



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 11:17 AM EDT

PDB ID : 1KBY / pdb_00001kby
Title : Structure of Photosynthetic Reaction Center with bacteriochlorophyll-bacteriopheophytin heterodimer
Authors : Camara-Artigas, A.; Magee, C.; Goetsch, A.; Allen, J.P.
Deposited on : 2001-11-07
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

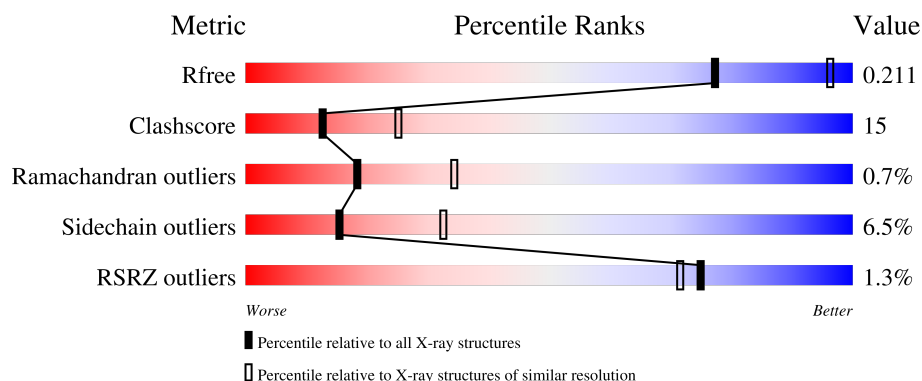
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	% 74% 23% .
2	M	307	2% 63% 32% ..
3	H	260	% 59% 25% 6% 9%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7220 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PHOTOSYNTHETIC REACTION CENTER PROTEIN L CHAIN.

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

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	0	0
			2406	1607	392	397	10			

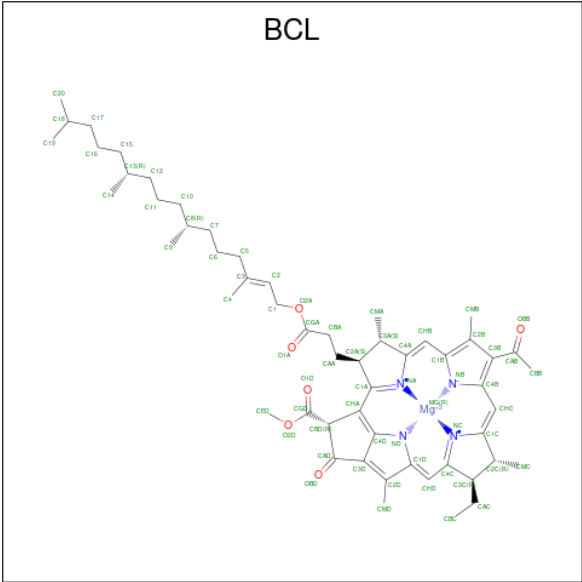
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	202	LEU	HIS	engineered mutation	UNP P02953

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER PROTEIN H CHAIN.

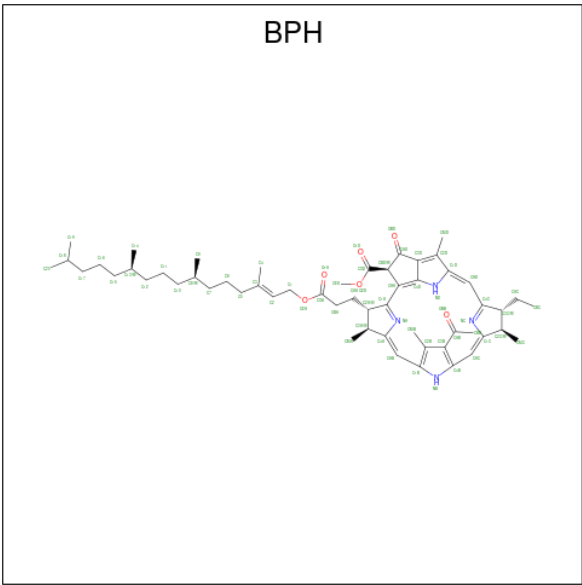
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	236	Total	C	N	O	S	0	0	0
			1794	1148	305	332	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



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

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

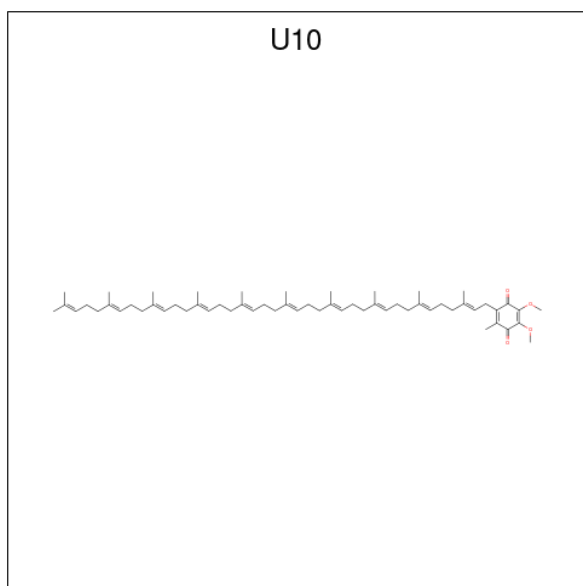
- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

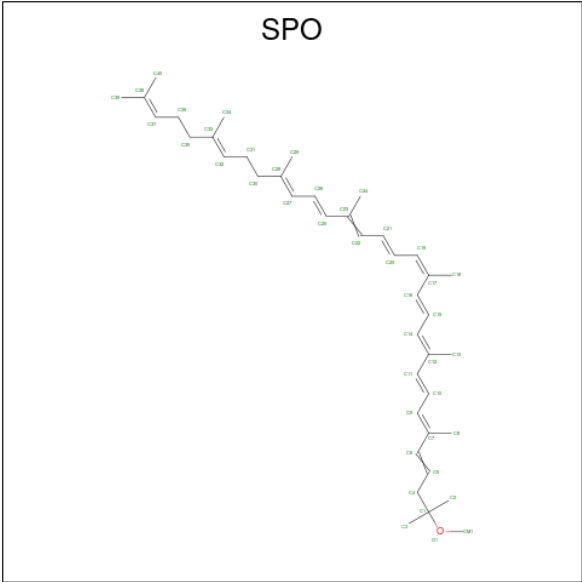
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Cl	0	0
			1	1		

- Molecule 8 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



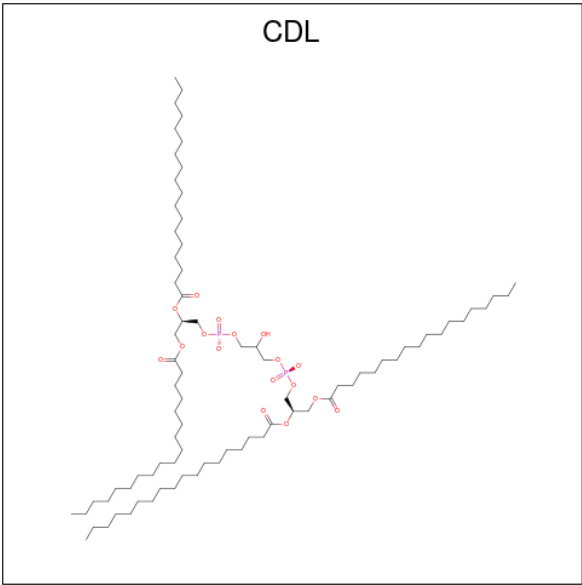
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 9 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).



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

- Molecule 10 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

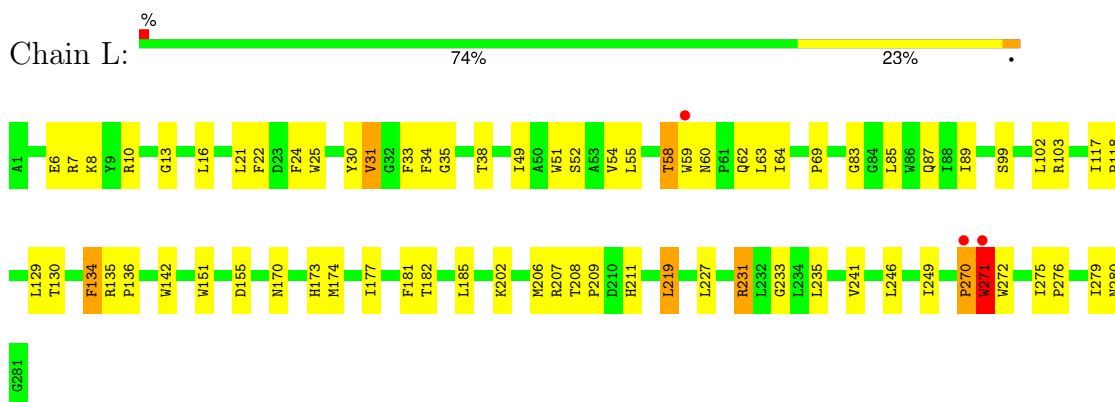
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	74	Total 74	O 74	0	0
11	M	71	Total 71	O 71	0	0
11	H	77	Total 77	O 77	0	0

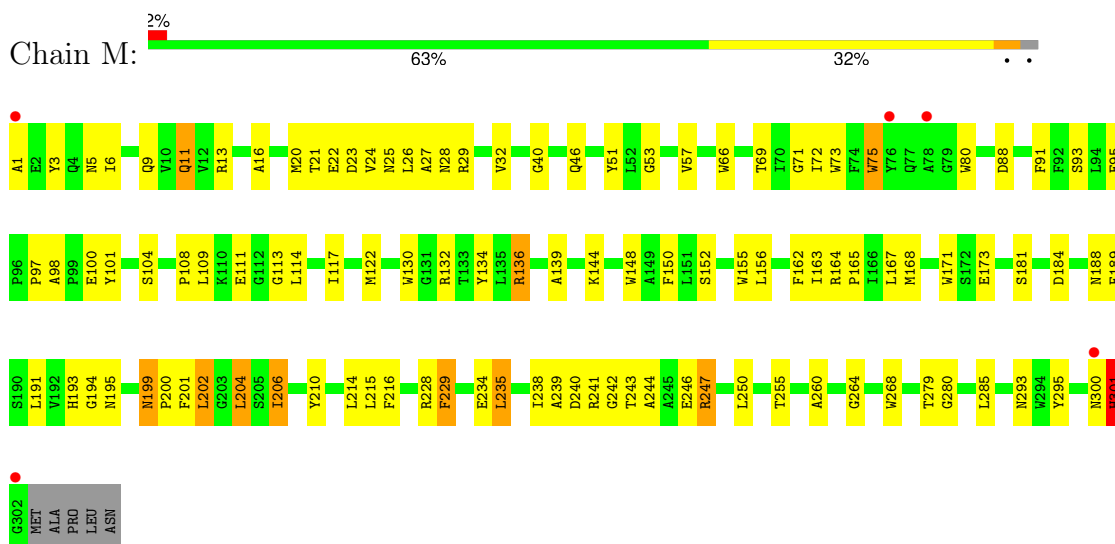
3 Residue-property plots [i](#)

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

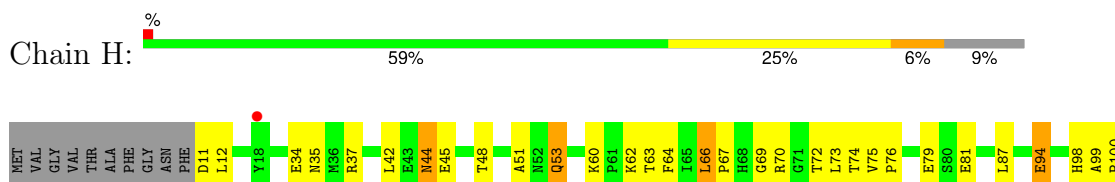
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER PROTEIN L CHAIN

