



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:15 PM UTC

PDB ID : 4N7K / pdb_00004n7k
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 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

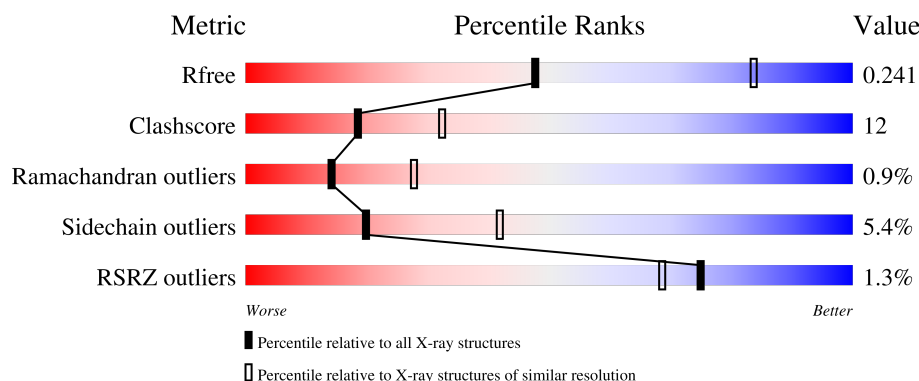
1 Overall quality at a glance

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% 81% 16% .
2	L	281	% 77% 21% .
3	M	303	2% 74% 25% .

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
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.

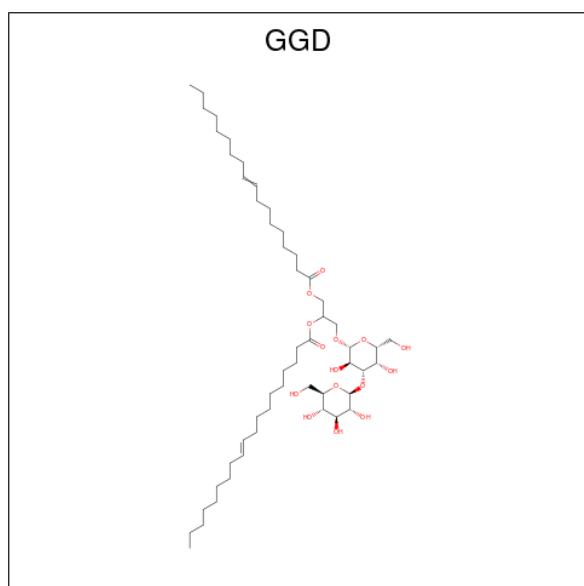
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	1	1
			2411	1607	396	398	10			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



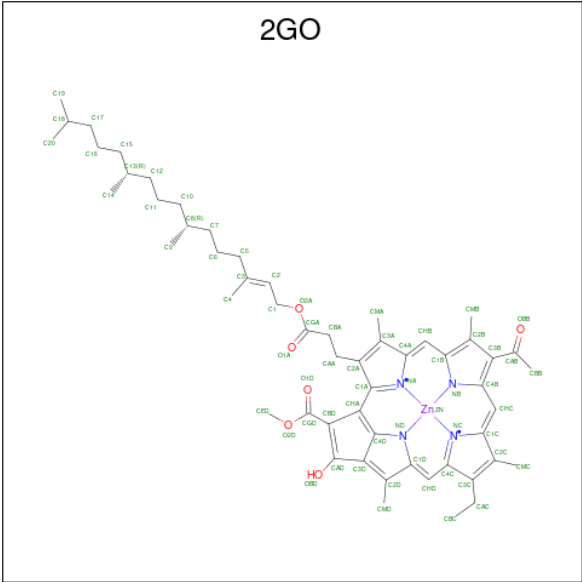
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

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



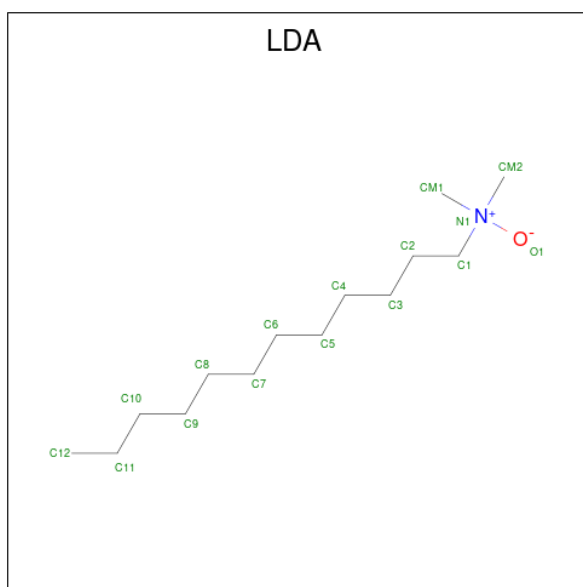
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			57	42	15		

- Molecule 6 is [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 (CCD ID: 2GO) (formula: C₅₅H₇₀N₄O₆Zn).



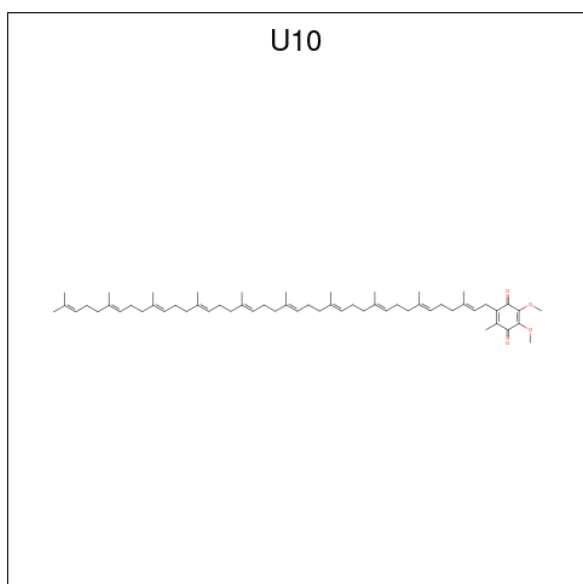
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	N	O	Zn	0	0
			66	55	4	6	1		
6	L	1	Total	C	N	O	Zn	0	0
			66	55	4	6	1		
6	L	1	Total	C	N	O	Zn	0	0
			66	55	4	6	1		
6	M	1	Total	C	N	O	Zn	0	0
			66	55	4	6	1		
6	M	1	Total	C	N	O	Zn	0	0
			66	55	4	6	1		
6	M	1	Total	C	N	O	Zn	0	0
			66	55	4	6	1		

- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



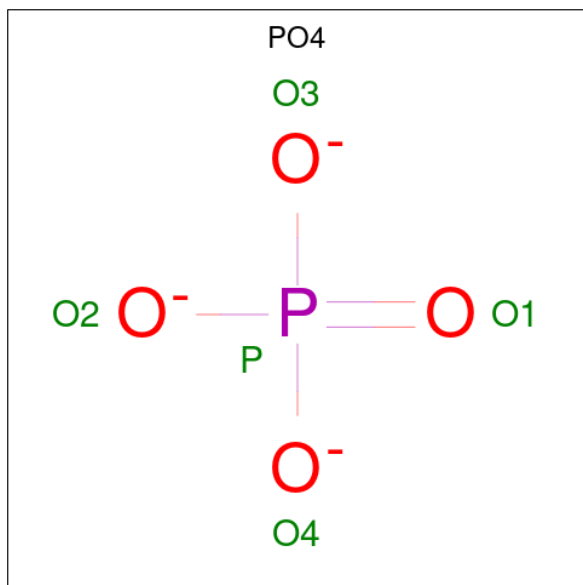
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		

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



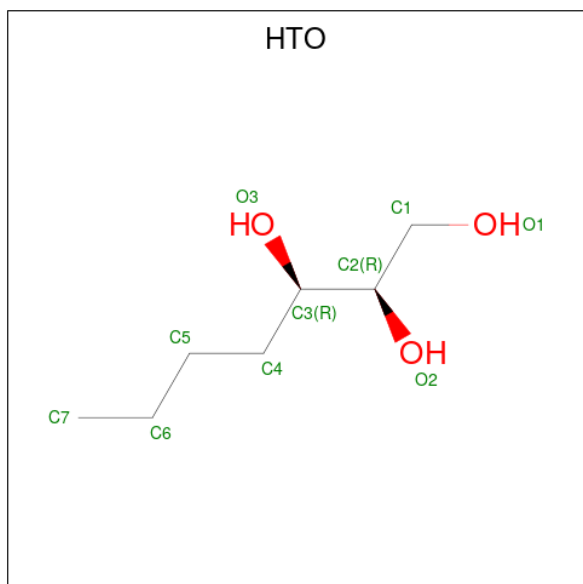
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		
8	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 9 is PHOSPHATE ION (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: $C_7H_{16}O_3$).

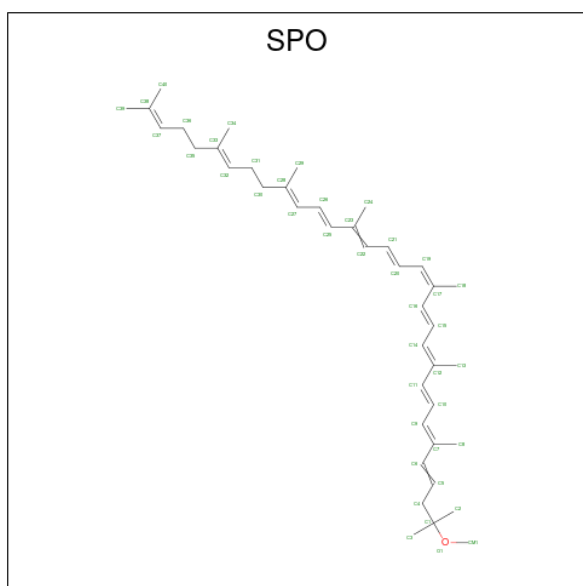


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		
10	L	1	Total	C	O	0	0
			10	7	3		

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

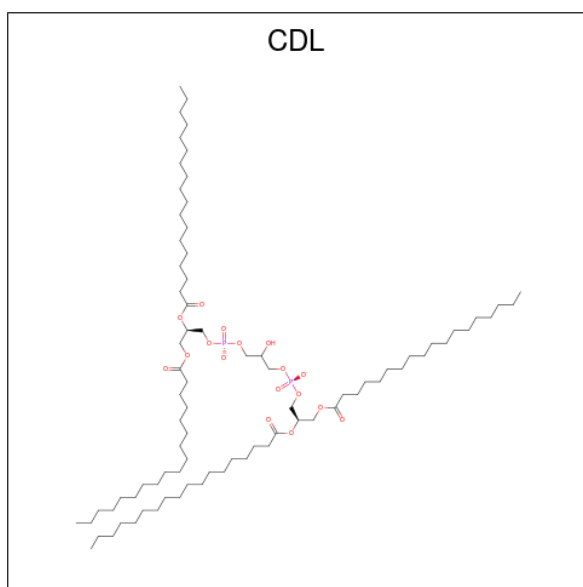
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).



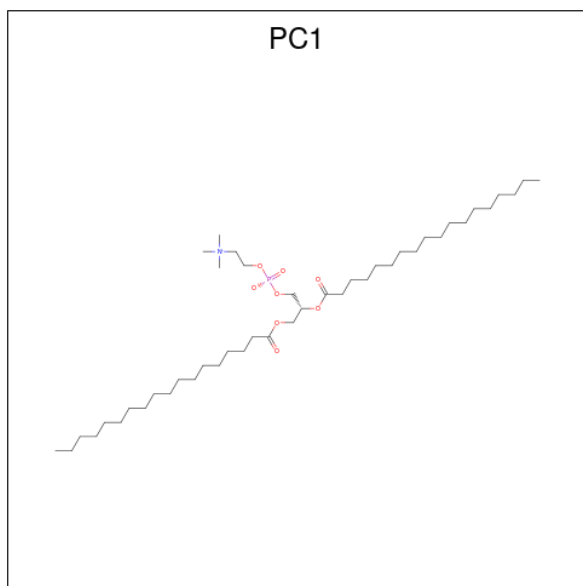
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 13 is CARDIOLIPIN (CCD ID: CDL) (formula: 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 (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		

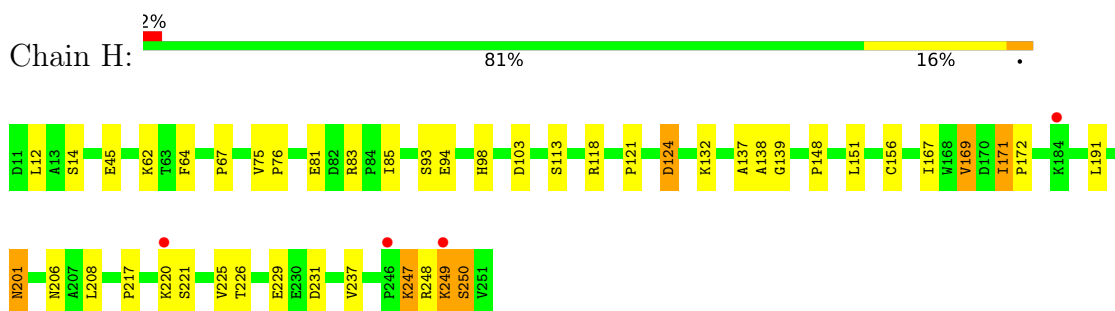
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	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

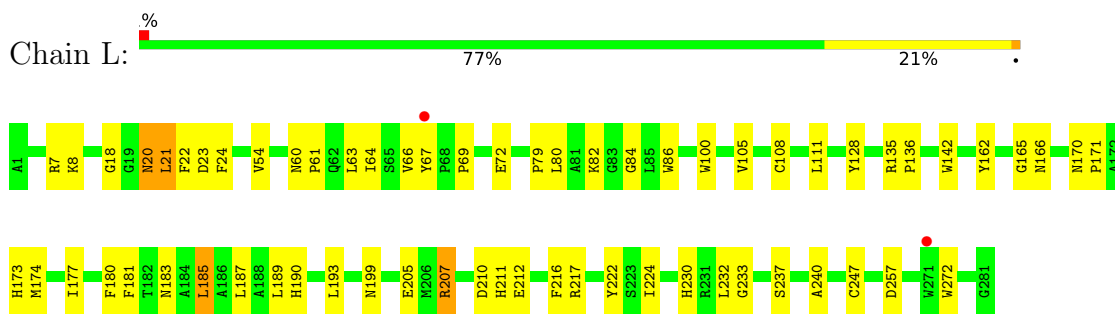
3 Residue-property plots

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.

