



## Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2023 – 01:45 PM EDT

PDB ID : 1RVJ  
Title : PHOTOSYNTHETIC REACTION CENTER DOUBLE MUTANT FROM RHODOBACTER SPHAEROIDES WITH ASP L213 REPLACED WITH ASN AND ARG H177 REPLACED WITH HIS  
Authors : Xu, Q.; Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher, G.  
Deposited on : 2003-12-14  
Resolution : 2.75 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](mailto: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>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (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)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

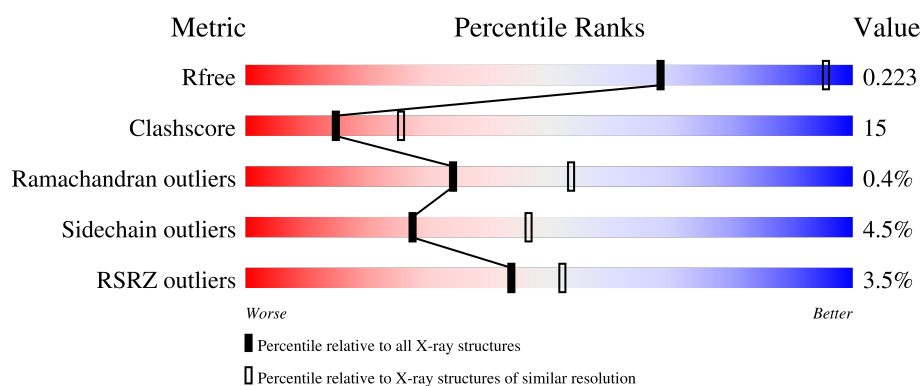
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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  $\geq 3$ , 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	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>
2	M	307	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 22%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>
3	H	260	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div>

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
10	LDA	M	863	-	-	-	X
5	BPH	L	856	X	-	-	-
5	BPH	M	855	X	-	-	-
6	U10	L	859	-	-	-	X

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 7210 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
			Total	C	N	O	S			
1	L	281	2232	1507	356	361	8	0	0	0

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
			Total	C	N	O	S			
2	M	301	2404	1605	393	396	10	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	307	ALA	-	cloning artifact	UNP P02953

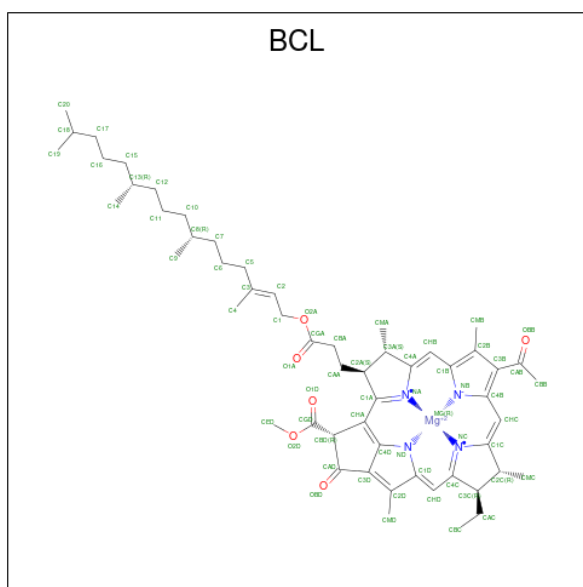
- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	238	1813	1160	310	334	9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

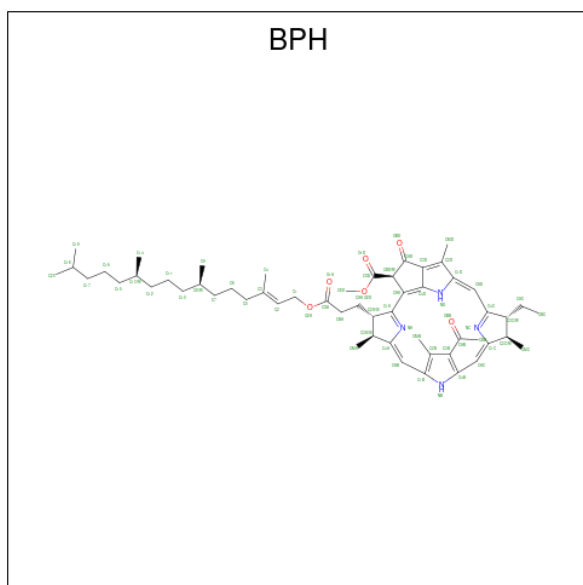
Chain	Residue	Modelled	Actual	Comment	Reference
H	8	GLN	GLY	engineered mutation	UNP P11846
H	177	HIS	ARG	engineered mutation	UNP P11846

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



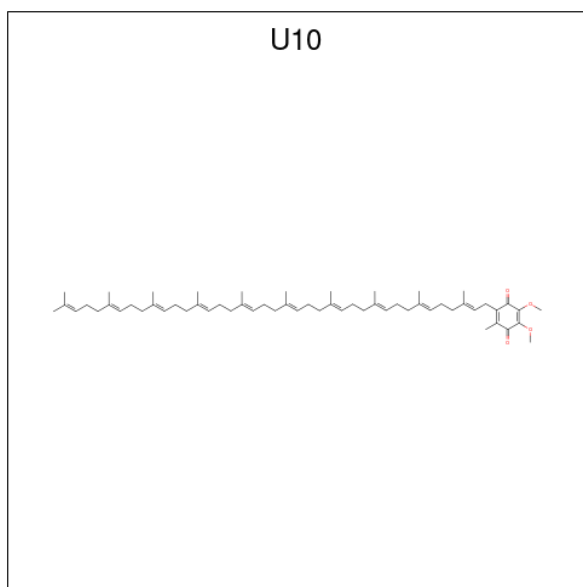
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Mg	N			O
4	L	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



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

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	L	1	44	40	4	0	0
6	M	1	48	44	4	0	0

- Molecule 7 is FE (II) ION (three-letter code: FE2) (formula: Fe).

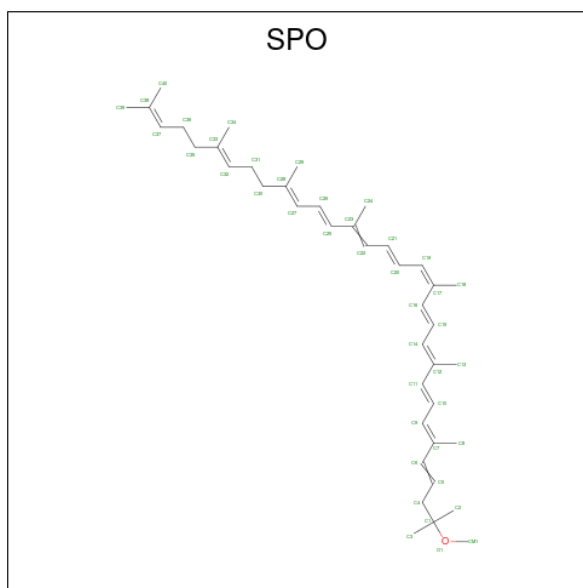
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
7	M	1	1	1	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

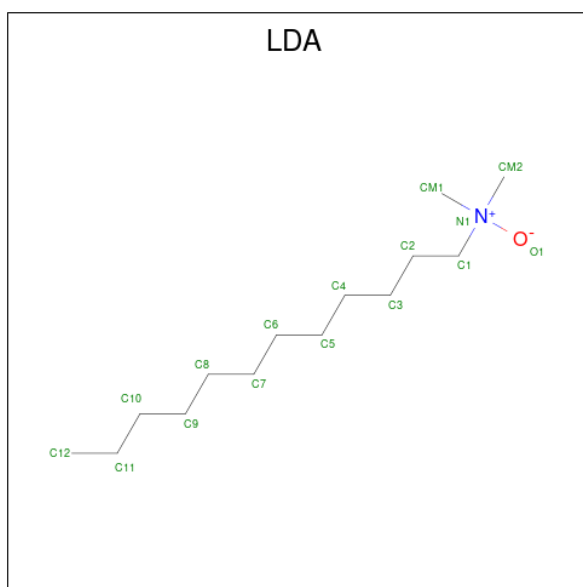
- Molecule 9 is SPHEROIDENE (three-letter code: SPO) (formula:  $C_{41}H_{60}O$ ).



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

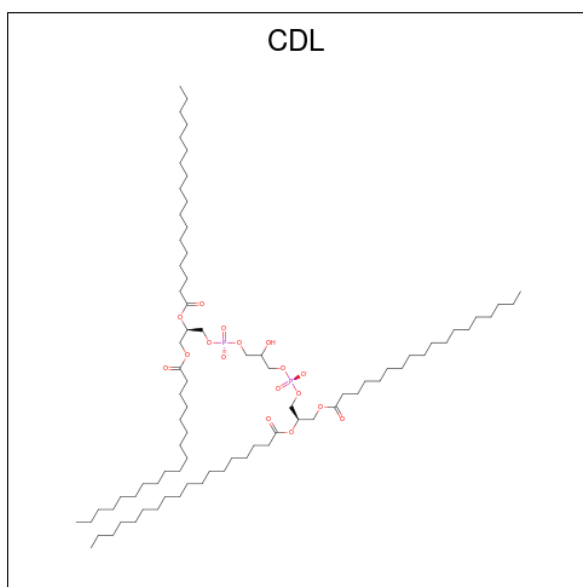
- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).





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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	O	P			
11	M	1	Total	69	50	17	2	0	0

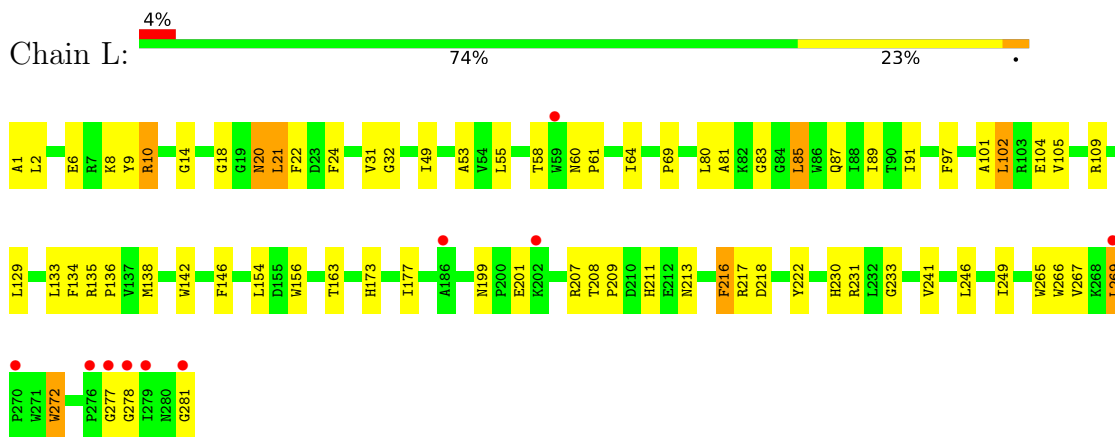
- Molecule 12 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
12	L	40	Total 40	O 40	0	0
12	M	43	Total 43	O 43	0	0
12	H	42	Total 42	O 42	0	0

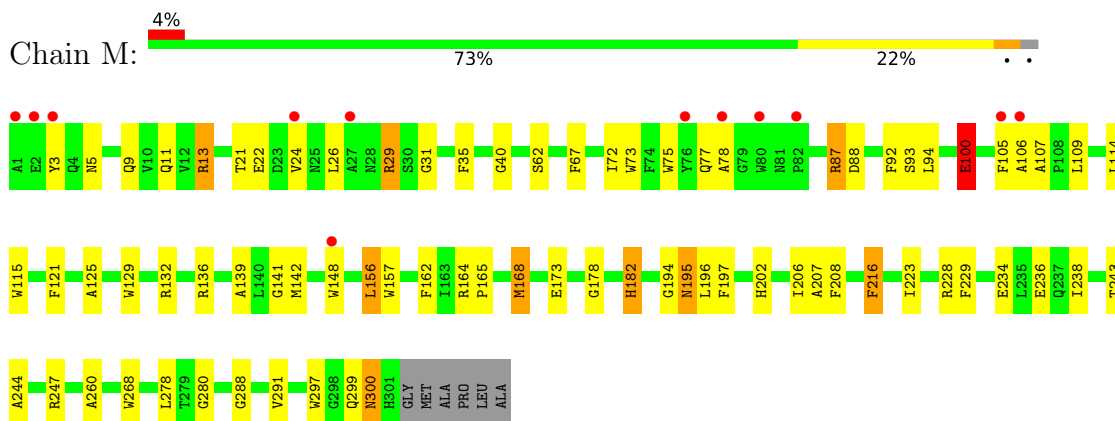
### 3 Residue-property plots

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

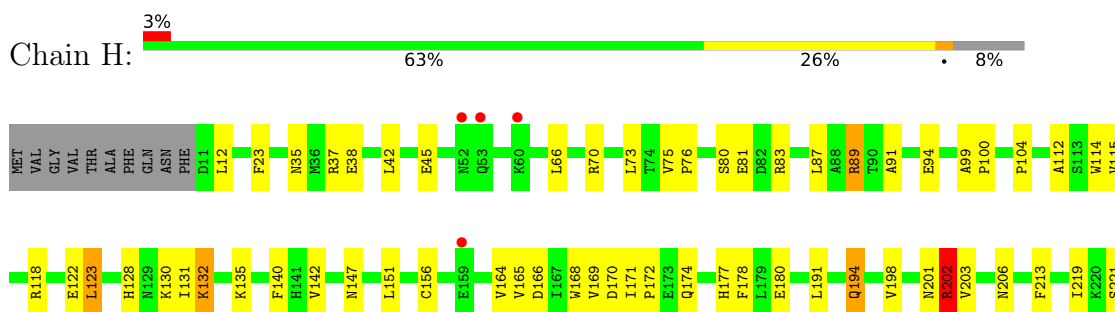
- Molecule 1: Reaction center protein L chain

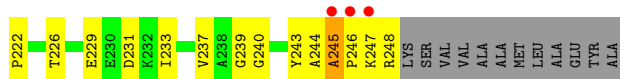


- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.24Å 138.24Å 184.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.00 – 2.75 39.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.00-2.75) 99.5 (39.00-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 2.77Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.218 , 0.237 0.204 , 0.223	Depositor DCC
$R_{free}$ test set	2685 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.7	Xtrriage
Anisotropy	0.093	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, CDL, SPO, PO4, FE2, U10, BPH, LDA

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	0.40	0/2320	0.59	0/3175
2	M	0.39	0/2496	0.57	0/3408
3	H	0.36	0/1862	0.63	0/2535
All	All	0.39	0/6678	0.60	0/9118

