wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2023 – 12:14 AM EDT

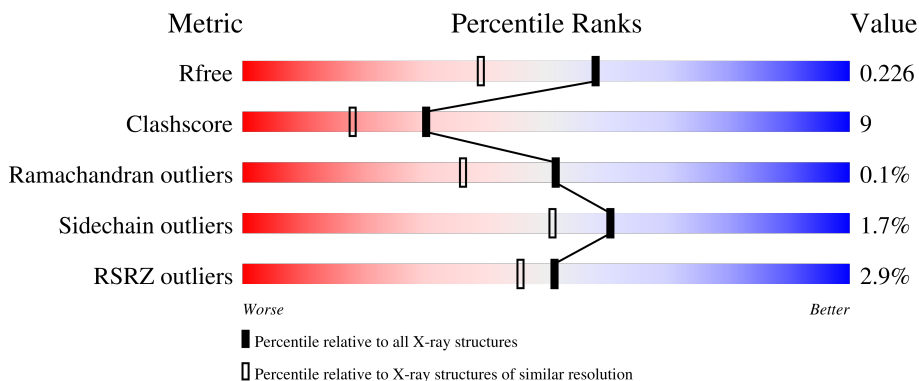|		
PDB ID	:	1RZH
Title	:	PHOTOSYNTHETIC REACTION CENTER DOUBLE MUTANT FROM RHODOBACTER SPHAEROIDES WITH ASP L213 REPLACED WITH ASN AND ARG M233 REPLACED WITH CYS IN THE CHARGE-NEUTRAL DQAQB STATE (TRIGONAL FORM)
Authors	:	Xu, Q.; Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher, G.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

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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 1.80 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.226
Clashscore		9
Ramachandran outliers		0.1%
Sidechain outliers		1.7%
RSRZ outliers		2.9%

Worse ← → *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	281	4% — 87% / 12% ·
2	M	307	3% — 80% / 18% ·
3	H	260	2% — 77% / 14% / 8%

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	GOL	M	867	-	X	-	-
4	BCL	M	851	X	-	-	-
5	BPH	L	856	X	-	-	-
5	BPH	M	855	X	-	-	-
6	U10	L	859[A]	-	-	-	X

2 Entry composition ⓘ

There are 14 unique types of molecules in this entry. The entry contains 7586 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total 2238	C 1510	N 357	O 363	S 8	0	1	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
2	M	301	Total 2399	C 1602	N 390	O 396	S 11	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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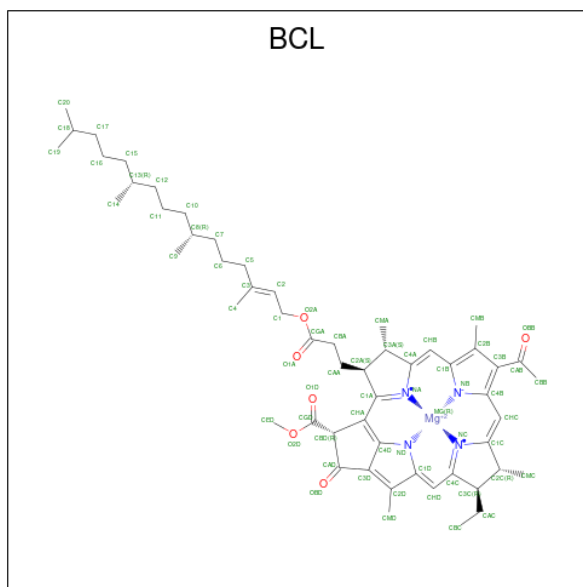
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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

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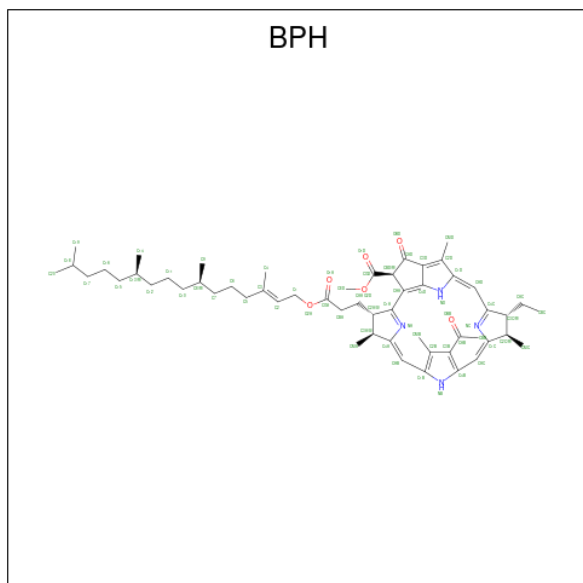
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total 65	C 55	N 4	O 6	0	0
5	M	1	Total 55	C 45	N 4	O 6	0	0

• Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).

