



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2023 – 06:24 AM EDT

PDB ID : 1Z9J
Title : Photosynthetic Reaction Center from Rhodobacter sphaeroides
Authors : Thielges, M.; Uyeda, G.; Camara-Artigas, A.; Kalman, L.; Williams, J.C.; Allen, J.P.
Deposited on : 2005-04-02
Resolution : 4.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

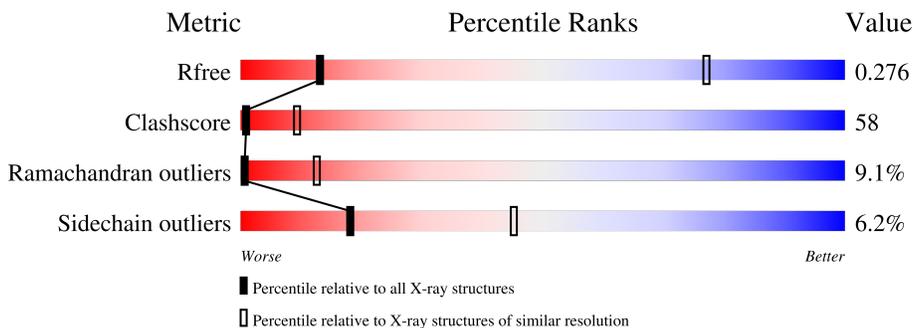
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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}	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	281	25% (green) 62% (yellow) 12% (orange) . (red)
2	B	307	26% (green) 62% (yellow) 10% (orange) .. (red)
3	C	260	36% (green) 49% (yellow) 7% (orange) 8% (grey)

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6957 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	A	281	2234	1507	357	362	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	HIS	LEU	engineered mutation	UNP P0C0Y8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	302	2415	1609	395	402	9	0	0	0

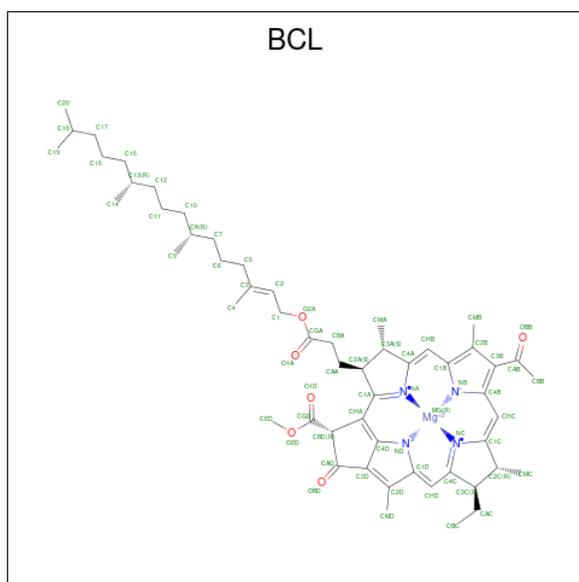
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	160	HIS	LEU	engineered mutation	UNP P0C0Y9
B	164	TYR	ARG	engineered mutation	UNP P0C0Y9
B	168	GLU	MET	engineered mutation	UNP P0C0Y9
B	197	HIS	PHE	engineered mutation	UNP P0C0Y9
B	288	ASP	GLY	engineered mutation	UNP P0C0Y9

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

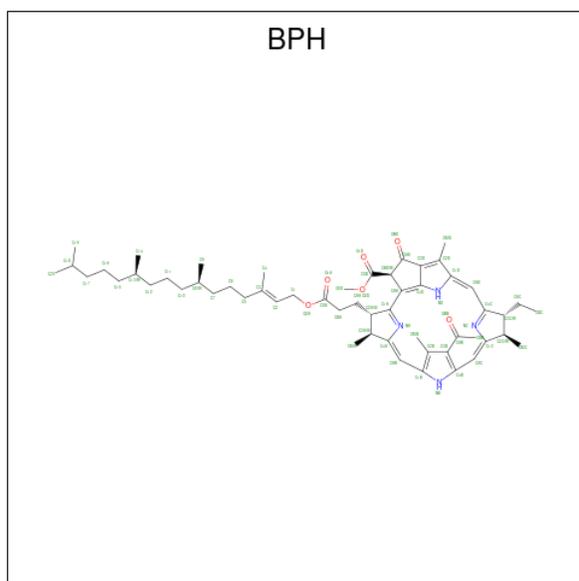
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	238	1814	1160	311	334	9	0	0	0

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



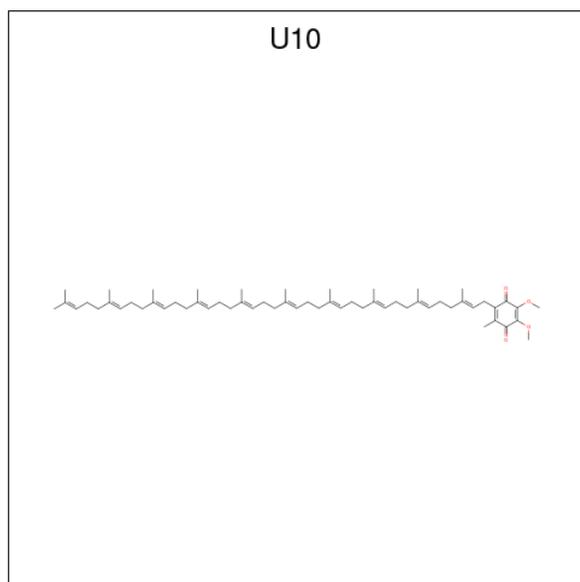
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Mg	N			O
4	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



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

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: C₅₉H₉₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			48	44	4		
6	B	1	Total	C	O	0	0
			48	44	4		

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

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

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Mn	0	0
			1	1		

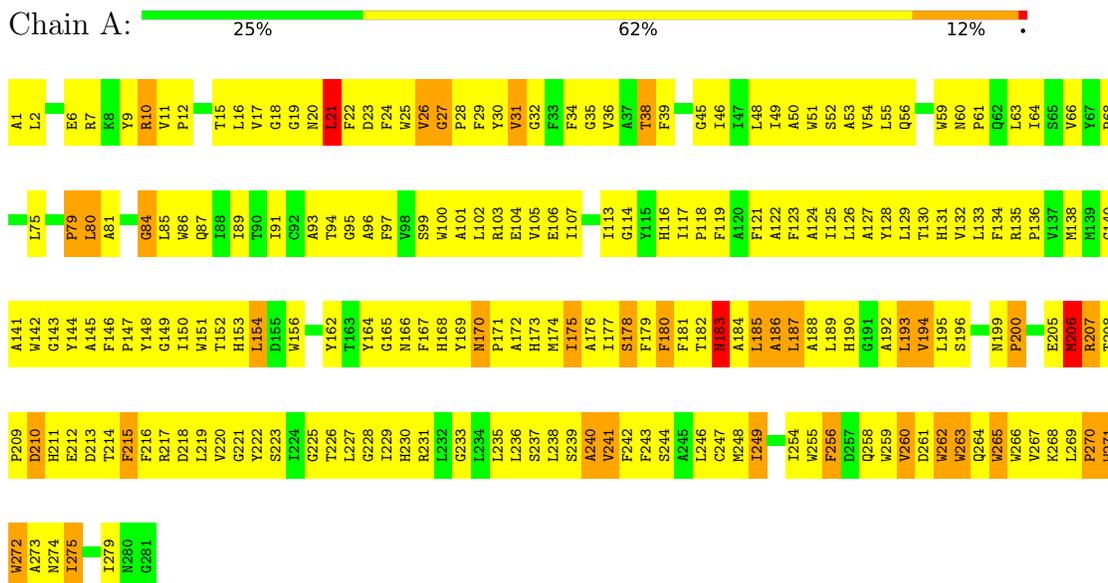
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	2	Total O 2 2	0	0