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2189	57	0
2	M	2404	0	2318	95	0
3	H	1813	0	1812	65	0
4	L	117	0	115	12	0
4	M	132	0	147	13	0
5	L	65	0	74	5	0
5	M	65	0	74	13	0
6	L	44	0	57	1	0
6	M	48	0	62	3	0
7	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	M	5	0	0	0	0
9	M	42	0	60	9	0
10	H	16	0	31	1	0
10	M	32	0	62	2	0
11	M	69	0	82	6	0
12	H	42	0	0	0	0
12	L	40	0	0	0	0
12	M	43	0	0	2	0
All	All	7210	0	7083	215	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 (215) 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)
5:M:855:BPH:H121	5:M:855:BPH:H9C1	1.40	0.99
2:M:300:ASN:N	2:M:300:ASN:HD22	1.64	0.93
1:L:241:VAL:HG21	5:L:856:BPH:HAC1	1.55	0.87
2:M:9:GLN:HE22	3:H:198:VAL:H	1.23	0.86
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.59	0.84
5:M:855:BPH:H9C1	5:M:855:BPH:C12	2.09	0.82
2:M:236:GLU:HG3	3:H:122:GLU:CD	2.06	0.76
2:M:13:ARG:HD2	2:M:35:PHE:CD2	2.20	0.75
2:M:228:ARG:HA	3:H:194:GLN:HG3	1.68	0.74
2:M:300:ASN:N	2:M:300:ASN:ND2	2.36	0.73
2:M:195:ASN:ND2	2:M:197:PHE:H	1.88	0.71
2:M:156:LEU:HD13	4:M:853:BCL:H43	1.73	0.71
6:M:858:U10:H202	10:H:862:LDA:H123	1.73	0.71
2:M:9:GLN:NE2	3:H:198:VAL:H	1.89	0.70
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.72	0.70
3:H:202:ARG:HG2	3:H:203:VAL:N	2.05	0.69
2:M:195:ASN:HD22	2:M:195:ASN:C	1.95	0.69
2:M:243:THR:O	2:M:247:ARG:HG3	1.93	0.68
2:M:75:TRP:HE1	9:M:860:SPO:H32A	1.57	0.68
2:M:278:LEU:HD21	11:M:900:CDL:H382	1.77	0.66
2:M:236:GLU:HG3	3:H:122:GLU:CG	2.26	0.66
2:M:207:ALA:HA	4:M:854:BCL:O1A	1.96	0.65
2:M:168:MET:HG2	2:M:173:GLU:HG3	1.79	0.65
1:L:265:TRP:O	1:L:269:LEU:HD13	1.99	0.63
3:H:132:LYS:HG3	3:H:171:ILE:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:194:GLY:O	2:M:195:ASN:HB3	1.99	0.63
3:H:245:ALA:HB3	3:H:246:PRO:HD3	1.80	0.62
1:L:218:ASP:OD1	2:M:29:ARG:HD2	1.99	0.62
2:M:67:PHE:CG	5:M:855:BPH:H9C2	2.34	0.62
1:L:207:ARG:HG2	2:M:142:MET:HG2	1.80	0.62
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.35	0.62
2:M:228:ARG:HA	3:H:194:GLN:CG	2.29	0.62
3:H:66:LEU:CD1	3:H:118:ARG:HH22	2.11	0.62
4:L:851:BCL:HBC1	4:M:853:BCL:CAD	2.30	0.61
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.35	0.61
5:M:855:BPH:H121	5:M:855:BPH:C9	2.24	0.61
1:L:105:VAL:O	1:L:109:ARG:HG3	2.01	0.61
2:M:9:GLN:HE22	3:H:198:VAL:N	1.95	0.61
2:M:236:GLU:HG3	3:H:122:GLU:HG3	1.82	0.60
3:H:132:LYS:HG3	3:H:171:ILE:CD1	2.31	0.60
1:L:231:ARG:HD2	2:M:5:ASN:O	2.01	0.60
1:L:18:GLY:O	1:L:21:LEU:HB2	2.02	0.60
3:H:140:PHE:CE2	3:H:174:GLN:HG2	2.37	0.60
3:H:191:LEU:HD11	3:H:213:PHE:HE2	1.67	0.60
2:M:75:TRP:NE1	9:M:860:SPO:H32A	2.17	0.60
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.84	0.59
2:M:13:ARG:O	3:H:140:PHE:HA	2.02	0.59
2:M:168:MET:CG	2:M:173:GLU:HG3	2.33	0.59
2:M:208:PHE:HE1	10:M:861:LDA:H111	1.68	0.59
1:L:1:ALA:O	1:L:2:LEU:HD12	2.04	0.58
2:M:228:ARG:CA	3:H:194:GLN:HG3	2.34	0.58
2:M:178:GLY:O	2:M:182:HIS:HB3	2.04	0.58
1:L:80:LEU:HB3	1:L:85:LEU:HD13	1.86	0.57
3:H:165:VAL:CG2	3:H:180:GLU:HG2	2.34	0.57
3:H:37:ARG:O	3:H:38:GLU:HG2	2.04	0.57
2:M:109:LEU:HB3	2:M:114:LEU:CD1	2.35	0.57
3:H:140:PHE:HE2	3:H:174:GLN:HG2	1.69	0.56
1:L:101:ALA:O	1:L:104:GLU:HB2	2.05	0.56
2:M:77:GLN:HE22	2:M:93:SER:H	1.52	0.56
2:M:5:ASN:HD22	3:H:194:GLN:HB3	1.69	0.56
2:M:299:GLN:C	2:M:300:ASN:HD22	2.09	0.56
1:L:14:GLY:O	1:L:109:ARG:HD3	2.05	0.56
3:H:165:VAL:O	3:H:166:ASP:HB2	2.05	0.56
4:M:854:BCL:HAA2	10:M:861:LDA:H32	1.87	0.56
2:M:109:LEU:HB3	2:M:114:LEU:HD13	1.87	0.55
1:L:87:GLN:O	1:L:91:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:60:ASN:O	1:L:64:ILE:HG13	2.07	0.55
1:L:230:HIS:CD2	2:M:223:ILE:HG13	2.42	0.54
3:H:201:ASN:O	3:H:202:ARG:HB3	2.07	0.54
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.42	0.54
1:L:207:ARG:HG3	1:L:211:HIS:CG	2.42	0.54
3:H:104:PRO:HB2	3:H:243:TYR:CE2	2.43	0.54
2:M:21:THR:CG2	2:M:26:LEU:HD11	2.36	0.54
9:M:860:SPO:HM12	9:M:860:SPO:H5	1.90	0.54
4:L:851:BCL:HBB2	9:M:860:SPO:H243	1.90	0.54
1:L:222:TYR:HA	12:M:1103:HOH:O	2.07	0.53
2:M:26:LEU:HD12	2:M:26:LEU:H	1.73	0.53
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.74	0.53
2:M:195:ASN:HD22	2:M:196:LEU:N	2.07	0.53
3:H:156:CYS:SG	3:H:248:ARG:HB2	2.49	0.52
3:H:89:ARG:HG2	3:H:91:ALA:O	2.10	0.52
2:M:234:GLU:O	2:M:238:ILE:HG13	2.10	0.52
4:L:852:BCL:H42	4:M:854:BCL:HBC2	1.91	0.52
1:L:241:VAL:CG2	5:L:856:BPH:HAC1	2.33	0.52
3:H:248:ARG:HB2	3:H:248:ARG:NH1	2.25	0.52
4:L:851:BCL:HBB1	2:M:157:TRP:HD1	1.74	0.51
4:M:854:BCL:H61	6:M:858:U10:H203	1.92	0.51
3:H:70:ARG:NH2	3:H:123:LEU:HD22	2.26	0.51
5:L:856:BPH:H7C2	4:M:854:BCL:H193	1.93	0.51
3:H:229:GLU:O	3:H:233:ILE:HG13	2.10	0.51
1:L:266:TRP:HE1	2:M:87:ARG:HA	1.76	0.51
2:M:280:GLY:HA2	4:M:853:BCL:HED2	1.93	0.51
5:M:855:BPH:C14	5:M:855:BPH:H172	2.40	0.50
2:M:125:ALA:HB1	5:M:855:BPH:H2	1.93	0.50
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.10	0.50
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.93	0.49
1:L:207:ARG:HG3	1:L:211:HIS:ND1	2.27	0.49
3:H:112:ALA:HB2	3:H:239:GLY:HA3	1.94	0.49
2:M:75:TRP:HE1	9:M:860:SPO:HM13	1.76	0.49
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.43	0.49
1:L:208:THR:H	1:L:211:HIS:CD2	2.31	0.48
2:M:195:ASN:ND2	2:M:195:ASN:C	2.64	0.48
5:M:855:BPH:C14	5:M:855:BPH:C17	2.90	0.48
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.49	0.48
2:M:67:PHE:CG	5:M:855:BPH:C9	2.96	0.48
1:L:49:ILE:HG12	1:L:89:ILE:HD13	1.95	0.48
2:M:164:ARG:O	2:M:168:MET:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:233:GLY:HA3	2:M:216:PHE:CE1	2.48	0.48
1:L:272:TRP:CE2	2:M:87:ARG:HB3	2.49	0.48
11:M:900:CDL:H381	3:H:23:PHE:CZ	2.49	0.48
4:L:851:BCL:HBC1	4:M:853:BCL:CB	2.43	0.47
1:L:1:ALA:HB1	3:H:42:LEU:HB3	1.96	0.47
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.95	0.47
3:H:170:ASP:O	3:H:174:GLN:N	2.48	0.47
1:L:69:PRO:HD2	1:L:142:TRP:HB2	1.97	0.47
1:L:6:GLU:OE2	1:L:10:ARG:HD3	2.15	0.47
1:L:267:VAL:HG13	2:M:87:ARG:HD2	1.96	0.47
4:L:852:BCL:H122	5:L:856:BPH:H3A	1.97	0.47
3:H:130:LYS:HG2	3:H:131:ILE:HD12	1.96	0.47
2:M:195:ASN:HD22	2:M:197:PHE:H	1.59	0.47
2:M:73:TRP:NE1	2:M:77:GLN:NE2	2.62	0.46
2:M:67:PHE:CD1	5:M:855:BPH:H9C2	2.51	0.46
1:L:213:ASN:O	1:L:217:ARG:HB2	2.15	0.46
3:H:81:GLU:O	3:H:83:ARG:HG2	2.16	0.46
2:M:62:SER:HB3	2:M:121:PHE:O	2.14	0.46
2:M:100:GLU:H	2:M:100:GLU:HG3	1.48	0.46
3:H:245:ALA:HA	3:H:248:ARG:NH2	2.31	0.46
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.97	0.46
1:L:80:LEU:HD22	1:L:85:LEU:CD1	2.46	0.45
2:M:3:TYR:CD2	3:H:194:GLN:HA	2.50	0.45
1:L:208:THR:HB	1:L:209:PRO:HD2	1.99	0.45
2:M:129:TRP:O	2:M:132:ARG:HB3	2.17	0.45
5:M:855:BPH:H172	5:M:855:BPH:H142	1.98	0.45
1:L:216:PHE:HE1	12:M:1087:HOH:O	1.98	0.45
2:M:291:VAL:HG13	2:M:297:TRP:HB2	1.99	0.45
3:H:201:ASN:O	3:H:202:ARG:CB	2.64	0.45
1:L:102:LEU:HD12	1:L:102:LEU:HA	1.74	0.45
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.51	0.45
4:L:852:BCL:CGA	4:M:854:BCL:HBC1	2.47	0.45
2:M:78:ALA:HB2	2:M:92:PHE:CZ	2.52	0.45
3:H:170:ASP:HB2	3:H:177:HIS:HD2	1.81	0.45
3:H:45:GLU:HG3	3:H:94:GLU:OE2	2.17	0.44
1:L:55:LEU:HD13	1:L:81:ALA:HB2	1.98	0.44
3:H:131:ILE:C	3:H:132:LYS:HG2	2.36	0.44
3:H:191:LEU:HD11	3:H:213:PHE:CE2	2.51	0.44
1:L:85:LEU:O	1:L:89:ILE:HG13	2.18	0.44
4:L:851:BCL:H2C	4:L:851:BCL:HBC2	1.67	0.44
2:M:148:TRP:HB3	11:M:900:CDL:H741	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:855:BPH:C17	5:M:855:BPH:H141	2.46	0.44
3:H:244:ALA:O	3:H:246:PRO:N	2.51	0.44
2:M:148:TRP:CD1	11:M:900:CDL:OB6	2.71	0.44
4:L:851:BCL:CBB	9:M:860:SPO:H243	2.47	0.44
2:M:148:TRP:CE2	11:M:900:CDL:H511	2.52	0.44
1:L:20:ASN:HD22	1:L:20:ASN:N	2.16	0.44
1:L:211:HIS:HE1	2:M:22:GLU:OE1	1.99	0.44
2:M:87:ARG:HG3	2:M:88:ASP:N	2.33	0.44
3:H:99:ALA:HA	3:H:100:PRO:HD3	1.89	0.44
1:L:163:THR:O	1:L:163:THR:HG22	2.17	0.44
6:L:859:U10:H311	2:M:31:GLY:O	2.17	0.44
3:H:247:LYS:N	3:H:247:LYS:HD2	2.33	0.44
1:L:277:GLY:N	1:L:281:GLY:O	2.51	0.44
2:M:106:ALA:O	2:M:107:ALA:C	2.56	0.44
4:M:854:BCL:HBA2	4:M:854:BCL:H3A	1.75	0.44
2:M:105:PHE:CD2	2:M:105:PHE:N	2.86	0.43
2:M:168:MET:HE3	2:M:288:GLY:O	2.18	0.43
3:H:131:ILE:HA	3:H:169:VAL:O	2.17	0.43
1:L:278:GLY:HA2	2:M:77:GLN:O	2.19	0.43
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.18	0.43
2:M:24:VAL:HG11	2:M:29:ARG:NH1	2.34	0.43
1:L:53:ALA:HB1	1:L:58:THR:O	2.18	0.43
3:H:219:ILE:HA	3:H:229:GLU:OE2	2.18	0.43
2:M:182:HIS:CG	9:M:860:SPO:H181	2.54	0.43
3:H:75:VAL:HA	3:H:76:PRO:C	2.39	0.43
3:H:221:SER:HA	3:H:222:PRO:HD3	1.87	0.43
2:M:162:PHE:HB2	9:M:860:SPO:H291	2.00	0.42
2:M:3:TYR:HD2	3:H:194:GLN:HA	1.84	0.42
2:M:75:TRP:CD1	9:M:860:SPO:H32A	2.53	0.42
2:M:94:LEU:CD2	2:M:115:TRP:HB2	2.50	0.42
3:H:151:LEU:O	3:H:164:VAL:HG23	2.19	0.42
5:M:855:BPH:C12	5:M:855:BPH:C9	2.80	0.42
3:H:156:CYS:HB3	3:H:206:ASN:O	2.18	0.42
1:L:60:ASN:HA	1:L:61:PRO:HD3	1.84	0.42
2:M:157:TRP:HB2	4:M:853:BCL:H62	2.02	0.42
1:L:8:LYS:HE2	1:L:9:TYR:CZ	2.55	0.42
3:H:123:LEU:HA	3:H:128:HIS:O	2.20	0.42
1:L:83:GLY:O	1:L:87:GLN:HG3	2.19	0.42
1:L:272:TRP:CD2	2:M:87:ARG:HB3	2.54	0.42
4:L:852:BCL:H2C	4:M:853:BCL:H2C	2.01	0.42
2:M:24:VAL:HG22	2:M:139:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:851:BCL:HBB2	4:L:851:BCL:HHC	2.01	0.41
3:H:140:PHE:CE1	3:H:171:ILE:HG13	2.55	0.41
3:H:114:TRP:HE3	3:H:115:VAL:O	2.03	0.41
3:H:142:VAL:HG21	3:H:147:ASN:ND2	2.34	0.41
1:L:134:PHE:O	1:L:138:MET:HG3	2.20	0.41
2:M:132:ARG:O	2:M:136:ARG:HG2	2.20	0.41
1:L:97:PHE:CE1	4:L:852:BCL:H121	2.55	0.41
2:M:109:LEU:O	2:M:114:LEU:HD13	2.20	0.41
3:H:219:ILE:HD12	3:H:221:SER:O	2.21	0.41
1:L:201:GLU:HG3	2:M:141:GLY:O	2.21	0.41
3:H:171:ILE:HB	3:H:172:PRO:HD3	2.02	0.41
1:L:246:LEU:HA	1:L:249:ILE:HG22	2.02	0.41
5:L:856:BPH:HHB	5:L:856:BPH:HMB1	1.92	0.41
2:M:11:GLN:OE1	2:M:40:GLY:HA3	2.19	0.41
2:M:268:TRP:CD1	6:M:858:U10:H111	2.56	0.41
3:H:240:GLY:O	3:H:244:ALA:HB3	2.21	0.41
1:L:129:LEU:O	1:L:133:LEU:HB3	2.21	0.41
2:M:87:ARG:NE	2:M:88:ASP:OD1	2.55	0.40
1:L:31:VAL:HG12	1:L:32:GLY:N	2.36	0.40
2:M:72:ILE:HG23	2:M:73:TRP:N	2.37	0.40
2:M:67:PHE:CB	5:M:855:BPH:C9	2.99	0.40
3:H:169:VAL:CG1	3:H:170:ASP:N	2.84	0.40
3:H:233:ILE:O	3:H:237:VAL:HG23	2.22	0.40
1:L:20:ASN:HD22	1:L:20:ASN:H	1.70	0.40
1:L:146:PHE:HB3	1:L:156:TRP:CD2	2.57	0.40
1:L:199:ASN:O	11:M:900:CDL:H1	2.20	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%)	266 (95%)	13 (5%)	0	100	100
2	M	299/307 (97%)	285 (95%)	13 (4%)	1 (0%)	41	60
3	H	236/260 (91%)	227 (96%)	7 (3%)	2 (1%)	19	34
All	All	814/848 (96%)	778 (96%)	33 (4%)	3 (0%)	34	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	245	ALA
2	M	100	GLU
3	H	202	ARG