U10
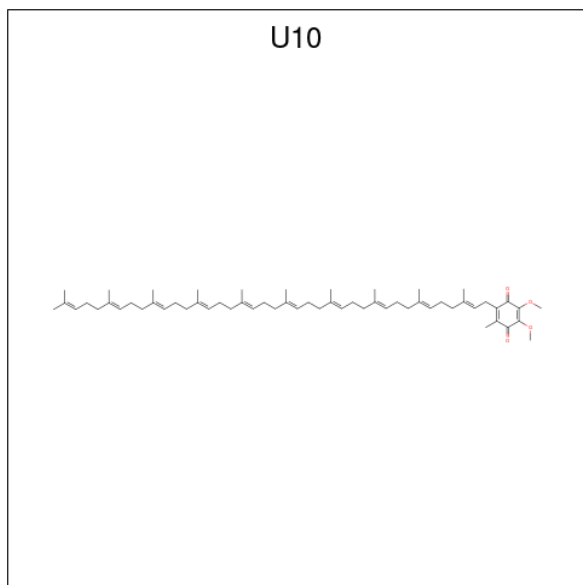
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total 33	C 29	O 4	0	1
6	M	1	Total 48	C 44	O 4	0	0

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

HTO

C1
O3
HO   OH O1
C2(R)
C3(R)
C5
OH
C4   O2
C7
C6
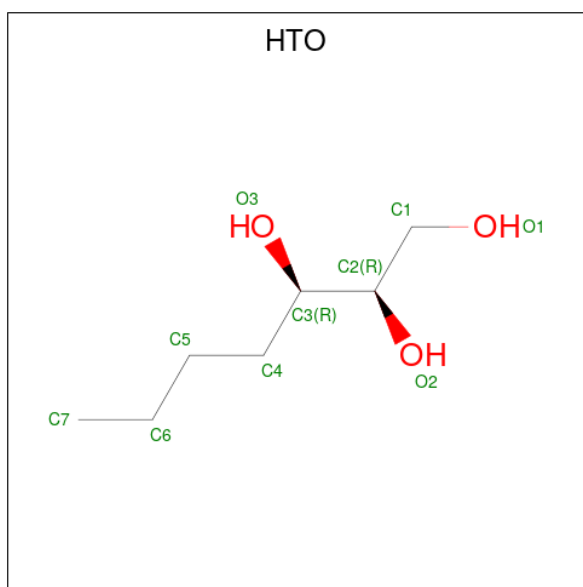
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total 10	C 7	O 3	0	0
7	L	1	Total 10	C 7	O 3	0	0

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

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

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

PO4

O3
O^-

O2 O^- — P $=$ O O1
P

O^-

O4
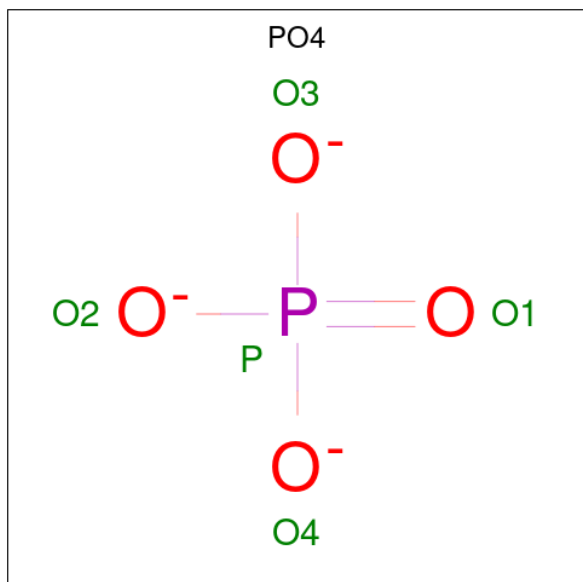
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
9	M	1	5	4	1	0	0

- Molecule 10 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).
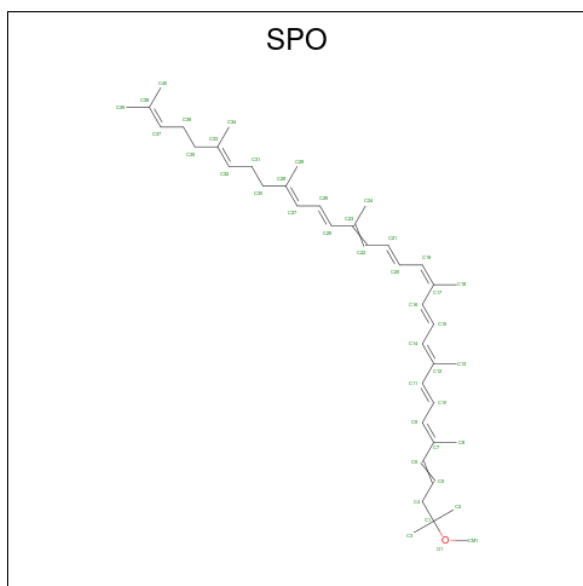
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	M	1	42	41	1	0	0

- Molecule 11 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).
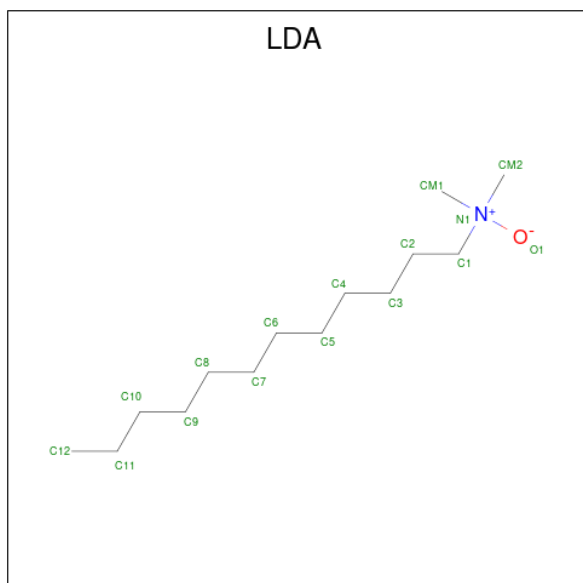
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	M	1	Total 16	C 14	N 1	O 1	0	0
11	M	1	Total 16	C 14	N 1	O 1	0	0
11	H	1	Total 16	C 14	N 1	O 1	0	0

