



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2023 – 04:20 AM EDT

PDB ID : 1Z9K
Title : Photosynthetic Reaction Center from Rhodobacter sphaeroides
Authors : Camara-Artigas, A.; Allen, J.P.
Deposited on : 2005-04-02
Resolution : 4.60 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

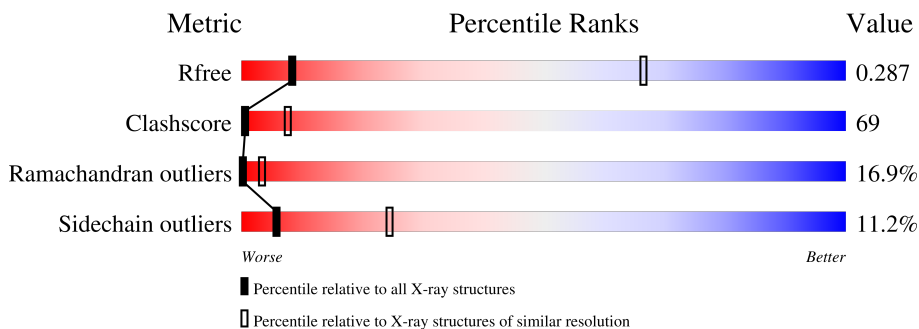
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 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	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)

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	21% (green) 58% (yellow) 20% (orange) . (red)
2	B	307	22% (green) 55% (yellow) 19% (orange) . . (red)
3	C	260	28% (green) 49% (yellow) 12% (orange) . 8% (grey)

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6946 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	2232	1507	355	362	8	0	0	0

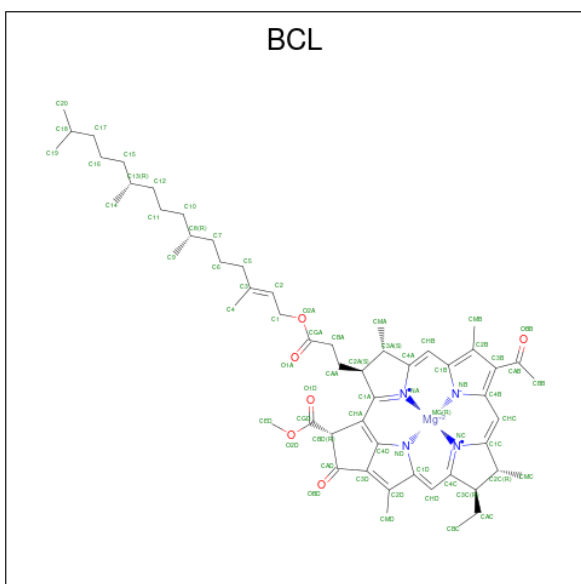
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	302	2408	1607	394	397	10	0	0	0

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

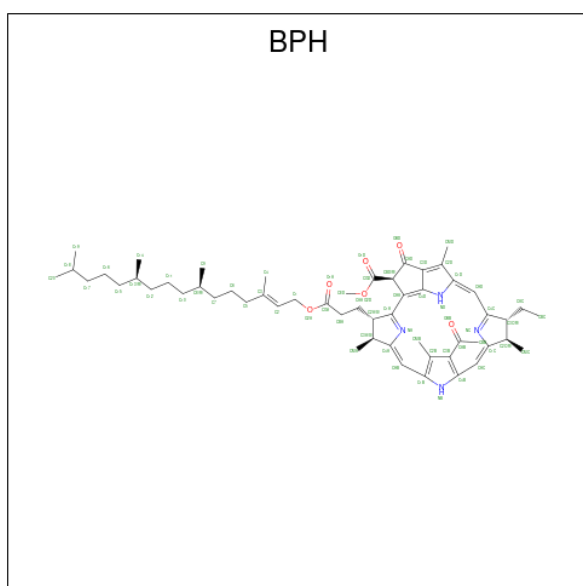
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	238	1814	1160	311	334	9	0	0	0

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



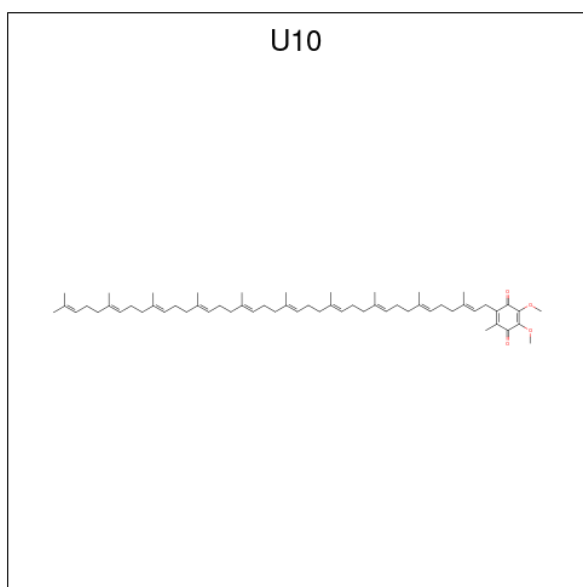
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- 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: $C_{59}H_{90}O_4$).



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		

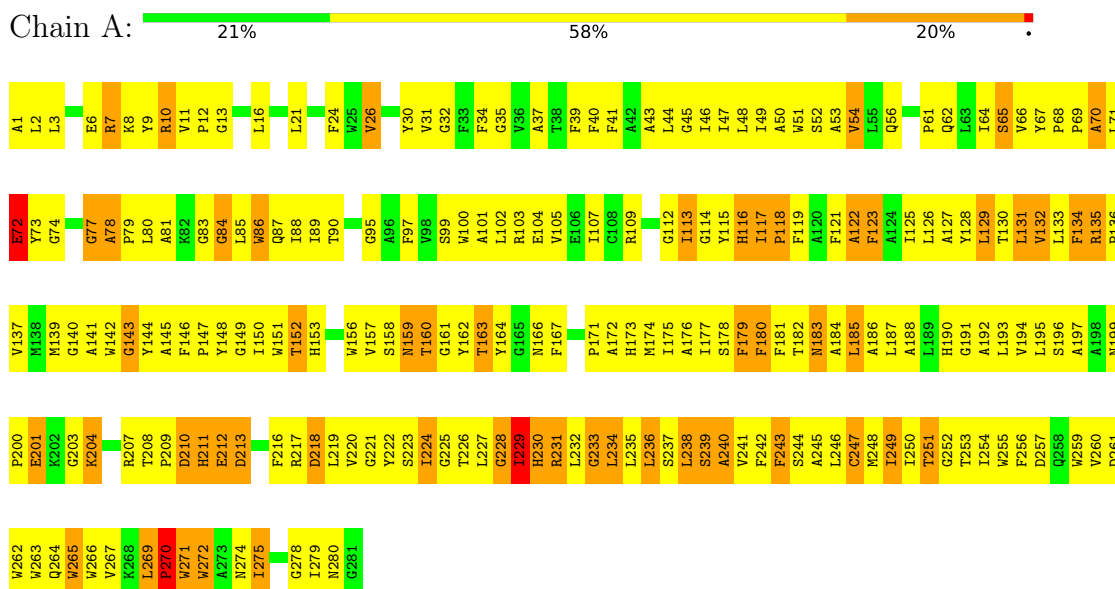
- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

