Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 12:14 AM EDT

PDB ID	:	1RZH
Title	:	PHOTOSYNTHETIC REACTION CENTER DOUBLE MUTANT FROM RHODOBACTER SPHAEROIDES WITH ASP L213 REPLACED WITH ASN AND ARG M233 REPLACED WITH CYS IN THE CHARGE-NEUTRAL DQAQB STATE (TRIGONAL FORM)
Authors	:	Xu, Q.; Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher, G.
Deposited on	:	2003-12-24
Resolution	:	1.80 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:

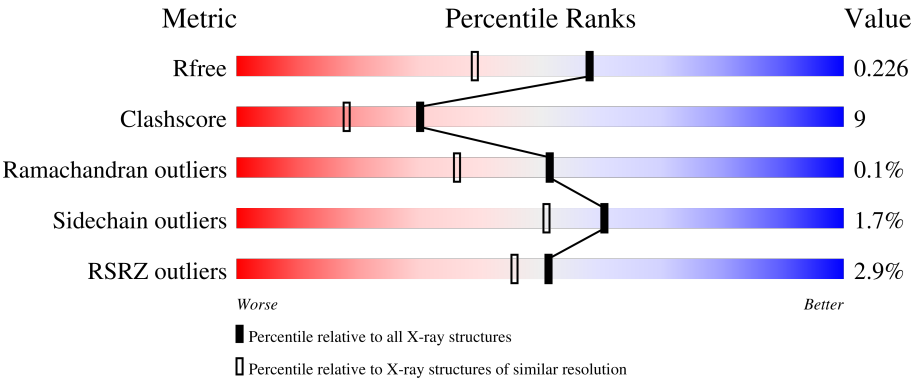
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	4% 87% 12%
2	M	307	3% 80% 18%
3	H	260	2% 77% 14% 8%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

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
13	GOL	M	867	-	X	-	-
4	BCL	M	851	X	-	-	-
5	BPH	L	856	X	-	-	-
5	BPH	M	855	X	-	-	-
6	U10	L	859[A]	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 7586 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	1	0
			2238	1510	357	363	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
			2399	1602	390	396	11			

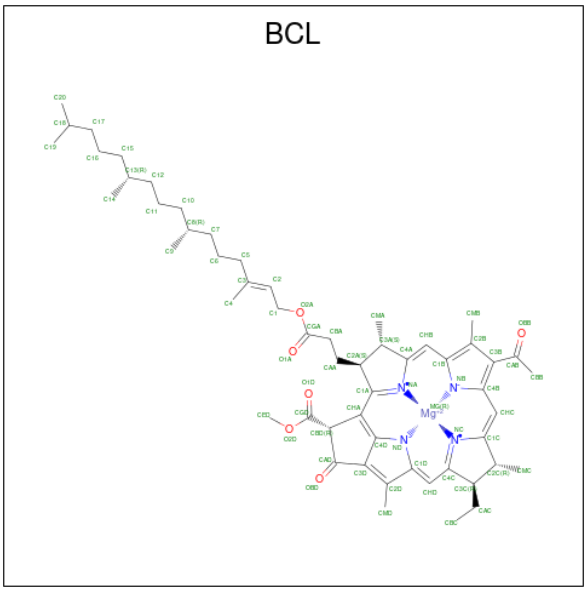
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	233	CYS	ARG	engineered mutation	UNP P02953

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

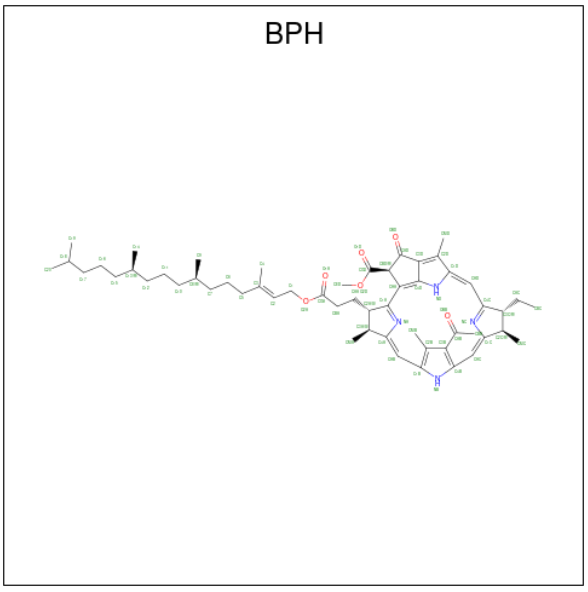
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	238	Total	C	N	O	S	0	1	0
			1822	1165	312	335	10			

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



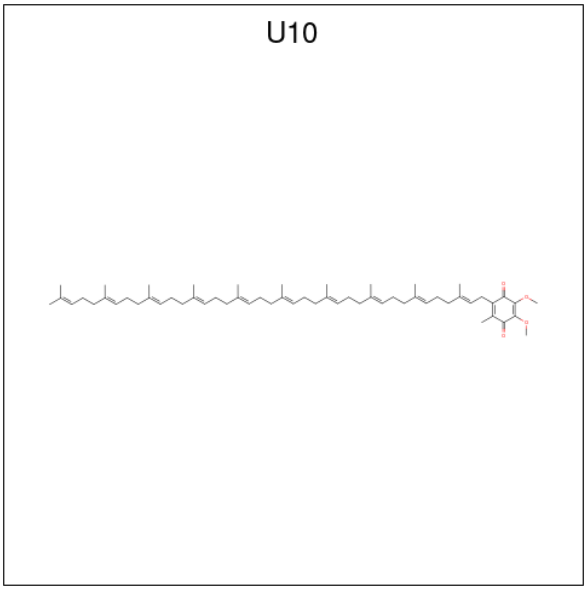
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



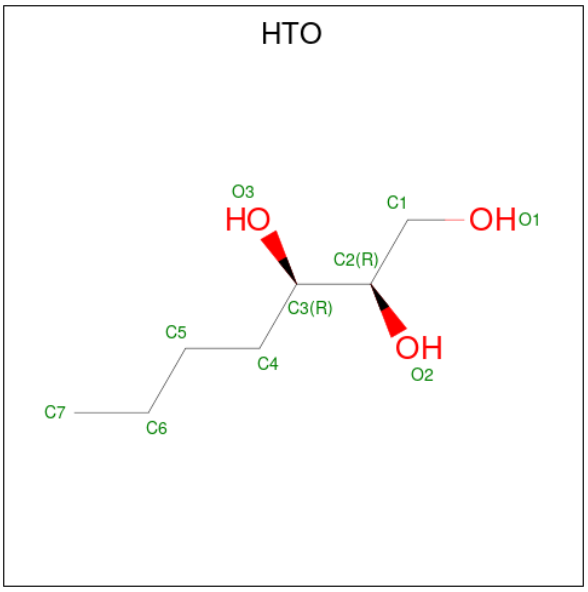
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C N O 65 55 4 6	0	0
5	M	1	Total C N O 55 45 4 6	0	0

- 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 33 29 4	0	1
6	M	1	Total C O 48 44 4	0	0

- Molecule 7 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).

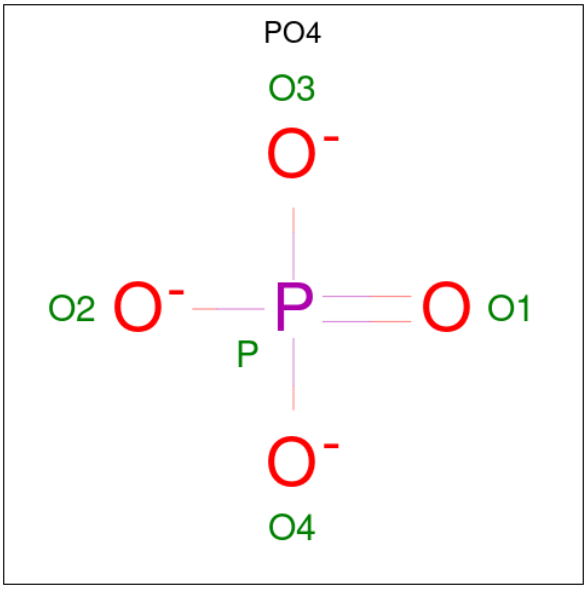


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C O 10 7 3	0	0
7	L	1	Total C O 10 7 3	0	0

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

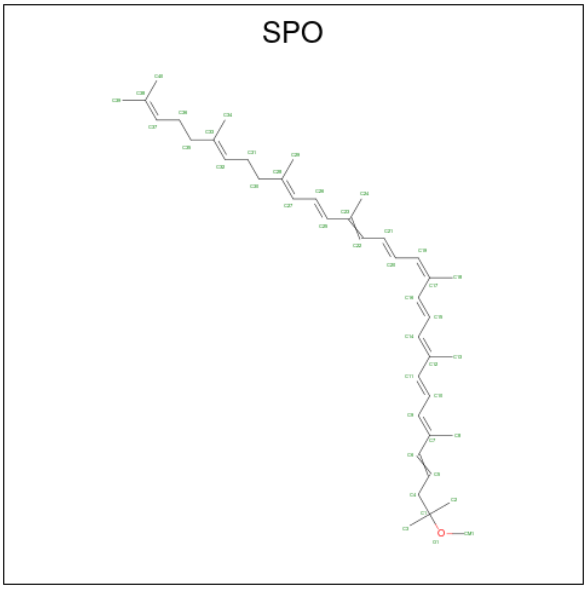
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total Fe 1 1	0	0

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



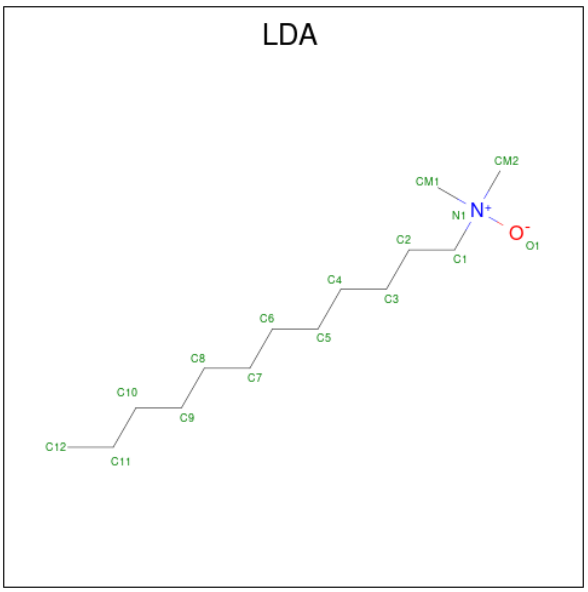
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total O P 5 4 1	0	0

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



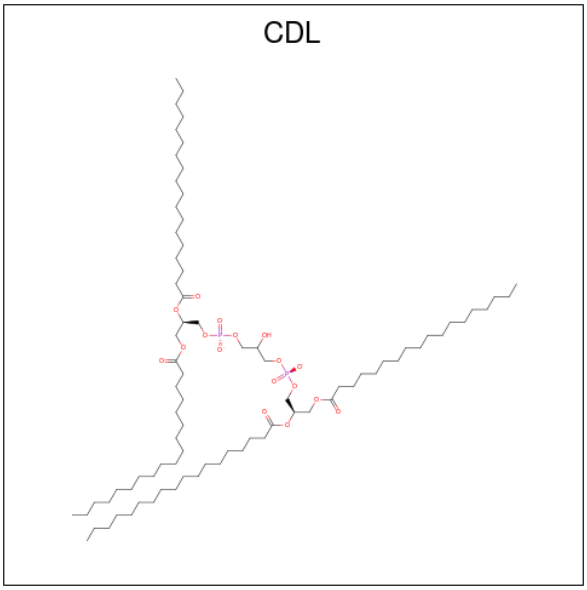
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total C O 42 41 1	0	0

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



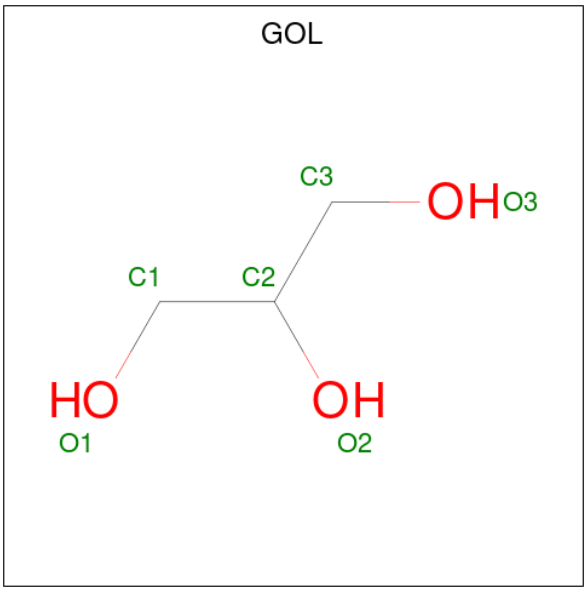
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	M	1	Total	C	N	O	0	0
			16	14	1	1		
11	M	1	Total	C	N	O	0	0
			16	14	1	1		
11	H	1	Total	C	N	O	0	0
			16	14	1	1		

- 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
			69	50	17	2		

- Molecule 13 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	M	1	Total	C	O	0	0
			6	3	3		

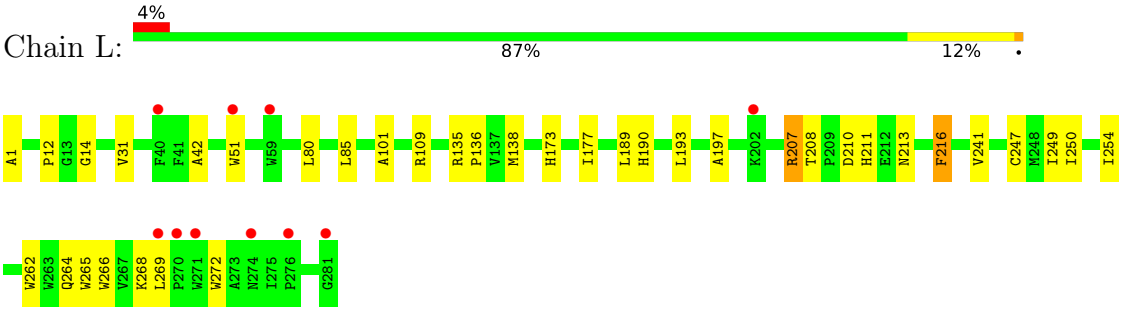
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	L	124	Total	O	0	2
			124	124		
14	M	138	Total	O	0	0
			138	138		
14	H	209	Total	O	0	0
			209	209		

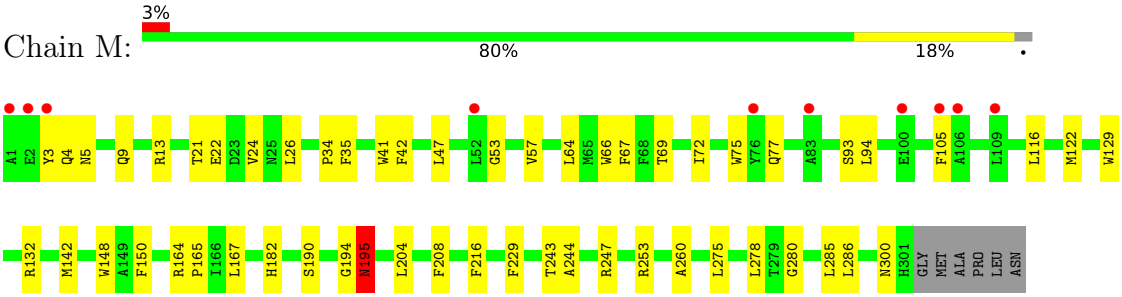
3 Residue-property plots (i)

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.