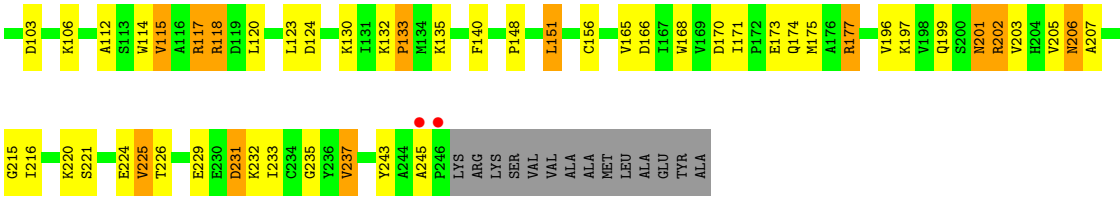


• Molecule 2: PHOTOSYNTHETIC REACTION CENTER PROTEIN M CHAIN



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER PROTEIN H CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.31Å 142.31Å 187.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.07 – 2.50 27.07 – 2.56	Depositor EDS
% Data completeness (in resolution range)	81.4 (27.07-2.50) 83.6 (27.07-2.56)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.57Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.195 , 0.224 0.196 , 0.211	Depositor DCC
R_{free} test set	6034 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7220	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, U10, CL, SPO, BPH, BCL, CDL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	L	0.49	0/2320	0.96	11/3175 (0.3%)
2	M	0.46	0/2497	0.91	7/3409 (0.2%)
3	H	0.46	0/1842	0.99	8/2509 (0.3%)
All	All	0.47	0/6659	0.95	26/9093 (0.3%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	66	LEU	CA-C-N	9.16	131.29	119.84
3	H	66	LEU	C-N-CA	9.16	131.29	119.84
1	L	6	GLU	N-CA-C	8.94	122.69	111.69
1	L	35	GLY	N-CA-C	-7.36	103.35	112.77
1	L	31	VAL	CA-C-N	-7.25	115.09	122.27
1	L	31	VAL	C-N-CA	-7.25	115.09	122.27
1	L	33	PHE	N-CA-C	-7.10	103.54	111.28
3	H	243	TYR	N-CA-C	6.95	119.88	111.82
2	M	202	LEU	N-CA-C	-6.72	104.04	111.36
1	L	59	TRP	N-CA-C	-6.31	103.72	112.30
3	H	133	PRO	N-CA-C	-6.31	101.35	111.38
1	L	13	GLY	N-CA-C	6.18	119.22	112.29
1	L	219	LEU	N-CA-C	6.06	117.75	111.03
1	L	31	VAL	CB-CA-C	-6.00	105.17	111.23
2	M	206	ILE	CB-CA-C	-5.97	104.32	111.97
3	H	67	PRO	N-CA-C	5.92	124.67	112.47
3	H	81	GLU	N-CA-C	-5.59	101.10	109.15
2	M	268	TRP	N-CA-C	-5.35	105.35	111.07
2	M	46	GLN	N-CA-C	5.30	118.18	109.76
2	M	229	PHE	N-CA-C	-5.25	104.31	111.56
3	H	44	ASN	N-CA-C	-5.17	103.10	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	134	PHE	N-CA-C	5.06	116.49	111.07
2	M	23	ASP	N-CA-C	-5.06	107.27	112.93
3	H	69	GLY	N-CA-C	-5.06	108.02	115.30
2	M	71	GLY	N-CA-C	5.04	119.84	113.24
1	L	231	ARG	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2187	62	0
2	M	2406	0	2325	81	0
3	H	1794	0	1792	68	0
4	L	198	0	222	14	0
5	L	130	0	152	14	0
5	M	65	0	76	9	0
6	M	1	0	0	0	0
7	M	1	0	0	0	0
8	M	48	0	63	2	0
9	M	42	0	60	1	0
10	M	81	0	106	1	0
11	H	77	0	0	1	0
11	L	74	0	0	2	0
11	M	71	0	0	3	0
All	All	7220	0	6983	213	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 15.

All (213) 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:271:TRP:H	1:L:271:TRP:CD1	1.68	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:272:TRP:HA	1:L:275:ILE:HD13	1.42	1.00
5:M:852:BPH:HAA2	5:M:852:BPH:HBD	1.47	0.96
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.45	0.95
1:L:34:PHE:O	1:L:38:THR:HG23	1.74	0.88
4:L:850:BCL:H93	5:M:852:BPH:H203	1.56	0.87
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.57	0.86
1:L:38:THR:HG22	1:L:99:SER:HB2	1.56	0.85
5:M:852:BPH:HAA2	5:M:852:BPH:CBD	2.02	0.83
2:M:202:LEU:O	2:M:206:ILE:HG12	1.79	0.81
1:L:58:THR:HG21	1:L:63:LEU:HD23	1.64	0.79
3:H:70:ARG:HH21	3:H:120:LEU:HB3	1.49	0.78
1:L:271:TRP:CD1	1:L:271:TRP:N	2.49	0.77
1:L:38:THR:HG22	1:L:99:SER:CB	2.15	0.76
1:L:271:TRP:H	1:L:271:TRP:HD1	1.30	0.75
2:M:206:ILE:HG23	5:M:852:BPH:HMB2	1.67	0.75
2:M:75:TRP:HD1	2:M:80:TRP:HA	1.52	0.74
1:L:181:PHE:CD2	5:L:854:BPH:HBB1	2.23	0.74
3:H:45:GLU:HG3	3:H:94:GLU:HG2	1.71	0.73
2:M:240:ASP:O	3:H:117:ARG:NH1	2.21	0.71
5:L:855:BPH:HBB2	2:M:210:TYR:HB3	1.73	0.70
3:H:70:ARG:NH2	3:H:120:LEU:HB3	2.07	0.70
4:L:850:BCL:H11	5:L:854:BPH:HBB2	1.74	0.69
2:M:199:ASN:C	2:M:199:ASN:HD22	2.00	0.68
2:M:72:ILE:HD12	2:M:73:TRP:N	2.08	0.68
3:H:201:ASN:H	3:H:201:ASN:HD22	1.41	0.68
1:L:211:HIS:CE1	2:M:20:MET:HE2	2.29	0.67
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.76	0.67
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.76	0.67
2:M:242:GLY:HA2	3:H:117:ARG:HD2	1.75	0.66
2:M:144:LYS:N	2:M:144:LYS:HD2	2.11	0.66
3:H:148:PRO:HA	3:H:151:LEU:HD22	1.77	0.66
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.77	0.65
1:L:51:TRP:O	1:L:54:VAL:HG22	1.96	0.65
1:L:7:ARG:NH1	3:H:98:HIS:CD2	2.65	0.64
2:M:11:GLN:OE1	2:M:40:GLY:HA3	1.96	0.64
1:L:7:ARG:HH12	3:H:98:HIS:CD2	2.16	0.63
2:M:243:THR:O	2:M:247:ARG:HG2	1.99	0.63
1:L:117:ILE:HB	1:L:118:PRO:HD3	1.81	0.63
3:H:70:ARG:HH12	3:H:123:LEU:HD11	1.63	0.62
2:M:241:ARG:HD3	2:M:246:GLU:HG2	1.80	0.62
1:L:275:ILE:HD12	1:L:275:ILE:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.34	0.62
2:M:168:MET:HG3	2:M:173:GLU:HG2	1.82	0.62
1:L:275:ILE:HD12	1:L:275:ILE:N	2.15	0.61
2:M:93:SER:HB2	2:M:181:SER:OG	2.00	0.61
2:M:75:TRP:CD1	2:M:80:TRP:HA	2.35	0.61
3:H:156:CYS:HB3	3:H:206:ASN:O	2.00	0.61
2:M:242:GLY:CA	3:H:117:ARG:HD2	2.30	0.61
3:H:148:PRO:O	3:H:151:LEU:HB2	2.00	0.61
2:M:164:ARG:HH12	2:M:173:GLU:HG3	1.66	0.61
2:M:199:ASN:ND2	2:M:201:PHE:H	1.99	0.60
3:H:70:ARG:NH1	3:H:123:LEU:HD11	2.17	0.60
3:H:37:ARG:NH2	3:H:60:LYS:O	2.35	0.60
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.85	0.59
1:L:241:VAL:HG21	5:L:855:BPH:HAC2	1.83	0.59
1:L:246:LEU:O	1:L:249:ILE:HG22	2.02	0.59
1:L:275:ILE:H	1:L:275:ILE:CD1	2.15	0.58
2:M:113:GLY:O	2:M:117:ILE:HD13	2.03	0.58
1:L:60:ASN:O	1:L:64:ILE:HG13	2.03	0.58
2:M:164:ARG:NH1	2:M:173:GLU:HG3	2.19	0.58
11:M:1152:HOH:O	3:H:118:ARG:HD3	2.03	0.58
1:L:30:TYR:O	1:L:103:ARG:NH1	2.37	0.57
3:H:130:LYS:HE3	3:H:170:ASP:OD2	2.04	0.57
4:L:850:BCL:CBB	4:L:850:BCL:HHC	2.34	0.57
2:M:101:TYR:O	2:M:104:SER:HB3	2.05	0.57
1:L:181:PHE:HB3	5:L:854:BPH:CBB	2.35	0.57
1:L:208:THR:HB	1:L:209:PRO:HD2	1.86	0.56
2:M:204:LEU:CB	2:M:279:THR:HG21	2.36	0.56
2:M:199:ASN:HD22	2:M:200:PRO:N	2.04	0.55
2:M:136:ARG:NE	2:M:136:ARG:HA	2.21	0.55
1:L:52:SER:HB2	1:L:85:LEU:HD13	1.89	0.55
1:L:181:PHE:HB3	5:L:854:BPH:HBB2	1.88	0.55
1:L:103:ARG:HG3	11:L:1016:HOH:O	2.07	0.55
5:L:854:BPH:H4C2	5:M:852:BPH:H141	1.88	0.55
3:H:202:ARG:HG2	3:H:203:VAL:N	2.21	0.55
4:L:850:BCL:HHC	4:L:850:BCL:HBB3	1.90	0.54
3:H:133:PRO:HG3	3:H:168:TRP:CZ2	2.42	0.54
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.08	0.53
3:H:103:ASP:HB3	3:H:106:LYS:HB2	1.91	0.53
1:L:22:PHE:O	1:L:31:VAL:O	2.27	0.53
2:M:22:GLU:HB3	2:M:139:ALA:O	2.08	0.53
1:L:246:LEU:C	1:L:246:LEU:HD13	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:54:VAL:HG23	1:L:55:LEU:N	2.25	0.52
2:M:204:LEU:HB3	2:M:279:THR:HG21	1.91	0.52
3:H:201:ASN:HD22	3:H:201:ASN:N	2.03	0.52
3:H:45:GLU:CG	3:H:94:GLU:HG2	2.37	0.52
2:M:152:SER:O	2:M:155:TRP:HB3	2.10	0.52
3:H:135:LYS:HE2	3:H:166:ASP:OD2	2.10	0.52
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.45	0.52
1:L:174:MET:HB3	4:L:850:BCL:O1D	2.09	0.52
3:H:221:SER:HB3	3:H:224:GLU:HG2	1.92	0.52
2:M:53:GLY:O	2:M:57:VAL:HG23	2.11	0.51
2:M:1:ALA:HB3	3:H:197:LYS:NZ	2.25	0.51
2:M:163:ILE:O	2:M:167:LEU:HG	2.10	0.51
3:H:42:LEU:N	3:H:53:GLN:OE1	2.43	0.51
1:L:182:THR:OG1	4:L:850:BCL:H42	2.10	0.51
5:L:855:BPH:HHC	5:L:855:BPH:HBB3	1.92	0.50
3:H:133:PRO:HG3	3:H:168:TRP:CE2	2.46	0.50
3:H:233:ILE:O	3:H:237:VAL:HG13	2.11	0.50
2:M:134:TYR:CE2	2:M:144:LYS:HG2	2.47	0.50
2:M:72:ILE:HD12	2:M:72:ILE:C	2.36	0.50
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.47	0.50
3:H:207:ALA:HB1	3:H:237:VAL:O	2.11	0.50
2:M:130:TRP:HD1	2:M:150:PHE:CD2	2.30	0.49
4:L:853:BCL:HAA2	4:L:853:BCL:HBD	1.95	0.48
11:M:1055:HOH:O	3:H:34:GLU:HG3	2.13	0.48
1:L:103:ARG:NH2	2:M:255:THR:O	2.46	0.48
3:H:201:ASN:H	3:H:201:ASN:ND2	2.07	0.48
2:M:24:VAL:HG11	2:M:29:ARG:NH1	2.28	0.48
3:H:75:VAL:HA	3:H:76:PRO:C	2.38	0.48
2:M:13:ARG:O	3:H:140:PHE:HA	2.14	0.48
2:M:25:ASN:OD1	2:M:27:ALA:HB3	2.13	0.48
1:L:280:ASN:ND2	2:M:88:ASP:OD1	2.46	0.48
2:M:194:GLY:O	2:M:195:ASN:HB3	2.12	0.47
1:L:83:GLY:O	1:L:87:GLN:HG3	2.15	0.47
2:M:239:ALA:O	3:H:73:LEU:HD22	2.14	0.47
3:H:11:ASP:HB2	11:H:1139:HOH:O	2.14	0.47
3:H:70:ARG:NH1	3:H:123:LEU:CD1	2.77	0.47
4:L:851:BCL:HAA2	4:L:853:BCL:HBC1	1.96	0.47
1:L:275:ILE:N	1:L:275:ILE:CD1	2.76	0.47
2:M:199:ASN:C	2:M:199:ASN:ND2	2.71	0.47
3:H:44:ASN:ND2	3:H:48:THR:HG22	2.30	0.47
1:L:58:THR:HG21	1:L:63:LEU:CD2	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:231:ARG:HD2	2:M:6:ILE:O	2.15	0.47
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.96	0.47
2:M:97:PRO:CG	2:M:171:TRP:HB2	2.43	0.46
1:L:219:LEU:HD12	2:M:132:ARG:NH1	2.30	0.46
2:M:228:ARG:HG3	2:M:229:PHE:CE1	2.50	0.46
3:H:45:GLU:CD	3:H:94:GLU:HG2	2.40	0.46
2:M:293:ASN:OD1	2:M:295:TYR:HB3	2.16	0.46
8:M:857:U10:H222	8:M:857:U10:H201	1.66	0.46
3:H:63:THR:HA	3:H:73:LEU:O	2.16	0.46
3:H:168:TRP:CZ3	3:H:225:VAL:HG22	2.50	0.46
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.97	0.46
4:L:853:BCL:H193	5:L:855:BPH:H111	1.96	0.46
1:L:22:PHE:HA	1:L:24:PHE:HE2	1.81	0.45
3:H:34:GLU:OE2	3:H:37:ARG:NH1	2.49	0.45
2:M:300:ASN:O	2:M:301:HIS:C	2.59	0.45
4:L:851:BCL:CAA	4:L:853:BCL:HBC1	2.46	0.45
2:M:1:ALA:HB3	3:H:197:LYS:HZ3	1.80	0.45
2:M:109:LEU:HD12	2:M:109:LEU:N	2.32	0.45
3:H:175:MET:HE1	3:H:177:ARG:NH2	2.31	0.45
1:L:38:THR:HG22	1:L:99:SER:HB3	1.97	0.45
1:L:85:LEU:O	1:L:89:ILE:HG13	2.17	0.45
2:M:204:LEU:HB2	2:M:279:THR:HG21	1.98	0.45
3:H:34:GLU:O	3:H:37:ARG:HG3	2.17	0.45
3:H:199:GLN:OE1	3:H:202:ARG:HD2	2.17	0.45
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.52	0.45
3:H:132:LYS:HD2	3:H:171:ILE:CD1	2.46	0.45
2:M:28:ASN:HB2	2:M:51:TYR:CE2	2.52	0.44
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.17	0.44
11:M:1077:HOH:O	3:H:70:ARG:HD3	2.17	0.44
1:L:130:THR:HA	1:L:134:PHE:HB2	2.00	0.44
1:L:206:MET:HE3	3:H:64:PHE:CD1	2.52	0.44
2:M:101:TYR:CD1	2:M:101:TYR:N	2.85	0.44
3:H:115:VAL:HG13	3:H:231:ASP:OD2	2.18	0.44
2:M:229:PHE:HB2	2:M:244:ALA:HB2	2.00	0.44
2:M:134:TYR:CD1	2:M:134:TYR:C	2.96	0.44
1:L:170:ASN:HB3	1:L:173:HIS:CB	2.48	0.44
2:M:75:TRP:HZ3	9:M:859:SPO:O1	2.01	0.44
3:H:99:ALA:HA	3:H:100:PRO:HD3	1.85	0.44
1:L:270:PRO:HB2	1:L:271:TRP:HD1	1.83	0.43
2:M:189:PHE:O	2:M:193:HIS:HD2	2.01	0.43
2:M:162:PHE:C	2:M:165:PRO:HD2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:34:PHE:HB2	11:L:1016:HOH:O	2.18	0.43
2:M:184:ASP:O	2:M:188:ASN:HB2	2.18	0.43
1:L:60:ASN:HB3	1:L:63:LEU:HB2	2.00	0.43
2:M:11:GLN:HE21	2:M:11:GLN:HB2	1.66	0.43
3:H:173:GLU:O	3:H:174:GLN:C	2.62	0.43
8:M:857:U10:H271	8:M:857:U10:H251	1.71	0.43
3:H:165:VAL:O	3:H:166:ASP:HB2	2.17	0.43
1:L:8:LYS:HA	3:H:87:LEU:HD11	2.01	0.42
3:H:45:GLU:HG3	3:H:94:GLU:CG	2.44	0.42
4:L:851:BCL:HAA2	4:L:851:BCL:HBD	2.01	0.42
2:M:109:LEU:HA	2:M:113:GLY:HA3	2.01	0.42
1:L:227:LEU:O	1:L:231:ARG:HG3	2.19	0.42
3:H:148:PRO:HA	3:H:151:LEU:CD2	2.46	0.42
2:M:234:GLU:O	2:M:238:ILE:HG13	2.20	0.42
1:L:202:LYS:H	1:L:202:LYS:HG3	1.54	0.42
1:L:279:ILE:HG21	2:M:91:PHE:HB3	2.01	0.42
5:L:854:BPH:HBB3	5:L:854:BPH:HHC	2.02	0.42
1:L:62:GLN:NE2	1:L:151:TRP:HE1	2.18	0.42
1:L:170:ASN:HB3	1:L:173:HIS:HB3	2.02	0.42
3:H:215:GLY:O	3:H:216:ILE:C	2.61	0.42
3:H:112:ALA:HA	3:H:235:GLY:O	2.20	0.42
5:L:854:BPH:H7C2	5:M:852:BPH:H192	2.01	0.41
3:H:114:TRP:CZ2	3:H:232:LYS:HE2	2.54	0.41
3:H:44:ASN:HD22	3:H:48:THR:HG22	1.84	0.41
1:L:272:TRP:HA	1:L:275:ILE:CD1	2.30	0.41
2:M:235:LEU:HD12	2:M:235:LEU:HA	1.82	0.41
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.20	0.41
2:M:280:GLY:O	5:M:852:BPH:HED3	2.20	0.41
3:H:62:LYS:O	3:H:74:THR:HA	2.20	0.41
4:L:851:BCL:H122	5:L:855:BPH:H3A	2.03	0.41
4:L:850:BCL:HMB2	5:L:854:BPH:HMB2	2.03	0.41
2:M:148:TRP:CD2	10:M:5000:CDL:H511	2.56	0.41
2:M:98:ALA:HB1	2:M:100:GLU:OE1	2.20	0.41
2:M:199:ASN:HD22	2:M:201:PHE:H	1.68	0.41
3:H:124:ASP:OD1	3:H:124:ASP:C	2.64	0.41
2:M:242:GLY:O	2:M:246:GLU:HG3	2.20	0.41
3:H:66:LEU:N	3:H:66:LEU:HD23	2.36	0.41
1:L:233:GLY:HA3	2:M:216:PHE:CE1	2.55	0.41
5:L:854:BPH:H8	5:M:852:BPH:H191	2.03	0.41
3:H:118:ARG:HB3	3:H:120:LEU:HD23	2.02	0.41
1:L:10:ARG:NH2	1:L:25:TRP:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:132:LYS:HD2	3:H:171:ILE:HD11	2.03	0.41
4:L:850:BCL:HBB3	4:L:850:BCL:CHC	2.48	0.41
2:M:73:TRP:CE3	2:M:114:LEU:HD12	2.56	0.40
5:M:852:BPH:HBC2	5:M:852:BPH:H2C	1.95	0.40
2:M:69:THR:O	2:M:72:ILE:HG13	2.21	0.40
1:L:49:ILE:HG13	1:L:89:ILE:HD13	2.03	0.40
1:L:275:ILE:HA	1:L:276:PRO:HD3	1.96	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%)	262 (94%)	15 (5%)	2 (1%)	18	34
2	M	300/307 (98%)	286 (95%)	13 (4%)	1 (0%)	36	55
3	H	234/260 (90%)	222 (95%)	9 (4%)	3 (1%)	9	18
All	All	813/848 (96%)	770 (95%)	37 (5%)	6 (1%)	18	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	301	HIS
3	H	220	LYS
3	H	51	ALA
1	L	270	PRO
1	L	271	TRP
3	H	245	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	220/220 (100%)	210 (96%)	10 (4%)	24	49
2	M	236/240 (98%)	220 (93%)	16 (7%)	14	31
3	H	191/208 (92%)	175 (92%)	16 (8%)	10	22
All	All	647/668 (97%)	605 (94%)	42 (6%)	15	32