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).
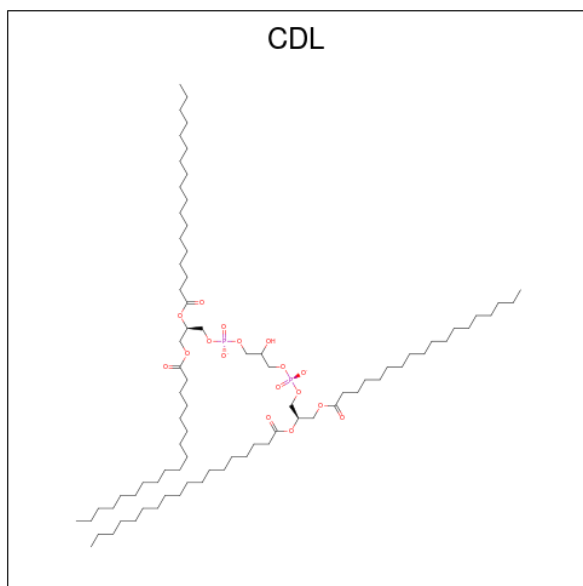
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	M	1	Total 69	C 50	O 17	P 2	0	0

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

GOL

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

- Molecule 14 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	L	124	Total 124	O 124	0	2
14	M	138	Total 138	O 138	0	0
14	H	209	Total 209	O 209	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.
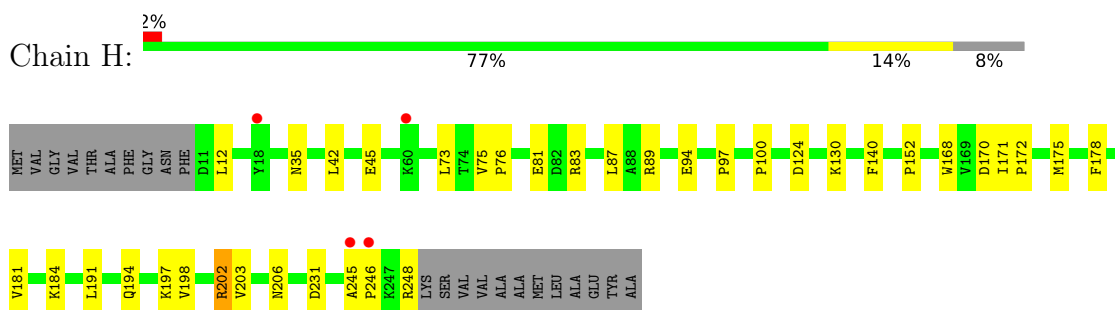
• Molecule 1: Reaction center protein L chain
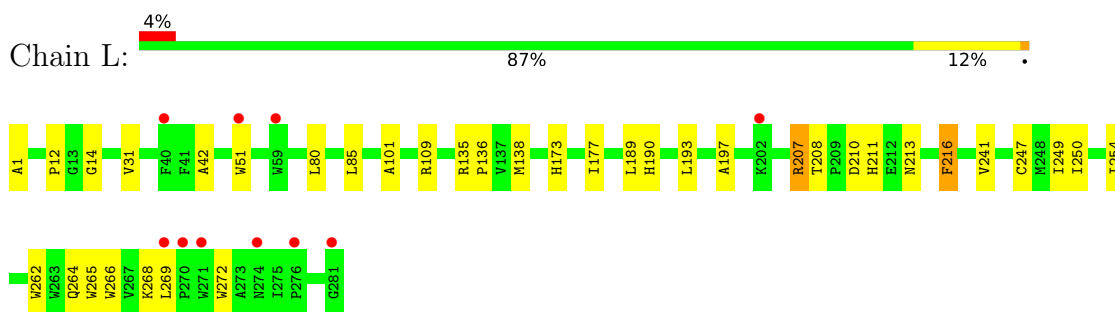
• Molecule 2: Reaction center protein M chain
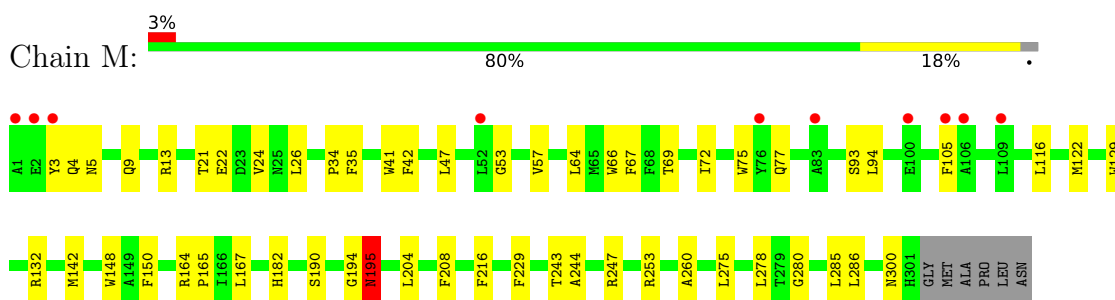
• Molecule 3: Reaction center protein H chain