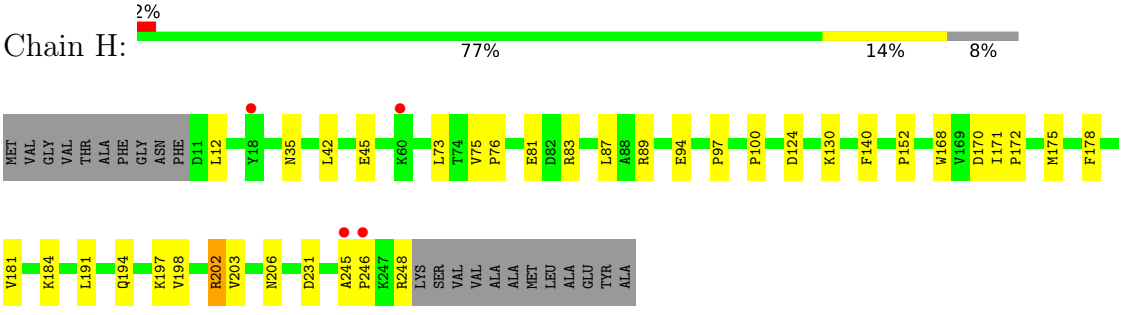
• Molecule 1: Reaction center protein L chain



• Molecule 2: Reaction center protein M chain



• Molecule 3: Reaction center protein H chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.35Å 139.35Å 184.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.31 – 1.80 39.31 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.31-1.80) 98.3 (39.31-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 1.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.233 0.214 , 0.226	Depositor DCC
R_{free} test set	9418 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.2	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7586	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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: U10, GOL, LDA, HTO, CDL, PO4, SPO, FE2, BPH, BCL

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	0.36	0/2326	0.55	0/3183
2	M	0.35	0/2491	0.53	0/3402
3	H	0.30	0/1870	0.59	0/2544
All	All	0.34	0/6687	0.56	0/9129

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

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	2238	0	2193	36	0
2	M	2399	0	2310	53	0
3	H	1822	0	1826	29	0
4	L	132	0	148	4	0
4	M	132	0	148	21	0
5	L	65	0	74	5	0
5	M	55	0	53	3	0
6	L	33	0	39	8	0
6	M	48	0	61	3	0
7	L	20	0	32	2	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	5	0	0	0	0
10	M	42	0	60	7	0
11	H	16	0	31	2	0
11	M	32	0	62	5	0
12	M	69	0	82	2	0
13	M	6	0	4	0	0
14	H	209	0	0	1	0
14	L	124	0	0	0	0
14	M	138	0	0	0	0
All	All	7586	0	7123	132	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 9.

All (132) 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)
4:M:851:BCL:C9	4:M:851:BCL:H121	1.41	1.43
4:M:851:BCL:C12	4:M:851:BCL:H91	1.36	1.39
1:L:241:VAL:HG21	5:L:856:BPH:HAC1	1.46	0.97
4:M:851:BCL:H91	4:M:851:BCL:H122	1.54	0.90
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.53	0.90
3:H:206:ASN:HD21	3:H:248:ARG:HD3	1.49	0.76
2:M:13:ARG:HD2	2:M:35:PHE:CD2	2.21	0.76
1:L:216:PHE:CG	6:L:859[A]:U10:H3M2	2.21	0.74
4:M:851:BCL:H121	4:M:851:BCL:H92	1.67	0.72
4:M:851:BCL:H112	4:M:853:BCL:H171	1.72	0.72
1:L:189:LEU:HB3	6:L:859[A]:U10:H4M3	1.74	0.70
3:H:89:ARG:NH1	3:H:94:GLU:HG2	2.07	0.70
2:M:77:GLN:HE22	2:M:93:SER:H	1.38	0.70
2:M:9:GLN:NE2	3:H:198:VAL:H	1.90	0.68
2:M:9:GLN:HE22	3:H:198:VAL:H	1.43	0.67
4:M:851:BCL:C9	4:M:851:BCL:C12	2.16	0.66
4:M:853:BCL:CBB	4:M:853:BCL:HMB1	2.27	0.65
4:M:851:BCL:H121	4:M:851:BCL:H91	0.66	0.64
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.78	0.64
2:M:64:LEU:HD23	5:M:855:BPH:H9C3	1.79	0.64
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.80	0.63
1:L:193:LEU:HD22	6:L:859[A]:U10:H3M3	1.79	0.62
3:H:202:ARG:HG2	3:H:203:VAL:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:41:TRP:CG	11:M:863:LDA:HM13	2.36	0.61
3:H:181:VAL:HG21	3:H:191:LEU:HD12	1.83	0.61
2:M:75:TRP:HE1	10:M:860:SPO:HM13	1.66	0.61
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.82	0.60
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.37	0.60
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.84	0.59
2:M:286:LEU:HD21	3:H:12:LEU:HD12	1.83	0.59
4:M:851:BCL:HMB1	4:M:851:BCL:CBB	2.32	0.59
1:L:266:TRP:O	1:L:269:LEU:HD23	2.02	0.59
2:M:69:THR:O	2:M:72:ILE:HG22	2.02	0.59
2:M:148:TRP:HB3	12:M:900:CDL:H741	1.85	0.58
4:M:851:BCL:HMB1	4:M:851:BCL:HBB2	1.85	0.58
1:L:211:HIS:HE1	2:M:22:GLU:OE1	1.86	0.58
1:L:207:ARG:HG2	2:M:142:MET:HG2	1.84	0.58
1:L:189:LEU:CB	6:L:859[A]:U10:H4M3	2.34	0.57
1:L:241:VAL:CG2	5:L:856:BPH:HAC1	2.30	0.56
4:M:853:BCL:HMB1	4:M:853:BCL:HBB3	1.88	0.56
1:L:265:TRP:O	1:L:269:LEU:HD22	2.05	0.56
4:L:854:BCL:HMB1	4:L:854:BCL:HBB2	1.87	0.56
1:L:208:THR:H	1:L:211:HIS:CD2	2.24	0.56
2:M:204:LEU:HG	11:M:861:LDA:HM22	1.88	0.56
2:M:105:PHE:HD1	2:M:116:LEU:HD13	1.73	0.54
4:L:854:BCL:H61	6:M:858:U10:H203	1.89	0.54
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.88	0.54
1:L:193:LEU:CD2	6:L:859[A]:U10:H3M3	2.38	0.53
3:H:206:ASN:HD21	3:H:248:ARG:CD	2.21	0.53
2:M:253:ARG:HH12	11:H:862:LDA:HM23	1.73	0.52
1:L:31:VAL:HG22	6:M:858:U10:H403	1.91	0.52
2:M:253:ARG:HH12	11:H:862:LDA:CM2	2.21	0.52
1:L:51:TRP:CZ3	1:L:80:LEU:HD13	2.46	0.51
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.46	0.51
1:L:216:PHE:CD1	6:L:859[A]:U10:H3M2	2.45	0.51
3:H:81:GLU:O	3:H:83:ARG:HG2	2.11	0.50
7:L:866:HTO:H61	6:M:858:U10:H23	1.92	0.50
2:M:275:LEU:HD23	2:M:278:LEU:HD23	1.94	0.50
1:L:189:LEU:HB3	6:L:859[A]:U10:C4M	2.40	0.49
2:M:9:GLN:HE22	3:H:197:LYS:HA	1.76	0.49
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.48	0.48
4:L:852:BCL:H122	5:L:856:BPH:H3A	1.95	0.48
2:M:24:VAL:O	2:M:26:LEU:HD12	2.13	0.48
3:H:75:VAL:HA	3:H:76:PRO:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:194:GLY:O	2:M:195:ASN:HB3	2.13	0.48
2:M:167:LEU:HD12	2:M:285:LEU:HD11	1.95	0.48
3:H:45:GLU:HG3	3:H:94:GLU:OE2	2.14	0.48
1:L:266:TRP:HA	1:L:269:LEU:CD2	2.43	0.47
2:M:26:LEU:HD12	2:M:26:LEU:N	2.29	0.47
3:H:152:PRO:HG2	3:H:202:ARG:HB2	1.96	0.47
1:L:14:GLY:O	1:L:109:ARG:HD3	2.15	0.47
2:M:53:GLY:O	2:M:57:VAL:HG23	2.15	0.47
2:M:190:SER:HB2	4:M:853:BCL:H3C	1.97	0.47
1:L:208:THR:H	1:L:211:HIS:HD2	1.63	0.46
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.15	0.46
1:L:138:MET:SD	1:L:249:ILE:HD11	2.56	0.46
10:M:860:SPO:HM12	10:M:860:SPO:H5	1.97	0.46
2:M:26:LEU:HD12	2:M:26:LEU:H	1.81	0.46
1:L:264:GLN:O	1:L:268:LYS:HG2	2.16	0.46
2:M:150:PHE:N	5:M:855:BPH:HMD3	2.31	0.46
2:M:286:LEU:CD2	3:H:12:LEU:HD12	2.45	0.45
4:M:851:BCL:H102	4:M:851:BCL:H61	1.40	0.45
3:H:12:LEU:HD13	3:H:12:LEU:O	2.15	0.45
2:M:13:ARG:O	3:H:140:PHE:HA	2.17	0.45
2:M:41:TRP:CD2	11:M:863:LDA:CM1	3.00	0.45
4:M:853:BCL:HHC	4:M:853:BCL:OBB	2.17	0.45
3:H:245:ALA:HA	3:H:248:ARG:NH2	2.32	0.45
1:L:42:ALA:HA	5:L:856:BPH:H9C3	1.97	0.44
2:M:300:ASN:N	2:M:300:ASN:HD22	2.14	0.44
2:M:194:GLY:O	2:M:195:ASN:CB	2.66	0.44
1:L:51:TRP:CE3	1:L:85:LEU:HD21	2.53	0.44
10:M:860:SPO:H15	10:M:860:SPO:H131	1.82	0.43
2:M:243:THR:O	2:M:247:ARG:HG3	2.18	0.43
3:H:130:LYS:NZ	3:H:170:ASP:OD2	2.52	0.43
1:L:262:TRP:O	1:L:265:TRP:HD1	2.02	0.43
1:L:12:PRO:HG3	3:H:97:PRO:HB2	2.00	0.43
4:M:851:BCL:H192	10:M:860:SPO:H81	2.01	0.43
4:M:851:BCL:C19	10:M:860:SPO:C8	2.97	0.43
3:H:194:GLN:H	3:H:194:GLN:CD	2.22	0.43
2:M:182:HIS:CG	10:M:860:SPO:H181	2.54	0.42
2:M:208:PHE:CE1	11:M:861:LDA:H92	2.54	0.42
2:M:190:SER:CB	4:M:853:BCL:H3C	2.49	0.42
1:L:250:ILE:HB	1:L:254:ILE:HD11	2.01	0.42
4:L:854:BCL:C4A	4:L:854:BCL:HBA1	2.49	0.42
2:M:67:PHE:CG	5:M:855:BPH:H9C2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:210:ASP:OD1	3:H:124:ASP:HB2	2.20	0.42
3:H:184:LYS:HD3	14:H:913:HOH:O	2.20	0.42
1:L:208:THR:OG1	1:L:211:HIS:HD2	2.03	0.42
2:M:34:PRO:HG2	2:M:47:LEU:HD22	2.01	0.42
2:M:280:GLY:O	4:M:853:BCL:HED3	2.20	0.42
1:L:101:ALA:CB	7:L:865:HTO:H72	2.50	0.42
2:M:42:PHE:HB2	11:M:863:LDA:H72	2.01	0.41
2:M:129:TRP:O	2:M:132:ARG:HB3	2.19	0.41
2:M:75:TRP:HE1	10:M:860:SPO:H32A	1.86	0.41
2:M:195:ASN:C	2:M:195:ASN:HD22	2.24	0.41
4:M:851:BCL:C4	4:M:851:BCL:H72	2.49	0.41
4:M:851:BCL:OBB	4:M:851:BCL:HHC	2.21	0.41
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.55	0.41
1:L:1:ALA:HB1	3:H:42:LEU:HB3	2.02	0.41
1:L:197:ALA:HA	1:L:207:ARG:HB2	2.02	0.41
3:H:168:TRP:HB2	3:H:178:PHE:HB2	2.02	0.41
2:M:300:ASN:N	2:M:300:ASN:ND2	2.68	0.41
2:M:148:TRP:CE2	12:M:900:CDL:H511	2.56	0.41
3:H:89:ARG:HH12	3:H:94:GLU:HG2	1.82	0.41
4:M:851:BCL:C4	4:M:851:BCL:C7	2.99	0.40
1:L:190:HIS:HA	6:L:859[A]:U10:H4M1	2.04	0.40
2:M:4:GLN:HA	2:M:4:GLN:OE1	2.21	0.40
1:L:213:ASN:HD22	1:L:213:ASN:HA	1.73	0.40
2:M:26:LEU:H	2:M:26:LEU:CD1	2.34	0.40
3:H:245:ALA:N	3:H:246:PRO:CD	2.84	0.40
1:L:269:LEU:HD13	1:L:269:LEU:HA	1.92	0.40
5:L:856:BPH:OBB	5:L:856:BPH:HHC	2.21	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	280/281 (100%)	273 (98%)	7 (2%)	0	100 100
2	M	299/307 (97%)	292 (98%)	6 (2%)	1 (0%)	41 27
3	H	237/260 (91%)	236 (100%)	1 (0%)	0	100 100
All	All	816/848 (96%)	801 (98%)	14 (2%)	1 (0%)	51 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	ASN

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	221/220 (100%)	217 (98%)	4 (2%)	59 48
2	M	236/240 (98%)	233 (99%)	3 (1%)	69 62
3	H	194/208 (93%)	190 (98%)	4 (2%)	53 42
All	All	651/668 (98%)	640 (98%)	11 (2%)	60 51

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	207	ARG
1	L	216	PHE
1	L	247	CYS
1	L	272	TRP
2	M	94	LEU
2	M	195	ASN
2	M	216	PHE
3	H	73	LEU
3	H	175	MET
3	H	202	ARG
3	H	231	ASP