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	16	LEU
1	L	21	LEU
1	L	58	THR
1	L	102	LEU
1	L	129	LEU
1	L	155	ASP
1	L	185	LEU
1	L	207	ARG
1	L	235	LEU
1	L	271	TRP
2	M	9	GLN
2	M	11	GLN
2	M	75	TRP
2	M	95	GLU
2	M	136	ARG
2	M	156	LEU
2	M	191	LEU
2	M	199	ASN
2	M	204	LEU
2	M	214	LEU
2	M	215	LEU
2	M	235	LEU
2	M	247	ARG
2	M	250	LEU
2	M	285	LEU
2	M	301	HIS

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Mol	Chain	Res	Type
3	H	12	LEU
3	H	53	GLN
3	H	72	THR
3	H	79	GLU
3	H	94	GLU
3	H	115	VAL
3	H	117	ARG
3	H	118	ARG
3	H	151	LEU
3	H	177	ARG
3	H	201	ASN
3	H	202	ARG
3	H	206	ASN
3	H	225	VAL
3	H	231	ASP
3	H	237	VAL

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

Mol	Chain	Res	Type
1	L	62	GLN
1	L	159	ASN
1	L	264	GLN
2	M	77	GLN
2	M	193	HIS
2	M	199	ASN
2	M	299	GLN
3	H	32	GLN
3	H	44	ASN
3	H	98	HIS
3	H	201	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	BPH	L	855	-	59,70,70	1.88	11 (18%)	59,101,101	2.51	18 (30%)
10	CDL	M	5000	-	80,80,99	0.73	1 (1%)	86,92,111	0.95	6 (6%)
4	BCL	L	851	1	69,74,74	1.42	9 (13%)	79,115,115	1.63	16 (20%)
8	U10	M	857	-	48,48,63	2.49	14 (29%)	60,61,79	2.11	20 (33%)
9	SPO	M	859	-	41,41,41	3.32	24 (58%)	47,50,50	2.76	15 (31%)
5	BPH	L	854	-	59,70,70	1.89	13 (22%)	59,101,101	2.44	16 (27%)
5	BPH	M	852	-	59,70,70	1.96	14 (23%)	59,101,101	3.25	24 (40%)
4	BCL	L	850	2	69,74,74	2.27	16 (23%)	79,115,115	4.68	26 (32%)
4	BCL	L	853	1	69,74,74	1.48	11 (15%)	79,115,115	1.94	23 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BPH	L	855	-	-	8/37/105/105	0/5/6/6
10	CDL	M	5000	-	-	33/91/91/110	-
4	BCL	L	851	1	-	5/41/137/137	-
8	U10	M	857	-	-	15/45/69/87	0/1/1/1
9	SPO	M	859	-	-	12/47/47/47	-
5	BPH	L	854	-	-	7/37/105/105	0/5/6/6
5	BPH	M	852	-	-	9/37/105/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	L	850	2	-	7/41/137/137	-
4	BCL	L	853	1	-	8/41/137/137	-

