Full wwPDB X-ray Structure Validation Report (i)

Mar 8, 2026 – 05:16 PM UTC

PDB ID	:	1M3X / pdb_00001m3x
Title	:	Photosynthetic Reaction Center From Rhodobacter Sphaeroides
Authors	:	Camara-Artigas, A.; Brune, D.; Allen, J.P.
Deposited on	:	2002-07-01
Resolution	:	2.55 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 (i) 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 (i)) were used in the production of this report:

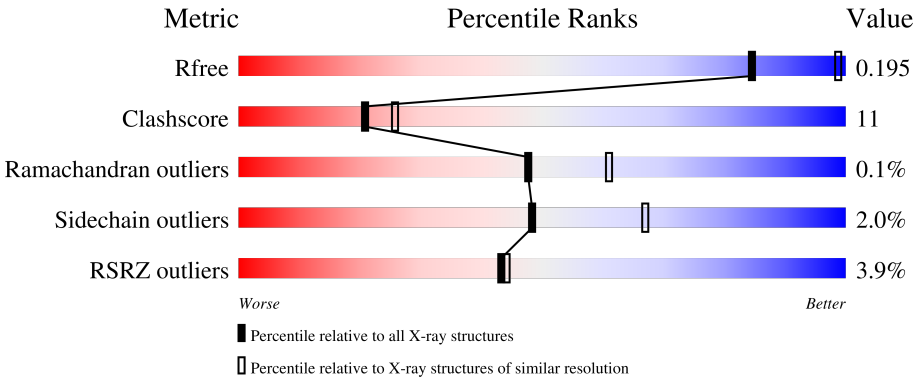
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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 <=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	L	281	5% 84% 15%
2	M	307	4% 75% 22%
3	H	260	2% 76% 15% 8%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 7323 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 Photosynthetic Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

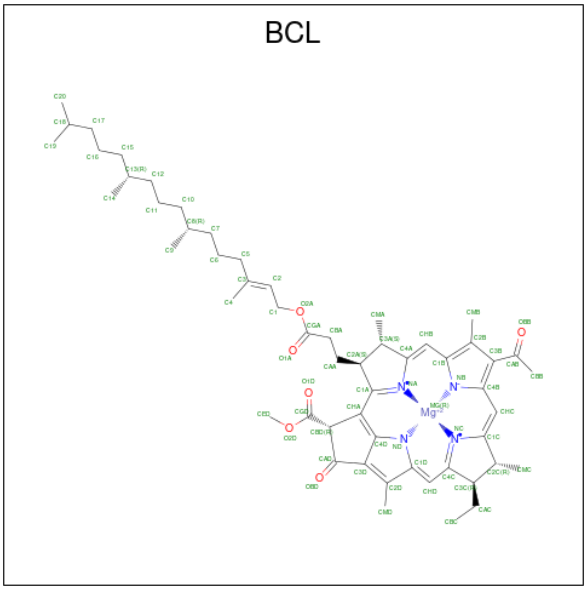
- Molecule 2 is a protein called Photosynthetic Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	0	0
			2408	1607	394	397	10			

- Molecule 3 is a protein called Photosynthetic Reaction center protein H chain.

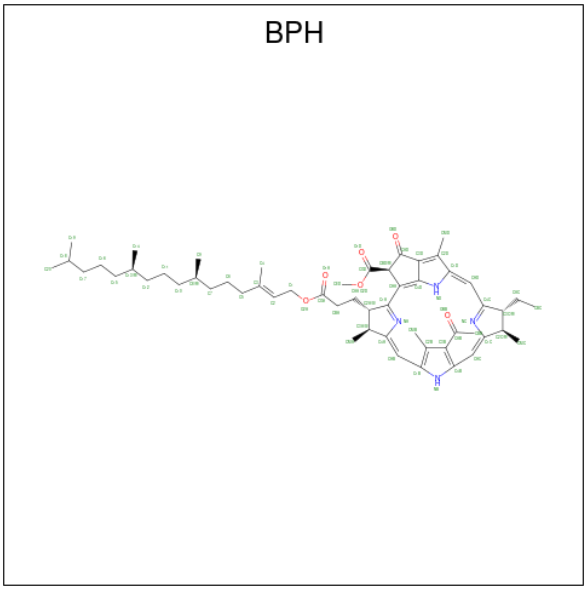
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	238	Total	C	N	O	S	0	0	0
			1814	1160	311	334	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



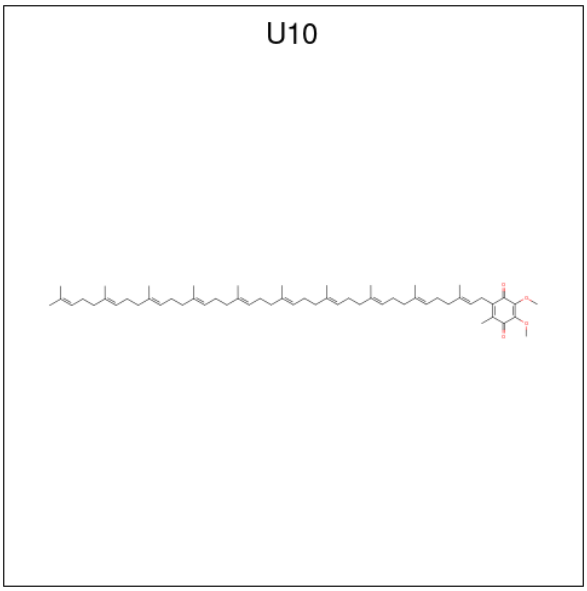
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			52	41	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



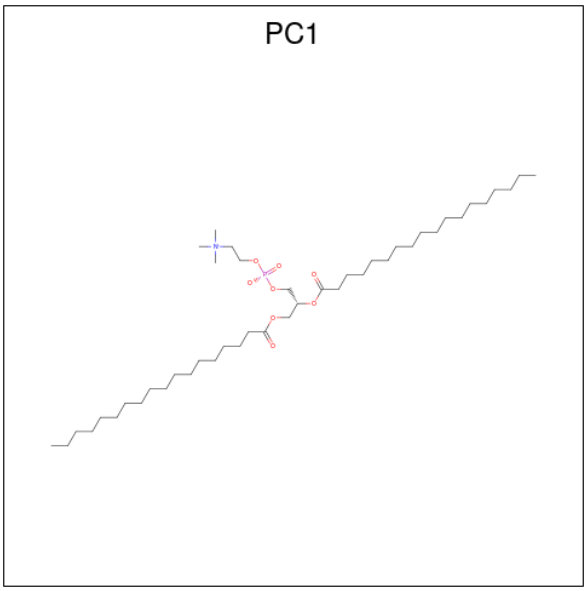
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C O 13 9 4	0	0
6	M	1	Total C O 48 44 4	0	0

- Molecule 7 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



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

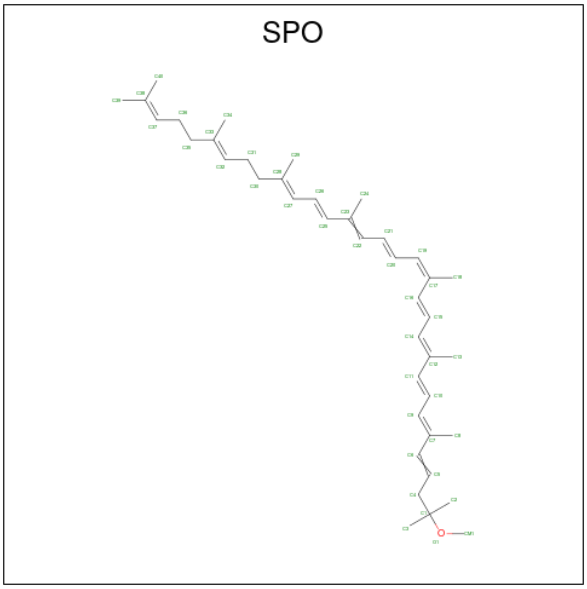
- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

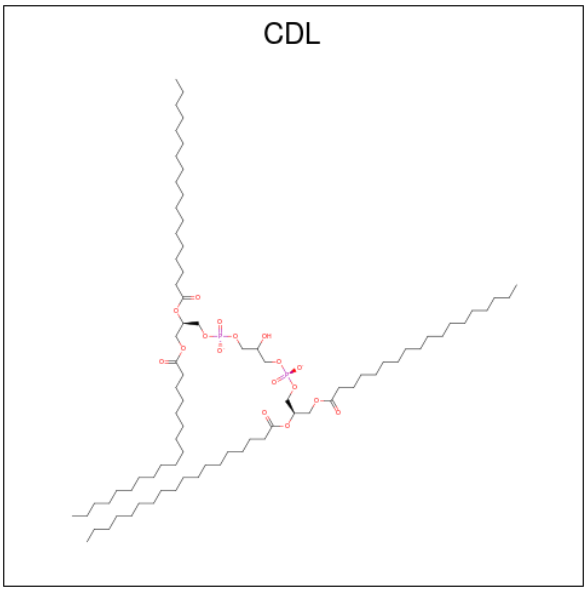
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total Cl 1 1	0	0

- Molecule 10 is SPHEROIDENE (CCD ID: SPO) (formula: $C_{41}H_{60}O$).



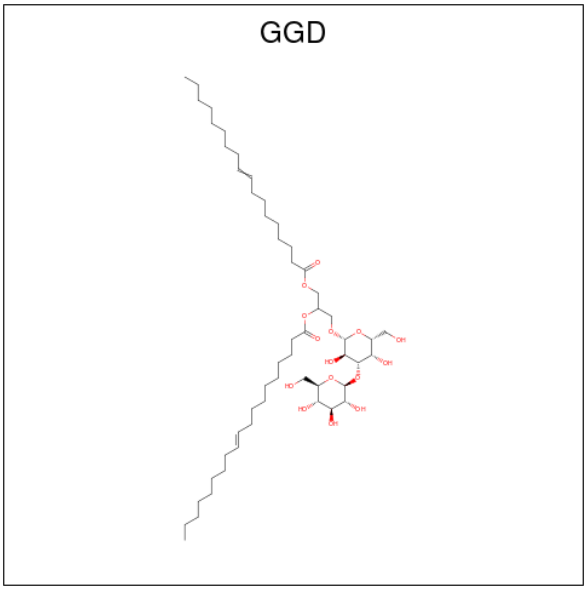
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total C O 42 41 1	0	0

- Molecule 11 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 12 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: $C_{52}H_{94}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			57	42	15		

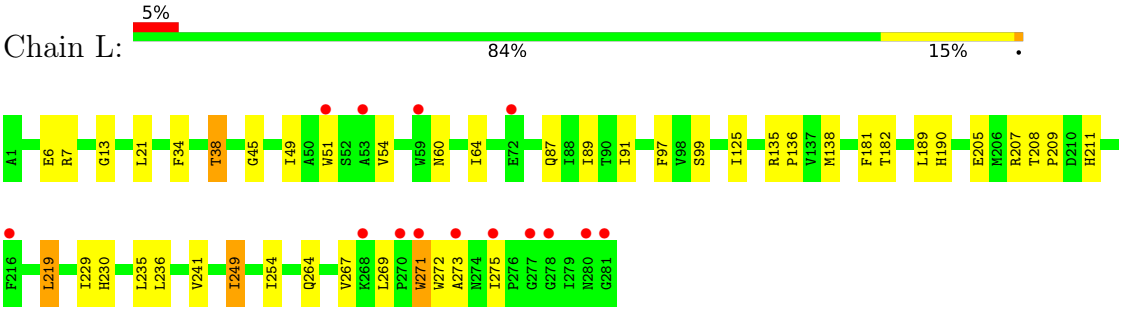
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	L	63	Total O 63 63	0	0
13	M	68	Total O 68 68	0	0
13	H	72	Total O 72 72	0	0

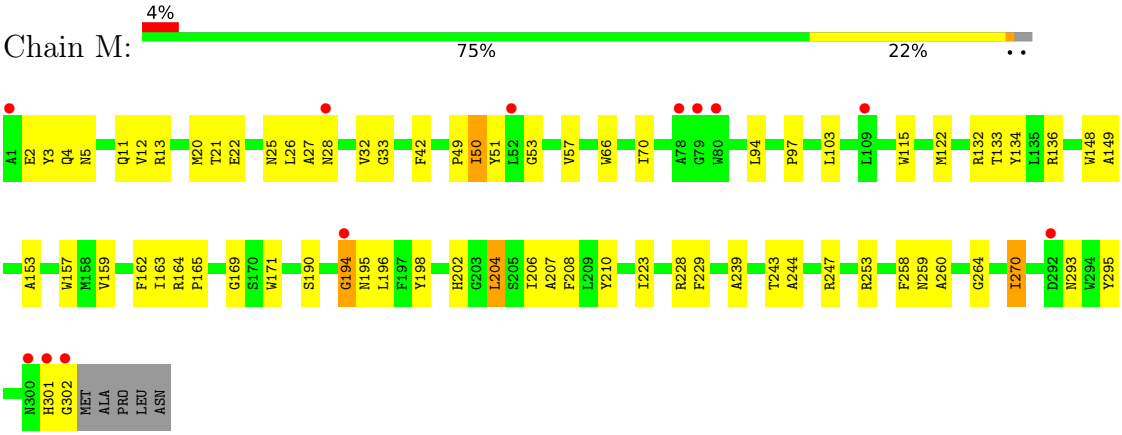
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

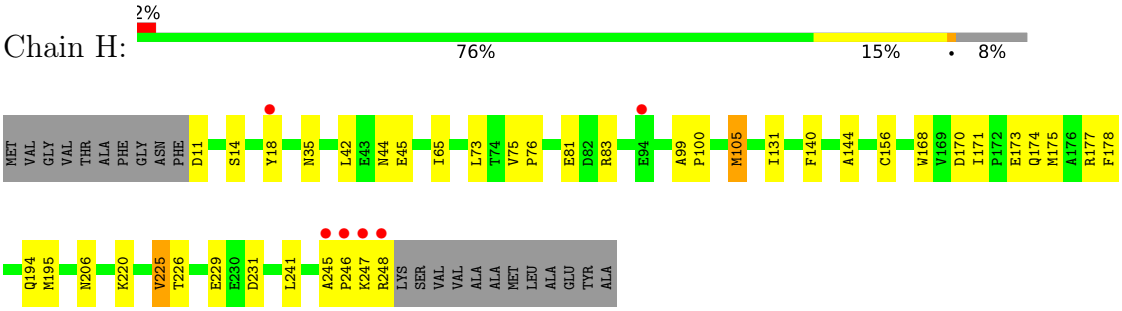
• Molecule 1: Photosynthetic Reaction center protein L chain



• Molecule 2: Photosynthetic Reaction center protein M chain



• Molecule 3: Photosynthetic Reaction center protein H chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.80Å 141.80Å 187.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.91 – 2.55 29.91 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.2 (29.91-2.55) 96.8 (29.91-2.55)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.54Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.185 , 0.209 0.181 , 0.195	Depositor DCC
R_{free} test set	6974 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 67.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7323	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FE, BCL, PC1, SPO, CDL, CL, BPH, U10, GGD