4 Data and refinement statistics ⓘ

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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	L	0.36	0/2326	0.55	0/3183
2	M	0.35	0/2491	0.53	0/3402
3	H	0.30	0/1870	0.59	0/2544
All	All	0.34	0/6687	0.56	0/9129

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2238	0	2193	36	0
2	M	2399	0	2310	53	0
3	H	1822	0	1826	29	0
4	L	132	0	148	4	0
4	M	132	0	148	21	0
5	L	65	0	74	5	0
5	M	55	0	53	3	0
6	L	33	0	39	8	0
6	M	48	0	61	3	0
7	L	20	0	32	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	M	1	0	0	0	0
9	M	5	0	0	0	0
10	M	42	0	60	7	0
11	H	16	0	31	2	0
11	M	32	0	62	5	0
12	M	69	0	82	2	0
13	M	6	0	4	0	0
14	H	209	0	0	1	0
14	L	124	0	0	0	0
14	M	138	0	0	0	0
All	All	7586	0	7123	132	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 132 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:851:BCL:C9	4:M:851:BCL:H121	1.41	1.43
4:M:851:BCL:C12	4:M:851:BCL:H91	1.36	1.39
1:L:241:VAL:HG21	5:L:856:BPH:HAC1	1.46	0.97
4:M:851:BCL:H91	4:M:851:BCL:H122	1.54	0.90
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.53	0.90

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	280/281 (100%)	273 (98%)	7 (2%)	0	100	100
2	M	299/307 (97%)	292 (98%)	6 (2%)	1 (0%)	41	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	237/260 (91%)	236 (100%)	1 (0%)	0	100	100
All	All	816/848 (96%)	801 (98%)	14 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	ASN

5.3.2 Protein sidechains ⓘ

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

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

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

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	73	LEU
3	H	175	MET
3	H	231	ASP
3	H	202	ARG
2	M	94	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	300	ASN
3	H	206	ASN
2	M	9	GLN
2	M	77	GLN

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Mol	Chain	Res	Type
2	M	195	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
11	LDA	M	861	-	12,15,15	2.14	1 (8%)	14,17,17	1.60	4 (28%)
7	HTO	L	865	-	9,9,9	1.31	1 (11%)	10,10,10	0.37	0
9	PO4	M	864	-	4,4,4	1.72	1 (25%)	6,6,6	0.43	0
4	BCL	L	852	-	58,74,74	1.24	5 (8%)	69,115,115	1.85	19 (27%)
10	SPO	M	860	-	40,41,41	3.41	23 (57%)	47,50,50	4.12	16 (34%)
4	BCL	M	851	-	58,74,74	1.57	10 (17%)	69,115,115	2.55	27 (39%)
11	LDA	H	862	-	12,15,15	2.15	1 (8%)	14,17,17	1.76	4 (28%)
5	BPH	M	855	-	41,60,70	1.87	10 (24%)	40,89,101	2.96	18 (45%)
7	HTO	L	866	-	9,9,9	1.31	1 (11%)	10,10,10	0.37	0
11	LDA	M	863	-	12,15,15	2.03	1 (8%)	14,17,17	1.68	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
13	GOL	M	867	-	5,5,5	4.51	5 (100%)	5,5,5	5.78	3 (60%)
4	BCL	L	854	-	58,74,74	1.63	15 (25%)	69,115,115	2.21	23 (33%)
4	BCL	M	853	-	58,74,74	1.78	11 (18%)	69,115,115	2.69	20 (28%)
12	CDL	M	900	-	68,68,99	0.74	2 (2%)	74,80,111	0.96	4 (5%)
5	BPH	L	856	-	51,70,70	1.74	10 (19%)	52,101,101	2.65	18 (34%)
6	U10	M	858	-	48,48,63	2.13	18 (37%)	58,61,79	3.30	18 (31%)
6	U10	L	859[A]	-	33,33,63	2.06	11 (33%)	40,43,79	1.94	12 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	LDA	M	861	-	-	6/13/13/13	-
7	HTO	L	865	-	-	7/10/10/10	-
4	BCL	L	852	-	-	4/37/137/137	-
10	SPO	M	860	-	-	13/47/47/47	-
4	BCL	M	851	-	2/2/21/25	19/37/137/137	-
11	LDA	H	862	-	-	6/13/13/13	-
5	BPH	M	855	-	1/1/16/22	11/25/93/105	0/5/6/6
7	HTO	L	866	-	-	8/10/10/10	-
11	LDA	M	863	-	-	3/13/13/13	-
13	GOL	M	867	-	-	2/4/4/4	-
4	BCL	L	854	-	-	8/37/137/137	-
4	BCL	M	853	-	-	3/37/137/137	-
12	CDL	M	900	-	-	22/79/79/110	-
5	BPH	L	856	-	2/2/18/22	8/37/105/105	0/5/6/6
6	U10	M	858	-	-	10/45/69/87	0/1/1/1
6	U10	L	859[A]	-	-	4/27/51/87	0/1/1/1

The worst 5 of 126 bond length outliers are listed below:

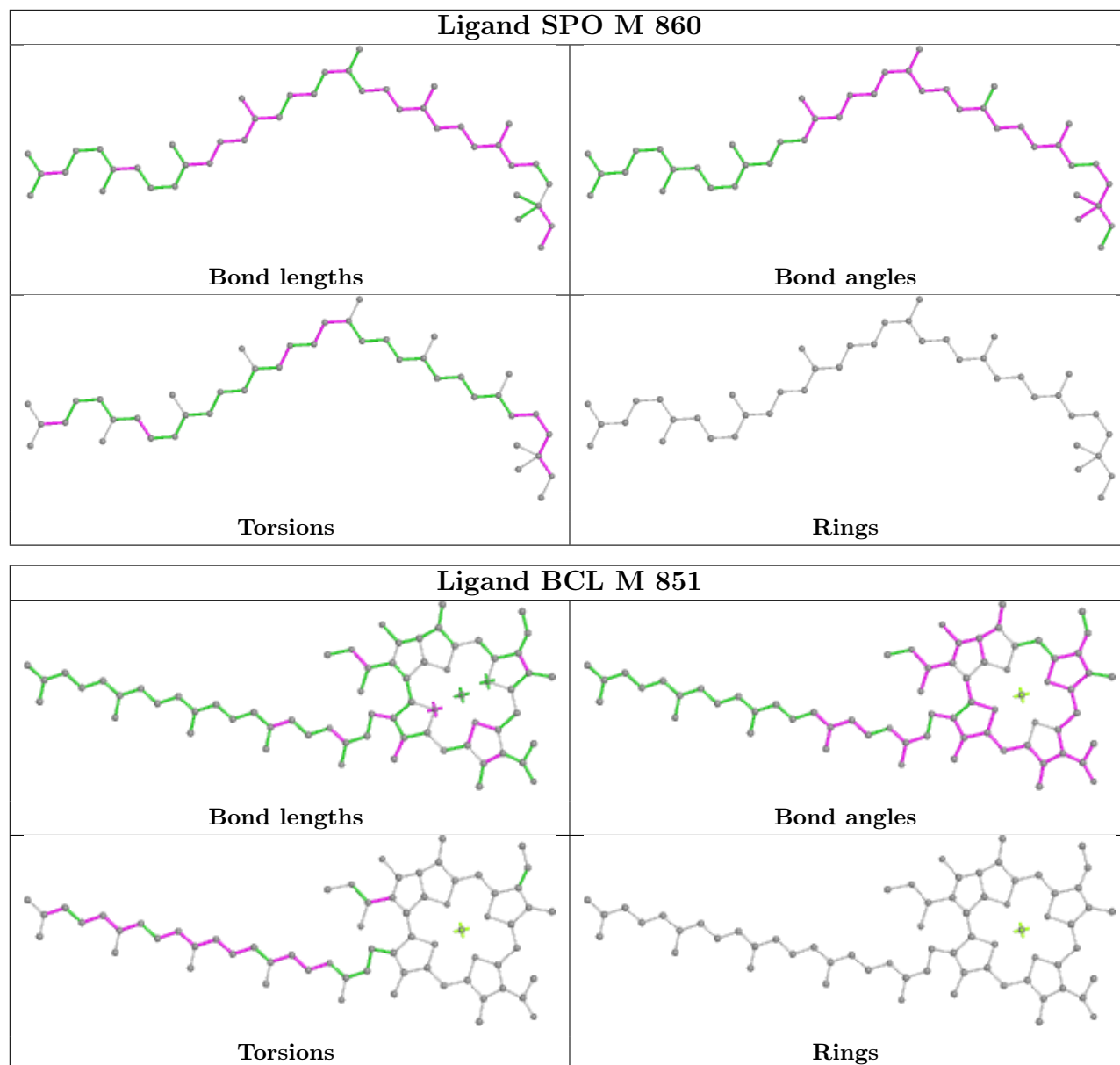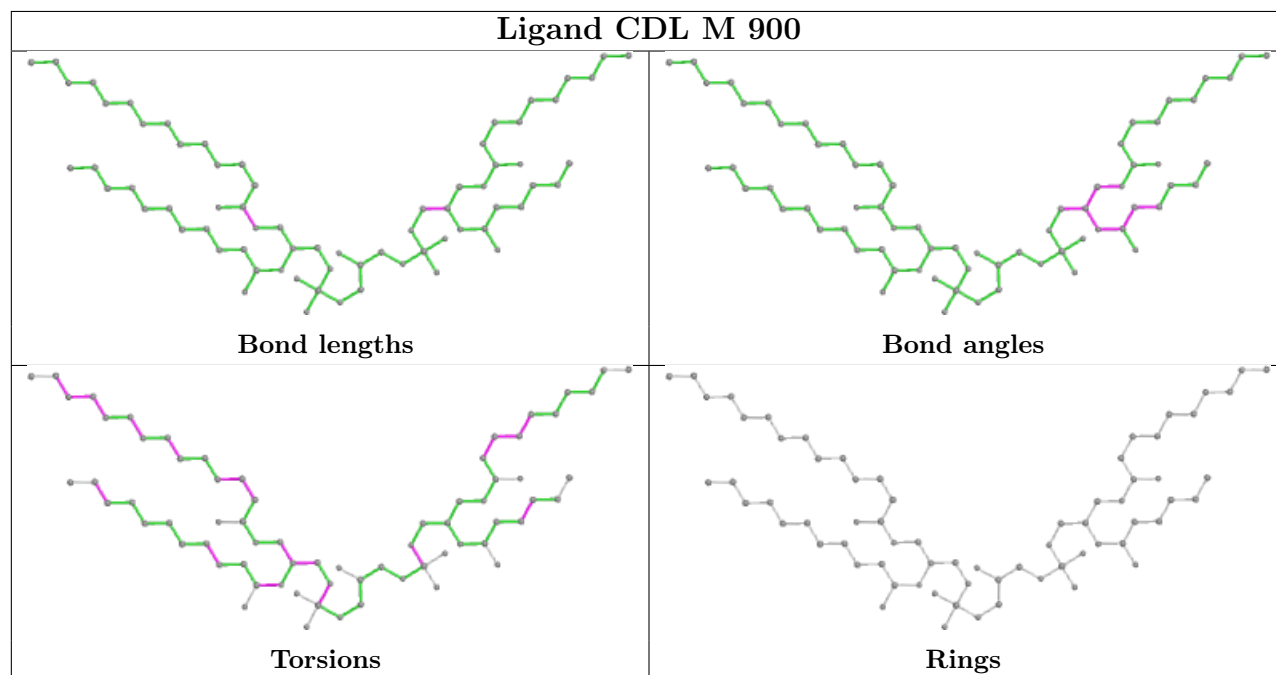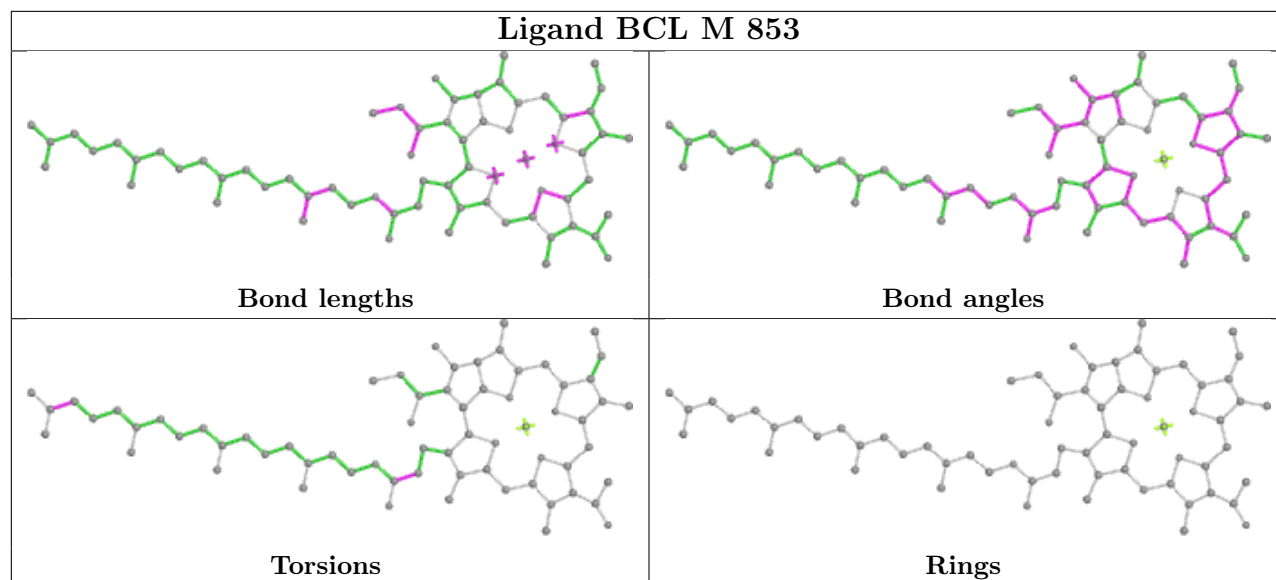| Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	860	SPO	C6-C5	8.77	1.54	1.32
10	M	860	SPO	C10-C11	7.87	1.54	1.34
10	M	860	SPO	C15-C16	7.63	1.54	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	867	GOL	C3-C2	-7.34	1.21	1.51
11	H	862	LDA	O1-N1	-7.24	1.25	1.42