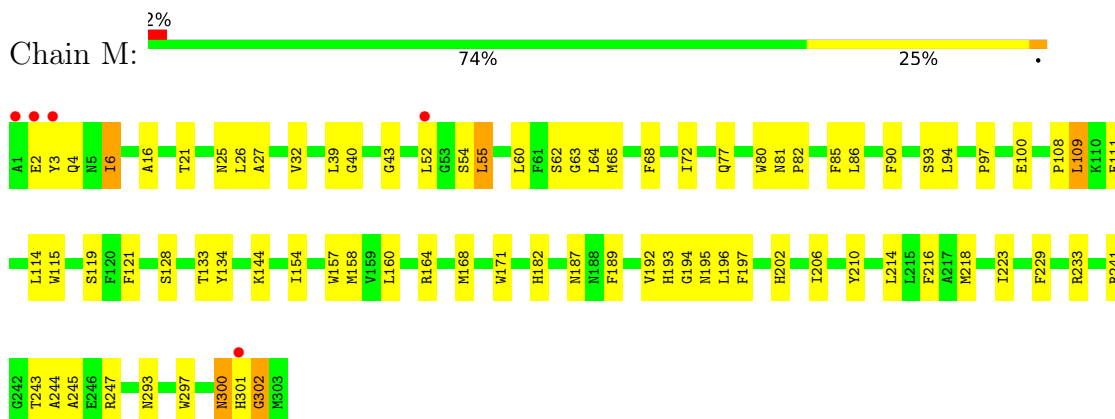
- Molecule 1: Reaction Center H Chain



- 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 36.91 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.0 (36.91-2.85) 96.0 (36.91-2.85)	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 (4.85%)	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)	0.31 , 53.3	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	0.95	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: CDL, PC1, LDA, GOL, GGD, HTO, SPO, U10, PO4, FE, 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	0.76	0/1929	1.04	0/2619
2	L	0.69	0/2339	0.96	1/3203 (0.0%)
3	M	0.72	0/2508	1.02	3/3424 (0.1%)
All	All	0.72	0/6776	1.01	4/9246 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	81	ASN	CA-C-N	9.68	129.31	119.24
3	M	81	ASN	C-N-CA	9.68	129.31	119.24
3	M	160	LEU	N-CA-C	5.95	117.44	111.07
2	L	210	ASP	N-CA-C	-5.71	105.14	111.36

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	63	0
3	M	2411	0	2319	63	0
4	H	24	0	32	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	18	0	24	3	0
5	H	57	0	68	2	0
6	L	198	0	207	15	0
6	M	198	0	207	27	0
7	L	48	0	93	0	0
7	M	32	0	62	1	0
8	L	46	0	46	13	0
8	M	48	0	63	3	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	178	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 (178) 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: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:CBB	6:M:402:2GO:H19	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:174:MET:HE2	6:M:401:2GO:H3	1.63	0.80
3:M:300:ASN:C	3:M:302:GLY:H	1.93	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H19	6:M:402:2GO:H22	1.70	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
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:81:GLU:OE1	2:L:8:LYS:NZ	2.27	0.67
1:H:248:ARG:HA	1:H:249[A]:LYS:HB3	1.76	0.67
3:M:63:GLY:HA3	6:M:406:2GO:H40	1.75	0.67
3:M:108:PRO:HG2	3:M:111:GLU:HB2	1.77	0.67
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:H21	6:M:402:2GO:H19	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:O3	8:L:306[B]:U10:H4M2	1.96	0.63
3:M:189:PHE:O	3:M:193:HIS:HD2	1.81	0.63
6:L:301:2GO:H8	3:M:206:ILE:HD13	1.82	0.62
1:H:132:LYS:HD2	1:H:171:ILE:HD13	1.82	0.62
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
3:M:300:ASN:C	3:M:302:GLY:N	2.56	0.59
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:H21	6:L:301:2GO:H19	1.85	0.59
6:M:401:2GO:H22	6:M:402:2GO:H37	1.84	0.59
1:H:201:ASN:H	1:H:201:ASN:HD22	1.49	0.59
2:L:20:ASN:H	2:L:20:ASN:ND2	1.99	0.58
6:M:402:2GO:H31	6:M:402:2GO:CBD	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
15:H:401:HOH:O	13:M:409:CDL:HA32	2.05	0.57
2:L:190:HIS:HA	8:L:306[A]:U10:O2	2.05	0.57
1:H:62:LYS:HE2	1:H:64:PHE:CZ	2.41	0.56
3:M:218:MET:HE2	8:M:407:U10:H1M1	1.86	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
1:H:75:VAL:HA	1:H:76:PRO:C	2.33	0.54
2:L:22:PHE:HA	2:L:24:PHE:CE2	2.43	0.53
6:L:301:2GO:CMD	3:M:206:ILE:HD13	2.38	0.53
2:L:189:LEU:HD23	6:M:406:2GO:H8	1.91	0.53
3:M:4:GLN:NE2	3:M:4:GLN:HA	2.24	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: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
3:M:189:PHE:O	3:M:193:HIS:CD2	2.62	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
6:L:305:2GO:H19	6:L:305:2GO:CBB	2.38	0.50
3:M:90:PHE:N	3:M:90:PHE:HD1	2.10	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG12	3:M:192:VAL:O	2.12	0.48
2:L:166:ASN:OD1	2:L:166:ASN:C	2.56	0.48
3:M:97:PRO:HG2	3:M:171:TRP:HB2	1.95	0.48
2:L:174:MET:HE2	6:M:401:2GO:CED	2.38	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:H381	13:M:409:CDL:H421	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
2:L:82:LYS:HE2	9:L:308:PO4:O1	2.16	0.46
6:L:301:2GO:H13	6:L:307:2GO:CGA	2.45	0.46
3:M:134:TYR:CE2	3:M:144:LYS:HG3	2.51	0.45
1:H:45:GLU:HG3	1:H:94:GLU:CD	2.41	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
2:L:232:LEU:HD21	8:L:306[B]:U10:H1M2	1.98	0.44
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
3:M:164:ARG:NH2	3:M:168:MET:HE2	2.33	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:173:HIS:CE1	2:L:177:ILE:HD11	2.52	0.44
2:L:177:ILE:HD13	6:M:401:2GO:H8	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O2	8:L:306[B]:U10:H3M3	2.18	0.43
2:L:63:LEU:O	2:L:64:ILE:C	2.62	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:67:PRO:HA	2:L:205:GLU:OE1	2.18	0.42
1:H:124:ASP:HB2	1:H:172:PRO:HG3	2.02	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
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:115:TRP:O	3:M:119:SER:OG	2.37	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
1:H:103:ASP:OD1	1:H:103:ASP:C	2.64	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
3:M:157:TRP:CE3	3:M:158:MET:HG2	2.56	0.41
2:L:79:PRO:O	2:L:80:LEU:C	2.64	0.41
2:L:66:VAL:O	2:L:86:TRP:HD1	2.03	0.40
3:M:40:GLY:HA2	3:M:43:GLY:O	2.21	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:H22	6:L:305:2GO:CHC	2.41	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%)	7	17
2	L	281/281 (100%)	262 (93%)	17 (6%)	2 (1%)	18	35
3	M	302/303 (100%)	277 (92%)	23 (8%)	2 (1%)	18	35
All	All	828/825 (100%)	769 (93%)	51 (6%)	8 (1%)	14	25

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 [i](#)

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%)	12	26
2	L	221/220 (100%)	214 (97%)	7 (3%)	34	59
3	M	237/237 (100%)	222 (94%)	15 (6%)	16	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	657/653 (101%)	620 (94%)	37 (6%)	20	40

All (37) 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	169	VAL
1	H	171	ILE
1	H	191	LEU
1	H	201	ASN
1	H	217	PRO
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	54	VAL
2	L	72	GLU
2	L	185	LEU
2	L	207	ARG
2	L	247	CYS
3	M	6	ILE
3	M	39	LEU
3	M	52	LEU
3	M	54	SER
3	M	55	LEU
3	M	60	LEU
3	M	72	ILE
3	M	94	LEU
3	M	100	GLU
3	M	109	LEU
3	M	133	THR
3	M	154	ILE
3	M	182	HIS
3	M	214	LEU
3	M	300	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
1	H	141	HIS
1	H	201	ASN
2	L	20	ASN
2	L	159	ASN
2	L	183	ASN
2	L	258	GLN
3	M	4	GLN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	300	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
6	2GO	M	401	3	73,74,74	2.25	23 (31%)	91,115,115	3.43	34 (37%)
4	GOL	H	303	-	5,5,5	0.53	0	5,5,5	0.45	0
8	U10	M	407	-	48,48,63	1.51	4 (8%)	60,61,79	1.52	12 (20%)
7	LDA	L	302	-	13,15,15	2.00	1 (7%)	14,17,17	0.61	0
14	PC1	M	410	-	42,42,53	1.17	2 (4%)	48,50,61	2.48	11 (22%)
4	GOL	H	301	-	5,5,5	0.43	0	5,5,5	0.56	0
8	U10	L	306[A]	-	23,23,63	2.12	2 (8%)	30,31,79	1.41	5 (16%)
7	LDA	L	303	-	13,15,15	1.95	1 (7%)	14,17,17	0.45	0
10	HTO	L	309	-	9,9,9	0.79	0	10,10,10	0.82	0
13	CDL	M	409	-	80,80,99	3.97	5 (6%)	86,92,111	1.27	8 (9%)
6	2GO	M	406	-	73,74,74	2.24	24 (32%)	91,115,115	3.49	39 (42%)
7	LDA	M	404	-	13,15,15	2.07	2 (15%)	14,17,17	0.60	0
5	GGD	H	305	-	58,58,68	1.04	3 (5%)	72,72,82	1.53	12 (16%)
9	PO4	L	308	-	4,4,4	1.03	0	6,6,6	0.40	0
6	2GO	L	307	2	73,74,74	2.22	23 (31%)	91,115,115	3.53	38 (41%)
4	GOL	H	304	-	5,5,5	0.45	0	5,5,5	0.60	0
7	LDA	M	403	-	13,15,15	2.04	1 (7%)	14,17,17	0.71	0
4	GOL	H	302	-	5,5,5	0.80	0	5,5,5	1.11	0
6	2GO	L	305	-	73,74,74	2.34	24 (32%)	91,115,115	3.40	43 (47%)
10	HTO	L	310	-	9,9,9	0.74	0	10,10,10	0.60	0
4	GOL	L	312	-	5,5,5	0.34	0	5,5,5	0.45	0
6	2GO	L	301	2	73,74,74	2.28	23 (31%)	91,115,115	3.47	46 (50%)
8	U10	L	306[B]	-	23,23,63	1.99	2 (8%)	30,31,79	1.36	5 (16%)
12	SPO	M	408	-	41,41,41	0.79	0	47,50,50	1.55	12 (25%)
6	2GO	M	402	3	73,74,74	2.18	25 (34%)	91,115,115	3.70	39 (42%)
7	LDA	L	304	-	13,15,15	2.00	1 (7%)	14,17,17	0.63	0
4	GOL	L	311	-	5,5,5	0.44	0	5,5,5	0.42	0
4	GOL	L	313	-	5,5,5	0.36	0	5,5,5	0.58	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
6	2GO	M	401	3	-	14/41/97/97	-
4	GOL	H	303	-	-	3/4/4/4	-
8	U10	M	407	-	-	9/45/69/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LDA	L	302	-	-	6/13/13/13	-
14	PC1	M	410	-	-	23/46/46/57	-
4	GOL	H	301	-	-	3/4/4/4	-
8	U10	L	306[A]	-	-	3/15/39/87	0/1/1/1
7	LDA	L	303	-	-	5/13/13/13	-
10	HTO	L	309	-	-	6/10/10/10	-
13	CDL	M	409	-	-	50/91/91/110	-
6	2GO	M	406	-	-	20/41/97/97	-
7	LDA	M	404	-	-	6/13/13/13	-
5	GGD	H	305	-	-	12/47/87/97	0/2/2/2
6	2GO	L	307	2	-	7/41/97/97	-
4	GOL	H	304	-	-	2/4/4/4	-
7	LDA	M	403	-	-	4/13/13/13	-
4	GOL	H	302	-	-	2/4/4/4	-
6	2GO	L	305	-	-	18/41/97/97	-
10	HTO	L	310	-	-	3/10/10/10	-
4	GOL	L	312	-	-	4/4/4/4	-
6	2GO	L	301	2	-	13/41/97/97	-
8	U10	L	306[B]	-	-	5/15/39/87	0/1/1/1
12	SPO	M	408	-	-	10/47/47/47	-
6	2GO	M	402	3	-	12/41/97/97	-
7	LDA	L	304	-	-	7/13/13/13	-
4	GOL	L	311	-	-	2/4/4/4	-
4	GOL	L	313	-	-	2/4/4/4	-

All (166) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	409	CDL	C35-C34	33.75	3.19	1.51
8	L	306[A]	U10	C6-C1	8.69	1.50	1.35
8	L	306[B]	U10	C6-C1	8.29	1.50	1.35
8	M	407	U10	C6-C1	7.28	1.48	1.35
7	M	403	LDA	O1-N1	-6.98	1.25	1.42
7	L	304	LDA	O1-N1	-6.96	1.25	1.42
6	L	305	2GO	C2A-C3A	6.96	1.51	1.36
6	L	307	2GO	C3C-C2C	6.96	1.51	1.36
6	L	305	2GO	C3C-C2C	6.91	1.51	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	404	LDA	O1-N1	-6.88	1.25	1.42
7	L	302	LDA	O1-N1	-6.82	1.25	1.42
7	L	303	LDA	O1-N1	-6.78	1.25	1.42
6	L	301	2GO	O2D-CGD	6.76	1.48	1.33
6	L	301	2GO	C3C-C2C	6.69	1.51	1.36
6	M	406	2GO	C2A-C3A	6.68	1.51	1.36
6	L	301	2GO	C2A-C3A	6.62	1.51	1.36
6	L	307	2GO	C2A-C3A	6.46	1.50	1.36
6	M	401	2GO	C3C-C2C	6.32	1.50	1.36
6	L	305	2GO	O2D-CGD	6.24	1.46	1.33
6	M	402	2GO	C2A-C3A	6.06	1.49	1.36
6	M	402	2GO	C3C-C2C	5.87	1.49	1.36
6	M	401	2GO	C2A-C3A	5.63	1.48	1.36
6	M	406	2GO	C3C-C2C	5.62	1.48	1.36
6	M	401	2GO	O2D-CGD	5.45	1.45	1.33
6	L	307	2GO	O2D-CGD	5.38	1.45	1.33
6	M	402	2GO	O2D-CGD	5.20	1.44	1.33
6	M	406	2GO	O2D-CGD	5.10	1.44	1.33
6	L	301	2GO	O2A-CGA	5.07	1.48	1.33
13	M	409	CDL	OB6-CB5	4.99	1.48	1.34
6	M	401	2GO	O2A-CGA	4.95	1.47	1.33
13	M	409	CDL	OB8-CB7	4.89	1.47	1.33
14	M	410	PC1	O31-C31	4.75	1.47	1.33
13	M	409	CDL	OA6-CA5	4.72	1.47	1.34
6	M	406	2GO	O2A-CGA	4.71	1.47	1.33
14	M	410	PC1	O21-C21	4.66	1.47	1.34
13	M	409	CDL	OA8-CA7	4.65	1.46	1.33
6	M	401	2GO	CHD-C1D	4.62	1.47	1.38
6	L	305	2GO	O2A-CGA	4.59	1.46	1.33
6	M	402	2GO	O2A-CGA	4.53	1.46	1.33
6	M	402	2GO	CHD-C1D	4.49	1.47	1.38
6	M	401	2GO	C1A-NA	-4.45	1.28	1.38
6	M	401	2GO	C3D-C4D	-4.44	1.34	1.44
6	L	305	2GO	C4C-C3C	4.42	1.52	1.45
5	H	305	GGD	OC8-CC7	4.41	1.46	1.33
6	L	307	2GO	O2A-CGA	4.34	1.46	1.33
6	L	307	2GO	C1A-NA	-4.31	1.29	1.38
6	M	406	2GO	C3D-C4D	-4.27	1.34	1.44
6	M	402	2GO	C3D-C4D	-4.25	1.34	1.44
5	H	305	GGD	OC6-CC5	4.17	1.46	1.34
6	L	305	2GO	C3D-C4D	-4.15	1.34	1.44
6	L	307	2GO	C3D-C4D	-4.09	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	301	2GO	C1A-NA	-4.07	1.29	1.38
6	L	305	2GO	CHD-C1D	4.04	1.46	1.38
6	M	406	2GO	CHA-C1A	3.98	1.50	1.41
6	M	406	2GO	CHD-C1D	3.95	1.46	1.38
8	M	407	U10	C4-C3	3.93	1.50	1.36
6	L	301	2GO	C3D-C4D	-3.93	1.35	1.44
6	M	401	2GO	CHB-C1B	3.83	1.48	1.39
6	L	301	2GO	CHB-C1B	3.80	1.47	1.39
6	L	305	2GO	C3D-C2D	3.79	1.49	1.39
6	M	401	2GO	CHD-C4C	3.78	1.47	1.39
6	M	406	2GO	CHD-C4C	3.75	1.47	1.39
6	L	305	2GO	CHD-C4C	3.73	1.47	1.39
8	L	306[A]	U10	C4-C3	3.70	1.49	1.36
6	L	305	2GO	C1A-NA	-3.69	1.30	1.38
6	L	305	2GO	C3B-C4B	3.68	1.48	1.41
6	L	305	2GO	CHB-C1B	3.66	1.47	1.39
6	M	401	2GO	C3B-C4B	3.65	1.48	1.41
6	M	401	2GO	C4C-C3C	3.65	1.51	1.45
6	L	307	2GO	C3B-C4B	3.62	1.48	1.41
6	M	402	2GO	CHD-C4C	3.61	1.47	1.39
6	L	301	2GO	C4C-C3C	3.60	1.51	1.45
6	M	406	2GO	CHC-C4B	3.60	1.47	1.39
6	M	406	2GO	CHB-C1B	3.60	1.47	1.39
6	M	406	2GO	C3B-C4B	3.59	1.48	1.41
6	M	406	2GO	C1A-C2A	3.59	1.52	1.45
6	M	406	2GO	C3D-C2D	3.56	1.48	1.39
6	L	301	2GO	C1C-C2C	3.50	1.51	1.44
6	L	307	2GO	CHD-C1D	3.50	1.45	1.38
6	L	307	2GO	CHB-C1B	3.50	1.47	1.39
6	L	305	2GO	C4A-C3A	3.49	1.51	1.44
6	M	406	2GO	C1A-NA	-3.48	1.30	1.38
6	L	305	2GO	C1A-C2A	3.47	1.52	1.45
6	L	307	2GO	C4C-NC	-3.44	1.30	1.37
8	L	306[B]	U10	C4-C3	3.44	1.48	1.36
6	L	301	2GO	C4C-NC	-3.42	1.30	1.37
6	M	401	2GO	C3D-C2D	3.37	1.48	1.39
6	M	406	2GO	C1C-C2C	3.36	1.51	1.44
6	L	301	2GO	C3B-C4B	3.29	1.47	1.41
6	L	301	2GO	C1A-C2A	3.23	1.52	1.45
6	M	402	2GO	CHA-C1A	3.23	1.48	1.41
6	L	305	2GO	CHC-C4B	3.23	1.46	1.39
6	L	307	2GO	CHD-C4C	3.23	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	305	2GO	C1C-C2C	3.21	1.51	1.44
6	L	307	2GO	C1C-C2C	3.20	1.51	1.44
6	L	307	2GO	C3D-C2D	3.20	1.47	1.39
6	M	406	2GO	C4C-C3C	3.20	1.50	1.45
6	M	402	2GO	C1A-NA	-3.17	1.31	1.38
6	M	402	2GO	C1C-NC	-3.17	1.32	1.38
6	M	402	2GO	C3D-C2D	3.14	1.47	1.39
6	M	406	2GO	C4A-C3A	3.14	1.50	1.44
6	M	402	2GO	CHC-C1C	-3.13	1.32	1.38
6	M	401	2GO	C4C-NC	-3.12	1.30	1.37
6	M	401	2GO	C1C-C2C	3.12	1.50	1.44
6	M	402	2GO	C3B-C4B	3.11	1.47	1.41
6	L	307	2GO	C4C-C3C	3.08	1.50	1.45
6	M	402	2GO	C1A-C2A	3.08	1.51	1.45
6	M	406	2GO	C4C-NC	-3.06	1.30	1.37
6	L	301	2GO	C4A-C3A	3.06	1.50	1.44
6	L	307	2GO	C1A-C2A	3.00	1.51	1.45
6	L	307	2GO	C4A-C3A	3.00	1.50	1.44
6	M	402	2GO	CHB-C1B	2.97	1.46	1.39
6	M	401	2GO	CHC-C1C	-2.97	1.32	1.38
6	L	307	2GO	CHB-C4A	-2.97	1.32	1.38
6	M	401	2GO	C1A-C2A	2.96	1.51	1.45
6	M	401	2GO	C4A-C3A	2.96	1.50	1.44
6	M	402	2GO	C4C-NC	-2.94	1.31	1.37
6	M	402	2GO	C4A-C3A	2.93	1.50	1.44
6	M	402	2GO	CHC-C4B	2.91	1.45	1.39
6	L	301	2GO	C3D-C2D	2.89	1.46	1.39
6	L	307	2GO	CHC-C4B	2.84	1.45	1.39
6	L	301	2GO	CHA-C1A	2.84	1.47	1.41
6	L	301	2GO	CHC-C1C	-2.78	1.32	1.38
6	M	402	2GO	CHB-C4A	-2.78	1.32	1.38
6	M	402	2GO	C4C-C3C	2.74	1.49	1.45
6	L	301	2GO	CHD-C4C	2.73	1.45	1.39
6	M	402	2GO	C1C-C2C	2.72	1.50	1.44
6	L	301	2GO	CHD-C1D	2.70	1.43	1.38
6	L	301	2GO	C1B-C2B	2.69	1.49	1.43
6	L	305	2GO	CHA-C1A	2.69	1.47	1.41
6	L	305	2GO	CHC-C1C	-2.66	1.33	1.38
6	L	305	2GO	C4C-NC	-2.63	1.31	1.37
6	M	406	2GO	CHA-C4D	2.61	1.46	1.40
7	M	404	LDA	C1-N1	-2.61	1.48	1.51
6	L	305	2GO	C1B-C2B	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	406	2GO	CHC-C1C	-2.47	1.33	1.38
6	L	301	2GO	C1D-ND	-2.47	1.32	1.38
6	L	307	2GO	CHC-C1C	-2.46	1.33	1.38
6	L	307	2GO	C1B-C2B	2.45	1.48	1.43
6	M	402	2GO	C4B-NB	-2.41	1.32	1.38
6	M	401	2GO	C1D-C2D	2.40	1.50	1.45
8	M	407	U10	C33-C34	2.39	1.38	1.33
6	M	401	2GO	C4B-NB	-2.38	1.33	1.38
6	L	305	2GO	CHA-C4D	2.34	1.46	1.40
6	L	307	2GO	CHA-C1A	2.32	1.46	1.41
6	L	305	2GO	C3D-CAD	2.31	1.49	1.43
8	M	407	U10	C31-C29	2.30	1.56	1.51
6	M	401	2GO	C1B-C2B	2.27	1.48	1.43
6	L	305	2GO	CHB-C4A	-2.27	1.33	1.38
6	M	402	2GO	C1D-ND	-2.26	1.33	1.38
6	M	402	2GO	C1B-C2B	2.25	1.48	1.43
6	M	406	2GO	C1B-C2B	2.24	1.48	1.43
5	H	305	GGD	OA1-CA1	2.22	1.43	1.40
6	L	301	2GO	CHC-C4B	2.20	1.44	1.39
6	M	401	2GO	CHB-C4A	-2.17	1.34	1.38
6	M	406	2GO	C1D-C2D	2.16	1.49	1.45
6	L	301	2GO	CHB-C4A	-2.14	1.34	1.38
6	L	305	2GO	C1D-C2D	2.14	1.49	1.45
6	L	307	2GO	C3D-CAD	2.09	1.49	1.43
6	M	402	2GO	CHA-C4D	2.08	1.45	1.40
6	M	401	2GO	C3D-CAD	2.06	1.49	1.43
6	L	307	2GO	C4B-NB	-2.06	1.33	1.38
6	M	406	2GO	OBD-CAD	-2.06	1.26	1.33
6	L	301	2GO	C4A-NA	-2.05	1.34	1.38
6	M	401	2GO	CHC-C4B	2.05	1.44	1.39
6	M	406	2GO	CHB-C4A	-2.04	1.34	1.38