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	857	U10	C6-C1	10.46	1.54	1.35
4	L	850	BCL	C1B-NB	-10.32	1.24	1.37
9	M	859	SPO	C15-C16	9.17	1.58	1.34
4	L	850	BCL	C3B-C4B	8.54	1.58	1.41
5	L	855	BPH	C3A-C2A	-8.38	1.47	1.54
9	M	859	SPO	C10-C11	7.13	1.53	1.34
5	L	854	BPH	C3A-C2A	-7.00	1.48	1.54
9	M	859	SPO	C6-C5	6.79	1.50	1.32
5	M	852	BPH	C3B-C2B	5.71	1.49	1.39
9	M	859	SPO	C21-C20	5.39	1.51	1.36
5	L	854	BPH	C3D-C2D	5.15	1.48	1.39
5	L	855	BPH	C3D-C2D	5.11	1.48	1.39
8	M	857	U10	C4-C3	5.00	1.54	1.36
9	M	859	SPO	C26-C25	4.89	1.47	1.34
8	M	857	U10	C7-C8	-4.78	1.43	1.50
9	M	859	SPO	C13-C12	4.69	1.60	1.50
5	M	852	BPH	C3D-CAD	-4.60	1.39	1.47
4	L	850	BCL	C3D-C2D	4.59	1.51	1.39
4	L	853	BCL	C2-C3	4.44	1.43	1.33
4	L	850	BCL	C3B-CAB	4.42	1.60	1.46
5	M	852	BPH	C2-C3	4.35	1.43	1.33
4	L	850	BCL	C3B-C2B	4.31	1.57	1.42
4	L	851	BCL	C3D-C2D	4.25	1.50	1.39
9	M	859	SPO	O1-CM1	4.11	1.56	1.43
5	L	855	BPH	C3B-C2B	4.08	1.46	1.39
5	L	854	BPH	C3B-C4B	4.06	1.48	1.41
4	L	850	BCL	C2-C3	4.04	1.42	1.33
9	M	859	SPO	C15-C14	3.99	1.55	1.43
5	M	852	BPH	CMB-C2B	3.85	1.59	1.51
8	M	857	U10	C6-C5	3.80	1.57	1.46
5	L	854	BPH	C3B-C2B	3.79	1.46	1.39
5	M	852	BPH	CHA-CBD	3.78	1.56	1.51
5	M	852	BPH	O2A-CGA	-3.77	1.22	1.33
8	M	857	U10	C7-C6	3.77	1.58	1.51
4	L	853	BCL	C3D-C2D	3.74	1.49	1.39
5	M	852	BPH	C3B-C4B	3.71	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	855	BPH	C3B-C4B	3.70	1.47	1.41
9	M	859	SPO	C35-C33	3.63	1.58	1.51
4	L	850	BCL	C4B-NB	-3.62	1.33	1.37
4	L	853	BCL	CMB-C2B	3.52	1.58	1.50
5	L	855	BPH	CMB-C2B	3.50	1.58	1.51
4	L	850	BCL	CHC-C4B	3.49	1.47	1.39
5	M	852	BPH	C2C-C3C	-3.43	1.51	1.54
9	M	859	SPO	C4-C5	-3.43	1.45	1.50
9	M	859	SPO	C32-C33	3.42	1.40	1.33
4	L	851	BCL	CMB-C2B	3.42	1.57	1.50
5	L	854	BPH	C2-C3	3.41	1.40	1.33
9	M	859	SPO	C10-C9	3.32	1.53	1.43
5	L	854	BPH	CMB-C2B	3.28	1.58	1.51
4	L	853	BCL	C3C-C4C	-3.27	1.47	1.51
4	L	853	BCL	C3B-CAB	3.26	1.56	1.46
8	M	857	U10	C33-C34	3.25	1.40	1.33
9	M	859	SPO	C31-C32	-3.21	1.40	1.50
5	M	852	BPH	C3D-C2D	3.21	1.45	1.39
9	M	859	SPO	C11-C12	-3.20	1.39	1.46
9	M	859	SPO	C37-C38	3.18	1.42	1.32
4	L	851	BCL	C1D-C2D	-3.17	1.39	1.45
5	M	852	BPH	C3B-CAB	3.16	1.57	1.49
4	L	851	BCL	C3B-CAB	3.11	1.56	1.46
4	L	851	BCL	C2-C3	3.10	1.40	1.33
9	M	859	SPO	C8-C7	3.09	1.57	1.50
9	M	859	SPO	O1-C1	3.09	1.58	1.41
4	L	851	BCL	CBB-CAB	3.07	1.56	1.50
8	M	857	U10	C28-C29	3.06	1.40	1.33
5	L	855	BPH	C3D-CAD	-3.05	1.41	1.47
8	M	857	U10	C23-C24	2.95	1.39	1.33
8	M	857	U10	C18-C19	2.90	1.39	1.33
8	M	857	U10	C13-C14	2.89	1.39	1.33
5	L	854	BPH	C3D-CAD	-2.79	1.42	1.47
4	L	850	BCL	CMB-C2B	2.78	1.56	1.50
4	L	850	BCL	CBB-CAB	2.77	1.55	1.50
5	M	852	BPH	C1B-C2B	2.72	1.42	1.39
4	L	851	BCL	C3B-C4B	2.72	1.46	1.41
4	L	851	BCL	CMD-C2D	2.69	1.56	1.50
5	L	854	BPH	CMD-C2D	2.66	1.56	1.51
8	M	857	U10	O4-C4	2.64	1.43	1.36
5	M	852	BPH	O2A-C1	-2.63	1.39	1.46
5	L	855	BPH	C2-C3	2.62	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	859	SPO	C29-C28	2.61	1.57	1.50
4	L	853	BCL	C1D-C2D	-2.61	1.40	1.45
9	M	859	SPO	C24-C23	2.59	1.56	1.50
5	L	854	BPH	C2C-C3C	-2.59	1.52	1.54
4	L	853	BCL	CMD-C2D	2.58	1.56	1.50
4	L	853	BCL	CBB-CAB	2.53	1.55	1.50
9	M	859	SPO	C14-C12	2.52	1.41	1.35
10	M	5000	CDL	CB3-CB4	2.51	1.58	1.50
8	M	857	U10	C38-C39	2.50	1.39	1.32
5	L	854	BPH	C4D-CHA	2.49	1.43	1.39
4	L	850	BCL	C1D-C2D	-2.49	1.40	1.45
5	L	855	BPH	CMD-C2D	2.46	1.56	1.51
4	L	853	BCL	C3B-C4B	2.45	1.46	1.41
5	L	855	BPH	O2A-CGA	-2.41	1.26	1.33
5	M	852	BPH	CMD-C2D	2.38	1.56	1.51
4	L	850	BCL	C3A-C2A	-2.36	1.48	1.54
8	M	857	U10	C36-C34	2.32	1.56	1.51
4	L	850	BCL	CMD-C2D	2.31	1.55	1.50
4	L	853	BCL	MG-NB	2.29	2.10	2.05
5	M	852	BPH	C4-C3	2.28	1.56	1.50
9	M	859	SPO	C25-C23	-2.28	1.41	1.46
4	L	853	BCL	C3A-C2A	-2.23	1.48	1.54
4	L	850	BCL	O2D-CGD	-2.21	1.27	1.33
4	L	850	BCL	OBD-CAD	2.13	1.26	1.22
9	M	859	SPO	C6-C7	-2.12	1.41	1.46
5	L	855	BPH	C4-C3	2.10	1.55	1.50
4	L	850	BCL	MG-NB	2.08	2.09	2.05
9	M	859	SPO	C19-C17	2.08	1.40	1.35
4	L	851	BCL	O2A-CGA	-2.07	1.27	1.33
5	L	854	BPH	C4A-C3A	-2.06	1.47	1.51
8	M	857	U10	O3-C3	2.06	1.41	1.36
5	L	854	BPH	C5-C3	2.04	1.55	1.51
5	L	854	BPH	O2D-CGD	-2.03	1.28	1.33
9	M	859	SPO	C18-C17	2.03	1.54	1.50
5	L	855	BPH	OBD-CAD	2.02	1.24	1.22