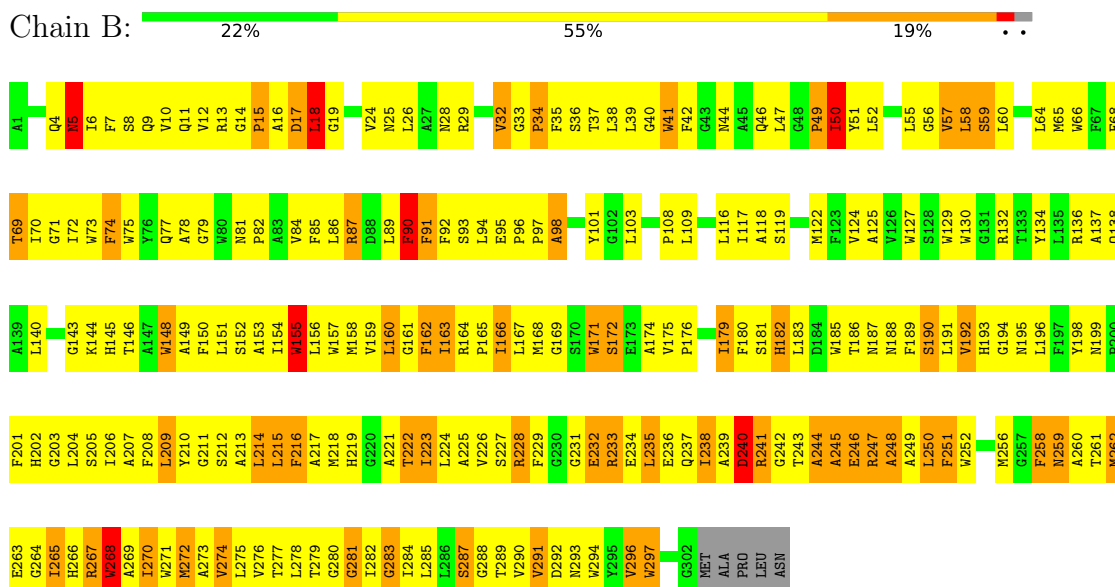
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

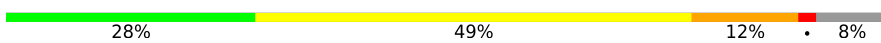
- Molecule 1: Reaction center protein L chain

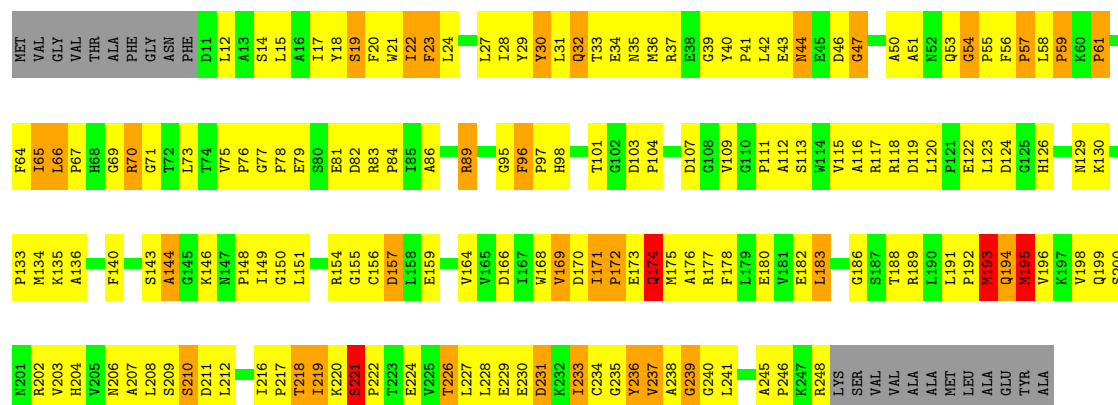


- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain

Chain C:  28% 49% 12% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	207.80Å 207.80Å 107.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 4.60 24.90 – 4.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-4.60) 91.4 (24.90-4.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 4.24Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.330 , 0.330 0.253 , 0.287	Depositor DCC
R_{free} test set	2066 reflections (8.55%)	wwPDB-VP
Wilson B-factor (Å ²)	174.1	Xtrriage
Anisotropy	0.410	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6946	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 3.13% 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: FE, BPH, BCL, U10, MN

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	0.52	0/2320	0.71	1/3175 (0.0%)
2	B	0.52	0/2500	0.75	1/3413 (0.0%)
3	C	0.55	0/1862	0.75	0/2534
All	All	0.53	0/6682	0.74	2/9122 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	52	LEU	CA-CB-CG	5.58	128.15	115.30
1	A	231	ARG	N-CA-C	-5.07	97.31	111.00

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	2232	0	2187	370	0
2	B	2408	0	2321	435	0
3	C	1814	0	1818	229	0
4	A	132	0	148	19	0
4	B	132	0	148	16	0
5	A	65	0	76	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	65	0	76	13	0
6	A	48	0	63	4	0
6	B	48	0	63	15	0
7	B	1	0	0	0	0
8	C	1	0	0	0	0
All	All	6946	0	6900	951	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 69.

The worst 5 of 951 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:50:ILE:HD13	2:B:51:TYR:H	1.08	1.08
1:A:187:LEU:HD21	2:B:269:ALA:HB1	1.31	1.06
1:A:179:PHE:O	1:A:240:ALA:HB2	1.57	1.05
3:C:170:ASP:HB2	3:C:177:ARG:HE	1.22	1.03
2:B:159:VAL:HA	2:B:163:ILE:HB	1.36	1.03

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	A	279/281 (99%)	149 (53%)	76 (27%)	54 (19%)	0	2
2	B	300/307 (98%)	164 (55%)	84 (28%)	52 (17%)	0	3
3	C	236/260 (91%)	144 (61%)	60 (25%)	32 (14%)	0	4
All	All	815/848 (96%)	457 (56%)	220 (27%)	138 (17%)	0	3

5 of 138 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	21	LEU
1	A	73	TYR
1	A	113	ILE
1	A	143	GLY

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%)	197 (90%)	23 (10%)	7 26
2	B	236/240 (98%)	203 (86%)	33 (14%)	3 19
3	C	193/208 (93%)	176 (91%)	17 (9%)	10 33
All	All	649/668 (97%)	576 (89%)	73 (11%)	6 24