All (304) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	307	2GO	CAC-C3C-C4C	-12.38	108.68	124.79
6	M	402	2GO	CAA-C2A-C3A	-11.98	105.43	127.87
6	M	402	2GO	CAC-C3C-C4C	-11.71	109.56	124.79
6	M	406	2GO	CAC-C3C-C2C	-11.07	107.22	127.56
6	M	406	2GO	CAC-C3C-C4C	-10.33	111.35	124.79
6	M	402	2GO	CMC-C2C-C1C	-9.70	109.88	125.03
6	M	401	2GO	C2A-C1A-NA	9.64	116.62	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	301	2GO	CMA-C3A-C4A	-9.61	110.01	125.03
6	L	307	2GO	CMC-C2C-C1C	-9.23	110.61	125.03
6	M	406	2GO	CAA-C2A-C3A	-9.12	110.79	127.87
6	M	402	2GO	CAC-C3C-C2C	-8.97	111.08	127.56
14	M	410	PC1	C15-N-C13	-8.97	85.42	108.98
6	L	307	2GO	C4A-C3A-C2A	-8.92	97.60	106.98
6	L	307	2GO	CAA-C2A-C3A	-8.88	111.23	127.87
6	L	305	2GO	CMC-C2C-C1C	-8.83	111.24	125.03
14	M	410	PC1	C15-N-C14	-8.75	85.98	108.98
6	M	401	2GO	CAC-C3C-C2C	-8.71	111.55	127.56
6	L	301	2GO	CAC-C3C-C4C	-8.68	113.49	124.79
6	M	401	2GO	CAA-C2A-C3A	-8.54	111.87	127.87
6	M	406	2GO	CMA-C3A-C4A	-8.47	111.81	125.03
6	L	305	2GO	CMA-C3A-C4A	-8.20	112.22	125.03
6	L	301	2GO	CMC-C2C-C1C	-8.14	112.31	125.03
6	M	401	2GO	CMC-C2C-C1C	-8.05	112.45	125.03
6	L	307	2GO	C2A-C1A-NA	7.93	115.29	109.15
6	M	401	2GO	CAC-C3C-C4C	-7.86	114.56	124.79
6	L	301	2GO	CAA-C2A-C3A	-7.85	113.17	127.87
6	M	401	2GO	CMA-C3A-C4A	-7.77	112.90	125.03
6	M	401	2GO	CMA-C3A-C2A	-7.73	105.24	126.15
6	L	305	2GO	CAC-C3C-C2C	-7.70	113.41	127.56
6	M	402	2GO	CMA-C3A-C4A	-7.68	113.03	125.03
6	L	305	2GO	CAA-C2A-C3A	-7.56	113.71	127.87
6	L	301	2GO	CHD-C4C-C3C	-7.54	113.78	124.77
6	L	305	2GO	CHA-CBD-CAD	-7.49	100.04	107.06
6	M	402	2GO	CHA-CBD-CGD	-7.40	101.44	125.24
6	L	301	2GO	CAC-C3C-C2C	-7.34	114.08	127.56
6	M	401	2GO	C1C-C2C-C3C	-7.33	99.27	106.98
6	M	401	2GO	CMD-C2D-C1D	7.29	137.56	124.73
6	L	305	2GO	C2A-C1A-NA	7.19	114.72	109.15
6	L	305	2GO	C1C-C2C-C3C	-7.04	99.57	106.98
6	M	406	2GO	CMC-C2C-C3C	-6.96	107.32	126.15
6	L	301	2GO	CMD-C2D-C1D	6.94	136.96	124.73
6	M	406	2GO	CHD-C4C-C3C	-6.93	114.67	124.77
6	L	307	2GO	CMD-C2D-C1D	6.92	136.91	124.73
6	L	301	2GO	C1C-C2C-C3C	-6.75	99.88	106.98
6	M	402	2GO	C1C-C2C-C3C	-6.67	99.96	106.98
6	M	402	2GO	C2A-C1A-NA	6.65	114.30	109.15
6	M	402	2GO	CHD-C4C-C3C	-6.63	115.11	124.77
6	L	301	2GO	C2A-C1A-NA	6.61	114.27	109.15
6	L	307	2GO	C1C-C2C-C3C	-6.60	100.04	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	307	2GO	CHD-C4C-C3C	-6.60	115.16	124.77
6	L	305	2GO	CAC-C3C-C4C	-6.59	116.21	124.79
6	M	406	2GO	CHA-CBD-CAD	-6.58	100.90	107.06
6	M	406	2GO	C4A-C3A-C2A	-6.47	100.17	106.98
6	M	406	2GO	CMD-C2D-C1D	6.35	135.91	124.73
6	M	401	2GO	CHA-C1A-C2A	-6.31	118.62	128.14
6	M	402	2GO	CMA-C3A-C2A	-6.21	109.36	126.15
6	M	402	2GO	CMC-C2C-C3C	-6.14	109.53	126.15
6	M	402	2GO	CMD-C2D-C1D	6.12	135.51	124.73
6	L	305	2GO	C4A-C3A-C2A	-6.12	100.54	106.98
6	L	307	2GO	CMA-C3A-C4A	-6.06	115.57	125.03
6	L	307	2GO	CAC-C3C-C2C	-6.03	116.49	127.56
6	L	307	2GO	CAA-C2A-C1A	-5.98	111.54	128.30
13	M	409	CDL	C36-C35-C34	5.98	144.58	114.37
6	M	406	2GO	C1C-C2C-C3C	-5.97	100.70	106.98
6	L	301	2GO	CHA-C1A-C2A	-5.93	119.20	128.14
6	L	305	2GO	CMD-C2D-C1D	5.92	135.15	124.73
6	L	307	2GO	CMA-C3A-C2A	-5.89	110.22	126.15
6	L	305	2GO	C2B-C1B-NB	5.82	116.33	109.02
6	M	401	2GO	C1A-C2A-C3A	-5.82	98.95	106.63
6	L	301	2GO	CMA-C3A-C2A	-5.81	110.44	126.15
8	M	407	U10	C30-C29-C31	5.81	125.31	115.23
6	M	406	2GO	C2B-C1B-NB	5.77	116.26	109.02
6	M	402	2GO	C2B-C1B-NB	5.75	116.24	109.02
6	M	402	2GO	CHA-CBD-CAD	-5.72	101.70	107.06
6	L	301	2GO	CAD-CBD-CGD	-5.68	106.06	126.64
6	M	406	2GO	C2A-C1A-NA	5.67	113.55	109.15
6	L	307	2GO	CHA-CBD-CAD	-5.61	101.80	107.06
6	L	307	2GO	CHA-C1A-C2A	-5.58	119.72	128.14
6	M	401	2GO	CMC-C2C-C3C	-5.57	111.08	126.15
6	M	402	2GO	CAD-CBD-CGD	-5.55	106.52	126.64
14	M	410	PC1	O21-C21-C22	5.55	123.49	111.48
14	M	410	PC1	C15-N-C12	-5.53	87.94	109.91
6	L	305	2GO	CAD-CBD-CGD	-5.50	106.71	126.64
6	M	401	2GO	CHA-CBD-CAD	-5.47	101.94	107.06
6	L	305	2GO	CHA-C1A-C2A	-5.46	119.91	128.14
6	M	402	2GO	CHA-C1A-C2A	-5.44	119.93	128.14
6	L	305	2GO	CAA-C2A-C1A	-5.42	113.12	128.30
6	L	305	2GO	CHD-C4C-C3C	-5.33	117.00	124.77
6	L	301	2GO	C1A-C2A-C3A	-5.32	99.62	106.63
6	L	305	2GO	O2D-CGD-CBD	5.31	121.36	111.82
6	M	406	2GO	CMC-C2C-C1C	-5.30	116.75	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	402	2GO	CAA-C2A-C1A	-5.26	113.56	128.30
6	M	406	2GO	CMA-C3A-C2A	-5.25	111.96	126.15
6	M	406	2GO	CAD-CBD-CGD	-5.24	107.66	126.64
6	L	301	2GO	CAA-C2A-C1A	-5.23	113.66	128.30
6	L	305	2GO	CMA-C3A-C2A	-5.22	112.03	126.15
6	L	301	2GO	CMC-C2C-C3C	-5.20	112.07	126.15
6	M	401	2GO	C2C-C1C-NC	5.19	115.75	109.06
6	L	307	2GO	C2C-C1C-NC	5.11	115.65	109.06
6	L	307	2GO	C2B-C1B-NB	5.10	115.43	109.02
6	L	301	2GO	CHA-CBD-CAD	-5.10	102.28	107.06
6	L	307	2GO	CMC-C2C-C3C	-5.10	112.36	126.15
13	M	409	CDL	OA6-CA5-C11	5.07	122.44	111.48
6	L	305	2GO	C2C-C1C-NC	5.03	115.54	109.06
6	L	301	2GO	C4A-C3A-C2A	-4.94	101.78	106.98
6	L	305	2GO	CMC-C2C-C3C	-4.91	112.88	126.15
6	M	406	2GO	C2C-C1C-NC	4.87	115.33	109.06
6	M	406	2GO	O2D-CGD-CBD	4.85	120.55	111.82
6	M	401	2GO	C4A-C3A-C2A	-4.82	101.91	106.98
6	L	305	2GO	C1A-C2A-C3A	-4.74	100.38	106.63
6	M	402	2GO	C4A-C3A-C2A	-4.72	102.01	106.98
6	M	402	2GO	C4C-C3C-C2C	-4.70	100.05	106.89
6	L	305	2GO	CHA-CBD-CGD	-4.69	110.17	125.24
6	M	401	2GO	CHD-C4C-C3C	-4.66	117.98	124.77
6	M	406	2GO	C1A-C2A-C3A	-4.59	100.57	106.63
6	L	301	2GO	C2B-C1B-NB	4.57	114.76	109.02
6	M	406	2GO	CAA-C2A-C1A	-4.57	115.51	128.30
6	M	401	2GO	O2D-CGD-CBD	4.49	119.89	111.82
5	H	305	GGD	CA4-CA3-CA2	4.46	117.05	110.86
6	L	301	2GO	C2C-C1C-NC	4.46	114.80	109.06
6	M	401	2GO	C2B-C1B-NB	4.40	114.55	109.02
14	M	410	PC1	C14-N-C13	4.38	120.48	108.98
13	M	409	CDL	OB6-CB5-C51	4.35	120.90	111.48
6	M	406	2GO	CHD-C1D-ND	-4.35	117.62	124.82
6	L	301	2GO	CED-O2D-CGD	4.35	123.91	115.85
6	L	301	2GO	C4C-C3C-C2C	-4.30	100.63	106.89
5	H	305	GGD	CA1-CA2-CA3	4.30	117.59	110.11
6	M	401	2GO	CAD-CBD-CGD	-4.24	111.26	126.64
6	L	301	2GO	C3D-C2D-C1D	-4.19	100.12	105.83
6	M	402	2GO	C3D-C2D-C1D	-4.14	100.18	105.83
6	M	406	2GO	CHA-CBD-CGD	-4.14	111.93	125.24
6	L	307	2GO	C3A-C4A-NA	4.13	114.38	109.06
6	M	401	2GO	CAA-C2A-C1A	-4.11	116.79	128.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	305	2GO	CHD-C1D-ND	-3.99	118.22	124.82
6	M	402	2GO	C2C-C1C-NC	3.98	114.19	109.06
6	L	307	2GO	C1A-C2A-C3A	-3.98	101.38	106.63
6	M	401	2GO	C1-O2A-CGA	3.96	126.23	116.65
6	M	406	2GO	CHA-C1A-C2A	-3.88	122.28	128.14
6	M	406	2GO	C1-O2A-CGA	3.87	126.02	116.65
6	L	307	2GO	C4-C3-C5	3.83	121.87	115.23
5	H	305	GGD	CA3-CA4-CA5	3.79	117.65	109.57
6	M	402	2GO	C3A-C4A-NA	3.69	113.82	109.06
6	L	301	2GO	C1-O2A-CGA	3.69	125.58	116.65
6	M	406	2GO	C3D-C2D-C1D	-3.69	100.80	105.83
6	M	402	2GO	O2A-CGA-CBA	3.67	123.02	111.83
5	H	305	GGD	OC6-CC5-C14	3.66	119.40	111.48
6	M	402	2GO	CHD-C1D-ND	-3.62	118.83	124.82
6	M	402	2GO	C1A-C2A-C3A	-3.57	101.92	106.63
12	M	408	SPO	C4-C5-C6	-3.57	119.90	124.91
6	L	307	2GO	CAD-CBD-CGD	-3.57	113.71	126.64
6	L	305	2GO	CHC-C1C-C2C	-3.56	116.84	126.95
6	L	307	2GO	CHC-C1C-C2C	-3.53	116.91	126.95
6	L	301	2GO	CHC-C1C-C2C	-3.46	117.12	126.95
5	H	305	GGD	OA5-CA1-CA2	3.42	117.39	110.37
6	L	301	2GO	C3C-C4C-NC	3.40	116.51	110.16
6	L	307	2GO	CHD-C1D-ND	-3.37	119.25	124.82
12	M	408	SPO	C20-C19-C17	-3.36	122.56	127.28
6	L	307	2GO	C3D-C2D-C1D	-3.36	101.25	105.83
6	L	307	2GO	C3C-C4C-NC	3.35	116.42	110.16
6	M	402	2GO	O2D-CGD-O1D	-3.35	117.11	123.50
6	M	401	2GO	C3A-C4A-NA	3.33	113.36	109.06
6	L	301	2GO	CHD-C1D-ND	-3.33	119.31	124.82
6	M	401	2GO	CHA-CBD-CGD	-3.33	114.54	125.24
6	L	301	2GO	O1D-CGD-CBD	-3.32	118.58	124.60
6	L	305	2GO	C3A-C4A-NA	3.30	113.31	109.06
6	M	401	2GO	CHC-C1C-C2C	-3.28	117.62	126.95
6	L	305	2GO	O2A-CGA-CBA	3.27	121.80	111.83
6	M	401	2GO	CHD-C1D-ND	-3.27	119.42	124.82
6	M	406	2GO	C3C-C4C-NC	3.24	116.21	110.16
6	L	307	2GO	O2A-CGA-CBA	3.24	121.71	111.83
6	L	305	2GO	CMB-C2B-C1B	3.17	130.25	125.42
8	M	407	U10	C1M-C1-C6	-3.14	119.28	124.45
6	L	301	2GO	O2D-CGD-CBD	3.14	117.46	111.82
5	H	305	GGD	CA1-OA5-CA5	3.08	119.73	113.72
6	M	401	2GO	C3D-C4D-ND	3.07	116.24	110.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	401	2GO	CMD-C2D-C3D	-3.05	120.69	127.69
6	L	305	2GO	O2A-CGA-O1A	-3.05	116.00	123.63
12	M	408	SPO	C21-C22-C23	-3.04	123.01	127.28
6	M	406	2GO	C3A-C4A-NA	3.03	112.97	109.06
5	H	305	GGD	OB5-CB5-CB4	3.03	115.16	109.70
6	M	406	2GO	CHC-C1C-C2C	-3.03	118.35	126.95
6	M	401	2GO	C3D-C2D-C1D	-3.00	101.73	105.83
6	M	402	2GO	C3C-C4C-NC	3.00	115.76	110.16
6	L	301	2GO	CHA-CBD-CGD	-2.99	115.61	125.24
6	L	301	2GO	C1D-CHD-C4C	-2.98	119.68	126.02
6	L	305	2GO	O2D-CGD-O1D	-2.98	117.81	123.50
6	L	305	2GO	C3D-C2D-C1D	-2.98	101.77	105.83
6	L	307	2GO	O2A-CGA-O1A	-2.98	116.18	123.63
6	L	307	2GO	C4C-C3C-C2C	-2.97	102.56	106.89
6	M	402	2GO	CHB-C4A-C3A	-2.97	118.51	126.95
14	M	410	PC1	O31-C31-C32	2.97	120.89	111.83
6	L	307	2GO	CHB-C4A-C3A	-2.94	118.58	126.95
5	H	305	GGD	CB3-CB4-CB5	2.93	115.55	110.23
6	L	305	2GO	CED-O2D-CGD	2.91	121.25	115.85
6	L	301	2GO	C4-C3-C5	2.90	120.26	115.23
6	L	305	2GO	C4C-C3C-C2C	-2.89	102.68	106.89
8	L	306[A]	U10	C10-C9-C8	-2.86	116.29	123.63
14	M	410	PC1	O21-C21-O22	-2.85	117.05	123.70
8	M	407	U10	C4M-O4-C4	2.84	126.47	116.47
6	L	301	2GO	CHD-C4C-NC	2.82	129.70	124.77
6	M	406	2GO	C4C-C3C-C2C	-2.80	102.82	106.89
6	L	301	2GO	C3D-C4D-ND	2.78	115.70	110.51
6	M	402	2GO	O2A-CGA-O1A	-2.76	116.73	123.63
6	M	406	2GO	CMB-C2B-C1B	2.75	129.61	125.42
6	L	305	2GO	CBB-CAB-C3B	-2.75	114.61	120.40
6	M	402	2GO	C3D-C4D-ND	2.73	115.60	110.51
8	L	306[B]	U10	C10-C9-C11	2.72	119.95	115.23
8	M	407	U10	C25-C24-C26	2.72	119.95	115.23
13	M	409	CDL	OA6-CA5-OA7	-2.71	117.37	123.70
6	L	305	2GO	C3D-C4D-ND	2.71	115.55	110.51
6	L	301	2GO	CMB-C2B-C1B	2.70	129.53	125.42
12	M	408	SPO	C13-C12-C11	2.68	122.19	118.09
6	L	307	2GO	O2D-CGD-CBD	2.67	116.62	111.82
8	L	306[B]	U10	C1M-C1-C6	-2.67	120.07	124.45
6	M	402	2GO	CED-O2D-CGD	2.66	120.79	115.85
6	L	307	2GO	C3D-C4D-ND	2.66	115.47	110.51
12	M	408	SPO	C40-C38-C39	2.63	120.65	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	301	2GO	C5-C3-C2	-2.63	115.27	121.17
6	L	307	2GO	O2D-CGD-O1D	-2.61	118.51	123.50
6	M	401	2GO	O1D-CGD-CBD	-2.60	119.88	124.60
13	M	409	CDL	OA8-CA7-C31	2.58	119.71	111.83
6	M	406	2GO	C3D-C4D-ND	2.56	115.29	110.51
6	L	305	2GO	C1-C2-C3	-2.56	122.00	126.20
12	M	408	SPO	C26-C27-C28	-2.56	124.09	127.69
6	L	307	2GO	CMD-C2D-C3D	-2.56	121.83	127.69
8	L	306[A]	U10	C1M-C1-C6	-2.55	120.27	124.45
8	M	407	U10	C32-C31-C29	2.54	121.61	113.19
6	M	402	2GO	CHD-C4C-NC	2.50	129.13	124.77
6	L	307	2GO	C1D-CHD-C4C	-2.49	120.72	126.02
6	L	301	2GO	C11-C12-C13	-2.49	107.69	115.97
6	M	406	2GO	CHD-C4C-NC	2.48	129.11	124.77
6	M	406	2GO	O2A-CGA-CBA	2.48	119.40	111.83
8	M	407	U10	C20-C19-C21	2.46	119.50	115.23
6	M	406	2GO	O2D-CGD-O1D	-2.44	118.84	123.50
8	L	306[A]	U10	C7-C6-C1	-2.43	120.72	124.89
12	M	408	SPO	C29-C28-C30	2.43	119.45	115.23
6	M	406	2GO	CHB-C4A-C3A	-2.43	120.04	126.95
14	M	410	PC1	C13-N-C12	2.43	119.56	109.91
14	M	410	PC1	O21-C2-C3	2.43	117.05	108.34
6	M	402	2GO	O2D-CGD-CBD	2.42	116.18	111.82
13	M	409	CDL	OB8-CB7-C71	2.42	119.20	111.83
14	M	410	PC1	O31-C31-O32	-2.40	117.61	123.63
12	M	408	SPO	C14-C15-C16	-2.38	116.30	123.20
8	L	306[A]	U10	C3M-O3-C3	2.38	124.84	116.47
6	M	402	2GO	CMB-C2B-C1B	2.37	129.03	125.42
6	M	401	2GO	CHB-C4A-C3A	-2.37	120.22	126.95
6	M	402	2GO	CHC-C1C-C2C	-2.36	120.23	126.95
6	M	401	2GO	C1-C2-C3	2.36	130.07	126.20
6	M	401	2GO	C1D-CHD-C4C	-2.36	121.01	126.02
6	L	307	2GO	C1-O2A-CGA	2.34	122.31	116.65
6	M	401	2GO	CMB-C2B-C1B	2.34	128.97	125.42
8	M	407	U10	C15-C14-C16	2.33	119.28	115.23
6	M	402	2GO	CHC-C4B-C3B	-2.33	122.46	131.72
6	L	301	2GO	C2D-C1D-ND	2.32	113.88	110.35
6	L	301	2GO	CHB-C4A-C3A	-2.31	120.39	126.95
6	L	301	2GO	O2A-CGA-CBA	2.26	118.73	111.83
6	L	301	2GO	CHC-C1C-NC	2.26	127.66	124.75
6	L	305	2GO	CHB-C4A-C3A	-2.26	120.53	126.95
5	H	305	GGD	OC8-CC6-CC4	2.25	114.89	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	305	GGD	OC8-CC7-C31	2.25	118.70	111.83
6	M	402	2GO	CHB-C4A-NA	2.25	127.65	124.75
14	M	410	PC1	C14-N-C12	2.24	118.81	109.91
5	H	305	GGD	OC6-CC5-OC7	-2.24	118.47	123.70
6	L	305	2GO	CHD-C4C-NC	2.23	128.67	124.77
13	M	409	CDL	OA8-CA7-OA9	-2.23	118.04	123.63
8	M	407	U10	C6-C1-C2	2.23	120.93	119.17
8	L	306[A]	U10	C10-C9-C11	2.22	119.08	115.23
6	L	305	2GO	C3C-C4C-NC	2.21	114.30	110.16
6	L	301	2GO	CHB-C4A-NA	2.21	127.60	124.75
6	M	406	2GO	O1D-CGD-CBD	-2.20	120.61	124.60
6	L	301	2GO	C16-C17-C18	-2.19	106.14	115.94
8	M	407	U10	C17-C18-C19	-2.19	122.60	127.62
12	M	408	SPO	C8-C7-C6	2.19	121.44	118.09
6	M	401	2GO	C4-C3-C2	-2.19	118.01	123.63
6	L	305	2GO	CHC-C1C-NC	2.17	127.54	124.75
6	L	301	2GO	CHC-C4B-C3B	-2.17	123.11	131.72
6	L	301	2GO	C3A-C4A-NA	2.16	111.84	109.06
6	M	406	2GO	CED-O2D-CGD	2.15	119.84	115.85
12	M	408	SPO	C24-C23-C25	2.14	121.36	118.09
12	M	408	SPO	C40-C38-C37	-2.14	116.23	122.66
12	M	408	SPO	C34-C33-C35	2.13	118.93	115.23
8	M	407	U10	C30-C29-C28	-2.13	118.16	123.63
6	M	402	2GO	C1-C2-C3	-2.11	122.73	126.20
8	L	306[B]	U10	C16-C14-C15	2.11	119.44	114.59
8	L	306[B]	U10	C7-C8-C9	-2.10	123.21	126.83
6	L	305	2GO	O1D-CGD-CBD	-2.09	120.81	124.60
6	M	402	2GO	C1D-CHD-C4C	-2.09	121.58	126.02
5	H	305	GGD	OA5-CA5-CA6	2.09	111.61	106.44
6	L	301	2GO	CMD-C2D-C3D	-2.09	122.90	127.69
13	M	409	CDL	OB8-CB7-OB9	-2.08	118.42	123.63
8	M	407	U10	C31-C29-C28	-2.07	116.52	121.17
8	M	407	U10	C7-C6-C1	-2.07	121.34	124.89
8	L	306[B]	U10	C7-C6-C1	-2.07	121.35	124.89
6	L	307	2GO	CHC-C1C-NC	2.06	127.41	124.75
6	L	307	2GO	CHD-C4C-NC	2.05	128.35	124.77
6	M	406	2GO	C3B-C2B-C1B	-2.05	99.86	106.40
6	M	406	2GO	OB8-CAB-CBB	2.04	124.34	119.77
6	L	305	2GO	CMD-C2D-C3D	-2.03	123.03	127.69
6	M	406	2GO	CHB-C1B-C2B	-2.03	121.54	127.43
6	L	305	2GO	CHD-C1D-C2D	2.01	129.67	125.49
6	L	307	2GO	C11-C10-C8	-2.01	109.29	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	301	2GO	C6-C5-C3	-2.01	108.58	113.47
6	L	305	2GO	OBB-CAB-CBB	2.01	124.27	119.77
6	L	305	2GO	C1-O2A-CGA	2.00	121.50	116.65