The worst 5 of 190 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	860	SPO	C2-C1-C4	-20.56	79.29	110.86
6	M	858	U10	C32-C33-C34	18.38	171.91	127.66
4	M	853	BCL	C1C-NC-C4C	12.01	112.11	106.71
5	M	855	BPH	O2D-CGD-CBD	11.49	125.55	111.00
10	M	860	SPO	C3-C1-C4	-11.47	93.25	110.86

All (5) chirality outliers are listed below:

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

5 of 134 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	851	BCL	C1-C2-C3-C4
5	L	856	BPH	C4C-C3C-CAC-CBC
5	L	856	BPH	C2C-C3C-CAC-CBC
5	L	856	BPH	O2A-C1-C2-C3
5	M	855	BPH	O2A-C1-C2-C3

There are no ring outliers.

15 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	861	LDA	2	0
7	L	865	HTO	1	0
4	L	852	BCL	1	0
10	M	860	SPO	7	0
4	M	851	BCL	15	0
11	H	862	LDA	2	0
5	M	855	BPH	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	866	HTO	1	0
11	M	863	LDA	3	0
4	L	854	BCL	3	0
4	M	853	BCL	7	0
12	M	900	CDL	2	0
5	L	856	BPH	5	0
6	M	858	U10	3	0
6	L	859[A]	U10	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand BCL L 852

Bond lengths

Bond angles

Torsions

Rings

Ligand SPO M 860

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL M 851

Bond lengths

Bond angles

Torsions

Rings

Ligand BPH M 855

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL L 854

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL M 853

Bond lengths

Bond angles

Torsions

Rings

Ligand CDL M 900

Bond lengths

Bond angles

Torsions

Rings