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	23	PHE
3	C	233	ILE
3	C	65	ILE
3	C	206	ASN
2	B	18	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	145	HIS
2	B	188	ASN
3	C	206	ASN
3	C	126	HIS
2	B	5	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
5	BPH	B	854	-	51,70,70	1.72	7 (13%)	52,101,101	1.84	10 (19%)
6	U10	B	856	-	48,48,63	2.32	13 (27%)	58,61,79	1.99	19 (32%)
6	U10	A	857	-	48,48,63	2.75	18 (37%)	58,61,79	1.84	19 (32%)
4	BCL	A	850	2	58,74,74	1.87	12 (20%)	69,115,115	2.17	22 (31%)
4	BCL	B	852	2	58,74,74	1.48	6 (10%)	69,115,115	1.90	13 (18%)
5	BPH	A	855	-	51,70,70	1.61	7 (13%)	52,101,101	1.91	12 (23%)
4	BCL	B	853	1	58,74,74	1.58	11 (18%)	69,115,115	1.94	14 (20%)
4	BCL	A	851	1	58,74,74	1.53	10 (17%)	69,115,115	2.01	13 (18%)

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	B	854	-	-	11/37/105/105	0/5/6/6
6	U10	B	856	-	-	14/45/69/87	0/1/1/1
6	U10	A	857	-	-	15/45/69/87	0/1/1/1
4	BCL	A	850	2	-	8/37/137/137	-
4	BCL	B	852	2	-	12/37/137/137	-
5	BPH	A	855	-	-	10/37/105/105	0/5/6/6
4	BCL	B	853	1	-	7/37/137/137	-
4	BCL	A	851	1	-	8/37/137/137	-

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	857	U10	C6-C1	11.71	1.56	1.35
6	B	856	U10	C6-C1	9.26	1.52	1.35
4	B	852	BCL	C3D-C2D	5.70	1.49	1.39
4	B	853	BCL	C3B-C2B	5.29	1.48	1.39
6	A	857	U10	C7-C6	5.28	1.60	1.51

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	851	BCL	CAD-C3D-C4D	-8.17	103.92	108.47
4	B	853	BCL	CMB-C2B-C1B	-6.88	117.90	128.46
4	A	851	BCL	CMB-C2B-C1B	-6.70	118.17	128.46
4	B	852	BCL	CAD-C3D-C4D	-6.50	104.85	108.47
4	B	852	BCL	CMB-C2B-C1B	-6.43	118.58	128.46

There are no chirality outliers.

5 of 85 torsion outliers are listed below:

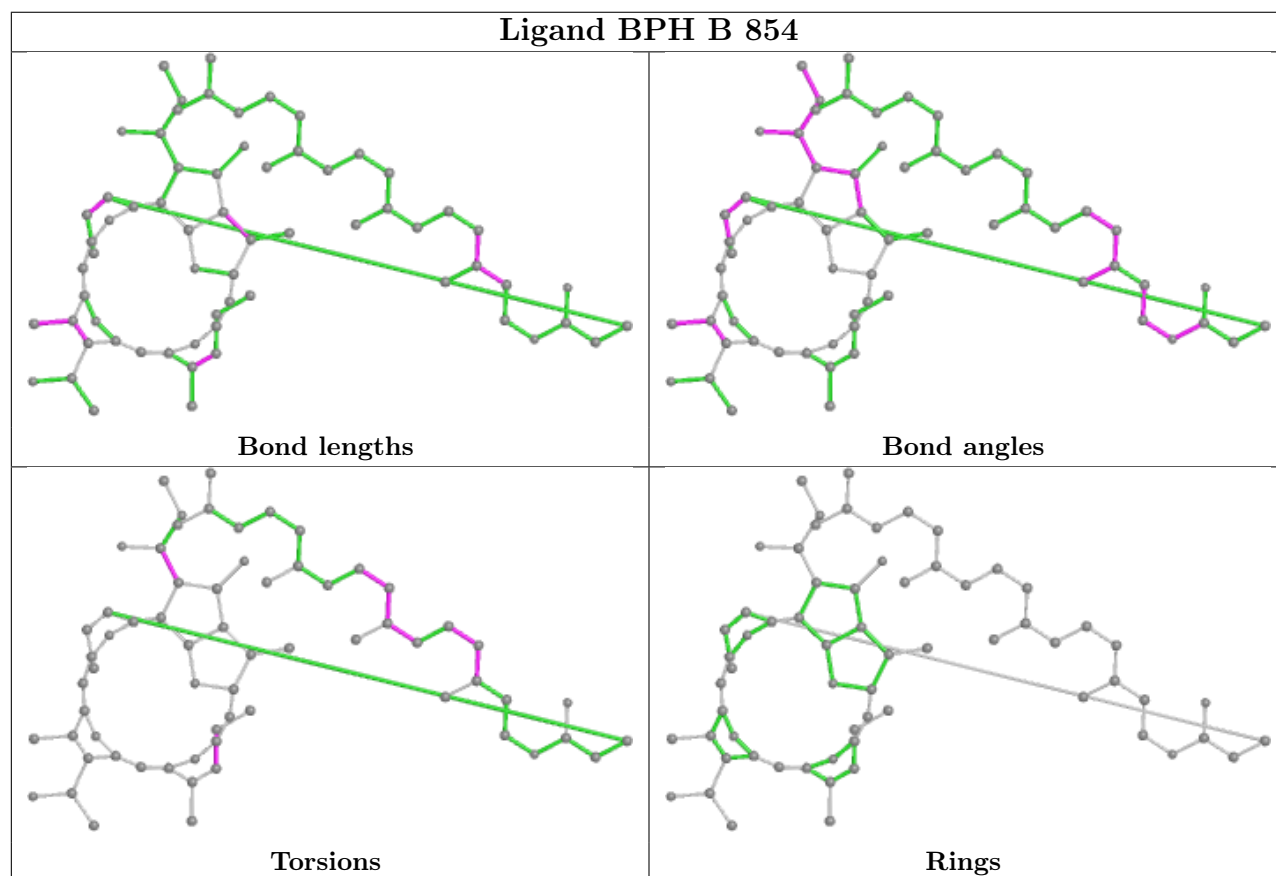
Mol	Chain	Res	Type	Atoms
4	B	852	BCL	C4-C3-C5-C6
5	A	855	BPH	C4C-C3C-CAC-CBC
5	A	855	BPH	C2C-C3C-CAC-CBC
5	A	855	BPH	C6-C7-C8-C9
5	B	854	BPH	C4C-C3C-CAC-CBC