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	L	0.45	0/2320	0.89	4/3175 (0.1%)
2	M	0.44	0/2500	0.87	1/3413 (0.0%)
3	H	0.43	1/1862 (0.1%)	0.88	1/2534 (0.0%)
All	All	0.44	1/6682 (0.0%)	0.88	6/9122 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	171	ILE	CA-CB	5.25	1.57	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	6	GLU	N-CA-C	9.25	121.44	111.36
1	L	7	ARG	N-CA-C	6.29	118.94	111.33
2	M	194	GLY	N-CA-C	-5.98	99.00	113.18
3	H	44	ASN	N-CA-C	-5.50	102.62	110.59
1	L	13	GLY	N-CA-C	5.47	118.42	112.29
1	L	219	LEU	N-CA-C	5.28	116.84	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2187	49	0
2	M	2408	0	2321	69	0
3	H	1814	0	1818	39	0
4	L	184	0	191	11	0
4	M	66	0	74	3	0
5	L	65	0	76	5	0
5	M	65	0	76	6	0
6	L	13	0	9	2	0
6	M	48	0	63	3	0
7	L	43	0	60	8	0
8	M	1	0	0	0	0
9	M	1	0	0	0	0
10	M	42	0	60	0	0
11	M	81	0	106	0	0
12	M	57	0	65	16	0
13	H	72	0	0	3	0
13	L	63	0	0	1	0
13	M	68	0	0	1	0
All	All	7323	0	7106	158	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (158) 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)
7:L:901:PC1:C1	7:L:901:PC1:C2	1.74	1.64
7:L:901:PC1:C1	7:L:901:PC1:O11	1.74	1.35
1:L:271:TRP:H	1:L:271:TRP:CD1	1.88	0.86
2:M:202:HIS:O	2:M:206:ILE:HD13	1.78	0.84
7:L:901:PC1:C1	7:L:901:PC1:P	2.76	0.74
2:M:207:ALA:CB	12:M:902:GGD:OB3	2.36	0.73
2:M:253:ARG:HH22	12:M:902:GGD:C24	2.01	0.73
2:M:50:ILE:HD13	2:M:51:TYR:N	2.02	0.73
1:L:97:PHE:HB3	1:L:125:ILE:HD12	1.69	0.73
7:L:901:PC1:C1	7:L:901:PC1:C3	2.66	0.73
3:H:14:SER:O	3:H:18:TYR:HD1	1.72	0.73
1:L:49:ILE:HD13	1:L:89:ILE:HD13	1.70	0.72
1:L:34:PHE:O	1:L:38:THR:HG23	1.89	0.72
1:L:219:LEU:HD12	2:M:132:ARG:NH1	2.06	0.71
2:M:207:ALA:HB1	12:M:902:GGD:OB3	1.91	0.70
2:M:50:ILE:HD13	2:M:51:TYR:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.73	0.69
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.75	0.68
4:L:853:BCL:HBA1	12:M:902:GGD:OB3	1.94	0.67
1:L:241:VAL:HG21	5:L:855:BPH:HAC2	1.76	0.67
1:L:271:TRP:CD1	1:L:271:TRP:N	2.61	0.65
2:M:195:ASN:HB3	2:M:198:TYR:CD2	2.32	0.64
1:L:51:TRP:O	1:L:54:VAL:HG22	1.97	0.64
1:L:235:LEU:HD22	2:M:42:PHE:CZ	2.32	0.64
5:L:855:BPH:HBB2	2:M:210:TYR:HB3	1.80	0.63
2:M:228:ARG:HB3	3:H:195:MET:HE3	1.80	0.63
2:M:204:LEU:O	2:M:207:ALA:HB3	1.98	0.63
1:L:97:PHE:HB3	1:L:125:ILE:CD1	2.29	0.62
3:H:156:CYS:HB2	3:H:248:ARG:HG3	1.82	0.60
1:L:219:LEU:HA	2:M:132:ARG:HH12	1.65	0.60
12:M:902:GGD:C24	3:H:42:LEU:HD11	2.31	0.60
2:M:32:VAL:HG22	2:M:49:PRO:HD3	1.84	0.59
2:M:302:GLY:HA2	3:H:11:ASP:OD1	2.01	0.59
1:L:38:THR:HG22	1:L:99:SER:HB3	1.85	0.59
7:L:901:PC1:C2	7:L:901:PC1:H11	2.18	0.59
2:M:11:GLN:HB2	3:H:144:ALA:HB3	1.84	0.59
1:L:45:GLY:O	1:L:49:ILE:HG12	2.04	0.58
1:L:38:THR:HG22	1:L:99:SER:CB	2.35	0.57
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.85	0.57
2:M:207:ALA:HB2	12:M:902:GGD:OB3	2.04	0.57
5:L:855:BPH:HBB3	5:L:855:BPH:HHC	1.87	0.56
3:H:156:CYS:SG	3:H:248:ARG:HB2	2.46	0.56
12:M:902:GGD:C24	3:H:42:LEU:HD21	2.36	0.56
1:L:190:HIS:HB2	1:L:229:ILE:HD11	1.88	0.55
4:L:850:BCL:HBB2	4:M:852:BCL:H111	1.88	0.55
1:L:219:LEU:HD12	2:M:132:ARG:HH11	1.72	0.55
4:L:853:BCL:H193	5:L:855:BPH:H111	1.88	0.55
3:H:105:MET:HA	3:H:105:MET:HE2	1.87	0.55
2:M:243:THR:O	2:M:247:ARG:HG3	2.07	0.54
3:H:131:ILE:HD13	3:H:170:ASP:HA	1.89	0.54
2:M:190:SER:O	2:M:194:GLY:O	2.25	0.54
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.08	0.54
2:M:13:ARG:O	3:H:140:PHE:HA	2.07	0.54
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.90	0.54
2:M:253:ARG:HB2	2:M:259:ASN:HD22	1.72	0.54
2:M:208:PHE:CE1	12:M:902:GGD:OA4	2.61	0.53
1:L:181:PHE:HB3	5:M:854:BPH:CBB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:28:ASN:HB2	2:M:51:TYR:CE1	2.43	0.53
6:M:857:U10:H202	12:M:902:GGD:HC31	1.90	0.53
1:L:211:HIS:CE1	2:M:20:MET:HE2	2.44	0.53
1:L:264:GLN:HA	1:L:267:VAL:CG1	2.39	0.53
2:M:208:PHE:HE1	12:M:902:GGD:OA4	1.92	0.53
2:M:25:ASN:OD1	2:M:27:ALA:HB3	2.09	0.52
2:M:258:PHE:CE1	12:M:902:GGD:H151	2.44	0.52
1:L:189:LEU:HB3	6:L:858:U10:H4M3	1.91	0.52
1:L:272:TRP:HA	1:L:275:ILE:HG12	1.92	0.52
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.09	0.52
3:H:65:ILE:HD12	3:H:65:ILE:N	2.24	0.52
3:H:220:LYS:HE3	13:H:1054:HOH:O	2.10	0.52
1:L:49:ILE:CD1	1:L:89:ILE:HD13	2.37	0.52
1:L:219:LEU:O	2:M:132:ARG:NH1	2.41	0.52
3:H:45:GLU:HG3	13:H:1081:HOH:O	2.09	0.52
1:L:254:ILE:C	1:L:254:ILE:HD12	2.36	0.51
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.46	0.51
1:L:181:PHE:CD2	5:M:854:BPH:HBB1	2.45	0.51
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.46	0.51
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.92	0.51
7:L:901:PC1:C2	7:L:901:PC1:H12	2.18	0.51
1:L:190:HIS:HB2	1:L:229:ILE:CD1	2.41	0.50
2:M:94:LEU:HD21	2:M:115:TRP:HA	1.93	0.50
1:L:181:PHE:HB3	5:M:854:BPH:HBB2	1.94	0.50
1:L:60:ASN:O	1:L:64:ILE:HG12	2.10	0.50
3:H:81:GLU:O	3:H:83:ARG:HG2	2.12	0.50
1:L:269:LEU:HD12	1:L:272:TRP:CZ2	2.47	0.50
2:M:149:ALA:HB2	2:M:270:ILE:HD11	1.94	0.49
1:L:219:LEU:HD11	2:M:133:THR:HG22	1.95	0.49
3:H:75:VAL:HA	3:H:76:PRO:C	2.38	0.49
2:M:253:ARG:NH2	12:M:902:GGD:C24	2.74	0.49
3:H:248:ARG:HG2	3:H:248:ARG:O	2.12	0.49
1:L:219:LEU:HA	2:M:132:ARG:NH1	2.27	0.48
1:L:34:PHE:O	1:L:38:THR:CG2	2.60	0.48
1:L:235:LEU:HD22	2:M:42:PHE:HZ	1.78	0.48
7:L:901:PC1:C1	7:L:901:PC1:H2	2.19	0.48
3:H:245:ALA:HB3	3:H:246:PRO:HD3	1.95	0.48
3:H:248:ARG:HB2	3:H:248:ARG:NH1	2.29	0.47
4:L:851:BCL:H122	5:L:855:BPH:H3A	1.97	0.47
2:M:228:ARG:CZ	3:H:195:MET:HE1	2.45	0.47
3:H:175:MET:HE1	3:H:177:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:241:LEU:HB2	13:H:1089:HOH:O	2.15	0.47
1:L:138:MET:SD	1:L:249:ILE:HD11	2.55	0.46
4:L:850:BCL:HAA2	4:L:850:BCL:HBD	1.98	0.46
2:M:21:THR:HG23	2:M:26:LEU:HD21	1.95	0.46
1:L:208:THR:HB	1:L:209:PRO:HD2	1.98	0.46
6:M:857:U10:H222	6:M:857:U10:H201	1.59	0.46
2:M:208:PHE:HE1	12:M:902:GGD:HO41	1.57	0.45
2:M:208:PHE:HE1	12:M:902:GGD:HA62	1.81	0.45
1:L:230:HIS:CD2	2:M:223:ILE:HG13	2.52	0.45
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.98	0.45
3:H:245:ALA:C	3:H:247:LYS:H	2.23	0.45
1:L:235:LEU:HD23	7:L:901:PC1:C2B	2.47	0.45
1:L:219:LEU:C	2:M:132:ARG:HH12	2.24	0.45
1:L:229:ILE:O	1:L:229:ILE:HG12	2.16	0.45
1:L:219:LEU:CA	2:M:132:ARG:HH12	2.29	0.45
4:M:852:BCL:HAA2	4:M:852:BCL:HBD	1.98	0.45
2:M:153:ALA:HB2	5:M:854:BPH:HAC1	1.98	0.44
2:M:32:VAL:HG12	2:M:33:GLY:O	2.16	0.44
2:M:132:ARG:O	2:M:136:ARG:HG2	2.17	0.44
3:H:131:ILE:CD1	3:H:177:ARG:HD2	2.47	0.44
3:H:194:GLN:H	3:H:194:GLN:CD	2.26	0.44
4:L:853:BCL:HBA1	12:M:902:GGD:CB3	2.47	0.44
2:M:162:PHE:C	2:M:165:PRO:HD2	2.43	0.44
3:H:156:CYS:SG	3:H:248:ARG:HA	2.58	0.44
4:L:850:BCL:H11	5:M:854:BPH:HBB2	2.01	0.43
2:M:66:TRP:O	2:M:70:ILE:HG12	2.18	0.43
2:M:239:ALA:O	3:H:73:LEU:HD22	2.17	0.43
4:L:850:BCL:HBB1	2:M:157:TRP:CD1	2.54	0.43
2:M:53:GLY:O	2:M:57:VAL:HG23	2.18	0.43
2:M:159:VAL:HA	2:M:163:ILE:HB	1.99	0.43
3:H:206:ASN:O	3:H:248:ARG:HD3	2.19	0.43
1:L:205:GLU:HG3	13:L:1122:HOH:O	2.18	0.43
2:M:293:ASN:OD1	2:M:295:TYR:HB3	2.19	0.43
2:M:202:HIS:O	2:M:206:ILE:CD1	2.58	0.42
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.54	0.42
1:L:229:ILE:HD12	6:L:858:U10:O4	2.19	0.42
4:L:853:BCL:H61	6:M:857:U10:H203	2.01	0.42
2:M:2:GLU:HG3	2:M:4:GLN:NE2	2.34	0.42
2:M:134:TYR:C	2:M:134:TYR:CD1	2.97	0.42
1:L:269:LEU:HD12	1:L:272:TRP:HZ2	1.84	0.42
3:H:99:ALA:HA	3:H:100:PRO:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:168:TRP:CZ3	3:H:225:VAL:HG22	2.54	0.42
4:L:850:BCL:H2	5:M:854:BPH:CMB	2.50	0.42
1:L:87:GLN:O	1:L:91:ILE:HG12	2.21	0.41
2:M:49:PRO:HG2	13:M:1045:HOH:O	2.19	0.41
2:M:103:LEU:HG	2:M:169:GLY:O	2.20	0.41
1:L:182:THR:HG22	1:L:236:LEU:HD13	2.03	0.41
2:M:195:ASN:HB3	2:M:198:TYR:CE2	2.55	0.41
4:L:851:BCL:H112	4:L:853:BCL:HBB2	2.03	0.41
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.21	0.41
2:M:228:ARG:CB	3:H:195:MET:HE3	2.49	0.41
4:M:852:BCL:HBC2	4:M:852:BCL:H2C	1.94	0.41
12:M:902:GGD:OC7	12:M:902:GGD:HC32	2.21	0.41
2:M:21:THR:O	2:M:22:GLU:C	2.64	0.41
3:H:173:GLU:O	3:H:174:GLN:C	2.64	0.41
1:L:269:LEU:O	1:L:273:ALA:HB2	2.21	0.40
3:H:156:CYS:HB3	3:H:206:ASN:O	2.21	0.40
2:M:302:GLY:HA2	3:H:11:ASP:CG	2.46	0.40
1:L:190:HIS:ND1	1:L:229:ILE:HD13	2.37	0.40
3:H:131:ILE:HD12	3:H:177:ARG:HD2	2.03	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	L	279/281 (99%)	267 (96%)	12 (4%)	0	100 100
2	M	300/307 (98%)	289 (96%)	10 (3%)	1 (0%)	36 45
3	H	236/260 (91%)	227 (96%)	9 (4%)	0	100 100
All	All	815/848 (96%)	783 (96%)	31 (4%)	1 (0%)	48 61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	301	HIS

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	L	220/220 (100%)	215 (98%)	5 (2%)	44	62
2	M	236/240 (98%)	231 (98%)	5 (2%)	47	66
3	H	193/208 (93%)	190 (98%)	3 (2%)	55	73
All	All	649/668 (97%)	636 (98%)	13 (2%)	48	67

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	38	THR
1	L	207	ARG
1	L	249	ILE
1	L	271	TRP
2	M	12	VAL
2	M	50	ILE
2	M	196	LEU
2	M	204	LEU
2	M	270	ILE
3	H	105	MET
3	H	225	VAL
3	H	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	258	GLN
1	L	274	ASN
2	M	4	GLN
2	M	188	ASN