There are no chirality outliers.

All (251) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	301	GOL	O1-C1-C2-O2
4	H	301	GOL	O1-C1-C2-C3
4	H	302	GOL	C1-C2-C3-O3
4	H	303	GOL	C1-C2-C3-O3
4	H	304	GOL	O1-C1-C2-C3
4	L	311	GOL	C1-C2-C3-O3
4	L	312	GOL	O1-C1-C2-C3
4	L	312	GOL	C1-C2-C3-O3
4	L	313	GOL	O1-C1-C2-C3
5	H	305	GGD	OC7-CC5-OC6-CC4
5	H	305	GGD	C14-CC5-OC6-CC4
6	L	305	2GO	C1A-C2A-CAA-CBA
6	L	307	2GO	C1A-C2A-CAA-CBA
6	M	401	2GO	C3A-C2A-CAA-CBA
6	M	406	2GO	C4B-C3B-CAB-CBB
6	M	406	2GO	C4B-C3B-CAB-OBB
6	M	406	2GO	C2B-C3B-CAB-CBB
6	M	406	2GO	C2B-C3B-CAB-OBB
7	L	304	LDA	C2-C1-N1-O1
7	L	304	LDA	C2-C1-N1-CM1
7	L	304	LDA	C2-C1-N1-CM2
7	M	403	LDA	C2-C1-N1-CM1
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
10	L	310	HTO	O1-C1-C2-O2
10	L	310	HTO	O1-C1-C2-C3
12	M	408	SPO	O1-C1-C4-C5
12	M	408	SPO	C2-C1-C4-C5
12	M	408	SPO	C3-C1-C4-C5
12	M	408	SPO	C5-C6-C7-C9
13	M	409	CDL	CA3-OA5-PA1-OA2
13	M	409	CDL	CA3-OA5-PA1-OA3