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	220/220 (100%)	211 (96%)	9 (4%)	30	50
2	M	236/239 (99%)	226 (96%)	10 (4%)	30	49
3	H	193/209 (92%)	183 (95%)	10 (5%)	23	39
All	All	649/668 (97%)	620 (96%)	29 (4%)	27	46

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	10	ARG
1	L	20	ASN
1	L	21	LEU
1	L	85	LEU
1	L	102	LEU
1	L	154	LEU
1	L	216	PHE
1	L	269	LEU
1	L	272	TRP
2	M	13	ARG

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Mol	Chain	Res	Type
2	M	29	ARG
2	M	87	ARG
2	M	100	GLU
2	M	156	LEU
2	M	168	MET
2	M	182	HIS
2	M	195	ASN
2	M	216	PHE
2	M	300	ASN
3	H	12	LEU
3	H	73	LEU
3	H	80	SER
3	H	89	ARG
3	H	123	LEU
3	H	132	LYS
3	H	135	LYS
3	H	194	GLN
3	H	202	ARG
3	H	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	20	ASN
1	L	87	GLN
1	L	211	HIS
1	L	264	GLN
2	M	5	ASN
2	M	9	GLN
2	M	77	GLN
2	M	195	ASN
2	M	300	ASN
3	H	177	HIS
3	H	194	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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
4	BCL	M	853	-	58,74,74	1.31	7 (12%)	69,115,115	2.74	25 (36%)
11	CDL	M	900	-	68,68,99	1.33	8 (11%)	74,80,111	1.74	15 (20%)
6	U10	M	858	-	48,48,63	2.10	16 (33%)	58,61,79	3.24	16 (27%)
10	LDA	M	863	-	12,15,15	2.19	1 (8%)	14,17,17	1.65	3 (21%)
4	BCL	L	852	-	58,74,74	1.25	4 (6%)	69,115,115	1.97	23 (33%)
10	LDA	H	862	-	12,15,15	2.04	1 (8%)	14,17,17	1.77	4 (28%)
4	BCL	M	854	-	58,74,74	1.28	9 (15%)	69,115,115	2.38	19 (27%)
8	PO4	M	864	-	4,4,4	1.62	0	6,6,6	0.43	0
4	BCL	L	851	-	43,59,74	1.54	6 (13%)	51,97,115	2.42	16 (31%)
6	U10	L	859	-	44,44,63	1.65	10 (22%)	53,56,79	1.30	5 (9%)
5	BPH	L	856	-	51,70,70	1.73	11 (21%)	52,101,101	2.68	18 (34%)
9	SPO	M	860	-	40,41,41	3.47	24 (60%)	47,50,50	4.16	14 (29%)
10	LDA	M	861	-	12,15,15	2.13	1 (8%)	14,17,17	1.64	4 (28%)
5	BPH	M	855	-	51,70,70	1.93	10 (19%)	52,101,101	2.81	21 (40%)

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
4	BCL	M	853	-	-	12/37/137/137	-
11	CDL	M	900	-	-	23/79/79/110	-
6	U10	M	858	-	-	10/45/69/87	0/1/1/1
10	LDA	M	863	-	-	7/13/13/13	-
4	BCL	L	852	-	-	2/37/137/137	-
10	LDA	H	862	-	-	7/13/13/13	-
4	BCL	M	854	-	-	8/37/137/137	-
4	BCL	L	851	-	-	1/19/119/137	-
6	U10	L	859	-	-	15/41/65/87	0/1/1/1
5	BPH	L	856	-	2/2/18/22	15/37/105/105	0/5/6/6
9	SPO	M	860	-	-	14/47/47/47	-
10	LDA	M	861	-	-	7/13/13/13	-
5	BPH	M	855	-	2/2/18/22	17/37/105/105	0/5/6/6

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	860	SPO	C6-C5	8.89	1.55	1.32
9	M	860	SPO	C10-C11	8.16	1.55	1.34
9	M	860	SPO	C15-C16	7.55	1.54	1.34
10	M	863	LDA	O1-N1	-7.39	1.24	1.42
10	M	861	LDA	O1-N1	-6.94	1.25	1.42
10	H	862	LDA	O1-N1	-6.86	1.26	1.42
5	M	855	BPH	C2C-C3C	-6.69	1.48	1.54
9	M	860	SPO	C27-C28	6.09	1.40	1.34
5	M	855	BPH	C11-C10	-5.47	1.28	1.52
5	L	856	BPH	C11-C10	-5.35	1.29	1.52
9	M	860	SPO	C21-C20	5.24	1.49	1.36
9	M	860	SPO	C26-C25	5.11	1.47	1.34
6	M	858	U10	O4-C4	5.07	1.49	1.36
6	M	858	U10	C7-C8	-4.83	1.43	1.50
4	L	851	BCL	C3C-C4C	-4.74	1.45	1.51
5	M	855	BPH	O2D-CGD	4.72	1.44	1.33
5	L	856	BPH	C2C-C3C	-4.71	1.50	1.54
5	M	855	BPH	O2A-CGA	4.54	1.46	1.33
5	L	856	BPH	O2A-CGA	4.30	1.45	1.33
6	M	858	U10	C28-C29	4.24	1.43	1.33
9	M	860	SPO	C14-C12	4.12	1.41	1.35
9	M	860	SPO	C9-C7	4.06	1.41	1.35
6	M	858	U10	C33-C34	3.98	1.42	1.33
9	M	860	SPO	C19-C17	3.94	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	859	U10	C6-C1	3.91	1.42	1.35
9	M	860	SPO	O1-CM1	3.86	1.55	1.43
4	M	853	BCL	MG-NA	3.83	2.15	2.06
11	M	900	CDL	CA3-CA4	3.76	1.62	1.50
6	M	858	U10	C6-C1	3.74	1.42	1.35
5	M	855	BPH	C3A-C2A	-3.72	1.51	1.54
11	M	900	CDL	OA8-CA7	3.68	1.44	1.33
5	L	856	BPH	O2D-CGD	3.62	1.42	1.33
11	M	900	CDL	OA6-CA4	3.48	1.55	1.46
4	L	852	BCL	C1B-NB	3.37	1.38	1.35
6	M	858	U10	C13-C14	3.36	1.41	1.33
4	L	852	BCL	MG-NA	3.26	2.14	2.06
4	L	851	BCL	C1B-NB	3.22	1.38	1.35
11	M	900	CDL	C11-CA5	3.19	1.60	1.50
5	M	855	BPH	C1A-C2A	3.19	1.55	1.51
4	L	851	BCL	MG-NA	3.16	2.13	2.06
9	M	860	SPO	C10-C9	3.10	1.53	1.43
6	L	859	U10	C8-C9	3.04	1.40	1.33
5	L	856	BPH	O2D-CED	-3.02	1.38	1.45
4	M	854	BCL	MG-NC	-3.00	1.99	2.06
6	M	858	U10	C37-C38	-3.00	1.40	1.50
4	L	851	BCL	MG-NC	-2.96	1.99	2.06
11	M	900	CDL	OA6-CA5	2.95	1.42	1.34
9	M	860	SPO	O1-C1	2.94	1.58	1.41
6	M	858	U10	O3-C3	2.87	1.43	1.36
6	L	859	U10	C18-C19	2.86	1.39	1.33
11	M	900	CDL	OA8-CA6	2.85	1.51	1.45
9	M	860	SPO	C32-C33	2.84	1.39	1.33
6	L	859	U10	C3-C2	-2.83	1.40	1.48
6	L	859	U10	C28-C29	2.83	1.39	1.33
6	M	858	U10	C23-C24	2.83	1.39	1.33
4	M	853	BCL	C1B-NB	2.82	1.37	1.35
6	M	858	U10	O3-C3M	-2.81	1.38	1.45
9	M	860	SPO	C26-C27	2.80	1.52	1.43
6	L	859	U10	C7-C8	-2.80	1.46	1.50
9	M	860	SPO	C37-C38	2.80	1.40	1.32
5	L	856	BPH	C2-C3	2.80	1.39	1.33
5	L	856	BPH	C1A-C2A	2.75	1.55	1.51
9	M	860	SPO	C13-C12	2.73	1.56	1.50
9	M	860	SPO	C8-C7	2.69	1.56	1.50
5	M	855	BPH	C2-C3	2.69	1.39	1.33
6	L	859	U10	C33-C34	2.66	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	860	SPO	C11-C12	-2.65	1.40	1.45
9	M	860	SPO	C24-C23	2.64	1.56	1.50
5	M	855	BPH	O2D-CED	-2.62	1.39	1.45
5	L	856	BPH	C3A-C2A	-2.61	1.52	1.54
6	M	858	U10	C36-C34	2.58	1.56	1.51
9	M	860	SPO	C25-C23	-2.56	1.40	1.45
5	M	855	BPH	CAA-C2A	2.56	1.59	1.54
6	L	859	U10	C13-C14	2.55	1.39	1.33
4	M	853	BCL	C2-C3	-2.55	1.26	1.33
9	M	860	SPO	C15-C14	2.54	1.51	1.43
11	M	900	CDL	OB2-CB2	-2.53	1.35	1.44
4	M	854	BCL	C1B-NB	2.52	1.37	1.35
5	L	856	BPH	O1D-CGD	2.50	1.27	1.21
9	M	860	SPO	C35-C33	2.49	1.56	1.51
6	L	859	U10	C23-C24	2.47	1.38	1.33
6	L	859	U10	C4-C5	-2.47	1.41	1.48
5	L	856	BPH	CHA-CBD	2.42	1.55	1.52
4	M	854	BCL	CBB-CAB	2.40	1.56	1.49
4	M	854	BCL	C3D-CAD	-2.37	1.40	1.46
9	M	860	SPO	C6-C7	-2.34	1.40	1.45
6	M	858	U10	C31-C29	2.32	1.56	1.51
4	M	853	BCL	C3C-C4C	-2.26	1.48	1.51
6	M	858	U10	C30-C29	2.26	1.56	1.50
6	M	858	U10	C15-C14	2.26	1.56	1.50
4	M	854	BCL	MG-NA	2.24	2.11	2.06
4	L	852	BCL	C3C-C4C	-2.22	1.48	1.51
4	L	852	BCL	CBB-CAB	2.21	1.56	1.49
4	M	854	BCL	C4-C3	2.20	1.56	1.50
4	M	853	BCL	C3A-C2A	2.17	1.60	1.54
4	M	854	BCL	C3C-C4C	-2.15	1.48	1.51
11	M	900	CDL	PB2-OB5	2.14	1.68	1.59
6	M	858	U10	C8-C9	2.14	1.38	1.33
4	M	853	BCL	CBB-CAB	2.14	1.56	1.49
5	M	855	BPH	CHA-CBD	2.13	1.54	1.52
4	M	854	BCL	C4B-CHC	-2.12	1.35	1.41
6	M	858	U10	C18-C19	2.11	1.38	1.33
9	M	860	SPO	C22-C23	2.11	1.38	1.35
4	L	851	BCL	C3D-CAD	-2.10	1.40	1.46
4	M	853	BCL	MG-NC	-2.10	2.01	2.06
4	M	854	BCL	C6-C5	2.09	1.59	1.52
4	L	851	BCL	C4-C3	2.03	1.55	1.50
5	L	856	BPH	CAA-C2A	2.03	1.58	1.54