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Mol	Chain	Res	Type
2	M	259	ASN
2	M	299	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	BPH	M	854	-	59,70,70	1.84	13 (22%)	59,101,101	2.41	16 (27%)
6	U10	L	858	-	13,13,63	3.10	6 (46%)	16,18,79	1.57	5 (31%)
4	BCL	L	851	-	69,74,74	1.39	11 (15%)	79,115,115	1.66	16 (20%)
4	BCL	L	850	-	55,60,74	1.52	10 (18%)	61,98,115	1.99	20 (32%)
7	PC1	L	901	-	42,42,53	2.45	13 (30%)	48,50,61	1.71	11 (22%)
10	SPO	M	859	-	41,41,41	3.33	22 (53%)	47,50,50	2.77	16 (34%)
12	GGD	M	902	-	58,58,68	2.98	20 (34%)	72,72,82	4.38	34 (47%)
6	U10	M	857	-	48,48,63	2.42	13 (27%)	60,61,79	2.15	20 (33%)
4	BCL	L	853	-	69,74,74	1.50	12 (17%)	79,115,115	2.03	24 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	CDL	M	900	-	80,80,99	0.67	2 (2%)	86,92,111	0.92	5 (5%)
4	BCL	M	852	-	69,74,74	1.33	8 (11%)	79,115,115	1.74	18 (22%)
5	BPH	L	855	-	59,70,70	1.79	9 (15%)	59,101,101	2.56	18 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BPH	M	854	-	-	7/37/105/105	0/5/6/6
6	U10	L	858	-	-	2/4/24/87	0/1/1/1
4	BCL	L	851	-	-	5/41/137/137	-
4	BCL	L	850	-	-	3/25/121/137	-
7	PC1	L	901	-	-	15/46/46/57	-
10	SPO	M	859	-	-	14/47/47/47	-
12	GGD	M	902	-	-	27/47/87/97	0/2/2/2
6	U10	M	857	-	-	14/45/69/87	0/1/1/1
4	BCL	L	853	-	-	5/41/137/137	-
11	CDL	M	900	-	-	28/91/91/110	-
4	BCL	M	852	-	-	8/41/137/137	-
5	BPH	L	855	-	-	9/37/105/105	0/5/6/6

All (139) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	902	GGD	OC6-CC4	-12.98	1.16	1.46
6	M	857	U10	C6-C1	9.89	1.52	1.35
10	M	859	SPO	C15-C16	9.23	1.58	1.34
6	L	858	U10	C6-C1	8.44	1.52	1.35
12	M	902	GGD	OA1-CC3	8.39	1.58	1.43
7	L	901	PC1	O11-C1	7.97	1.74	1.44
7	L	901	PC1	C1-C2	7.64	1.74	1.50
5	L	855	BPH	C3A-C2A	-7.62	1.48	1.54
10	M	859	SPO	C10-C11	7.08	1.53	1.34
5	M	854	BPH	C3A-C2A	-6.95	1.48	1.54
10	M	859	SPO	C6-C5	6.86	1.51	1.32
12	M	902	GGD	OB5-CB5	6.04	1.59	1.44
10	M	859	SPO	C21-C20	5.61	1.51	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	902	GGD	OC6-CC5	5.28	1.49	1.34
7	L	901	PC1	O21-C21	5.20	1.49	1.34
5	M	854	BPH	C3D-C2D	4.99	1.48	1.39
12	M	902	GGD	OB4-CB4	4.94	1.55	1.43
10	M	859	SPO	C26-C25	4.85	1.47	1.34
6	M	857	U10	C4-C3	4.70	1.53	1.36
10	M	859	SPO	C13-C12	4.61	1.60	1.50
6	M	857	U10	C7-C8	-4.59	1.43	1.50
4	L	853	BCL	C2-C3	4.52	1.43	1.33
6	L	858	U10	C4-C3	4.39	1.52	1.36
12	M	902	GGD	OB5-CB1	4.34	1.53	1.41
4	L	851	BCL	C3D-C2D	4.31	1.50	1.39
12	M	902	GGD	C24-C23	-4.30	1.31	1.49
12	M	902	GGD	OB2-CB2	4.24	1.53	1.43
5	L	855	BPH	C3D-C2D	4.11	1.46	1.39
7	L	901	PC1	O31-C31	4.07	1.45	1.33
10	M	859	SPO	C15-C14	4.03	1.55	1.43
12	M	902	GGD	OB6-CB6	-4.02	1.25	1.42
4	L	853	BCL	C3D-C2D	4.02	1.50	1.39
4	L	850	BCL	C2-C3	4.00	1.42	1.33
6	M	857	U10	C7-C6	3.95	1.58	1.51
5	L	855	BPH	C3B-C4B	3.92	1.47	1.41
10	M	859	SPO	O1-CM1	3.88	1.55	1.43
4	M	852	BCL	C3D-C2D	3.86	1.49	1.39
6	M	857	U10	C6-C5	3.82	1.57	1.46
4	L	850	BCL	C3D-C2D	3.80	1.49	1.39
5	L	855	BPH	C3B-C2B	3.79	1.46	1.39
10	M	859	SPO	C35-C33	3.66	1.58	1.51
5	M	854	BPH	C3B-C2B	3.64	1.45	1.39
12	M	902	GGD	C31-CC7	3.64	1.61	1.50
10	M	859	SPO	C4-C5	-3.64	1.44	1.50
4	L	851	BCL	CMB-C2B	3.60	1.58	1.50
10	M	859	SPO	C32-C33	3.55	1.41	1.33
12	M	902	GGD	CA4-CA5	3.53	1.60	1.53
6	L	858	U10	C6-C5	3.47	1.54	1.44
12	M	902	GGD	C39-C38	3.45	1.51	1.31
10	M	859	SPO	C10-C9	3.42	1.53	1.43
5	M	854	BPH	CMB-C2B	3.41	1.58	1.51
6	M	857	U10	C28-C29	3.41	1.40	1.33
5	L	855	BPH	C3D-CAD	-3.40	1.41	1.47
6	M	857	U10	C18-C19	3.39	1.40	1.33
4	L	853	BCL	CMB-C2B	3.37	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	850	BCL	CMB-C2B	3.35	1.57	1.50
10	M	859	SPO	C11-C12	-3.32	1.38	1.46
7	L	901	PC1	P-O12	-3.29	1.40	1.55
5	M	854	BPH	C3B-C4B	3.28	1.46	1.41
4	M	852	BCL	CMB-C2B	3.25	1.57	1.50
10	M	859	SPO	C37-C38	3.24	1.42	1.32
6	M	857	U10	C33-C34	3.20	1.40	1.33
4	L	850	BCL	C3B-C4B	3.17	1.47	1.41
4	M	852	BCL	C2-C3	3.16	1.40	1.33
7	L	901	PC1	P-O14	3.13	1.61	1.50
4	L	851	BCL	C2-C3	3.12	1.40	1.33
10	M	859	SPO	O1-C1	3.12	1.59	1.41
4	M	852	BCL	CMD-C2D	3.11	1.57	1.50
10	M	859	SPO	C31-C32	-3.09	1.41	1.50
10	M	859	SPO	C8-C7	3.06	1.57	1.50
5	L	855	BPH	CMB-C2B	3.05	1.57	1.51
5	M	854	BPH	C2-C3	3.05	1.40	1.33
4	M	852	BCL	CBB-CAB	2.99	1.56	1.50
5	M	854	BPH	C3D-CAD	-2.99	1.42	1.47
6	M	857	U10	C13-C14	2.96	1.39	1.33
6	M	857	U10	C23-C24	2.95	1.39	1.33
7	L	901	PC1	O22-C21	2.94	1.31	1.22
4	L	853	BCL	C3A-C2A	-2.93	1.46	1.54
4	L	851	BCL	CBB-CAB	2.93	1.55	1.50
4	M	852	BCL	C3B-CAB	2.90	1.55	1.46
4	L	853	BCL	C3C-C4C	-2.87	1.48	1.51
12	M	902	GGD	CB4-CB5	2.84	1.59	1.53
12	M	902	GGD	C15-C14	2.84	1.62	1.52
5	L	855	BPH	C2-C3	2.84	1.39	1.33
4	L	853	BCL	C3B-C4B	2.79	1.46	1.41
4	L	851	BCL	CMD-C2D	2.78	1.56	1.50
4	L	850	BCL	C3B-CAB	2.76	1.55	1.46
10	M	859	SPO	C29-C28	2.75	1.57	1.50
4	L	851	BCL	C1D-C2D	-2.75	1.39	1.45
4	L	850	BCL	CBB-CAB	2.74	1.55	1.50
4	L	853	BCL	CBB-CAB	2.73	1.55	1.50
5	M	854	BPH	CMD-C2D	2.71	1.57	1.51
5	M	854	BPH	C2C-C3C	-2.70	1.52	1.54
12	M	902	GGD	OC7-CC5	2.65	1.30	1.22
4	L	851	BCL	C3B-C4B	2.62	1.46	1.41
7	L	901	PC1	C2A-C29	2.62	1.67	1.51
6	M	857	U10	C38-C39	2.60	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	902	GGD	CC6-CC4	-2.59	1.42	1.50
4	M	852	BCL	C1D-C2D	-2.54	1.40	1.45
4	L	851	BCL	C3B-CAB	2.53	1.54	1.46
5	L	855	BPH	O2A-CGA	-2.53	1.26	1.33
12	M	902	GGD	OB3-CB3	-2.53	1.36	1.43
10	M	859	SPO	C24-C23	2.53	1.55	1.50
7	L	901	PC1	O31-C3	2.51	1.50	1.45
4	M	852	BCL	C3B-C4B	2.51	1.46	1.41
4	L	853	BCL	CMD-C2D	2.51	1.55	1.50
4	L	853	BCL	C3B-CAB	2.50	1.54	1.46
4	L	853	BCL	CAA-CBA	-2.47	1.45	1.52
7	L	901	PC1	P-O11	-2.47	1.49	1.59
12	M	902	GGD	OB1-CA3	2.46	1.50	1.43
5	L	855	BPH	CMD-C2D	2.43	1.56	1.51
6	L	858	U10	C4-C5	2.43	1.52	1.46
4	L	851	BCL	C3C-C4C	-2.41	1.48	1.51
6	M	857	U10	O4-C4	2.40	1.42	1.36
7	L	901	PC1	C3-C2	2.40	1.58	1.50
5	M	854	BPH	C4D-CHA	2.40	1.43	1.39
5	M	854	BPH	CBD-CGD	2.39	1.55	1.52
4	L	850	BCL	C3A-C2A	-2.39	1.48	1.54
10	M	859	SPO	C14-C12	2.39	1.41	1.35
12	M	902	GGD	OA1-CA1	-2.37	1.36	1.40
4	L	851	BCL	CAC-C3C	2.30	1.58	1.54
5	M	854	BPH	C1A-C2A	2.25	1.54	1.51
4	L	853	BCL	C1D-C2D	-2.24	1.40	1.45
7	L	901	PC1	C12-N	-2.23	1.44	1.51
4	L	850	BCL	O2D-CGD	-2.21	1.27	1.33
10	M	859	SPO	C19-C17	2.20	1.40	1.35
4	L	850	BCL	C1D-C2D	-2.19	1.41	1.45
4	L	850	BCL	CMD-C2D	2.17	1.55	1.50
11	M	900	CDL	OA8-CA7	2.17	1.39	1.33
10	M	859	SPO	C25-C23	-2.17	1.41	1.46
6	L	858	U10	O4-C4	2.16	1.42	1.36
12	M	902	GGD	C22-C23	2.13	1.45	1.29
6	M	857	U10	O3-C3	2.12	1.41	1.36
4	L	851	BCL	O2A-CGA	-2.12	1.27	1.33
5	M	854	BPH	O2A-CGA	-2.11	1.27	1.33
7	L	901	PC1	O21-C2	2.08	1.51	1.46
4	L	853	BCL	MG-NB	2.05	2.09	2.05
11	M	900	CDL	CB3-CB4	2.05	1.57	1.50
6	L	858	U10	C1-C2	2.04	1.50	1.47