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

Mol	Chain	Res	Type
1	L	87	GLN
1	L	211	HIS
1	L	213	ASN
2	M	9	GLN
2	M	77	GLN
2	M	195	ASN
2	M	299	GLN
2	M	300	ASN
3	H	206	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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	$\#\|Z\| > 2$
11	LDA	M	861	-	12,15,15	2.14	1 (8%)	14,17,17	1.60	4 (28%)
7	HTO	L	865	-	9,9,9	1.31	1 (11%)	10,10,10	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	PO4	M	864	-	4,4,4	1.72	1 (25%)	6,6,6	0.43	0
4	BCL	L	852	-	58,74,74	1.24	5 (8%)	69,115,115	1.85	19 (27%)
10	SPO	M	860	-	40,41,41	3.41	23 (57%)	47,50,50	4.12	16 (34%)
4	BCL	M	851	-	58,74,74	1.57	10 (17%)	69,115,115	2.55	27 (39%)
11	LDA	H	862	-	12,15,15	2.15	1 (8%)	14,17,17	1.76	4 (28%)
5	BPH	M	855	-	41,60,70	1.87	10 (24%)	40,89,101	2.96	18 (45%)
7	HTO	L	866	-	9,9,9	1.31	1 (11%)	10,10,10	0.37	0
11	LDA	M	863	-	12,15,15	2.03	1 (8%)	14,17,17	1.68	4 (28%)
13	GOL	M	867	-	5,5,5	4.51	5 (100%)	5,5,5	5.78	3 (60%)
4	BCL	L	854	-	58,74,74	1.63	15 (25%)	69,115,115	2.21	23 (33%)
4	BCL	M	853	-	58,74,74	1.78	11 (18%)	69,115,115	2.69	20 (28%)
12	CDL	M	900	-	68,68,99	0.74	2 (2%)	74,80,111	0.96	4 (5%)
5	BPH	L	856	-	51,70,70	1.74	10 (19%)	52,101,101	2.65	18 (34%)
6	U10	M	858	-	48,48,63	2.13	18 (37%)	58,61,79	3.30	18 (31%)
6	U10	L	859[A]	-	33,33,63	2.06	11 (33%)	40,43,79	1.94	12 (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
11	LDA	M	861	-	-	6/13/13/13	-
7	HTO	L	865	-	-	7/10/10/10	-
4	BCL	L	852	-	-	4/37/137/137	-
10	SPO	M	860	-	-	13/47/47/47	-
4	BCL	M	851	-	2/2/21/25	19/37/137/137	-
11	LDA	H	862	-	-	6/13/13/13	-
5	BPH	M	855	-	1/1/16/22	11/25/93/105	0/5/6/6
7	HTO	L	866	-	-	8/10/10/10	-
11	LDA	M	863	-	-	3/13/13/13	-
13	GOL	M	867	-	-	2/4/4/4	-
4	BCL	L	854	-	-	8/37/137/137	-
4	BCL	M	853	-	-	3/37/137/137	-
12	CDL	M	900	-	-	22/79/79/110	-
5	BPH	L	856	-	2/2/18/22	8/37/105/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	U10	M	858	-	-	10/45/69/87	0/1/1/1
6	U10	L	859[A]	-	-	4/27/51/87	0/1/1/1

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	860	SPO	C6-C5	8.77	1.54	1.32
10	M	860	SPO	C10-C11	7.87	1.54	1.34
10	M	860	SPO	C15-C16	7.63	1.54	1.34
13	M	867	GOL	C3-C2	-7.34	1.21	1.51
11	H	862	LDA	O1-N1	-7.24	1.25	1.42
11	M	861	LDA	O1-N1	-7.08	1.25	1.42
5	M	855	BPH	C2C-C3C	-6.84	1.48	1.54
11	M	863	LDA	O1-N1	-6.78	1.26	1.42
4	M	853	BCL	MG-NA	5.92	2.20	2.06
10	M	860	SPO	C27-C28	5.57	1.39	1.34
5	L	856	BPH	C11-C10	-5.44	1.28	1.52
5	L	856	BPH	C2C-C3C	-5.35	1.49	1.54
4	M	853	BCL	C4B-NB	5.22	1.39	1.35
4	L	854	BCL	O2D-CGD	5.20	1.45	1.33
10	M	860	SPO	C21-C20	5.11	1.49	1.36
6	M	858	U10	O4-C4	4.93	1.48	1.36
4	M	853	BCL	O2D-CGD	4.87	1.45	1.33
10	M	860	SPO	C26-C25	4.82	1.47	1.34
6	L	859[A]	U10	O4-C4	4.77	1.48	1.36
4	M	851	BCL	O2D-CGD	4.75	1.44	1.33
6	M	858	U10	C37-C38	-4.73	1.35	1.50
13	M	867	GOL	O1-C1	4.53	1.61	1.42
4	M	851	BCL	MG-NA	4.48	2.16	2.06
6	M	858	U10	C33-C34	4.44	1.43	1.33
4	L	854	BCL	MG-NA	4.37	2.16	2.06
10	M	860	SPO	C14-C12	4.31	1.41	1.35
4	M	853	BCL	C1B-NB	4.24	1.39	1.35
10	M	860	SPO	O1-CM1	4.06	1.56	1.43
5	M	855	BPH	O2A-CGA	4.02	1.45	1.33
5	M	855	BPH	O2D-CGD	3.94	1.42	1.33
6	L	859[A]	U10	C13-C14	3.93	1.42	1.33
4	M	851	BCL	C1B-NB	3.93	1.38	1.35
5	L	856	BPH	O2A-CGA	3.88	1.44	1.33
5	L	856	BPH	O2D-CGD	3.86	1.42	1.33
4	M	851	BCL	O2A-CGA	3.72	1.44	1.33
4	L	852	BCL	C1B-NB	3.72	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	860	SPO	C19-C17	3.70	1.40	1.35
6	M	858	U10	C6-C1	3.57	1.41	1.35
6	M	858	U10	O3-C3	3.57	1.45	1.36
4	L	854	BCL	C1B-NB	3.56	1.38	1.35
6	M	858	U10	C7-C8	-3.56	1.45	1.50
10	M	860	SPO	C9-C7	3.55	1.40	1.35
6	M	858	U10	C13-C14	3.54	1.41	1.33
6	L	859[A]	U10	C6-C1	3.49	1.41	1.35
13	M	867	GOL	O3-C3	3.45	1.57	1.42
6	L	859[A]	U10	O3-C3	3.38	1.45	1.36
4	M	853	BCL	MG-NC	3.31	2.14	2.06
4	M	853	BCL	O2A-CGA	3.31	1.43	1.33
6	L	859[A]	U10	C7-C8	-3.25	1.46	1.50
6	M	858	U10	C31-C29	3.20	1.57	1.51
4	M	853	BCL	C2-C3	3.20	1.40	1.33
4	M	851	BCL	C4B-NB	3.16	1.38	1.35
5	M	855	BPH	CHA-CBD	3.13	1.55	1.52
6	L	859[A]	U10	C23-C24	3.08	1.41	1.32
6	L	859[A]	U10	C8-C9	3.04	1.40	1.33
7	L	866	HTO	C3-C2	3.02	1.60	1.52
4	L	852	BCL	MG-NA	3.02	2.13	2.06
7	L	865	HTO	C3-C2	3.01	1.60	1.52
10	M	860	SPO	C25-C23	-2.95	1.39	1.45
10	M	860	SPO	C32-C33	2.91	1.40	1.33
10	M	860	SPO	O1-C1	2.91	1.57	1.41
4	L	854	BCL	C4B-NB	2.90	1.37	1.35
4	L	854	BCL	C2C-C3C	-2.89	1.46	1.54
6	L	859[A]	U10	O3-C3M	-2.86	1.38	1.45
10	M	860	SPO	C10-C9	2.86	1.52	1.43
10	M	860	SPO	C37-C38	2.85	1.40	1.32
13	M	867	GOL	C1-C2	-2.80	1.40	1.51
6	L	859[A]	U10	C18-C19	2.77	1.39	1.33
13	M	867	GOL	O2-C2	-2.76	1.35	1.43
5	M	855	BPH	C2-C3	2.75	1.39	1.33
10	M	860	SPO	C8-C7	2.75	1.56	1.50
10	M	860	SPO	C15-C14	2.72	1.51	1.43
4	L	854	BCL	O2A-CGA	2.71	1.41	1.33
5	L	856	BPH	C2-C3	2.71	1.39	1.33
4	M	851	BCL	CAA-C2A	2.71	1.59	1.54
10	M	860	SPO	C24-C23	2.70	1.56	1.50
10	M	860	SPO	C26-C27	2.68	1.51	1.43
10	M	860	SPO	C13-C12	2.67	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	860	SPO	C11-C12	-2.66	1.40	1.45
5	L	856	BPH	C1A-C2A	2.63	1.54	1.51
5	M	855	BPH	O2D-CED	-2.60	1.39	1.45
4	L	854	BCL	CAA-C2A	2.58	1.58	1.54
5	L	856	BPH	CHA-CBD	2.56	1.55	1.52
4	L	854	BCL	CMC-C2C	2.56	1.58	1.53
5	M	855	BPH	C1A-C2A	2.56	1.54	1.51
5	L	856	BPH	O2D-CED	-2.54	1.39	1.45
6	M	858	U10	O3-C3M	-2.54	1.39	1.45
4	L	852	BCL	C4-C3	2.54	1.57	1.50
4	L	854	BCL	C2-C3	2.52	1.39	1.33
6	M	858	U10	C8-C9	2.51	1.39	1.33
6	M	858	U10	C23-C24	2.50	1.39	1.33
6	M	858	U10	C18-C19	2.49	1.39	1.33
5	M	855	BPH	C3A-C2A	-2.46	1.52	1.54
4	L	854	BCL	C3B-C2B	-2.43	1.35	1.39
6	M	858	U10	C28-C29	2.42	1.38	1.33
4	M	851	BCL	CMA-C3A	2.41	1.58	1.53
4	L	852	BCL	CBB-CAB	2.41	1.56	1.49
6	M	858	U10	C25-C24	2.39	1.56	1.50
4	M	851	BCL	C2-C3	2.37	1.38	1.33
5	L	856	BPH	C3A-C2A	-2.36	1.52	1.54
4	L	854	BCL	O1D-CGD	2.36	1.27	1.21
6	M	858	U10	C15-C14	2.34	1.56	1.50
6	L	859[A]	U10	C15-C14	2.34	1.56	1.50
4	M	851	BCL	C2C-C3C	-2.34	1.47	1.54
10	M	860	SPO	C6-C7	-2.33	1.40	1.45
10	M	860	SPO	C22-C23	2.32	1.38	1.35
4	M	853	BCL	O2D-CED	-2.32	1.39	1.45
6	L	859[A]	U10	C7-C6	2.32	1.55	1.51
6	M	858	U10	C36-C34	2.32	1.56	1.51
4	M	851	BCL	C3B-C2B	-2.28	1.35	1.39
5	M	855	BPH	O1D-CGD	2.27	1.26	1.21
5	L	856	BPH	CAA-C2A	2.22	1.59	1.54
6	M	858	U10	C30-C29	2.19	1.56	1.50
12	M	900	CDL	OA8-CA7	2.17	1.39	1.33
4	L	854	BCL	CMB-C2B	2.14	1.56	1.51
12	M	900	CDL	CB3-CB4	2.10	1.57	1.50
4	M	853	BCL	C3C-C4C	2.06	1.54	1.51
6	M	858	U10	C6-C5	2.05	1.52	1.46
5	M	855	BPH	CAA-C2A	2.05	1.58	1.54
4	L	854	BCL	CMA-C3A	2.05	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	853	BCL	C4-C3	2.05	1.55	1.50
4	L	854	BCL	O2D-CED	-2.04	1.40	1.45
4	M	853	BCL	O1D-CGD	2.02	1.26	1.21
9	M	864	PO4	P-O3	-2.01	1.48	1.54
4	L	854	BCL	CAC-C3C	2.01	1.57	1.54
4	L	852	BCL	C3D-CAD	-2.00	1.41	1.46