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	860	SPO	C2-C1-C4	-20.82	78.90	110.86
6	M	858	U10	C32-C33-C34	18.38	171.91	127.66
4	M	853	BCL	C1-C2-C3	12.78	148.15	126.04
5	L	856	BPH	O2D-CGD-CBD	11.80	125.95	111.00
5	M	855	BPH	O2D-CGD-CBD	11.75	125.89	111.00
9	M	860	SPO	C3-C1-C4	-11.70	92.89	110.86
4	M	854	BCL	CAC-C3C-C4C	-10.41	89.47	112.58
4	L	851	BCL	CBC-CAC-C3C	-8.20	95.21	113.47
6	M	858	U10	C27-C28-C29	8.11	147.19	127.66
5	M	855	BPH	C1-C2-C3	6.48	137.26	126.04
9	M	860	SPO	C15-C14-C12	-6.10	118.61	127.31
6	M	858	U10	C3M-O3-C3	6.01	137.78	116.47
4	M	853	BCL	C5-C3-C2	-6.01	108.95	121.12
9	M	860	SPO	C20-C21-C22	-5.97	111.25	123.47
4	M	854	BCL	O2A-C1-C2	-5.78	93.44	108.64
4	L	851	BCL	CAD-C3D-C4D	-5.74	105.27	108.47
4	M	853	BCL	C4-C3-C5	5.66	124.79	115.27
5	L	856	BPH	CBC-CAC-C3C	5.61	125.06	113.77
9	M	860	SPO	C25-C23-C22	-5.39	110.67	118.94
4	L	852	BCL	C4A-NA-C1A	-5.30	104.32	106.71
4	M	854	BCL	C2C-C3C-C4C	5.30	109.27	101.34
11	M	900	CDL	OB6-CB5-C51	5.17	122.65	111.50
11	M	900	CDL	OB8-CB6-CB4	5.09	123.25	108.43
5	M	855	BPH	C7-C6-C5	4.98	126.88	113.36
4	M	853	BCL	CAD-C3D-C4D	-4.94	105.71	108.47
4	L	852	BCL	CAD-C3D-C4D	-4.91	105.73	108.47
5	L	856	BPH	C1-C2-C3	4.83	134.40	126.04
4	M	854	BCL	C1-O2A-CGA	4.82	129.09	116.44
5	L	856	BPH	C6-C5-C3	4.74	125.88	113.45
11	M	900	CDL	OA2-PA1-OA3	-4.73	90.60	109.07
4	M	853	BCL	C16-C15-C13	-4.71	100.69	115.92
5	M	855	BPH	O1D-CGD-CBD	-4.70	116.91	124.74
11	M	900	CDL	CB2-C1-CA2	-4.63	99.17	112.79
5	M	855	BPH	CED-O2D-CGD	4.53	126.18	115.94
4	L	851	BCL	CMD-C2D-C3D	4.45	133.00	124.68
6	M	858	U10	C36-C34-C33	4.37	129.97	121.12
4	M	853	BCL	OBB-CAB-CBB	-4.33	110.42	120.17
4	M	854	BCL	OBB-CAB-CBB	-4.33	110.43	120.17
4	L	851	BCL	C1-C2-C3	-4.32	119.75	126.75
4	L	851	BCL	C4A-NA-C1A	-4.27	104.78	106.71
4	M	854	BCL	CMD-C2D-C3D	4.23	132.59	124.68
5	L	856	BPH	O2D-CGD-O1D	-4.17	115.68	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	852	BCL	OBB-CAB-CBB	-4.17	110.78	120.17
5	L	856	BPH	C11-C10-C8	4.01	128.89	115.92
9	M	860	SPO	C24-C23-C25	3.99	124.36	118.08
4	M	853	BCL	CMD-C2D-C3D	3.98	132.13	124.68
4	L	851	BCL	OBB-CAB-CBB	-3.95	111.28	120.17
5	M	855	BPH	CBC-CAC-C3C	3.92	121.66	113.77
4	M	854	BCL	C1C-NC-C4C	3.91	108.47	106.71
4	L	852	BCL	CMD-C2D-C3D	3.88	131.94	124.68
5	L	856	BPH	CED-O2D-CGD	3.88	124.71	115.94
4	L	851	BCL	C2C-C3C-C4C	3.87	107.13	101.34
6	M	858	U10	O5-C5-C6	-3.85	114.80	121.55
5	L	856	BPH	O1D-CGD-CBD	-3.84	118.34	124.74
5	M	855	BPH	C6-C5-C3	3.77	123.33	113.45
9	M	860	SPO	C18-C17-C19	-3.72	117.71	122.92
4	L	852	BCL	OBD-CAD-CBD	-3.70	120.61	125.89
5	M	855	BPH	C11-C10-C8	3.68	127.83	115.92
4	L	852	BCL	C1-C2-C3	-3.64	119.74	126.04
4	M	853	BCL	OBD-CAD-CBD	-3.64	120.69	125.89
4	M	854	BCL	C4A-NA-C1A	-3.63	105.07	106.71
10	H	862	LDA	CM1-N1-C1	-3.63	102.61	110.23
11	M	900	CDL	OA5-PA1-OA3	-3.61	94.95	109.07
9	M	860	SPO	C1-C4-C5	3.59	122.57	113.06
6	M	858	U10	C31-C29-C28	3.55	128.31	121.12
4	M	853	BCL	CMB-C2B-C3B	3.54	131.30	124.68
4	M	854	BCL	C11-C12-C13	-3.52	104.53	115.92
4	M	854	BCL	CAD-C3D-C4D	-3.51	106.51	108.47
4	L	852	BCL	CMB-C2B-C3B	3.51	131.25	124.68
9	M	860	SPO	C15-C16-C17	-3.48	116.65	126.42
4	L	851	BCL	CAC-C3C-C4C	-3.47	104.87	112.58
4	M	853	BCL	CMB-C2B-C1B	-3.46	123.14	128.46
4	L	851	BCL	CAA-C2A-C3A	-3.44	103.36	112.78
6	M	858	U10	C30-C29-C31	-3.43	109.50	115.27
4	M	853	BCL	C12-C11-C10	-3.43	97.48	113.24
5	M	855	BPH	O2D-CGD-O1D	-3.42	117.16	123.84
4	L	851	BCL	OBD-CAD-CBD	-3.38	121.06	125.89
11	M	900	CDL	CB6-CB4-CB3	-3.38	103.81	111.79
4	M	854	BCL	C3C-C2C-C1C	-3.34	96.47	101.87
9	M	860	SPO	C3-C1-C2	3.34	116.65	110.37
5	L	856	BPH	CMB-C2B-C3B	3.28	130.81	124.68
6	M	858	U10	C20-C19-C21	-3.25	109.81	115.27
11	M	900	CDL	O1-C1-CA2	-3.25	98.17	109.56
6	L	859	U10	C25-C24-C26	3.24	120.72	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	856	BPH	CMA-C3A-C4A	-3.23	107.29	114.38
4	M	853	BCL	C2C-C3C-C4C	3.23	106.18	101.34
10	M	861	LDA	CM1-N1-C1	-3.18	103.55	110.23
11	M	900	CDL	OB6-CB5-OB7	-3.14	116.12	123.70
5	M	855	BPH	C4C-C3C-C2C	3.12	105.81	102.84
5	L	856	BPH	C1C-C2C-C3C	3.12	105.81	102.84
9	M	860	SPO	C6-C7-C9	-3.12	114.16	118.94
4	L	851	BCL	C1C-NC-C4C	3.11	108.11	106.71
10	M	863	LDA	C5-C4-C3	-3.06	98.88	114.42
5	L	856	BPH	C4C-C3C-C2C	3.06	105.75	102.84
4	M	853	BCL	O2A-C1-C2	-3.03	100.68	108.64
6	M	858	U10	C31-C32-C33	3.00	121.75	111.88
4	M	853	BCL	O2A-CGA-CBA	2.99	121.29	111.91
4	L	852	BCL	O2D-CGD-CBD	-2.97	105.99	111.27
11	M	900	CDL	OB2-PB2-OB3	2.97	120.67	109.07
6	M	858	U10	O2-C2-C3	-2.97	114.64	120.93
4	M	853	BCL	C20-C18-C19	-2.96	96.85	110.51
4	M	854	BCL	CBB-CAB-C3B	2.96	129.14	120.34
5	M	855	BPH	C1C-C2C-C3C	2.93	105.63	102.84
4	L	852	BCL	CMB-C2B-C1B	-2.92	123.98	128.46
4	L	852	BCL	O1D-CGD-CBD	2.91	130.45	124.48
5	M	855	BPH	CMB-C2B-C3B	2.90	130.11	124.68
9	M	860	SPO	C8-C7-C6	2.89	122.63	118.08
5	M	855	BPH	CAA-C2A-C3A	-2.86	104.95	112.78
6	L	859	U10	C30-C29-C31	2.84	120.05	115.27
10	M	863	LDA	C9-C8-C7	-2.83	100.06	114.42
5	L	856	BPH	C7-C6-C5	-2.81	105.73	113.36
6	L	859	U10	C35-C34-C36	2.80	119.18	115.98
4	M	853	BCL	CBB-CAB-C3B	2.80	128.64	120.34
5	M	855	BPH	CMA-C3A-C4A	-2.79	108.27	114.38
4	M	853	BCL	C7-C6-C5	-2.78	105.81	113.36
4	L	851	BCL	CHA-C1A-NA	-2.77	120.05	126.40
4	M	853	BCL	C4A-NA-C1A	-2.77	105.46	106.71
10	M	861	LDA	CM2-N1-C1	2.77	116.05	110.23
4	M	854	BCL	OBD-CAD-CBD	-2.77	121.94	125.89
10	H	862	LDA	O1-N1-C1	2.76	116.04	109.27
6	M	858	U10	C35-C34-C36	-2.74	110.65	115.27
5	M	855	BPH	OBD-CAD-CBD	-2.74	121.80	125.82
4	M	853	BCL	CHA-C1A-NA	-2.69	120.23	126.40
6	L	859	U10	C7-C8-C9	-2.67	122.35	126.79
4	M	853	BCL	C1-O2A-CGA	-2.66	109.46	116.44
4	L	852	BCL	C7-C6-C5	-2.66	106.13	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	851	BCL	C3D-CAD-CBD	2.66	111.11	107.61
4	L	852	BCL	CBB-CAB-C3B	2.65	128.21	120.34
4	M	853	BCL	CAC-C3C-C4C	-2.61	106.79	112.58
5	M	855	BPH	CMD-C2D-C3D	2.61	129.55	124.68
6	L	859	U10	C3M-O3-C3	2.58	125.61	116.47
4	L	851	BCL	CHD-C4C-NC	2.51	127.87	125.08
4	M	853	BCL	CED-O2D-CGD	2.51	121.61	115.94
6	M	858	U10	C21-C19-C18	2.51	126.19	121.12
4	L	852	BCL	CHA-C1A-NA	-2.51	120.66	126.40
6	M	858	U10	C1-C6-C5	-2.50	117.23	119.58
4	M	854	BCL	C14-C13-C15	-2.50	102.23	111.29
5	M	855	BPH	C5-C3-C2	-2.49	116.07	121.12
4	L	852	BCL	CAA-C2A-C3A	-2.49	105.96	112.78
11	M	900	CDL	OA4-PA1-OA3	-2.49	99.94	112.24
10	H	862	LDA	CM2-N1-C1	2.48	115.44	110.23
10	M	861	LDA	O1-N1-C1	2.46	115.30	109.27
4	L	851	BCL	CMB-C2B-C3B	2.45	129.26	124.68
11	M	900	CDL	OA4-PA1-OA2	2.45	119.11	107.75
11	M	900	CDL	OA4-PA1-OA5	2.44	119.07	107.75
9	M	860	SPO	C10-C9-C7	-2.43	123.84	127.31
4	M	854	BCL	CHA-C1A-NA	-2.43	120.84	126.40
5	L	856	BPH	O2A-CGA-O1A	-2.42	117.48	123.59
4	M	854	BCL	CMB-C2B-C3B	2.42	129.21	124.68
4	L	852	BCL	CAC-C3C-C4C	-2.41	107.23	112.58
4	L	852	BCL	C16-C15-C13	-2.41	108.13	115.92
4	L	852	BCL	C11-C12-C13	-2.41	108.13	115.92
4	L	852	BCL	C2C-C3C-C4C	2.40	104.94	101.34
5	M	855	BPH	C6-C7-C8	-2.40	108.15	115.92
10	H	862	LDA	C9-C8-C7	-2.40	102.26	114.42
10	M	863	LDA	O1-N1-C1	2.39	115.12	109.27
4	M	854	BCL	CBA-CAA-C2A	2.36	120.82	113.86
4	L	852	BCL	C3D-CAD-CBD	2.33	110.68	107.61
9	M	860	SPO	C20-C19-C17	-2.33	123.99	127.31
5	M	855	BPH	C4-C3-C5	2.32	119.18	115.27
4	L	851	BCL	CBB-CAB-C3B	2.32	127.22	120.34
6	M	858	U10	C7-C8-C9	2.31	130.64	126.79
5	M	855	BPH	CMA-C3A-C2A	-2.31	104.71	113.99
4	L	852	BCL	CED-O2D-CGD	2.25	121.03	115.94
6	M	858	U10	C16-C14-C13	2.25	125.67	121.12
11	M	900	CDL	OA6-CA5-C11	2.25	116.34	111.50
5	M	855	BPH	O2A-CGA-O1A	-2.24	117.94	123.59
5	L	856	BPH	CAA-C2A-C3A	-2.23	106.66	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	854	BCL	CMB-C2B-C1B	-2.22	125.05	128.46
5	L	856	BPH	CMA-C3A-C2A	-2.22	105.06	113.99
4	L	852	BCL	CBC-CAC-C3C	-2.18	108.62	113.47
4	M	853	BCL	O2A-CGA-O1A	-2.17	118.12	123.59
4	L	852	BCL	O2A-C1-C2	-2.12	103.05	108.64
11	M	900	CDL	C52-C51-CB5	2.10	121.26	113.62
6	M	858	U10	C7-C6-C5	-2.09	115.96	118.48
4	M	854	BCL	C3D-CAD-CBD	2.09	110.36	107.61
5	L	856	BPH	C4A-C3A-C2A	2.05	104.79	102.84
4	L	852	BCL	CBA-CAA-C2A	2.05	119.92	113.86
4	M	853	BCL	C6-C5-C3	2.03	118.79	113.45
5	L	856	BPH	CMD-C2D-C3D	2.01	128.44	124.68
10	M	861	LDA	C9-C8-C7	-2.01	104.24	114.42
4	M	853	BCL	C3D-CAD-CBD	2.00	110.24	107.61
11	M	900	CDL	OB6-CB4-CB6	2.00	115.66	108.40