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	902	GGD	CB1-OB1-CA3	20.16	165.77	117.98
12	M	902	GGD	OA1-CC3-CC4	16.36	150.62	110.82
10	M	859	SPO	C25-C23-C22	-11.15	101.47	119.01
5	L	855	BPH	C4D-CHA-CBD	-9.86	103.72	108.45
12	M	902	GGD	CC4-OC6-CC5	9.59	140.74	117.80
5	M	854	BPH	C4D-CHA-CBD	-8.91	104.18	108.45
12	M	902	GGD	C32-C31-CC7	7.89	142.59	113.69
12	M	902	GGD	C15-C14-CC5	7.65	141.73	113.69
4	L	853	BCL	CAA-C2A-C1A	-7.34	87.93	111.97
12	M	902	GGD	CC3-OA1-CA1	-7.21	98.34	113.80
12	M	902	GGD	CA1-CA2-CA3	-6.92	98.08	110.11
6	M	857	U10	C7-C6-C5	6.66	126.26	118.52
12	M	902	GGD	C21-C22-C23	-6.54	80.89	130.48
5	M	854	BPH	C1-O2A-CGA	6.12	131.47	116.65
5	M	854	BPH	O2D-CGD-CBD	6.11	117.66	110.95
5	L	855	BPH	C1-O2A-CGA	5.88	130.90	116.65
12	M	902	GGD	OB1-CA3-CA2	-5.82	92.45	107.23
5	L	855	BPH	C3D-C4D-ND	5.64	114.94	107.71
5	L	855	BPH	C4-C3-C5	5.42	124.63	115.23
5	L	855	BPH	O2D-CGD-CBD	5.39	116.87	110.95
5	M	854	BPH	C3D-C4D-ND	5.39	114.62	107.71
10	M	859	SPO	C20-C21-C22	-5.38	112.50	123.52
10	M	859	SPO	C26-C27-C28	-5.38	120.12	127.69
10	M	859	SPO	C18-C17-C19	-5.23	114.34	122.82
4	M	852	BCL	C4D-CHA-C1A	5.10	127.33	121.24
12	M	902	GGD	OC6-CC4-CC6	5.06	126.51	108.34
6	M	857	U10	C7-C6-C1	-4.96	116.39	124.89
12	M	902	GGD	OC8-CC7-C31	4.90	126.78	111.83
12	M	902	GGD	CC6-OC8-CC7	4.89	135.00	117.12
4	L	850	BCL	CAA-C2A-C1A	-4.86	96.05	111.97
12	M	902	GGD	OB1-CA3-CA4	4.77	119.35	107.23
4	L	850	BCL	CMB-C2B-C1B	-4.71	118.25	125.42
4	L	853	BCL	CHC-C4B-NB	-4.63	117.10	124.05
6	M	857	U10	C15-C14-C16	4.57	123.16	115.23
4	L	851	BCL	CMB-C2B-C1B	-4.54	118.51	125.42
5	M	854	BPH	CMB-C2B-C3B	4.46	133.59	124.68
4	L	850	BCL	CHC-C4B-NB	-4.44	117.39	124.05
4	L	853	BCL	CMB-C2B-C1B	-4.36	118.78	125.42
5	L	855	BPH	O1D-CGD-CBD	-4.31	118.19	124.72
6	M	857	U10	C10-C9-C8	-4.29	112.61	123.63
5	L	855	BPH	CMB-C2B-C3B	4.29	133.25	124.68
5	M	854	BPH	O1D-CGD-CBD	-4.28	118.24	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	855	BPH	C6-C5-C3	4.28	123.89	113.47
4	M	852	BCL	CED-O2D-CGD	4.27	125.61	115.92
6	M	857	U10	C15-C14-C13	-4.22	112.79	123.63
4	M	852	BCL	CHC-C4B-NB	-4.22	117.72	124.05
4	L	851	BCL	CED-O2D-CGD	4.22	125.48	115.92
4	M	852	BCL	CMB-C2B-C1B	-4.21	119.00	125.42
4	L	851	BCL	CHC-C4B-NB	-4.19	117.77	124.05
4	L	853	BCL	CAA-C2A-C3A	-4.14	101.80	113.00
12	M	902	GGD	OC8-CC6-CC4	4.11	120.25	108.40
12	M	902	GGD	OC6-CC4-CC3	4.05	122.87	108.34
4	L	853	BCL	C4A-NA-C1A	4.03	108.52	106.68
5	M	854	BPH	C2B-C1B-NB	4.01	112.33	109.43
10	M	859	SPO	C4-C5-C6	-3.99	119.31	124.91
7	L	901	PC1	O21-C21-C22	3.98	120.10	111.48
5	L	855	BPH	C2B-C1B-NB	3.98	112.31	109.43
10	M	859	SPO	C24-C23-C22	-3.97	116.38	122.82
4	L	853	BCL	CED-O2D-CGD	3.96	124.91	115.92
7	L	901	PC1	O21-C21-O22	-3.95	114.47	123.70
4	L	850	BCL	C4D-CHA-C1A	3.93	125.93	121.24
5	M	854	BPH	C4-C3-C5	3.89	121.98	115.23
7	L	901	PC1	P-O13-C11	3.82	139.45	121.26
4	M	852	BCL	C6-C5-C3	3.80	122.72	113.47
10	M	859	SPO	C11-C12-C14	-3.79	113.05	119.01
10	M	859	SPO	C15-C14-C12	-3.72	122.06	127.28
12	M	902	GGD	OC6-CC5-C14	3.64	119.35	111.48
4	L	851	BCL	C4D-CHA-C1A	3.63	125.58	121.24
12	M	902	GGD	OB5-CB5-CB6	3.63	115.43	106.44
4	L	851	BCL	C2A-C3A-C4A	3.62	107.71	101.87
4	L	853	BCL	C3D-C4D-ND	3.57	115.80	109.99
12	M	902	GGD	CB6-CB5-CB4	-3.57	104.26	113.02
7	L	901	PC1	C25-C24-C23	-3.56	96.38	114.37
4	L	850	BCL	C3D-C4D-ND	3.55	115.76	109.99
4	L	850	BCL	CED-O2D-CGD	3.55	123.97	115.92
11	M	900	CDL	OB8-CB6-CB4	3.49	118.44	108.40
5	L	855	BPH	C4D-ND-C1D	-3.48	104.70	108.87
7	L	901	PC1	O21-C2-C1	3.43	120.65	108.34
6	M	857	U10	C7-C8-C9	3.43	132.73	126.83
4	L	853	BCL	O2A-CGA-CBA	3.39	122.16	111.83
5	L	855	BPH	C5-C3-C2	-3.36	113.63	121.17
6	L	858	U10	O5-C5-C4	-3.29	116.62	121.66
6	M	857	U10	C25-C24-C23	-3.29	115.18	123.63
4	L	853	BCL	C4D-CHA-C1A	3.28	125.16	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	852	BCL	C3D-C4D-ND	3.25	115.27	109.99
10	M	859	SPO	C8-C7-C9	3.25	128.07	122.82
12	M	902	GGD	OB5-CB5-CB4	-3.24	103.86	109.70
12	M	902	GGD	CB4-CB3-CB2	3.24	116.51	110.83
7	L	901	PC1	C24-C23-C22	3.18	124.81	113.13
12	M	902	GGD	OC9-CC7-C31	-3.17	111.39	123.78
6	M	857	U10	C35-C34-C33	-3.15	115.53	123.63
10	M	859	SPO	C15-C16-C17	-3.15	117.72	126.36
4	L	850	BCL	C2A-C3A-C4A	3.14	106.95	101.87
6	M	857	U10	C11-C9-C8	3.14	128.22	121.17
4	M	852	BCL	C2A-C3A-C4A	3.12	106.91	101.87
5	M	854	BPH	C4D-ND-C1D	-3.12	105.14	108.87
12	M	902	GGD	CB3-CB4-CB5	-3.11	104.60	110.23
12	M	902	GGD	OC6-CC5-OC7	-3.10	116.45	123.70
4	M	852	BCL	CHA-C1A-NA	-3.07	119.44	126.39
4	L	851	BCL	C3D-C4D-ND	3.06	114.96	109.99
4	M	852	BCL	C4D-C3D-CAD	-3.06	104.78	108.11
4	L	851	BCL	OBD-CAD-C3D	-3.01	121.38	128.42
4	L	853	BCL	OBD-CAD-C3D	-2.99	121.42	128.42
7	L	901	PC1	C28-C27-C26	-2.97	99.37	114.37
5	M	854	BPH	C3D-CAD-CBD	2.96	111.50	107.61
4	L	850	BCL	CBA-CAA-C2A	2.95	122.57	113.79
4	M	852	BCL	C4A-NA-C1A	2.93	108.02	106.68
4	M	852	BCL	OBD-CAD-C3D	-2.91	121.61	128.42
4	L	853	BCL	C3A-C2A-C1A	2.90	105.69	101.34
6	L	858	U10	C1M-C1-C2	2.88	119.39	117.41
5	M	854	BPH	C4A-C3A-C2A	2.87	105.57	102.84
5	L	855	BPH	C4A-C3A-C2A	2.86	105.56	102.84
4	L	853	BCL	CBA-CAA-C2A	2.83	122.22	113.79
4	L	853	BCL	C2A-C1A-CHA	2.82	128.76	123.87
4	L	850	BCL	CMD-C2D-C1D	2.81	129.67	124.73
4	L	851	BCL	CHA-C1A-NA	-2.80	120.06	126.39
10	M	859	SPO	C16-C17-C19	2.78	123.39	119.01
12	M	902	GGD	OB5-CB1-CB2	-2.78	104.65	110.37
6	M	857	U10	C20-C19-C18	-2.77	116.51	123.63
6	M	857	U10	C25-C24-C26	2.76	120.02	115.23
10	M	859	SPO	C18-C17-C16	2.74	122.27	118.09
4	L	850	BCL	C4A-NA-C1A	2.72	107.92	106.68
4	M	852	BCL	CMD-C2D-C1D	2.71	129.51	124.73
7	L	901	PC1	O12-P-O11	2.71	119.83	107.57
12	M	902	GGD	C37-C38-C39	-2.70	104.61	124.83
4	L	853	BCL	O2D-CGD-CBD	2.69	115.94	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	850	BCL	CMB-C2B-C3B	2.68	134.13	125.67
4	L	850	BCL	OBD-CAD-C3D	-2.66	122.19	128.42
5	L	855	BPH	C3B-C4B-NB	2.66	111.92	108.05
12	M	902	GGD	C36-C35-C34	-2.66	100.93	114.37
4	L	853	BCL	CMB-C2B-C3B	2.64	133.98	125.67
4	L	851	BCL	CMB-C2B-C3B	2.63	133.97	125.67
6	M	857	U10	C4M-O4-C4	2.63	125.70	116.47
6	M	857	U10	O5-C5-C4	-2.62	115.48	121.03
12	M	902	GGD	OA5-CA5-CA4	2.60	114.39	109.70
5	M	854	BPH	O2A-C1-C2	-2.57	98.22	108.11
4	L	853	BCL	CMD-C2D-C1D	2.57	129.25	124.73
5	L	855	BPH	CED-O2D-CGD	2.56	121.73	115.92
4	L	851	BCL	C2A-C1A-CHA	2.56	128.30	123.87
4	L	853	BCL	C2A-C3A-C4A	2.55	105.98	101.87
5	M	854	BPH	CED-O2D-CGD	2.54	121.67	115.92
5	M	854	BPH	C3B-C4B-NB	2.54	111.74	108.05
4	L	853	BCL	C4D-C3D-CAD	-2.53	105.36	108.11
4	L	851	BCL	CBC-CAC-C3C	2.52	118.75	113.41
7	L	901	PC1	C2B-C2A-C29	2.51	130.34	113.36
4	L	851	BCL	C4D-C3D-CAD	-2.51	105.38	108.11
4	L	850	BCL	CMD-C2D-C3D	-2.48	122.00	127.69
4	L	853	BCL	O1D-CGD-CBD	-2.47	119.64	124.52
4	M	852	BCL	CMB-C2B-C3B	2.46	133.44	125.67
12	M	902	GGD	OB1-CB1-OB5	2.46	117.17	110.69
4	L	850	BCL	CHA-C1A-NA	-2.46	120.82	126.39
11	M	900	CDL	CB4-OB6-CB5	2.44	123.63	117.80
10	M	859	SPO	C13-C12-C11	2.43	121.80	118.09
6	M	857	U10	C30-C29-C31	2.43	119.45	115.23
4	L	853	BCL	C6-C5-C3	2.43	119.38	113.47
4	L	850	BCL	C4D-C3D-CAD	-2.43	105.47	108.11
5	L	855	BPH	C3D-CAD-CBD	2.41	110.78	107.61
4	L	850	BCL	C2A-C1A-CHA	2.39	128.02	123.87
4	L	851	BCL	C6-C5-C3	2.36	119.22	113.47
5	L	855	BPH	C2D-C1D-ND	2.36	111.13	109.43
4	L	851	BCL	CMA-C3A-C2A	-2.36	104.87	113.98
12	M	902	GGD	CA3-CA4-CA5	2.35	114.58	109.57
4	L	851	BCL	CMD-C2D-C1D	2.34	128.85	124.73
6	M	857	U10	C1-C6-C5	-2.34	117.35	119.62
6	M	857	U10	C1M-C1-C6	-2.33	120.62	124.45
12	M	902	GGD	OB3-CB3-CB4	-2.32	104.92	110.38
6	M	857	U10	C35-C34-C36	2.31	119.25	115.23
4	L	853	BCL	C2C-C3C-C4C	2.31	104.80	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	859	SPO	C10-C9-C7	-2.31	124.03	127.28
7	L	901	PC1	C3-C2-C1	-2.28	106.47	111.78
12	M	902	GGD	C16-C15-C14	2.27	121.48	113.13
6	M	857	U10	C10-C9-C11	2.27	119.17	115.23
10	M	859	SPO	C8-C7-C6	-2.27	114.62	118.09
6	M	857	U10	C21-C19-C18	2.26	126.24	121.17
11	M	900	CDL	CB6-CB4-CB3	-2.26	106.52	111.78
4	M	852	BCL	C2A-C1A-CHA	2.25	127.78	123.87
4	L	850	BCL	O2A-CGA-CBA	2.25	118.71	111.83
6	L	858	U10	C4M-O4-C4	2.25	124.38	116.47
4	M	852	BCL	C15-C13-C12	-2.23	100.77	112.07
5	M	854	BPH	OBD-CAD-C3D	-2.23	124.42	127.89
4	M	852	BCL	CMD-C2D-C3D	-2.21	122.61	127.69
4	L	850	BCL	O2D-CGD-CBD	2.21	115.08	111.23
4	L	851	BCL	O2A-CGA-CBA	2.20	118.55	111.83
7	L	901	PC1	C23-C22-C21	-2.20	105.64	113.69
6	L	858	U10	C1-C6-C5	-2.18	118.10	122.65
5	L	855	BPH	CMA-C3A-C2A	-2.18	105.72	114.13
4	L	850	BCL	O1D-CGD-CBD	-2.16	120.25	124.52
4	L	853	BCL	CHA-C4D-ND	-2.16	128.08	132.55
12	M	902	GGD	C35-C34-C33	-2.14	103.53	114.37
4	M	852	BCL	CGD-CBD-CAD	-2.12	103.99	110.85
5	L	855	BPH	OBD-CAD-C3D	-2.12	124.59	127.89
6	M	857	U10	C8-C7-C6	-2.11	106.89	112.08
10	M	859	SPO	C9-C10-C11	-2.10	117.11	123.20
4	L	853	BCL	CMD-C2D-C3D	-2.10	122.88	127.69
11	M	900	CDL	C52-C51-CB5	2.09	121.35	113.69
4	L	850	BCL	C2C-C3C-C4C	2.07	104.44	101.34
6	L	858	U10	C6-C5-C4	2.04	121.33	115.39
4	M	852	BCL	O2A-CGA-CBA	2.03	118.01	111.83
11	M	900	CDL	O1-C1-CA2	-2.03	102.69	109.70
12	M	902	GGD	C20-C21-C22	2.03	123.94	112.60
5	M	854	BPH	C6-C5-C3	2.02	118.40	113.47
12	M	902	GGD	OB1-CB1-CB2	-2.01	103.13	108.09
4	L	853	BCL	CHA-C1A-NA	-2.00	121.86	126.39

There are no chirality outliers.

All (137) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	851	BCL	C2C-C3C-CAC-CBC
4	L	851	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
4	L	853	BCL	CHA-CBD-CGD-O2D
4	M	852	BCL	C2-C3-C5-C6
4	M	852	BCL	C4-C3-C5-C6
5	L	855	BPH	C4C-C3C-CAC-CBC
5	L	855	BPH	C6-C7-C8-C9
5	M	854	BPH	C4C-C3C-CAC-CBC
5	M	854	BPH	C2C-C3C-CAC-CBC
6	M	857	U10	C1-C6-C7-C8
6	M	857	U10	C5-C6-C7-C8
6	M	857	U10	C19-C21-C22-C23
7	L	901	PC1	C11-O13-P-O12
7	L	901	PC1	C1-O11-P-O13
7	L	901	PC1	C22-C21-O21-C2
10	M	859	SPO	C21-C22-C23-C24
11	M	900	CDL	CA3-OA5-PA1-OA2
11	M	900	CDL	CA3-OA5-PA1-OA3
11	M	900	CDL	CA3-OA5-PA1-OA4
12	M	902	GGD	CC4-CC3-OA1-CA1
12	M	902	GGD	CC3-CC4-OC6-CC5
12	M	902	GGD	C19-C20-C21-C22
10	M	859	SPO	C36-C37-C38-C39
10	M	859	SPO	C36-C37-C38-C40
7	L	901	PC1	O22-C21-O21-C2
6	M	857	U10	C20-C19-C21-C22
10	M	859	SPO	C20-C21-C22-C23
5	L	855	BPH	C4-C3-C5-C6
5	M	854	BPH	C4-C3-C5-C6
6	M	857	U10	C15-C14-C16-C17
6	M	857	U10	C25-C24-C26-C27
5	L	855	BPH	C2-C3-C5-C6
5	M	854	BPH	C2-C3-C5-C6
6	M	857	U10	C13-C14-C16-C17
6	M	857	U10	C18-C19-C21-C22
6	M	857	U10	C23-C24-C26-C27
12	M	902	GGD	OA5-CA5-CA6-OA6
10	M	859	SPO	C33-C35-C36-C37
12	M	902	GGD	OA5-CA1-OA1-CC3
12	M	902	GGD	CA2-CA1-OA1-CC3
10	M	859	SPO	C24-C23-C25-C26
6	M	857	U10	C9-C11-C12-C13
7	L	901	PC1	C11-C12-N-C15
4	L	850	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
12	M	902	GGD	CA4-CA5-CA6-OA6
7	L	901	PC1	C11-C12-N-C13
4	M	852	BCL	C15-C16-C17-C18
7	L	901	PC1	C28-C29-C2A-C2B
11	M	900	CDL	C78-C79-C80-C81
12	M	902	GGD	C31-C32-C33-C34
4	L	851	BCL	C2A-CAA-CBA-CGA
7	L	901	PC1	C31-C32-C33-C34
11	M	900	CDL	CB7-C71-C72-C73
5	L	855	BPH	C3-C5-C6-C7
12	M	902	GGD	C40-C41-C42-C43
11	M	900	CDL	C36-C37-C38-C39
11	M	900	CDL	C39-C40-C41-C42
7	L	901	PC1	C11-C12-N-C14
11	M	900	CDL	C34-C35-C36-C37
7	L	901	PC1	C35-C36-C37-C38
12	M	902	GGD	C35-C36-C37-C38
10	M	859	SPO	C1-C4-C5-C6
12	M	902	GGD	OB5-CB5-CB6-OB6
11	M	900	CDL	C31-C32-C33-C34
11	M	900	CDL	C11-C12-C13-C14
11	M	900	CDL	C17-C18-C19-C20
5	L	855	BPH	C2C-C3C-CAC-CBC
11	M	900	CDL	C11-CA5-OA6-CA4
10	M	859	SPO	C2-C1-C4-C5
10	M	859	SPO	C3-C1-C4-C5
12	M	902	GGD	CC3-CC4-CC6-OC8
4	L	853	BCL	C5-C6-C7-C8
11	M	900	CDL	CA7-C31-C32-C33
5	L	855	BPH	C8-C10-C11-C12
11	M	900	CDL	C38-C39-C40-C41
12	M	902	GGD	C32-C31-CC7-OC8
7	L	901	PC1	C37-C38-C39-C3A
12	M	902	GGD	C37-C38-C39-C40
11	M	900	CDL	OA5-CA3-CA4-CA6
4	M	852	BCL	C11-C10-C8-C7
5	L	855	BPH	C6-C7-C8-C10
11	M	900	CDL	C55-C56-C57-C58
12	M	902	GGD	C17-C18-C19-C20
7	L	901	PC1	C3A-C3B-C3C-C3D
12	M	902	GGD	CA4-CA3-OB1-CB1
12	M	902	GGD	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
11	M	900	CDL	C80-C81-C82-C83
11	M	900	CDL	C71-C72-C73-C74
11	M	900	CDL	C20-C21-C22-C23
12	M	902	GGD	OA1-CC3-CC4-OC6
4	M	852	BCL	C11-C10-C8-C9
4	L	853	BCL	C15-C16-C17-C18
11	M	900	CDL	C21-C22-C23-C24
11	M	900	CDL	OA7-CA5-OA6-CA4
11	M	900	CDL	C72-C73-C74-C75
11	M	900	CDL	OA5-CA3-CA4-OA6
11	M	900	CDL	CA3-CA4-CA6-OA8
10	M	859	SPO	O1-C1-C4-C5
7	L	901	PC1	O13-C11-C12-N
11	M	900	CDL	C51-C52-C53-C54
12	M	902	GGD	C36-C37-C38-C39
12	M	902	GGD	C38-C39-C40-C41
12	M	902	GGD	CA2-CA3-OB1-CB1
6	L	858	U10	C5-C4-O4-C4M
4	L	853	BCL	CHA-CBD-CGD-O1D
7	L	901	PC1	C1-O11-P-O14
12	M	902	GGD	C41-C42-C43-C44
11	M	900	CDL	C54-C55-C56-C57
12	M	902	GGD	C39-C40-C41-C42
12	M	902	GGD	C32-C31-CC7-OC9
5	M	854	BPH	C11-C10-C8-C9
6	M	857	U10	C5-C4-O4-C4M
10	M	859	SPO	C18-C17-C19-C20
4	L	850	BCL	C4-C3-C5-C6
12	M	902	GGD	CC6-CC4-OC6-CC5
10	M	859	SPO	C16-C17-C19-C20
5	M	854	BPH	C11-C10-C8-C7
4	L	851	BCL	C15-C16-C17-C18
6	M	857	U10	C29-C31-C32-C33
5	M	854	BPH	C2A-CAA-CBA-CGA
11	M	900	CDL	C19-C20-C21-C22
5	L	855	BPH	CHA-CBD-CGD-O1D
10	M	859	SPO	C9-C10-C11-C12
4	M	852	BCL	CAA-CBA-CGA-O2A
12	M	902	GGD	C32-C33-C34-C35
4	L	853	BCL	C14-C13-C15-C16
6	L	858	U10	C3-C4-O4-C4M
4	L	850	BCL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
6	M	857	U10	C14-C16-C17-C18
4	M	852	BCL	C3-C5-C6-C7
6	M	857	U10	C12-C11-C9-C10
11	M	900	CDL	C40-C41-C42-C43
4	M	852	BCL	C12-C13-C15-C16
10	M	859	SPO	C17-C19-C20-C21
4	L	851	BCL	CAD-CBD-CGD-O2D
7	L	901	PC1	O21-C21-C22-C23
12	M	902	GGD	C20-C21-C22-C23