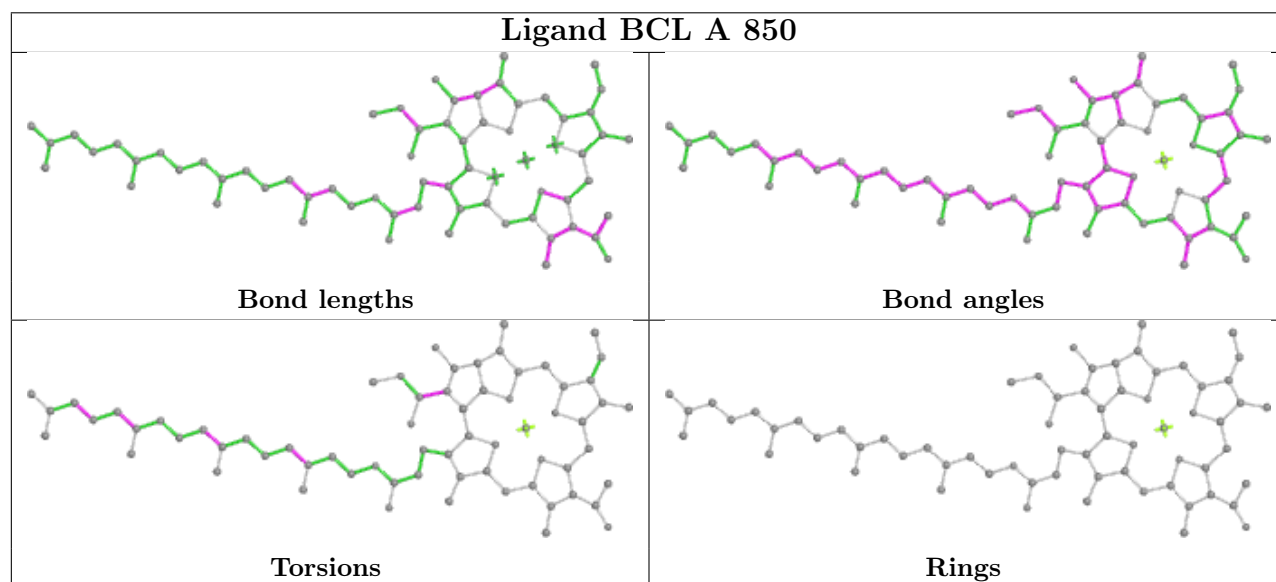
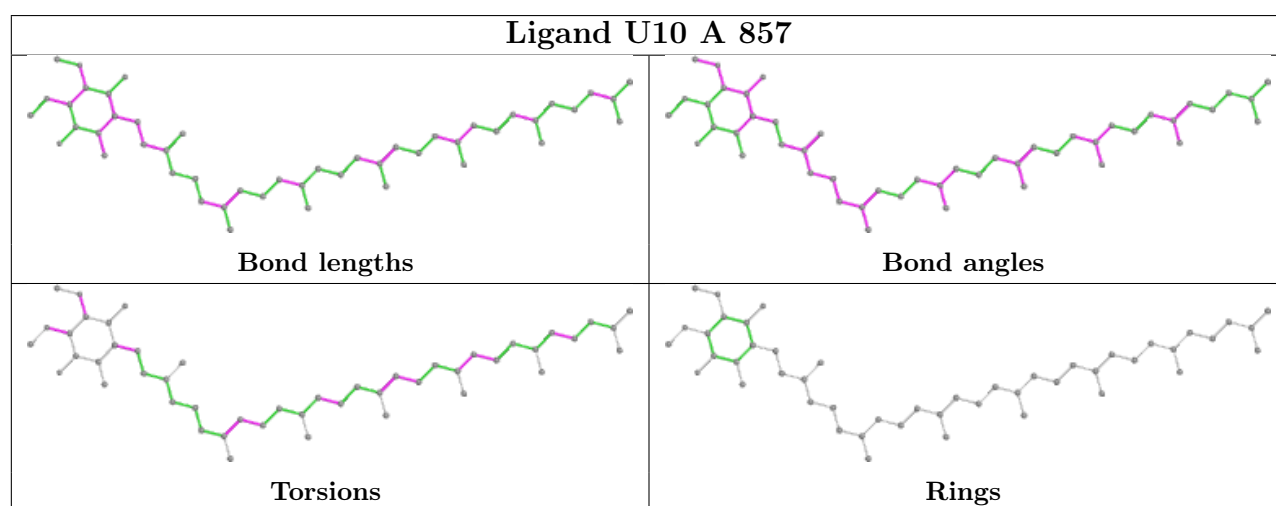
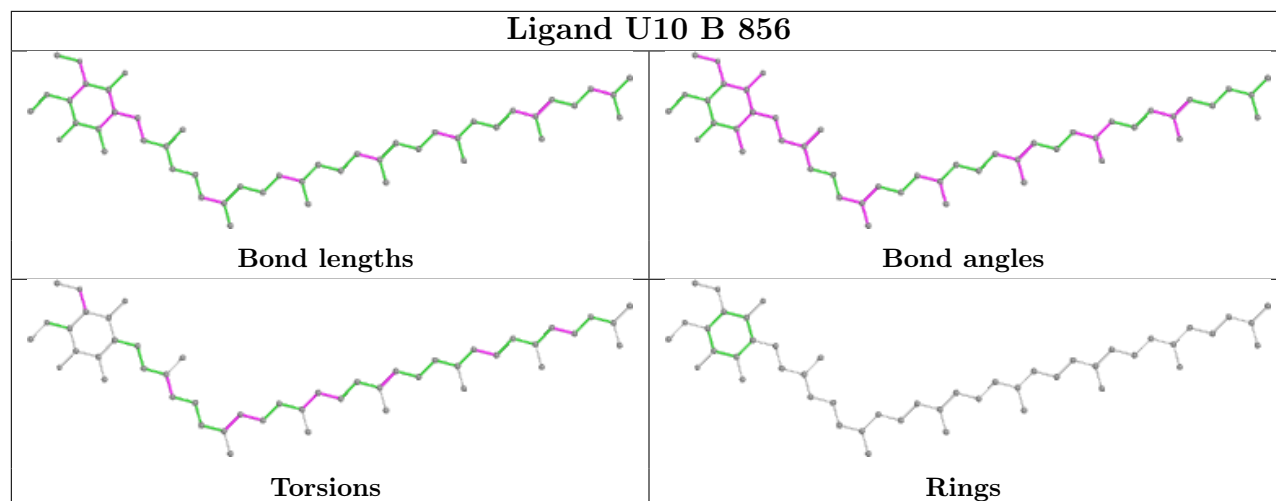
There are no ring outliers.