All (4) chirality outliers are listed below:

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

All (138) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	853	BCL	C2-C3-C5-C6
4	M	853	BCL	C4-C3-C5-C6
4	M	854	BCL	C1A-C2A-CAA-CBA
4	M	854	BCL	C3A-C2A-CAA-CBA
5	L	856	BPH	O2A-C1-C2-C3
5	M	855	BPH	O2A-C1-C2-C3
5	M	855	BPH	C1-C2-C3-C4
6	L	859	U10	C28-C29-C31-C32
6	L	859	U10	C29-C31-C32-C33
6	M	858	U10	C32-C33-C34-C35
6	M	858	U10	C32-C33-C34-C36
9	M	860	SPO	C4-C5-C6-C7
9	M	860	SPO	C36-C37-C38-C39
10	M	863	LDA	C2-C1-N1-CM1
10	M	863	LDA	C2-C1-N1-CM2

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Mol	Chain	Res	Type	Atoms
11	M	900	CDL	CA3-OA5-PA1-OA4
5	M	855	BPH	C8-C10-C11-C12
9	M	860	SPO	C36-C37-C38-C40
5	L	856	BPH	CBD-CGD-O2D-CED
4	M	853	BCL	C15-C16-C17-C18
4	M	853	BCL	C3-C5-C6-C7
6	L	859	U10	C30-C29-C31-C32
4	M	854	BCL	C2A-CAA-CBA-CGA
5	M	855	BPH	C1-C2-C3-C5
11	M	900	CDL	O1-C1-CB2-OB2
9	M	860	SPO	C33-C35-C36-C37
11	M	900	CDL	CA2-C1-CB2-OB2
5	M	855	BPH	C11-C12-C13-C14
5	L	856	BPH	O1D-CGD-O2D-CED
4	M	853	BCL	C8-C10-C11-C12
6	L	859	U10	C14-C16-C17-C18
6	L	859	U10	C19-C21-C22-C23
6	M	858	U10	C24-C26-C27-C28
4	M	854	BCL	C15-C16-C17-C18
11	M	900	CDL	CB2-OB2-PB2-OB5
10	M	861	LDA	C11-C10-C9-C8
11	M	900	CDL	C71-C72-C73-C74
11	M	900	CDL	C11-C12-C13-C14
5	L	856	BPH	C16-C17-C18-C20
10	M	863	LDA	C6-C7-C8-C9
10	H	862	LDA	C6-C7-C8-C9
5	L	856	BPH	C8-C10-C11-C12
5	L	856	BPH	C10-C11-C12-C13
5	L	856	BPH	C16-C17-C18-C19
10	M	861	LDA	C4-C5-C6-C7
5	M	855	BPH	C15-C16-C17-C18
10	M	863	LDA	C1-C2-C3-C4
5	M	855	BPH	C16-C17-C18-C19
10	M	861	LDA	C2-C3-C4-C5
11	M	900	CDL	C31-C32-C33-C34
9	M	860	SPO	C4-C1-O1-CM1
11	M	900	CDL	C17-C18-C19-C20
6	M	858	U10	C35-C34-C36-C37
10	M	863	LDA	C9-C10-C11-C12
5	M	855	BPH	C16-C17-C18-C20
9	M	860	SPO	C3-C1-O1-CM1
9	M	860	SPO	C2-C1-C4-C5

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Mol	Chain	Res	Type	Atoms
5	L	856	BPH	C12-C13-C15-C16
5	M	855	BPH	C11-C12-C13-C15
5	L	856	BPH	C14-C13-C15-C16
5	M	855	BPH	C6-C7-C8-C9
11	M	900	CDL	C51-C52-C53-C54
10	M	861	LDA	C9-C10-C11-C12
11	M	900	CDL	CA7-C31-C32-C33
6	L	859	U10	C12-C11-C9-C10
6	M	858	U10	C33-C34-C36-C37
4	M	853	BCL	O2A-C1-C2-C3
11	M	900	CDL	C40-C41-C42-C43
6	L	859	U10	C2-C3-O3-C3M
6	L	859	U10	C12-C11-C9-C8
11	M	900	CDL	OA7-CA5-OA6-CA4
5	M	855	BPH	C6-C7-C8-C10
10	H	862	LDA	C9-C10-C11-C12
4	M	853	BCL	CAD-CBD-CGD-O2D
4	M	854	BCL	CAD-CBD-CGD-O2D
5	L	856	BPH	CAD-CBD-CGD-O2D
11	M	900	CDL	CA3-CA4-CA6-OA8
11	M	900	CDL	C11-CA5-OA6-CA4
10	M	861	LDA	C2-C1-N1-CM1
10	M	861	LDA	C2-C1-N1-CM2
10	H	862	LDA	C2-C1-N1-CM1
10	H	862	LDA	C2-C1-N1-CM2
6	M	858	U10	C30-C29-C31-C32
5	L	856	BPH	C2C-C3C-CAC-CBC
10	H	862	LDA	C1-C2-C3-C4
6	M	858	U10	C28-C29-C31-C32
11	M	900	CDL	CA2-OA2-PA1-OA4
11	M	900	CDL	CA3-OA5-PA1-OA3
11	M	900	CDL	CB2-OB2-PB2-OB3
11	M	900	CDL	CB2-OB2-PB2-OB4
6	M	858	U10	C34-C36-C37-C38
6	M	858	U10	C5-C4-O4-C4M
6	L	859	U10	C33-C34-C36-C37
10	M	861	LDA	C2-C1-N1-O1
10	H	862	LDA	C2-C1-N1-O1
4	M	853	BCL	C12-C13-C15-C16
5	L	856	BPH	C4C-C3C-CAC-CBC
5	M	855	BPH	C14-C13-C15-C16
11	M	900	CDL	CA3-OA5-PA1-OA2

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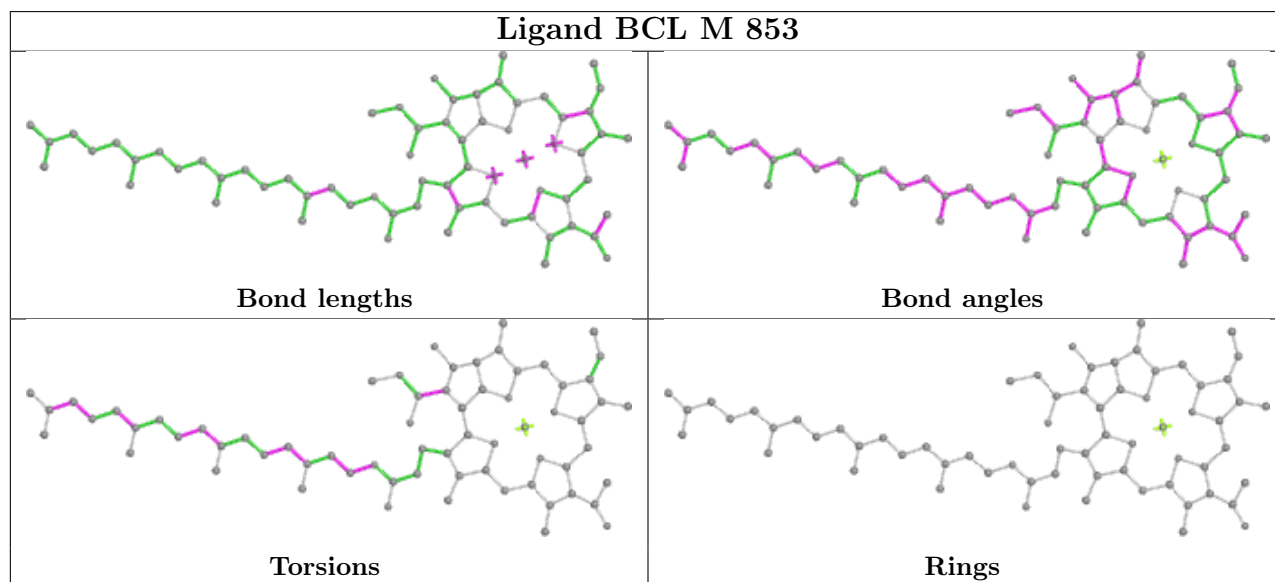
Mol	Chain	Res	Type	Atoms
9	M	860	SPO	C3-C1-C4-C5
4	M	853	BCL	C11-C10-C8-C7
10	M	863	LDA	C4-C5-C6-C7
5	M	855	BPH	C4-C3-C5-C6
4	L	852	BCL	C15-C16-C17-C18
6	L	859	U10	C15-C14-C16-C17
4	M	853	BCL	C14-C13-C15-C16
5	L	856	BPH	C6-C7-C8-C9
11	M	900	CDL	CB7-C71-C72-C73
9	M	860	SPO	C18-C17-C19-C20
9	M	860	SPO	C20-C21-C22-C23
6	L	859	U10	C4-C3-O3-C3M
11	M	900	CDL	CA5-C11-C12-C13
9	M	860	SPO	C16-C17-C19-C20
9	M	860	SPO	C1-C4-C5-C6
4	M	854	BCL	C14-C13-C15-C16
6	L	859	U10	C35-C34-C36-C37
6	L	859	U10	C18-C19-C21-C22
5	L	856	BPH	C13-C15-C16-C17
10	H	862	LDA	C11-C10-C9-C8
5	L	856	BPH	C11-C12-C13-C15
6	L	859	U10	C13-C14-C16-C17
6	M	858	U10	C3-C4-O4-C4M
11	M	900	CDL	OA6-CA4-CA6-OA8
4	L	851	BCL	CAD-CBD-CGD-O2D
5	M	855	BPH	CAD-CBD-CGD-O2D
5	M	855	BPH	C13-C15-C16-C17
4	M	854	BCL	O2A-C1-C2-C3
4	L	852	BCL	C12-C13-C15-C16
5	M	855	BPH	C2C-C3C-CAC-CBC
4	M	854	BCL	C13-C15-C16-C17
4	M	853	BCL	C2-C1-O2A-CGA
11	M	900	CDL	CB3-OB5-PB2-OB3
9	M	860	SPO	C30-C31-C32-C33
4	M	853	BCL	C16-C17-C18-C19
5	M	855	BPH	C2-C3-C5-C6
10	M	863	LDA	C2-C1-N1-O1
9	M	860	SPO	C17-C19-C20-C21
6	L	859	U10	C25-C24-C26-C27

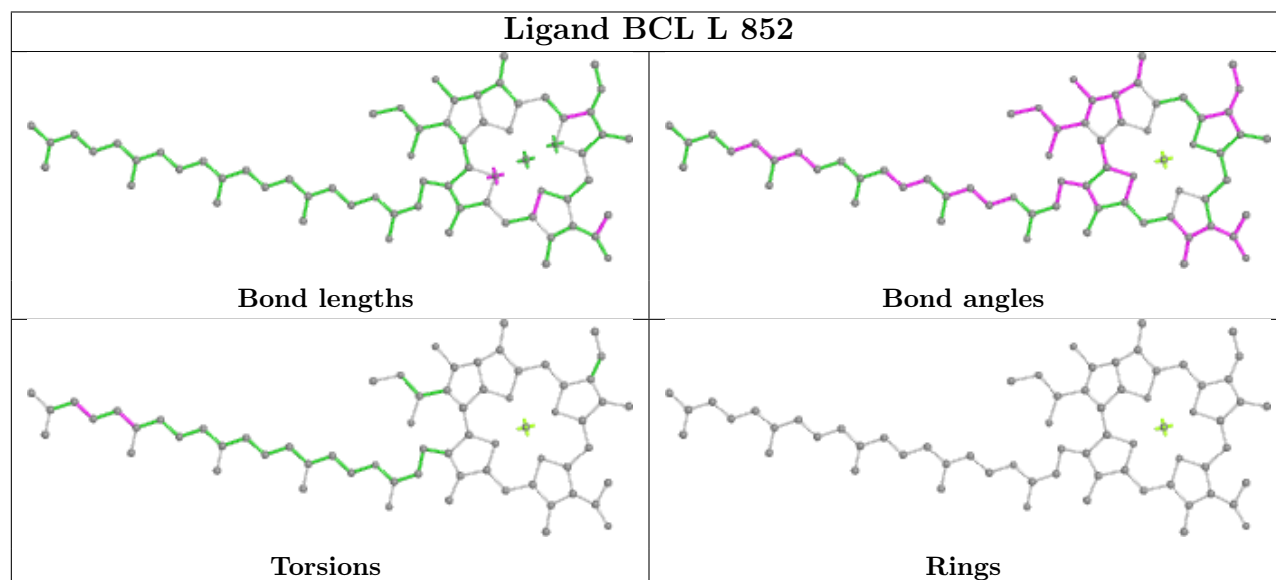
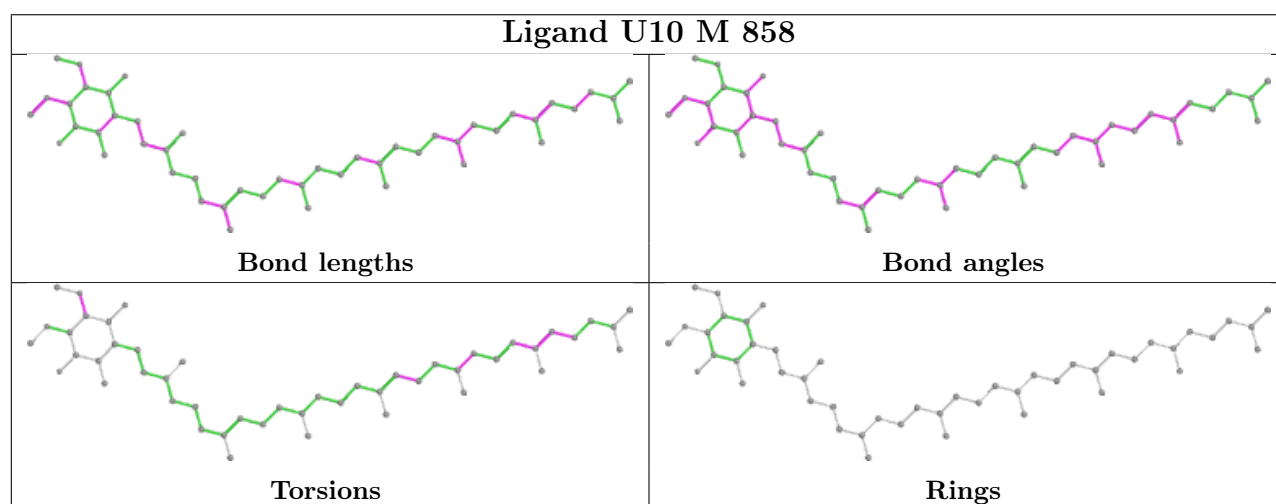
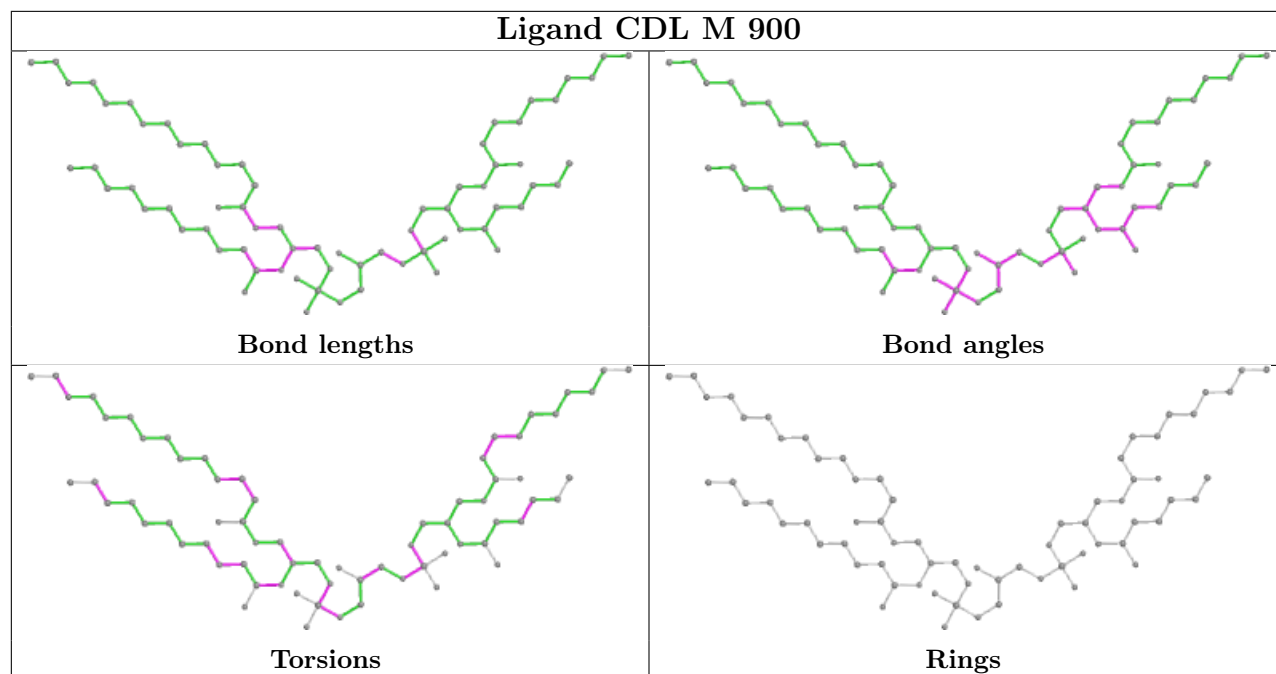
There are no ring outliers.