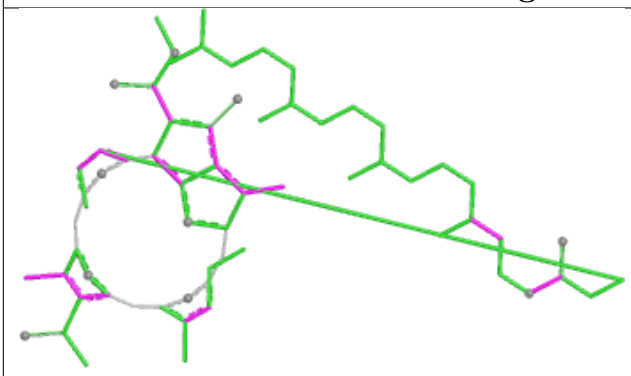
There are no ring outliers.

10 monomers are involved in 45 short contacts:

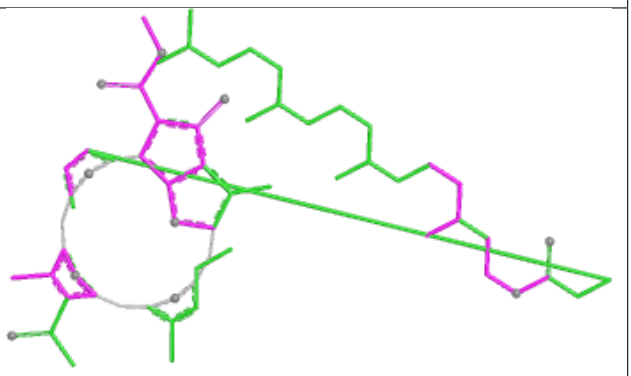
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	854	BPH	6	0
6	L	858	U10	2	0
4	L	851	BCL	2	0
4	L	850	BCL	5	0
7	L	901	PC1	8	0
12	M	902	GGD	16	0
6	M	857	U10	3	0
4	L	853	BCL	5	0
4	M	852	BCL	3	0
5	L	855	BPH	5	0

