6/6	0.87	0.15	86,95,99,102	0
10	HTO	L	307	10/10	0.88	0.24	84,101,113,113	0
13	CDL	M	410	81/100	0.89	0.21	64,96,144,149	0
7	U10	M	408	48/63	0.90	0.21	61,76,91,94	0
4	GOL	L	310	6/6	0.90	0.17	88,103,108,112	0
6	LDA	M	406	16/16	0.90	0.18	62,79,106,106	0
6	LDA	M	405	16/16	0.91	0.22	65,86,92,93	0
7	U10	L	304[A]	23/63	0.91	0.28	69,80,92,94	23
7	U10	L	304[B]	23/63	0.91	0.28	38,44,49,52	23
4	GOL	L	309	6/6	0.92	0.14	75,83,84,89	0
9	PO4	L	306	5/5	0.92	0.11	84,87,95,99	0
4	GOL	H	302	6/6	0.93	0.18	66,78,82,86	0
4	GOL	H	305	6/6	0.94	0.15	49,63,73,78	0
12	SPO	M	409	42/42	0.94	0.16	41,59,96,117	0
8	2GO	M	401	66/66	0.98	0.09	28,39,65,78	0
8	2GO	M	402	66/66	0.98	0.08	34,42,55,62	0
8	2GO	M	403	66/66	0.98	0.10	33,41,128,145	0
8	2GO	M	404	66/66	0.98	0.09	39,48,98,121	0
8	2GO	L	305	66/66	0.98	0.09	37,44,61,77	0
11	FE	M	407	1/1	1.00	0.04	40,40,40,40	0

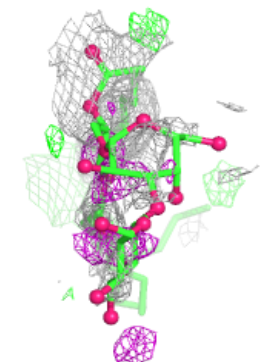
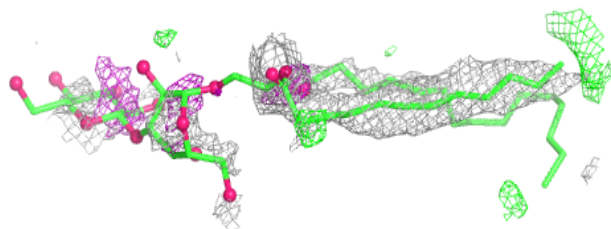
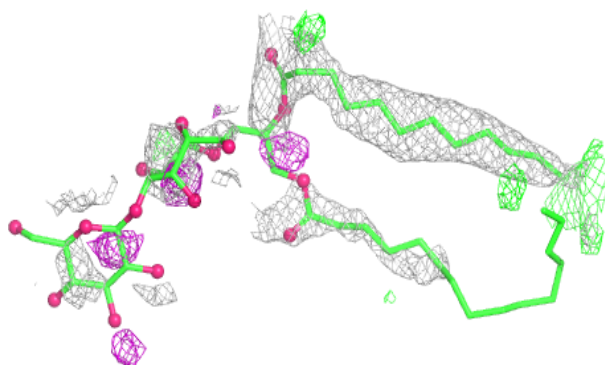
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PC1 M 411:

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

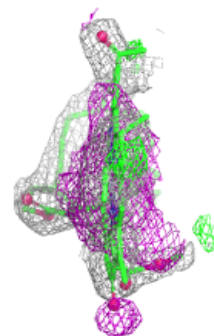
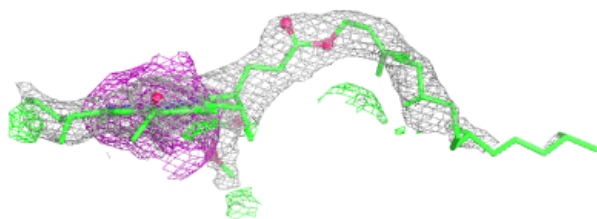
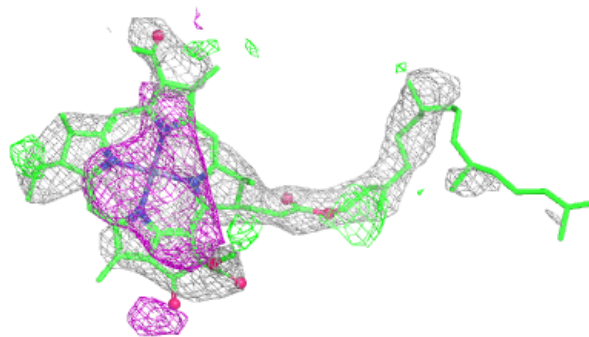
**Electron density around GGD H 306:**