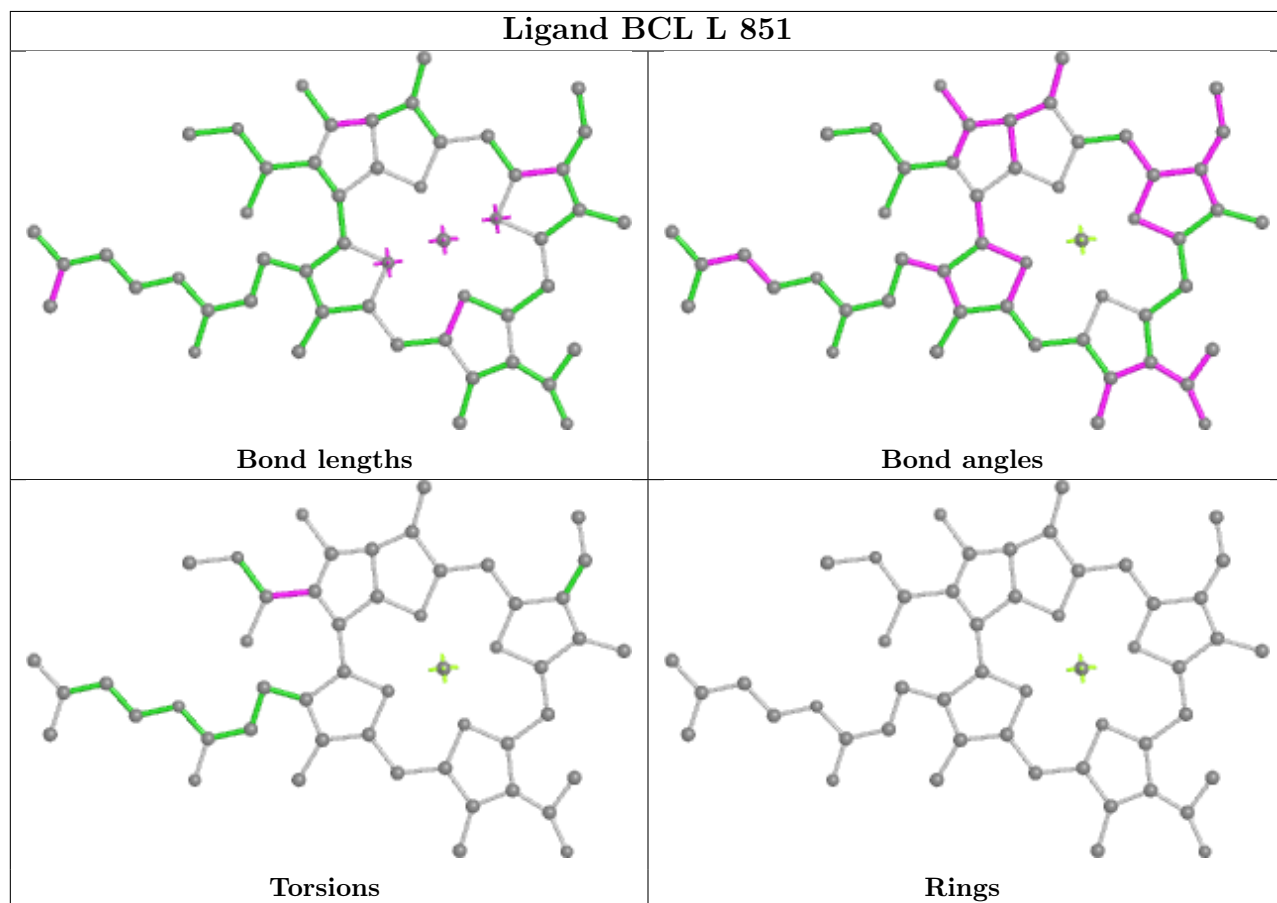
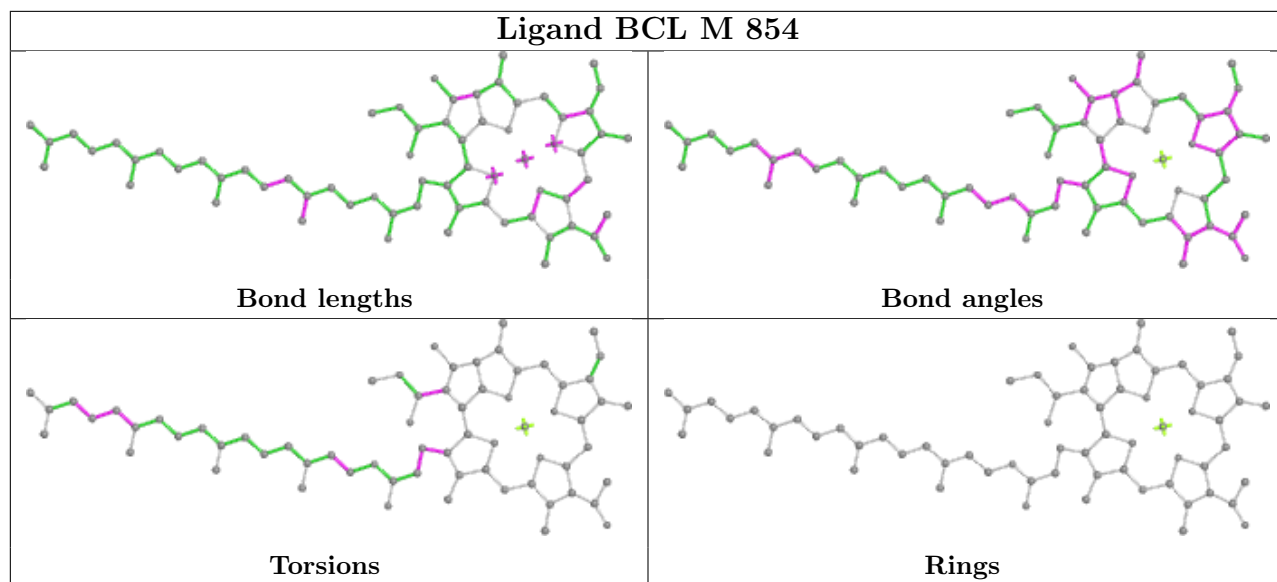
12 monomers are involved in 53 short contacts:

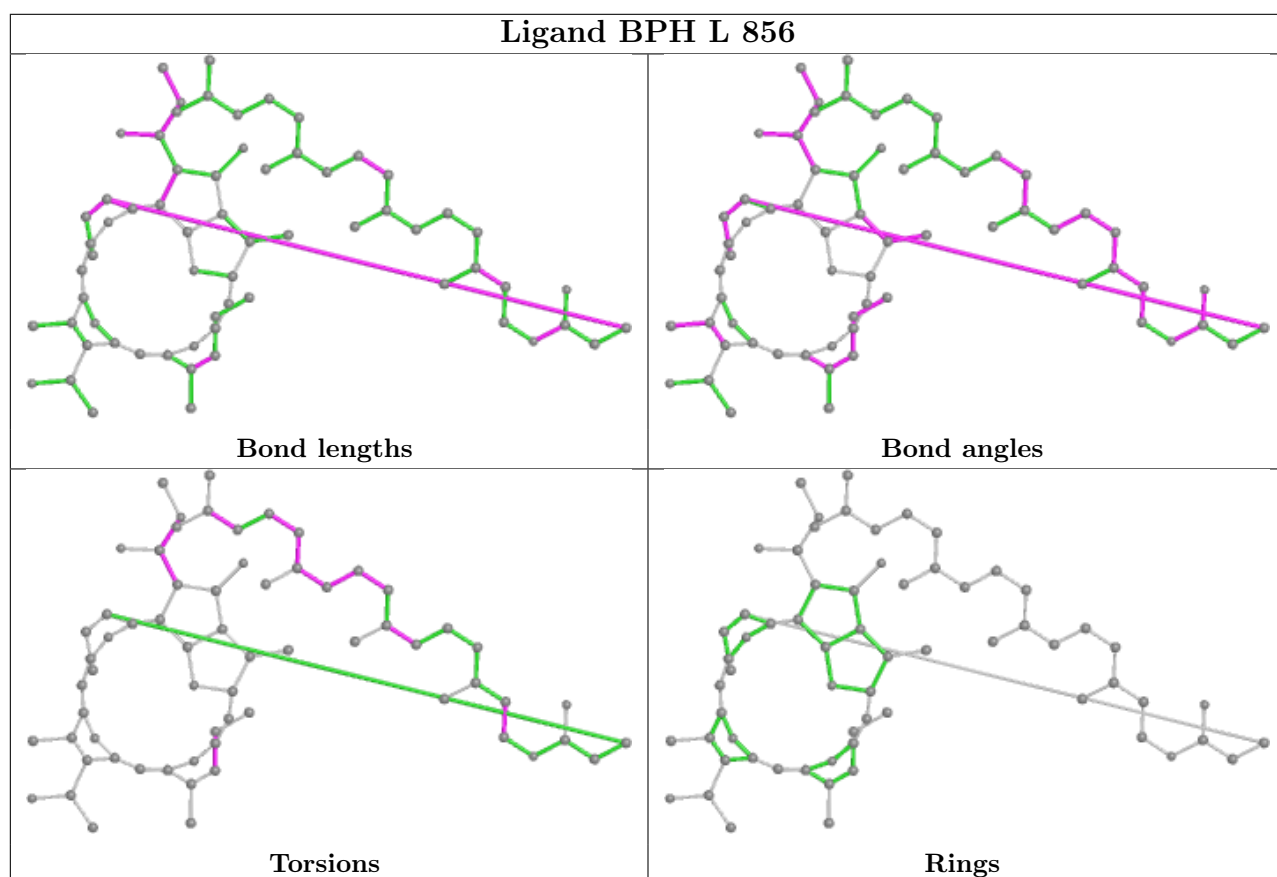
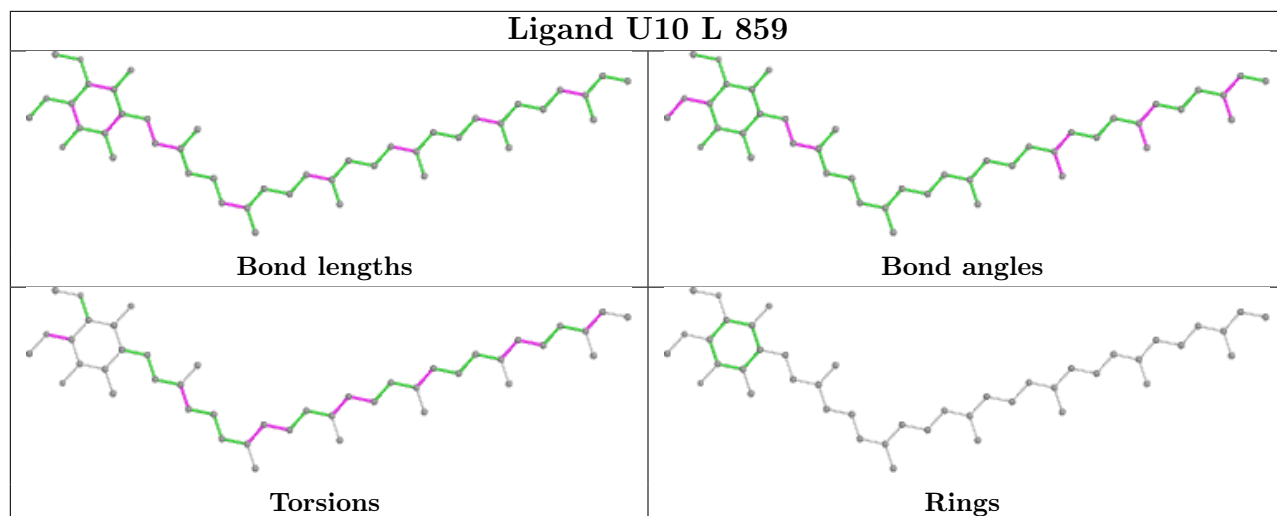
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	853	BCL	6	0
11	M	900	CDL	6	0
6	M	858	U10	3	0
4	L	852	BCL	5	0
10	H	862	LDA	1	0
4	M	854	BCL	7	0
4	L	851	BCL	7	0
6	L	859	U10	1	0
5	L	856	BPH	5	0
9	M	860	SPO	9	0
10	M	861	LDA	2	0
5	M	855	BPH	13	0