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	850	BCL	OBB-CAB-C3B	24.05	162.96	120.43
4	L	850	BCL	OBB-CAB-CBB	-18.59	78.14	119.77
4	L	850	BCL	CBB-CAB-C3B	-16.88	84.83	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	850	BCL	C3B-C4B-NB	12.63	126.43	109.76
5	M	852	BPH	C4D-CHA-CBD	-12.47	102.47	108.45
9	M	859	SPO	C25-C23-C22	-10.92	101.83	119.01
5	L	855	BPH	C4D-CHA-CBD	-9.23	104.03	108.45
5	L	854	BPH	C4D-CHA-CBD	-9.05	104.12	108.45
4	L	850	BCL	CHC-C4B-NB	-8.10	111.90	124.05
5	M	852	BPH	CBA-CAA-C2A	7.45	135.73	113.78
4	L	850	BCL	CMB-C2B-C1B	-6.74	115.16	125.42
5	L	854	BPH	C1-O2A-CGA	6.46	132.29	116.65
8	M	857	U10	C7-C6-C5	6.35	125.89	118.52
4	L	853	BCL	CAA-C2A-C1A	-6.30	91.32	111.97
5	L	854	BPH	O2D-CGD-CBD	6.14	117.69	110.95
5	L	855	BPH	C1-O2A-CGA	5.93	131.01	116.65
5	M	852	BPH	C1-O2A-CGA	5.84	130.79	116.65
5	M	852	BPH	C4-C3-C5	5.65	125.03	115.23
5	L	855	BPH	C3D-C4D-ND	5.61	114.89	107.71
5	L	855	BPH	O2D-CGD-CBD	5.42	116.90	110.95
9	M	859	SPO	C20-C21-C22	-5.41	112.44	123.52
5	L	854	BPH	C3D-C4D-ND	5.37	114.58	107.71
4	L	850	BCL	CAB-C3B-C2B	-5.36	116.61	127.74
5	L	855	BPH	C4-C3-C5	5.34	124.50	115.23
5	M	852	BPH	C3D-C4D-ND	5.28	114.47	107.71
5	M	852	BPH	C1-C2-C3	5.23	134.77	126.20
9	M	859	SPO	C18-C17-C19	-5.20	114.39	122.82
5	M	852	BPH	CMB-C2B-C3B	5.11	134.89	124.68
9	M	859	SPO	C26-C27-C28	-5.09	120.54	127.69
5	M	852	BPH	CAA-CBA-CGA	5.06	127.57	113.21
5	M	852	BPH	C5-C3-C2	-4.96	110.02	121.17
8	M	857	U10	C7-C6-C1	-4.89	116.50	124.89
5	M	852	BPH	C7-C6-C5	-4.85	100.34	113.26
5	M	852	BPH	C6-C5-C3	4.79	125.14	113.47
4	L	853	BCL	CMB-C2B-C1B	-4.68	118.29	125.42
5	L	854	BPH	CMB-C2B-C3B	4.67	134.01	124.68
4	L	851	BCL	CMB-C2B-C1B	-4.63	118.37	125.42
4	L	853	BCL	CHC-C4B-NB	-4.62	117.12	124.05
5	L	854	BPH	C2B-C1B-NB	4.61	112.76	109.43
8	M	857	U10	C15-C14-C16	4.60	123.20	115.23
4	L	850	BCL	CAA-C2A-C1A	-4.55	97.06	111.97
5	L	855	BPH	CMB-C2B-C3B	4.47	133.62	124.68
5	L	855	BPH	O1D-CGD-CBD	-4.35	118.13	124.72
5	L	854	BPH	O1D-CGD-CBD	-4.34	118.14	124.72
4	L	851	BCL	CHC-C4B-NB	-4.33	117.55	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	850	BCL	C3B-C2B-C1B	4.26	120.01	106.40
8	M	857	U10	C15-C14-C13	-4.22	112.80	123.63
9	M	859	SPO	C4-C5-C6	-4.17	119.05	124.91
4	L	850	BCL	C4A-NA-C1A	4.17	108.58	106.68
8	M	857	U10	C10-C9-C8	-4.15	112.98	123.63
5	L	855	BPH	C6-C5-C3	4.01	123.22	113.47
9	M	859	SPO	C11-C12-C14	-3.93	112.82	119.01
4	L	853	BCL	CED-O2D-CGD	3.93	124.83	115.92
9	M	859	SPO	C15-C14-C12	-3.92	121.78	127.28
4	L	851	BCL	CED-O2D-CGD	3.90	124.75	115.92
9	M	859	SPO	C24-C23-C22	-3.88	116.53	122.82
5	L	855	BPH	C2B-C1B-NB	3.84	112.21	109.43
5	M	852	BPH	C4D-ND-C1D	-3.84	104.27	108.87
4	L	850	BCL	C4D-CHA-C1A	3.78	125.76	121.24
4	L	853	BCL	C4D-CHA-C1A	3.75	125.72	121.24
5	M	852	BPH	C1A-C2A-C3A	-3.70	99.31	102.84
5	L	855	BPH	C5-C3-C2	-3.66	112.96	121.17
10	M	5000	CDL	OB8-CB6-CB4	3.65	118.92	108.40
5	M	852	BPH	O2D-CGD-CBD	3.65	114.96	110.95
4	L	853	BCL	C4A-NA-C1A	3.64	108.34	106.68
4	L	850	BCL	CED-O2D-CGD	3.63	124.14	115.92
9	M	859	SPO	C8-C7-C9	3.58	128.62	122.82
4	L	851	BCL	C2A-C3A-C4A	3.58	107.65	101.87
4	L	853	BCL	CBA-CAA-C2A	3.51	124.24	113.79
4	L	853	BCL	C3D-C4D-ND	3.48	115.64	109.99
4	L	851	BCL	C4D-CHA-C1A	3.45	125.36	121.24
5	M	852	BPH	C2B-C1B-NB	3.43	111.91	109.43
5	M	852	BPH	CAA-C2A-C3A	3.43	122.26	113.00
8	M	857	U10	C35-C34-C33	-3.42	114.84	123.63
4	L	850	BCL	C3D-C4D-ND	3.40	115.51	109.99
9	M	859	SPO	C15-C16-C17	-3.36	117.15	126.36
5	L	854	BPH	C4-C3-C5	3.35	121.04	115.23
5	L	855	BPH	C4D-ND-C1D	-3.26	104.97	108.87
5	M	852	BPH	C3B-C4B-NB	3.22	112.74	108.05
5	M	852	BPH	CED-O2D-CGD	3.19	123.16	115.92
5	L	854	BPH	C4D-ND-C1D	-3.11	105.15	108.87
4	L	850	BCL	C2A-C3A-C4A	3.07	106.83	101.87
5	M	852	BPH	O1D-CGD-CBD	-3.03	120.13	124.72
8	M	857	U10	C25-C24-C23	-3.02	115.87	123.63
4	L	850	BCL	C2A-C1A-CHA	3.01	129.09	123.87
4	L	851	BCL	OBD-CAD-C3D	-2.99	121.43	128.42
4	L	851	BCL	C3D-C4D-ND	2.98	114.83	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	857	U10	C25-C24-C26	2.98	120.40	115.23
5	L	854	BPH	C4A-C3A-C2A	2.95	105.64	102.84
5	L	854	BPH	C3D-CAD-CBD	2.94	111.48	107.61
5	L	855	BPH	CED-O2D-CGD	2.94	122.58	115.92
4	L	853	BCL	C2A-C3A-C4A	2.94	106.62	101.87
4	L	853	BCL	O2A-CGA-CBA	2.90	120.66	111.83
4	L	853	BCL	CMD-C2D-C1D	2.89	129.83	124.73
4	L	850	BCL	C6-C5-C3	2.89	120.52	113.47
4	L	853	BCL	OBD-CAD-C3D	-2.88	121.69	128.42
5	M	852	BPH	C4A-C3A-C2A	2.87	105.57	102.84
8	M	857	U10	C7-C8-C9	2.87	131.77	126.83
8	M	857	U10	C11-C9-C8	2.85	127.55	121.17
5	M	852	BPH	C2D-C1D-ND	2.81	111.46	109.43
9	M	859	SPO	C16-C17-C19	2.78	123.38	119.01
4	L	853	BCL	O2D-CGD-CBD	2.77	116.08	111.23
8	M	857	U10	C20-C19-C18	-2.75	116.57	123.63
5	M	852	BPH	C3D-CAD-CBD	2.73	111.21	107.61
4	L	851	BCL	CHA-C1A-NA	-2.72	120.22	126.39
9	M	859	SPO	C18-C17-C16	2.71	122.23	118.09
8	M	857	U10	C30-C29-C31	2.70	119.92	115.23
4	L	850	BCL	OBD-CAD-C3D	-2.70	122.11	128.42
5	L	855	BPH	C4A-C3A-C2A	2.68	105.39	102.84
8	M	857	U10	O5-C5-C4	-2.68	115.35	121.03
4	L	853	BCL	CMB-C2B-C3B	2.67	134.10	125.67
4	L	850	BCL	CBA-CAA-C2A	2.65	121.68	113.79
4	L	850	BCL	O2A-CGA-CBA	2.63	119.84	111.83
4	L	851	BCL	CMB-C2B-C3B	2.62	133.94	125.67
8	M	857	U10	C4M-O4-C4	2.61	125.64	116.47
9	M	859	SPO	C13-C12-C11	2.61	122.07	118.09
4	L	853	BCL	O1D-CGD-CBD	-2.61	119.38	124.52
5	L	854	BPH	O2A-C1-C2	-2.59	98.13	108.11
4	L	850	BCL	C4D-C3D-CAD	-2.58	105.31	108.11
5	L	854	BPH	CED-O2D-CGD	2.55	121.71	115.92
4	L	851	BCL	C2A-C1A-CHA	2.55	128.29	123.87
8	M	857	U10	C35-C34-C36	2.54	119.64	115.23
4	L	850	BCL	CHC-C4B-C3B	-2.54	121.63	131.72
4	L	850	BCL	CHA-C1A-NA	-2.54	120.65	126.39
4	L	851	BCL	C4D-C3D-CAD	-2.53	105.36	108.11
5	L	855	BPH	C3D-CAD-CBD	2.50	110.89	107.61
5	M	852	BPH	CMC-C2C-C1C	-2.46	109.31	114.61
5	L	855	BPH	C3B-C4B-NB	2.46	111.63	108.05
9	M	859	SPO	C9-C10-C11	-2.46	116.07	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	857	U10	C10-C9-C11	2.44	119.47	115.23
4	L	853	BCL	C4D-C3D-CAD	-2.44	105.46	108.11
4	L	853	BCL	CMD-C2D-C3D	-2.43	122.11	127.69
4	L	850	BCL	CMD-C2D-C1D	2.37	128.91	124.73
5	L	854	BPH	C3B-C4B-NB	2.33	111.44	108.05
10	M	5000	CDL	CB4-OB6-CB5	2.31	123.33	117.80
9	M	859	SPO	C8-C7-C6	-2.31	114.56	118.09
10	M	5000	CDL	OB6-CB5-C51	2.31	116.48	111.48
10	M	5000	CDL	CB6-CB4-CB3	-2.31	106.41	111.78
4	L	851	BCL	CBC-CAC-C3C	2.29	118.28	113.41
4	L	853	BCL	CHA-C1A-NA	-2.27	121.25	126.39
4	L	851	BCL	C4A-NA-C1A	2.26	107.71	106.68
4	L	853	BCL	C2C-C3C-C4C	2.26	104.72	101.34
4	L	853	BCL	C6-C5-C3	2.24	118.94	113.47
4	L	851	BCL	CMD-C2D-C1D	2.21	128.62	124.73
4	L	853	BCL	C2A-C1A-CHA	2.20	127.68	123.87
4	L	853	BCL	C3B-C4B-NB	2.18	112.64	109.76
4	L	853	BCL	CAA-C2A-C3A	-2.16	107.17	113.00
5	M	852	BPH	C6-C7-C8	2.14	123.06	115.97
8	M	857	U10	C1M-C1-C6	-2.13	120.94	124.45
5	L	855	BPH	CMA-C3A-C2A	-2.10	106.02	114.13
5	L	855	BPH	C2D-C1D-ND	2.08	110.94	109.43
5	L	855	BPH	OBD-CAD-C3D	-2.08	124.65	127.89
8	M	857	U10	C1-C6-C5	-2.07	117.61	119.62
5	L	854	BPH	OBD-CAD-C3D	-2.05	124.70	127.89
4	L	850	BCL	CHA-C4D-ND	-2.05	128.33	132.55
4	L	851	BCL	CMA-C3A-C2A	-2.04	106.08	113.98
5	L	854	BPH	CBB-CAB-C3B	-2.04	114.23	120.34
4	L	851	BCL	C6-C5-C3	2.02	118.38	113.47
10	M	5000	CDL	C52-C51-CB5	2.02	121.09	113.69
10	M	5000	CDL	OB6-CB5-OB7	-2.02	118.99	123.70
8	M	857	U10	C21-C19-C18	2.01	125.69	121.17
8	M	857	U10	C8-C7-C6	-2.01	107.13	112.08
4	L	850	BCL	CMD-C2D-C3D	-2.01	123.08	127.69
4	L	850	BCL	CAA-C2A-C3A	-2.00	107.59	113.00

There are no chirality outliers.

All (104) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
5	L	854	BPH	C4C-C3C-CAC-CBC
5	L	854	BPH	C2C-C3C-CAC-CBC
5	L	855	BPH	C4C-C3C-CAC-CBC
8	M	857	U10	C1-C6-C7-C8
8	M	857	U10	C5-C6-C7-C8
8	M	857	U10	C19-C21-C22-C23
9	M	859	SPO	C1-C4-C5-C6
9	M	859	SPO	C4-C5-C6-C7
9	M	859	SPO	C21-C22-C23-C24
9	M	859	SPO	C36-C37-C38-C40
10	M	5000	CDL	CA3-OA5-PA1-OA2
10	M	5000	CDL	CA3-OA5-PA1-OA3
10	M	5000	CDL	CA3-OA5-PA1-OA4
9	M	859	SPO	C36-C37-C38-C39
5	M	852	BPH	C3-C5-C6-C7
8	M	857	U10	C20-C19-C21-C22
8	M	857	U10	C18-C19-C21-C22
5	L	855	BPH	C3-C5-C6-C7
5	L	854	BPH	C4-C3-C5-C6
5	L	855	BPH	C4-C3-C5-C6
5	M	852	BPH	C4-C3-C5-C6
8	M	857	U10	C15-C14-C16-C17
8	M	857	U10	C25-C24-C26-C27
5	L	854	BPH	C2-C3-C5-C6
5	L	855	BPH	C2-C3-C5-C6
5	M	852	BPH	C2-C3-C5-C6
8	M	857	U10	C13-C14-C16-C17
8	M	857	U10	C23-C24-C26-C27
9	M	859	SPO	C33-C35-C36-C37
5	L	855	BPH	C6-C7-C8-C9
9	M	859	SPO	C24-C23-C25-C26
9	M	859	SPO	C20-C21-C22-C23
8	M	857	U10	C24-C26-C27-C28
8	M	857	U10	C29-C31-C32-C33
5	M	852	BPH	C8-C10-C11-C12
10	M	5000	CDL	CB7-C71-C72-C73
4	L	850	BCL	C5-C6-C7-C8
10	M	5000	CDL	C11-CA5-OA6-CA4
10	M	5000	CDL	OA7-CA5-OA6-CA4
4	L	850	BCL	C2A-CAA-CBA-CGA
10	M	5000	CDL	C17-C18-C19-C20
10	M	5000	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
10	M	5000	CDL	C39-C40-C41-C42
10	M	5000	CDL	CA5-C11-C12-C13
10	M	5000	CDL	C36-C37-C38-C39
10	M	5000	CDL	C52-C53-C54-C55
4	L	851	BCL	C2A-CAA-CBA-CGA
10	M	5000	CDL	C11-C12-C13-C14
4	L	853	BCL	C5-C6-C7-C8
8	M	857	U10	C9-C11-C12-C13
10	M	5000	CDL	C79-C80-C81-C82
5	L	855	BPH	C2C-C3C-CAC-CBC
5	L	855	BPH	C6-C7-C8-C10
10	M	5000	CDL	CA3-CA4-CA6-OA8
10	M	5000	CDL	C54-C55-C56-C57
4	L	850	BCL	C2B-C3B-CAB-CBB
10	M	5000	CDL	C76-C77-C78-C79
10	M	5000	CDL	C21-C22-C23-C24
10	M	5000	CDL	C55-C56-C57-C58
5	M	852	BPH	C11-C10-C8-C9
10	M	5000	CDL	OA5-CA3-CA4-CA6
5	M	852	BPH	C11-C10-C8-C7
10	M	5000	CDL	C38-C39-C40-C41
10	M	5000	CDL	OA5-CA3-CA4-OA6
5	L	855	BPH	C8-C10-C11-C12
4	L	850	BCL	C4B-C3B-CAB-CBB
9	M	859	SPO	C34-C33-C35-C36
5	M	852	BPH	C2C-C3C-CAC-CBC
10	M	5000	CDL	C34-C35-C36-C37
8	M	857	U10	C12-C11-C9-C10
10	M	5000	CDL	C33-C34-C35-C36
9	M	859	SPO	C32-C33-C35-C36
4	L	853	BCL	CHA-CBD-CGD-O1D
4	L	853	BCL	CHA-CBD-CGD-O2D
10	M	5000	CDL	CB2-OB2-PB2-OB4
4	L	850	BCL	C15-C16-C17-C18
5	L	854	BPH	C11-C10-C8-C9
5	L	854	BPH	C11-C10-C8-C7
9	M	859	SPO	C18-C17-C19-C20
4	L	853	BCL	C14-C13-C15-C16
10	M	5000	CDL	C40-C41-C42-C43
9	M	859	SPO	C16-C17-C19-C20
8	M	857	U10	C5-C4-O4-C4M
4	L	850	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
8	M	857	U10	C12-C11-C9-C8
4	L	850	BCL	C4-C3-C5-C6
10	M	5000	CDL	C78-C79-C80-C81
4	L	851	BCL	C5-C6-C7-C8
5	L	854	BPH	C2A-CAA-CBA-CGA
10	M	5000	CDL	C73-C74-C75-C76
4	L	853	BCL	C2A-CAA-CBA-CGA
4	L	853	BCL	C12-C13-C15-C16
10	M	5000	CDL	C52-C51-CB5-OB6
5	M	852	BPH	C6-C7-C8-C9
10	M	5000	CDL	C52-C51-CB5-OB7
10	M	5000	CDL	CA7-C31-C32-C33
4	L	851	BCL	CAD-CBD-CGD-O2D
4	L	853	BCL	C15-C16-C17-C18
10	M	5000	CDL	C72-C71-CB7-OB8
4	L	853	BCL	CAA-CBA-CGA-O2A
5	M	852	BPH	C10-C11-C12-C13
10	M	5000	CDL	C19-C20-C21-C22