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



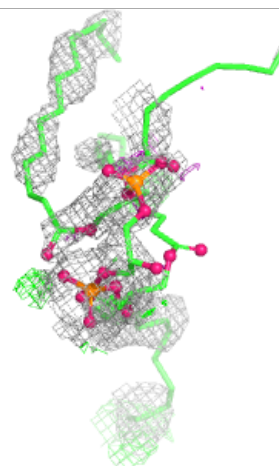
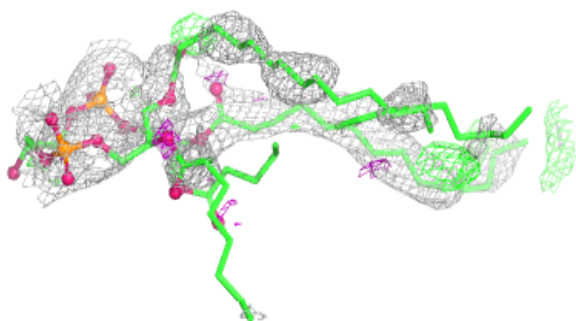
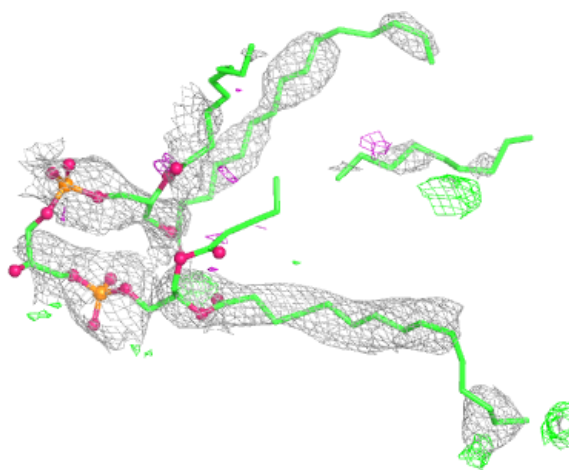
Electron density around 2GO L 311:

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



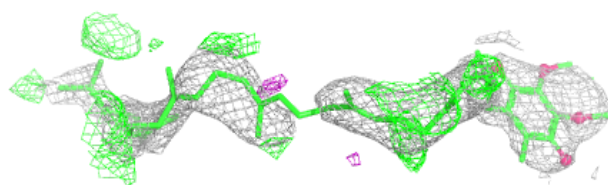
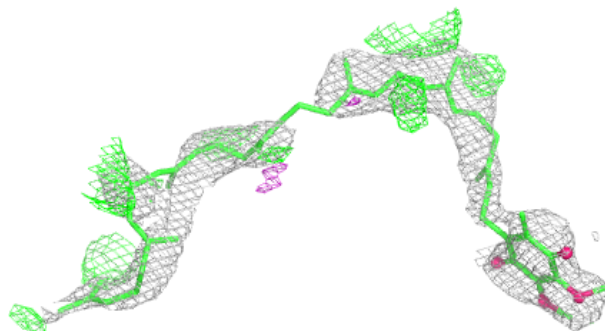
Electron density around CDL M 410:

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

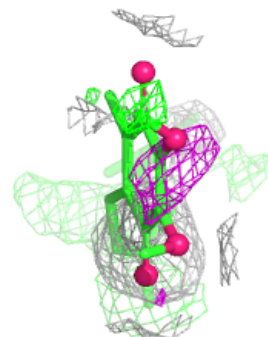
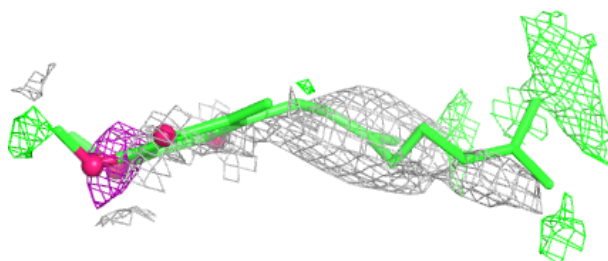
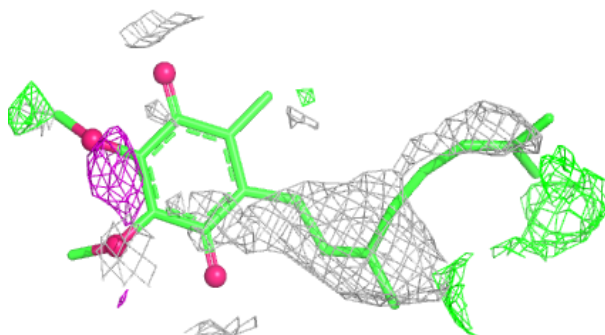