Ligand BPH L 856

Bond lengths

Bond angles

Torsions

Rings

Ligand U10 M 858

Bond lengths

Bond angles

Torsions

Rings

Ligand U10 L 859 (A)

Bond lengths

Bond angles

Torsions

Rings

5.7   Other polymers ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	L	281/281 (100%)	-0.09	10 (3%)	42	37	15, 22, 46, 59	0
2	M	301/307 (98%)	-0.02	10 (3%)	46	40	13, 25, 47, 63	0
3	H	238/260 (91%)	-0.28	4 (1%)	70	66	17, 25, 38, 51	0
All	All	820/848 (96%)	-0.12	24 (2%)	51	46	13, 24, 45, 63	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	10.2
1	L	281	GLY	4.9
1	L	51	TRP	4.2
1	L	276	PRO	3.7
2	M	2	GLU	3.6

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

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

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
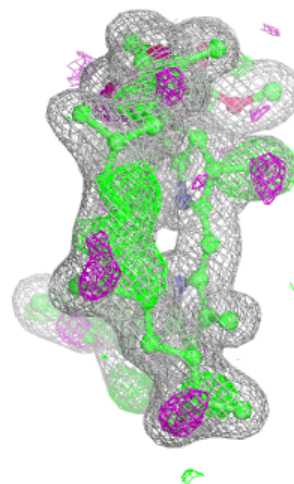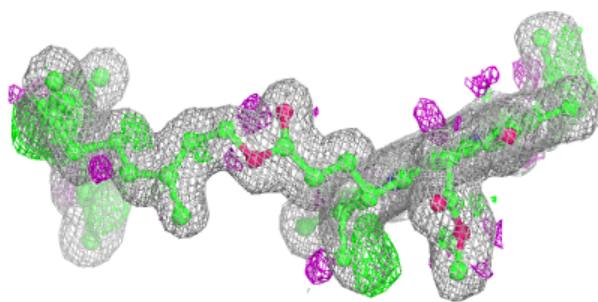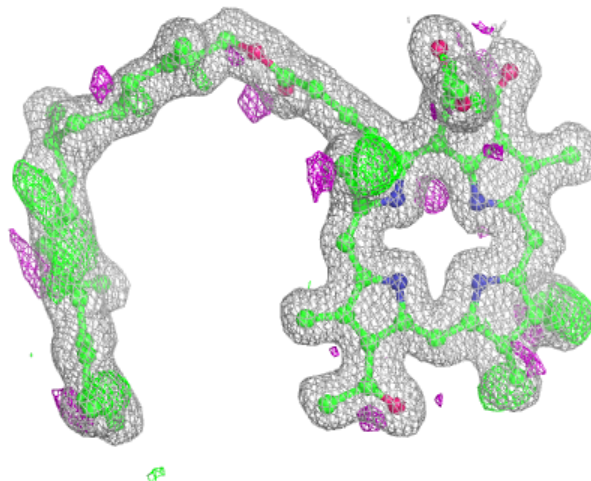
Electron density around CDL M 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
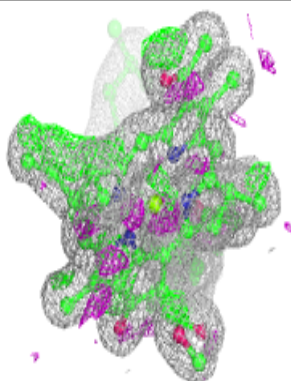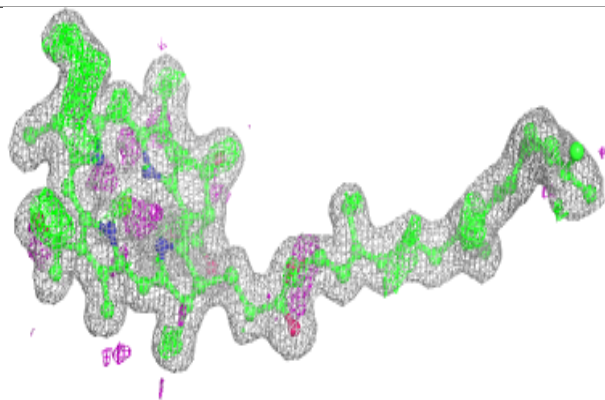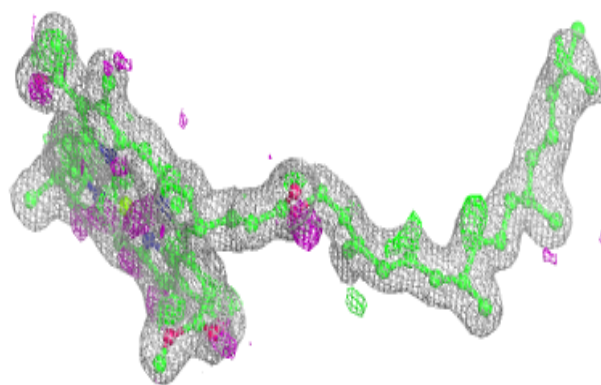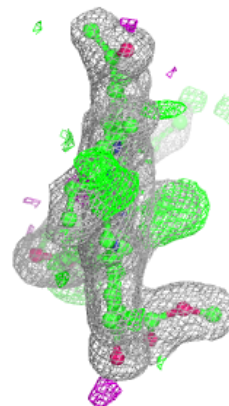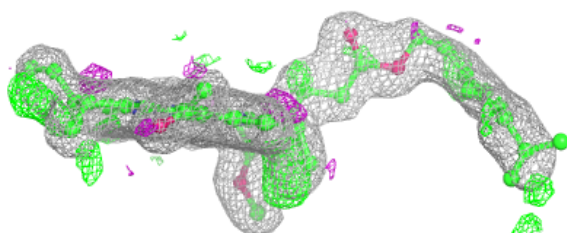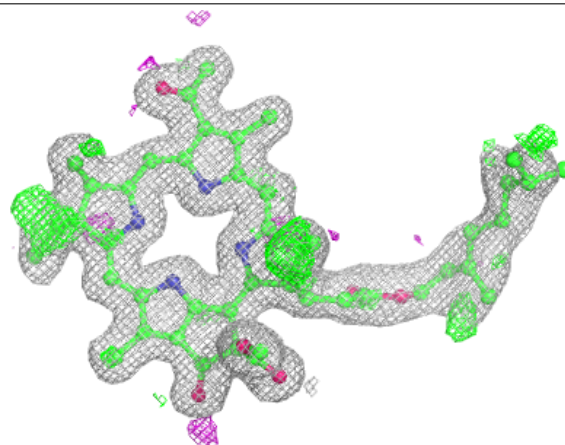mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
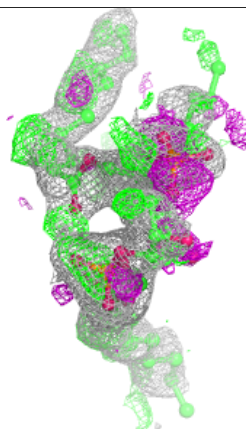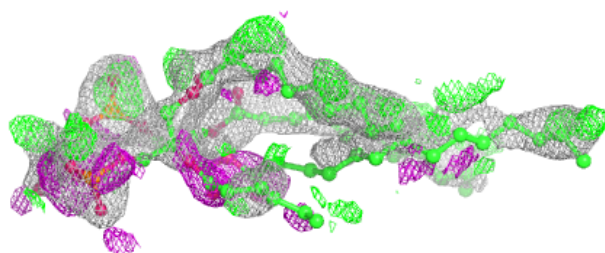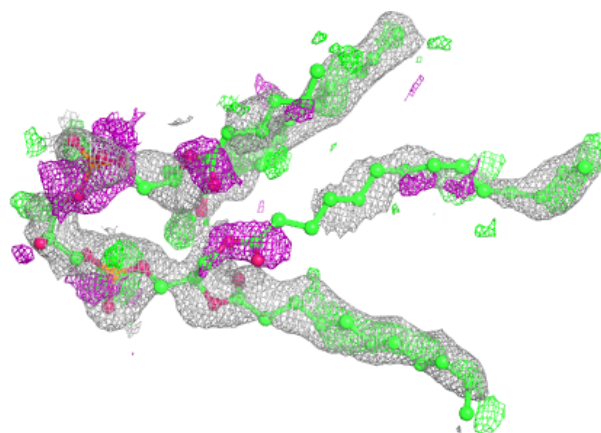
Electron density around U10 L 859 (A):