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

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Mol	Chain	Res	Type	Atoms
6	L	307	2GO	O1D-CGD-O2D-CED
6	M	401	2GO	C10-C11-C12-C13
8	M	407	U10	C30-C29-C31-C32
5	H	305	GGD	CA2-CA1-OA1-CC3
8	M	407	U10	C14-C16-C17-C18
8	M	407	U10	C24-C26-C27-C28
6	M	402	2GO	C3-C5-C6-C7
6	M	406	2GO	O2A-C1-C2-C3
14	M	410	PC1	C3-C2-O21-C21
8	M	407	U10	C28-C29-C31-C32
14	M	410	PC1	C11-C12-N-C13
6	L	301	2GO	O1D-CGD-O2D-CED
7	L	303	LDA	C6-C7-C8-C9
13	M	409	CDL	C71-C72-C73-C74
4	H	303	GOL	O2-C2-C3-O3
4	L	312	GOL	O2-C2-C3-O3
7	L	304	LDA	C4-C5-C6-C7
6	M	401	2GO	C16-C17-C18-C20
6	M	401	2GO	C16-C17-C18-C19
13	M	409	CDL	O1-C1-CA2-OA2
13	M	409	CDL	C17-C18-C19-C20
13	M	409	CDL	C51-C52-C53-C54
8	M	407	U10	C29-C31-C32-C33
5	H	305	GGD	C40-C41-C42-C43
7	L	304	LDA	C7-C8-C9-C10
7	L	302	LDA	C5-C6-C7-C8
13	M	409	CDL	C54-C55-C56-C57
14	M	410	PC1	C29-C2A-C2B-C2C
7	L	303	LDA	C5-C6-C7-C8
13	M	409	CDL	C16-C17-C18-C19
7	L	302	LDA	C6-C7-C8-C9
6	M	406	2GO	C8-C10-C11-C12
14	M	410	PC1	C22-C23-C24-C25
6	M	401	2GO	C4C-C3C-CAC-CBC
13	M	409	CDL	C20-C21-C22-C23
13	M	409	CDL	C35-C36-C37-C38
5	H	305	GGD	C34-C35-C36-C37
14	M	410	PC1	C27-C28-C29-C2A
13	M	409	CDL	C53-C54-C55-C56
7	L	302	LDA	C3-C4-C5-C6
7	L	302	LDA	C7-C8-C9-C10
6	L	307	2GO	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
7	M	403	LDA	C4-C5-C6-C7
13	M	409	CDL	C11-C12-C13-C14
5	H	305	GGD	OB5-CB5-CB6-OB6
6	L	301	2GO	C1A-C2A-CAA-CBA
4	H	302	GOL	O2-C2-C3-O3
4	H	304	GOL	O1-C1-C2-O2
6	L	301	2GO	C11-C12-C13-C15
6	M	406	2GO	C11-C12-C13-C15
13	M	409	CDL	C51-CB5-OB6-CB4
6	L	301	2GO	C11-C12-C13-C14
6	M	402	2GO	C11-C10-C8-C9
7	L	304	LDA	C5-C6-C7-C8
7	L	302	LDA	C2-C3-C4-C5
12	M	408	SPO	C4-C1-O1-CM1
13	M	409	CDL	C12-C13-C14-C15
6	L	301	2GO	CBD-CGD-O2D-CED
6	L	305	2GO	O2A-C1-C2-C3
7	M	403	LDA	C2-C3-C4-C5
13	M	409	CDL	C33-C34-C35-C36
7	L	303	LDA	C11-C10-C9-C8
7	M	403	LDA	C11-C10-C9-C8
13	M	409	CDL	C18-C19-C20-C21
13	M	409	CDL	C36-C37-C38-C39
12	M	408	SPO	C2-C1-O1-CM1
12	M	408	SPO	C3-C1-O1-CM1
10	L	309	HTO	C4-C5-C6-C7
14	M	410	PC1	C21-C22-C23-C24
6	M	402	2GO	C6-C7-C8-C9
6	M	406	2GO	C11-C12-C13-C14
7	M	404	LDA	C1-C2-C3-C4
6	M	406	2GO	C16-C17-C18-C20
7	L	302	LDA	C4-C5-C6-C7
14	M	410	PC1	C35-C36-C37-C38
6	M	402	2GO	C6-C7-C8-C10
6	M	402	2GO	C11-C10-C8-C7
13	M	409	CDL	C81-C82-C83-C84
5	H	305	GGD	CC5-C14-C15-C16
13	M	409	CDL	CA3-CA4-CA6-OA8
6	L	305	2GO	C3-C5-C6-C7
6	L	305	2GO	C16-C17-C18-C19
13	M	409	CDL	OB5-CB3-CB4-OB6
6	L	305	2GO	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	M	410	PC1	C2B-C2C-C2D-C2E
6	M	406	2GO	C4C-C3C-CAC-CBC
4	H	301	GOL	O2-C2-C3-O3
13	M	409	CDL	C39-C40-C41-C42
7	M	404	LDA	C9-C10-C11-C12
13	M	409	CDL	OB7-CB5-OB6-CB4
13	M	409	CDL	CB7-C71-C72-C73
6	L	301	2GO	C8-C10-C11-C12
13	M	409	CDL	C55-C56-C57-C58
6	L	305	2GO	C6-C7-C8-C10
6	M	406	2GO	C6-C7-C8-C10
12	M	408	SPO	C1-C4-C5-C6
6	L	305	2GO	C2B-C3B-CAB-CBB
6	L	305	2GO	C2B-C3B-CAB-OB
13	M	409	CDL	OA6-CA4-CA6-OA8
14	M	410	PC1	O21-C2-C3-O31
6	M	401	2GO	C11-C10-C8-C9
7	M	404	LDA	C3-C4-C5-C6
13	M	409	CDL	C73-C74-C75-C76
6	M	402	2GO	C16-C17-C18-C19
8	L	306[B]	U10	C2-C3-O3-C3M
5	H	305	GGD	C39-C40-C41-C42
13	M	409	CDL	OB5-CB3-CB4-CB6
6	L	301	2GO	C3-C5-C6-C7
6	L	301	2GO	C11-C10-C8-C7
14	M	410	PC1	C28-C29-C2A-C2B
5	H	305	GGD	C32-C33-C34-C35
6	L	305	2GO	C6-C7-C8-C9
6	M	406	2GO	C6-C7-C8-C9
14	M	410	PC1	C33-C34-C35-C36
6	M	406	2GO	C16-C17-C18-C19
7	L	304	LDA	C1-C2-C3-C4
6	L	305	2GO	O1D-CGD-O2D-CED
6	M	402	2GO	C5-C6-C7-C8
7	L	303	LDA	C3-C4-C5-C6
6	L	305	2GO	C8-C10-C11-C12
13	M	409	CDL	CB2-OB2-PB2-OB4
13	M	409	CDL	CB2-OB2-PB2-OB5
14	M	410	PC1	C11-O13-P-O14
6	L	305	2GO	CAD-CBD-CGD-O1D
6	L	307	2GO	CAD-CBD-CGD-O1D
6	M	401	2GO	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
6	M	402	2GO	CAD-CBD-CGD-O1D
6	M	406	2GO	CAD-CBD-CGD-O1D
13	M	409	CDL	C72-C73-C74-C75
7	L	303	LDA	C9-C10-C11-C12
6	L	305	2GO	CAD-CBD-CGD-O2D
6	M	402	2GO	CAD-CBD-CGD-O2D
8	L	306[A]	U10	C9-C11-C12-C13
6	L	301	2GO	C3A-C2A-CAA-CBA
8	L	306[B]	U10	C12-C11-C9-C10
8	M	407	U10	C25-C24-C26-C27
6	M	401	2GO	C11-C10-C8-C7
13	M	409	CDL	CB2-C1-CA2-OA2
13	M	409	CDL	CB3-CB4-CB6-OB8
6	L	305	2GO	C11-C10-C8-C9
4	H	303	GOL	O1-C1-C2-O2
10	L	309	HTO	C3-C4-C5-C6
8	M	407	U10	C31-C32-C33-C34
6	M	402	2GO	C11-C12-C13-C15
8	M	407	U10	C23-C24-C26-C27
6	L	305	2GO	CBD-CGD-O2D-CED
7	M	404	LDA	C2-C3-C4-C5
6	M	406	2GO	CAD-CBD-CGD-O2D
8	M	407	U10	C34-C36-C37-C38
10	L	310	HTO	C3-C4-C5-C6
13	M	409	CDL	C75-C76-C77-C78
14	M	410	PC1	C25-C26-C27-C28
6	M	406	2GO	C2-C1-O2A-CGA
5	H	305	GGD	OA5-CA1-OA1-CC3
14	M	410	PC1	C1-C2-C3-O31
13	M	409	CDL	C78-C79-C80-C81
6	L	301	2GO	CAD-CBD-CGD-O1D
7	M	404	LDA	C6-C7-C8-C9
6	L	305	2GO	C4B-C3B-CAB-CBB
6	M	401	2GO	CAD-CBD-CGD-O2D
6	L	301	2GO	C11-C10-C8-C9
6	L	305	2GO	C11-C10-C8-C7
13	M	409	CDL	C52-C51-CB5-OB6
8	L	306[B]	U10	C12-C11-C9-C8
12	M	408	SPO	C15-C16-C17-C18
6	M	401	2GO	C2C-C3C-CAC-CBC
13	M	409	CDL	C12-C11-CA5-OA6
6	M	401	2GO	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
5	H	305	GGD	C32-C31-CC7-OC8
6	M	401	2GO	C11-C12-C13-C15
6	L	301	2GO	CAD-CBD-CGD-O2D
6	L	307	2GO	CAD-CBD-CGD-O2D
13	M	409	CDL	C52-C51-CB5-OB7
7	M	404	LDA	C7-C8-C9-C10
13	M	409	CDL	C12-C11-CA5-OA7

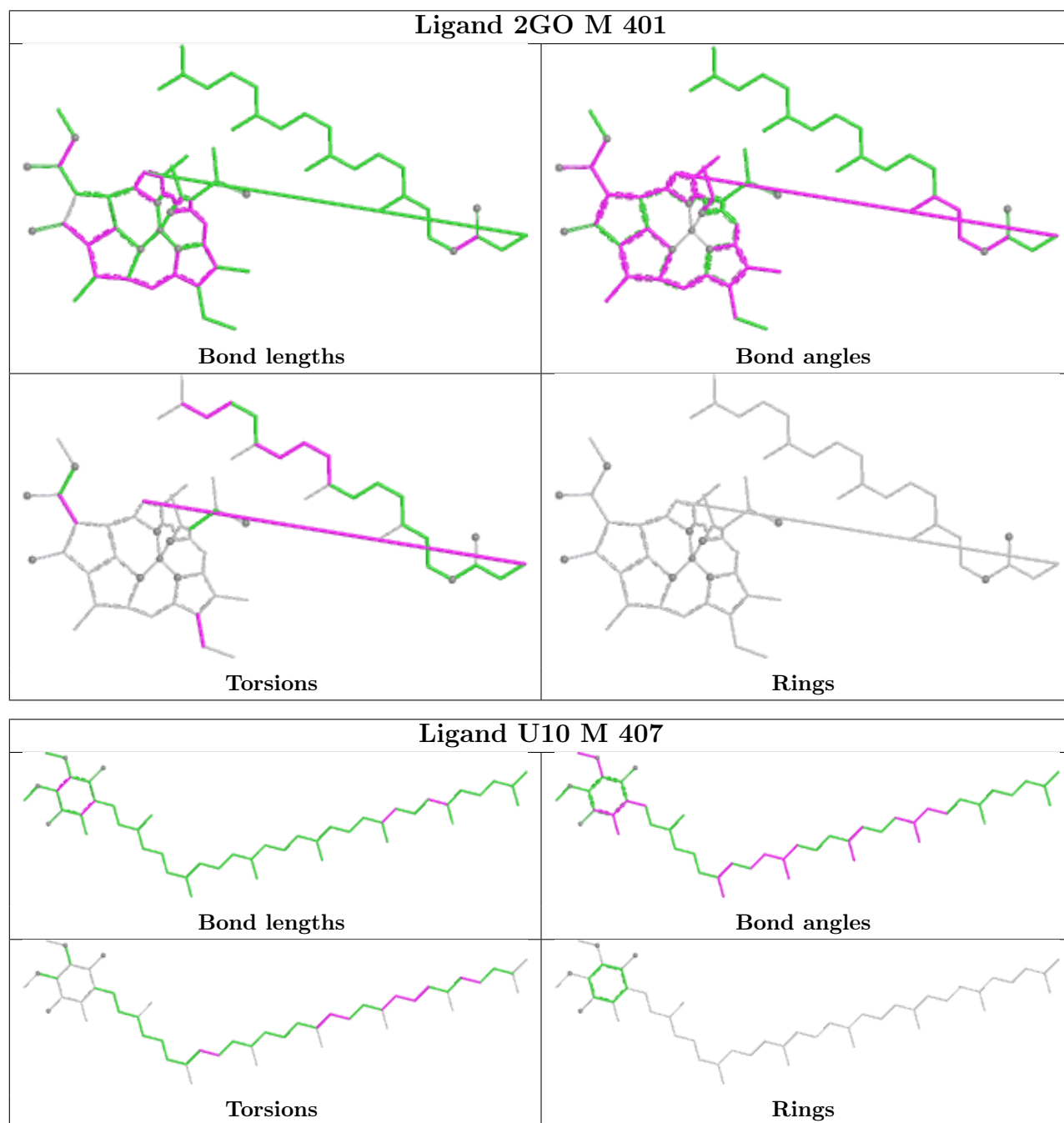
There are no ring outliers.

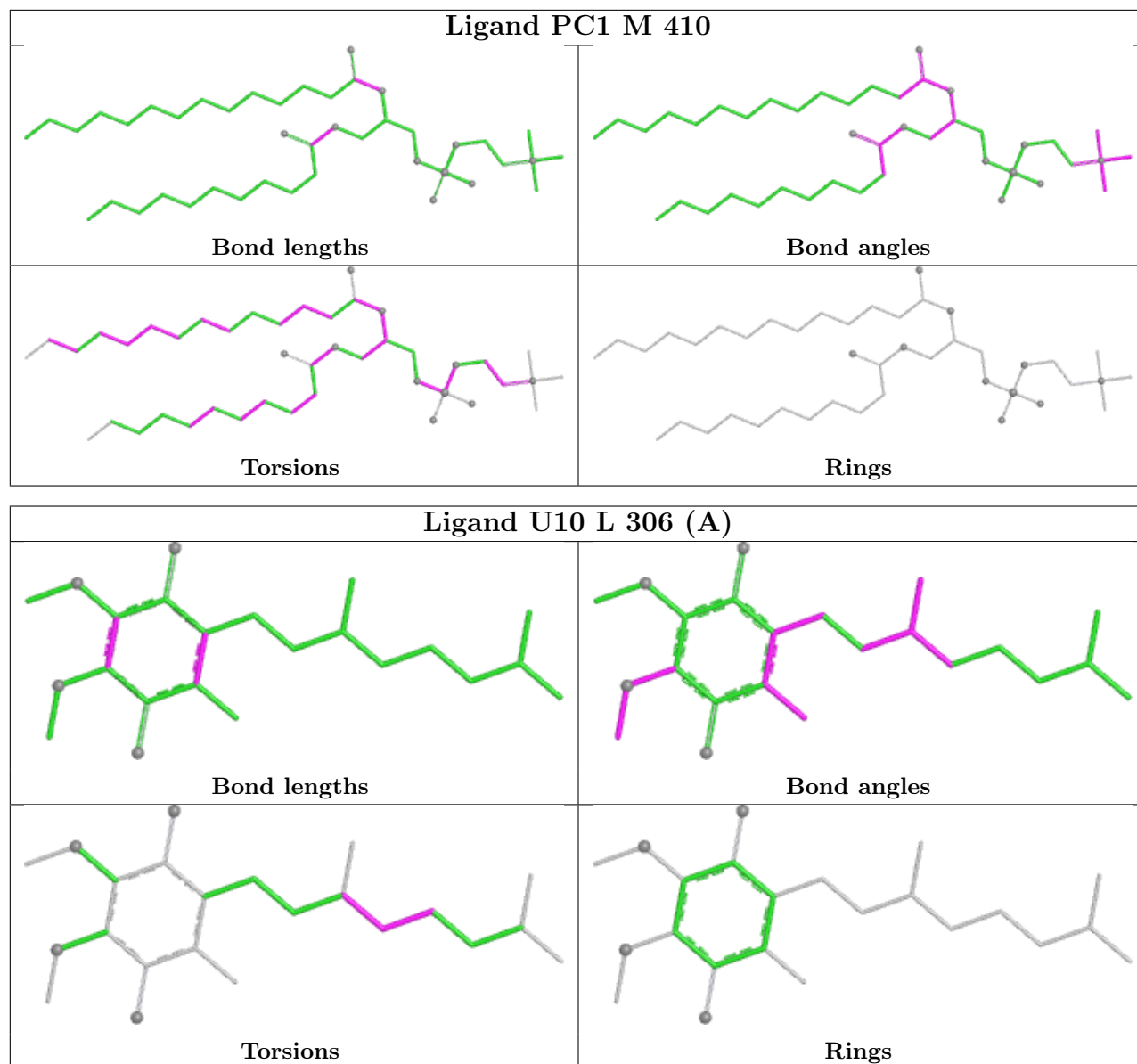
19 monomers are involved in 67 short contacts:

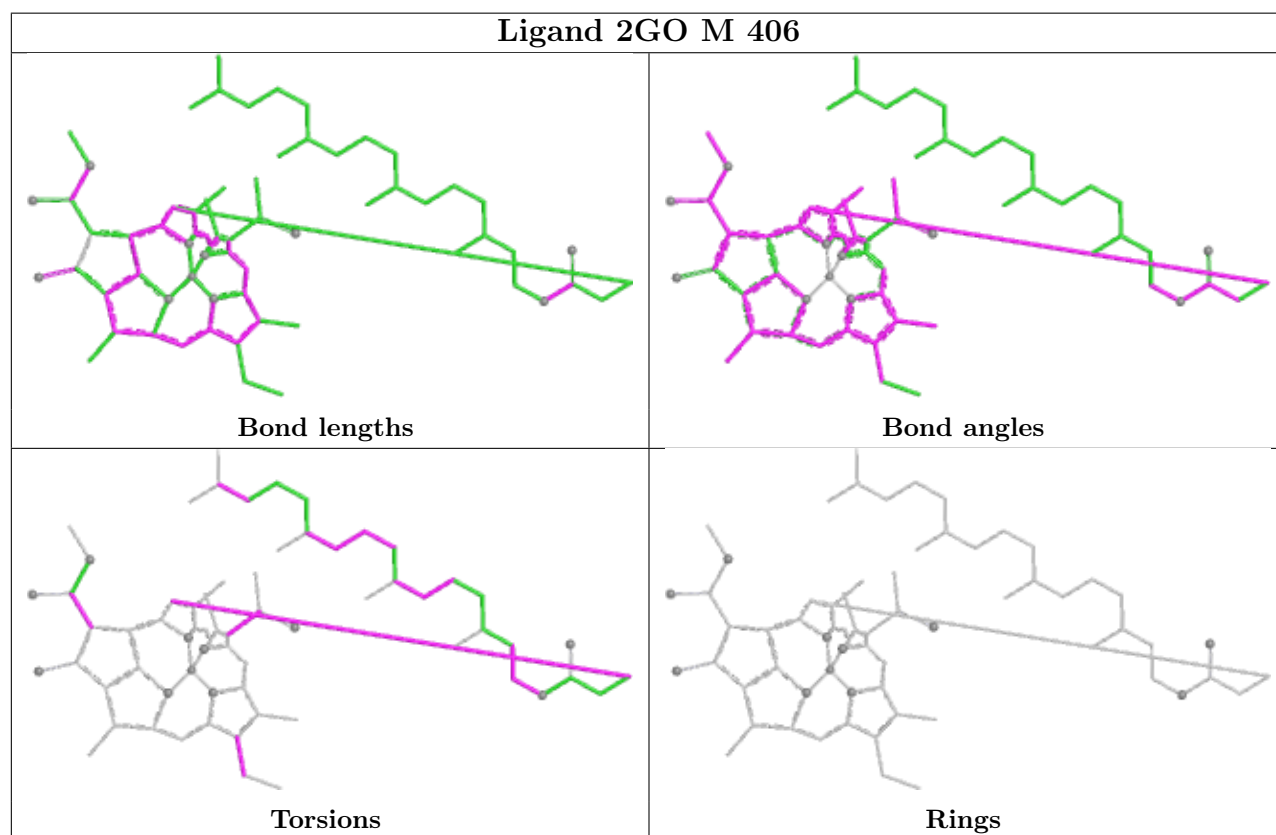
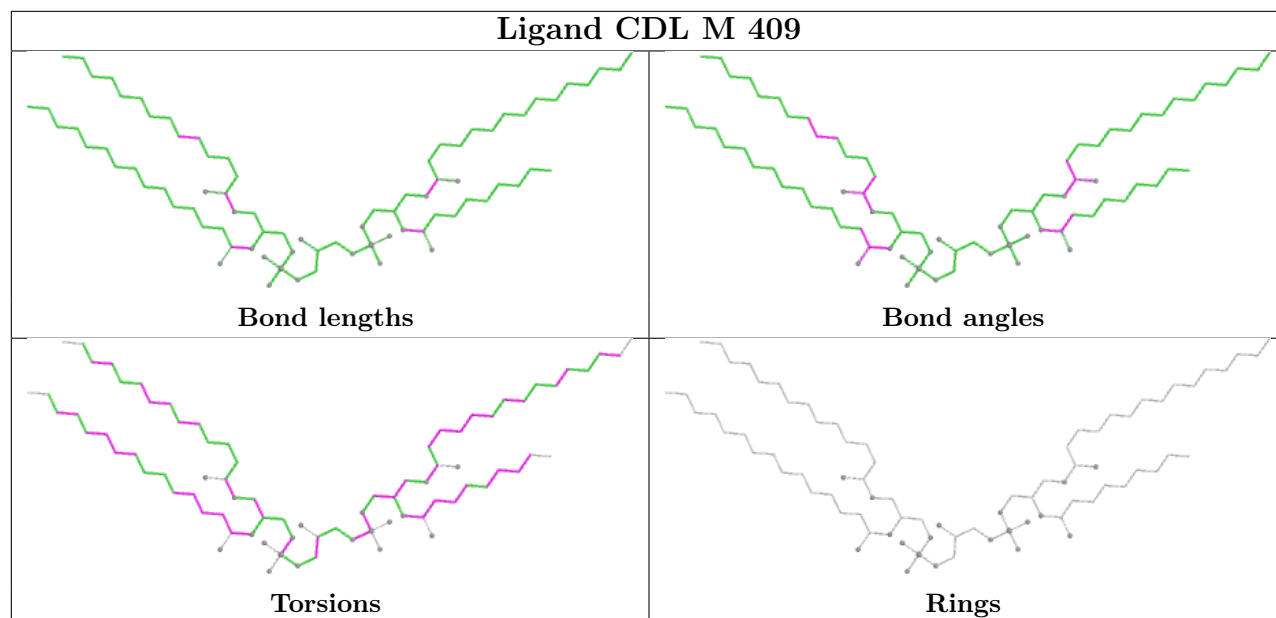
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	401	2GO	10	0
4	H	303	GOL	1	0
8	M	407	U10	3	0
4	H	301	GOL	1	0
8	L	306[A]	U10	7	0
13	M	409	CDL	2	0
6	M	406	2GO	8	0
5	H	305	GGD	2	0
9	L	308	PO4	1	0
6	L	307	2GO	2	0
7	M	403	LDA	1	0
6	L	305	2GO	8	0
4	L	312	GOL	1	0
6	L	301	2GO	6	0
8	L	306[B]	U10	6	0
12	M	408	SPO	5	0
6	M	402	2GO	10	0
4	L	311	GOL	1	0
4	L	313	GOL	1	0

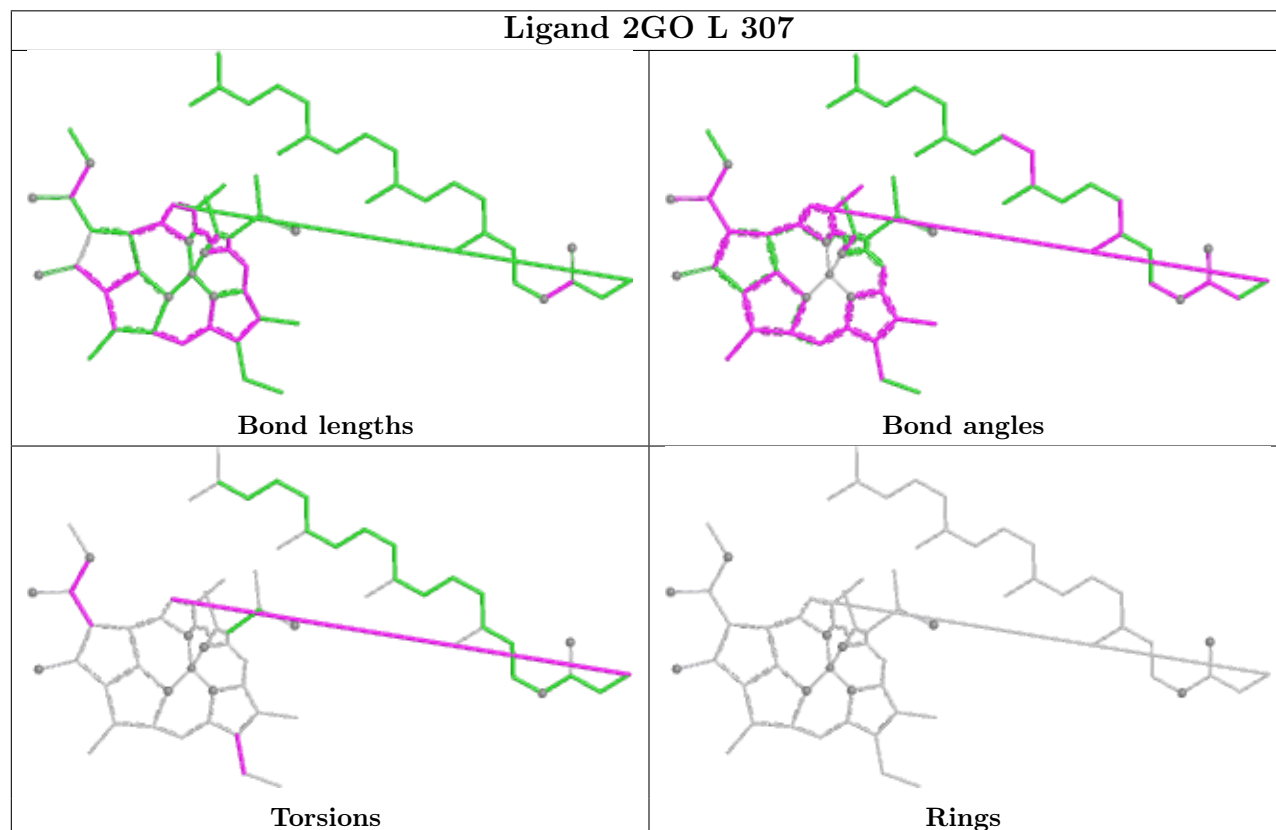
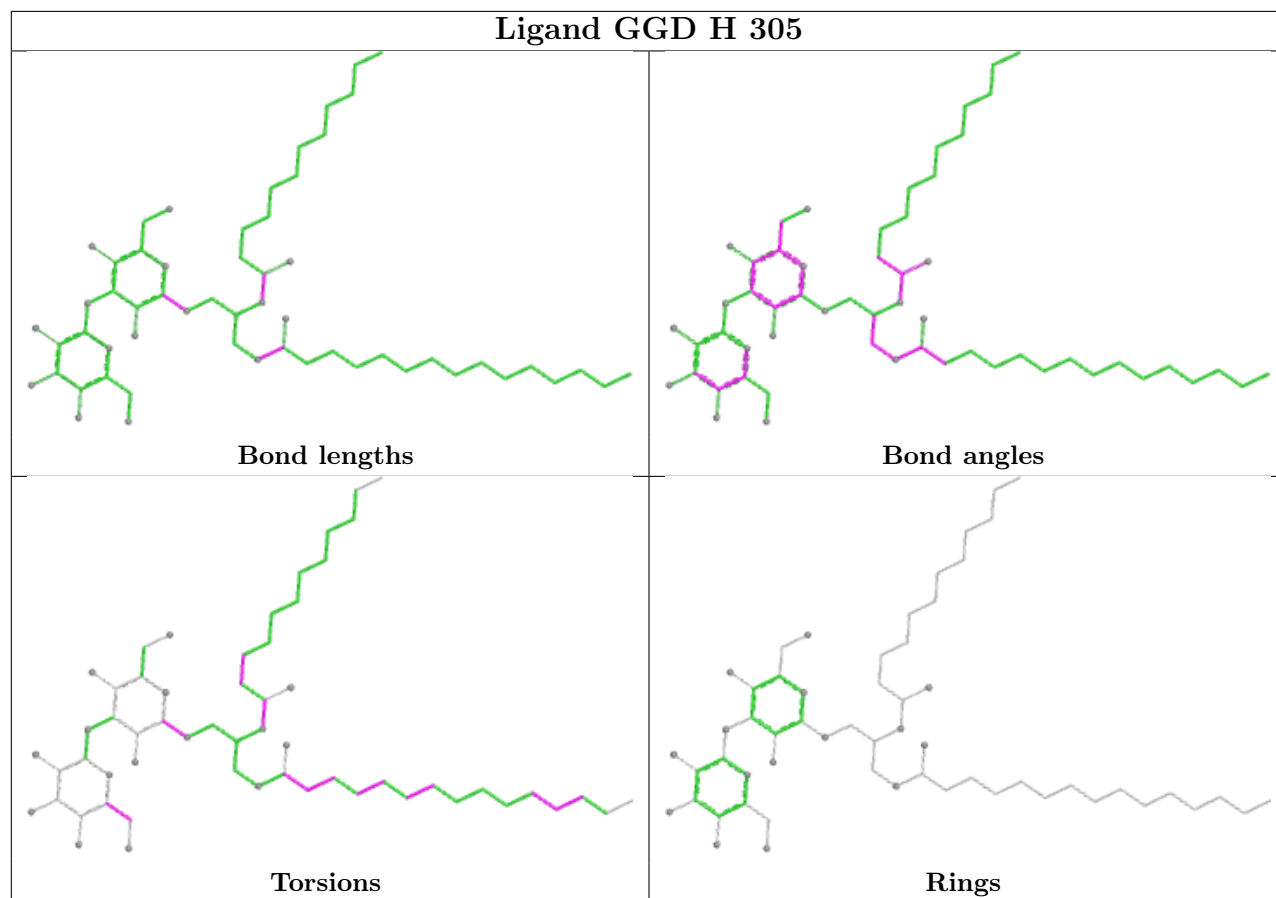
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