Electron density around U10 M 408:

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

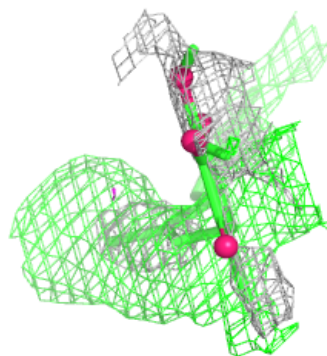
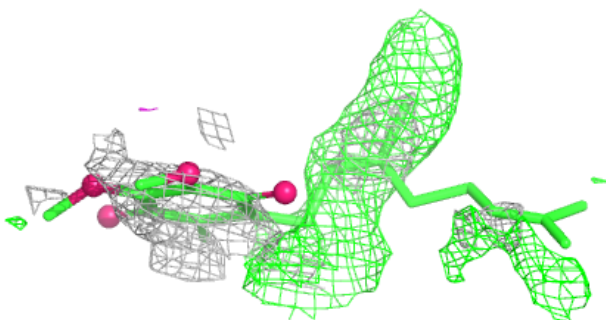
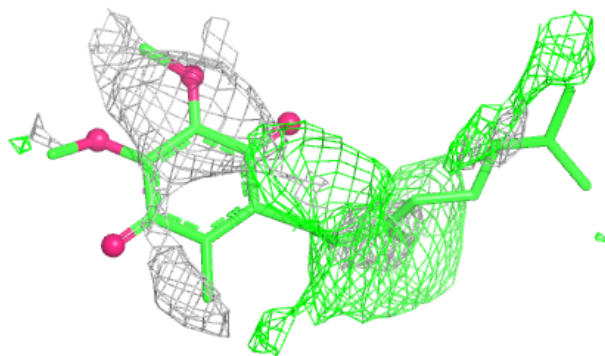
**Electron density around U10 L 304 (A):**

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

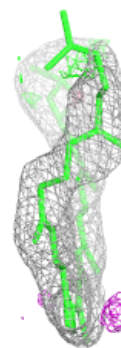
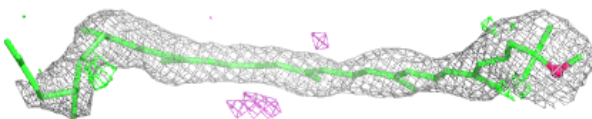
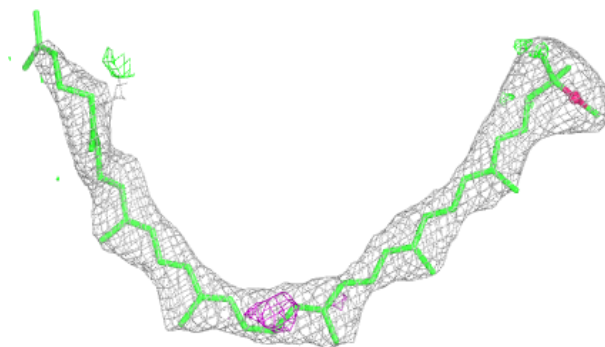


Electron density around U10 L 304 (B):

