



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 07:40 PM EDT

PDB ID : 1RY5
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT FROM
RHODOBACTER SPHAEROIDES WITH ASP L213 REPLACED WITH
ASN
Authors : Xu, Q.; Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher,
G.
Deposited on : 2003-12-19
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

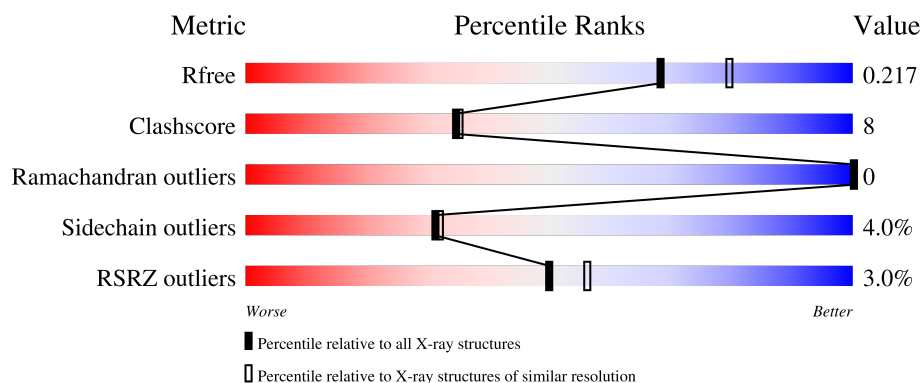
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

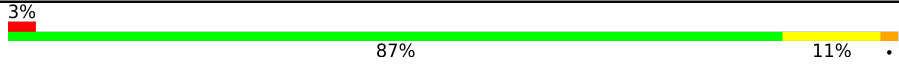
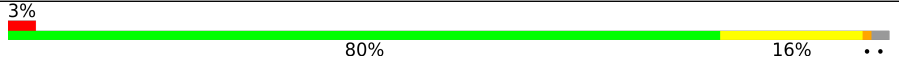

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	L	281	
2	M	307	
3	H	260	

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
5	BPH	L	856	X	-	-	-
7	GOL	L	866	-	X	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 7504 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	0	0
			2232	1507	356	361	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	213	ASN	ASP	engineered mutation	UNP P02954

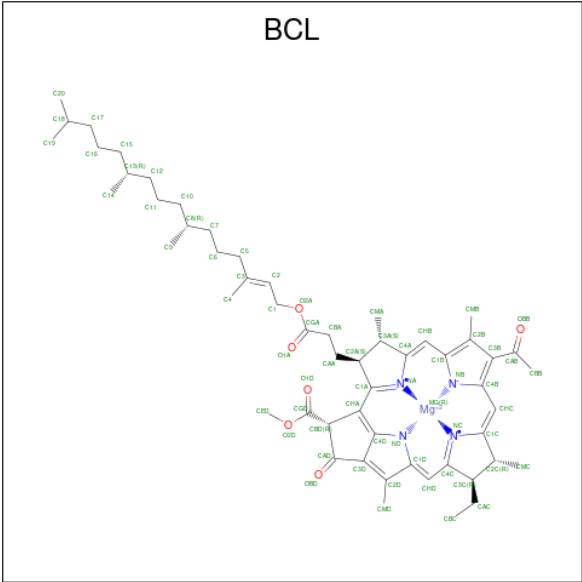
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	301	Total	C	N	O	S	0	0	0
			2404	1605	393	396	10			

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

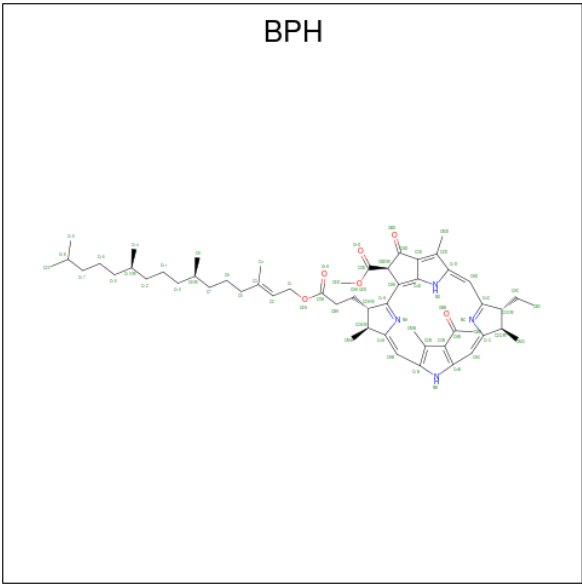
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	239	Total	C	N	O	S	0	1	0
			1832	1171	314	338	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			51	40	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 (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



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
			51	41	4	6		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			24	20	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

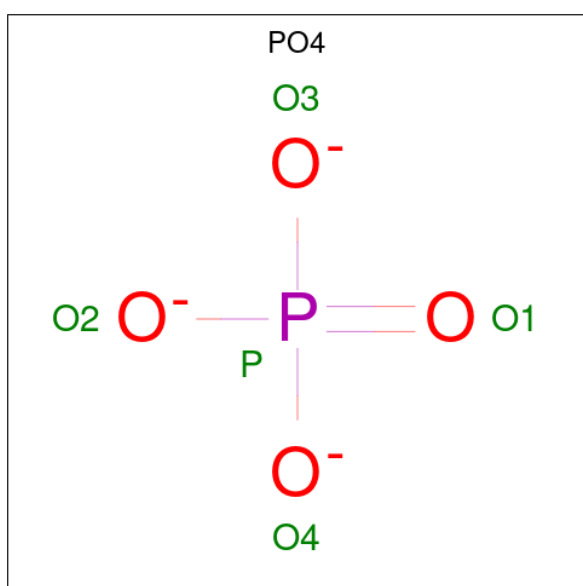


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is FE (II) ION (three-letter code: FE2) (formula: Fe).

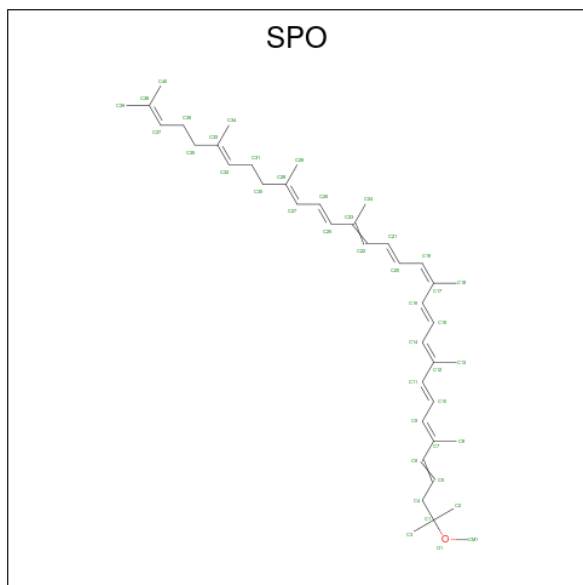
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



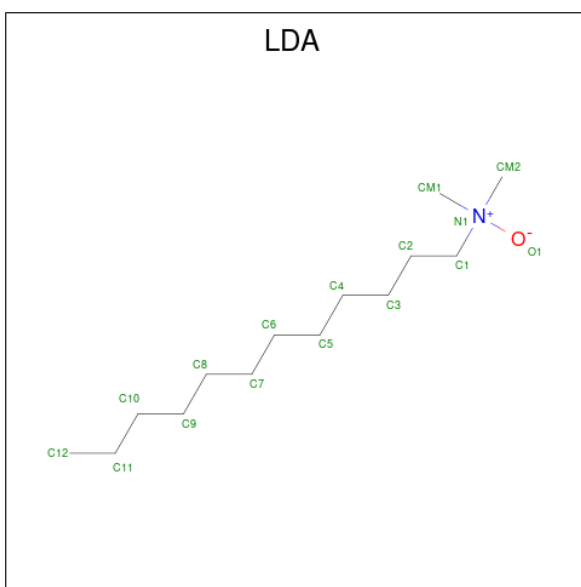
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	O	P	0	0
			5	4	1		
9	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 10 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



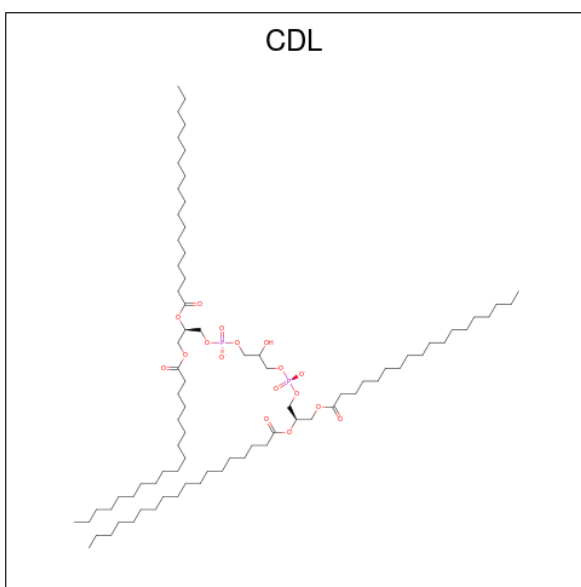
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 11 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 13 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	H	1	Total 1	K 1	0	0

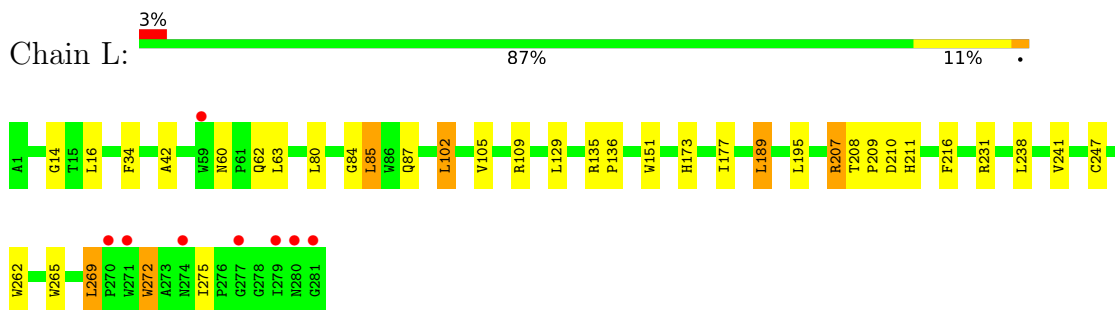
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	L	107	Total 107	O 107	0	0
14	M	130	Total 130	O 130	0	1
14	H	173	Total 173	O 173	0	1

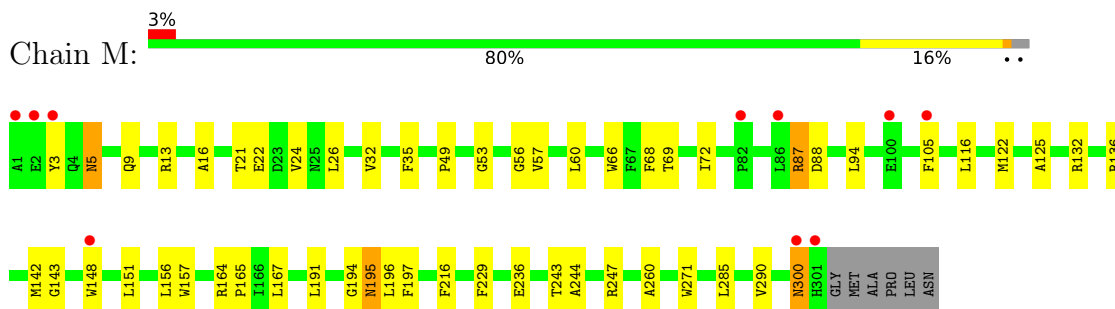
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

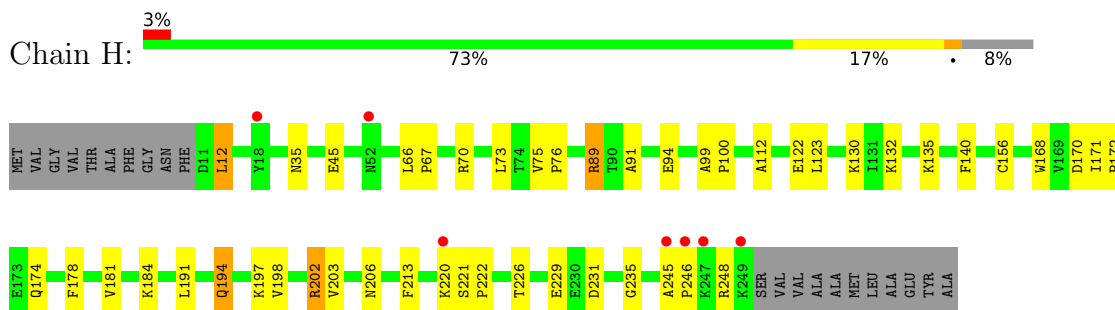
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.07Å 139.07Å 184.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.23 – 2.10 39.23 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.23-2.10) 98.8 (39.23-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.211 , 0.226 0.203 , 0.217	Depositor DCC
R_{free} test set	6001 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7504	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: BCL, PO4, CDL, K, U10, GOL, LDA, FE2, SPO, BPH

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	0.37	0/2320	0.55	0/3175
2	M	0.37	0/2496	0.53	0/3408
3	H	0.32	0/1880	0.59	0/2557
All	All	0.36	0/6696	0.56	0/9140

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2189	26	0
2	M	2404	0	2318	48	0
3	H	1832	0	1836	42	0
4	L	183	0	189	13	0
4	M	66	0	74	4	0
5	L	65	0	74	6	0
5	M	51	0	45	2	0
6	L	24	0	25	1	0
6	M	48	0	62	0	0
7	L	6	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	M	1	0	0	0	0
9	M	10	0	0	0	0
10	M	42	0	60	0	0
11	H	16	0	31	0	0
11	M	32	0	62	0	0
12	M	81	0	106	1	0
13	H	1	0	0	0	0
14	H	173	0	0	3	0
14	L	107	0	0	1	0
14	M	130	0	0	2	0
All	All	7504	0	7075	117	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 8.