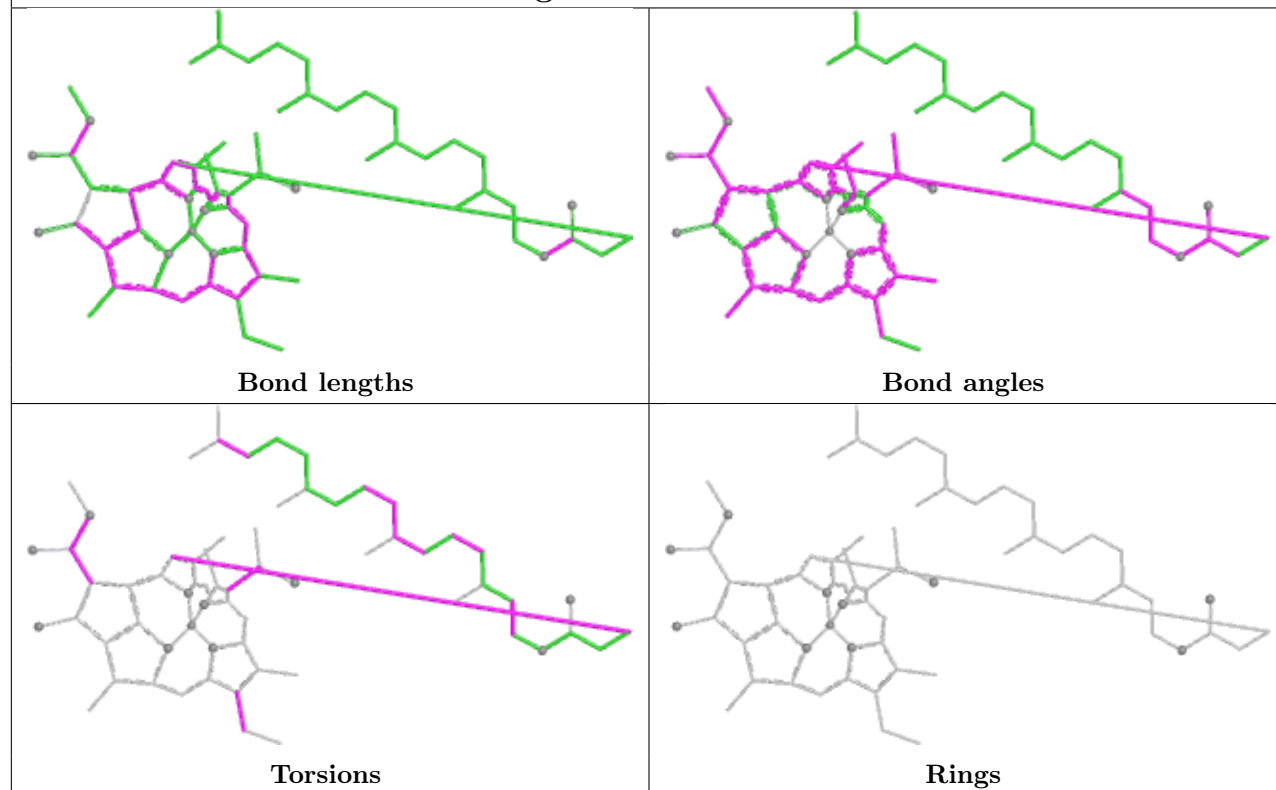




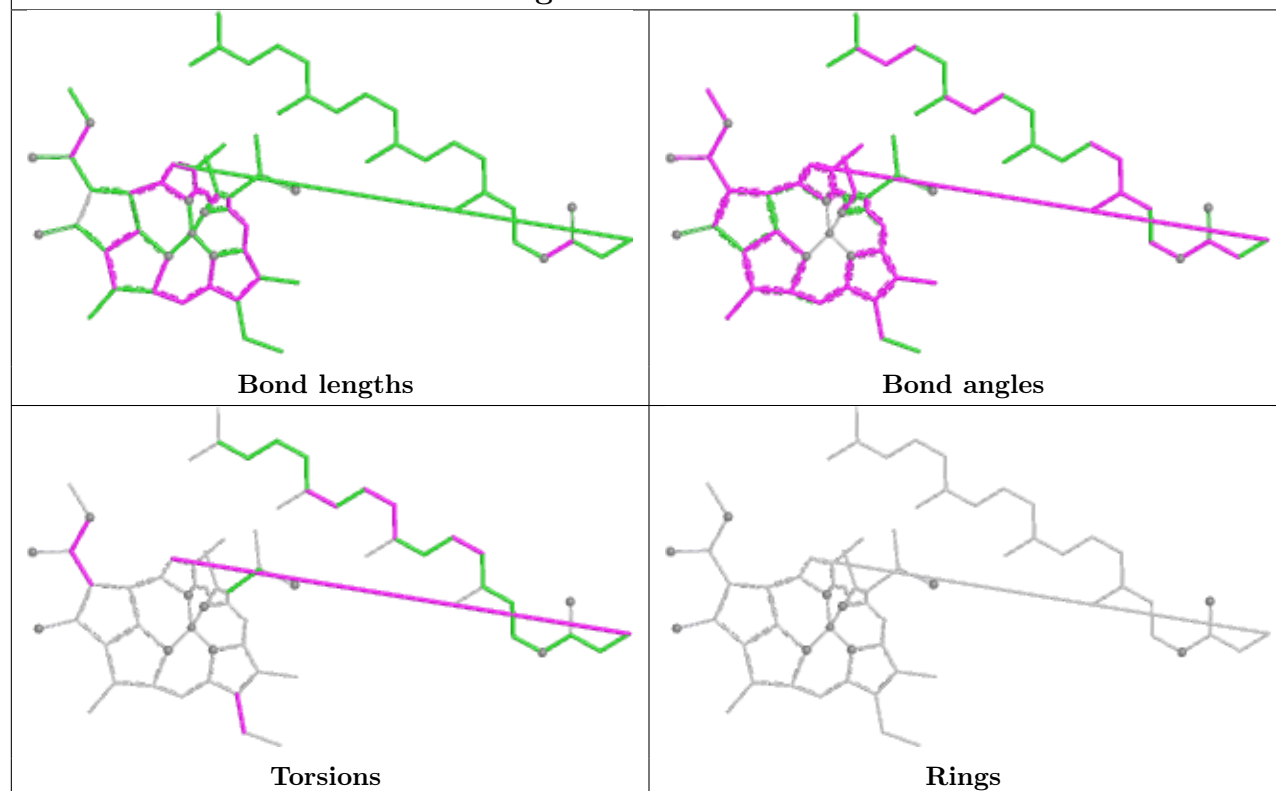


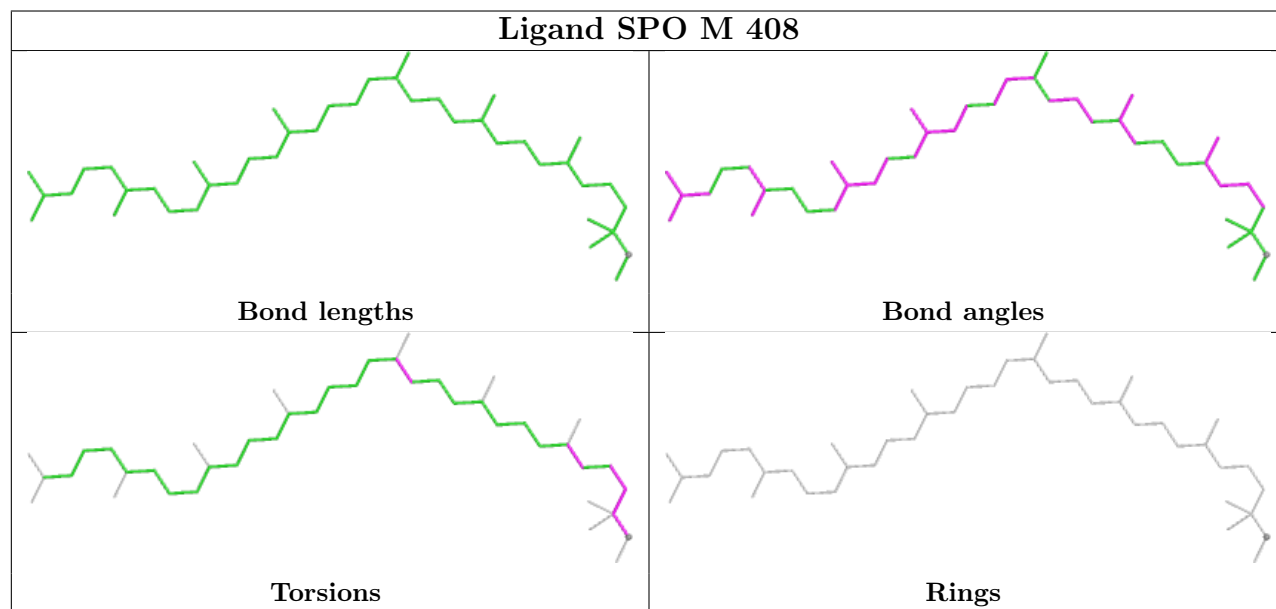
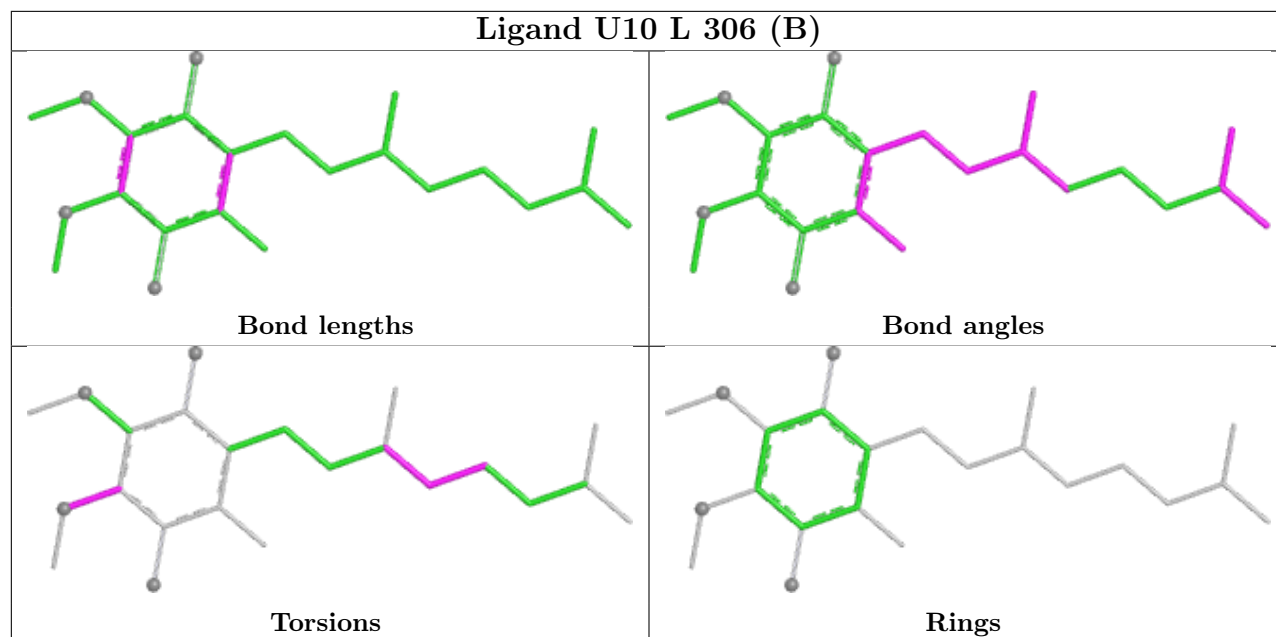


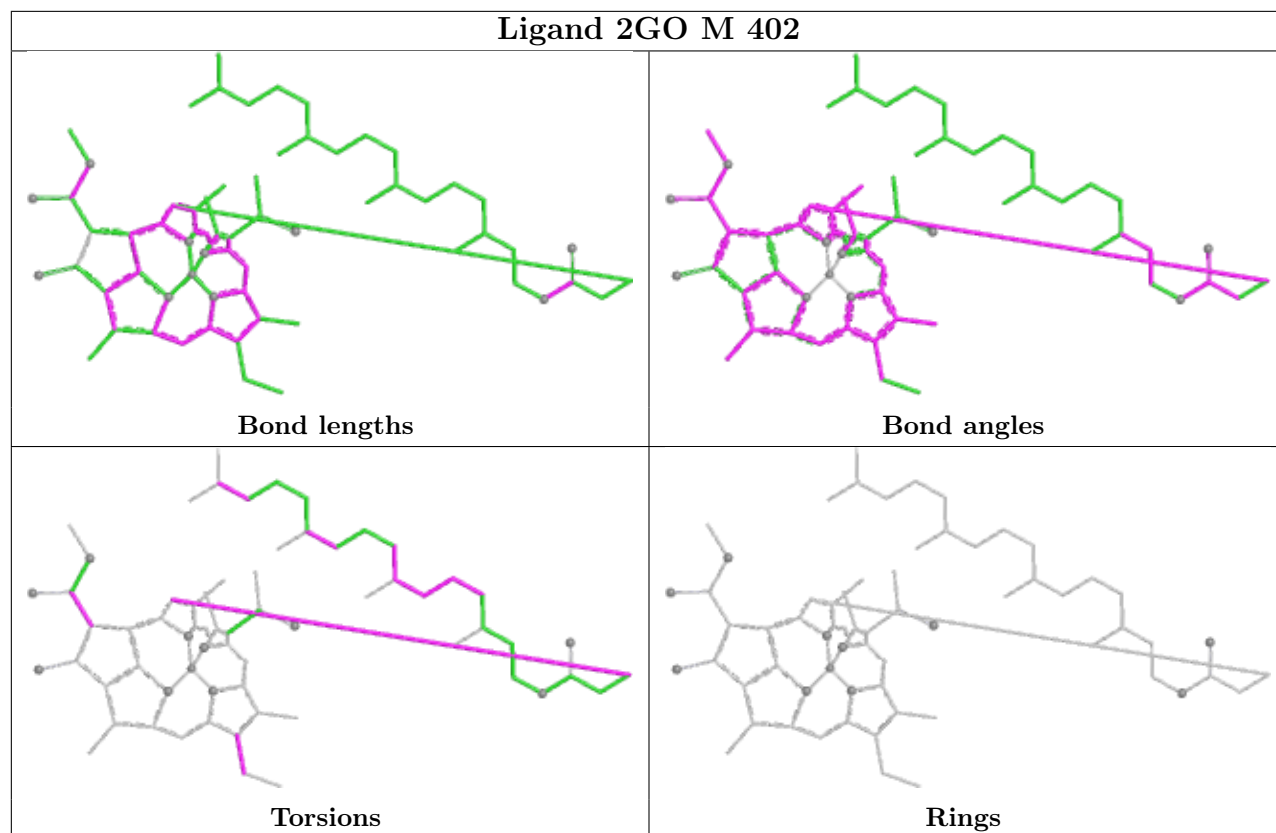
Ligand 2GO L 305



Ligand 2GO L 301







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%)	-0.40	4 (1%) 69 63	32, 53, 76, 161	8 (3%)
2	L	281/281 (100%)	-0.40	2 (0%) 84 80	37, 52, 79, 101	2 (0%)
3	M	303/303 (100%)	-0.30	5 (1%) 69 63	37, 55, 80, 123	7 (2%)
All	All	825/825 (100%)	-0.36	11 (1%) 75 68	32, 54, 80, 161	17 (2%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	12.8
3	M	2	GLU	7.2
1	H	249[A]	LYS	5.5
1	H	246	PRO	3.5
3	M	301	HIS	3.3
1	H	184	LYS	2.9
1	H	220[A]	LYS	2.7
3	M	3	TYR	2.7
3	M	52	LEU	2.5
2	L	271[A]	TRP	2.2
2	L	67	TYR	2.1

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 ⓘ

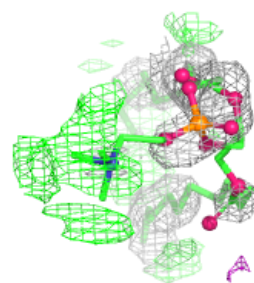
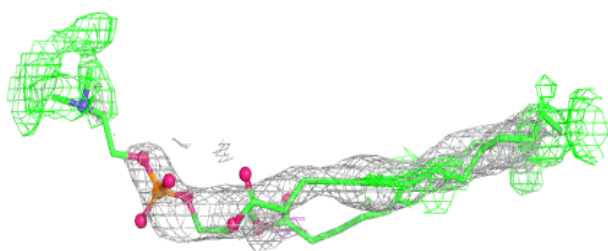
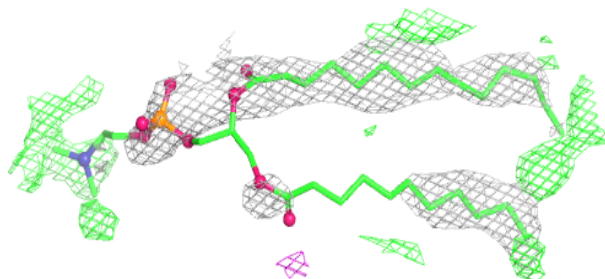
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.74	0.35	78,117,175,190	0
7	LDA	L	303	16/16	0.75	0.43	76,95,143,148	0
7	LDA	L	304	16/16	0.83	0.25	68,96,124,125	0
10	HTO	L	309	10/10	0.85	0.30	88,103,117,127	0
10	HTO	L	310	10/10	0.85	0.28	86,114,140,156	0
4	GOL	H	301	6/6	0.85	0.17	94,109,111,112	0
13	CDL	M	409	81/100	0.86	0.23	70,101,156,164	0
5	GGD	H	305	57/67	0.86	0.22	49,107,216,221	0
7	LDA	L	302	16/16	0.87	0.23	42,105,140,143	0
7	LDA	M	404	16/16	0.88	0.18	67,87,102,106	0
4	GOL	L	311	6/6	0.90	0.16	60,73,85,104	0
8	U10	L	306[A]	23/63	0.91	0.23	50,71,86,91	23
8	U10	L	306[B]	23/63	0.91	0.23	43,68,73,75	23
4	GOL	H	304	6/6	0.91	0.12	74,85,89,94	0
4	GOL	H	303	6/6	0.92	0.14	73,85,90,96	0
4	GOL	H	302	6/6	0.92	0.14	56,65,69,81	0
8	U10	M	407	48/63	0.93	0.15	43,54,99,111	0
12	SPO	M	408	42/42	0.94	0.16	46,64,98,112	0
6	2GO	M	406	66/66	0.94	0.15	60,76,135,142	0
4	GOL	L	313	6/6	0.94	0.10	84,89,93,93	0
9	PO4	L	308	5/5	0.95	0.07	97,97,98,98	0
4	GOL	L	312	6/6	0.95	0.11	87,88,92,95	0
7	LDA	M	403	16/16	0.95	0.13	42,60,67,68	0
6	2GO	L	305	66/66	0.97	0.09	31,47,56,58	0
6	2GO	M	402	66/66	0.98	0.08	39,50,75,86	0
6	2GO	L	301	66/66	0.98	0.08	29,39,59,68	0
6	2GO	L	307	66/66	0.98	0.09	35,48,59,63	0
6	2GO	M	401	66/66	0.98	0.10	35,47,88,92	0
11	FE	M	405	1/1	1.00	0.01	46,46,46,46	0

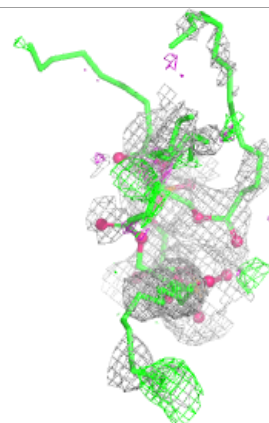
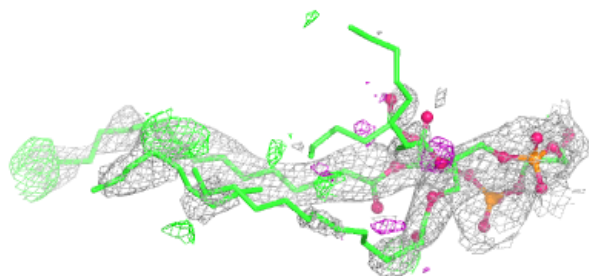
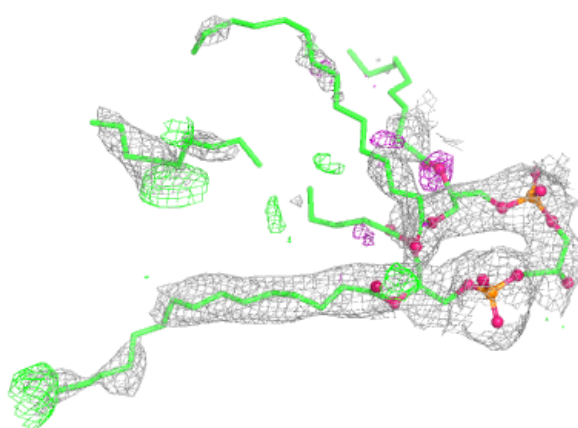
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