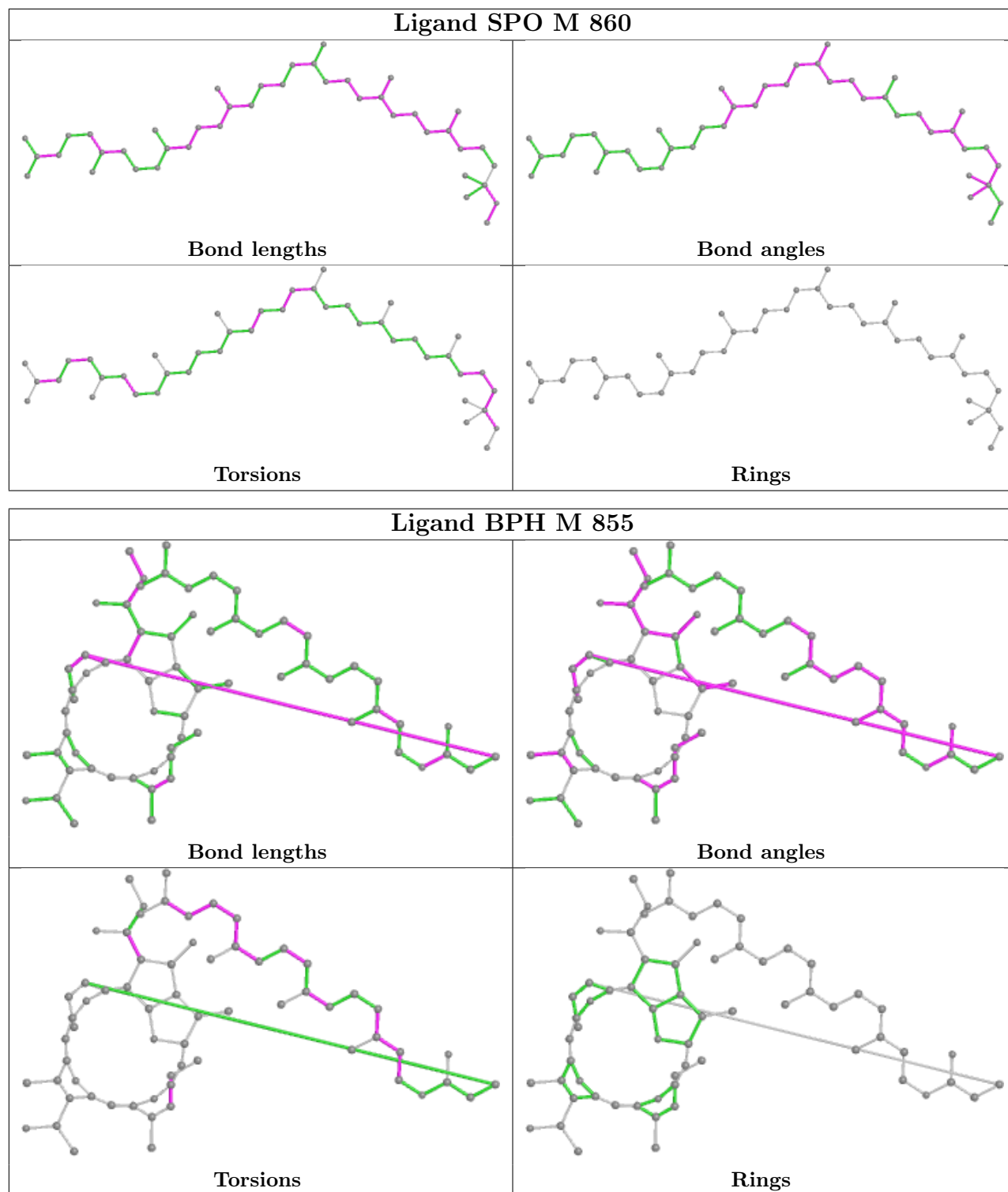
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	L	281/281 (100%)	-0.07	10 (3%) 42 51	40, 52, 77, 92	0
2	M	301/307 (98%)	0.00	12 (3%) 38 45	39, 55, 80, 112	0
3	H	238/260 (91%)	-0.04	7 (2%) 51 61	43, 55, 69, 111	0
All	All	820/848 (96%)	-0.04	29 (3%) 44 52	39, 54, 77, 112	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	6.7
3	H	246	PRO	6.4
1	L	277	GLY	5.0
3	H	245	ALA	4.5
2	M	3	TYR	4.2
3	H	247	LYS	3.9
1	L	281	GLY	3.3
2	M	76	TYR	3.2
1	L	59	TRP	3.1
2	M	80	TRP	3.1
1	L	276	PRO	3.0
1	L	270	PRO	3.0
3	H	53	GLN	2.7
2	M	27	ALA	2.7
1	L	279	ILE	2.6
2	M	2	GLU	2.4
2	M	106	ALA	2.3
3	H	52	ASN	2.2
3	H	60	LYS	2.2
1	L	202	LYS	2.2
1	L	269	LEU	2.2
2	M	105	PHE	2.2
1	L	278	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	M	82	PRO	2.1
3	H	159	GLU	2.1
2	M	24	VAL	2.1
2	M	148	TRP	2.1
1	L	186	ALA	2.0
2	M	78	ALA	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.

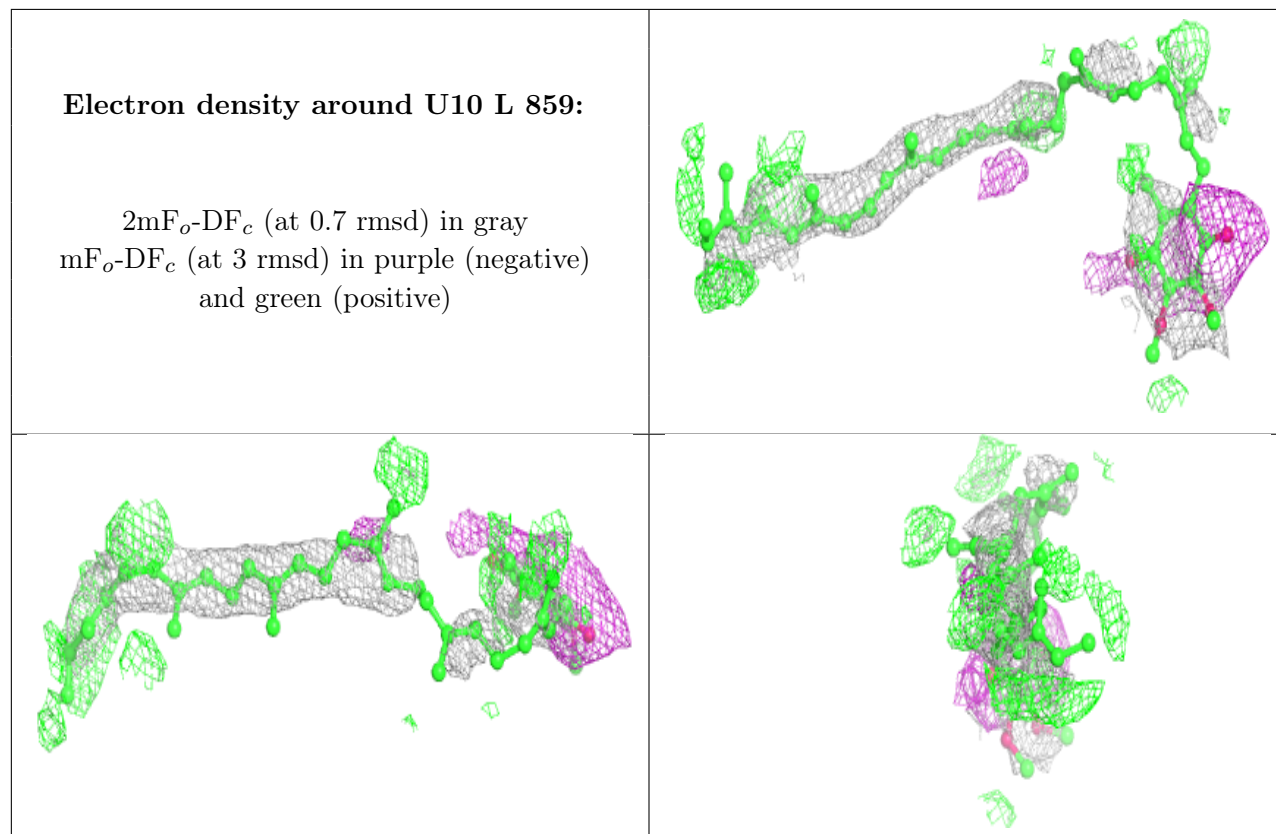
## 6.4 Ligands [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	U10	L	859	44/63	0.66	0.46	92,100,103,107	0
10	LDA	M	863	16/16	0.76	0.42	93,95,103,104	0
11	CDL	M	900	69/100	0.81	0.38	93,106,120,122	0
10	LDA	M	861	16/16	0.85	0.27	60,69,80,81	0
9	SPO	M	860	42/42	0.88	0.34	48,67,86,88	0
5	BPH	M	855	65/65	0.89	0.25	46,51,100,102	0
6	U10	M	858	48/63	0.91	0.27	47,59,84,85	0
10	LDA	H	862	16/16	0.93	0.23	66,68,78,79	0
8	PO4	M	864	5/5	0.93	0.14	91,93,94,94	0
4	BCL	L	852	66/66	0.95	0.18	38,49,52,53	0
4	BCL	M	854	66/66	0.95	0.18	35,40,62,64	0
5	BPH	L	856	65/65	0.95	0.20	37,43,52,54	0
4	BCL	L	851	51/66	0.95	0.23	39,45,68,70	0
4	BCL	M	853	66/66	0.96	0.21	44,50,63,70	0
7	FE2	M	857	1/1	0.99	0.16	45,45,45,45	0

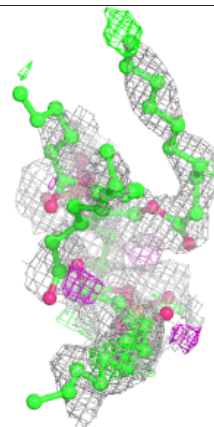
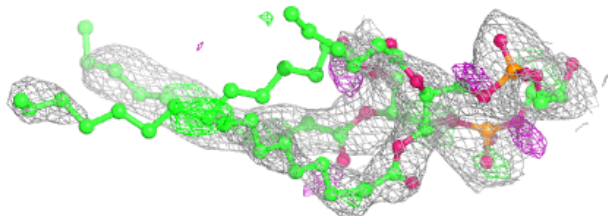
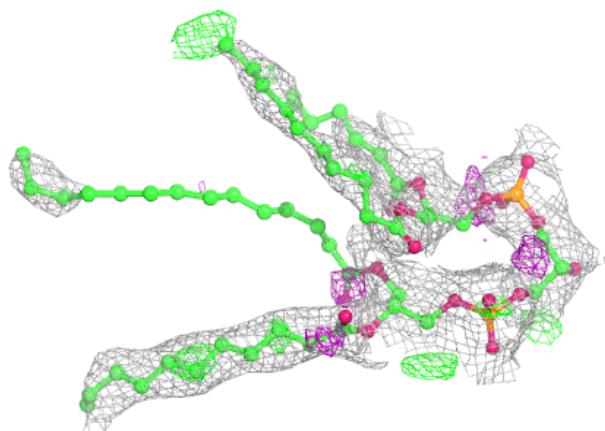
The following is a graphical depiction of the model fit to experimental electron density of all

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.