All (117) 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)
1:L:241:VAL:HG21	5:L:856:BPH:HAC2	1.35	1.03
2:M:157:TRP:HB2	4:M:853:BCL:H62	1.54	0.90
2:M:236:GLU:HG3	3:H:122:GLU:CD	1.98	0.84
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.65	0.78
2:M:13:ARG:HD2	2:M:35:PHE:CD2	2.23	0.74
3:H:194:GLN:H	3:H:194:GLN:NE2	1.88	0.72
3:H:89:ARG:HG3	14:H:875:HOH:O	1.92	0.69
3:H:245:ALA:HA	3:H:248:ARG:NH1	2.08	0.68
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.74	0.68
2:M:300:ASN:HD22	2:M:300:ASN:N	1.92	0.68
1:L:62:GLN:HE21	1:L:151:TRP:HE1	1.40	0.67
14:L:922:HOH:O	2:M:143:GLY:HA2	1.95	0.66
2:M:105:PHE:HD1	2:M:116:LEU:HD13	1.60	0.66
2:M:9:GLN:NE2	3:H:198:VAL:H	1.94	0.66
4:L:852:BCL:H42	4:L:854:BCL:HBC3	1.79	0.65
2:M:9:GLN:HE22	3:H:198:VAL:H	1.43	0.65
3:H:202:ARG:HG2	3:H:203:VAL:N	2.13	0.64
3:H:206:ASN:HD21	3:H:248:ARG:HD3	1.61	0.64
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.80	0.63
3:H:130:LYS:HE3	3:H:170:ASP:OD2	1.99	0.62
3:H:181:VAL:HG21	3:H:191:LEU:HD12	1.82	0.62
1:L:207:ARG:HG2	2:M:142:MET:HG2	1.83	0.61
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:60:ASN:CG	1:L:63:LEU:HD23	2.21	0.60
1:L:189:LEU:HG	1:L:216:PHE:HZ	1.67	0.60
2:M:136:ARG:NE	2:M:136:ARG:HA	2.19	0.58
2:M:13:ARG:O	3:H:140:PHE:HA	2.04	0.58
1:L:208:THR:H	1:L:211:HIS:CD2	2.22	0.57
1:L:231:ARG:HH21	2:M:5:ASN:ND2	2.01	0.57
1:L:62:GLN:NE2	1:L:151:TRP:HE1	2.01	0.57
3:H:112:ALA:HA	3:H:235:GLY:O	2.05	0.57
3:H:89:ARG:HG2	3:H:91:ALA:O	2.05	0.56
4:L:851:BCL:HBC1	4:M:853:BCL:HBD	1.87	0.56
2:M:26:LEU:H	2:M:26:LEU:HD12	1.70	0.56
3:H:140:PHE:CE2	3:H:174:GLN:HG2	2.40	0.56
2:M:60:LEU:HA	5:M:855:BPH:H4C2	1.88	0.55
3:H:45:GLU:HG3	3:H:94:GLU:OE2	2.06	0.55
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.88	0.55
2:M:236:GLU:HG3	3:H:122:GLU:CG	2.37	0.54
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.42	0.54
3:H:132:LYS:HG2	14:H:933:HOH:O	2.08	0.54
1:L:265:TRP:O	1:L:269:LEU:HD13	2.07	0.54
2:M:243:THR:O	2:M:247:ARG:HG3	2.08	0.53
3:H:140:PHE:HE2	3:H:174:GLN:HG2	1.74	0.52
1:L:105:VAL:O	1:L:109:ARG:HG3	2.10	0.52
4:L:854:BCL:HMA1	4:L:854:BCL:H121	1.92	0.52
1:L:14:GLY:O	1:L:109:ARG:HD3	2.10	0.51
1:L:80:LEU:HB3	1:L:85:LEU:HD13	1.93	0.51
4:L:851:BCL:HBC3	4:M:853:BCL:CAD	2.41	0.51
2:M:167:LEU:HD12	2:M:285:LEU:HD11	1.92	0.51
1:L:211:HIS:HE1	2:M:22:GLU:OE1	1.94	0.51
4:L:854:BCL:H151	5:L:856:BPH:H171	1.93	0.51
3:H:156:CYS:HB2	3:H:248:ARG:HG3	1.93	0.51
2:M:68:PHE:HA	14:M:1025:HOH:O	2.11	0.50
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.94	0.50
2:M:300:ASN:N	2:M:300:ASN:ND2	2.56	0.50
4:L:851:BCL:CBC	4:M:853:BCL:HBD	2.42	0.50
2:M:26:LEU:HD12	2:M:26:LEU:N	2.27	0.50
3:H:75:VAL:HA	3:H:76:PRO:C	2.33	0.49
2:M:194:GLY:O	2:M:195:ASN:HB3	2.11	0.49
6:L:859:U10:H3M1	14:M:923:HOH:O	2.13	0.49
1:L:16:LEU:HD23	1:L:109:ARG:NH1	2.27	0.48
3:H:245:ALA:HB3	3:H:246:PRO:HD3	1.94	0.48
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:236:GLU:HG3	3:H:122:GLU:HG3	1.95	0.48
2:M:125:ALA:HB1	5:M:855:BPH:H2	1.95	0.48
3:H:135:LYS:HD2	14:H:904:HOH:O	2.13	0.48
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.14	0.48
2:M:271:TRP:HH2	12:M:900:CDL:H342	1.78	0.47
3:H:194:GLN:H	3:H:194:GLN:HE21	1.59	0.47
1:L:208:THR:H	1:L:211:HIS:HD2	1.61	0.47
2:M:32:VAL:HG12	2:M:49:PRO:HD3	1.94	0.47
1:L:208:THR:HB	1:L:209:PRO:HD2	1.96	0.47
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.50	0.47
4:L:854:BCL:H193	4:L:854:BCL:H162	1.80	0.47
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.96	0.47
2:M:56:GLY:HA2	2:M:132:ARG:HD2	1.97	0.47
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.97	0.46
4:L:854:BCL:HBB3	5:L:856:BPH:H141	1.98	0.46
4:L:852:BCL:H122	5:L:856:BPH:H3A	1.97	0.46
2:M:69:THR:O	2:M:72:ILE:HG22	2.16	0.46
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.51	0.46
4:L:852:BCL:CGA	4:L:854:BCL:HBC1	2.46	0.46
2:M:195:ASN:HD22	2:M:195:ASN:C	2.19	0.46
2:M:24:VAL:O	2:M:26:LEU:HD12	2.16	0.46
4:L:852:BCL:HBD	4:L:854:BCL:HAC1	1.98	0.46
1:L:84:GLY:HA2	1:L:87:GLN:HE21	1.81	0.45
3:H:245:ALA:HA	3:H:248:ARG:HH12	1.81	0.45
1:L:34:PHE:CE1	1:L:102:LEU:HD23	2.52	0.45
1:L:238:LEU:HD23	5:L:856:BPH:CBC	2.47	0.45
3:H:170:ASP:OD1	3:H:172:PRO:HD2	2.17	0.44
3:H:184:LYS:N	3:H:184:LYS:HD2	2.32	0.44
3:H:206:ASN:HD21	3:H:248:ARG:CD	2.29	0.44
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.82	0.44
2:M:53:GLY:O	2:M:57:VAL:HG23	2.18	0.44
1:L:208:THR:HB	1:L:209:PRO:CD	2.48	0.43
3:H:66:LEU:HA	3:H:67:PRO:HD3	1.86	0.43
1:L:42:ALA:HA	5:L:856:BPH:H9C3	2.01	0.43
2:M:195:ASN:ND2	2:M:197:PHE:H	2.17	0.43
2:M:236:GLU:HG3	3:H:122:GLU:OE2	2.19	0.43
2:M:194:GLY:O	2:M:195:ASN:CB	2.67	0.43
2:M:26:LEU:H	2:M:26:LEU:CD1	2.31	0.42
2:M:290:VAL:HG11	3:H:12:LEU:HB3	2.01	0.42
3:H:99:ALA:HA	3:H:100:PRO:HD3	1.92	0.42
3:H:191:LEU:HD11	3:H:213:PHE:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:9:GLN:HE22	3:H:197:LYS:HA	1.83	0.42
4:L:851:BCL:HBC2	4:L:851:BCL:H2C	1.87	0.42
3:H:70:ARG:HH22	3:H:123:LEU:HD13	1.85	0.42
1:L:272:TRP:HA	1:L:275:ILE:HG13	2.01	0.42
2:M:56:GLY:O	2:M:60:LEU:HD13	2.20	0.41
3:H:220:LYS:HG3	3:H:229:GLU:OE2	2.19	0.41
1:L:60:ASN:CB	1:L:63:LEU:HD23	2.51	0.41
3:H:221:SER:HA	3:H:222:PRO:HD3	1.84	0.41
3:H:220:LYS:HB2	3:H:220:LYS:HE3	1.78	0.41
4:L:854:BCL:H141	4:L:854:BCL:H161	1.87	0.40
1:L:262:TRP:O	1:L:265:TRP:HD1	2.05	0.40
2:M:87:ARG:HG3	2:M:88:ASP:N	2.35	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%)	270 (97%)	9 (3%)	0	100	100
2	M	299/307 (97%)	292 (98%)	7 (2%)	0	100	100
3	H	238/260 (92%)	234 (98%)	4 (2%)	0	100	100
All	All	816/848 (96%)	796 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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%)	210 (96%)	10 (4%)	27	27
2	M	236/240 (98%)	226 (96%)	10 (4%)	30	30
3	H	195/208 (94%)	189 (97%)	6 (3%)	40	43
All	All	651/668 (98%)	625 (96%)	26 (4%)	31	32

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	85	LEU
1	L	102	LEU
1	L	129	LEU
1	L	189	LEU
1	L	195	LEU
1	L	207	ARG
1	L	210	ASP
1	L	247	CYS
1	L	269	LEU
1	L	272	TRP
2	M	5	ASN
2	M	87	ARG
2	M	94	LEU
2	M	151	LEU
2	M	156	LEU
2	M	191	LEU
2	M	195	ASN
2	M	196	LEU
2	M	216	PHE
2	M	300	ASN
3	H	12	LEU
3	H	73	LEU
3	H	89	ARG
3	H	194	GLN
3	H	202	ARG
3	H	231	ASP