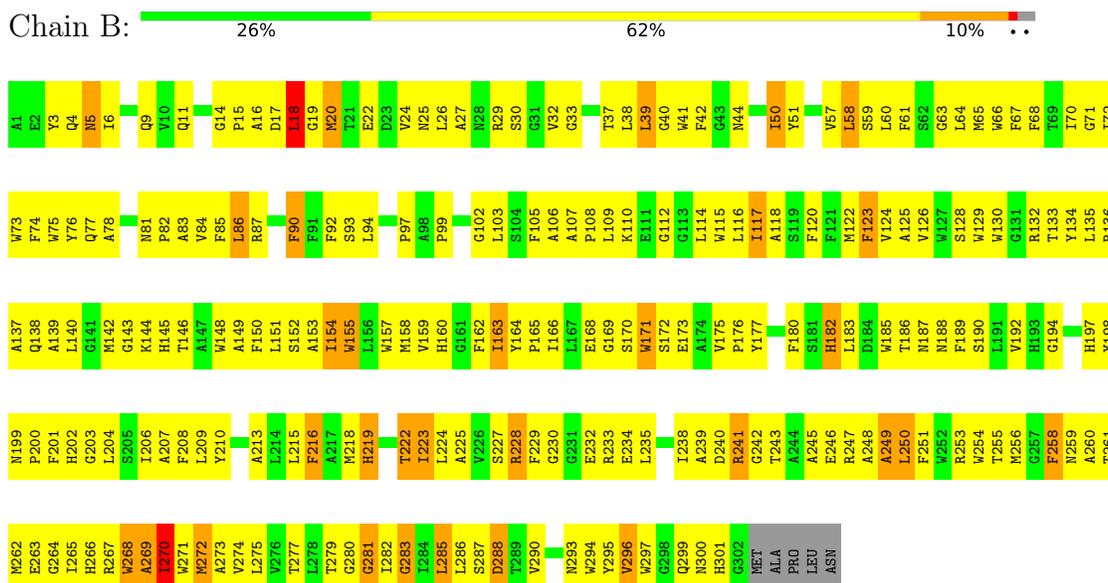
3 Residue-property plots

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. 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. 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.

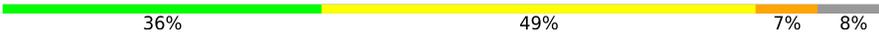
- Molecule 1: Reaction center protein L chain

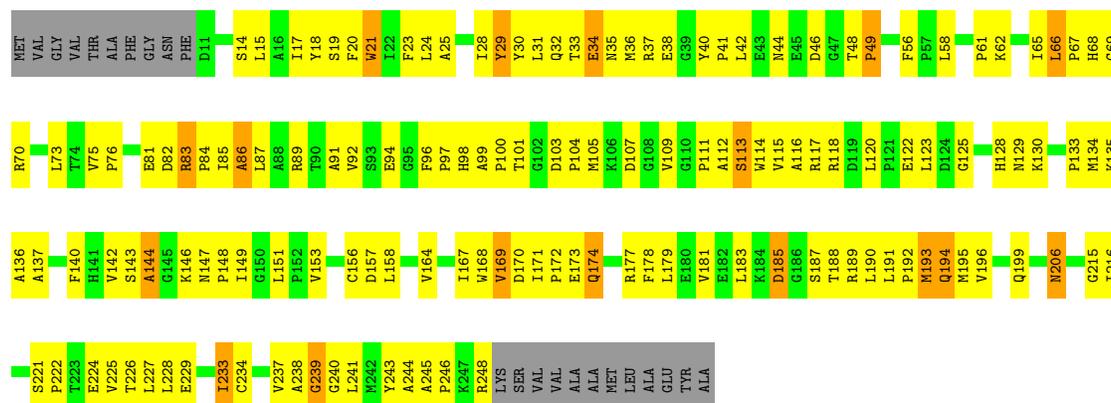


- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain

Chain C:  36% 49% 7% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	203.84Å 203.84Å 119.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 4.50 24.90 – 4.30	Depositor EDS
% Data completeness (in resolution range)	79.9 (19.96-4.50) 80.7 (24.90-4.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 4.24Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.299 , 0.338 0.221 , 0.276	Depositor DCC
R_{free} test set	712 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	145.2	Xtrriage
Anisotropy	0.494	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , -0.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6957	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	A	0.63	0/2323	0.80	1/3179 (0.0%)
2	B	0.63	0/2509	0.79	1/3428 (0.0%)
3	C	0.62	1/1862 (0.1%)	0.80	0/2534
All	All	0.62	1/6694 (0.0%)	0.80	2/9141 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	21	TRP	CB-CG	-5.17	1.41	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	GLY	N-CA-C	-5.09	100.38	113.10
2	B	285	LEU	CA-CB-CG	-5.03	103.73	115.30

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	A	2234	0	2183	329	0
2	B	2415	0	2309	368	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1814	0	1818	187	1
4	A	132	0	148	20	0
4	B	132	0	148	18	0
5	A	65	0	76	19	0
5	B	65	0	76	14	0
6	A	48	0	63	7	0
6	B	48	0	63	15	0
7	B	1	0	0	0	0
8	B	1	0	0	0	0
9	B	2	0	0	1	0
All	All	6957	0	6884	802	1

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 58.