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	860	SPO	C2-C1-C4	-20.56	79.29	110.86
6	M	858	U10	C32-C33-C34	18.38	171.91	127.66
4	M	853	BCL	C1C-NC-C4C	12.01	112.11	106.71
5	M	855	BPH	O2D-CGD-CBD	11.49	125.55	111.00
10	M	860	SPO	C3-C1-C4	-11.47	93.25	110.86
5	L	856	BPH	O2D-CGD-CBD	10.96	124.89	111.00
4	M	853	BCL	C4A-NA-C1A	10.64	111.49	106.71
13	M	867	GOL	O3-C3-C2	10.48	160.46	110.20
4	M	851	BCL	C1-C2-C3	7.85	139.61	126.04
13	M	867	GOL	O2-C2-C3	6.80	139.06	109.12
4	L	854	BCL	C4A-NA-C1A	6.44	109.60	106.71
6	L	859[A]	U10	C3M-O3-C3	6.32	138.85	116.47
6	M	858	U10	C27-C28-C29	6.31	142.84	127.66
10	M	860	SPO	C15-C14-C12	-6.19	118.47	127.31
4	M	853	BCL	O2D-CGD-CBD	6.13	122.16	111.27
4	L	854	BCL	O2D-CGD-CBD	6.12	122.15	111.27
4	M	851	BCL	OBB-CAB-C3B	5.96	130.56	119.99
4	M	851	BCL	C4-C3-C5	-5.96	105.25	115.27
10	M	860	SPO	C20-C21-C22	-5.92	111.34	123.47
5	M	855	BPH	C1-C2-C3	5.87	136.20	126.04
5	L	856	BPH	C1-C2-C3	5.73	135.96	126.04
6	M	858	U10	C3M-O3-C3	5.72	136.72	116.47
5	L	856	BPH	CBC-CAC-C3C	5.71	125.28	113.77
10	M	860	SPO	C25-C23-C22	-5.04	111.21	118.94
6	M	858	U10	C36-C37-C38	-4.98	95.52	111.88
6	M	858	U10	C37-C38-C39	4.91	144.53	127.75
6	M	858	U10	C31-C32-C33	4.73	127.42	111.88
4	M	851	BCL	OBD-CAD-CBD	-4.67	119.23	125.89
4	M	851	BCL	O2A-CGA-O1A	-4.62	111.94	123.59
4	M	851	BCL	O2A-CGA-CBA	4.60	126.34	111.91
4	L	854	BCL	C1C-NC-C4C	4.60	108.77	106.71
4	M	851	BCL	O2D-CGD-CBD	4.58	119.41	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	851	BCL	C4A-NA-C1A	4.54	108.75	106.71
5	M	855	BPH	O1D-CGD-CBD	-4.49	117.27	124.74
4	M	851	BCL	CAD-C3D-C4D	-4.46	105.98	108.47
4	L	852	BCL	CAD-C3D-C4D	-4.43	106.00	108.47
5	L	856	BPH	C6-C5-C3	4.35	124.86	113.45
5	M	855	BPH	CED-O2D-CGD	4.33	125.73	115.94
4	L	852	BCL	OBB-CAB-CBB	-4.23	110.64	120.17
6	M	858	U10	C36-C34-C33	4.23	129.67	121.12
4	M	853	BCL	CAD-C3D-C4D	-4.20	106.13	108.47
5	L	856	BPH	CED-O2D-CGD	4.18	125.39	115.94
5	L	856	BPH	O1D-CGD-CBD	-4.12	117.87	124.74
4	L	852	BCL	C1-C2-C3	-4.09	118.96	126.04
4	M	853	BCL	CAC-C3C-C2C	-4.04	104.17	114.26
4	M	851	BCL	C1C-NC-C4C	4.04	108.52	106.71
4	L	854	BCL	CMB-C2B-C1B	-4.03	122.27	128.46
5	M	855	BPH	CBC-CAC-C3C	3.98	121.79	113.77
6	M	858	U10	C35-C34-C36	-3.97	108.60	115.27
4	M	851	BCL	C5-C3-C2	3.94	129.08	121.12
4	M	851	BCL	CAA-C2A-C3A	-3.91	102.07	112.78
10	M	860	SPO	C24-C23-C25	3.90	124.23	118.08
6	L	859[A]	U10	O5-C5-C6	-3.88	114.74	121.55
4	L	854	BCL	C4B-CHC-C1C	-3.79	122.61	130.12
4	L	854	BCL	C1B-CHB-C4A	-3.79	122.62	130.12
10	M	860	SPO	C18-C17-C19	-3.78	117.63	122.92
4	L	852	BCL	CAA-C2A-C3A	-3.77	102.46	112.78
5	L	856	BPH	C11-C10-C8	3.72	127.94	115.92
4	M	851	BCL	C4B-C3B-CAB	-3.70	119.99	127.13
4	L	854	BCL	CAC-C3C-C2C	-3.69	105.05	114.26
4	L	852	BCL	C7-C6-C5	-3.65	103.45	113.36
4	L	854	BCL	OBB-CAB-C3B	3.63	126.43	119.99
10	M	860	SPO	C1-C4-C5	3.62	122.65	113.06
4	L	854	BCL	C4B-C3B-CAB	-3.62	120.14	127.13
4	L	854	BCL	CHC-C1C-NC	3.62	129.52	124.51
4	M	851	BCL	CMB-C2B-C1B	-3.60	122.93	128.46
5	M	855	BPH	C7-C6-C5	3.58	123.08	113.36
4	M	853	BCL	C1-C2-C3	-3.50	119.99	126.04
11	H	862	LDA	CM1-N1-C1	-3.43	103.02	110.23
10	M	860	SPO	C6-C7-C9	-3.43	113.67	118.94
12	M	900	CDL	OB8-CB6-CB4	3.43	118.41	108.43
5	M	855	BPH	O2D-CGD-O1D	-3.41	117.17	123.84
5	L	856	BPH	O2D-CGD-O1D	-3.39	117.21	123.84
5	M	855	BPH	C6-C5-C3	3.38	122.33	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	M	863	LDA	CM1-N1-C1	-3.36	103.17	110.23
4	L	852	BCL	CMB-C2B-C3B	3.36	130.96	124.68
10	M	860	SPO	C15-C16-C17	-3.36	116.98	126.42
4	L	852	BCL	CMD-C2D-C3D	3.35	130.95	124.68
4	L	852	BCL	C4A-NA-C1A	-3.35	105.20	106.71
10	M	860	SPO	C3-C1-C2	3.33	116.64	110.37
6	L	859[A]	U10	O2-C2-C3	-3.33	113.87	120.93
4	M	853	BCL	CHC-C1C-NC	3.31	129.09	124.51
4	L	854	BCL	O2D-CGD-O1D	-3.27	117.44	123.84
13	M	867	GOL	O1-C1-C2	3.24	125.74	110.20
10	M	860	SPO	C8-C7-C6	3.23	123.17	118.08
5	M	855	BPH	C1C-C2C-C3C	3.23	105.91	102.84
4	L	854	BCL	C1-O2A-CGA	3.22	124.90	116.44
4	M	851	BCL	OBB-CAB-CBB	-3.21	112.94	120.17
5	L	856	BPH	C4C-C3C-C2C	3.21	105.90	102.84
5	L	856	BPH	C1C-C2C-C3C	3.21	105.90	102.84
4	M	851	BCL	O2D-CGD-O1D	-3.21	117.56	123.84
5	L	856	BPH	CMA-C3A-C4A	-3.13	107.52	114.38
4	M	853	BCL	CAC-C3C-C4C	-3.13	105.65	112.58
4	L	852	BCL	CMB-C2B-C1B	-3.12	123.67	128.46
6	M	858	U10	C20-C19-C21	-3.12	110.02	115.27
6	M	858	U10	O5-C5-C6	-3.12	116.08	121.55
5	L	856	BPH	CMB-C2B-C3B	3.08	130.43	124.68
4	M	853	BCL	C4B-CHC-C1C	-3.06	124.06	130.12
6	M	858	U10	O2-C2-C3	-3.05	114.45	120.93
4	M	853	BCL	O2A-CGA-CBA	3.05	121.47	111.91
4	M	851	BCL	C4B-CHC-C1C	-3.04	124.10	130.12
4	M	851	BCL	C2C-C3C-C4C	3.02	105.87	101.34
6	L	859[A]	U10	C1-C6-C5	-3.02	116.74	119.58
4	L	854	BCL	CMB-C2B-C3B	2.99	130.28	124.68
11	H	862	LDA	O1-N1-C1	2.95	116.52	109.27
10	M	860	SPO	C20-C19-C17	-2.95	123.10	127.31
6	M	858	U10	C30-C29-C31	-2.95	110.31	115.27
5	M	855	BPH	CMA-C3A-C4A	-2.94	107.95	114.38
4	L	854	BCL	OBD-CAD-CBD	-2.91	121.74	125.89
5	M	855	BPH	C4C-C3C-C2C	2.91	105.61	102.84
4	L	852	BCL	OBD-CAD-CBD	-2.90	121.75	125.89
5	L	856	BPH	C7-C6-C5	-2.89	105.50	113.36
4	L	854	BCL	CAD-C3D-C4D	-2.89	106.86	108.47
6	L	859[A]	U10	C16-C14-C13	2.88	126.95	121.12
6	L	859[A]	U10	C20-C19-C21	-2.83	110.52	115.27
5	M	855	BPH	CMB-C2B-C3B	2.81	129.93	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	851	BCL	CMA-C3A-C2A	-2.80	102.54	113.83
11	M	861	LDA	CM1-N1-C1	-2.77	104.41	110.23
4	M	853	BCL	C5-C3-C2	2.71	126.60	121.12
4	M	853	BCL	O2D-CGD-O1D	-2.70	118.56	123.84
6	M	858	U10	C1-C6-C5	-2.67	117.07	119.58
4	M	853	BCL	O1D-CGD-CBD	-2.65	119.06	124.48
4	L	854	BCL	OBB-CAB-CBB	-2.65	114.21	120.17
11	M	863	LDA	O1-N1-C1	2.64	115.76	109.27
4	L	852	BCL	CBB-CAB-C3B	2.62	128.11	120.34
4	M	853	BCL	C4B-C3B-CAB	-2.59	122.13	127.13
11	M	861	LDA	O1-N1-C1	2.57	115.58	109.27
4	M	851	BCL	CMD-C2D-C3D	2.57	129.49	124.68
4	L	854	BCL	O2A-CGA-CBA	2.53	119.86	111.91
4	L	854	BCL	CAA-C2A-C3A	-2.49	105.95	112.78
4	L	852	BCL	C2C-C3C-C4C	2.49	105.07	101.34
4	L	852	BCL	O2D-CGD-CBD	-2.49	106.85	111.27
4	L	854	BCL	C3C-C2C-C1C	2.48	105.88	101.87
5	M	855	BPH	CMD-C2D-C3D	2.48	129.33	124.68
10	M	860	SPO	C10-C9-C7	-2.48	123.77	127.31
5	L	856	BPH	O2A-CGA-O1A	-2.48	117.33	123.59
11	H	862	LDA	CM2-N1-C1	2.47	115.42	110.23
5	L	856	BPH	OBD-CAD-CBD	-2.47	122.20	125.82
6	L	859[A]	U10	C17-C18-C19	2.43	133.51	127.66
5	M	855	BPH	C5-C3-C2	-2.43	116.20	121.12
4	L	852	BCL	CHA-C1A-NA	-2.42	120.85	126.40
6	M	858	U10	C31-C29-C28	2.41	125.99	121.12
5	L	856	BPH	CMD-C2D-C3D	2.40	129.16	124.68
6	L	859[A]	U10	C7-C6-C5	-2.40	115.59	118.48
11	M	863	LDA	C9-C8-C7	-2.39	102.30	114.42
12	M	900	CDL	CB4-OB6-CB5	2.39	123.67	117.79
4	L	854	BCL	CHB-C4A-NA	2.38	127.80	124.51
5	M	855	BPH	CAA-C2A-C3A	-2.38	106.27	112.78
4	M	853	BCL	C3C-C2C-C1C	2.38	105.71	101.87
5	L	856	BPH	CAA-C2A-C3A	-2.36	106.32	112.78
6	M	858	U10	C16-C14-C13	2.35	125.87	121.12
4	L	852	BCL	CAC-C3C-C4C	-2.34	107.38	112.58
11	M	863	LDA	CM2-N1-C1	2.33	115.13	110.23
11	H	862	LDA	C9-C8-C7	-2.32	102.63	114.42
4	M	853	BCL	OBD-CAD-CBD	-2.30	122.60	125.89
4	L	852	BCL	O1D-CGD-CBD	2.29	129.17	124.48
6	M	858	U10	C21-C19-C18	2.29	125.75	121.12
5	M	855	BPH	C4-C3-C5	2.29	119.12	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	851	BCL	C1B-CHB-C4A	-2.25	125.66	130.12
4	M	851	BCL	CHA-C1A-NA	-2.23	121.29	126.40
12	M	900	CDL	CB6-CB4-CB3	-2.23	106.53	111.79
4	L	852	BCL	C12-C11-C10	-2.21	103.07	113.24
4	L	852	BCL	C11-C12-C13	-2.18	108.86	115.92
5	M	855	BPH	O2A-CGA-O1A	-2.18	118.09	123.59
4	M	853	BCL	O2A-CGA-O1A	-2.17	118.12	123.59
4	L	854	BCL	O1D-CGD-CBD	-2.16	120.06	124.48
4	M	851	BCL	CMB-C2B-C3B	2.14	128.69	124.68
4	M	853	BCL	CMB-C2B-C1B	-2.13	125.18	128.46
6	M	858	U10	C41-C39-C38	-2.13	116.50	122.65
4	M	853	BCL	C1B-CHB-C4A	-2.12	125.91	130.12
12	M	900	CDL	C52-C51-CB5	2.12	121.34	113.62
4	M	853	BCL	C3A-C2A-C1A	2.12	104.52	101.34
6	M	858	U10	C6-C1-C2	2.11	120.85	119.18
10	M	860	SPO	C10-C11-C12	-2.11	120.48	126.42
6	L	859[A]	U10	C21-C19-C18	2.10	125.37	121.12
4	M	851	BCL	OBD-CAD-C3D	2.10	131.47	127.98
4	L	854	BCL	C2A-C3A-C4A	2.10	105.26	101.87
11	M	861	LDA	C9-C8-C7	-2.10	103.78	114.42
11	M	861	LDA	CM2-N1-C1	2.10	114.64	110.23
4	M	851	BCL	O1D-CGD-CBD	-2.09	120.21	124.48
6	L	859[A]	U10	C6-C1-C2	2.06	120.81	119.18
4	M	851	BCL	CMA-C3A-C4A	-2.05	106.26	111.77
5	M	855	BPH	CAC-C3C-C2C	-2.04	109.16	114.26
5	L	856	BPH	CAC-C3C-C4C	2.03	118.28	113.73
4	L	854	BCL	O2A-CGA-O1A	-2.03	118.48	123.59
4	M	851	BCL	C3C-C2C-C1C	2.02	105.13	101.87
6	L	859[A]	U10	C4-C3-C2	-2.01	116.73	120.68
10	M	860	SPO	O1-C1-C2	2.01	122.76	108.97
4	L	852	BCL	C16-C15-C13	-2.00	109.45	115.92
6	L	859[A]	U10	C8-C7-C6	2.00	117.44	112.05

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	851	BCL	C8
4	M	851	BCL	C13
5	L	856	BPH	C8
5	L	856	BPH	C13
5	M	855	BPH	C8

All (134) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	851	BCL	C1-C2-C3-C4
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	O2A-C1-C2-C3
5	M	855	BPH	C1-C2-C3-C4
5	M	855	BPH	C1-C2-C3-C5
6	L	859[A]	U10	C14-C16-C17-C18
6	M	858	U10	C32-C33-C34-C35
7	L	865	HTO	C1-C2-C3-O3
7	L	865	HTO	C1-C2-C3-C4
7	L	865	HTO	O2-C2-C3-O3
7	L	865	HTO	O2-C2-C3-C4
7	L	866	HTO	C1-C2-C3-O3
7	L	866	HTO	C1-C2-C3-C4
7	L	866	HTO	O2-C2-C3-O3
7	L	866	HTO	O2-C2-C3-C4
7	L	866	HTO	C3-C4-C5-C6
10	M	860	SPO	C4-C5-C6-C7
11	M	863	LDA	C2-C1-N1-CM2
12	M	900	CDL	CA3-OA5-PA1-OA3
12	M	900	CDL	CA3-OA5-PA1-OA4
13	M	867	GOL	C1-C2-C3-O3
4	M	851	BCL	C8-C10-C11-C12
4	M	851	BCL	C3-C5-C6-C7
5	M	855	BPH	C4-C3-C5-C6
4	M	851	BCL	C1-C2-C3-C5
10	M	860	SPO	C36-C37-C38-C39
6	M	858	U10	C32-C33-C34-C36
10	M	860	SPO	C36-C37-C38-C40
5	M	855	BPH	C2-C3-C5-C6
4	M	851	BCL	C11-C10-C8-C9
4	M	851	BCL	C13-C15-C16-C17
5	L	856	BPH	C8-C10-C11-C12
4	M	851	BCL	C5-C6-C7-C8
6	M	858	U10	C24-C26-C27-C28
12	M	900	CDL	CA3-OA5-PA1-OA2
5	L	856	BPH	C10-C11-C12-C13
11	M	861	LDA	C11-C10-C9-C8
5	M	855	BPH	C6-C7-C8-C10
12	M	900	CDL	C36-C37-C38-C39
12	M	900	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
5	L	856	BPH	C2-C3-C5-C6
4	L	854	BCL	C14-C13-C15-C16
12	M	900	CDL	CB7-C71-C72-C73
7	L	865	HTO	C2-C3-C4-C5
11	M	861	LDA	C4-C5-C6-C7
11	H	862	LDA	C11-C10-C9-C8
12	M	900	CDL	C34-C35-C36-C37
12	M	900	CDL	C31-C32-C33-C34
5	M	855	BPH	C6-C7-C8-C9
12	M	900	CDL	C11-C12-C13-C14
5	L	856	BPH	C4-C3-C5-C6
4	M	851	BCL	C6-C7-C8-C10
4	M	851	BCL	C12-C13-C15-C16
4	M	851	BCL	C14-C13-C15-C16
11	M	863	LDA	C4-C5-C6-C7
12	M	900	CDL	C38-C39-C40-C41
12	M	900	CDL	CA7-C31-C32-C33
7	L	865	HTO	O3-C3-C4-C5
12	M	900	CDL	C11-CA5-OA6-CA4
11	H	862	LDA	C9-C10-C11-C12
10	M	860	SPO	C4-C1-O1-CM1
13	M	867	GOL	O1-C1-C2-O2
4	L	854	BCL	C13-C15-C16-C17
10	M	860	SPO	C3-C1-O1-CM1
10	M	860	SPO	C2-C1-C4-C5
10	M	860	SPO	C3-C1-C4-C5
4	L	854	BCL	C12-C13-C15-C16
4	M	851	BCL	C11-C12-C13-C14
12	M	900	CDL	OA5-CA3-CA4-CA6
6	M	858	U10	C31-C32-C33-C34
7	L	866	HTO	O3-C3-C4-C5
12	M	900	CDL	C17-C18-C19-C20
12	M	900	CDL	C71-C72-C73-C74
12	M	900	CDL	CA3-CA4-CA6-OA8
6	M	858	U10	C25-C24-C26-C27
7	L	866	HTO	O1-C1-C2-O2
12	M	900	CDL	OA7-CA5-OA6-CA4
4	M	851	BCL	C2-C1-O2A-CGA
12	M	900	CDL	C72-C73-C74-C75
4	L	852	BCL	CAD-CBD-CGD-O2D
5	L	856	BPH	CAD-CBD-CGD-O2D
6	L	859[A]	U10	C2-C3-O3-C3M