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

Mol	Chain	Res	Type
1	L	62	GLN
1	L	87	GLN
1	L	211	HIS
1	L	213	ASN
2	M	5	ASN
2	M	9	GLN
2	M	195	ASN
2	M	300	ASN
3	H	194	GLN
3	H	206	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\# Z > 2$
7	GOL	L	866	-	5,5,5	4.53	5 (100%)	5,5,5	5.73	3 (60%)
4	BCL	L	854	-	58,74,74	1.34	6 (10%)	69,115,115	1.93	18 (26%)
5	BPH	M	855	-	50,56,70	1.42	8 (16%)	59,84,101	2.30	19 (32%)
11	LDA	M	863	-	12,15,15	2.12	1 (8%)	14,17,17	1.68	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BPH	L	856	-	64,70,70	1.48	9 (14%)	76,101,101	2.09	20 (26%)
10	SPO	M	860	-	40,41,41	3.48	23 (57%)	47,50,50	4.17	16 (34%)
12	CDL	M	900	-	80,80,99	0.81	2 (2%)	86,92,111	0.96	4 (4%)
4	BCL	M	853	-	58,74,74	1.22	5 (8%)	69,115,115	2.14	21 (30%)
6	U10	L	859	-	24,24,63	2.12	8 (33%)	29,32,79	2.13	11 (37%)
4	BCL	L	851	-	43,59,74	1.41	5 (11%)	51,97,115	2.30	17 (33%)
6	U10	M	858	-	48,48,63	1.99	14 (29%)	58,61,79	2.73	14 (24%)
11	LDA	H	861	-	12,15,15	2.08	1 (8%)	14,17,17	1.75	4 (28%)
11	LDA	M	862	-	12,15,15	2.09	1 (8%)	14,17,17	1.72	4 (28%)
4	BCL	L	852	-	58,74,74	1.26	5 (8%)	69,115,115	1.91	20 (28%)
9	PO4	M	865	-	4,4,4	1.68	0	6,6,6	0.42	0
9	PO4	M	864	-	4,4,4	1.66	0	6,6,6	0.43	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
7	GOL	L	866	-	-	3/4/4/4	-
4	BCL	L	854	-	-	14/37/137/137	-
5	BPH	M	855	-	-	8/38/89/105	0/5/6/6
11	LDA	M	863	-	-	7/13/13/13	-
5	BPH	L	856	-	2/2/18/22	11/54/105/105	0/5/6/6
10	SPO	M	860	-	-	12/47/47/47	-
12	CDL	M	900	-	-	27/91/91/110	-
4	BCL	M	853	-	-	12/37/137/137	-
6	U10	L	859	-	-	4/17/41/87	0/1/1/1
4	BCL	L	851	-	-	1/19/119/137	-
6	U10	M	858	-	-	5/45/69/87	0/1/1/1
11	LDA	H	861	-	-	5/13/13/13	-
11	LDA	M	862	-	-	6/13/13/13	-
4	BCL	L	852	-	-	4/37/137/137	-

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	860	SPO	C6-C5	9.08	1.55	1.32
10	M	860	SPO	C10-C11	8.26	1.55	1.34
10	M	860	SPO	C15-C16	7.80	1.54	1.34
7	L	866	GOL	C3-C2	-7.45	1.21	1.51
11	M	863	LDA	O1-N1	-7.06	1.25	1.42
11	M	862	LDA	O1-N1	-7.00	1.25	1.42
11	H	861	LDA	O1-N1	-6.98	1.25	1.42
5	L	856	BPH	C11-C10	-5.36	1.29	1.52
10	M	860	SPO	C21-C20	5.35	1.49	1.36
6	M	858	U10	O4-C4	5.23	1.49	1.36
10	M	860	SPO	C27-C28	5.17	1.39	1.34
10	M	860	SPO	C26-C25	4.74	1.46	1.34
10	M	860	SPO	C14-C12	4.61	1.41	1.35
7	L	866	GOL	O1-C1	4.55	1.61	1.42
6	L	859	U10	O4-C4	4.45	1.47	1.36
10	M	860	SPO	O1-CM1	4.32	1.56	1.43
10	M	860	SPO	C9-C7	4.31	1.41	1.35
5	M	855	BPH	O2A-CGA	4.11	1.45	1.33
6	L	859	U10	C13-C14	4.09	1.42	1.33
5	M	855	BPH	O2D-CGD	4.06	1.43	1.33
5	L	856	BPH	O2A-CGA	3.97	1.45	1.33
5	L	856	BPH	O2D-CGD	3.87	1.42	1.33
10	M	860	SPO	C19-C17	3.81	1.40	1.35
4	M	853	BCL	MG-NA	3.79	2.15	2.06
6	M	858	U10	C13-C14	3.57	1.41	1.33
6	L	859	U10	C7-C8	-3.56	1.45	1.50
6	M	858	U10	C7-C8	-3.53	1.45	1.50
4	L	852	BCL	C1B-NB	3.53	1.38	1.35
6	L	859	U10	O3-C3	3.52	1.45	1.36
4	L	854	BCL	MG-NA	3.51	2.14	2.06
4	M	853	BCL	C1B-NB	3.38	1.38	1.35
6	M	858	U10	C6-C1	3.33	1.41	1.35
4	L	852	BCL	MG-NA	3.32	2.14	2.06
7	L	866	GOL	O3-C3	3.28	1.56	1.42
6	M	858	U10	C23-C24	3.26	1.40	1.33
6	M	858	U10	O3-C3	3.24	1.44	1.36
4	L	854	BCL	C1B-NB	3.22	1.38	1.35
10	M	860	SPO	C10-C9	3.17	1.53	1.43
4	L	851	BCL	C1B-NB	3.10	1.38	1.35
6	L	859	U10	C6-C1	3.08	1.40	1.35
6	L	859	U10	C8-C9	3.02	1.40	1.33
10	M	860	SPO	C25-C23	-3.01	1.39	1.45
6	M	858	U10	O3-C3M	-3.00	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	851	BCL	MG-NA	3.00	2.13	2.06
10	M	860	SPO	C32-C33	2.94	1.40	1.33
6	L	859	U10	O3-C3M	-2.91	1.38	1.45
7	L	866	GOL	O2-C2	-2.86	1.34	1.43
10	M	860	SPO	C37-C38	2.85	1.40	1.32
10	M	860	SPO	O1-C1	2.81	1.57	1.41
12	M	900	CDL	OA8-CA7	2.79	1.41	1.33
10	M	860	SPO	C15-C14	2.79	1.52	1.43
5	L	856	BPH	C2-C3	2.77	1.39	1.33
6	M	858	U10	C8-C9	2.77	1.39	1.33
7	L	866	GOL	C1-C2	-2.76	1.40	1.51
10	M	860	SPO	C8-C7	2.72	1.56	1.50
4	L	851	BCL	C3C-C4C	-2.72	1.48	1.51
4	L	851	BCL	MG-NC	-2.68	1.99	2.06
6	M	858	U10	C38-C39	2.67	1.40	1.32
10	M	860	SPO	C13-C12	2.64	1.56	1.50
5	M	855	BPH	O2D-CED	-2.64	1.39	1.45
5	M	855	BPH	C2-C3	2.63	1.39	1.33
4	L	854	BCL	MG-NC	-2.61	2.00	2.06
6	M	858	U10	C18-C19	2.59	1.39	1.33
5	M	855	BPH	CAA-C2A	2.58	1.58	1.54
6	M	858	U10	C32-C33	-2.55	1.42	1.50
5	L	856	BPH	O2D-CED	-2.53	1.39	1.45
4	L	854	BCL	CAA-CBA	2.48	1.60	1.52
10	M	860	SPO	C26-C27	2.48	1.51	1.43
5	L	856	BPH	CAA-C2A	2.47	1.58	1.54
4	L	854	BCL	CAA-C2A	2.40	1.58	1.54
12	M	900	CDL	CB3-CB4	2.35	1.57	1.50
4	L	852	BCL	CBB-CAB	2.33	1.56	1.49
6	M	858	U10	C15-C14	2.33	1.56	1.50
6	M	858	U10	C28-C29	2.31	1.38	1.33
10	M	860	SPO	C11-C12	-2.31	1.41	1.45
4	M	853	BCL	CBB-CAB	2.30	1.56	1.49
6	L	859	U10	C15-C14	2.27	1.56	1.50
4	L	852	BCL	C4-C3	2.26	1.56	1.50
5	M	855	BPH	C2A-C1A	2.24	1.55	1.51
10	M	860	SPO	C24-C23	2.23	1.55	1.50
4	L	852	BCL	C3D-CAD	-2.21	1.40	1.46
10	M	860	SPO	C6-C7	-2.18	1.41	1.45
6	M	858	U10	C31-C29	2.13	1.55	1.51
5	M	855	BPH	C2C-C3C	-2.12	1.48	1.54
4	M	853	BCL	C4-C3	2.11	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	856	BPH	C2A-C1A	2.11	1.55	1.51
10	M	860	SPO	C22-C23	2.10	1.38	1.35
4	L	854	BCL	C4-C3	2.10	1.56	1.50
5	L	856	BPH	O1D-CGD	2.07	1.26	1.21
4	M	853	BCL	C3D-CAD	-2.07	1.40	1.46
4	L	851	BCL	C4-C3	2.06	1.55	1.50
5	M	855	BPH	C3D-C2D	-2.05	1.35	1.39
5	L	856	BPH	CHC-C1C	2.00	1.40	1.36