The worst 5 of 802 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)
2:B:64:LEU:HD21	5:B:854:BPH:H112	1.32	1.10
2:B:267:ARG:O	2:B:270:ILE:HG22	1.65	0.96
1:A:171:PRO:HA	1:A:174:MET:HG3	1.48	0.95
2:B:242:GLY:HA2	3:C:117:ARG:HD2	1.49	0.94
1:A:114:GLY:H	2:B:225:ALA:HB1	1.32	0.93

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:128:HIS:NE2	3:C:128:HIS:NE2[5_656]	2.18	0.02

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	A	279/281 (99%)	199 (71%)	51 (18%)	29 (10%)	0	9
2	B	300/307 (98%)	202 (67%)	69 (23%)	29 (10%)	0	11
3	C	236/260 (91%)	175 (74%)	45 (19%)	16 (7%)	1	17
All	All	815/848 (96%)	576 (71%)	165 (20%)	74 (9%)	1	12

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	80	LEU
1	A	186	ALA
1	A	200	PRO
1	A	215	PHE

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	A	220/220 (100%)	201 (91%)	19 (9%)	10	35
2	B	237/241 (98%)	223 (94%)	14 (6%)	19	47
3	C	193/208 (93%)	186 (96%)	7 (4%)	35	60
All	All	650/669 (97%)	610 (94%)	40 (6%)	18	45

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	188	ASN
3	C	169	VAL
2	B	197	HIS
2	B	270	ILE
3	C	206	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	44	ASN
3	C	68	HIS
3	C	206	ASN
3	C	129	ASN
2	B	202	HIS

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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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$
6	U10	B	856	-	48,48,63	2.43	13 (27%)	58,61,79	2.06	19 (32%)
5	BPH	B	854	-	51,70,70	1.84	10 (19%)	52,101,101	1.89	12 (23%)
6	U10	A	857	-	48,48,63	2.70	16 (33%)	58,61,79	2.07	18 (31%)
5	BPH	A	855	-	51,70,70	1.72	8 (15%)	52,101,101	1.82	10 (19%)
4	BCL	B	852	2	58,74,74	1.53	12 (20%)	69,115,115	2.00	16 (23%)
4	BCL	B	853	1	58,74,74	1.47	10 (17%)	69,115,115	2.10	22 (31%)
4	BCL	A	851	1	58,74,74	1.54	12 (20%)	69,115,115	1.82	11 (15%)
4	BCL	A	850	-	58,74,74	1.66	13 (22%)	69,115,115	1.98	17 (24%)

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
6	U10	B	856	-	-	12/45/69/87	0/1/1/1
5	BPH	B	854	-	-	8/37/105/105	0/5/6/6
6	U10	A	857	-	-	12/45/69/87	0/1/1/1
5	BPH	A	855	-	-	7/37/105/105	0/5/6/6
4	BCL	B	852	2	-	11/37/137/137	-
4	BCL	B	853	1	-	12/37/137/137	-
4	BCL	A	851	1	-	6/37/137/137	-
4	BCL	A	850	-	-	8/37/137/137	-

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	856	U10	C6-C1	10.41	1.54	1.35
6	A	857	U10	C6-C1	10.08	1.53	1.35
5	B	854	BPH	C2C-C3C	-5.73	1.49	1.54
5	B	854	BPH	C3A-C2A	-5.54	1.49	1.54
5	A	855	BPH	C3A-C2A	-5.52	1.49	1.54

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	853	BCL	CMB-C2B-C1B	-6.89	117.88	128.46
4	A	850	BCL	CMB-C2B-C1B	-6.70	118.16	128.46
4	B	853	BCL	CAA-C2A-C1A	-6.68	90.10	111.97
4	A	851	BCL	CMB-C2B-C1B	-6.64	118.25	128.46
4	B	852	BCL	CMB-C2B-C1B	-6.41	118.61	128.46

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

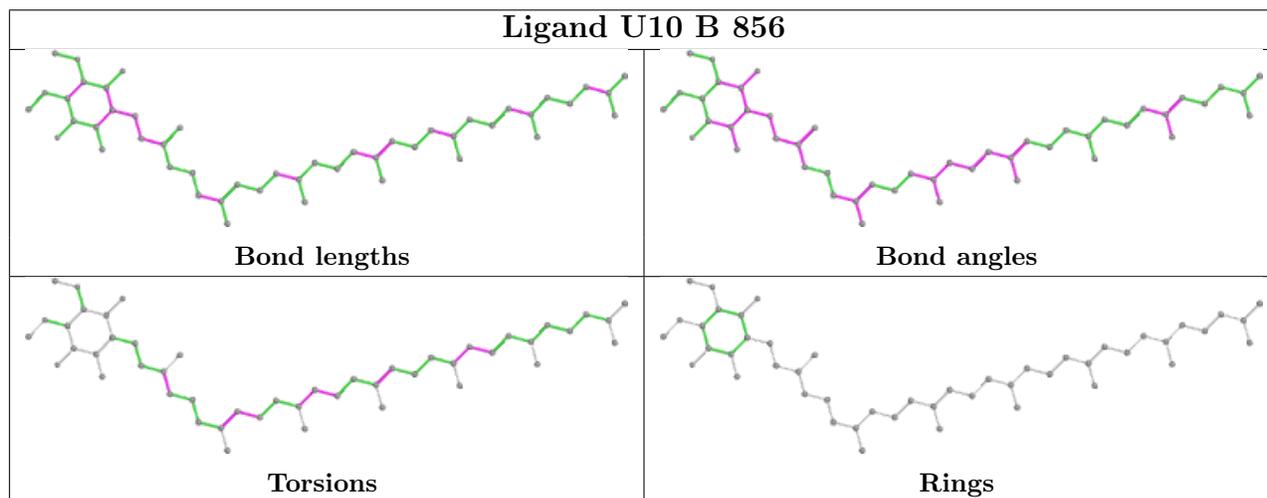
Mol	Chain	Res	Type	Atoms
4	A	850	BCL	C2C-C3C-CAC-CBC
4	A	850	BCL	C4C-C3C-CAC-CBC
4	B	852	BCL	C2C-C3C-CAC-CBC
4	B	852	BCL	C4C-C3C-CAC-CBC
5	A	855	BPH	C4C-C3C-CAC-CBC