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Mol	Chain	Res	Type	Atoms
4	M	853	BCL	C16-C17-C18-C19
11	M	861	LDA	C2-C1-N1-CM1
11	M	861	LDA	C2-C1-N1-CM2
11	H	862	LDA	C2-C1-N1-CM1
11	H	862	LDA	C2-C1-N1-CM2
12	M	900	CDL	C51-C52-C53-C54
4	L	854	BCL	C15-C16-C17-C18
4	L	854	BCL	C16-C17-C18-C20
11	M	861	LDA	C2-C1-N1-O1
11	H	862	LDA	C2-C1-N1-O1
4	L	852	BCL	C12-C13-C15-C16
12	M	900	CDL	OA5-CA3-CA4-OA6
5	M	855	BPH	C5-C6-C7-C8
4	L	854	BCL	C16-C17-C18-C19
4	M	851	BCL	C16-C17-C18-C19
4	L	852	BCL	C15-C16-C17-C18
7	L	865	HTO	C4-C5-C6-C7
6	M	858	U10	C34-C36-C37-C38
4	M	851	BCL	C6-C7-C8-C9
6	M	858	U10	C5-C4-O4-C4M
4	M	851	BCL	C16-C17-C18-C20
10	M	860	SPO	C20-C21-C22-C23
6	M	858	U10	C33-C34-C36-C37
5	M	855	BPH	C2-C1-O2A-CGA
11	H	862	LDA	C4-C5-C6-C7
10	M	860	SPO	C18-C17-C19-C20
10	M	860	SPO	C16-C17-C19-C20
6	M	858	U10	C36-C37-C38-C39
10	M	860	SPO	C1-C4-C5-C6
10	M	860	SPO	C17-C19-C20-C21
6	L	859[A]	U10	C20-C19-C21-C22
4	L	854	BCL	C4C-C3C-CAC-CBC
11	M	863	LDA	C2-C3-C4-C5
7	L	866	HTO	C4-C5-C6-C7
12	M	900	CDL	CB3-OB5-PB2-OB2
6	M	858	U10	C23-C24-C26-C27
4	L	852	BCL	C14-C13-C15-C16
4	L	854	BCL	CAD-CBD-CGD-O2D
4	M	851	BCL	CAD-CBD-CGD-O2D
5	M	855	BPH	CAD-CBD-CGD-O2D
6	L	859[A]	U10	C18-C19-C21-C22
4	M	851	BCL	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	M	853	BCL	C16-C17-C18-C20
4	M	851	BCL	CHA-CBD-CGD-O2D
11	M	861	LDA	C2-C3-C4-C5
12	M	900	CDL	C40-C41-C42-C43
10	M	860	SPO	C30-C31-C32-C33
4	M	851	BCL	C11-C10-C8-C7
4	M	853	BCL	CAA-CBA-CGA-O2A
5	M	855	BPH	C2A-CAA-CBA-CGA

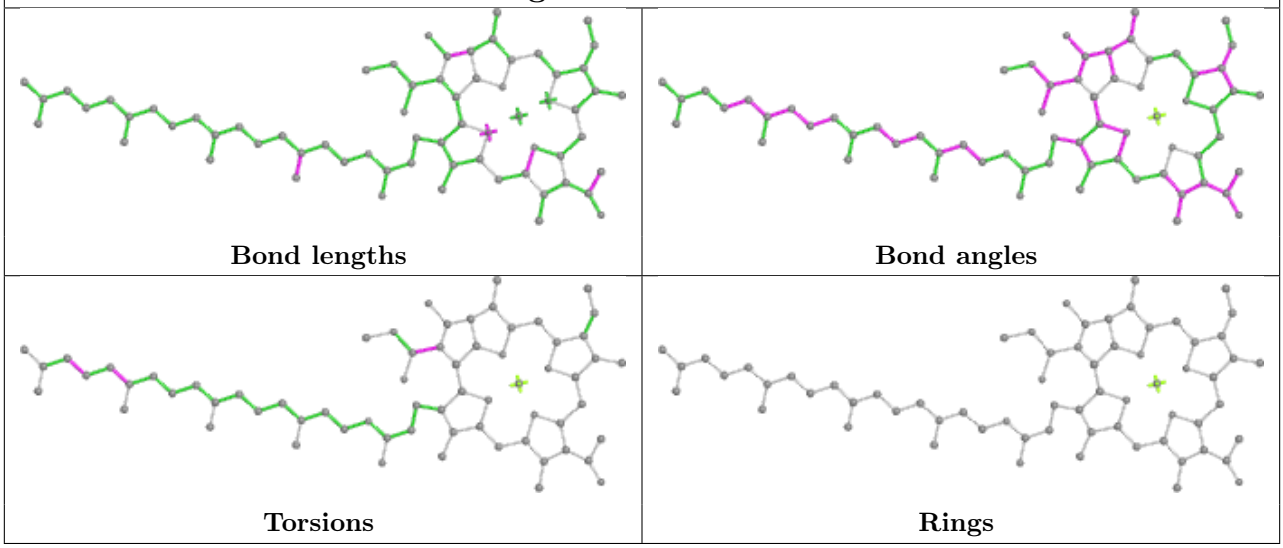
There are no ring outliers.

15 monomers are involved in 57 short contacts:

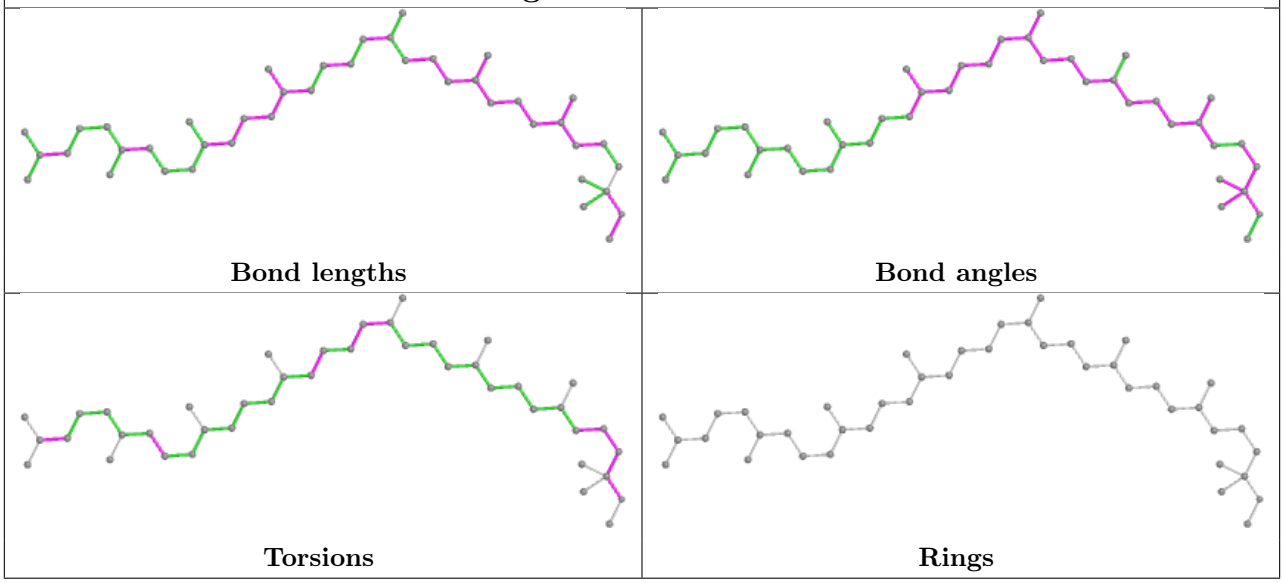
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	861	LDA	2	0
7	L	865	HTO	1	0
4	L	852	BCL	1	0
10	M	860	SPO	7	0
4	M	851	BCL	15	0
11	H	862	LDA	2	0
5	M	855	BPH	3	0
7	L	866	HTO	1	0
11	M	863	LDA	3	0
4	L	854	BCL	3	0
4	M	853	BCL	7	0
12	M	900	CDL	2	0
5	L	856	BPH	5	0
6	M	858	U10	3	0
6	L	859[A]	U10	8	0

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.