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	860	SPO	C3-C1-C4	-17.04	84.70	110.86
10	M	860	SPO	C2-C1-C4	-16.98	84.78	110.86
6	M	858	U10	C32-C33-C34	14.95	163.67	127.66
7	L	866	GOL	O3-C3-C2	10.29	159.56	110.20
5	M	855	BPH	O2D-CGD-CBD	8.18	125.80	111.27
5	L	856	BPH	O2D-CGD-CBD	7.84	125.20	111.27
7	L	866	GOL	O2-C2-C3	6.81	139.13	109.12
6	M	858	U10	C27-C28-C29	6.47	143.24	127.66
6	M	858	U10	C3M-O3-C3	6.39	139.11	116.47
4	M	853	BCL	C1-C2-C3	6.38	137.07	126.04
10	M	860	SPO	C15-C14-C12	-6.23	118.42	127.31
6	L	859	U10	C3M-O3-C3	6.20	138.43	116.47
5	M	855	BPH	C1-C2-C3	5.91	136.26	126.04
4	L	851	BCL	C4A-NA-C1A	-5.90	104.06	106.71
5	L	856	BPH	C1-C2-C3	5.79	136.05	126.04
10	M	860	SPO	C20-C21-C22	-5.72	111.77	123.47
4	L	851	BCL	C4D-C3D-CAD	-5.71	105.29	108.47
4	L	854	BCL	C4A-NA-C1A	-5.71	104.14	106.71
4	L	851	BCL	CAC-C3C-C4C	-5.69	99.94	112.58
4	M	853	BCL	C4D-C3D-CAD	-5.56	105.37	108.47
10	M	860	SPO	C25-C23-C22	-5.21	110.95	118.94
5	M	855	BPH	C4A-NA-C1A	5.16	112.31	108.14
4	L	854	BCL	C4D-C3D-CAD	-5.13	105.61	108.47
5	L	856	BPH	C4A-NA-C1A	4.55	111.81	108.14
4	L	852	BCL	C4D-C3D-CAD	-4.53	105.94	108.47
5	M	855	BPH	CED-O2D-CGD	4.47	126.05	115.94
4	M	853	BCL	C4-C3-C5	4.39	122.65	115.27
5	L	856	BPH	CED-O2D-CGD	4.34	125.75	115.94
4	L	851	BCL	C2C-C3C-C4C	4.33	107.82	101.34
4	L	852	BCL	C4A-NA-C1A	-4.32	104.76	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	853	BCL	C5-C3-C2	-4.31	112.40	121.12
5	L	856	BPH	C6-C5-C3	4.13	124.29	113.45
10	M	860	SPO	C24-C23-C25	4.13	124.58	118.08
4	L	854	BCL	OBB-CAB-CBB	-4.06	111.03	120.17
4	L	854	BCL	CMD-C2D-C3D	4.06	132.26	124.68
4	M	853	BCL	OBD-CAD-CBD	-4.05	120.10	125.89
4	L	852	BCL	OBB-CAB-CBB	-4.04	111.08	120.17
10	M	860	SPO	C18-C17-C19	-4.03	117.28	122.92
4	M	853	BCL	OBB-CAB-CBB	-4.03	111.11	120.17
4	L	851	BCL	OBB-CAB-CBB	-4.02	111.13	120.17
12	M	900	CDL	OB8-CB6-CB4	3.99	120.05	108.43
4	L	851	BCL	CMD-C2D-C3D	3.93	132.04	124.68
5	L	856	BPH	CBC-CAC-C3C	3.89	122.13	113.47
4	L	852	BCL	C1-C2-C3	-3.85	119.39	126.04
4	M	853	BCL	C11-C12-C13	-3.81	103.62	115.92
6	L	859	U10	O5-C5-C6	-3.77	114.94	121.55
4	L	852	BCL	CMB-C2B-C3B	3.75	131.69	124.68
5	L	856	BPH	C11-C10-C8	3.74	128.00	115.92
5	M	855	BPH	CBC-CAC-C3C	3.71	121.73	113.47
4	M	853	BCL	CMD-C2D-C3D	3.68	131.56	124.68
4	L	852	BCL	C7-C6-C5	-3.66	103.41	113.36
10	M	860	SPO	C3-C1-C2	3.66	117.25	110.37
5	L	856	BPH	O2D-CGD-O1D	-3.60	116.81	123.84
5	M	855	BPH	O1D-CGD-CBD	-3.59	117.13	124.48
11	H	861	LDA	CM1-N1-C1	-3.58	102.72	110.23
6	M	858	U10	O5-C5-C6	-3.55	115.33	121.55
4	L	851	BCL	OBD-CAD-CBD	-3.55	120.83	125.89
4	L	852	BCL	CMD-C2D-C3D	3.55	131.31	124.68
4	L	854	BCL	C11-C12-C13	-3.54	104.46	115.92
6	M	858	U10	C30-C29-C31	-3.54	109.32	115.27
11	M	862	LDA	CM1-N1-C1	-3.53	102.81	110.23
4	L	851	BCL	CMB-C2B-C3B	3.52	131.27	124.68
4	L	854	BCL	OBD-CAD-CBD	-3.48	120.92	125.89
5	M	855	BPH	O2D-CGD-O1D	-3.47	117.05	123.84
6	L	859	U10	O2-C2-C3	-3.47	113.57	120.93
11	M	863	LDA	CM1-N1-C1	-3.40	103.09	110.23
10	M	860	SPO	C15-C16-C17	-3.39	116.89	126.42
4	M	853	BCL	CMB-C2B-C3B	3.32	130.90	124.68
4	L	851	BCL	C1-C2-C3	-3.31	121.39	126.75
4	L	852	BCL	CMB-C2B-C1B	-3.30	123.40	128.46
7	L	866	GOL	O1-C1-C2	3.28	125.93	110.20
4	L	854	BCL	CMB-C2B-C3B	3.22	130.69	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	856	BPH	O1D-CGD-CBD	-3.20	117.94	124.48
12	M	900	CDL	CB4-OB6-CB5	3.16	125.57	117.79
4	L	854	BCL	C2C-C3C-C4C	3.14	106.05	101.34
4	L	852	BCL	CAC-C3C-C4C	-3.13	105.64	112.58
4	M	853	BCL	CMB-C2B-C1B	-3.09	123.71	128.46
4	L	852	BCL	OBD-CAD-CBD	-3.09	121.48	125.89
4	L	854	BCL	CAA-C2A-C3A	-3.05	104.42	112.78
4	L	851	BCL	CMB-C2B-C1B	-3.04	123.78	128.46
10	M	860	SPO	C6-C7-C9	-3.03	114.30	118.94
4	L	852	BCL	CAA-C2A-C3A	-2.99	104.58	112.78
4	L	854	BCL	C7-C6-C5	-2.96	105.33	113.36
10	M	860	SPO	C8-C7-C6	2.93	122.69	118.08
4	M	853	BCL	CHA-C1A-NA	-2.91	119.73	126.40
6	M	858	U10	C20-C19-C21	-2.91	110.38	115.27
4	L	851	BCL	CAA-C2A-C3A	-2.91	104.82	112.78
6	L	859	U10	C1-C6-C5	-2.88	116.87	119.58
5	L	856	BPH	C2C-C3C-C4C	2.86	105.62	101.34
4	L	851	BCL	CHA-C1A-NA	-2.85	119.86	126.40
11	H	861	LDA	O1-N1-C1	2.85	116.26	109.27
6	L	859	U10	C15-C14-C16	-2.85	112.73	115.98
5	M	855	BPH	C4D-CHA-C1A	-2.85	123.49	130.51
4	L	854	BCL	CHA-C1A-NA	-2.83	119.91	126.40
11	M	863	LDA	O1-N1-C1	2.82	116.20	109.27
11	M	862	LDA	O1-N1-C1	2.81	116.16	109.27
6	M	858	U10	O2-C2-C3	-2.80	114.98	120.93
5	M	855	BPH	C2C-C3C-C4C	2.80	105.54	101.34
5	M	855	BPH	CHD-C4C-NC	-2.79	121.89	125.20
4	M	853	BCL	CBB-CAB-C3B	2.77	128.58	120.34
5	L	856	BPH	C7-C6-C5	-2.76	105.86	113.36
4	L	854	BCL	CMB-C2B-C1B	-2.74	124.25	128.46
5	L	856	BPH	C3C-C2C-C1C	2.74	106.29	101.87
6	L	859	U10	C16-C14-C13	2.69	127.16	120.50
4	M	853	BCL	C16-C15-C13	-2.68	107.27	115.92
4	L	852	BCL	CHA-C1A-NA	-2.67	120.29	126.40
4	L	851	BCL	CBB-CAB-C3B	2.66	128.25	120.34
5	L	856	BPH	C4D-CHA-C1A	-2.66	123.95	130.51
4	M	853	BCL	C4A-NA-C1A	-2.66	105.51	106.71
4	M	853	BCL	C11-C10-C8	-2.63	107.43	115.92
10	M	860	SPO	C10-C9-C7	-2.62	123.57	127.31
4	M	853	BCL	CAA-C2A-C3A	-2.62	105.61	112.78
4	L	852	BCL	CBB-CAB-C3B	2.61	128.09	120.34
10	M	860	SPO	C1-C4-C5	2.60	119.94	113.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	855	BPH	C4-C3-C5	2.55	118.90	115.98
6	M	858	U10	C6-C1-C2	2.54	121.19	119.18
4	L	852	BCL	O2D-CGD-CBD	-2.54	106.76	111.27
4	L	851	BCL	C3C-C2C-C1C	-2.53	97.79	101.87
4	M	853	BCL	CED-O2D-CGD	2.53	121.65	115.94
5	L	856	BPH	O2A-CGA-O1A	-2.50	117.28	123.59
4	L	852	BCL	C11-C12-C13	-2.50	107.85	115.92
6	M	858	U10	C31-C29-C28	2.49	126.16	121.12
5	M	855	BPH	C2A-C1A-NA	-2.48	109.02	111.86
6	M	858	U10	C1-C6-C5	-2.47	117.26	119.58
4	L	854	BCL	CBB-CAB-C3B	2.46	127.64	120.34
6	M	858	U10	C16-C14-C13	2.46	126.08	121.12
4	L	852	BCL	O1D-CGD-CBD	2.45	129.50	124.48
5	M	855	BPH	CAA-C2A-C3A	-2.43	106.13	112.78
12	M	900	CDL	CB6-CB4-CB3	-2.43	106.05	111.79
11	M	862	LDA	CM2-N1-C1	2.41	115.29	110.23
5	M	855	BPH	C3C-C2C-C1C	2.39	105.73	101.87
4	L	854	BCL	C3D-CAD-CBD	2.39	110.75	107.61
4	L	854	BCL	C1-C2-C3	-2.39	121.91	126.04
11	H	861	LDA	CM2-N1-C1	2.37	115.21	110.23
5	M	855	BPH	CMD-C2D-C3D	2.34	129.06	124.68
6	M	858	U10	C21-C19-C18	2.33	125.83	121.12
5	L	856	BPH	CAA-C2A-C3A	-2.33	106.40	112.78
5	L	856	BPH	CHD-C4C-NC	-2.33	122.44	125.20
11	H	861	LDA	C9-C8-C7	-2.32	102.63	114.42
4	L	851	BCL	C3D-CAD-CBD	2.31	110.65	107.61
4	L	854	BCL	CAC-C3C-C4C	-2.31	107.46	112.58
5	L	856	BPH	CAC-C3C-C2C	-2.30	108.52	114.26
11	M	863	LDA	CM2-N1-C1	2.29	115.05	110.23
11	M	862	LDA	C9-C8-C7	-2.27	102.91	114.42
4	L	854	BCL	C12-C11-C10	-2.26	102.84	113.24
5	M	855	BPH	CBB-CAB-C3B	-2.26	115.59	120.43
12	M	900	CDL	C52-C51-CB5	2.26	121.84	113.62
4	L	852	BCL	CED-O2D-CGD	2.24	121.00	115.94
4	L	854	BCL	C16-C15-C13	-2.23	108.71	115.92
5	L	856	BPH	CMD-C2D-C3D	2.23	128.84	124.68
5	M	855	BPH	O2A-CGA-O1A	-2.20	118.04	123.59
6	L	859	U10	C6-C1-C2	2.19	120.91	119.18
4	M	853	BCL	C3D-CAD-CBD	2.19	110.49	107.61
4	L	852	BCL	C12-C11-C10	-2.19	103.19	113.24
10	M	860	SPO	C27-C26-C25	-2.18	116.42	123.22
11	M	863	LDA	C9-C8-C7	-2.17	103.39	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	856	BPH	OBD-CAD-CBD	-2.17	122.80	125.89
4	L	852	BCL	C2C-C3C-C4C	2.17	104.58	101.34
10	M	860	SPO	C20-C19-C17	-2.16	124.22	127.31
4	L	851	BCL	C1C-NC-C4C	2.16	107.67	106.71
5	M	855	BPH	OBD-CAD-CBD	-2.12	122.87	125.89
4	M	853	BCL	CAC-C3C-C2C	-2.09	109.03	114.26
6	L	859	U10	C8-C7-C6	2.08	117.64	112.05
6	M	858	U10	C7-C8-C9	2.07	130.25	126.79
5	M	855	BPH	C3A-C2A-C1A	2.07	104.12	101.64
6	M	858	U10	C31-C32-C33	2.06	118.65	111.88
10	M	860	SPO	O1-C1-C2	2.06	123.12	108.97
5	L	856	BPH	C5-C3-C2	-2.06	116.95	121.12
4	L	852	BCL	C16-C15-C13	-2.04	109.33	115.92
4	M	853	BCL	C7-C6-C5	-2.03	107.84	113.36
6	L	859	U10	C4-C3-C2	-2.03	116.69	120.68
4	M	853	BCL	C14-C13-C15	-2.03	103.95	111.29
4	L	851	BCL	CBC-CAC-C3C	-2.02	108.96	113.47
6	L	859	U10	C7-C6-C5	-2.02	116.05	118.48
6	L	859	U10	C1M-C1-C6	-2.01	121.12	124.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	856	BPH	C8
5	L	856	BPH	C13