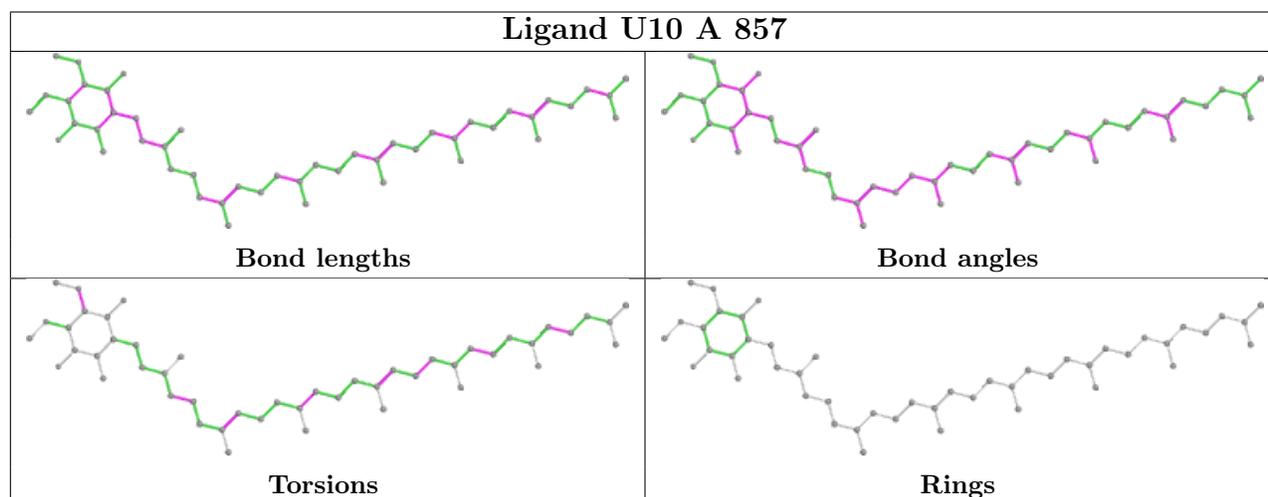
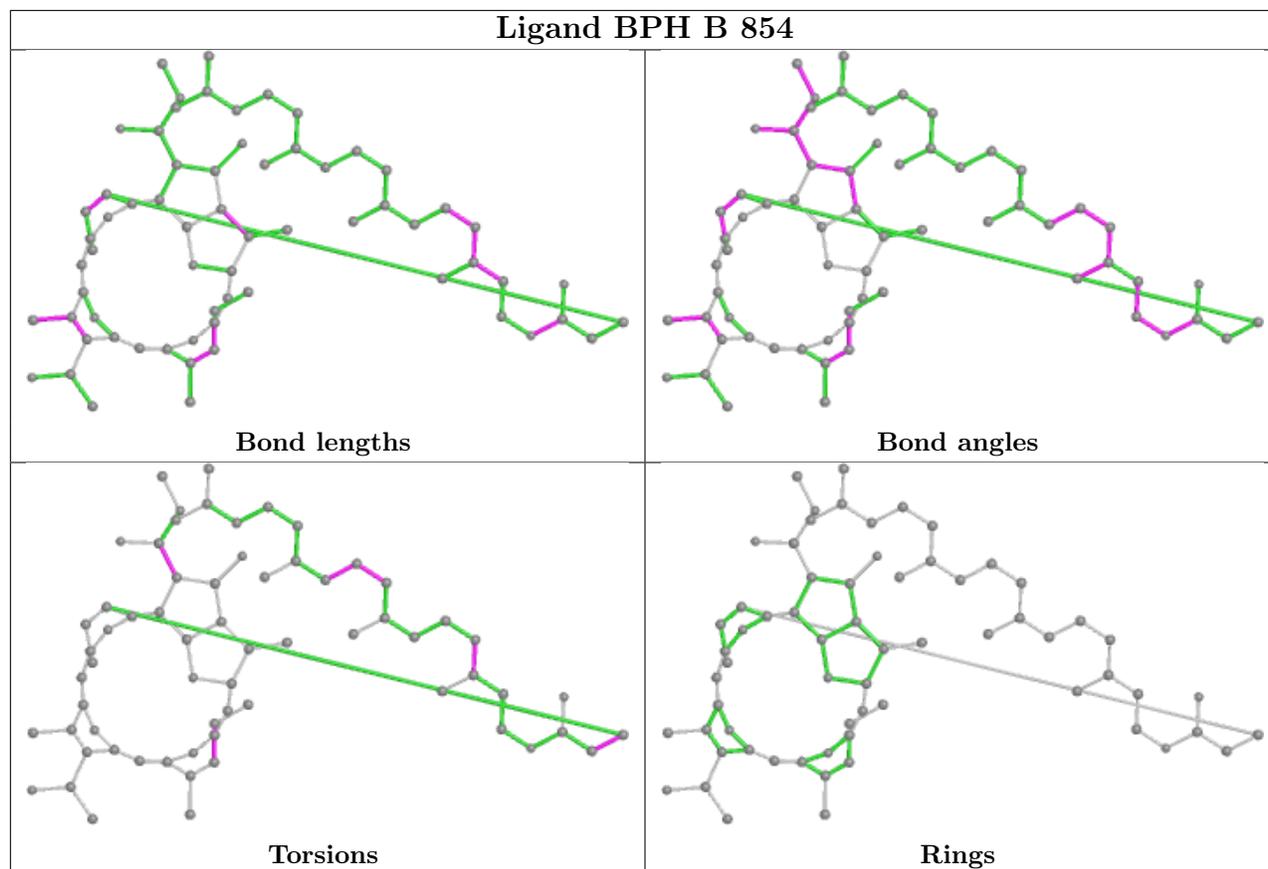
There are no ring outliers.