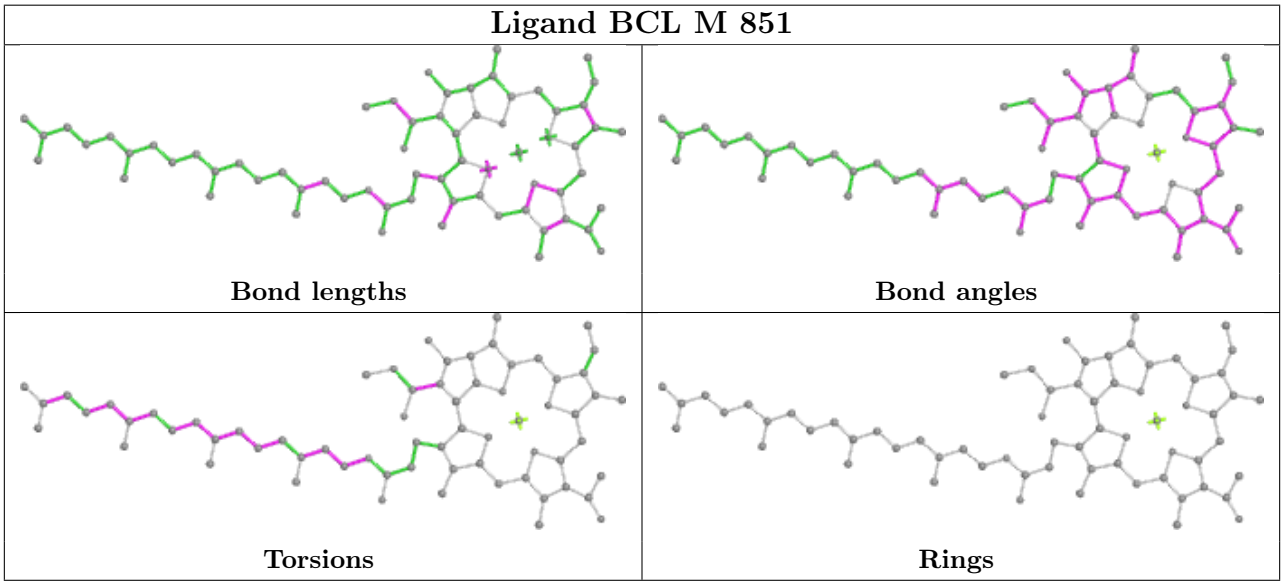
Ligand BCL L 852



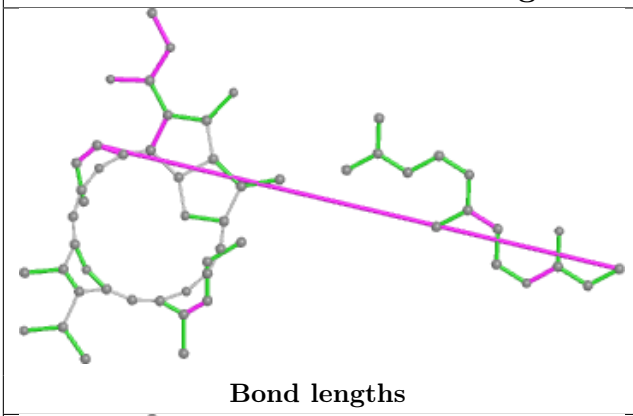
Ligand SPO M 860



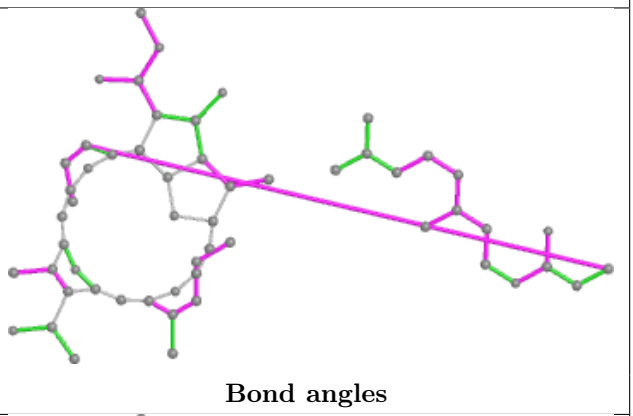
Ligand BCL M 851



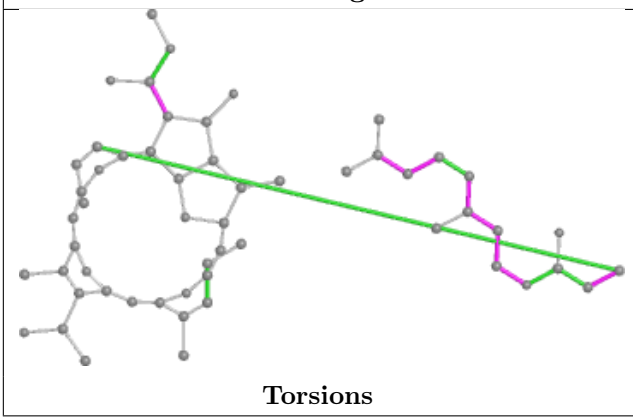
Ligand BPH M 855



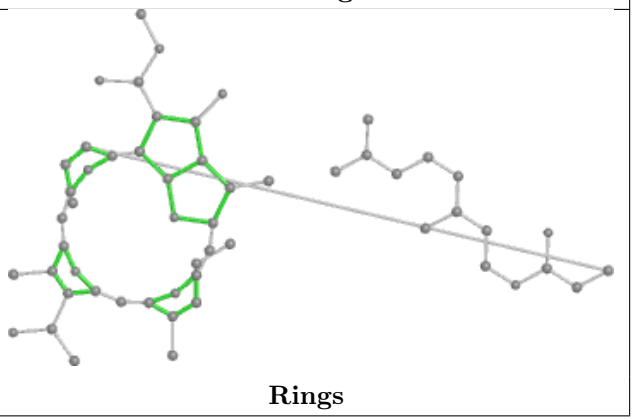
Bond lengths



Bond angles

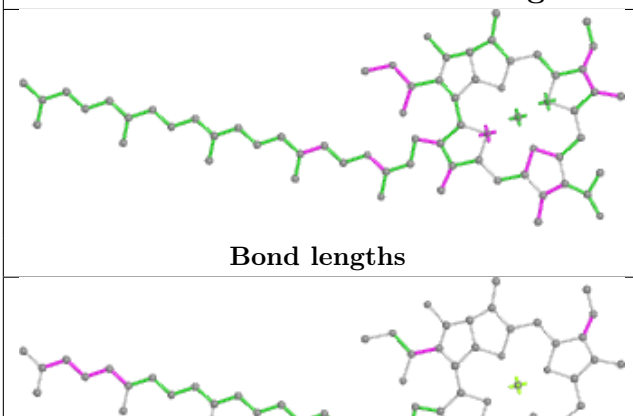


Torsions

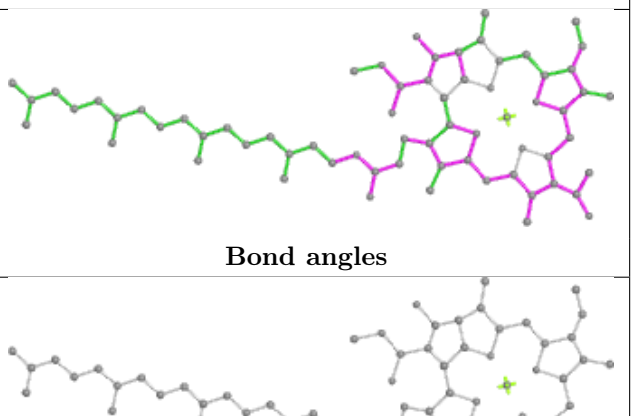


Rings

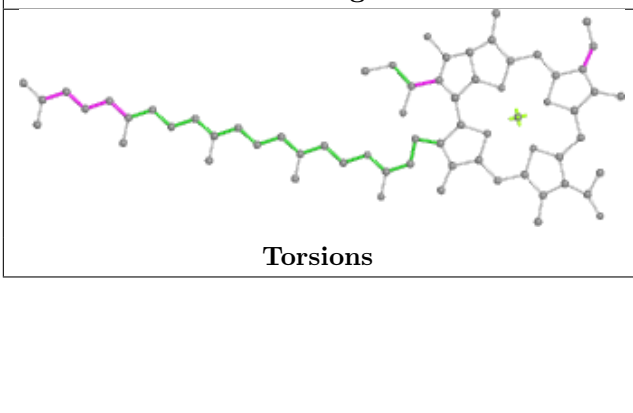
Ligand BCL L 854



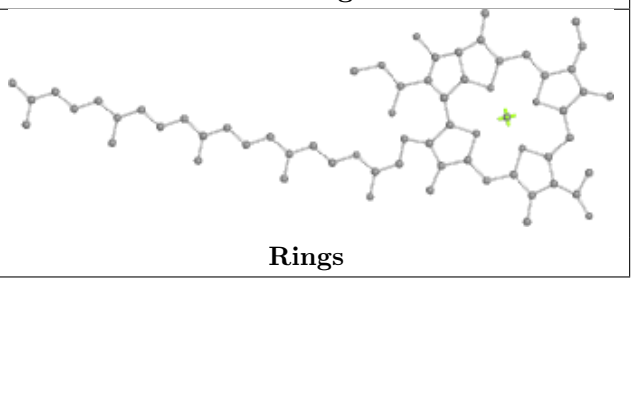
Bond lengths



Bond angles

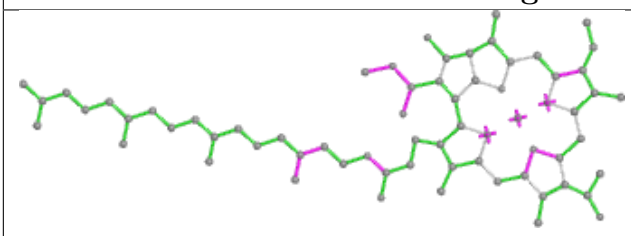


Torsions

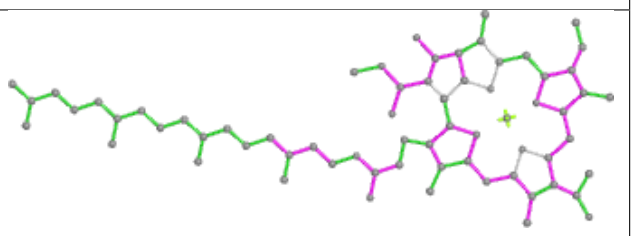


Rings

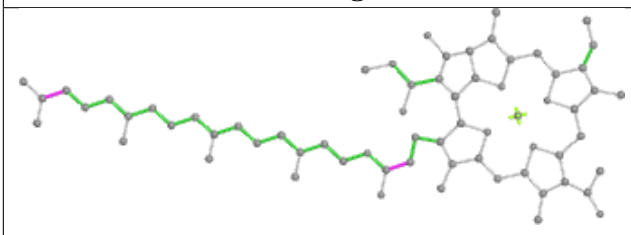
Ligand BCL M 853



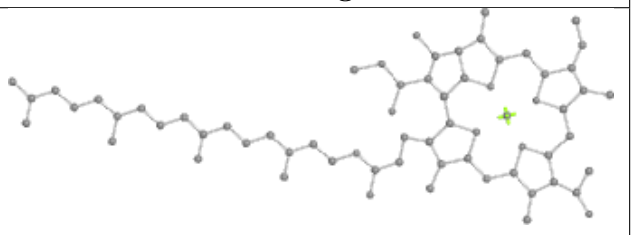
Bond lengths



Bond angles

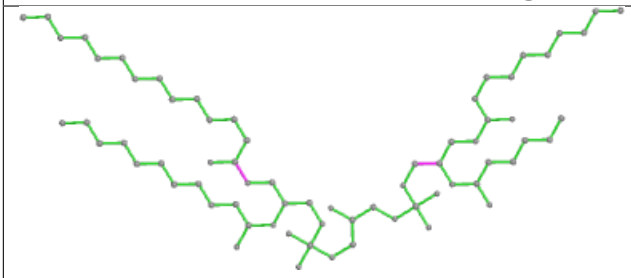


Torsions

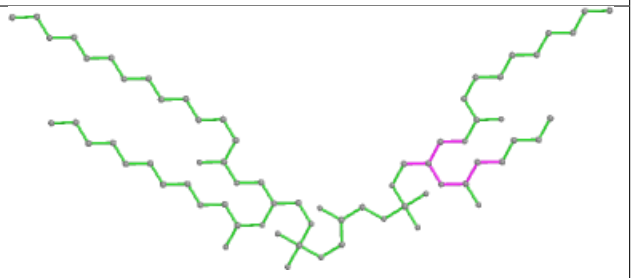


Rings

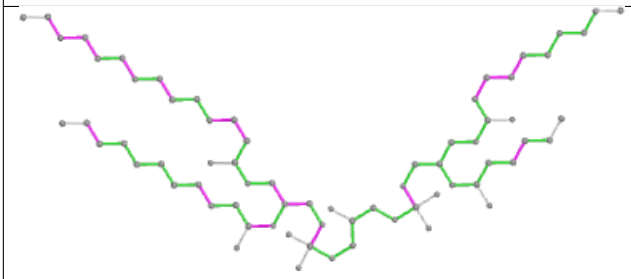
Ligand CDL M 900



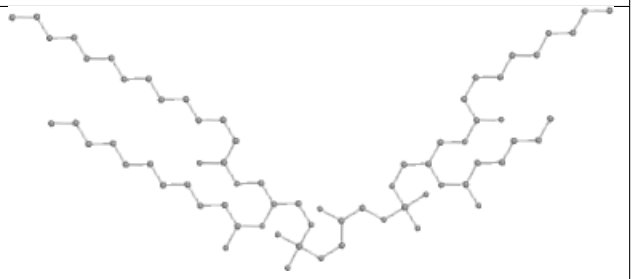
Bond lengths



Bond angles

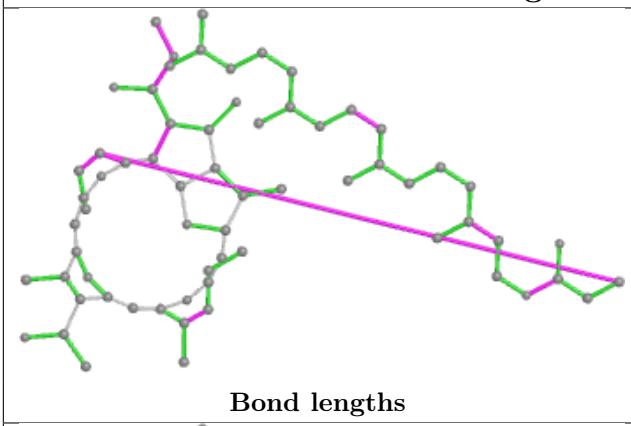


Torsions

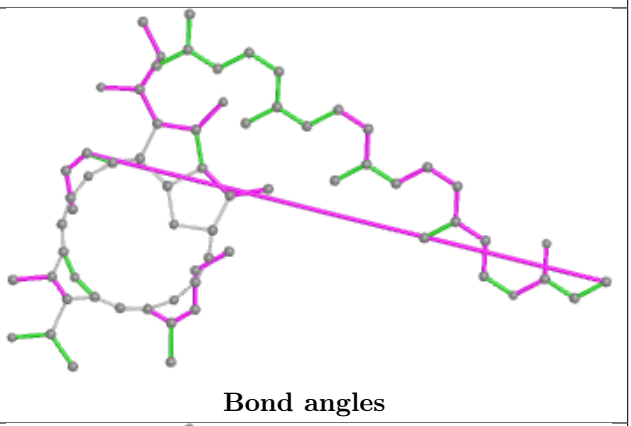


Rings

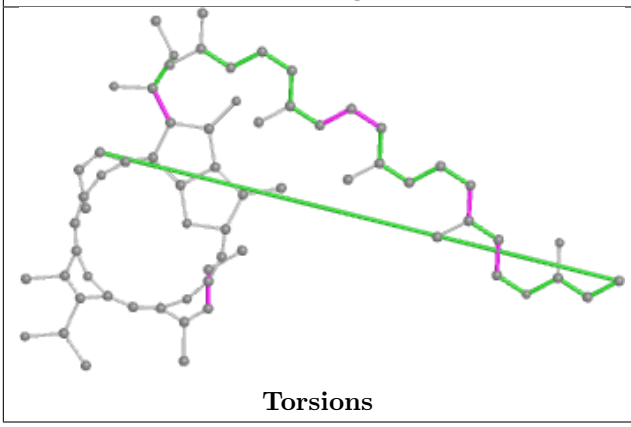
Ligand BPH L 856



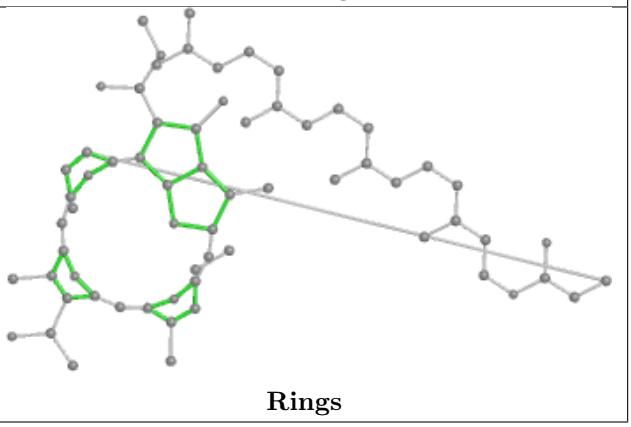
Bond lengths



Bond angles

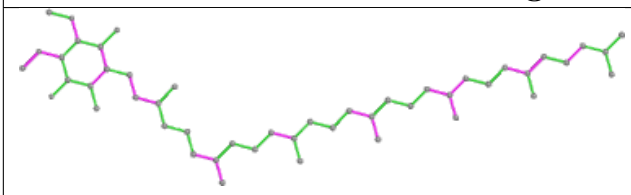


Torsions

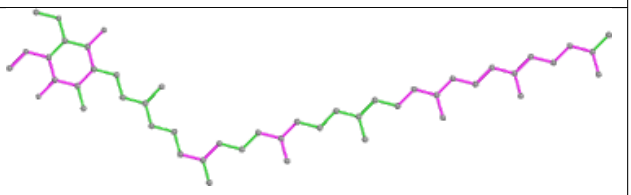


Rings

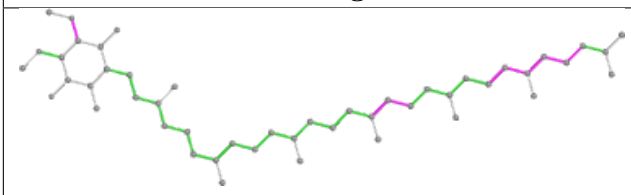
Ligand U10 M 858



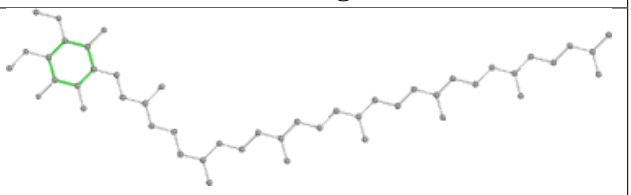
Bond lengths



Bond angles

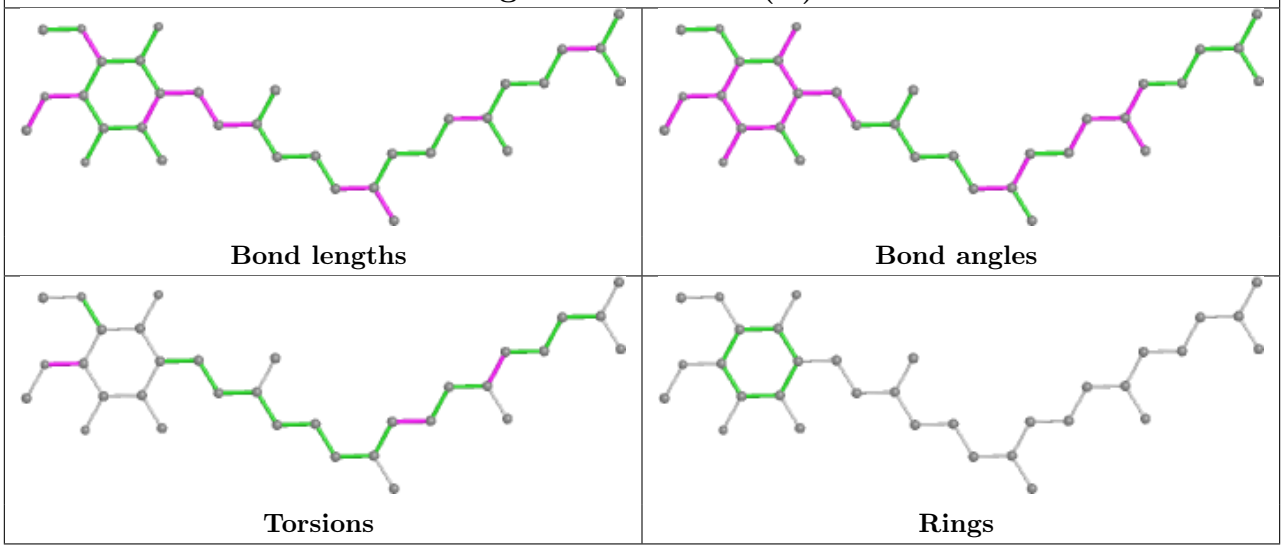


Torsions



Rings

Ligand U10 L 859 (A)



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, 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%)	-0.09	10 (3%) 42 37	15, 22, 46, 59	0
2	M	301/307 (98%)	-0.02	10 (3%) 46 40	13, 25, 47, 63	0
3	H	238/260 (91%)	-0.28	4 (1%) 70 66	17, 25, 38, 51	0
All	All	820/848 (96%)	-0.12	24 (2%) 51 46	13, 24, 45, 63	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	10.2
1	L	281	GLY	4.9
1	L	51	TRP	4.2
1	L	276	PRO	3.7
2	M	2	GLU	3.6
1	L	270	PRO	3.5
2	M	105	PHE	3.3
1	L	271	TRP	3.3
3	H	246	PRO	3.1
3	H	245	ALA	3.0
2	M	106	ALA	2.9
1	L	202	LYS	2.8
1	L	274	ASN	2.8
2	M	76	TYR	2.5
1	L	59	TRP	2.5
2	M	83	ALA	2.5
2	M	109	LEU	2.4
3	H	60	LYS	2.4
1	L	269	LEU	2.4
2	M	100	GLU	2.3
2	M	3	TYR	2.2
3	H	18	TYR	2.2
2	M	52	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	40	PHE	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, 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.