All (119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	854	BCL	C2C-C3C-CAC-CBC
5	L	856	BPH	C4C-C3C-CAC-CBC
5	L	856	BPH	C2C-C3C-CAC-CBC
5	L	856	BPH	O2A-C1-C2-C3
5	M	855	BPH	C4B-C3B-CAB-CBB
5	M	855	BPH	C4B-C3B-CAB-OB
5	M	855	BPH	C2B-C3B-CAB-CBB
5	M	855	BPH	C2B-C3B-CAB-OB
5	M	855	BPH	O2A-C1-C2-C3
5	M	855	BPH	C1-C2-C3-C4
6	L	859	U10	C15-C14-C16-C17
6	M	858	U10	C31-C32-C33-C34
7	L	866	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
10	M	860	SPO	C3-C1-O1-CM1
10	M	860	SPO	C4-C5-C6-C7
10	M	860	SPO	C33-C35-C36-C37
10	M	860	SPO	C36-C37-C38-C40
12	M	900	CDL	CA3-OA5-PA1-OA2
12	M	900	CDL	CA3-OA5-PA1-OA3
12	M	900	CDL	CA3-OA5-PA1-OA4
5	M	855	BPH	C1-C2-C3-C5
10	M	860	SPO	C36-C37-C38-C39
6	M	858	U10	C24-C26-C27-C28
12	M	900	CDL	CB7-C71-C72-C73
5	L	856	BPH	C8-C10-C11-C12
5	L	856	BPH	C10-C11-C12-C13
4	L	854	BCL	C16-C17-C18-C20
12	M	900	CDL	C11-C12-C13-C14
12	M	900	CDL	C78-C79-C80-C81
12	M	900	CDL	C20-C21-C22-C23
12	M	900	CDL	C34-C35-C36-C37
12	M	900	CDL	C11-CA5-OA6-CA4
11	H	861	LDA	C11-C10-C9-C8
12	M	900	CDL	C19-C20-C21-C22
12	M	900	CDL	OA7-CA5-OA6-CA4
11	M	862	LDA	C2-C3-C4-C5
11	M	863	LDA	C4-C5-C6-C7
5	L	856	BPH	C4-C3-C5-C6
5	L	856	BPH	C2-C3-C5-C6
11	M	863	LDA	C1-C2-C3-C4
11	M	863	LDA	C2-C3-C4-C5
4	M	853	BCL	C11-C10-C8-C9
4	M	853	BCL	C3-C5-C6-C7
4	L	854	BCL	C1A-C2A-CAA-CBA
12	M	900	CDL	CB3-OB5-PB2-OB2
4	L	854	BCL	C15-C16-C17-C18
12	M	900	CDL	OA5-CA3-CA4-CA6
10	M	860	SPO	C1-C4-C5-C6
12	M	900	CDL	CA3-CA4-CA6-OA8
11	H	861	LDA	C9-C10-C11-C12
12	M	900	CDL	C55-C56-C57-C58
12	M	900	CDL	C40-C41-C42-C43
12	M	900	CDL	C17-C18-C19-C20
11	M	862	LDA	C1-C2-C3-C4
4	L	854	BCL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
4	M	853	BCL	C11-C10-C8-C7
4	M	853	BCL	C14-C13-C15-C16
12	M	900	CDL	C21-C22-C23-C24
12	M	900	CDL	CA5-C11-C12-C13
4	M	853	BCL	C4-C3-C5-C6
7	L	866	GOL	O1-C1-C2-O2
12	M	900	CDL	OA5-CA3-CA4-OA6
12	M	900	CDL	C39-C40-C41-C42
4	L	852	BCL	C15-C16-C17-C18
4	L	854	BCL	C16-C17-C18-C19
5	L	856	BPH	C12-C13-C15-C16
10	M	860	SPO	C20-C21-C22-C23
4	L	852	BCL	CAD-CBD-CGD-O2D
5	L	856	BPH	CAD-CBD-CGD-O2D
11	M	862	LDA	C2-C1-N1-CM1
11	M	862	LDA	C2-C1-N1-CM2
11	M	863	LDA	C2-C1-N1-CM1
11	M	863	LDA	C2-C1-N1-CM2
11	H	861	LDA	C2-C1-N1-CM1
11	H	861	LDA	C2-C1-N1-CM2
12	M	900	CDL	OA6-CA4-CA6-OA8
12	M	900	CDL	C80-C81-C82-C83
7	L	866	GOL	O1-C1-C2-C3
4	M	853	BCL	C15-C16-C17-C18
12	M	900	CDL	CB3-OB5-PB2-OB4
11	M	863	LDA	C9-C10-C11-C12
6	L	859	U10	C13-C14-C16-C17
11	M	862	LDA	C2-C1-N1-O1
11	M	863	LDA	C2-C1-N1-O1
11	H	861	LDA	C2-C1-N1-O1
4	M	853	BCL	C11-C12-C13-C15
4	L	854	BCL	C11-C10-C8-C9
6	L	859	U10	C9-C11-C12-C13
4	M	853	BCL	C12-C13-C15-C16
4	M	853	BCL	C11-C12-C13-C14
5	L	856	BPH	C14-C13-C15-C16
6	M	858	U10	C5-C4-O4-C4M
4	M	853	BCL	C2-C3-C5-C6
10	M	860	SPO	C18-C17-C19-C20
4	L	852	BCL	C12-C13-C15-C16
4	L	854	BCL	C11-C10-C8-C7
10	M	860	SPO	C16-C17-C19-C20

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Mol	Chain	Res	Type	Atoms
6	M	858	U10	C30-C29-C31-C32
4	L	854	BCL	C4C-C3C-CAC-CBC
4	L	854	BCL	C13-C15-C16-C17
10	M	860	SPO	C4-C1-O1-CM1
11	M	862	LDA	C6-C7-C8-C9
4	M	853	BCL	CAA-CBA-CGA-O2A
4	L	854	BCL	C11-C12-C13-C14
4	L	851	BCL	CAD-CBD-CGD-O2D
5	M	855	BPH	CAD-CBD-CGD-O2D
12	M	900	CDL	C32-C31-CA7-OA8
4	L	854	BCL	CHA-CBD-CGD-O1D
4	L	854	BCL	CHA-CBD-CGD-O2D
10	M	860	SPO	C17-C19-C20-C21
4	L	852	BCL	C14-C13-C15-C16
6	L	859	U10	C5-C4-O4-C4M
4	L	854	BCL	C2A-CAA-CBA-CGA
10	M	860	SPO	C30-C31-C32-C33
5	L	856	BPH	C2-C1-O2A-CGA
12	M	900	CDL	C32-C31-CA7-OA9
4	M	853	BCL	CAA-CBA-CGA-O1A
12	M	900	CDL	CB2-OB2-PB2-OB4
6	M	858	U10	C28-C29-C31-C32

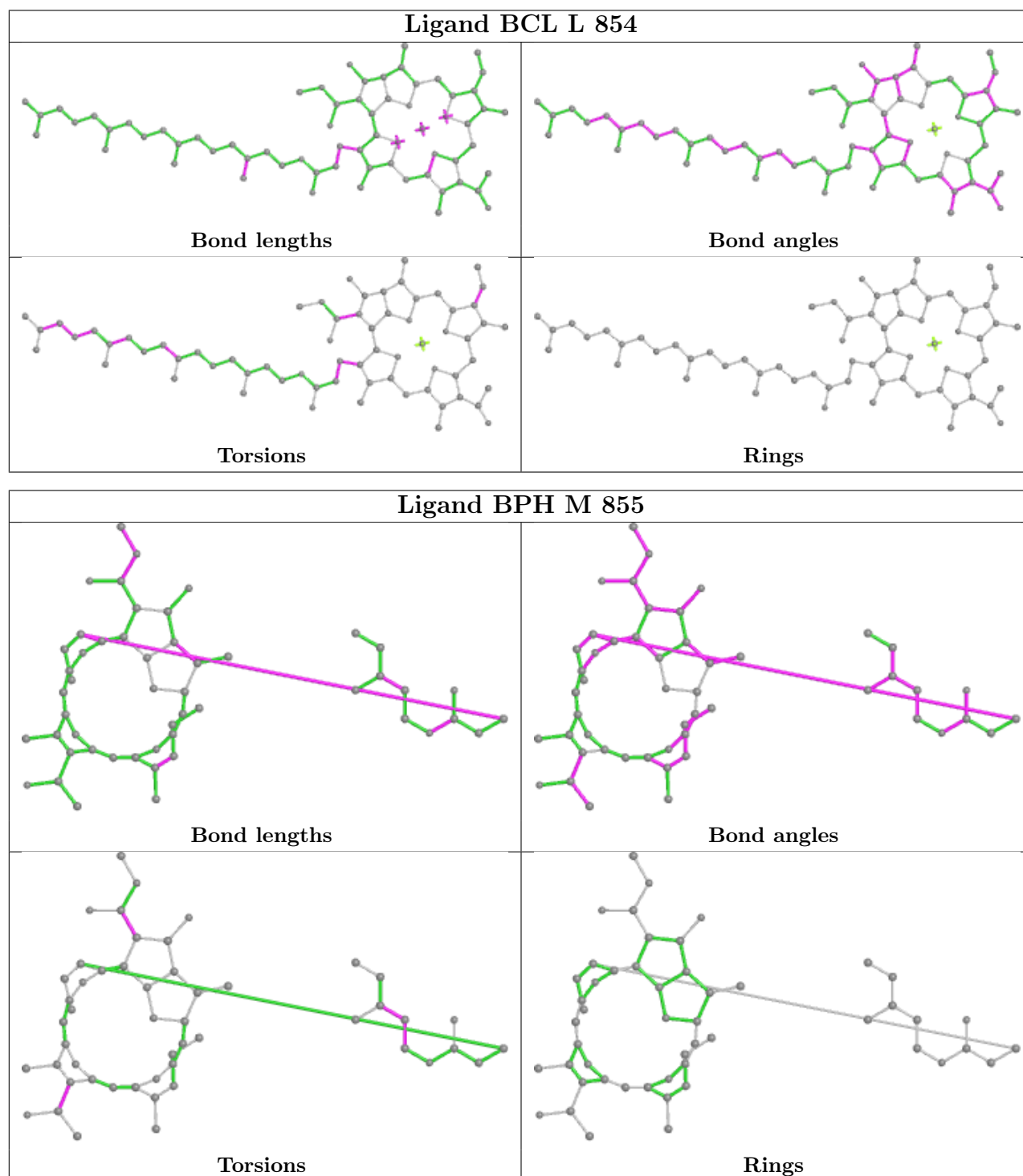
There are no ring outliers.

8 monomers are involved in 21 short contacts:

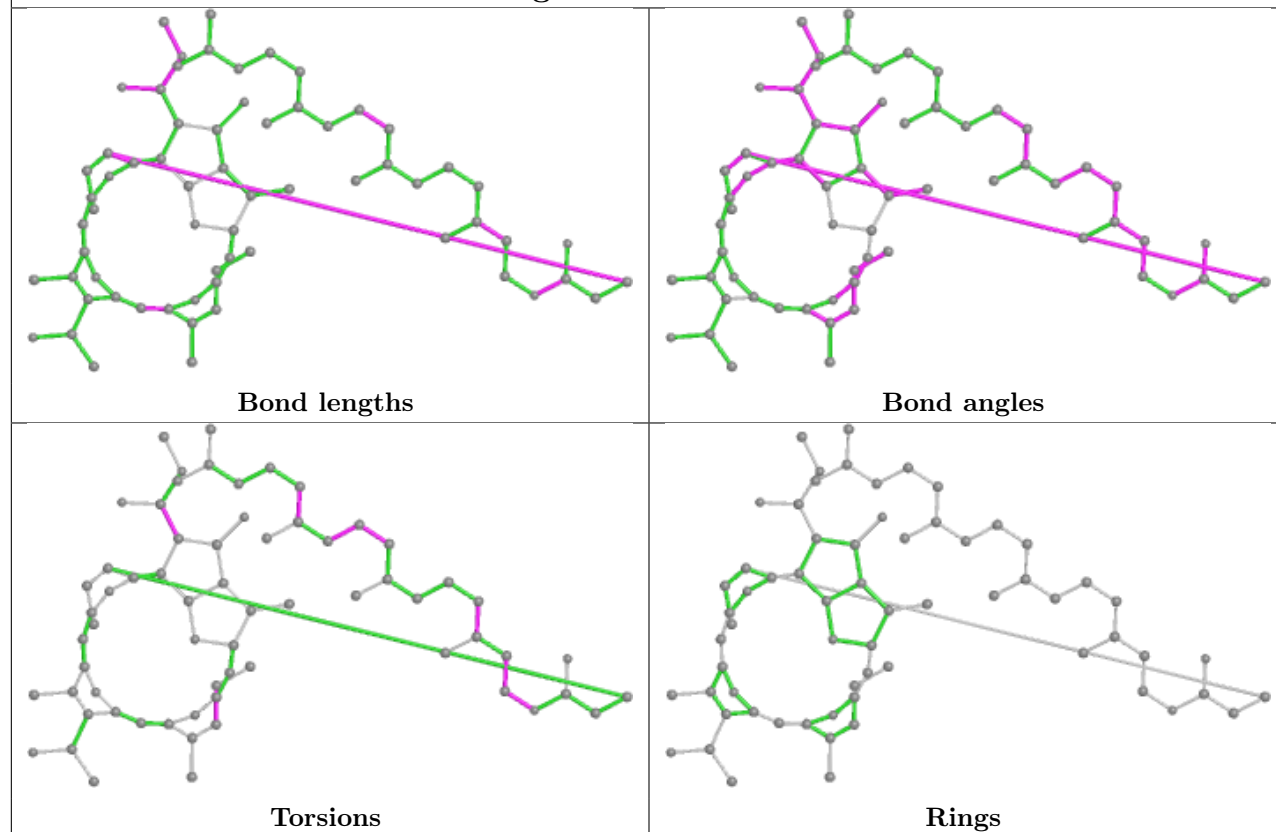
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	854	BCL	8	0
5	M	855	BPH	2	0
5	L	856	BPH	6	0
12	M	900	CDL	1	0
4	M	853	BCL	4	0
6	L	859	U10	1	0
4	L	851	BCL	4	0
4	L	852	BCL	4	0