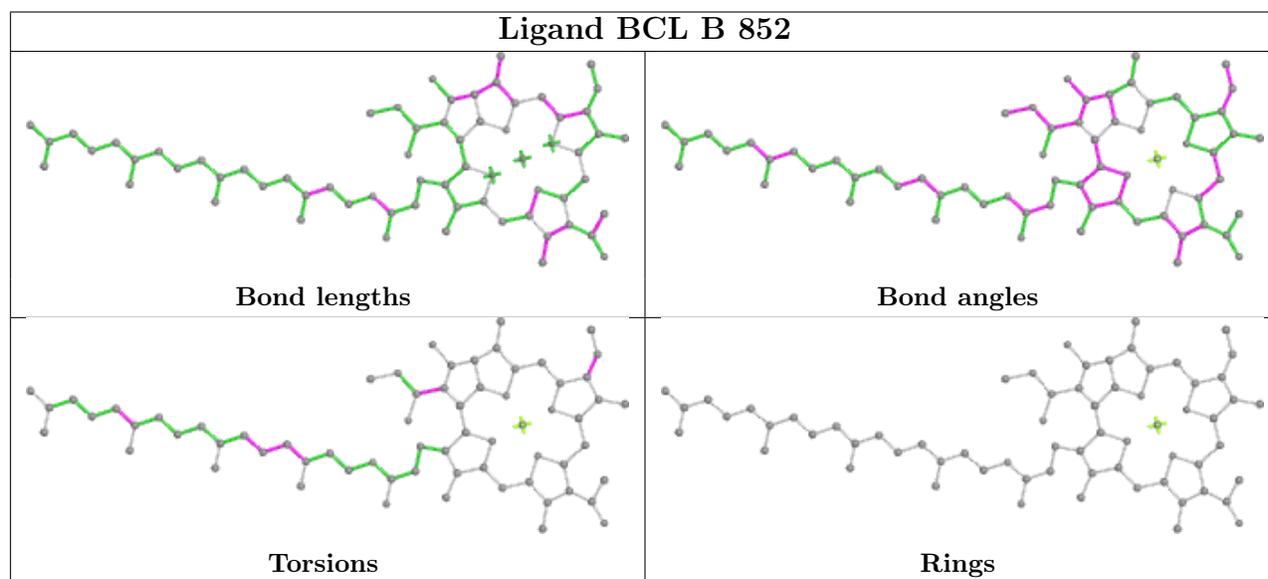
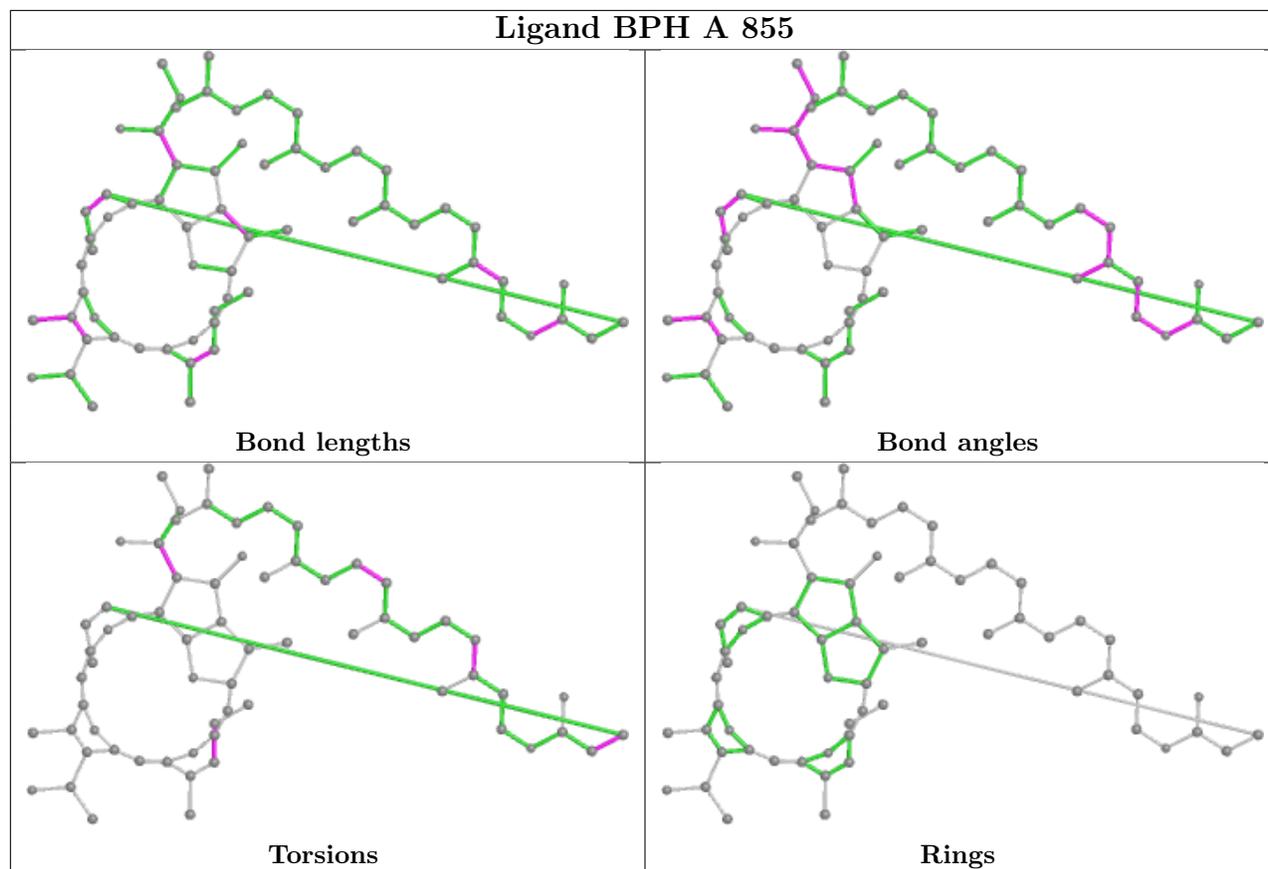
8 monomers are involved in 87 short contacts:

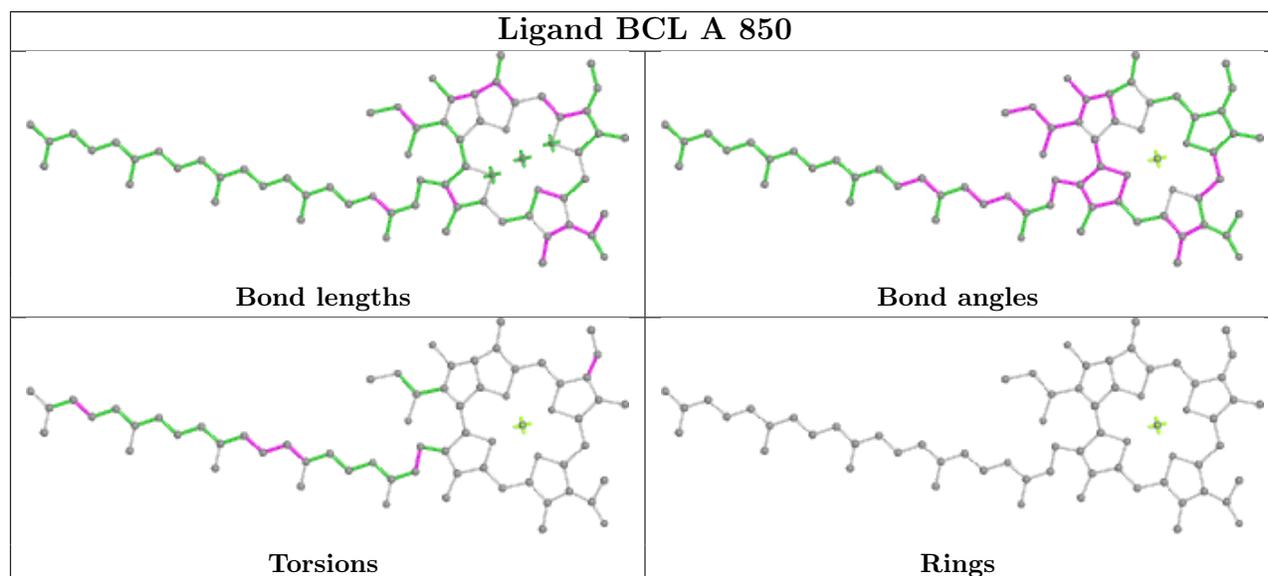
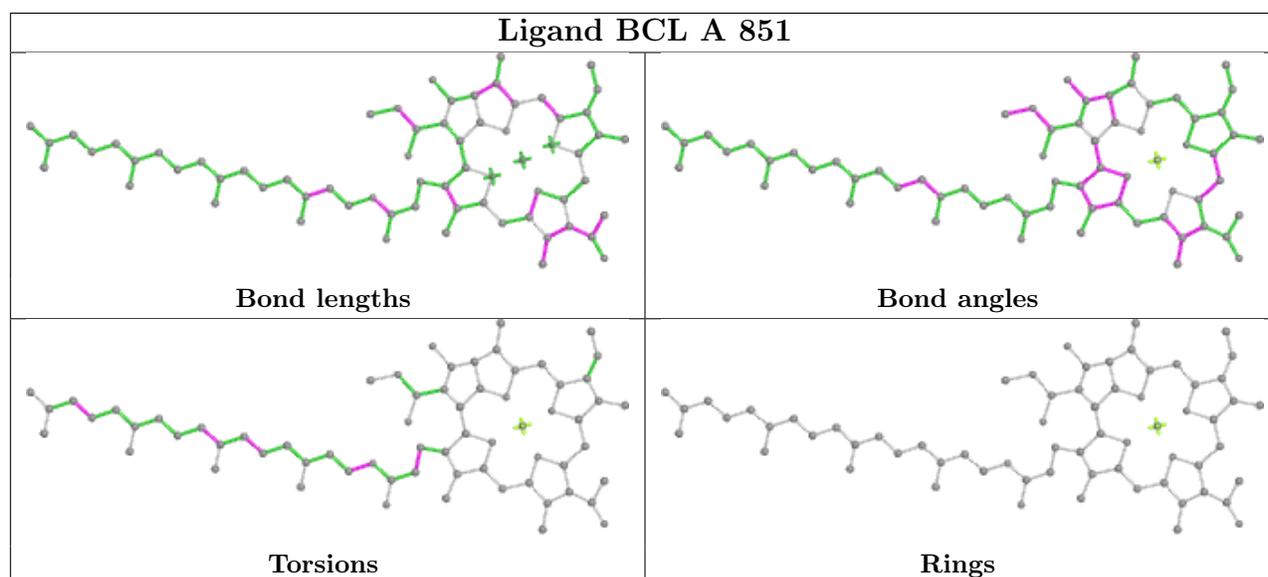
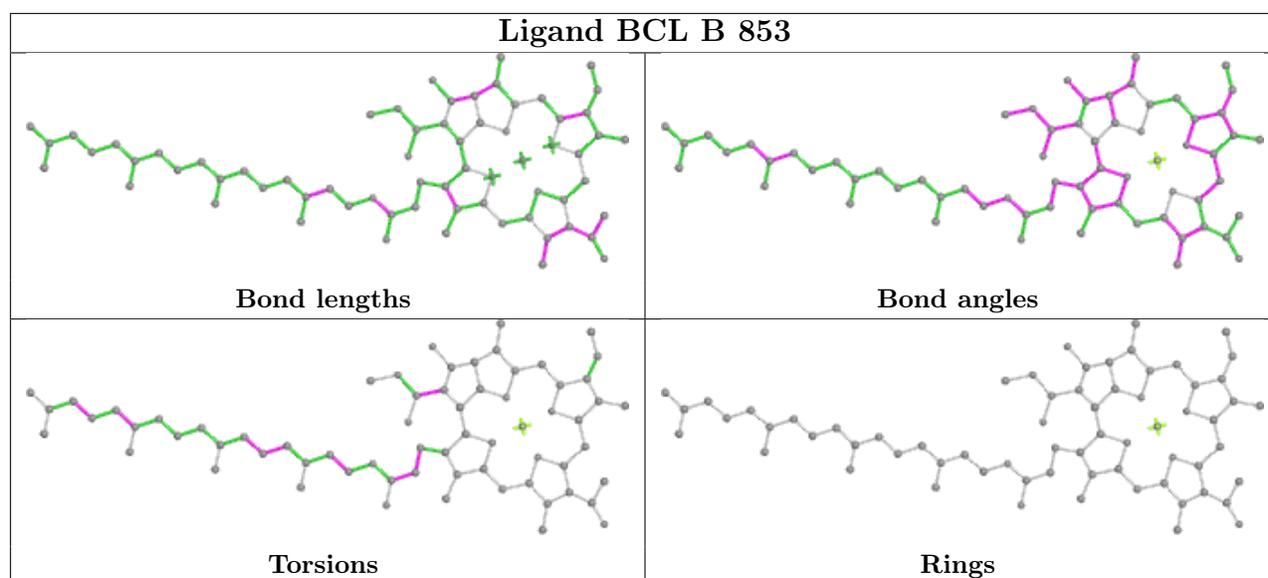
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	856	U10	15	0
5	B	854	BPH	14	0
6	A	857	U10	7	0
5	A	855	BPH	19	0
4	B	852	BCL	9	0
4	B	853	BCL	11	0
4	A	851	BCL	11	0
4	A	850	BCL	11	0

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

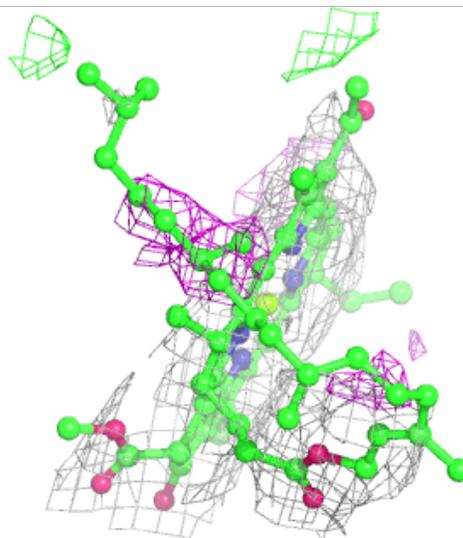
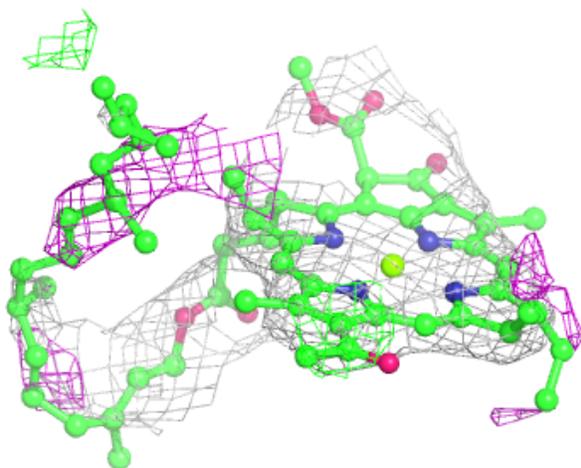
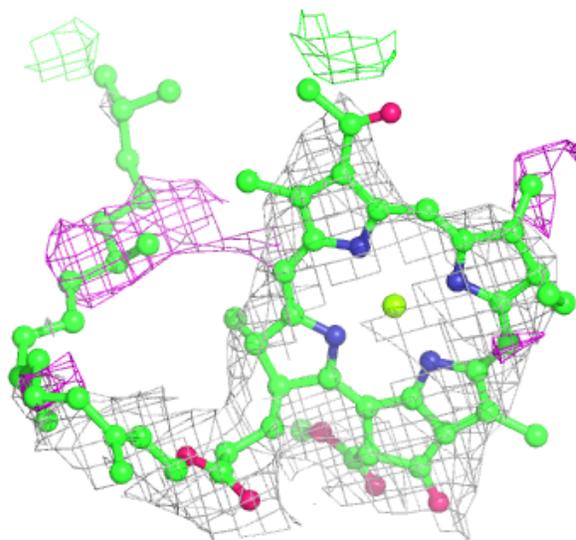
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