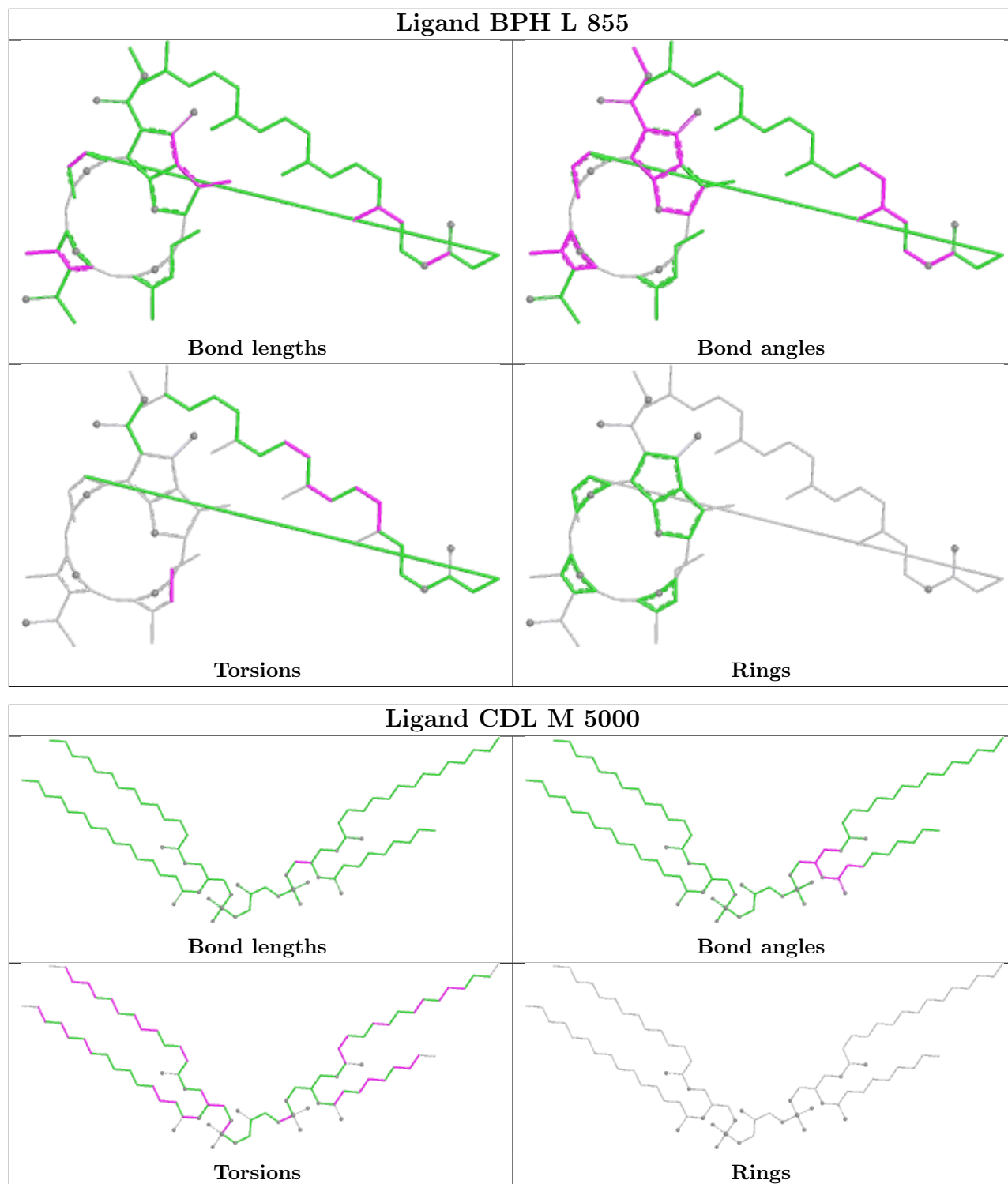
There are no ring outliers.

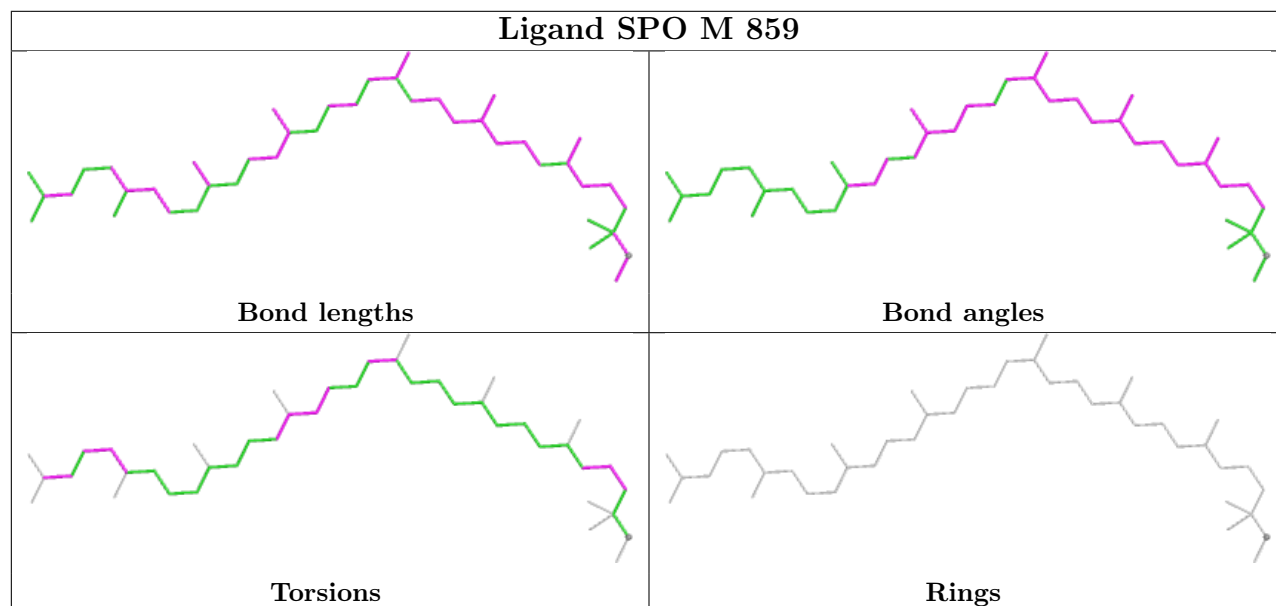
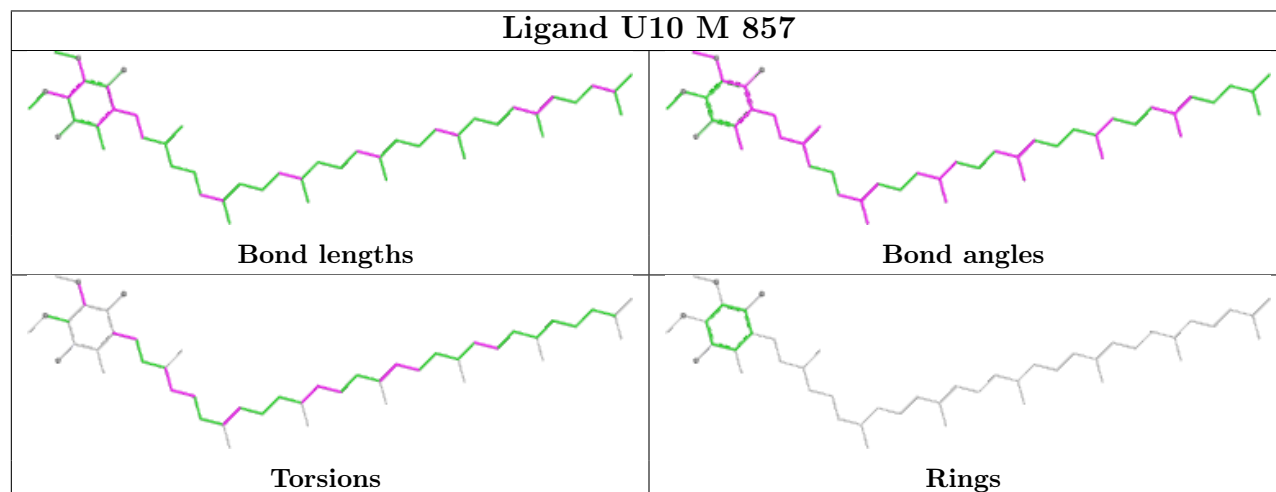
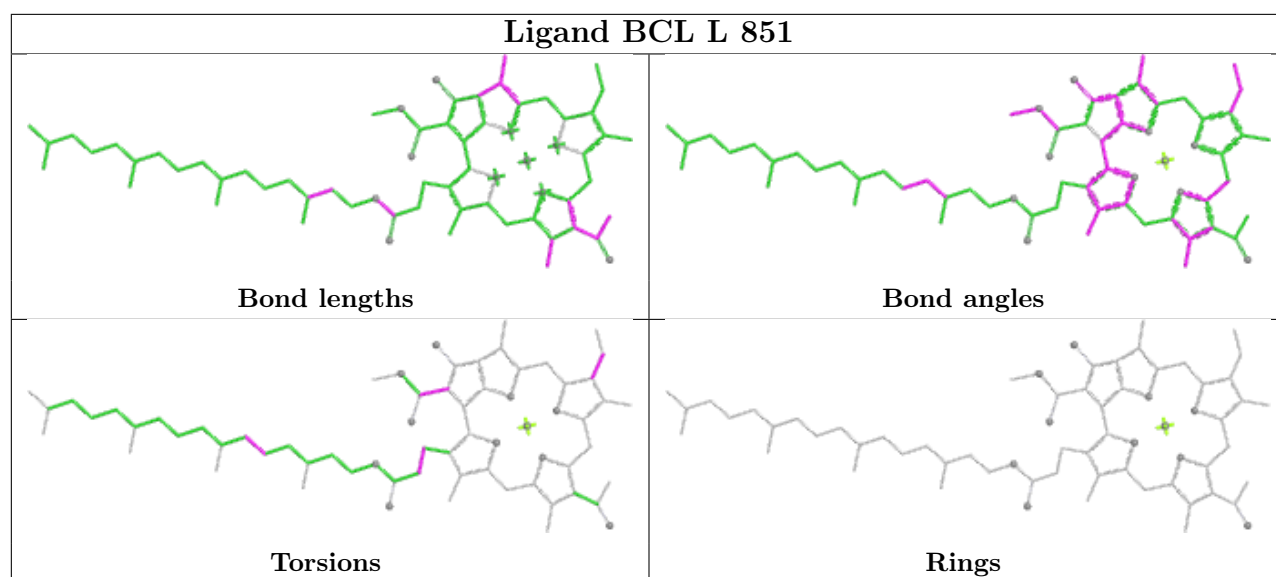
9 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	855	BPH	5	0
10	M	5000	CDL	1	0
4	L	851	BCL	4	0
8	M	857	U10	2	0
9	M	859	SPO	1	0
5	L	854	BPH	9	0
5	M	852	BPH	9	0
4	L	850	BCL	8	0
4	L	853	BCL	4	0