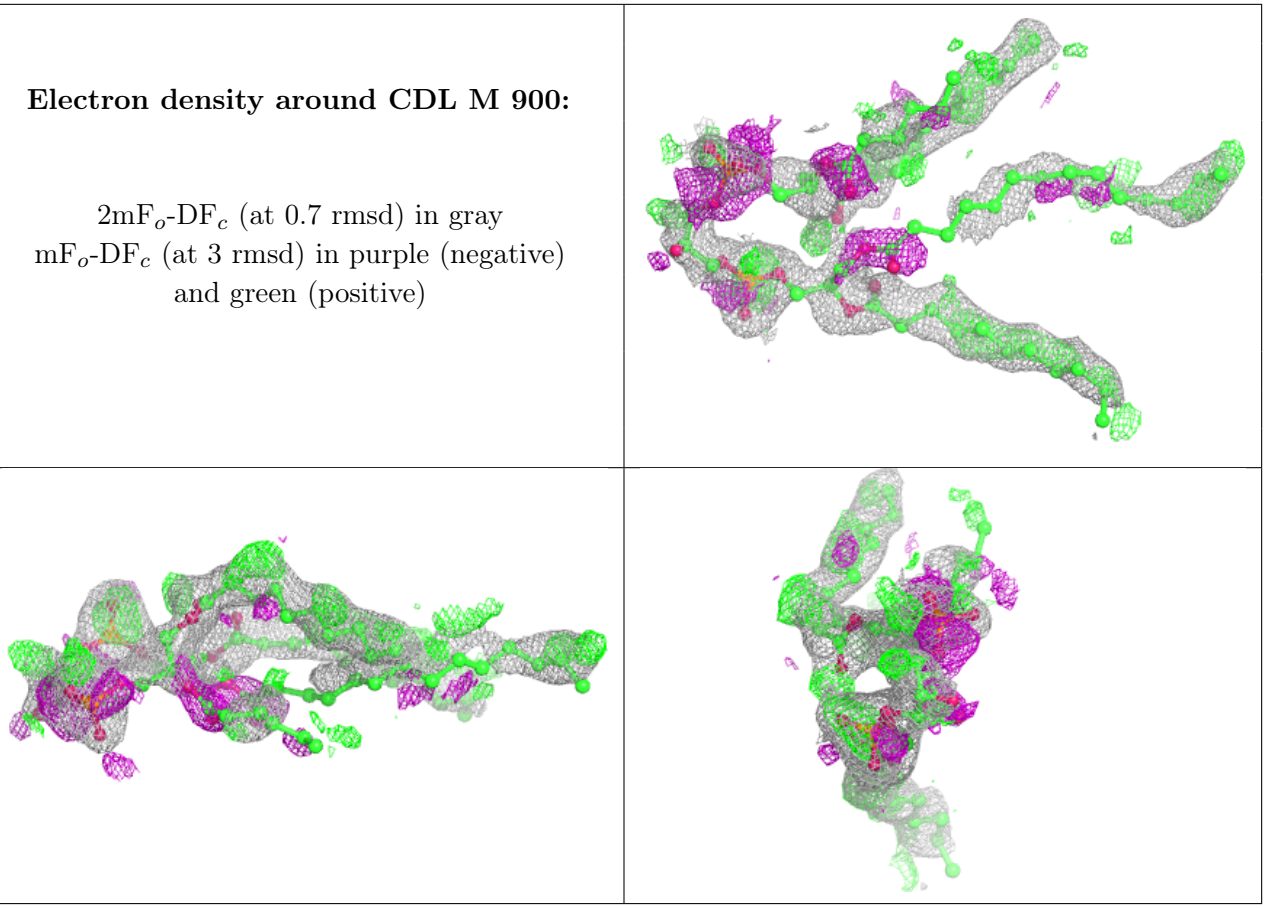
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	HTO	L	866	10/10	0.58	0.35	66,68,69,69	0
11	LDA	M	861	16/16	0.63	0.31	57,63,67,68	0
12	CDL	M	900	69/100	0.68	0.37	49,71,77,78	0
7	HTO	L	865	10/10	0.69	0.25	61,63,64,64	0
11	LDA	M	863	16/16	0.70	0.27	70,70,74,74	0
6	U10	L	859[A]	33/63	0.71	0.65	45,50,52,53	33
11	LDA	H	862	16/16	0.75	0.22	61,62,66,67	0
10	SPO	M	860	42/42	0.75	0.19	25,32,50,52	0
13	GOL	M	867	6/6	0.86	0.20	51,55,56,58	0
6	U10	M	858	48/63	0.89	0.19	16,29,61,63	0
9	PO4	M	864	5/5	0.89	0.17	72,73,73,73	0
4	BCL	M	851	66/66	0.91	0.16	17,22,66,68	0
5	BPH	L	856	65/65	0.92	0.12	13,17,33,36	0
4	BCL	M	853	66/66	0.92	0.14	13,18,38,44	0
5	BPH	M	855	55/65	0.93	0.13	19,22,63,66	0
4	BCL	L	854	66/66	0.93	0.12	12,17,40,44	0
4	BCL	L	852	66/66	0.93	0.12	15,17,29,32	0
8	FE2	M	857	1/1	0.98	0.09	14,14,14,14	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.

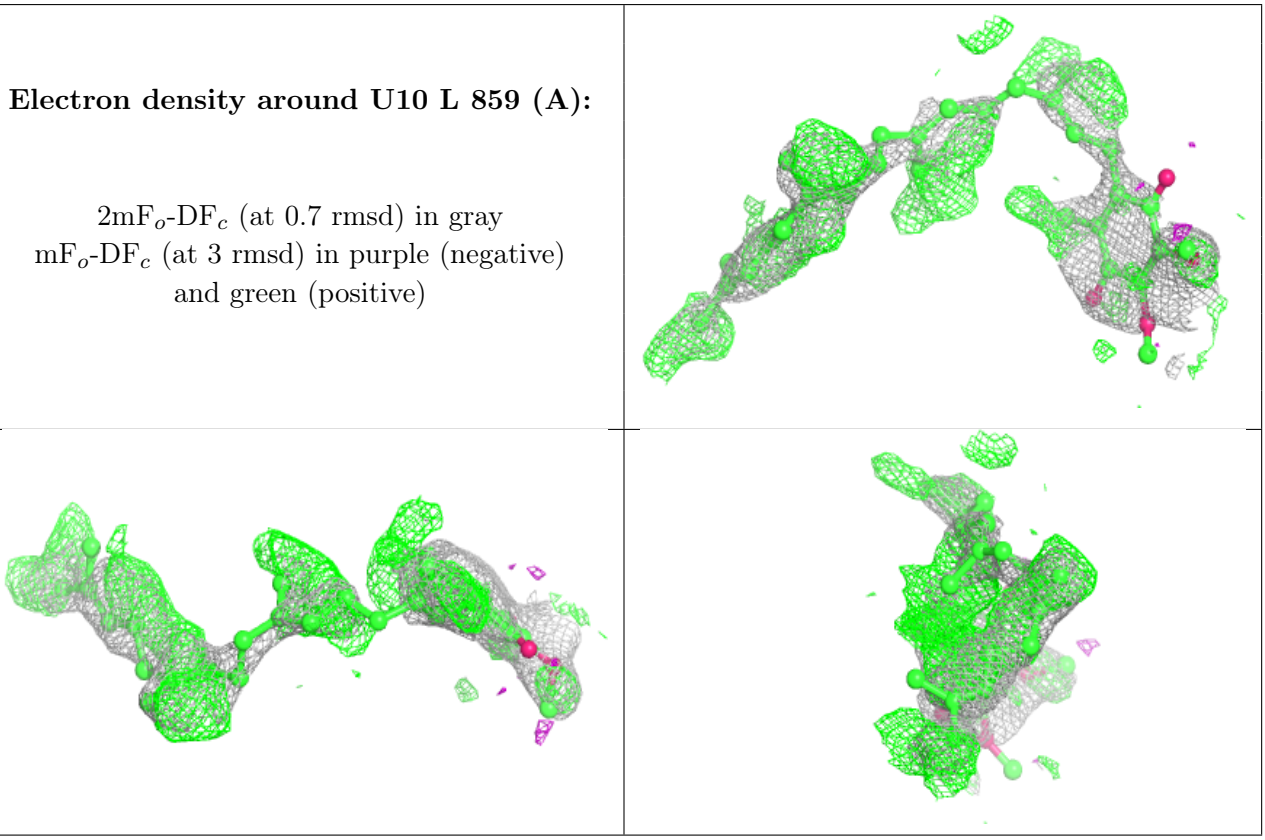
Electron density around CDL M 900:

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



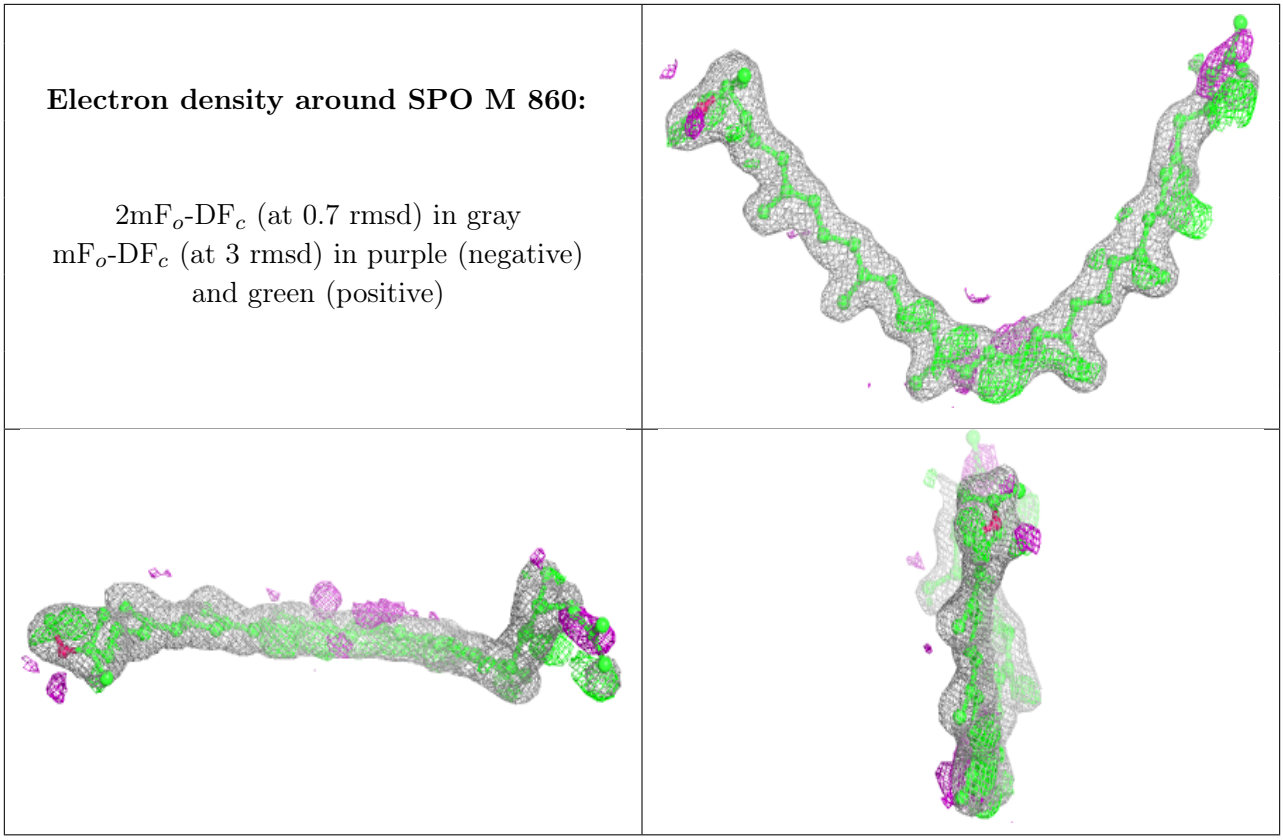
Electron density around U10 L 859 (A):

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



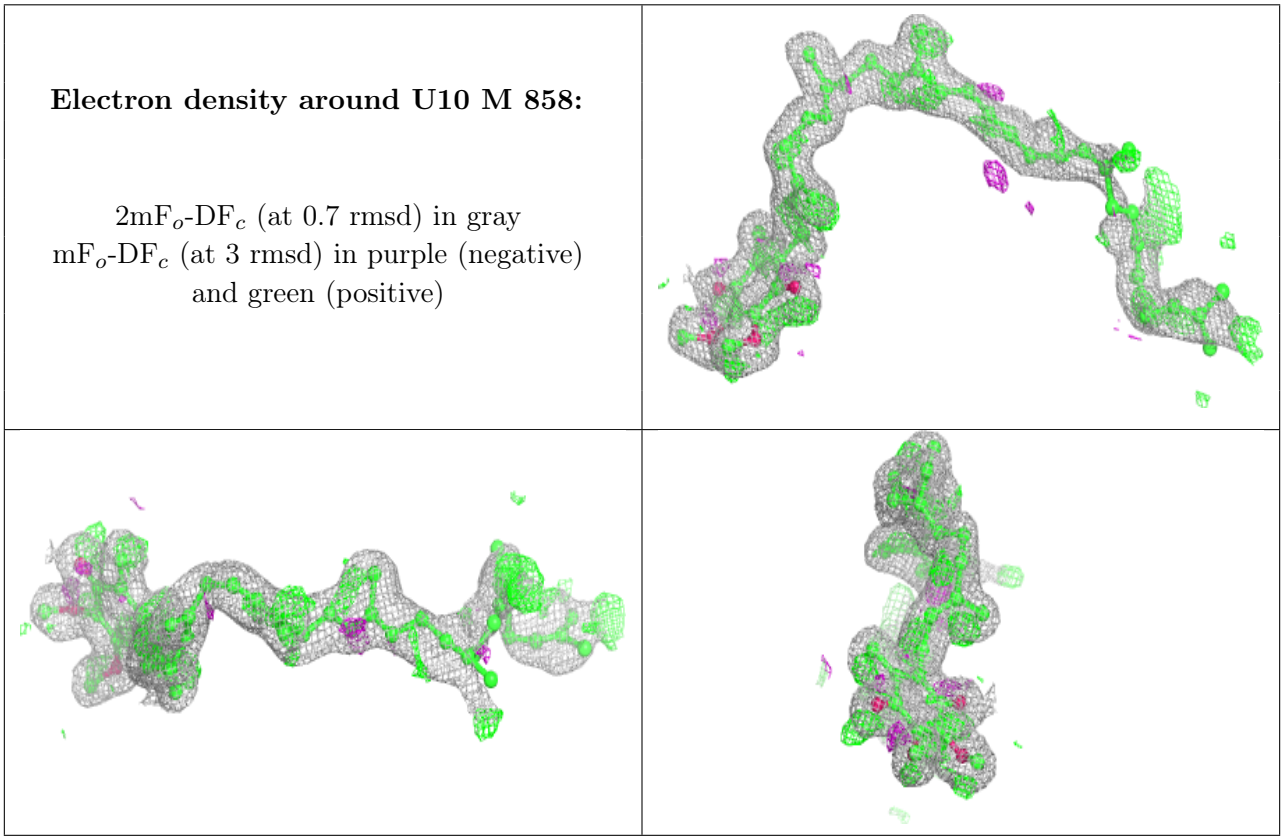
Electron density around SPO M 860:

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



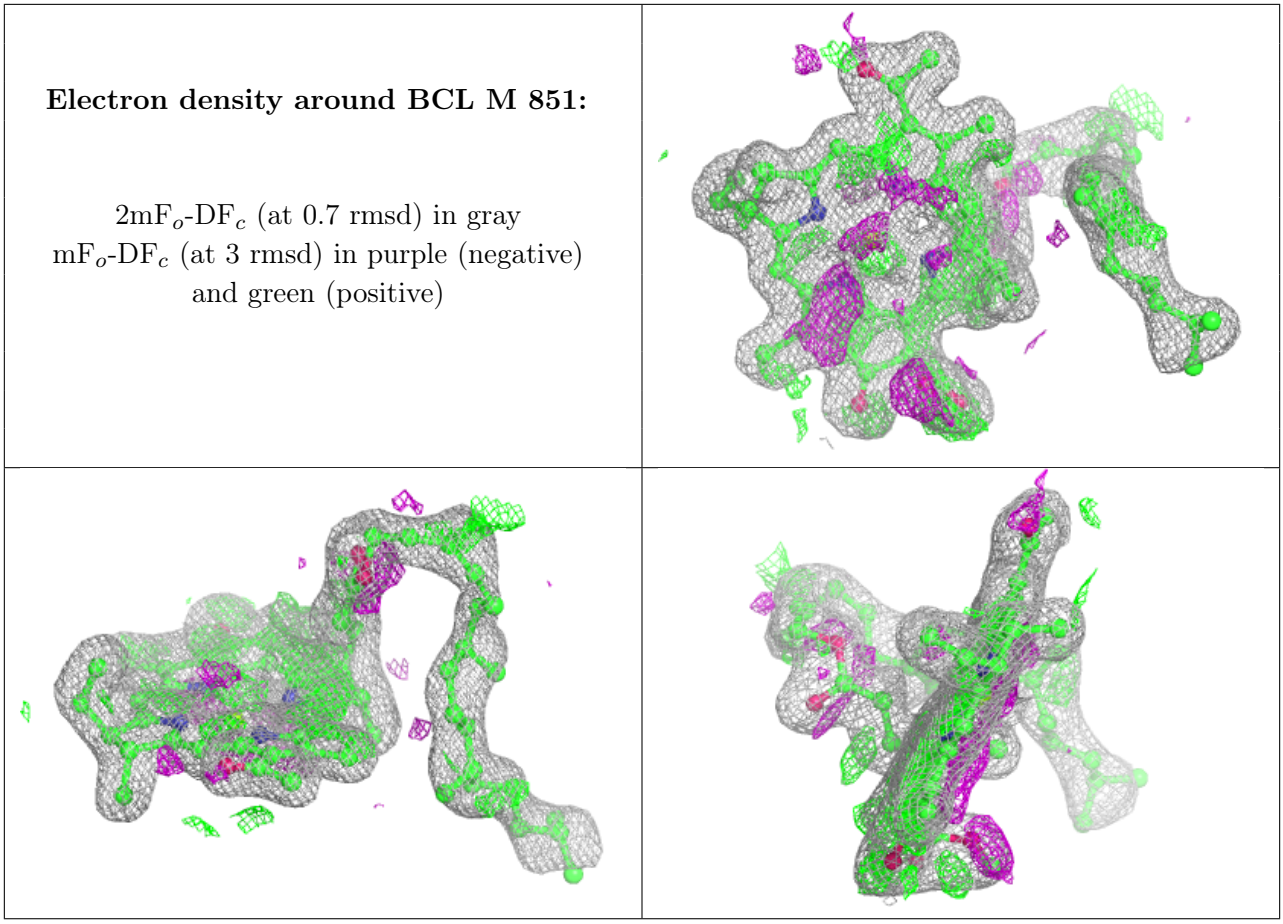
Electron density around U10 M 858:

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



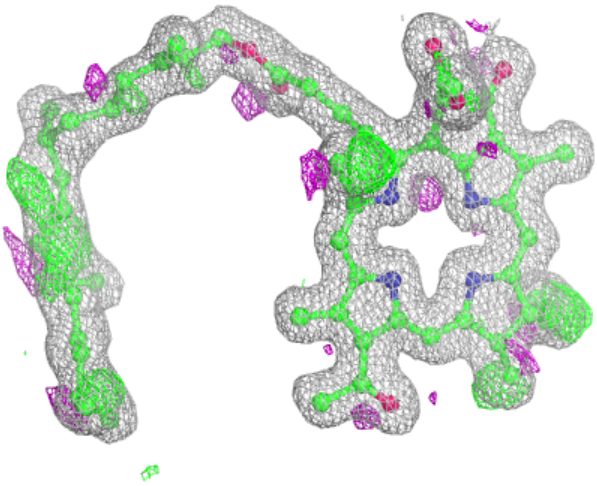
Electron density around BCL M 851:

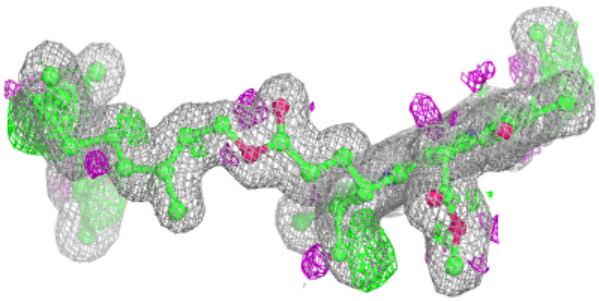
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BPH L 856:

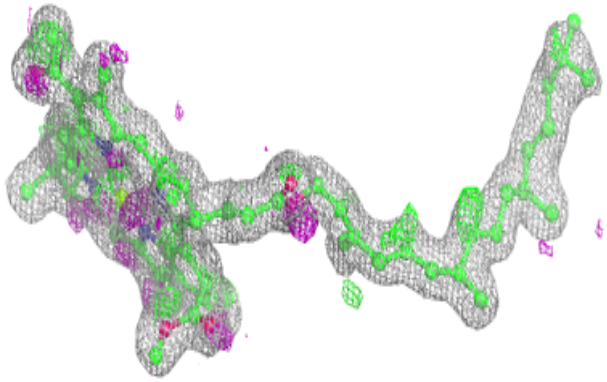
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

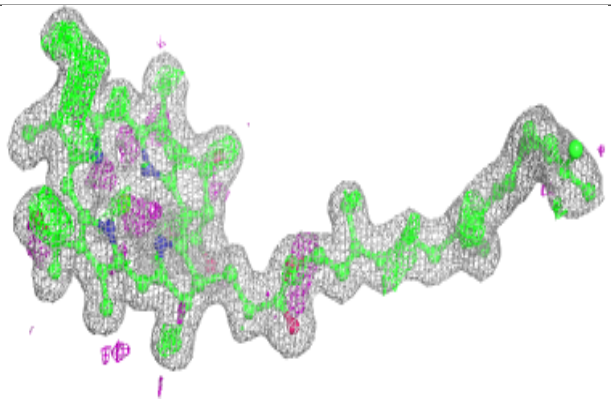




Electron density around BCL M 853:

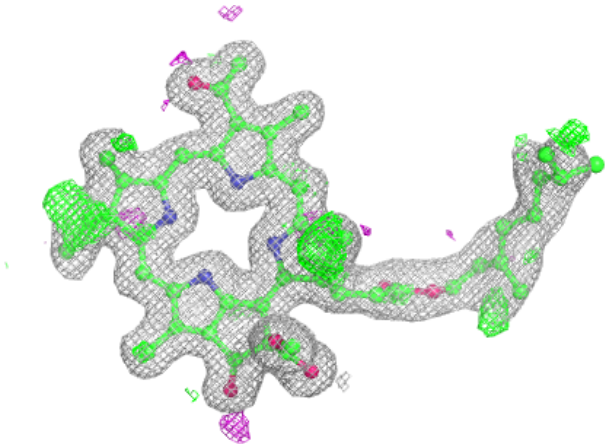
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

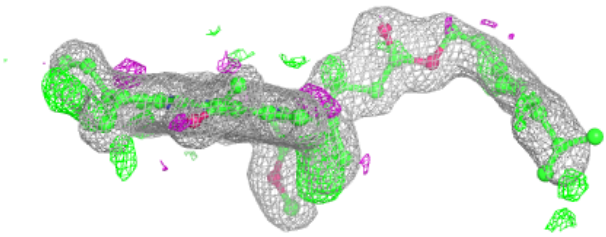


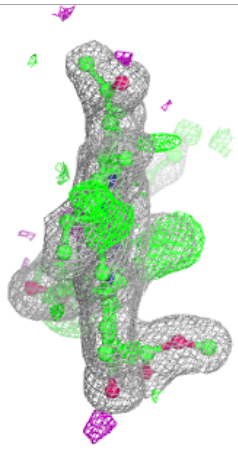


Electron density around BPH M 855:

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

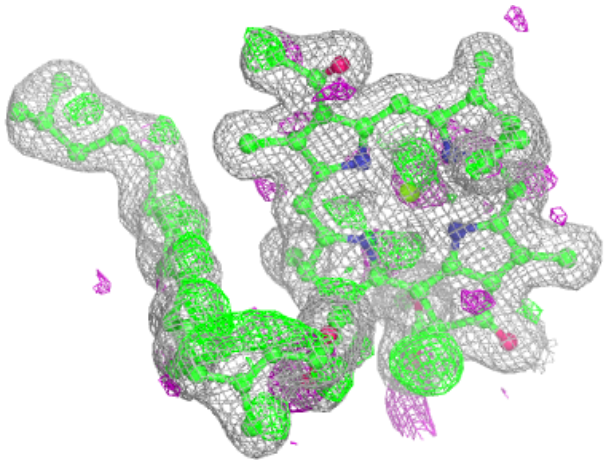


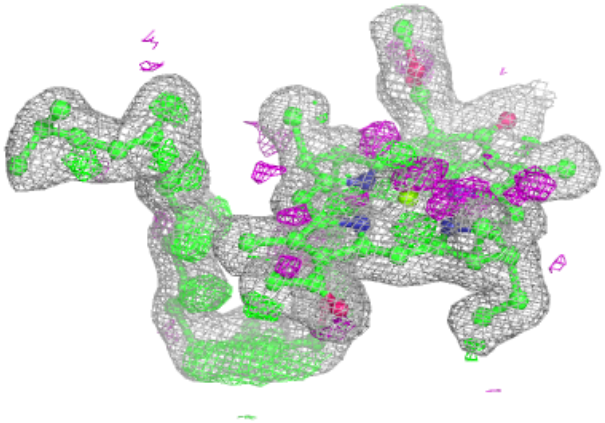


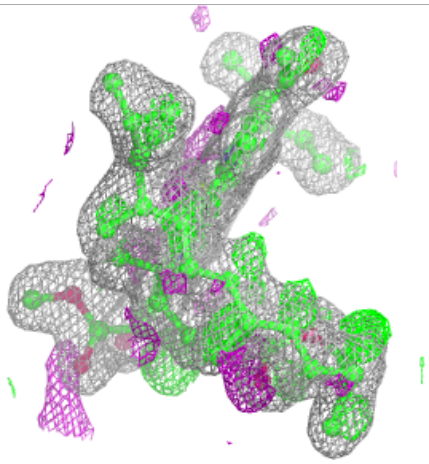


Electron density around BCL L 854:

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

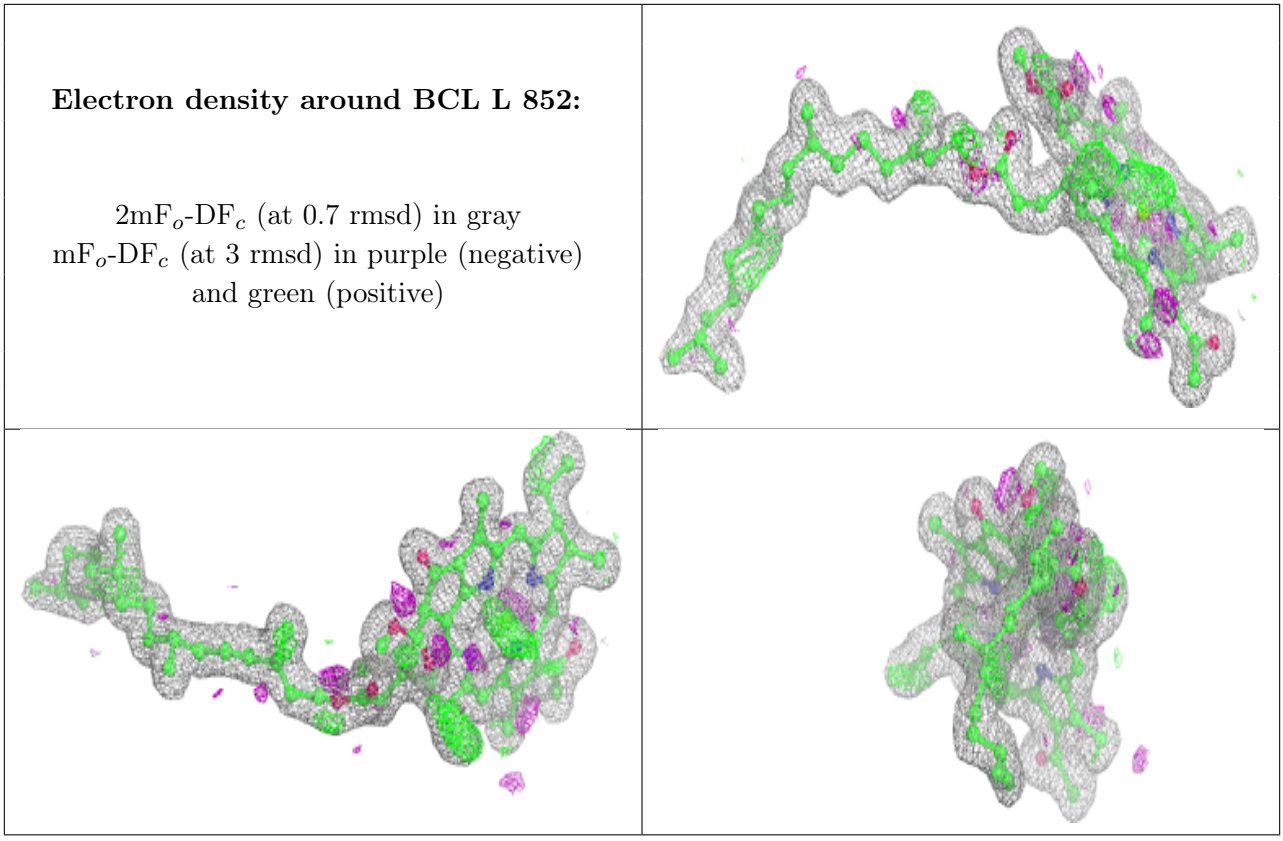






Electron density around BCL L 852:

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



6.5 Other polymers (i)

There are no such residues in this entry.