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

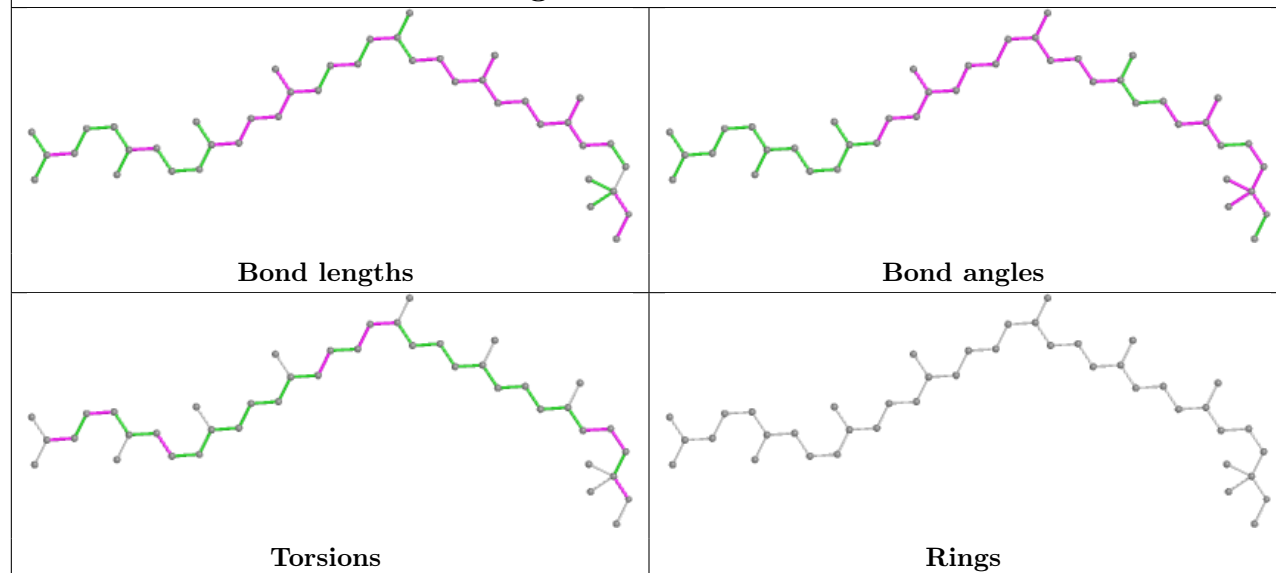
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

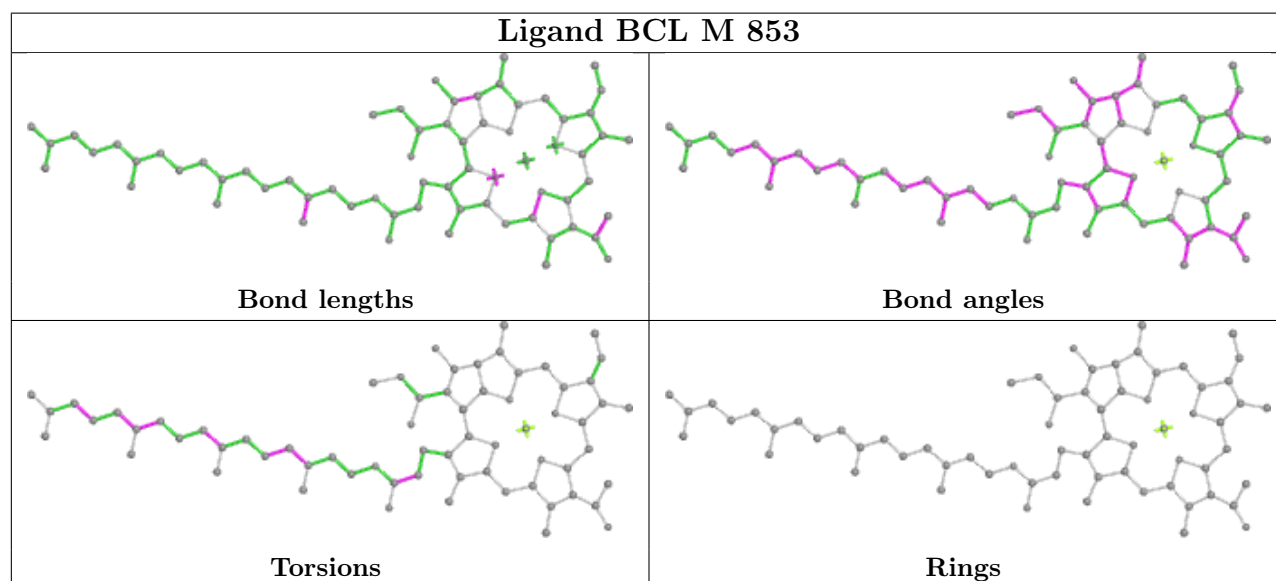
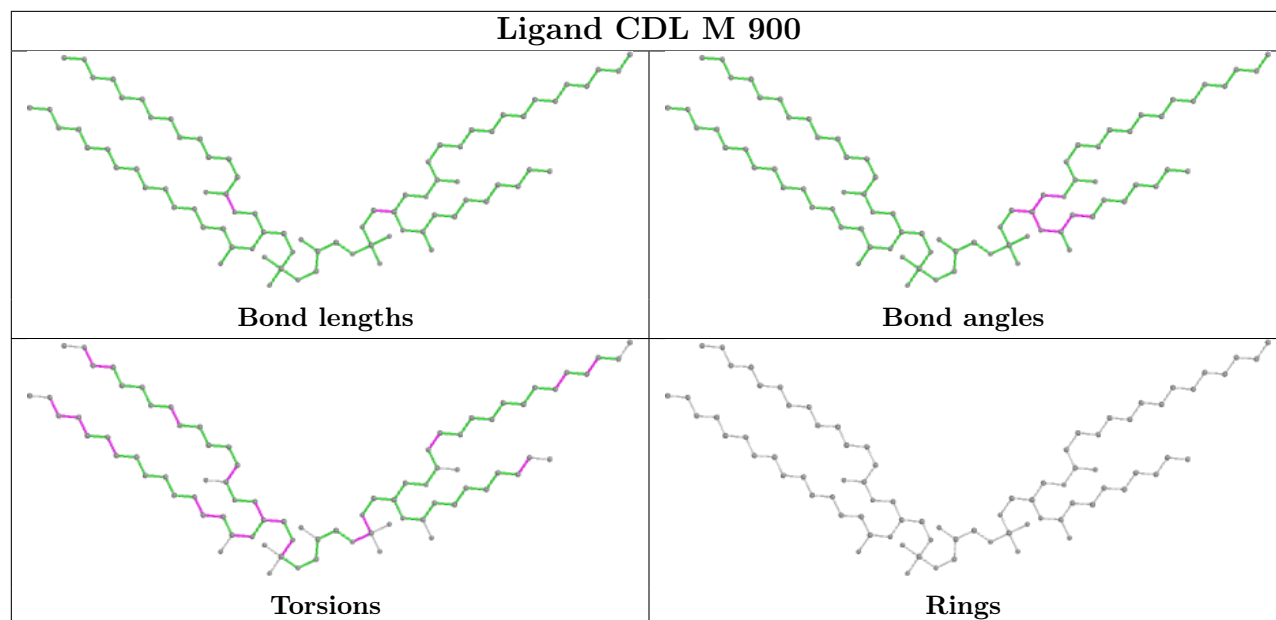