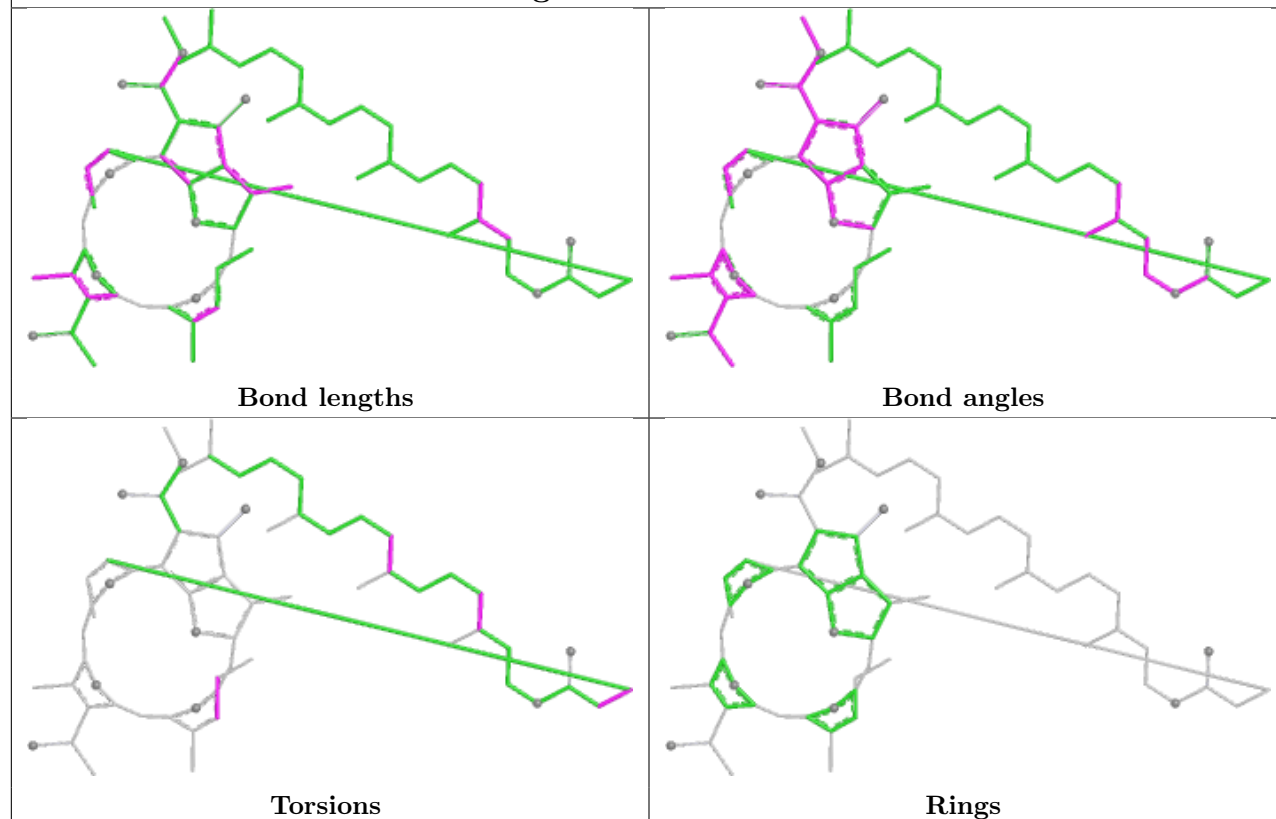
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

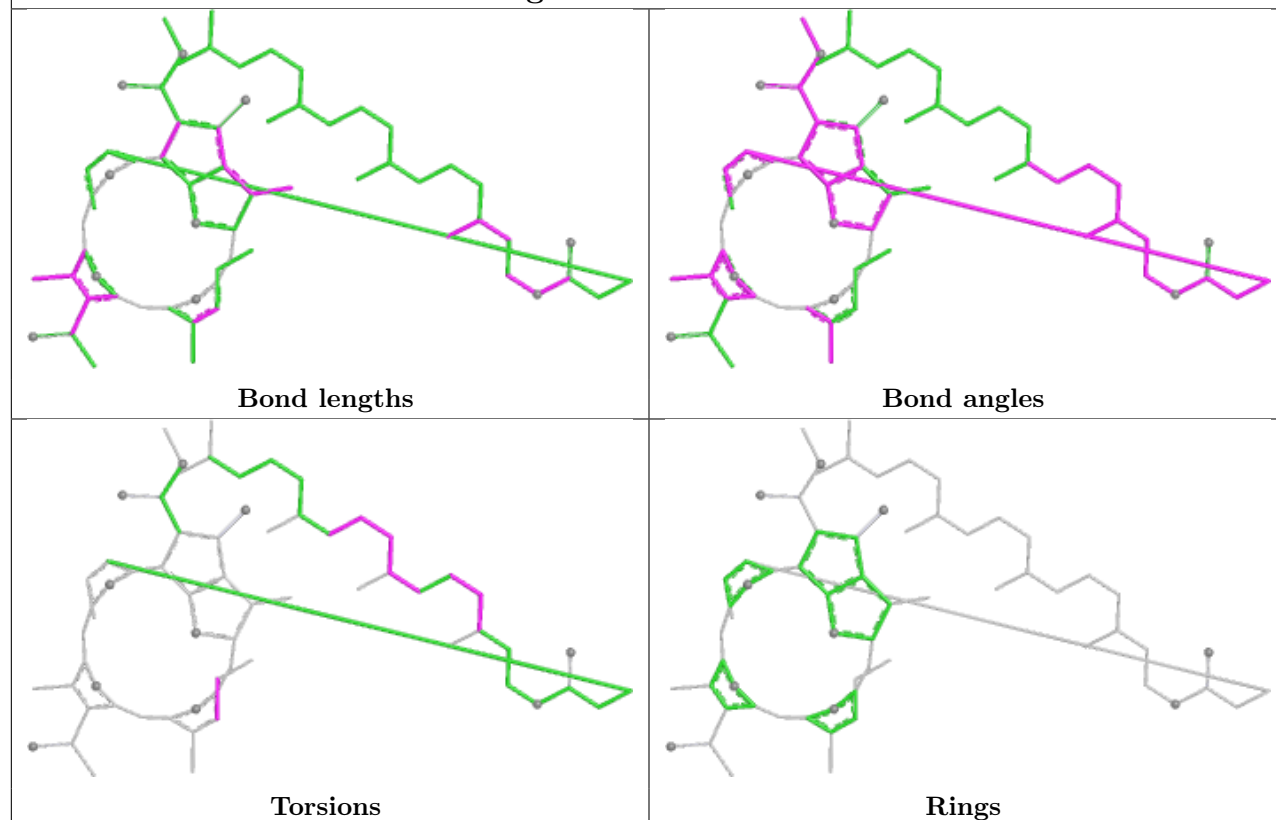


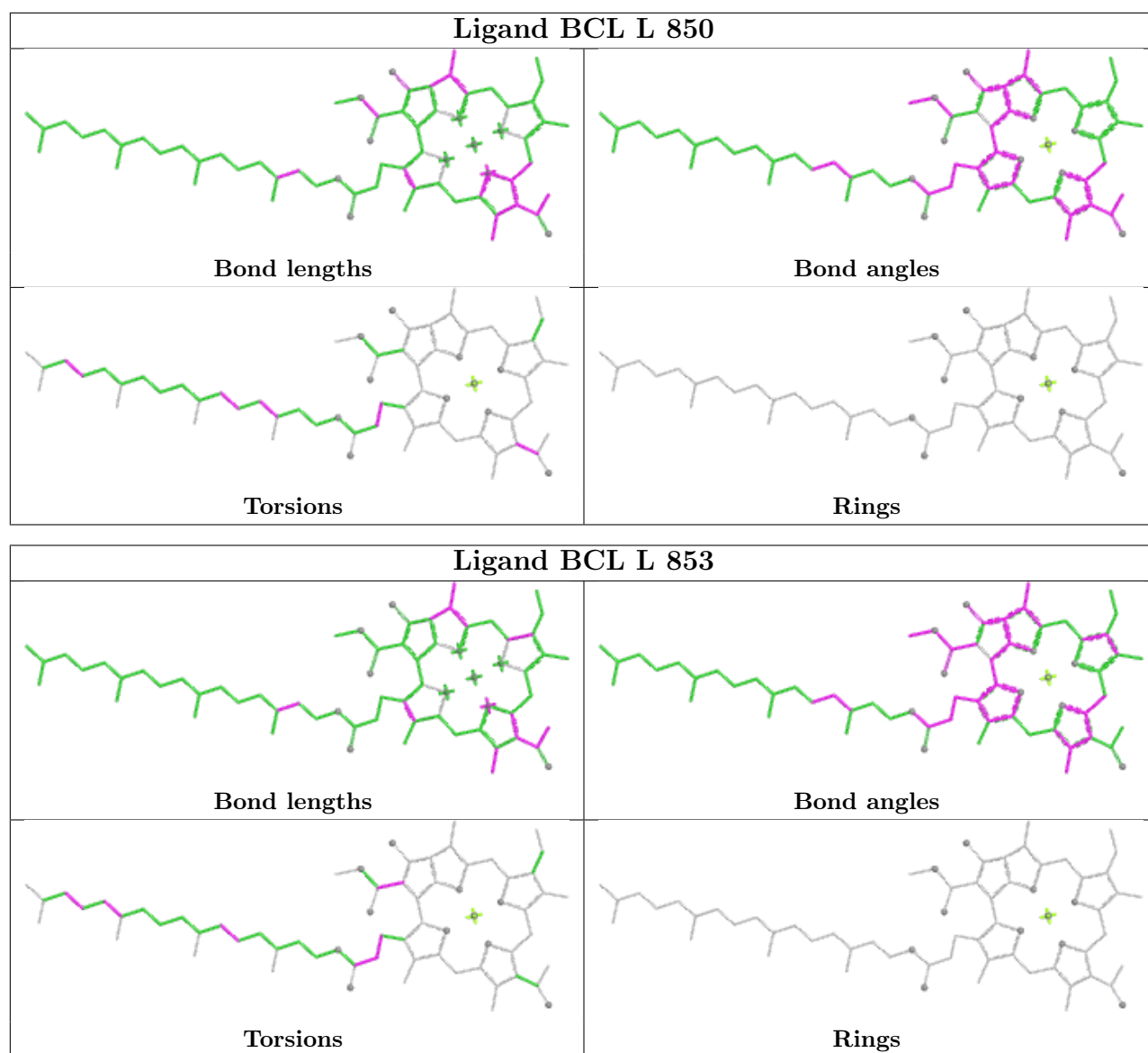


Ligand BPH L 854



Ligand BPH M 852





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	281/281 (100%)	-0.16	3 (1%) 78 75	24, 39, 73, 82	0
2	M	302/307 (98%)	-0.06	5 (1%) 69 65	23, 45, 74, 89	0
3	H	236/260 (90%)	-0.12	3 (1%) 75 71	28, 45, 65, 85	0
All	All	819/848 (96%)	-0.11	11 (1%) 75 71	23, 44, 72, 89	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	302	GLY	5.9
2	M	1	ALA	3.1
3	H	245	ALA	3.1
3	H	246	PRO	3.0
3	H	18	TYR	2.8
1	L	59	TRP	2.7
1	L	270	PRO	2.6
2	M	300	ASN	2.5
1	L	271	TRP	2.2
2	M	78	ALA	2.1
2	M	76	TYR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

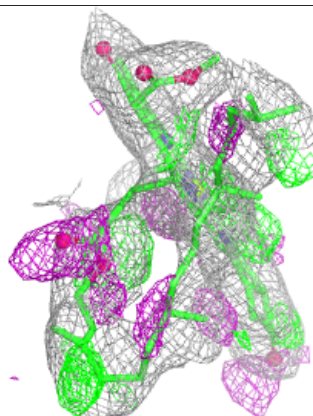
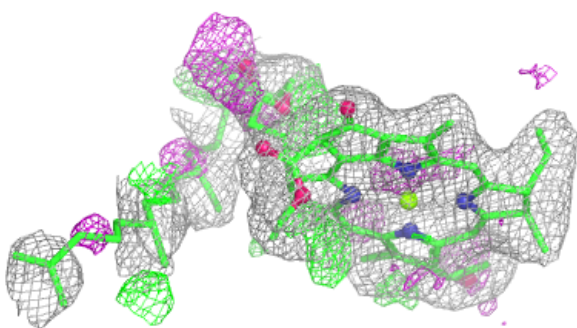
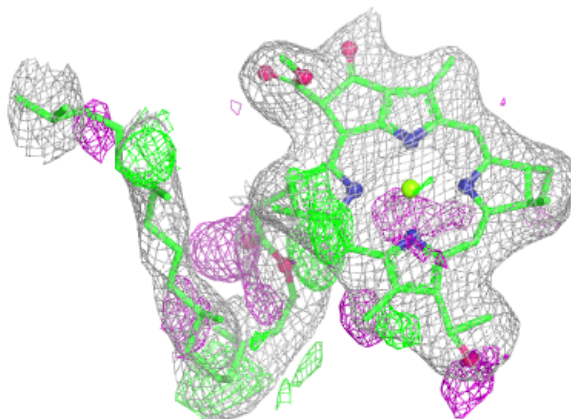
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CL	M	6000	1/1	0.77	0.16	100,100,100,100	0
4	BCL	L	850	66/66	0.89	0.16	35,46,96,98	0
10	CDL	M	5000	81/100	0.90	0.15	59,76,86,90	0
5	BPH	M	852	65/65	0.91	0.12	33,37,66,76	0
5	BPH	L	854	65/65	0.92	0.12	39,44,95,98	0
8	U10	M	857	48/63	0.92	0.13	41,51,69,70	0
4	BCL	L	853	66/66	0.92	0.11	24,30,60,66	0
9	SPO	M	859	42/42	0.93	0.14	47,62,74,75	0
5	BPH	L	855	65/65	0.93	0.10	26,35,46,53	0
4	BCL	L	851	66/66	0.95	0.09	30,37,47,60	0
6	FE	M	856	1/1	1.00	0.02	28,28,28,28	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.