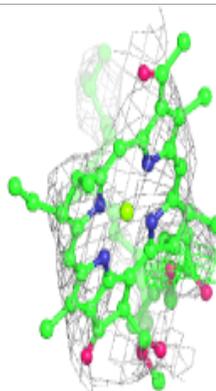
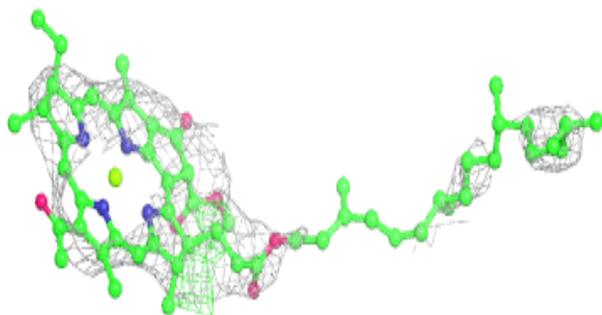
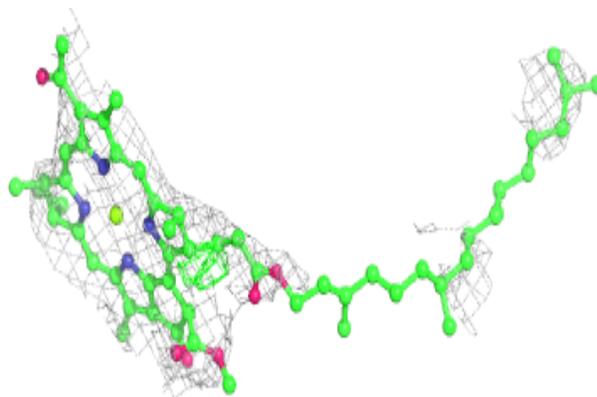
Electron density around BCL A 850:

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

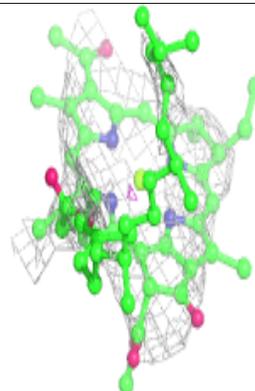
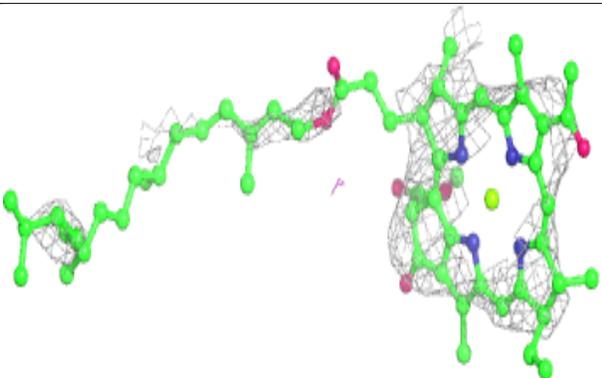
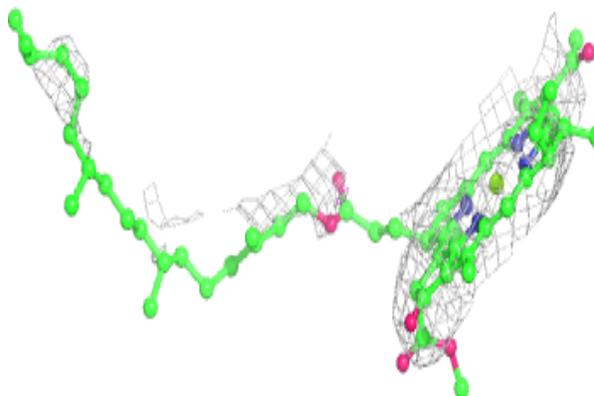


Electron density around BCL A 851:

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

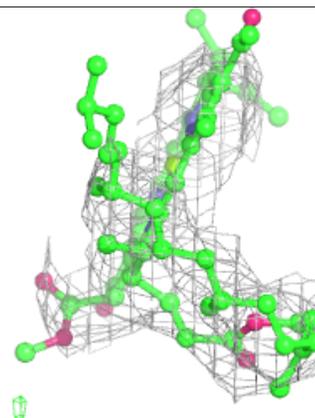
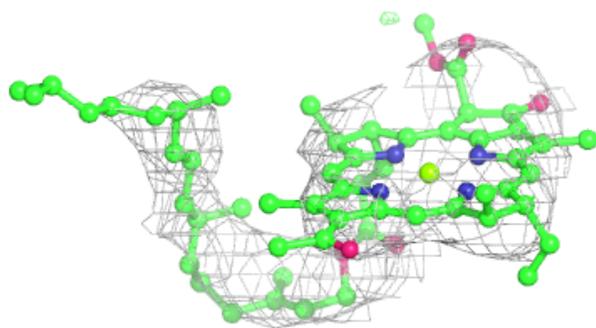
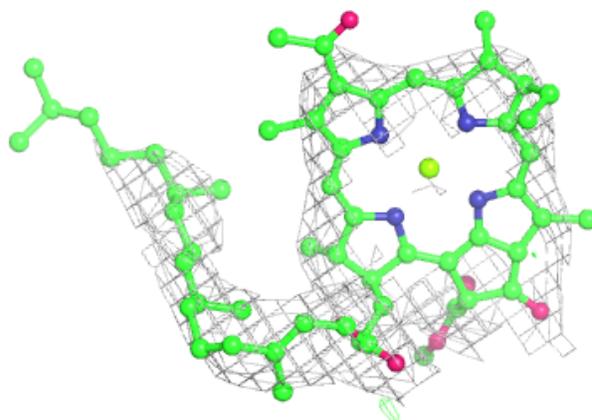
**Electron density around BCL B 852:**