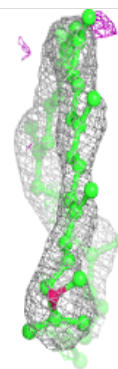
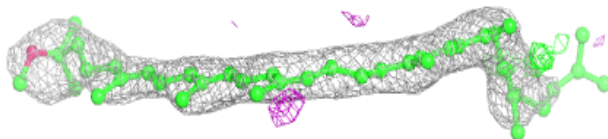
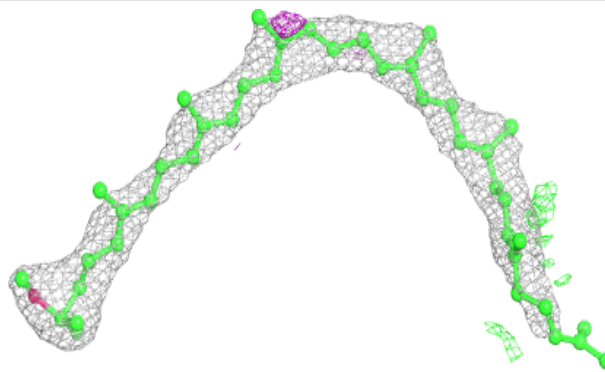


**Electron density around CDL M 900:**

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

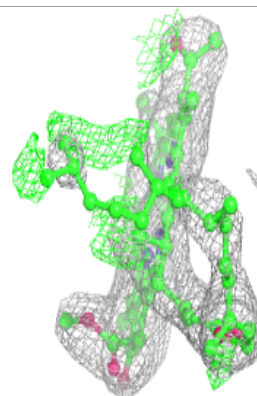
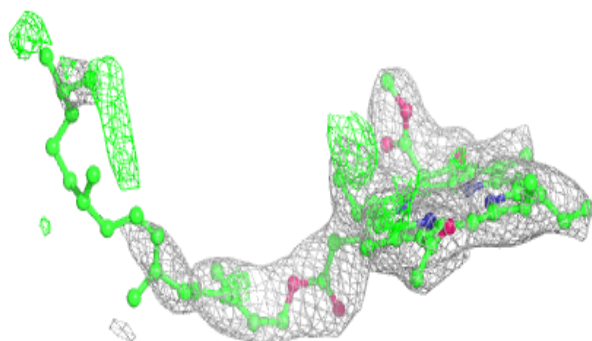
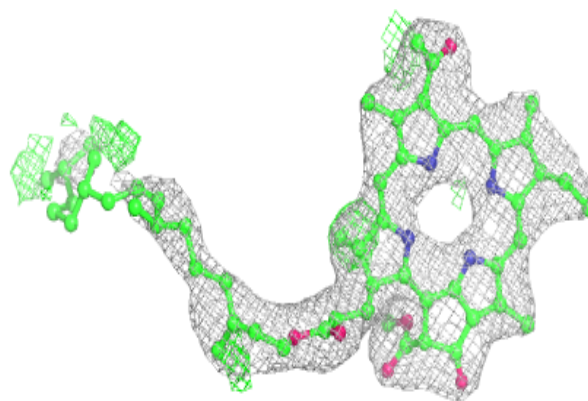
**Electron density around SPO M 860:**

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

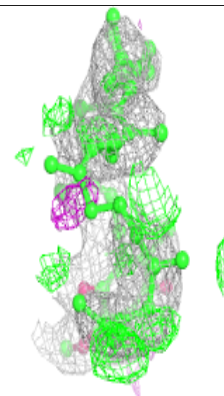
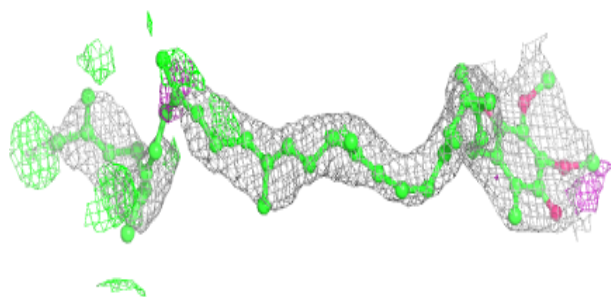
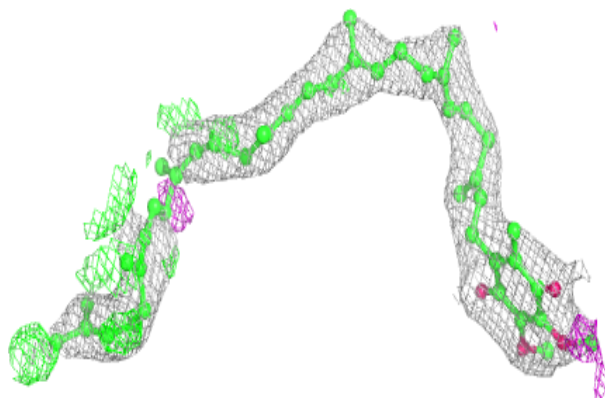


**Electron density around BPH M 855:**

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

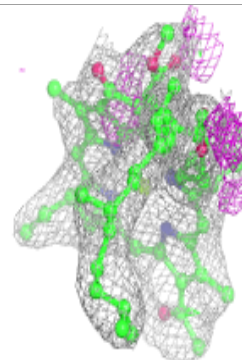
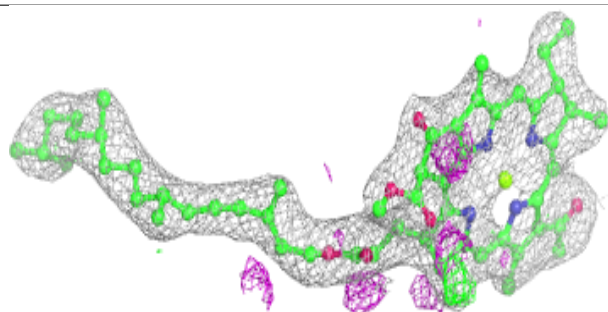
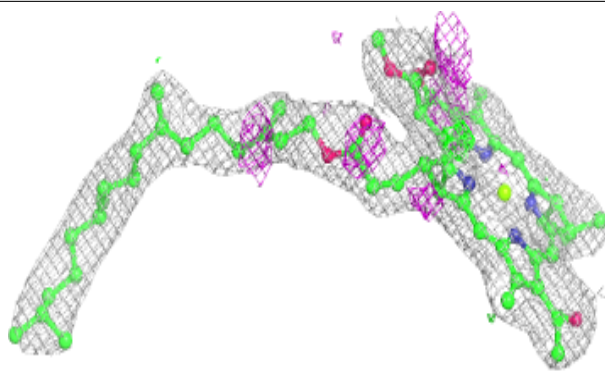
**Electron density around U10 M 858:**

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

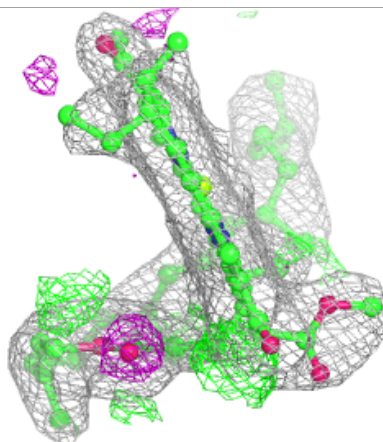
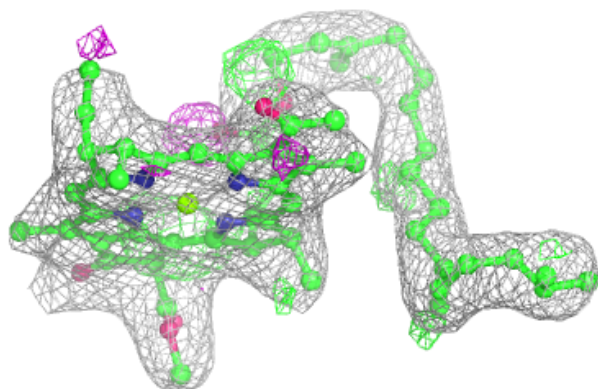
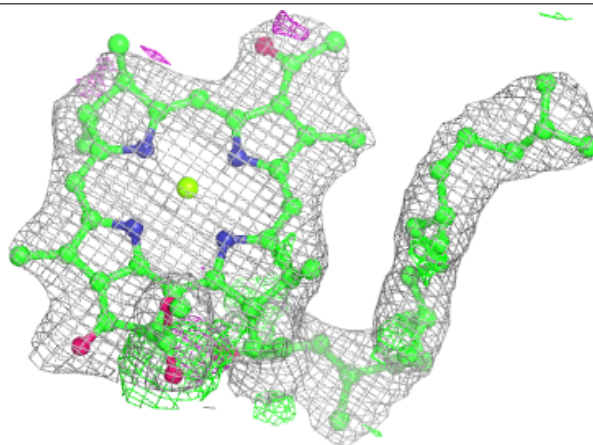


**Electron density around BCL L 852:**

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

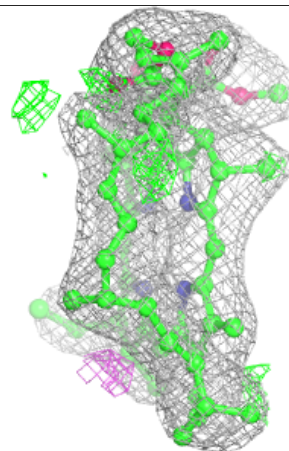
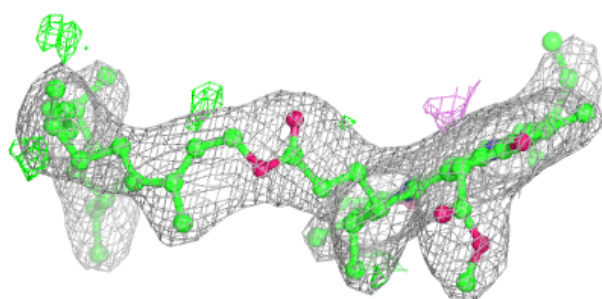
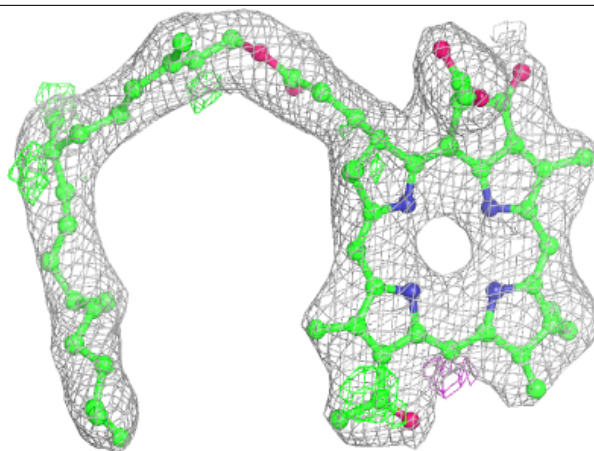
**Electron density around BCL M 854:**

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



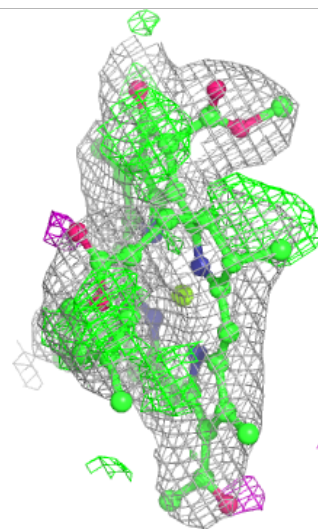
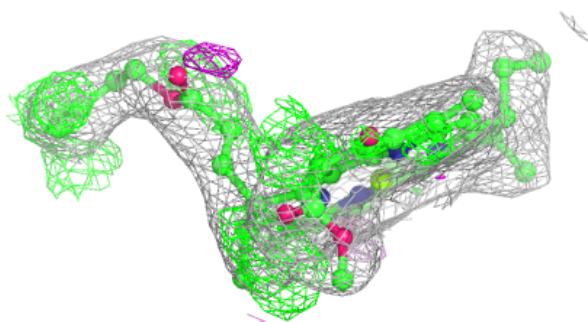
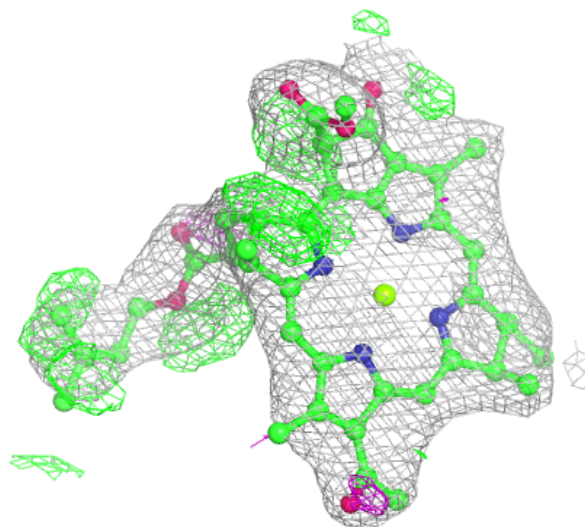
**Electron density around BPH L 856:**

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

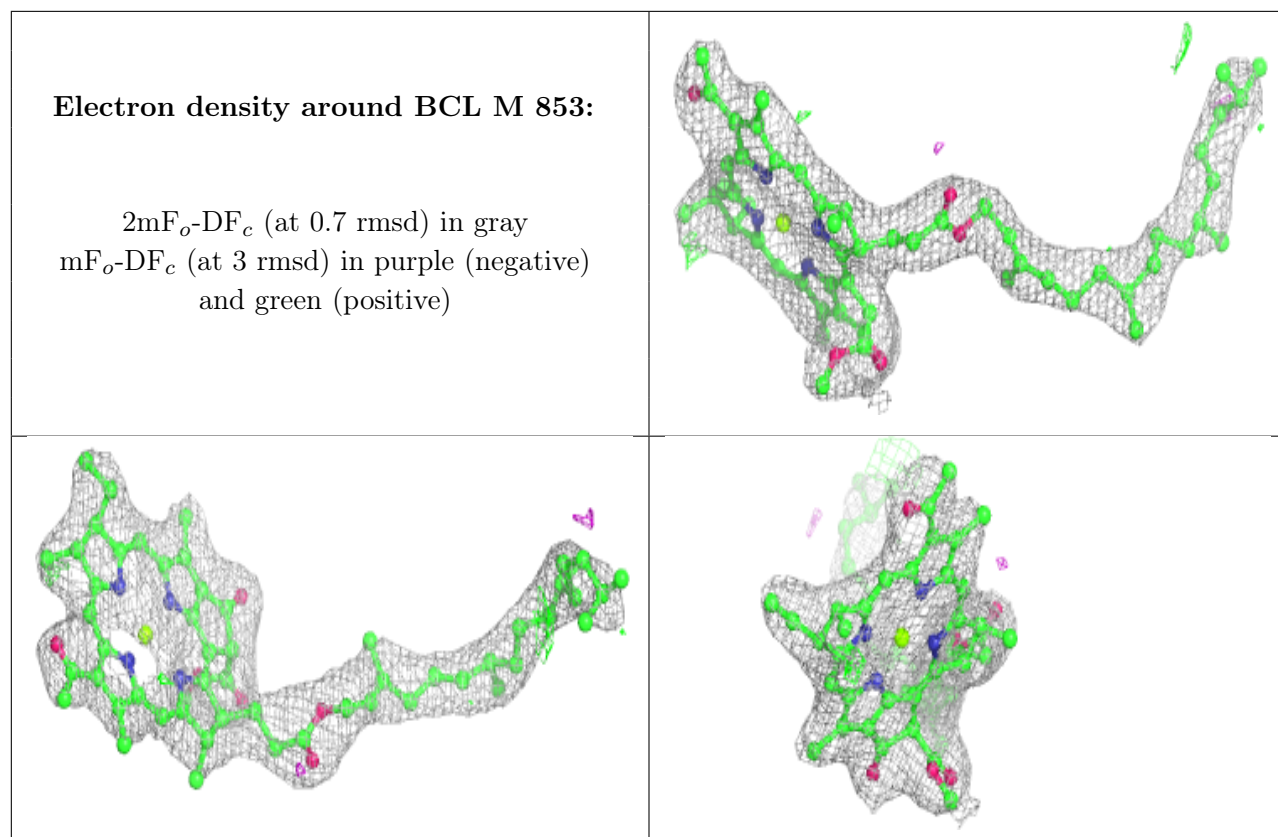


**Electron density around BCL L 851:**

$2mF_o-DF_c$  (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.