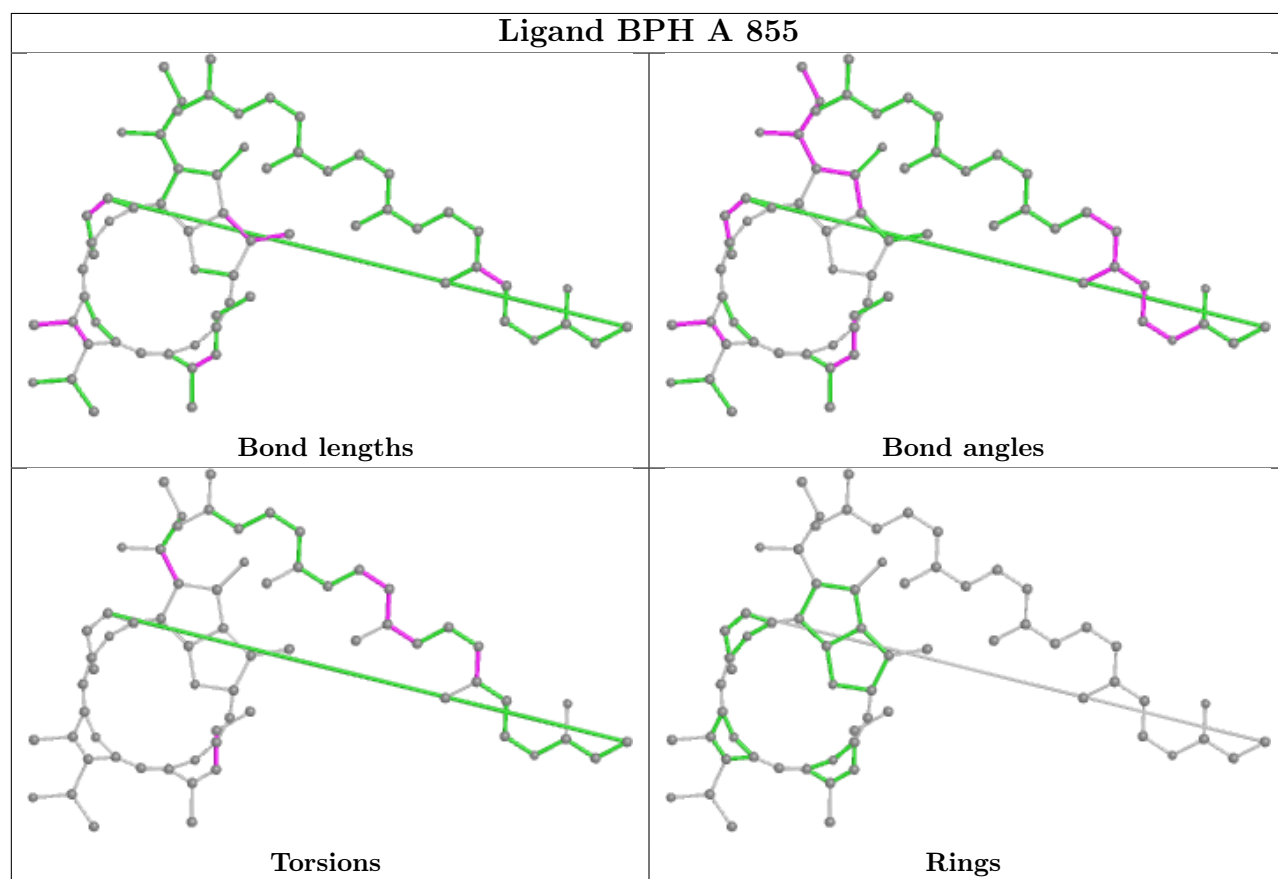
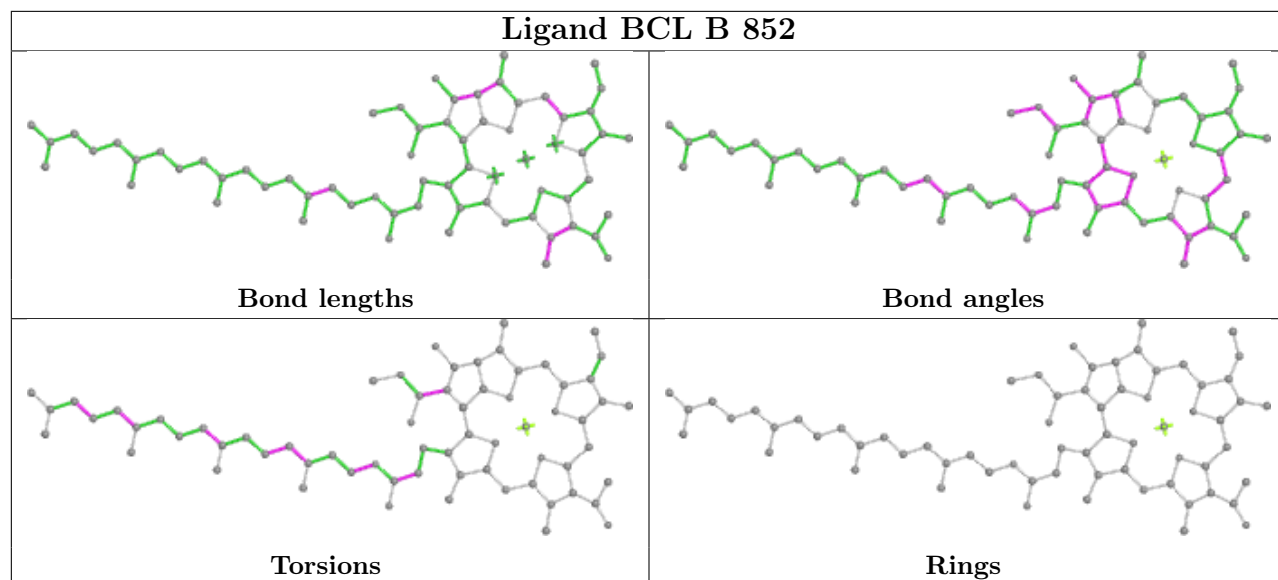
8 monomers are involved in 73 short contacts:

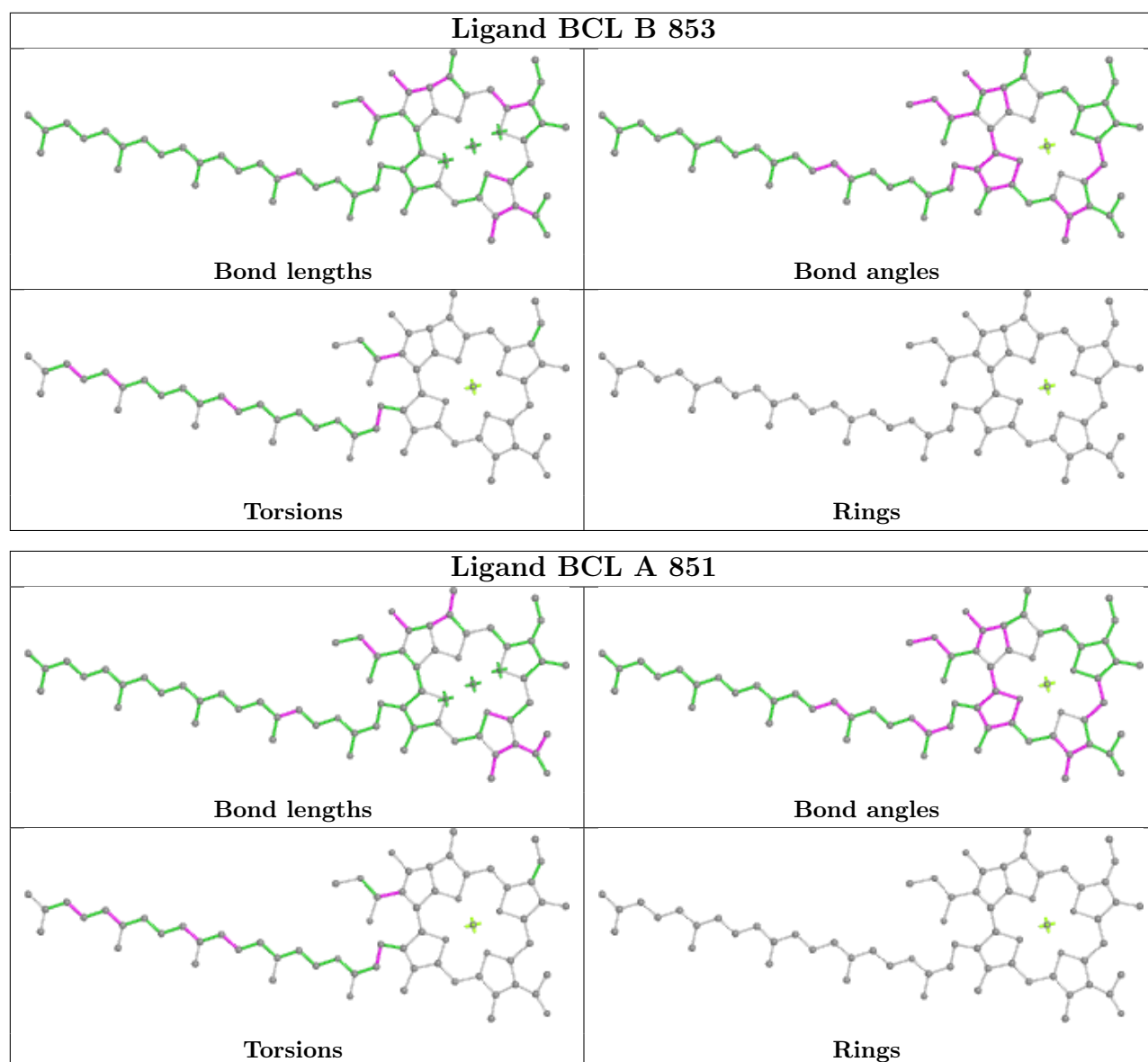
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	854	BPH	13	0
6	B	856	U10	15	0
6	A	857	U10	4	0
4	A	850	BCL	15	0
4	B	852	BCL	9	0
5	A	855	BPH	11	0
4	B	853	BCL	8	0
4	A	851	BCL	6	0

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.

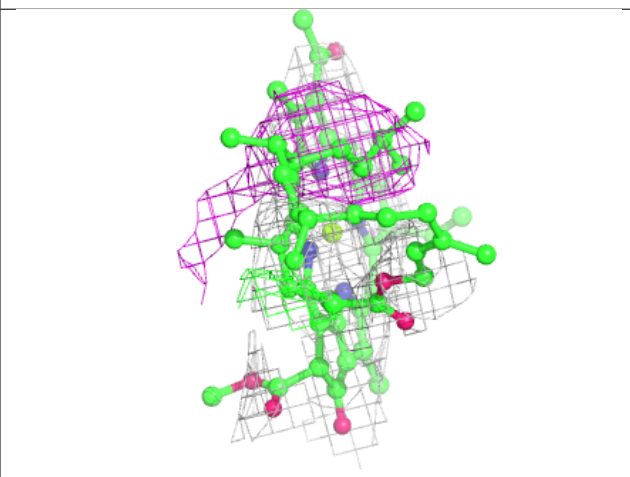
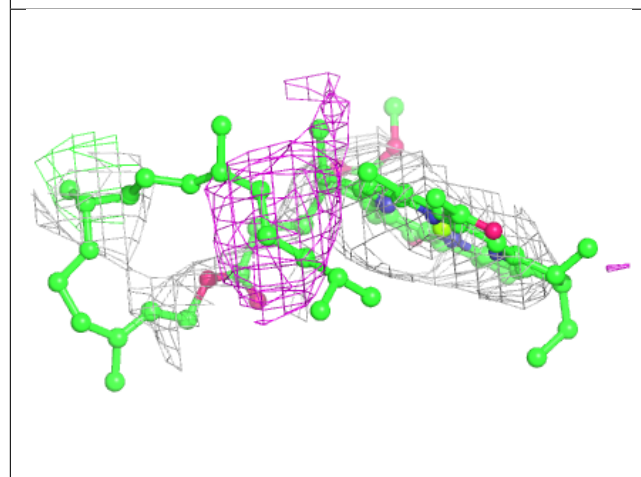
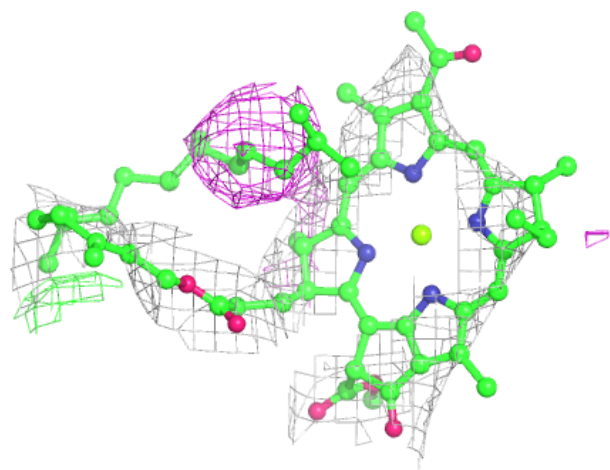
6.4 Ligands

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.

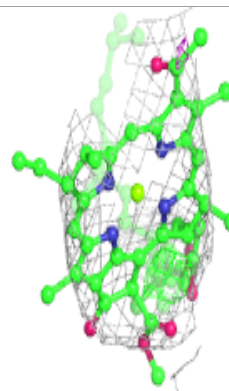
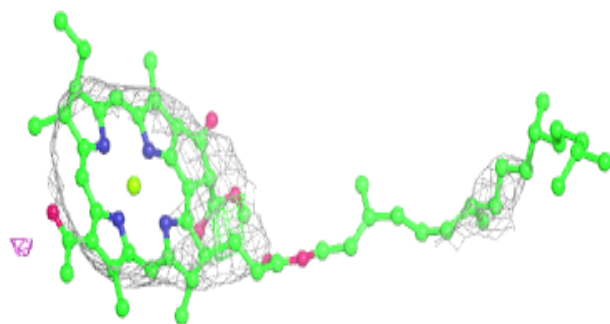
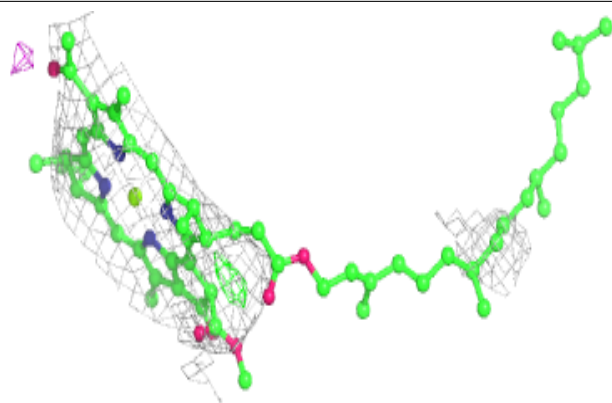
Electron density around BCL A 850:

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

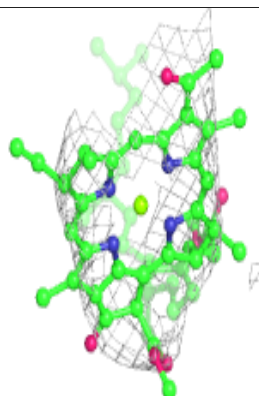
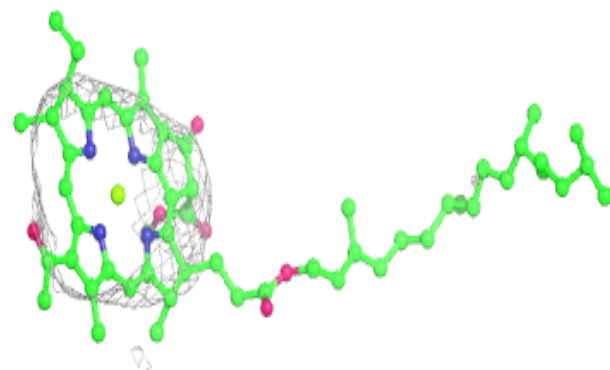
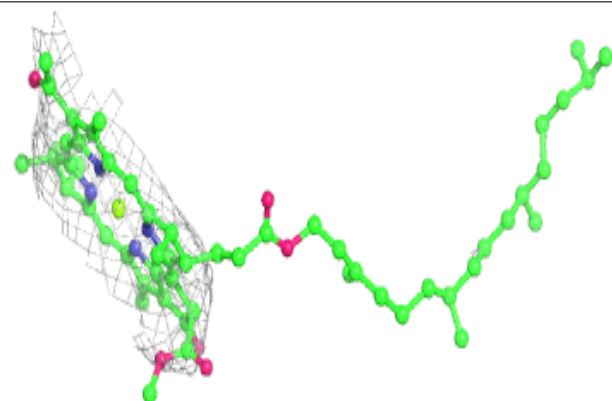


Electron density around BCL A 851:

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

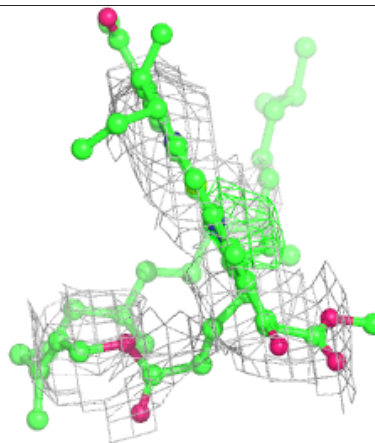
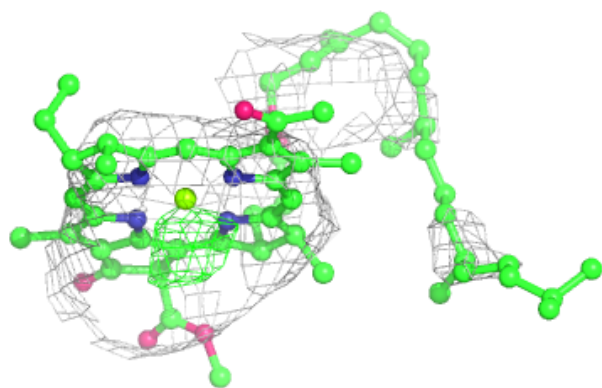
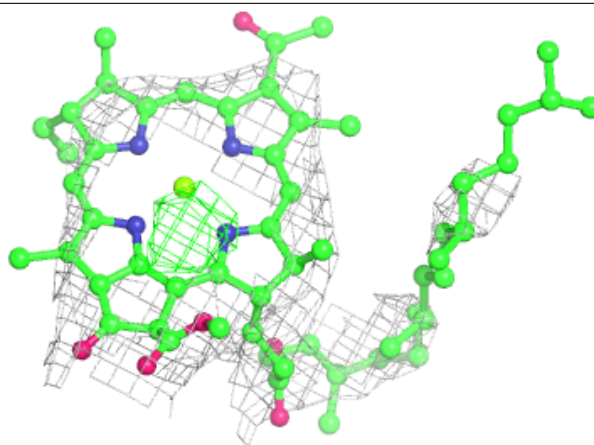
**Electron density around BCL B 852:**

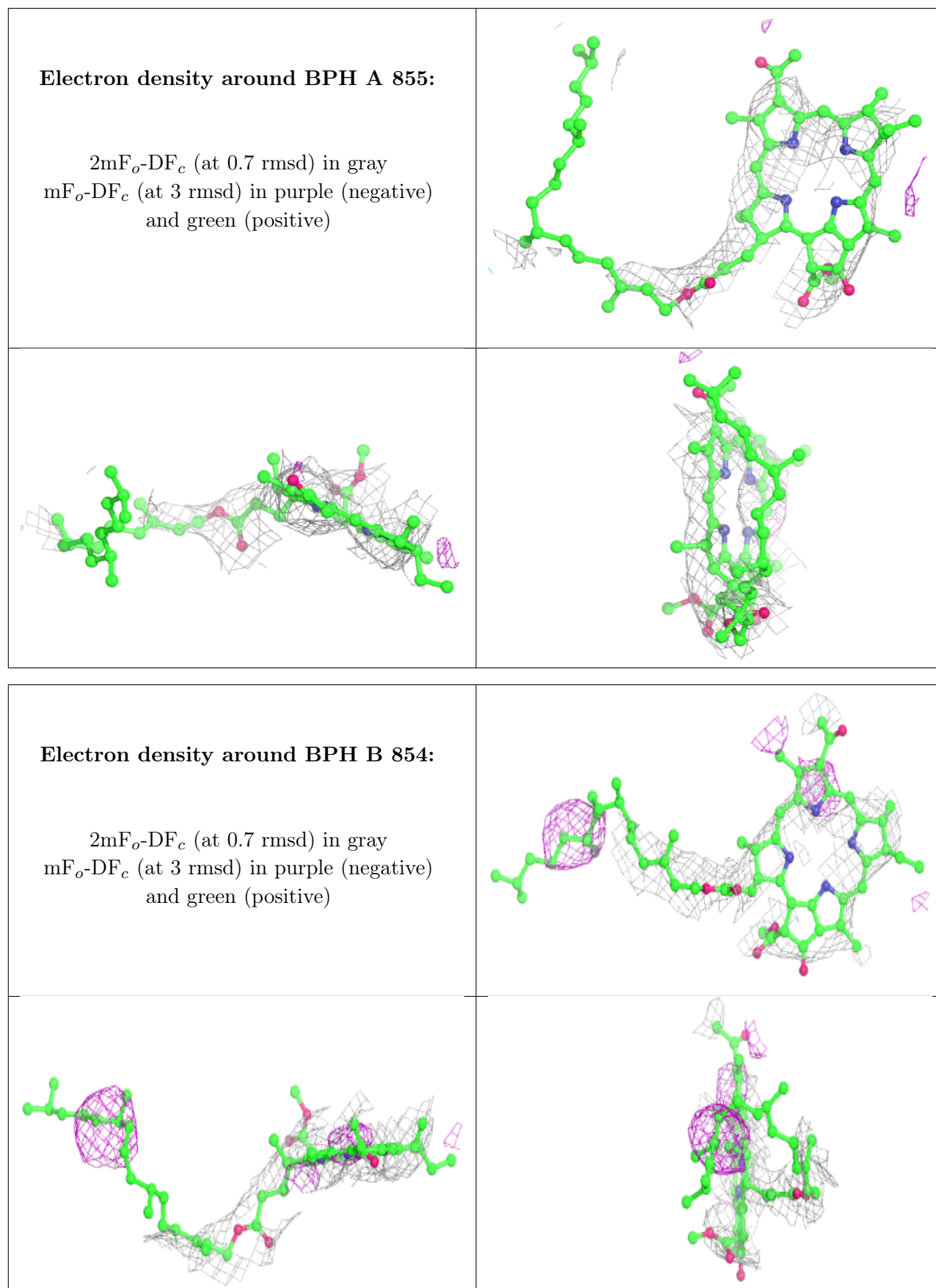
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCL B 853:

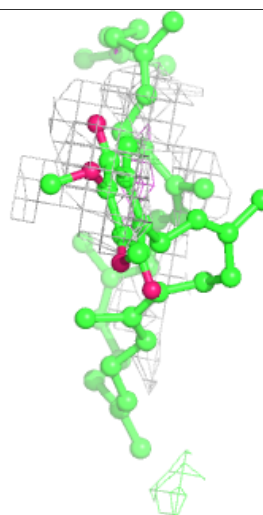
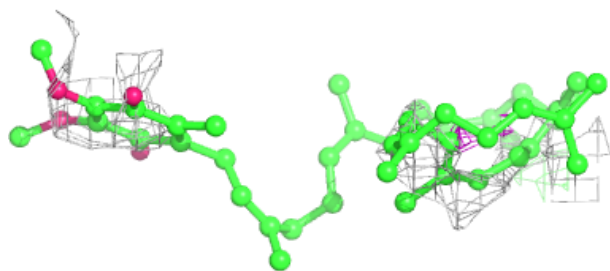
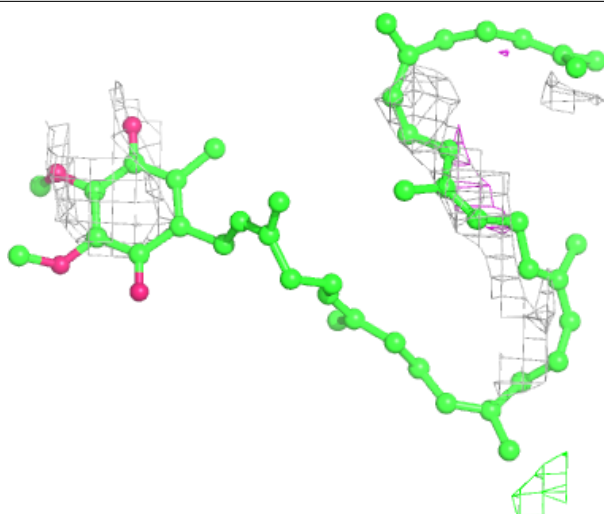
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

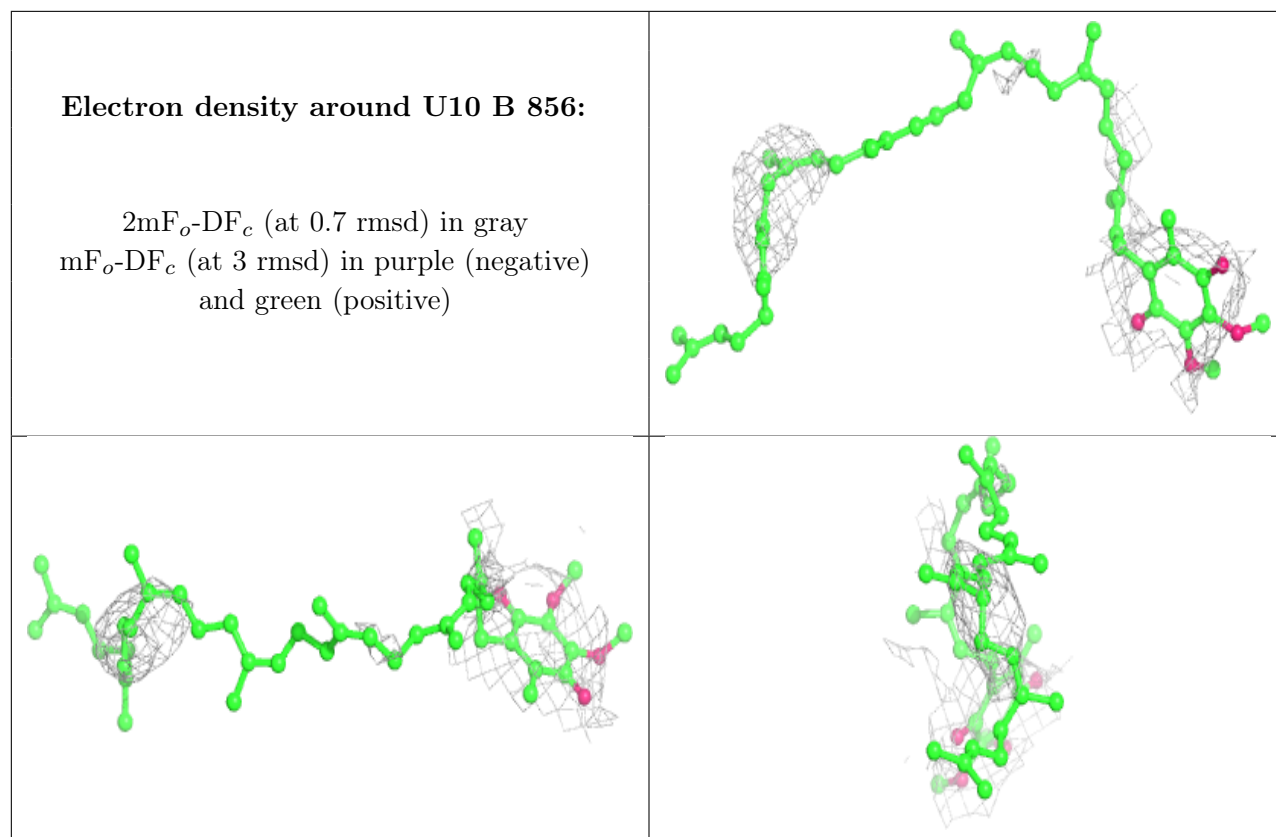




Electron density around U10 A 857:

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





6.5 Other polymers [i](#)

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