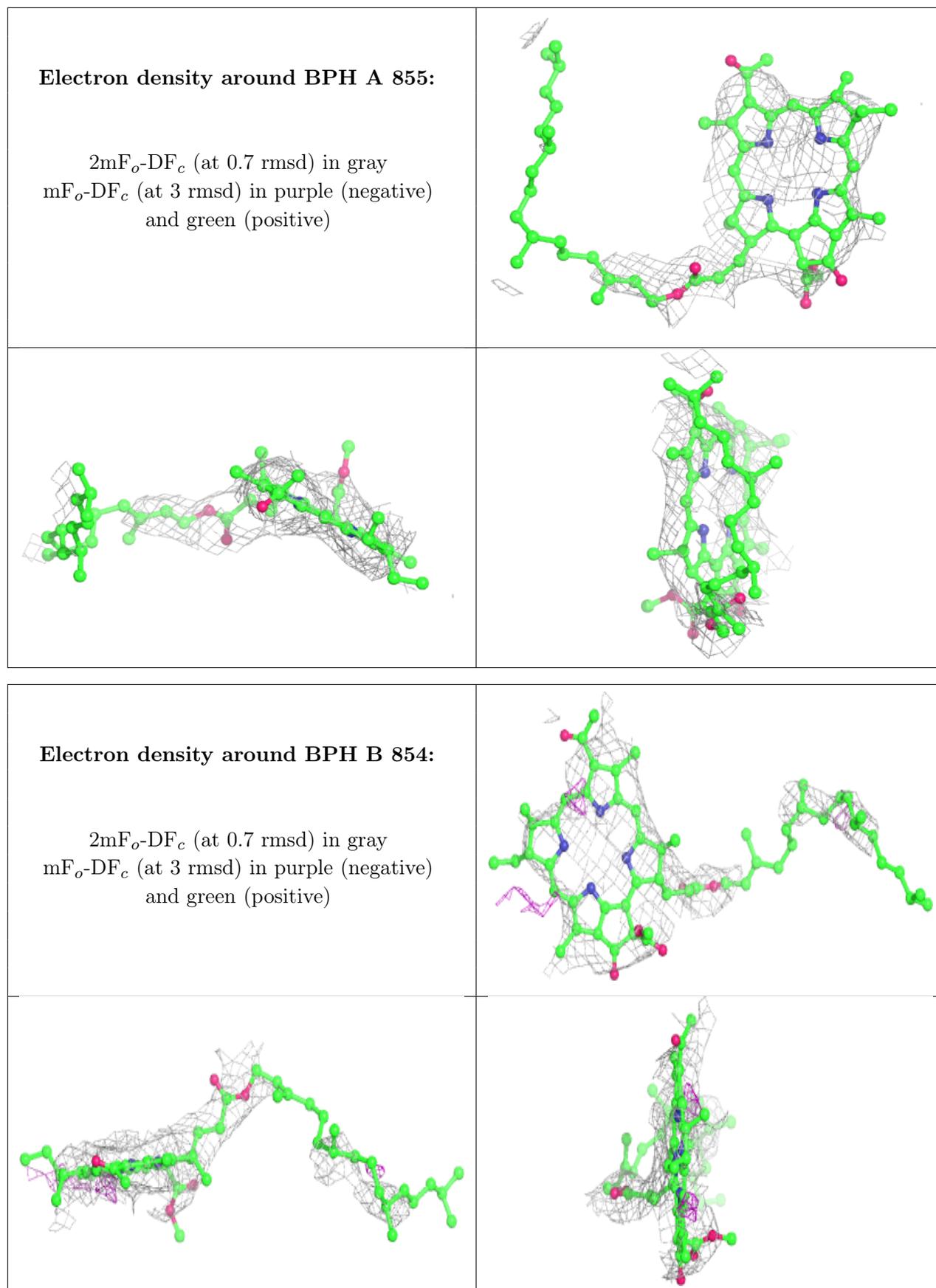
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCL B 853:

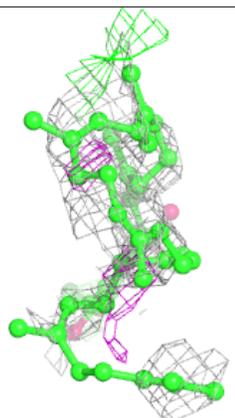
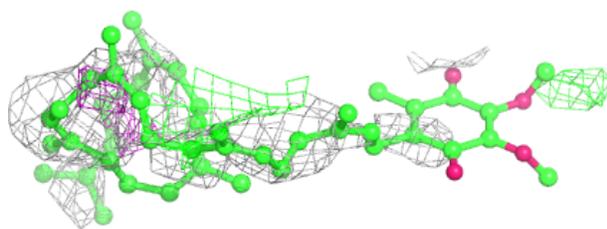
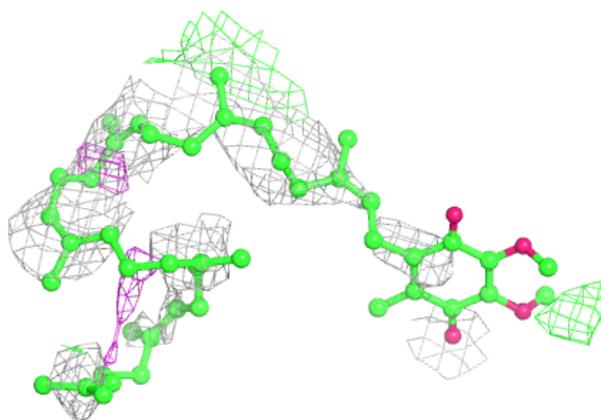
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



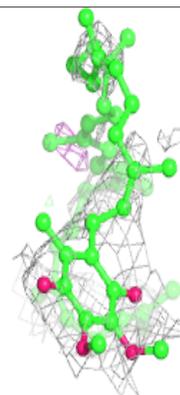
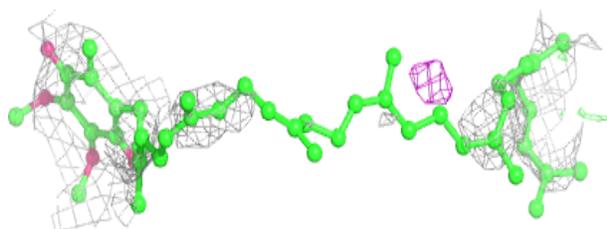
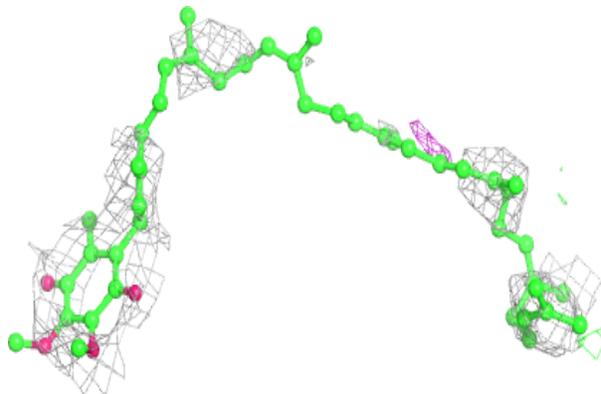


Electron density around U10 A 857:

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

**Electron density around U10 B 856:**

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



6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.