Ligand BPH L 856

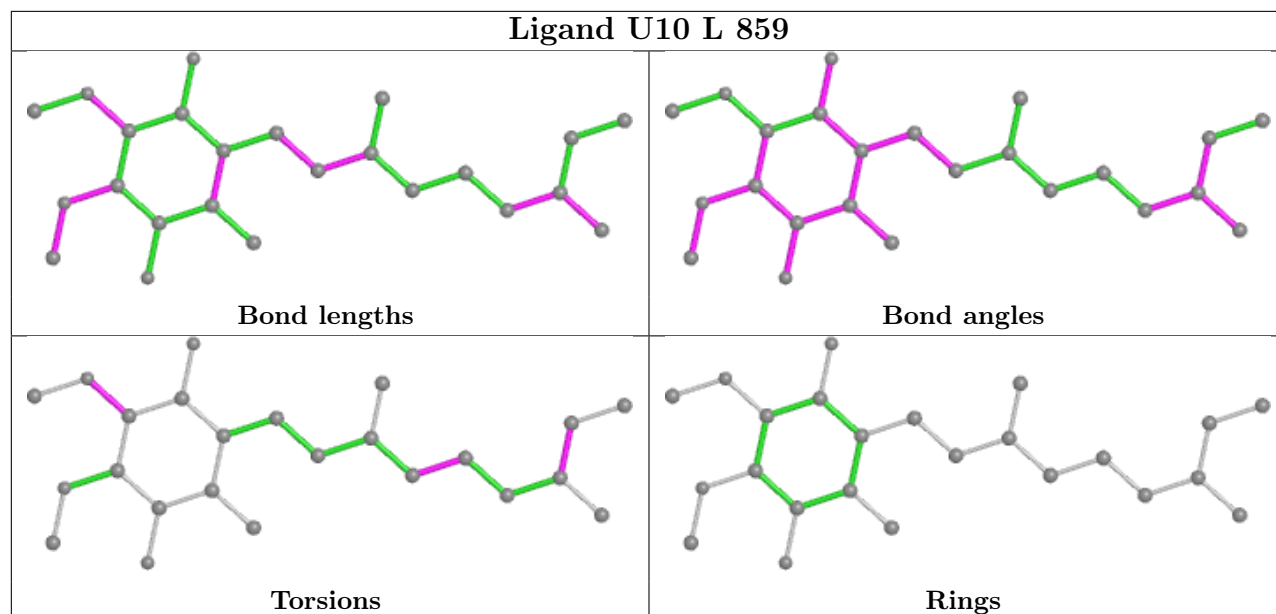


Ligand SPO M 860

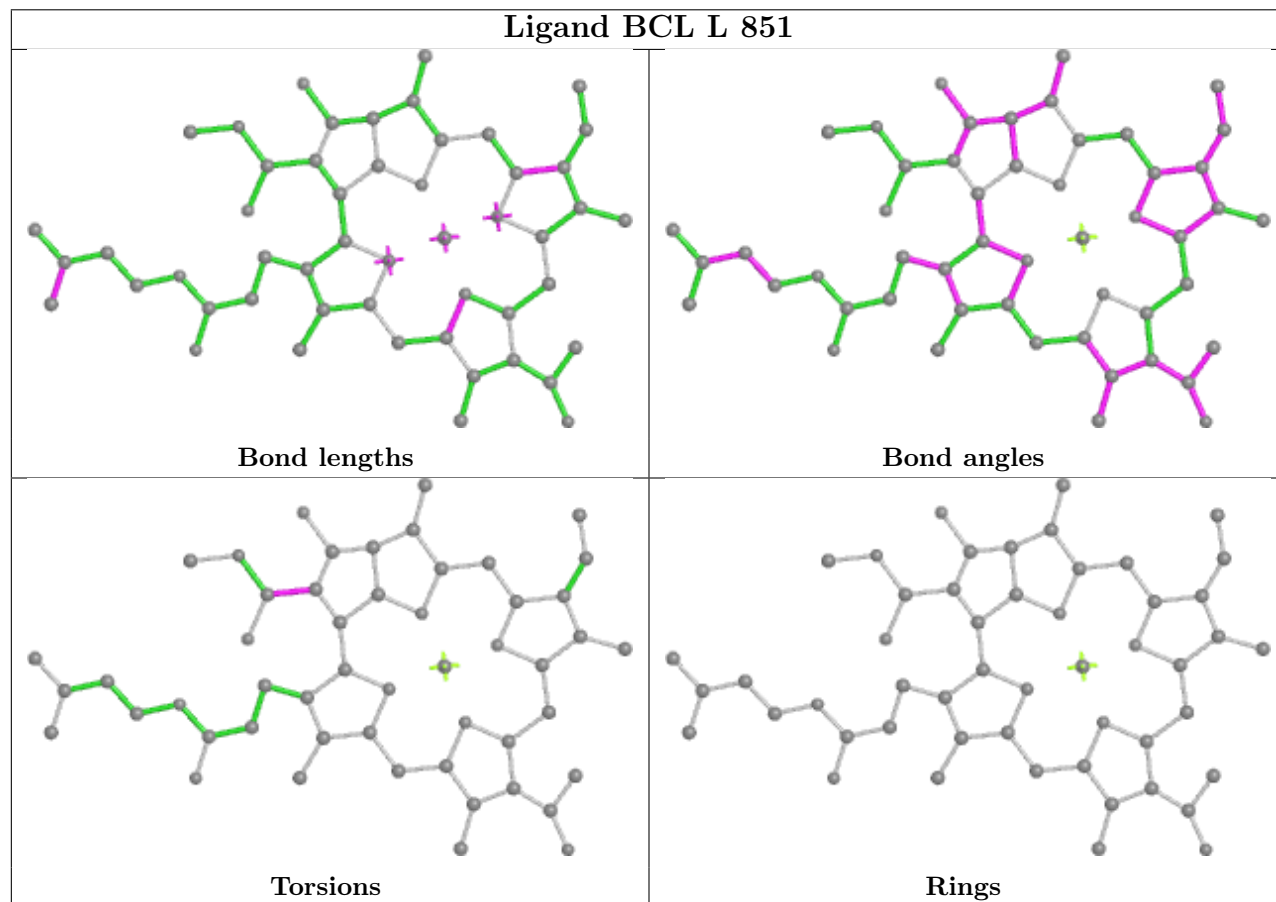


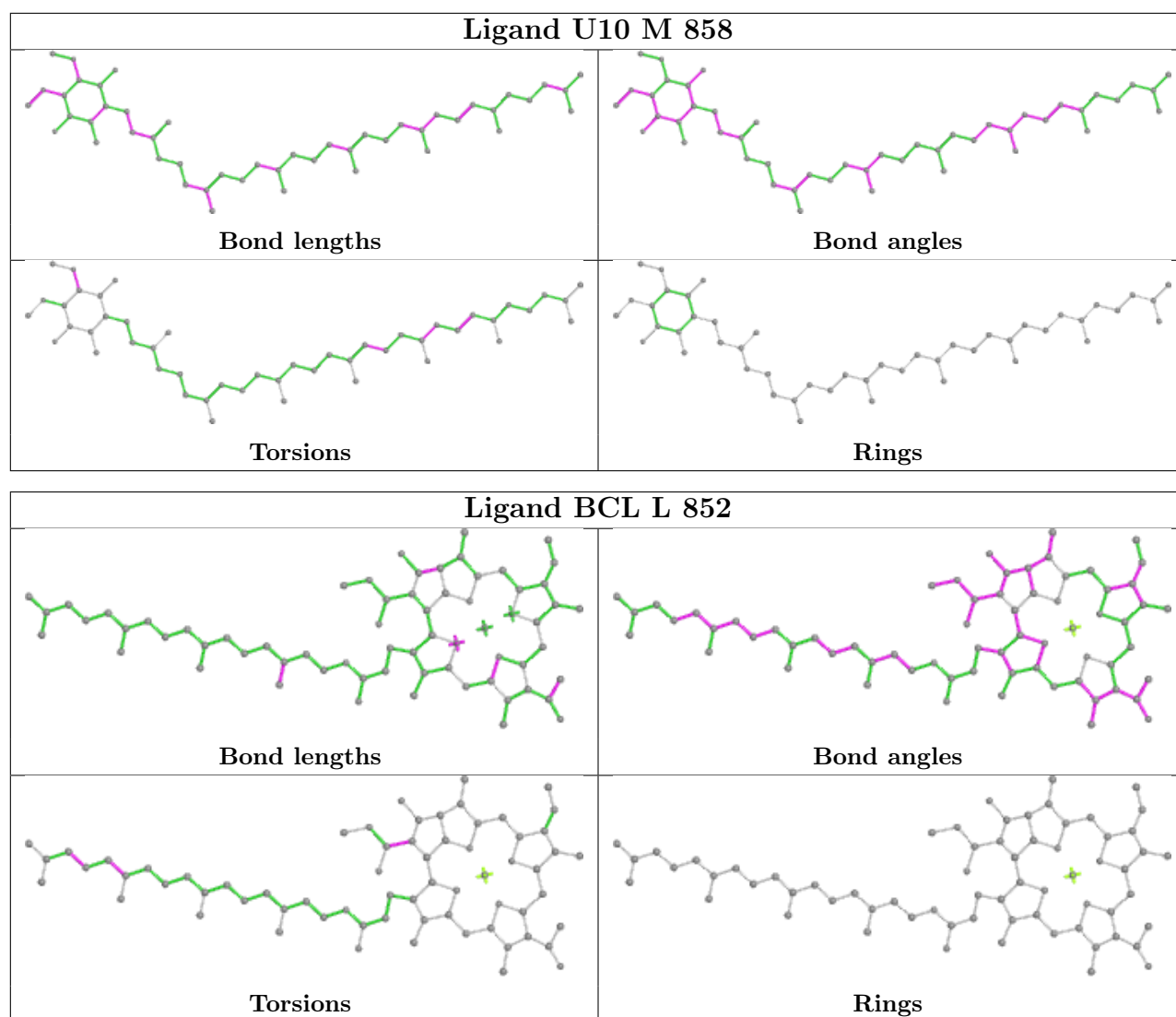


Ligand U10 L 859



Ligand BCL L 851





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 ⓘ

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, 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	L	281/281 (100%)	-0.28	8 (2%) 53 59	22, 31, 55, 82	0
2	M	301/307 (98%)	-0.13	10 (3%) 46 53	21, 35, 57, 78	0
3	H	239/260 (91%)	-0.32	7 (2%) 51 57	24, 35, 49, 84	0
All	All	821/848 (96%)	-0.24	25 (3%) 50 56	21, 34, 54, 84	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	9.5
1	L	59	TRP	4.4
2	M	3	TYR	4.3
3	H	249	LYS	4.3
1	L	277	GLY	4.0
1	L	279	ILE	3.8
3	H	245	ALA	3.7
2	M	301	HIS	3.6
2	M	2	GLU	3.6
3	H	18	TYR	2.9
1	L	271	TRP	2.9
2	M	100	GLU	2.9
2	M	82	PRO	2.8
1	L	280	ASN	2.8
1	L	270	PRO	2.8
2	M	148	TRP	2.7
3	H	247	LYS	2.7
1	L	281	GLY	2.6
3	H	52	ASN	2.4
2	M	86	LEU	2.3
2	M	105	PHE	2.2
3	H	246	PRO	2.1
1	L	274	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	M	300	ASN	2.1
3	H	220	LYS	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

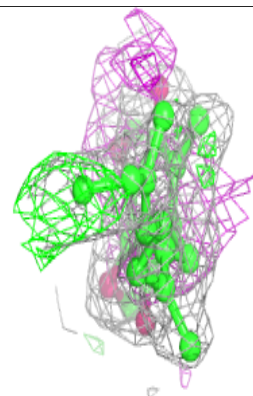
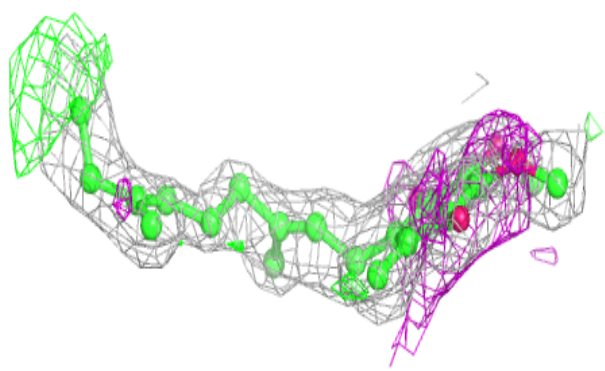
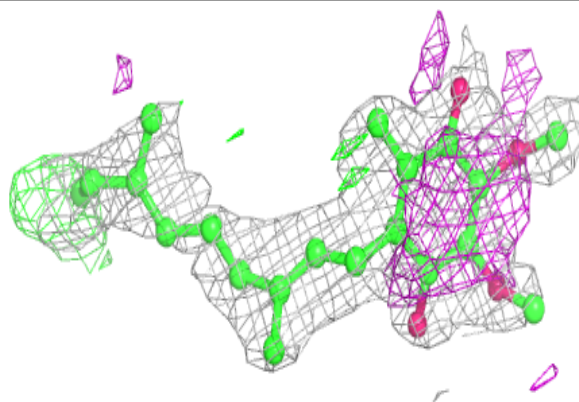
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	LDA	M	863	16/16	0.67	0.27	67,72,73,73	0
11	LDA	M	862	16/16	0.69	0.28	74,75,82,82	0
6	U10	L	859	24/63	0.69	0.28	43,53,58,58	0
12	CDL	M	900	81/100	0.79	0.27	61,75,84,86	0
10	SPO	M	860	42/42	0.80	0.20	34,46,62,64	0
11	LDA	H	861	16/16	0.84	0.17	63,65,68,69	0
7	GOL	L	866	6/6	0.86	0.12	47,52,53,54	0
6	U10	M	858	48/63	0.91	0.19	25,41,69,69	0
4	BCL	L	854	66/66	0.92	0.15	22,29,54,57	0
4	BCL	M	853	66/66	0.92	0.15	19,26,56,62	0
4	BCL	L	851	51/66	0.93	0.15	24,29,55,57	0
5	BPH	M	855	51/65	0.94	0.15	28,33,56,59	0
9	PO4	M	865	5/5	0.95	0.14	70,71,71,71	0
4	BCL	L	852	66/66	0.95	0.11	21,26,41,47	0
5	BPH	L	856	65/65	0.95	0.12	22,26,50,51	0
13	K	H	867	1/1	0.96	0.06	36,36,36,36	0
9	PO4	M	864	5/5	0.97	0.12	67,68,68,69	0
8	FE2	M	857	1/1	0.99	0.10	21,21,21,21	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.

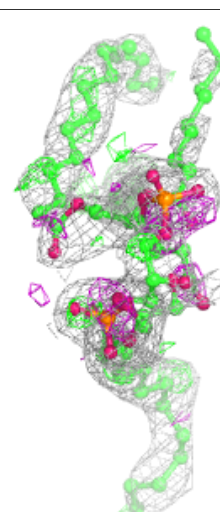
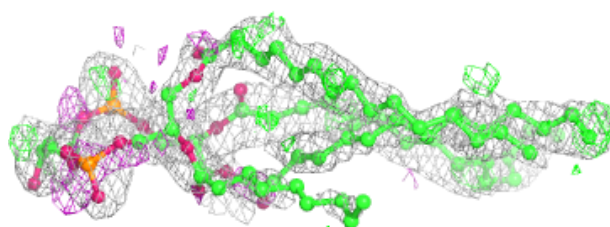
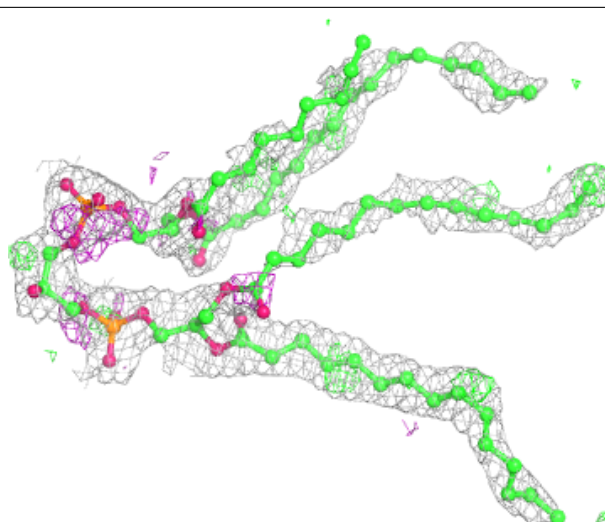
Electron density around U10 L 859:

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



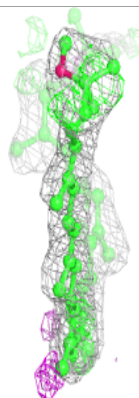
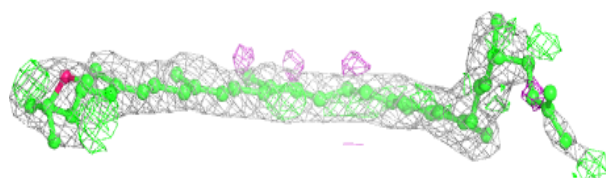
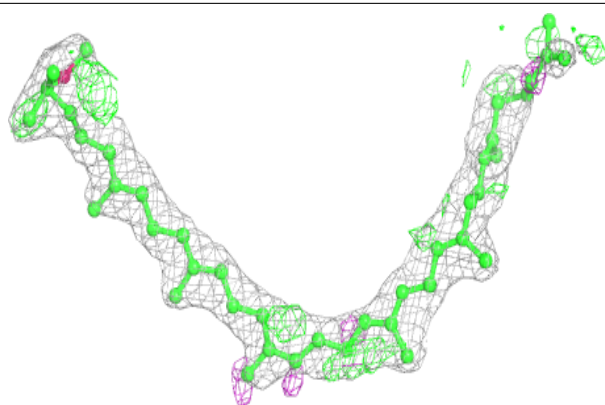
Electron density around CDL M 900:

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

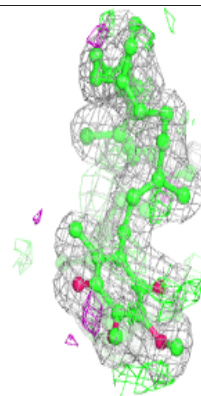
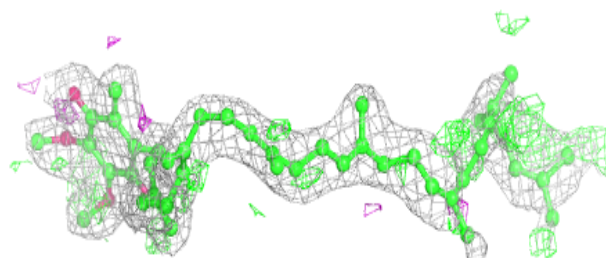
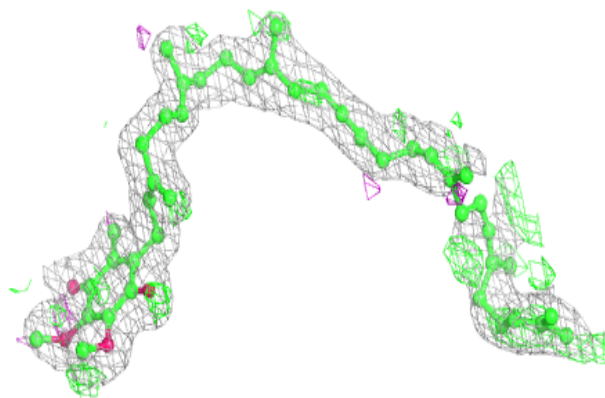


Electron density around SPO M 860:

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

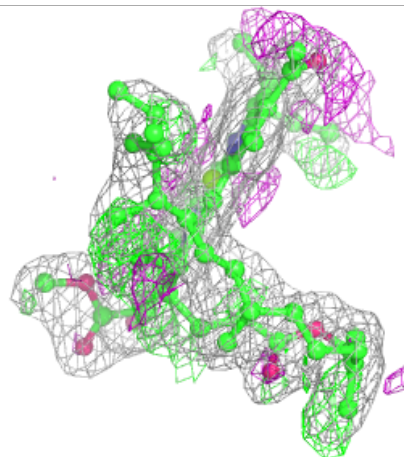
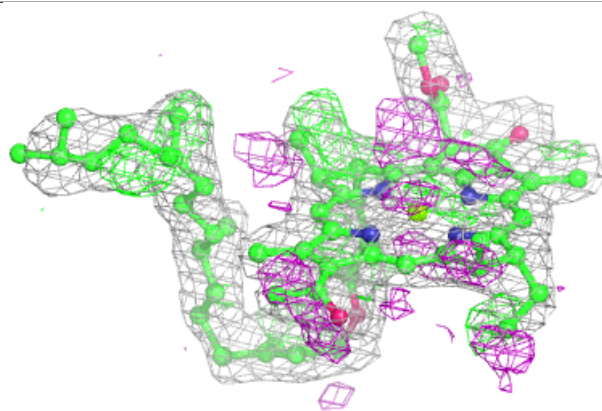
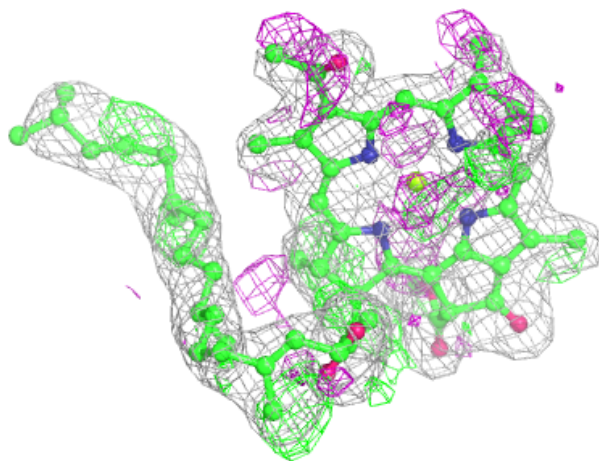
**Electron density around U10 M 858:**

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



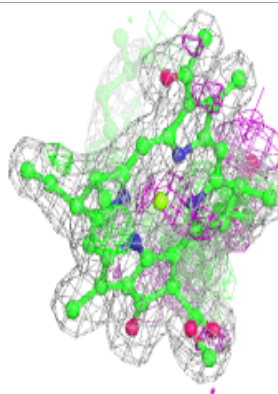
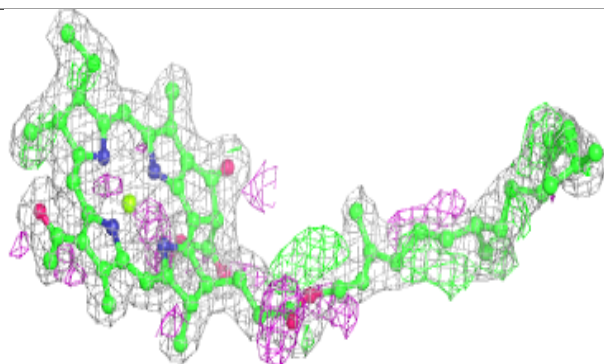
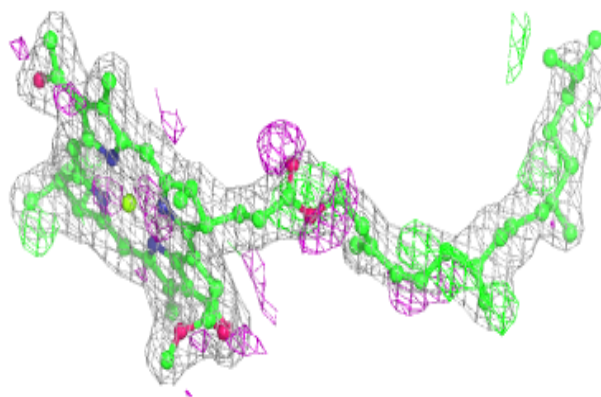
Electron density around BCL L 854:

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



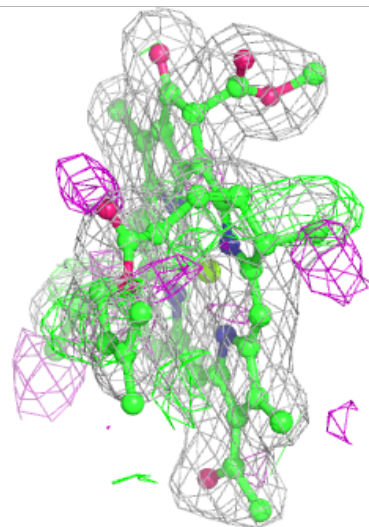
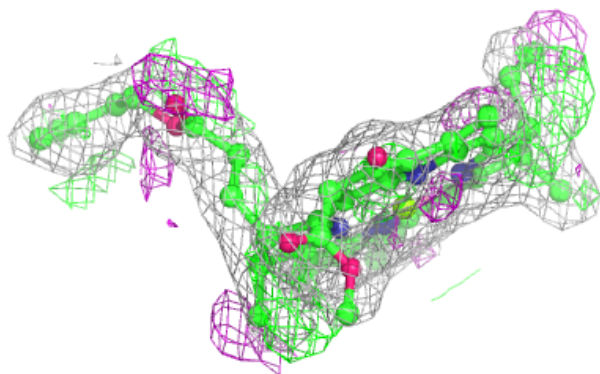
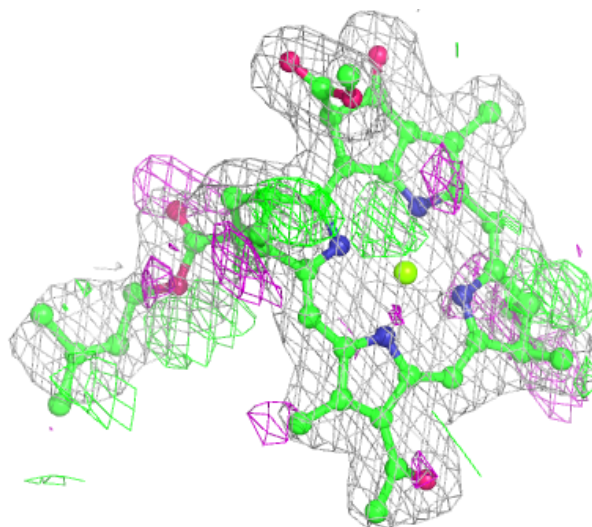
Electron density around BCL M 853:

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



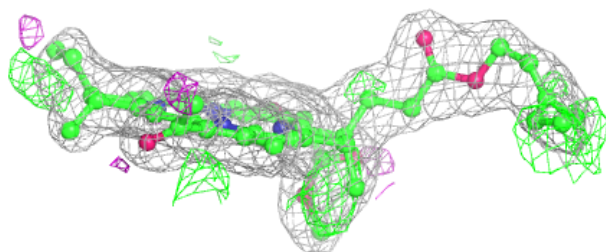
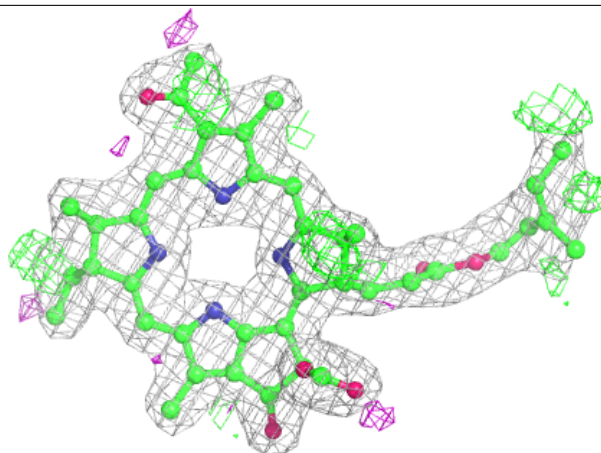
Electron density around BCL L 851:

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

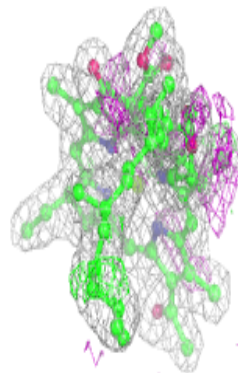
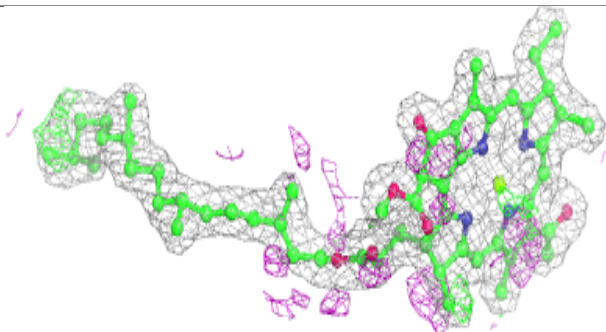
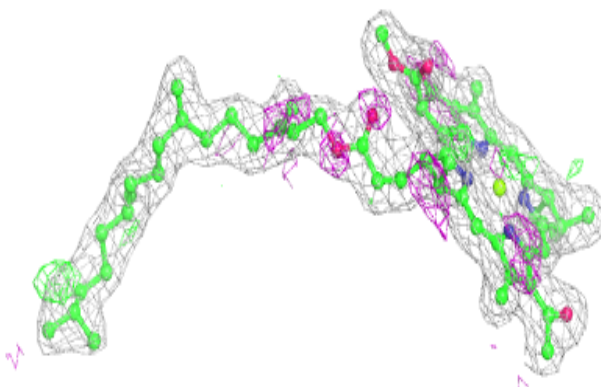


Electron density around BPH M 855:

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

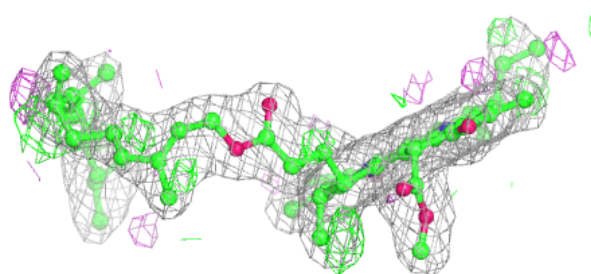
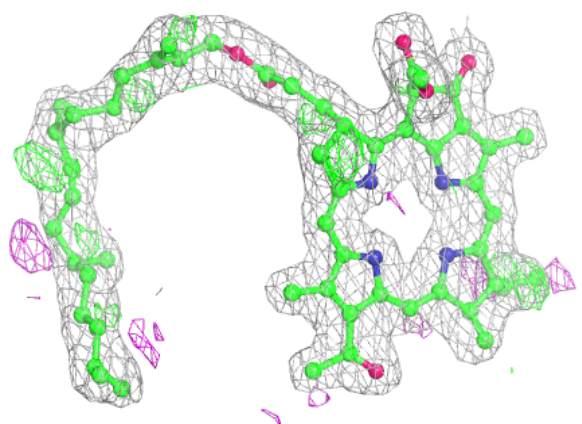
**Electron density around BCL L 852:**

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



Electron density around BPH L 856:

$2mF_o-DF_c$ (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.