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

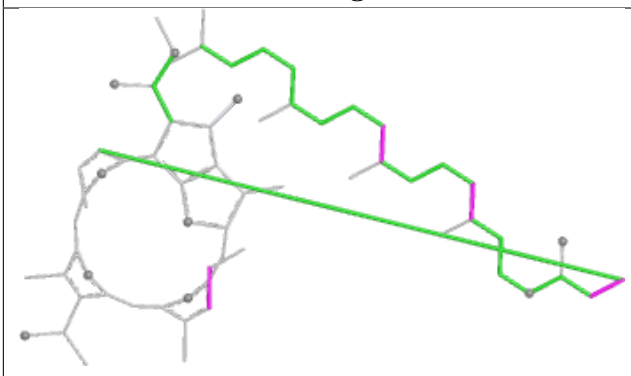
Ligand BPH M 854



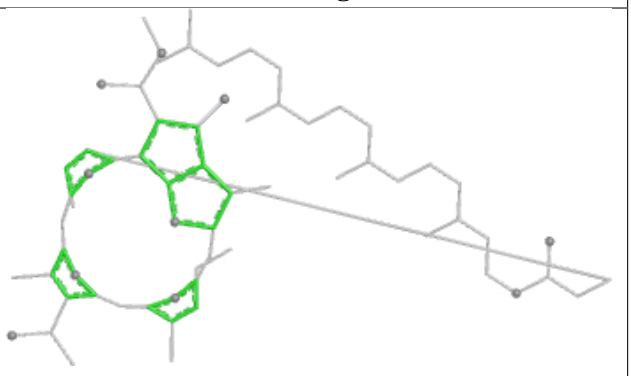
Bond lengths



Bond angles

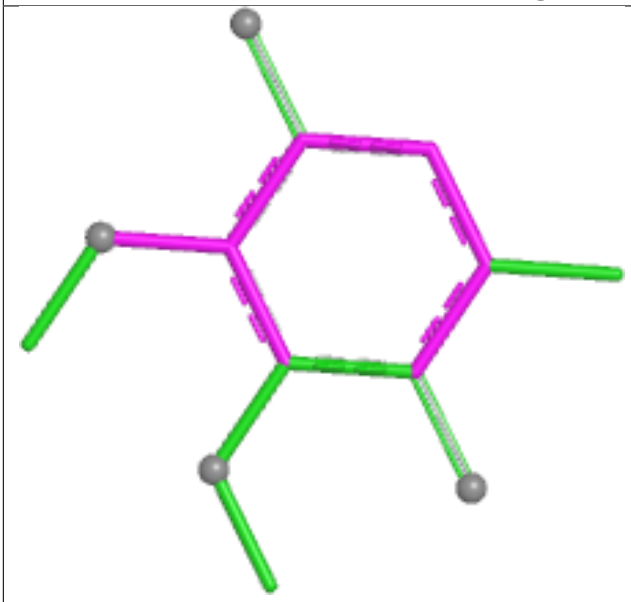


Torsions

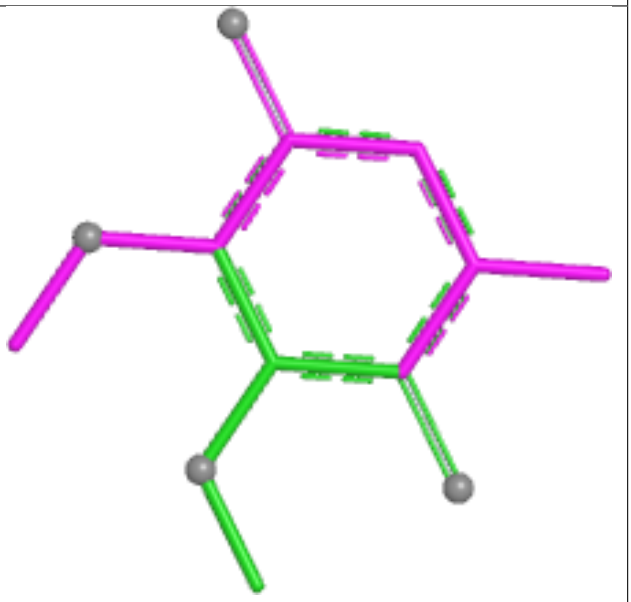


Rings

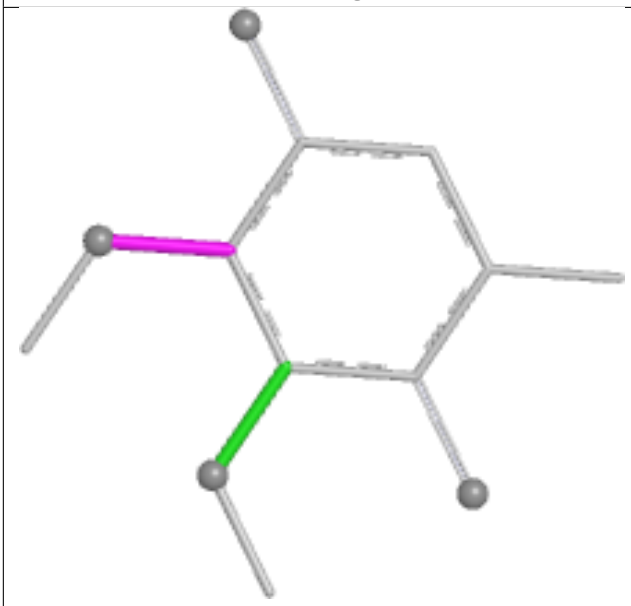
Ligand U10 L 858



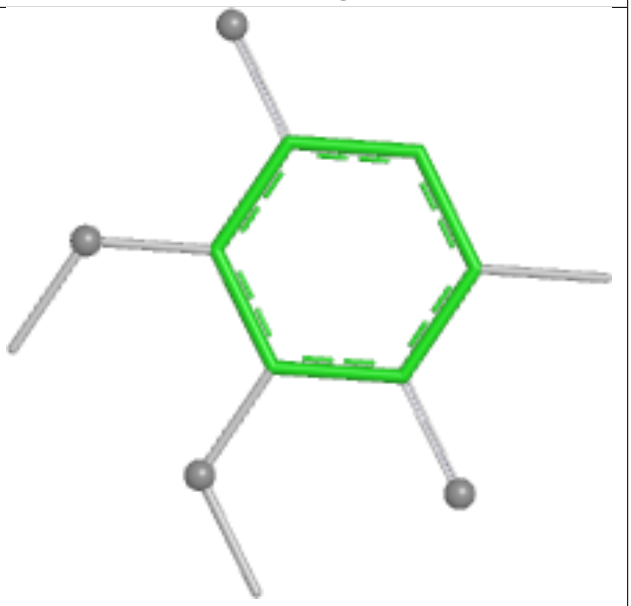
Bond lengths



Bond angles

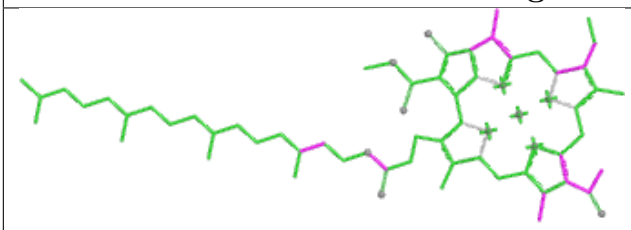


Torsions

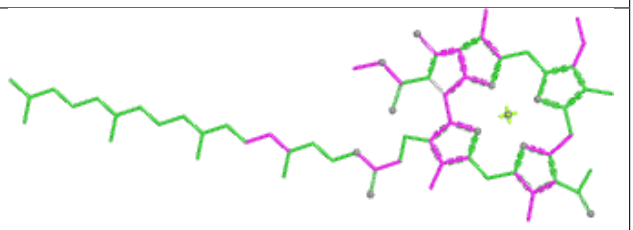


Rings

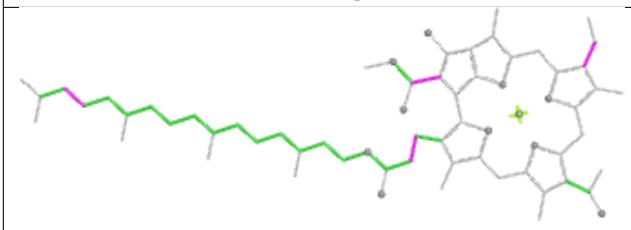
Ligand BCL L 851



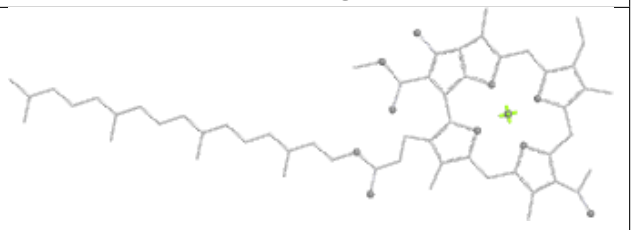
Bond lengths



Bond angles

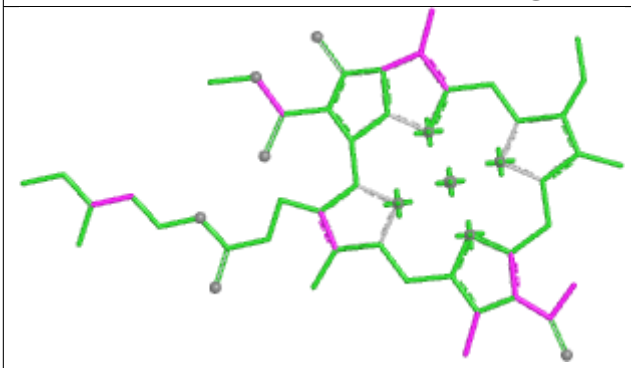


Torsions

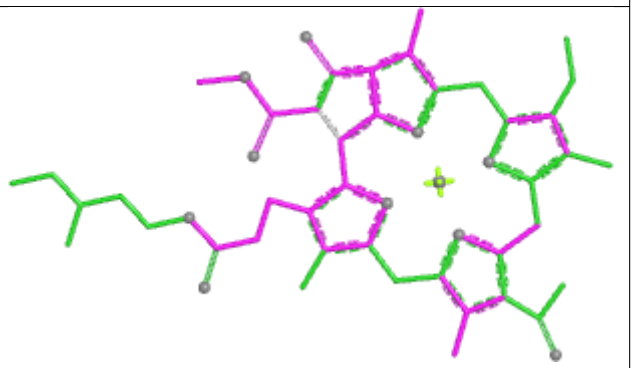


Rings

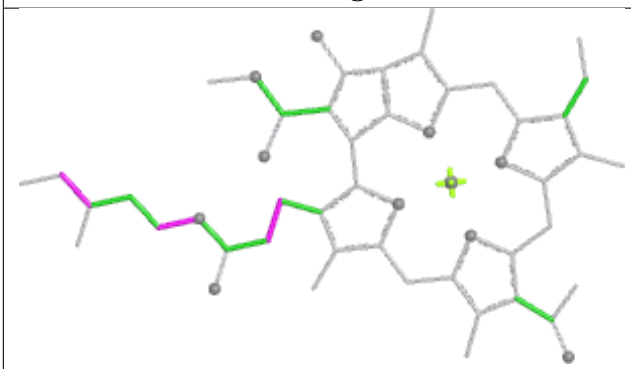
Ligand BCL L 850



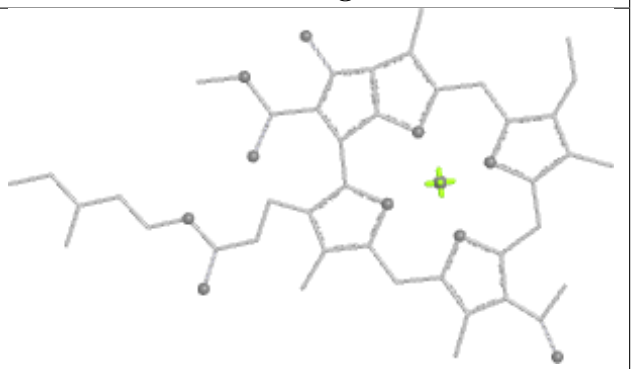
Bond lengths



Bond angles

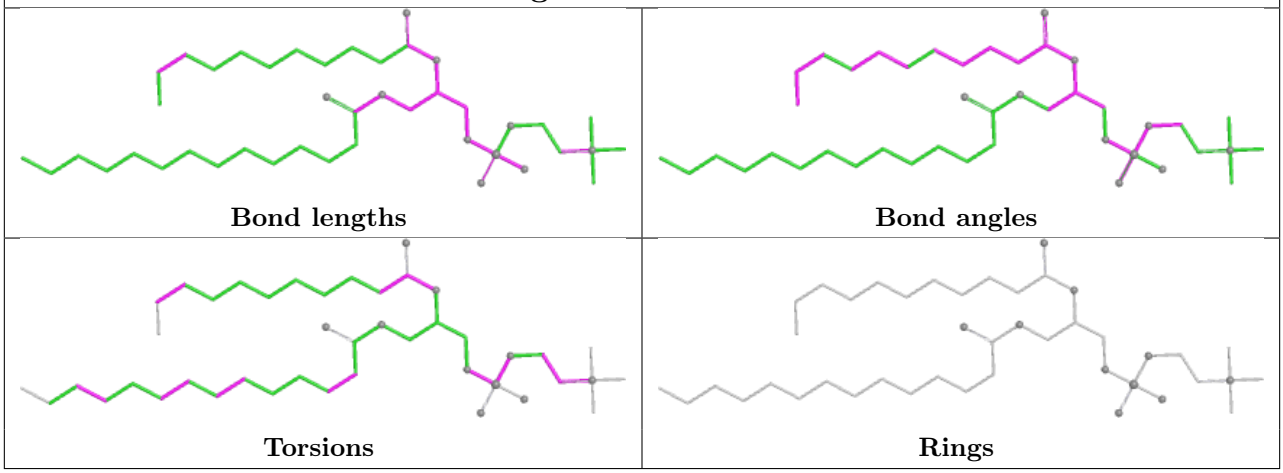


Torsions

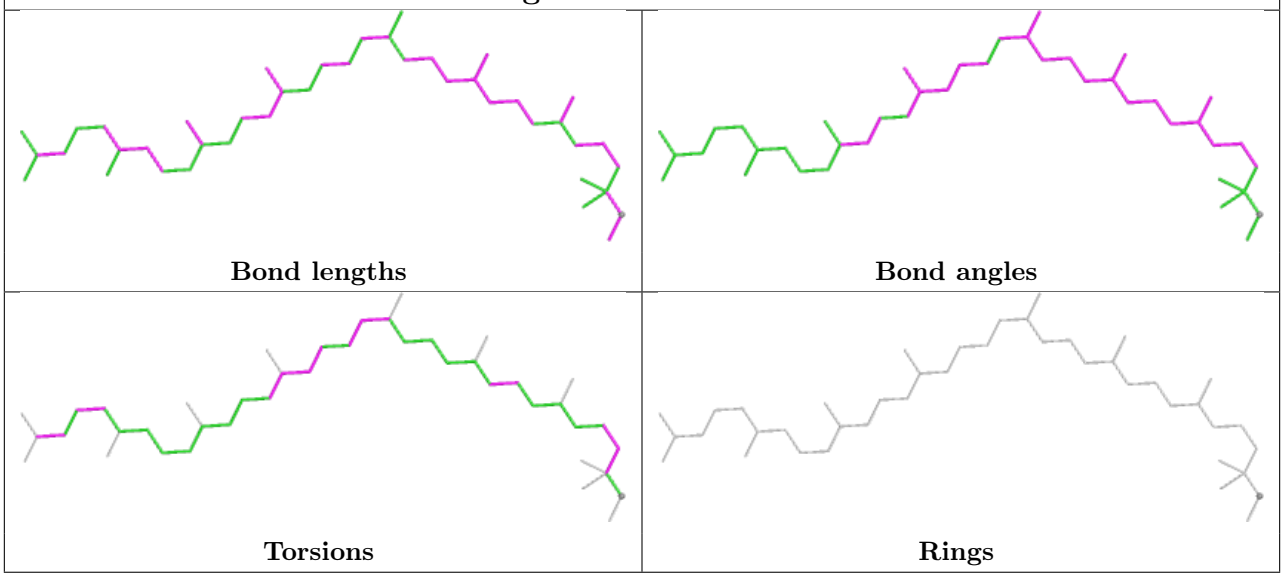


Rings

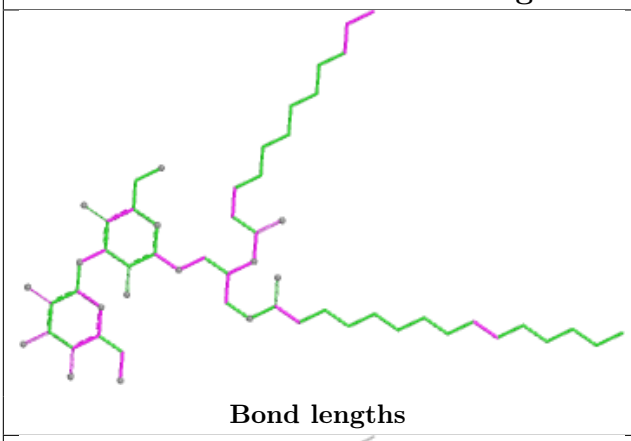
Ligand PC1 L 901



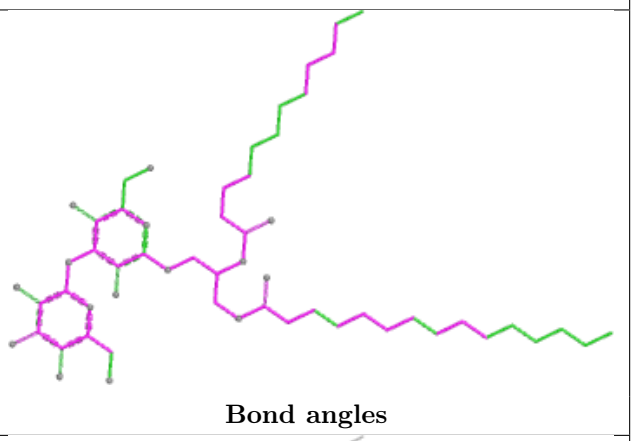
Ligand SPO M 859



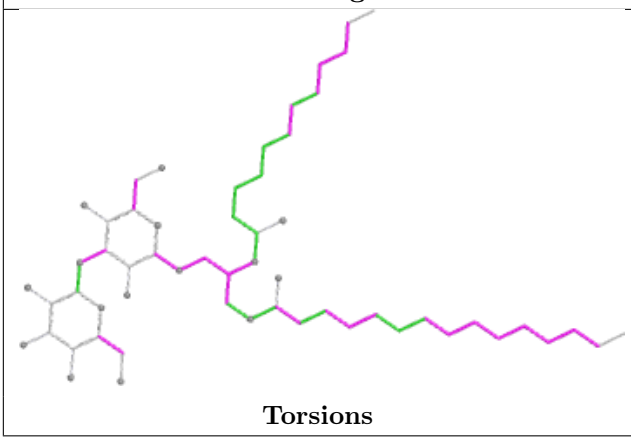
Ligand GGD M 902



Bond lengths



Bond angles



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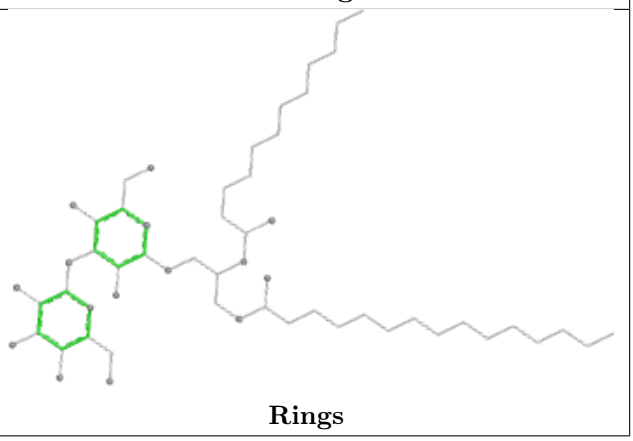
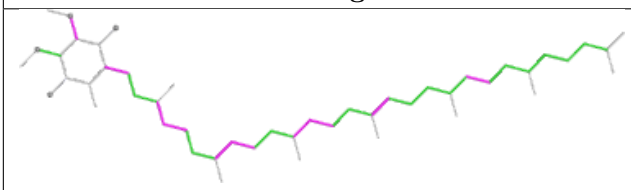