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

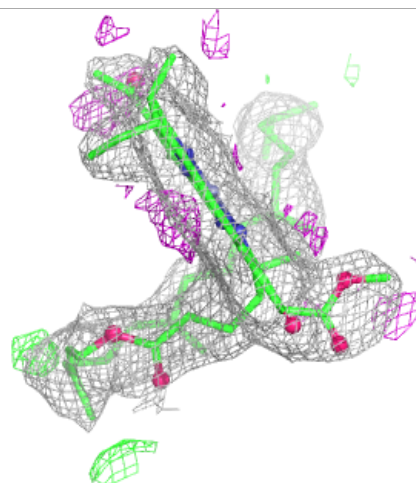
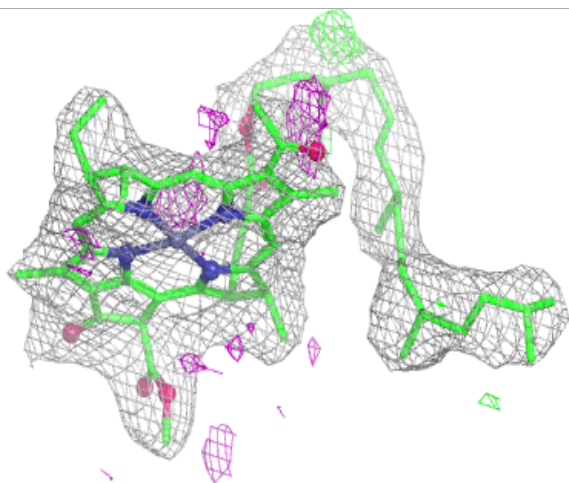
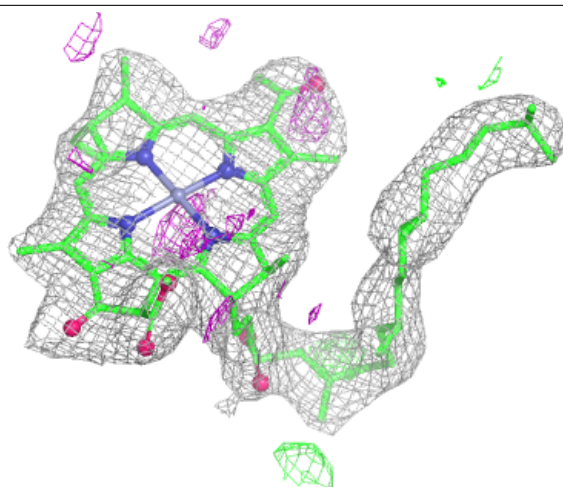
**Electron density around SPO M 409:**

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



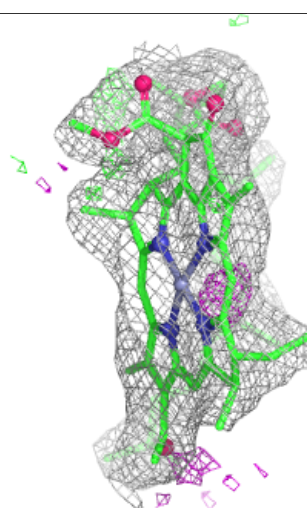
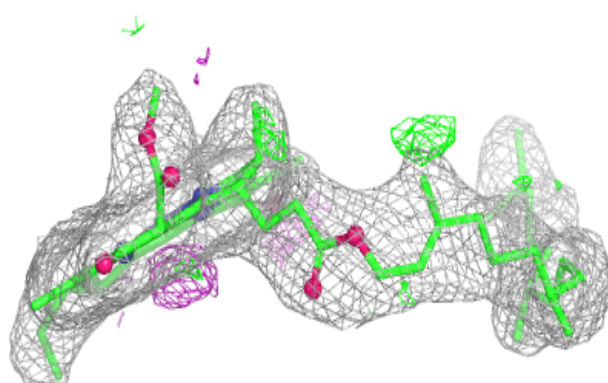
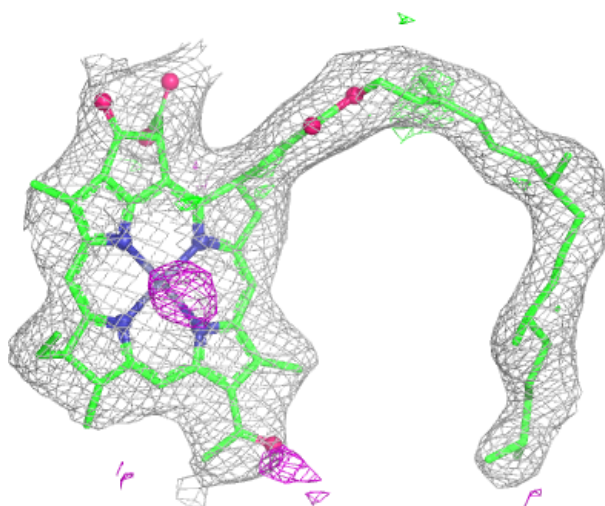
Electron density around 2GO M 401:

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



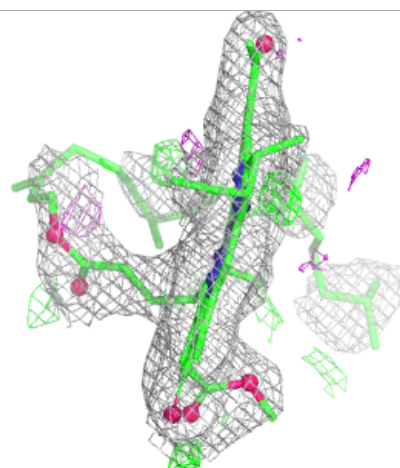
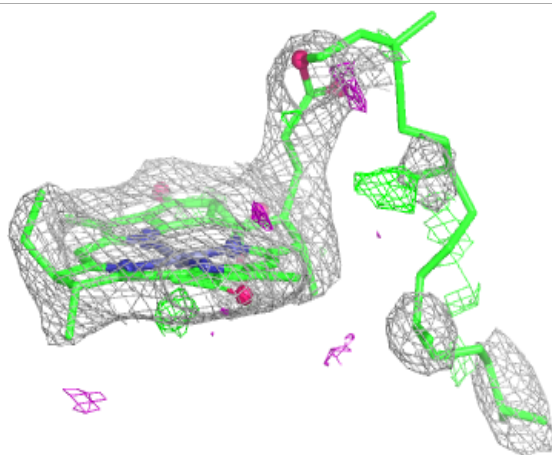
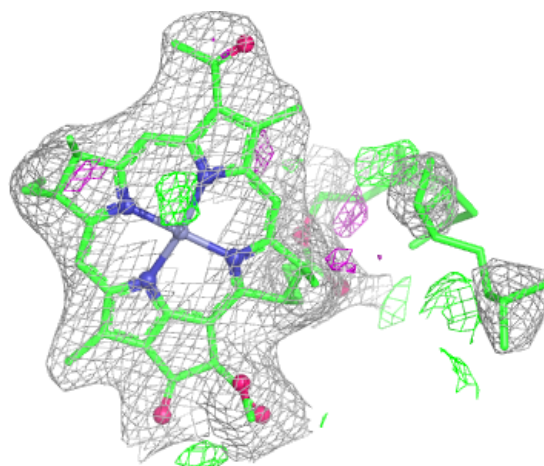
Electron density around 2GO M 402:

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



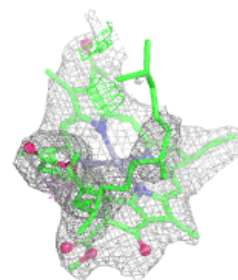
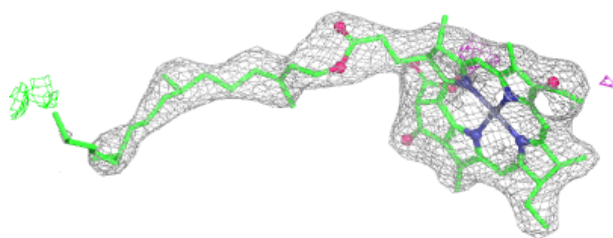
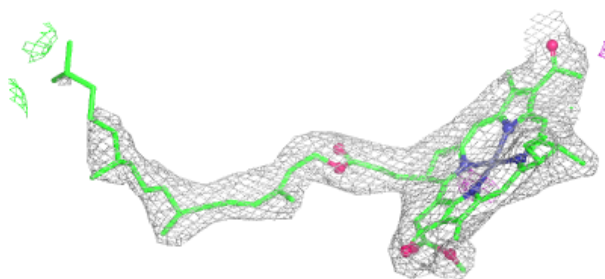
Electron density around 2GO M 403:

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

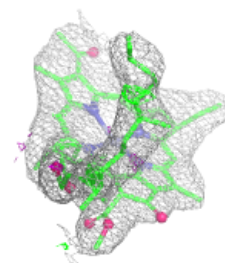
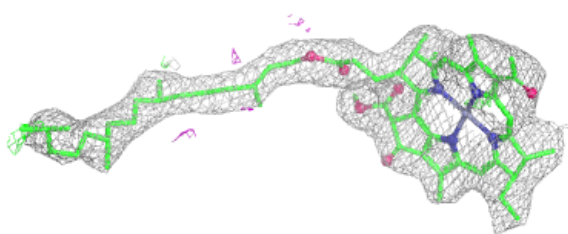
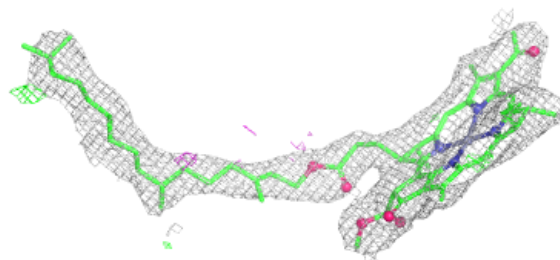


Electron density around 2GO M 404:

$2mF_o-DF_c$ (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.