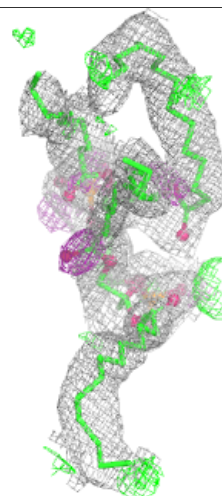
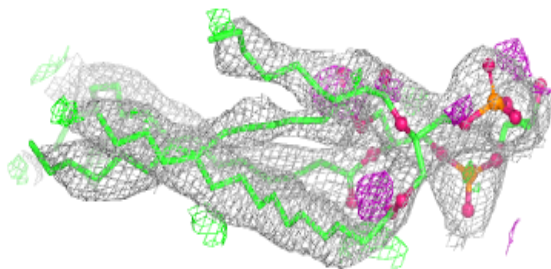
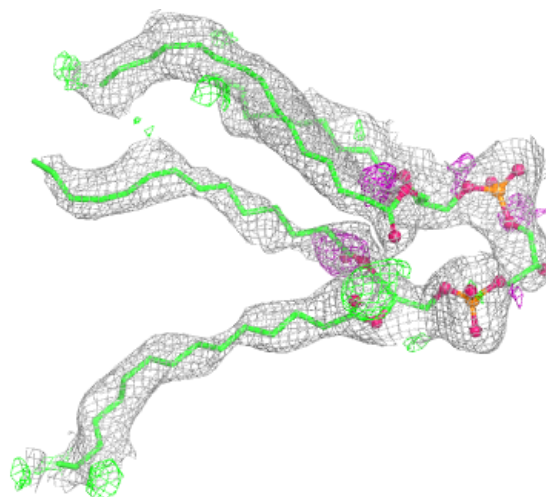
Electron density around BCL L 850:

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



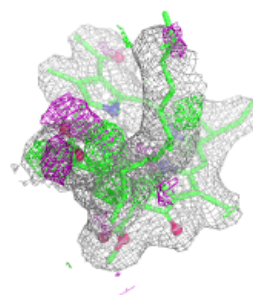
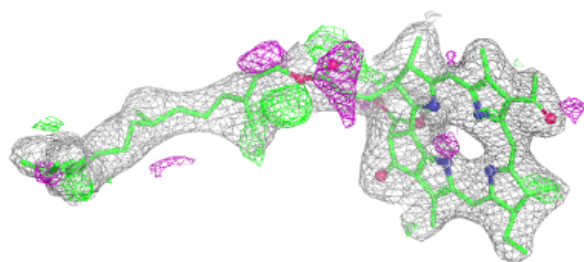
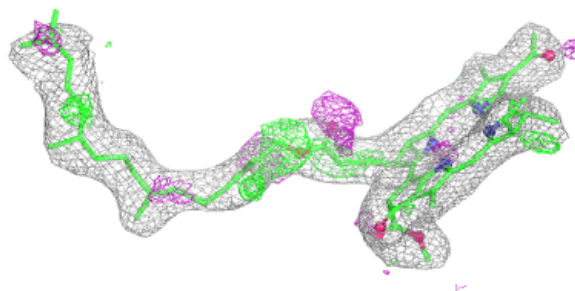
Electron density around CDL M 5000:

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

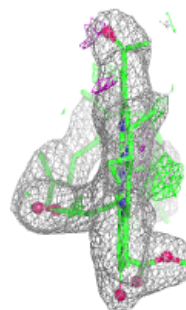
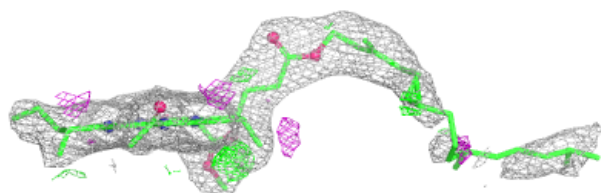
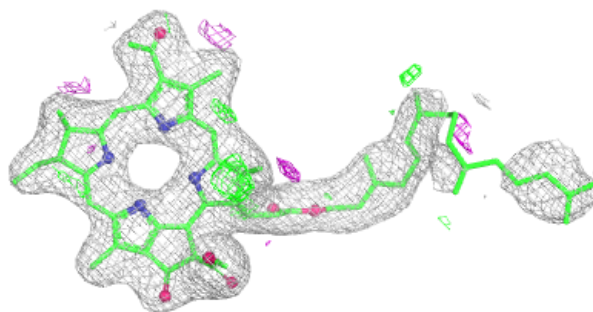


Electron density around BPH M 852:

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

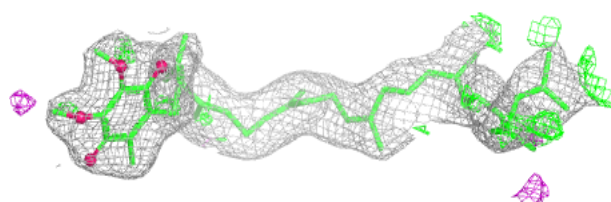
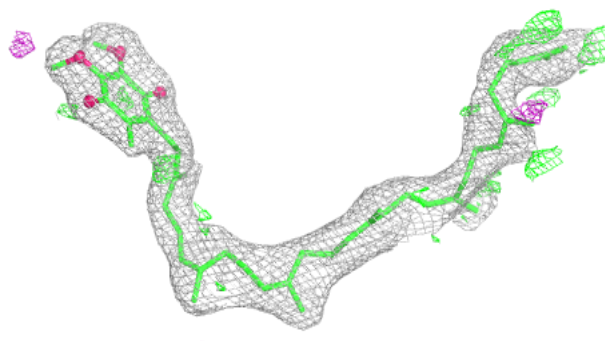
**Electron density around BPH L 854:**

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



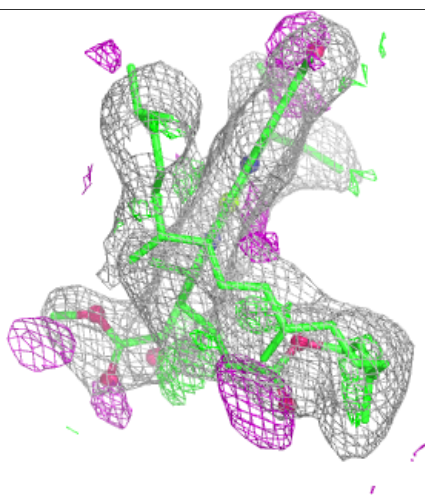
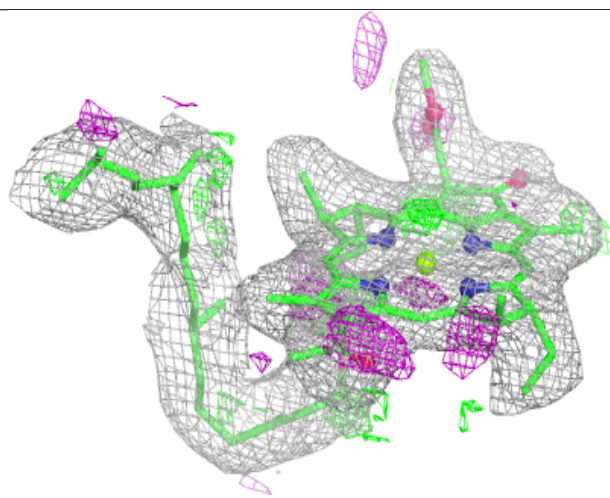
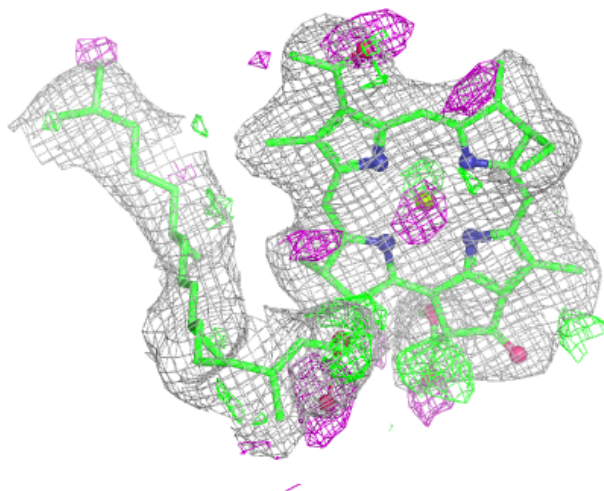
Electron density around U10 M 857:

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



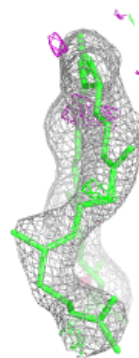
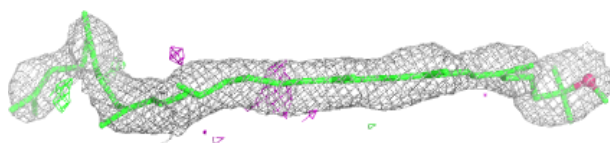
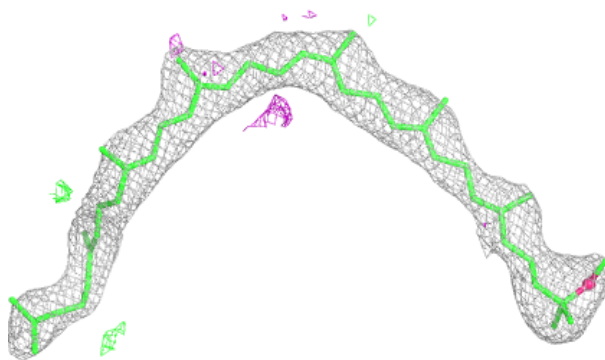
Electron density around BCL L 853:

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

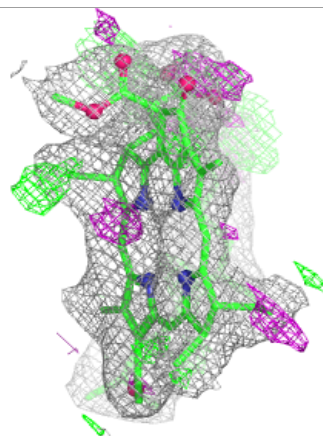
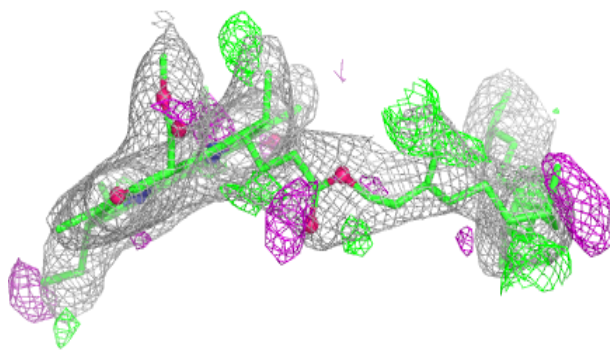
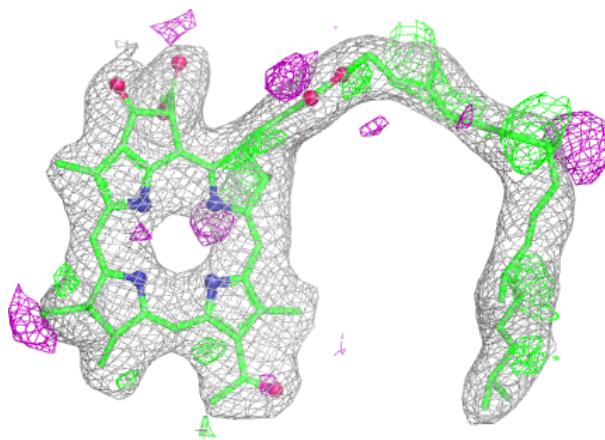


Electron density around SPO M 859:

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

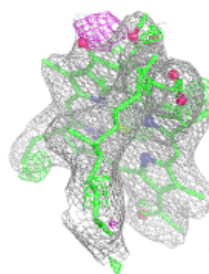
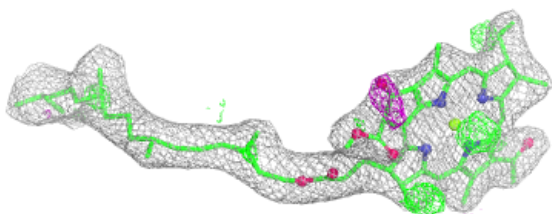
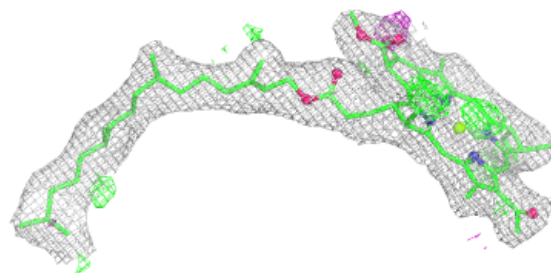
**Electron density around BPH L 855:**

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



Electron density around BCL L 851:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.