Rings

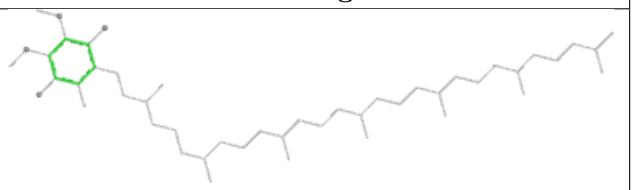
Ligand U10 M 857

Bond lengths

Bond angles

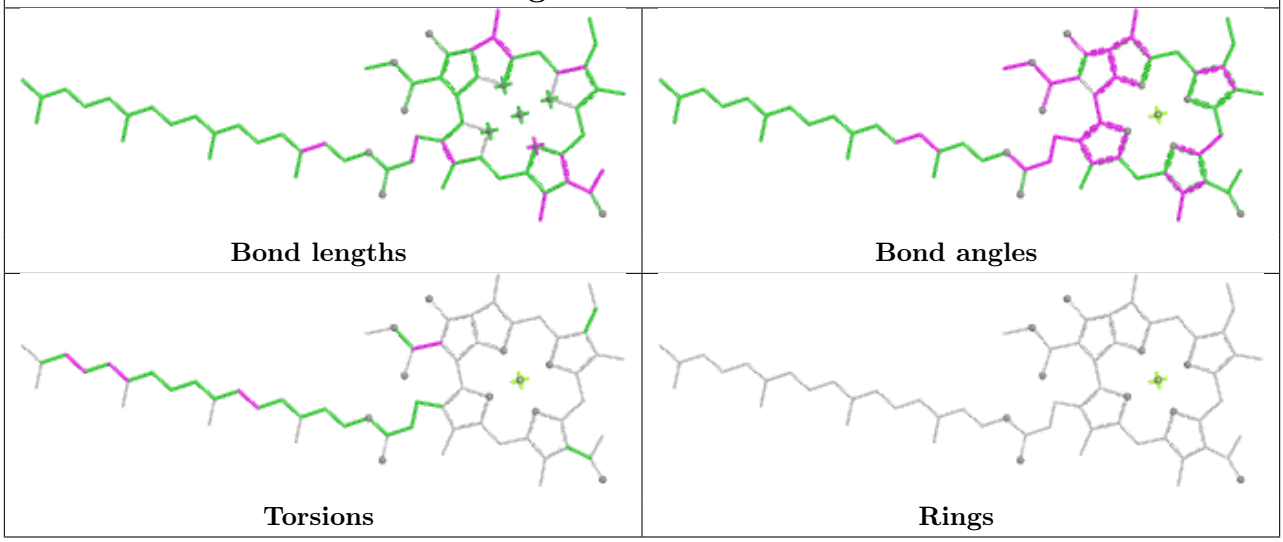


Torsions

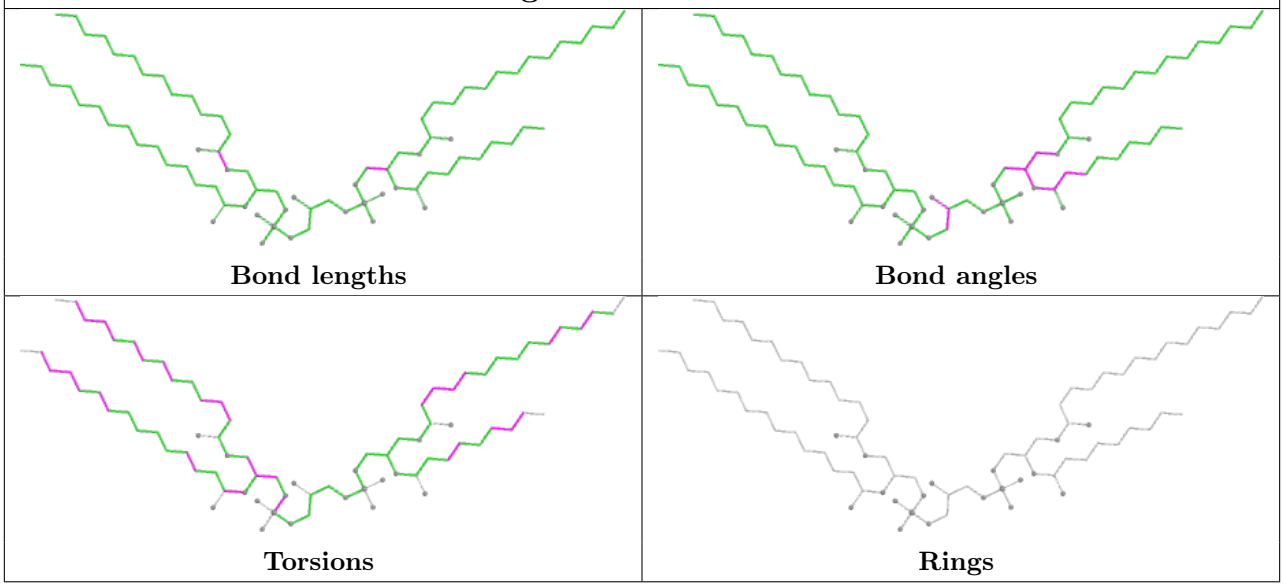


Rings

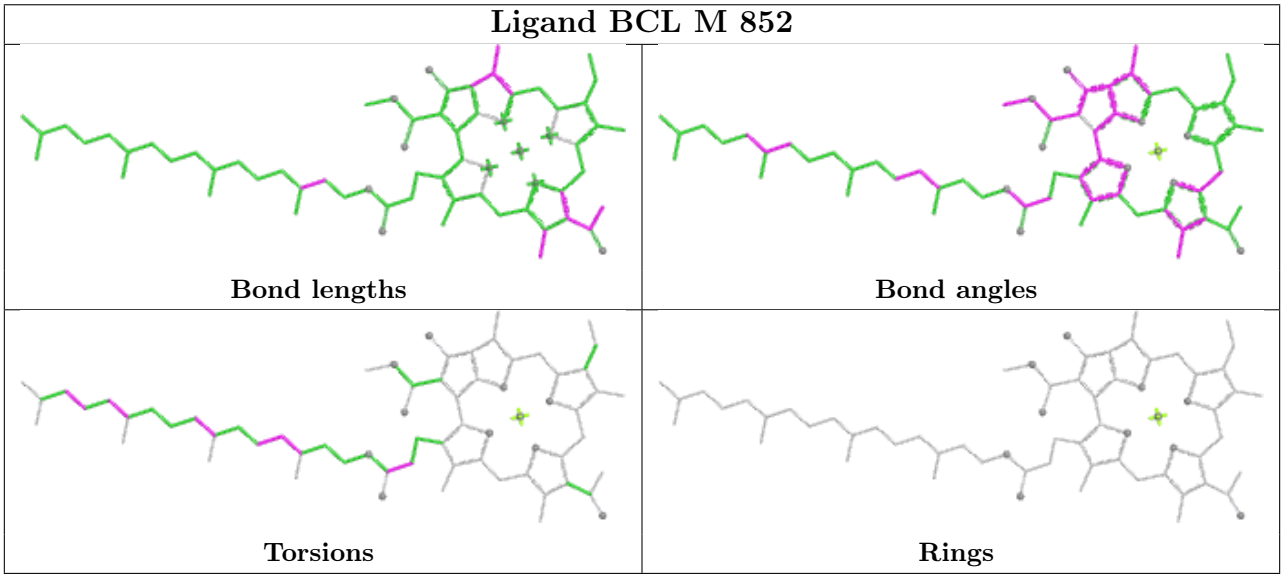
Ligand BCL L 853



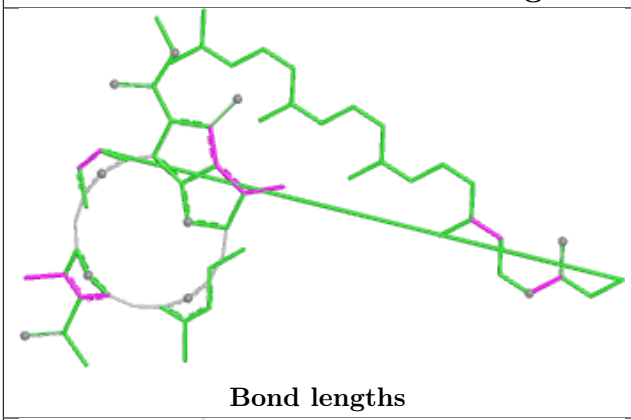
Ligand CDL M 900



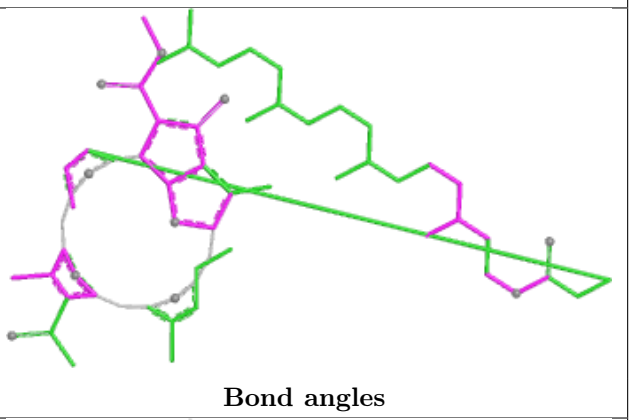
Ligand BCL M 852



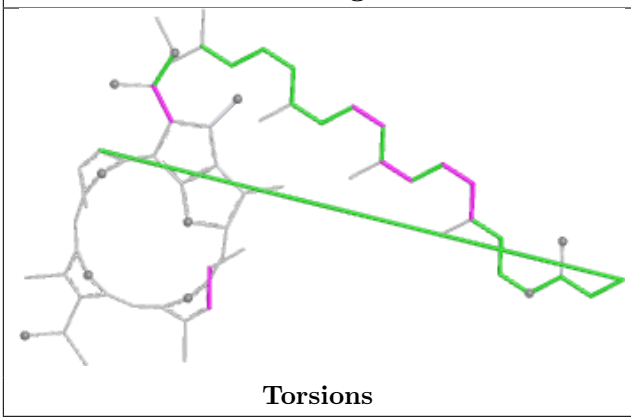
Ligand BPH L 855



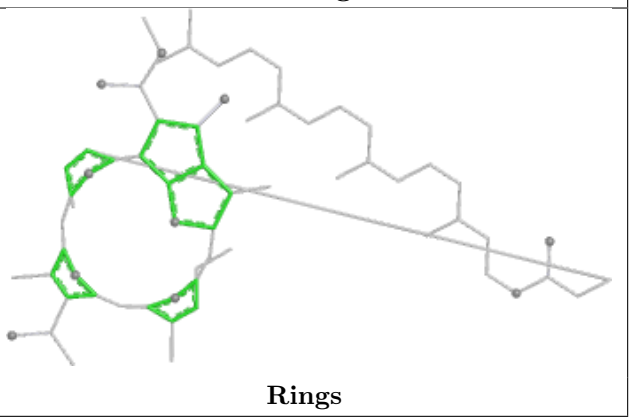
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	L	281/281 (100%)	-0.05	14 (4%) 34 33	15, 29, 64, 80	0
2	M	302/307 (98%)	0.06	12 (3%) 42 43	13, 34, 67, 79	0
3	H	238/260 (91%)	-0.11	6 (2%) 58 59	20, 33, 53, 80	0
All	All	821/848 (96%)	-0.03	32 (3%) 43 44	13, 32, 64, 80	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	302	GLY	6.0
3	H	18	TYR	5.5
2	M	1	ALA	5.3
3	H	246	PRO	4.5
1	L	271	TRP	3.9
1	L	281	GLY	3.8
1	L	275	ILE	3.4
2	M	292	ASP	3.2
3	H	247	LYS	3.2
2	M	301	HIS	3.1
3	H	245	ALA	3.0
3	H	248	ARG	3.0
2	M	52	LEU	2.9
2	M	300	ASN	2.8
2	M	28	ASN	2.8
2	M	79	GLY	2.7
1	L	59	TRP	2.7
1	L	270	PRO	2.7
1	L	273	ALA	2.7
1	L	268	LYS	2.6
1	L	72	GLU	2.5
2	M	194	GLY	2.5
3	H	94	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	51	TRP	2.4
1	L	278	GLY	2.4
2	M	109	LEU	2.3
1	L	216	PHE	2.2
1	L	53	ALA	2.2
2	M	78	ALA	2.2
1	L	280	ASN	2.1
1	L	277	GLY	2.1
2	M	80	TRP	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

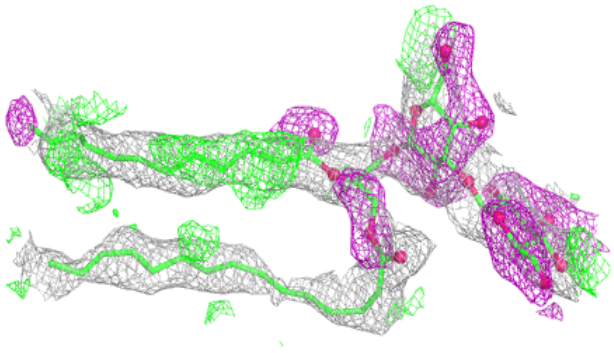
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

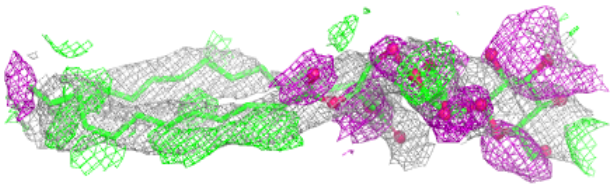
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	GGD	M	902	57/67	0.61	0.29	66,79,80,80	0
7	PC1	L	901	43/54	0.63	0.26	65,79,80,80	0
9	CL	M	2000	1/1	0.80	0.16	80,80,80,80	0
6	U10	L	858	13/63	0.82	0.42	55,56,57,59	13
11	CDL	M	900	81/100	0.88	0.18	55,67,78,80	0
4	BCL	L	850	52/66	0.91	0.13	23,28,54,56	0
10	SPO	M	859	42/42	0.92	0.14	34,47,65,68	0
5	BPH	M	854	65/65	0.92	0.14	30,35,80,80	0
6	U10	M	857	48/63	0.92	0.15	27,39,67,68	0
5	BPH	L	855	65/65	0.93	0.10	18,23,33,43	0
4	BCL	L	853	66/66	0.93	0.12	11,17,52,59	0
4	BCL	M	852	66/66	0.93	0.11	19,24,56,69	0
4	BCL	L	851	66/66	0.94	0.09	16,23,36,44	0
8	FE	M	856	1/1	1.00	0.04	18,18,18,18	0

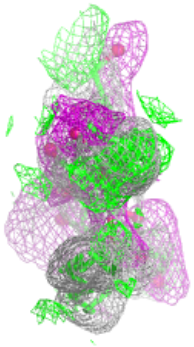
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GGD M 902:

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

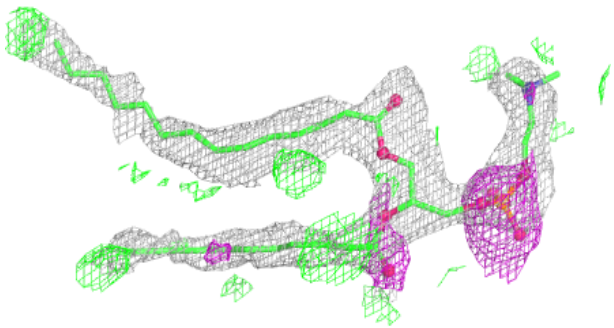


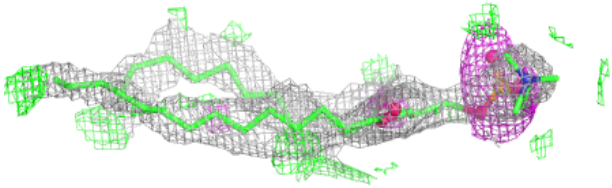


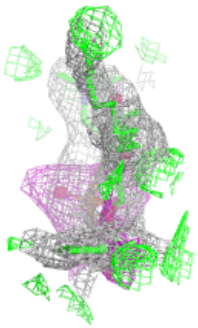


Electron density around PC1 L 901:

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

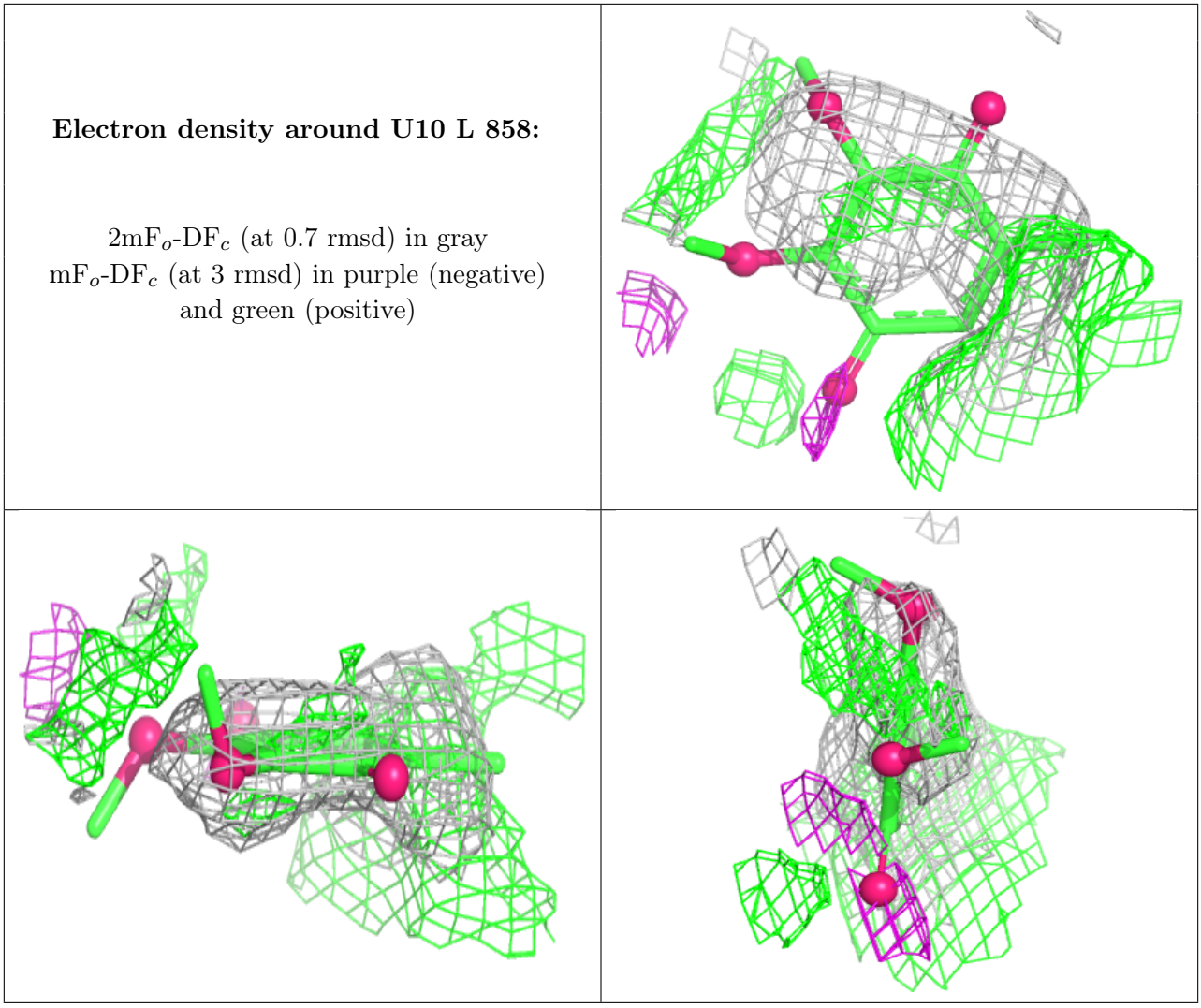






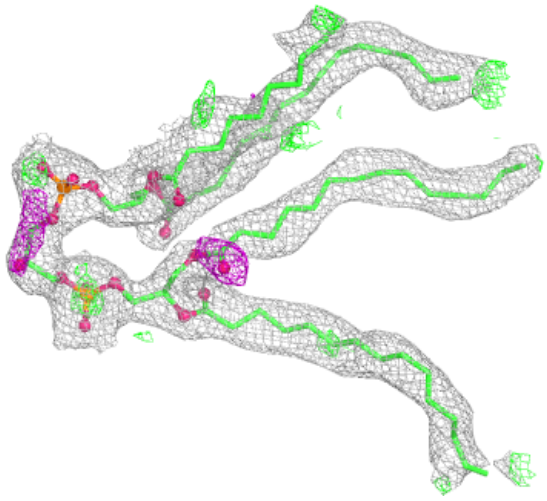
Electron density around U10 L 858:

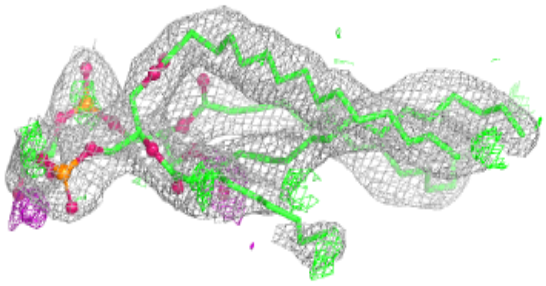
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

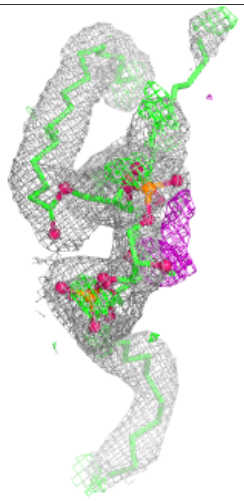


Electron density around CDL M 900:

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

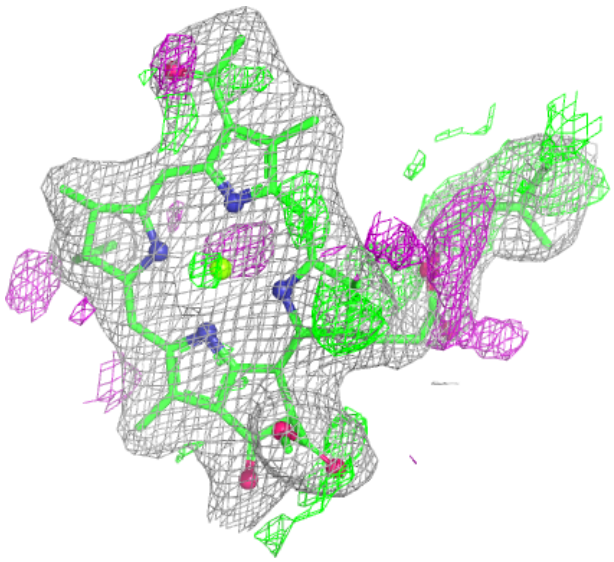


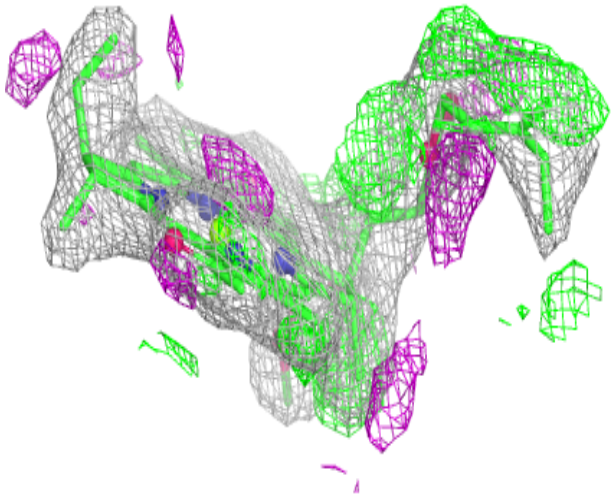


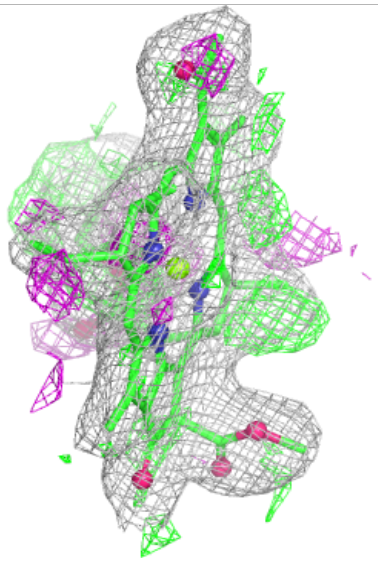


Electron density around BCL L 850:

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

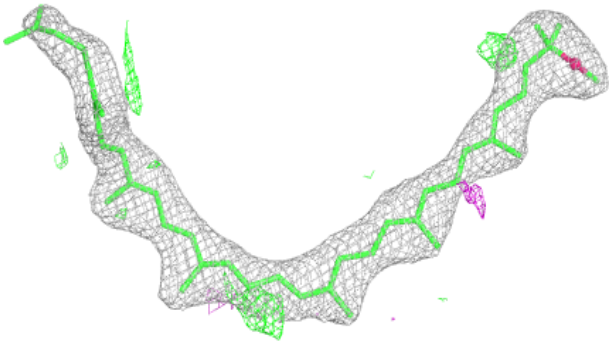


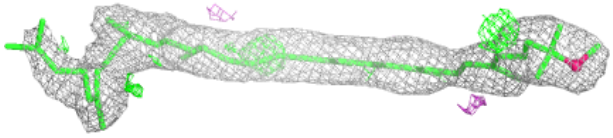


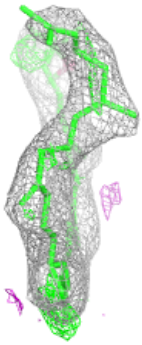


Electron density around SPO M 859:

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

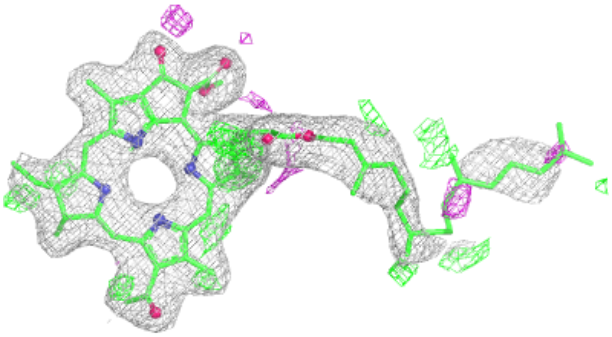


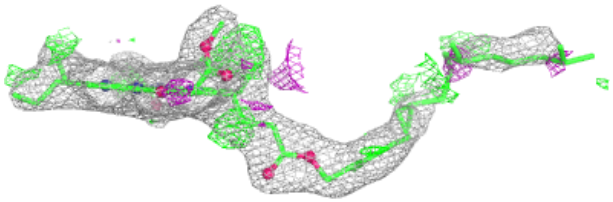


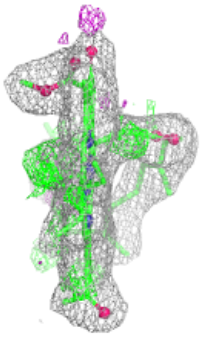


Electron density around BPH M 854:

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

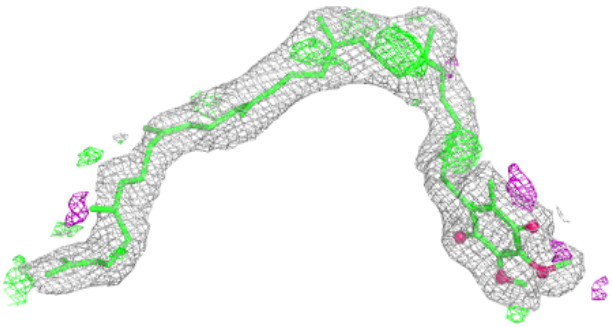


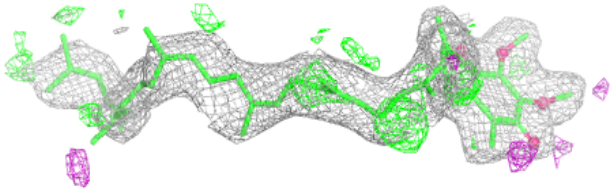


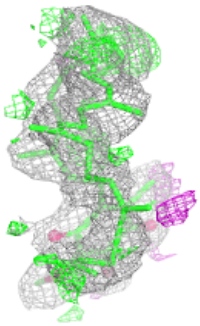


Electron density around U10 M 857:

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

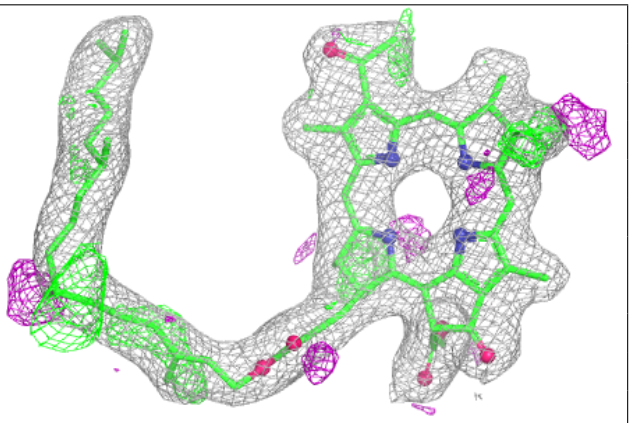


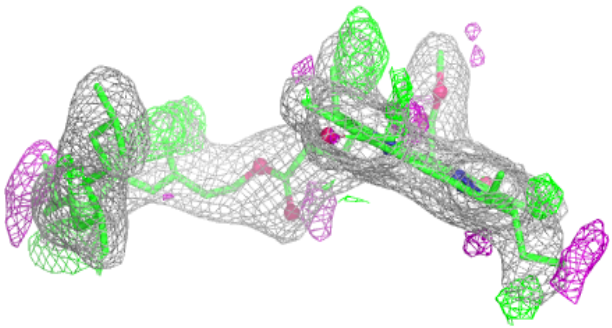


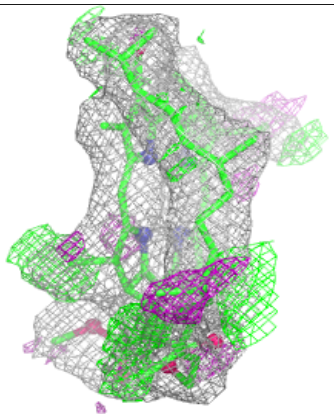


Electron density around BPH L 855:

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

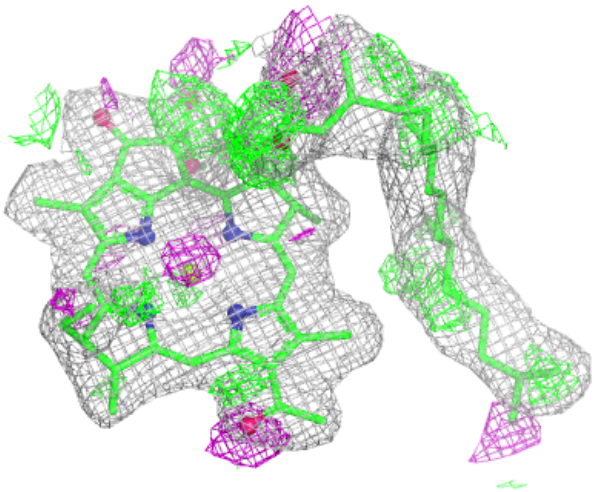


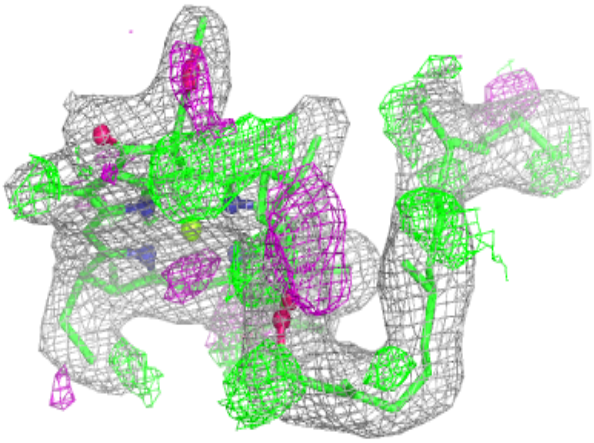


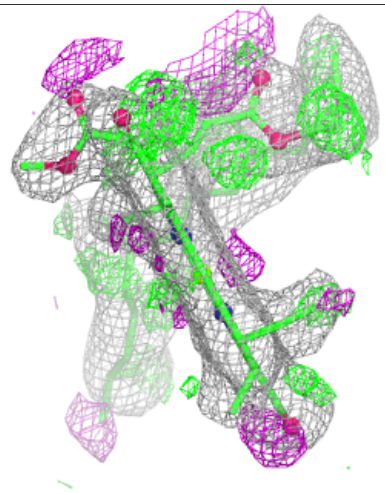


Electron density around BCL L 853:

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

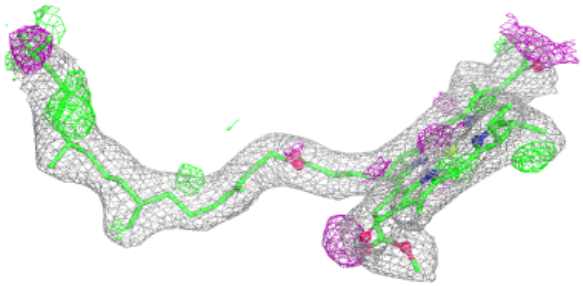


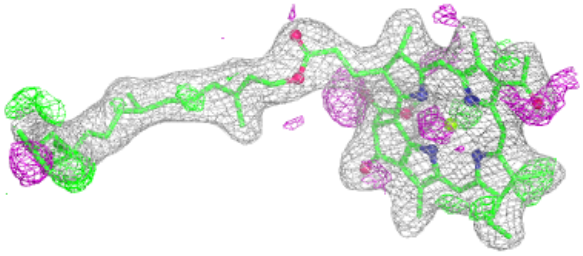


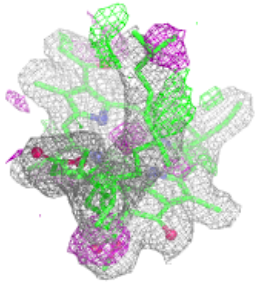


Electron density around BCL M 852:

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

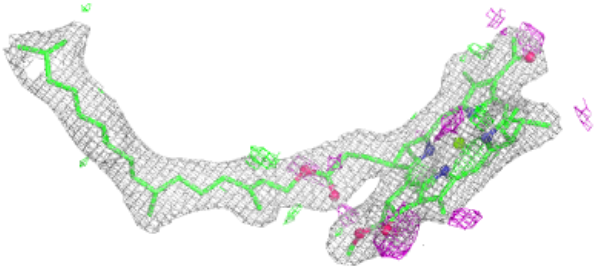


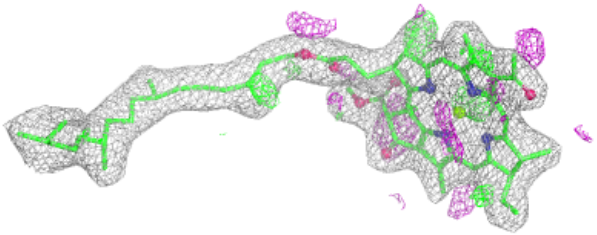


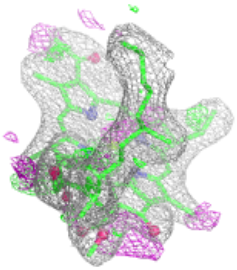


Electron density around BCL L 851:

$2mF_o$-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.