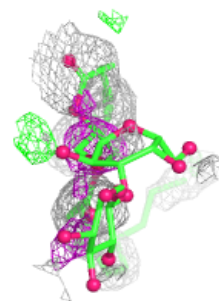
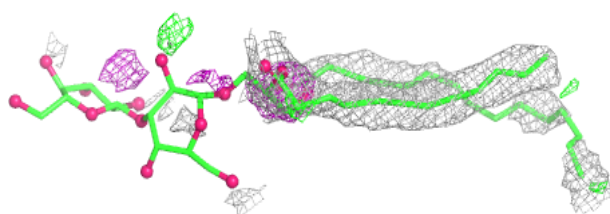
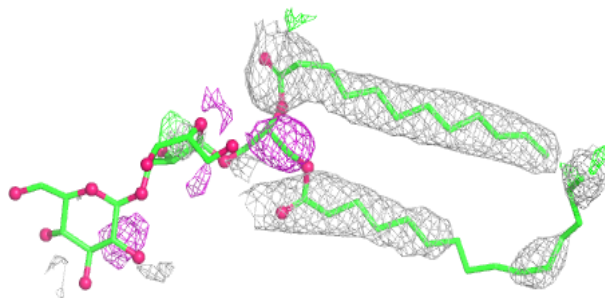
**Electron density around CDL M 409:**

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

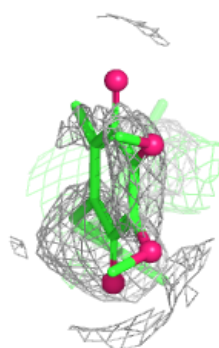
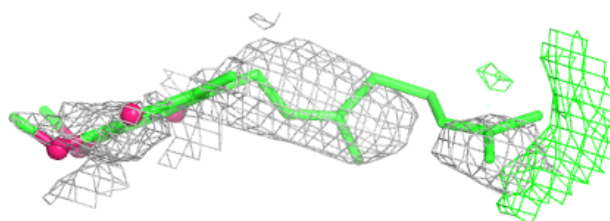
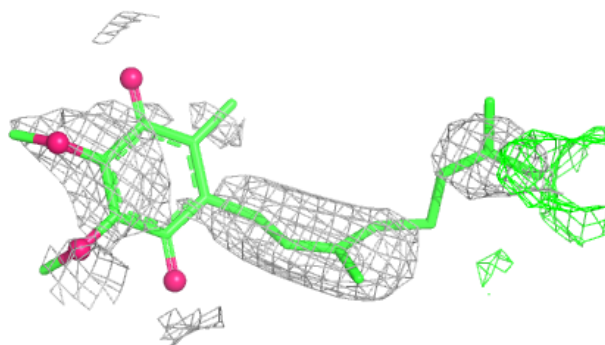


Electron density around GGD H 305:

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

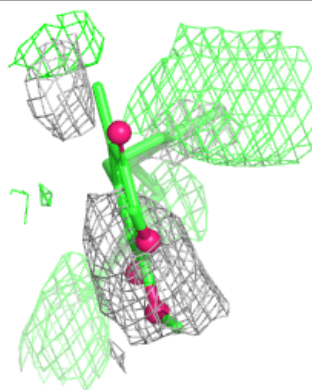
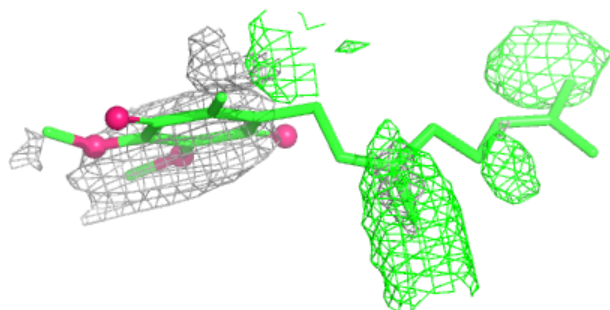
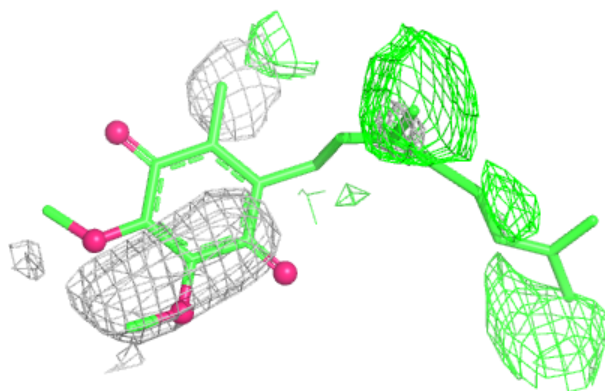
**Electron density around U10 L 306 (A):**

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

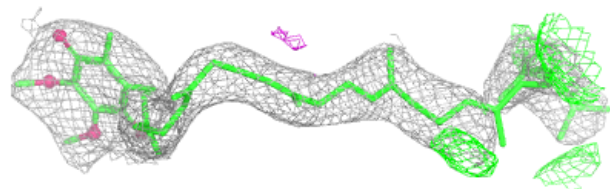
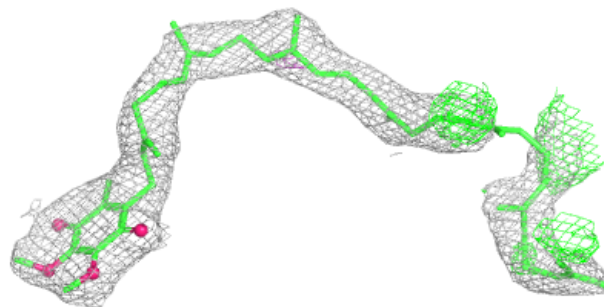


Electron density around U10 L 306 (B):

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

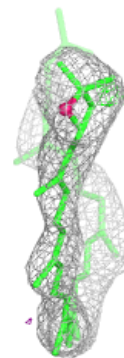
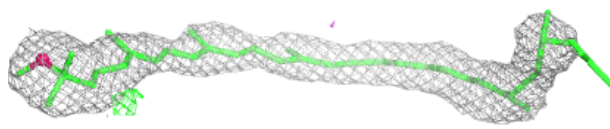
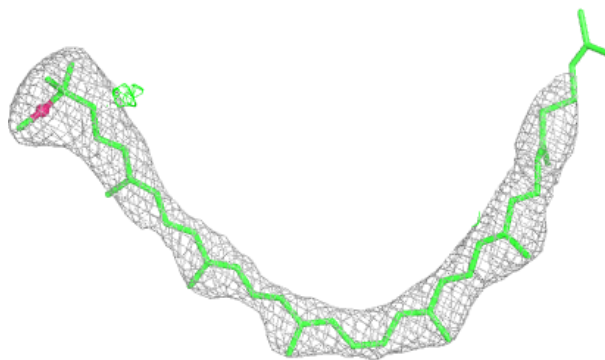
**Electron density around U10 M 407:**

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

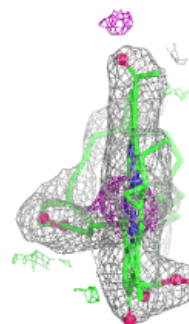
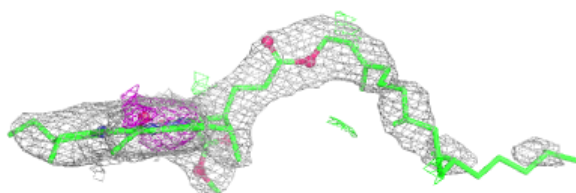
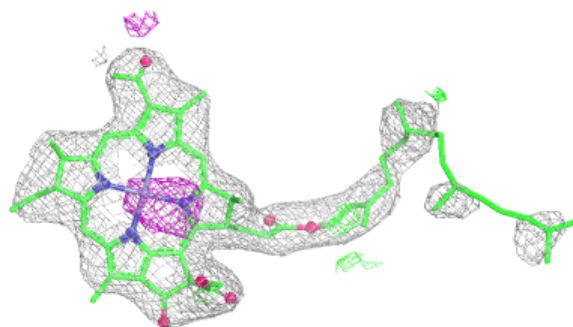


Electron density around SPO M 408:

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

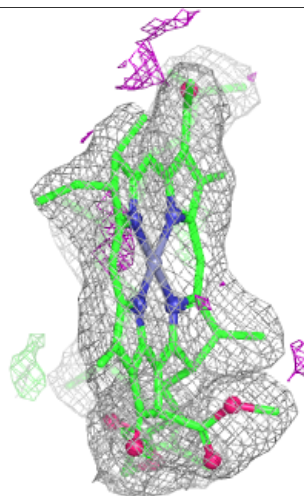
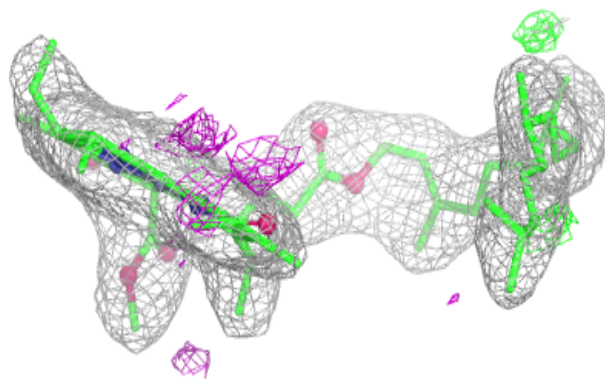
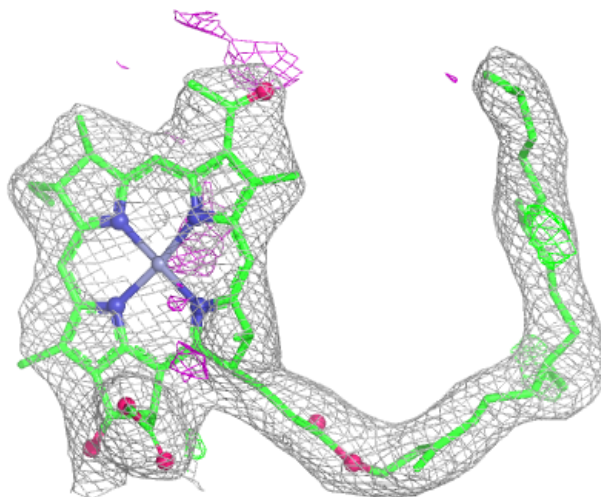
**Electron density around 2GO M 406:**

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



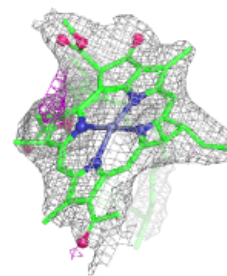
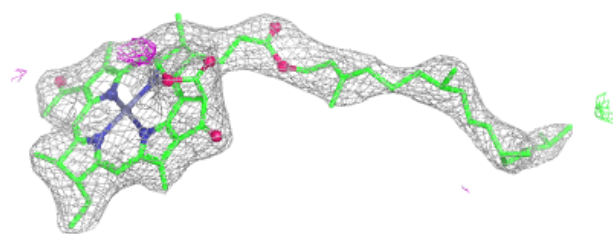
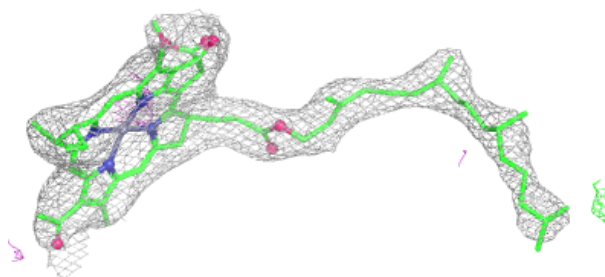
Electron density around 2GO L 305:

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

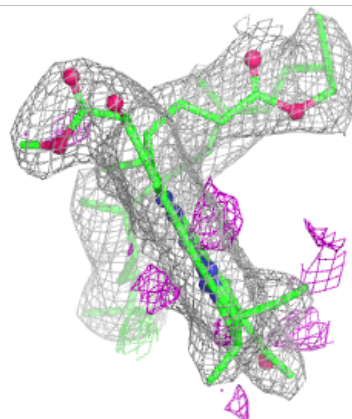
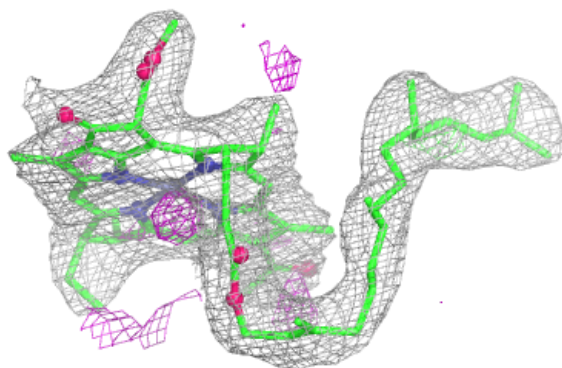
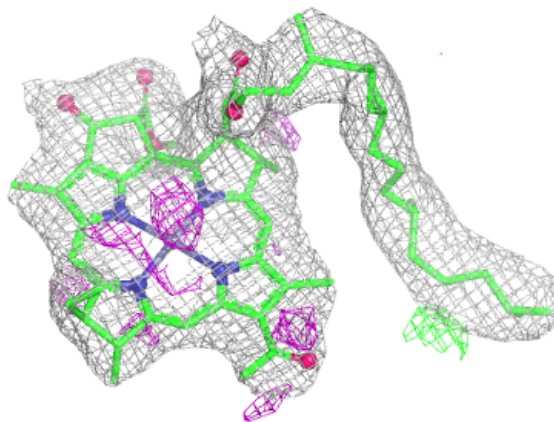


Electron density around 2GO M 402:

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

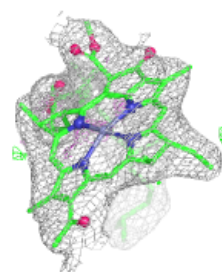
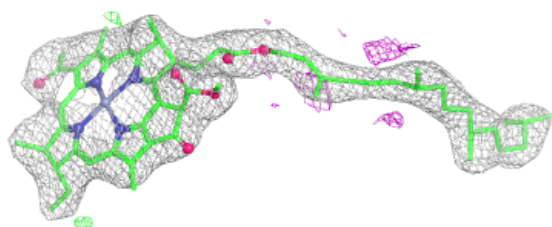
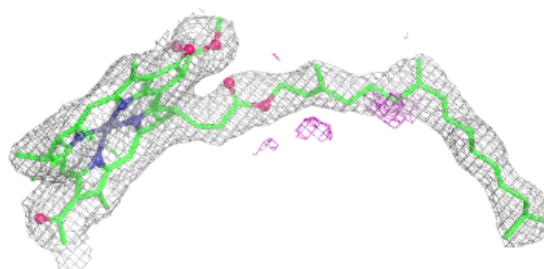
**Electron density around 2GO L 301:**

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

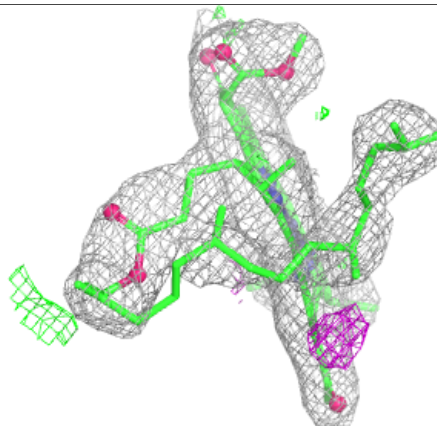
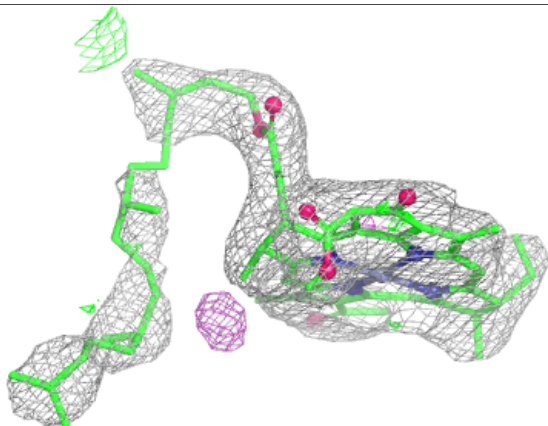
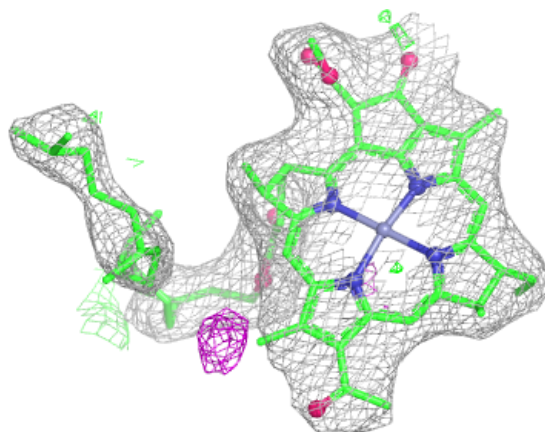


Electron density around 2GO L 307:

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

**Electron density around 2GO 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.