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

Electron density around SPO M 860:

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

Electron density around U10 M 858:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
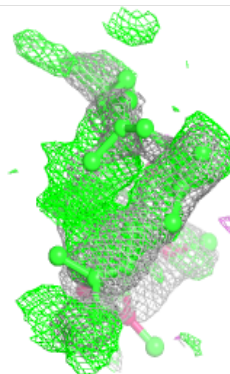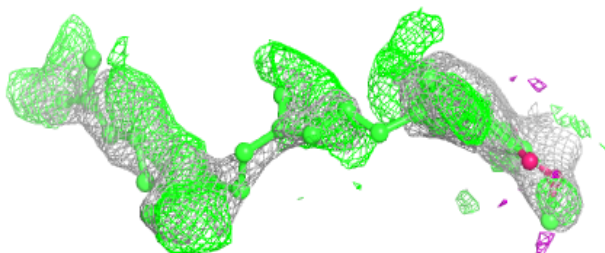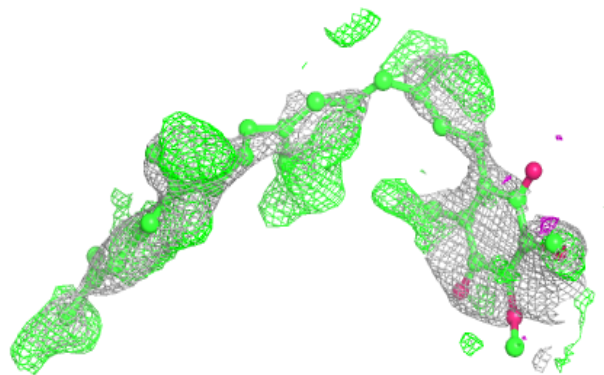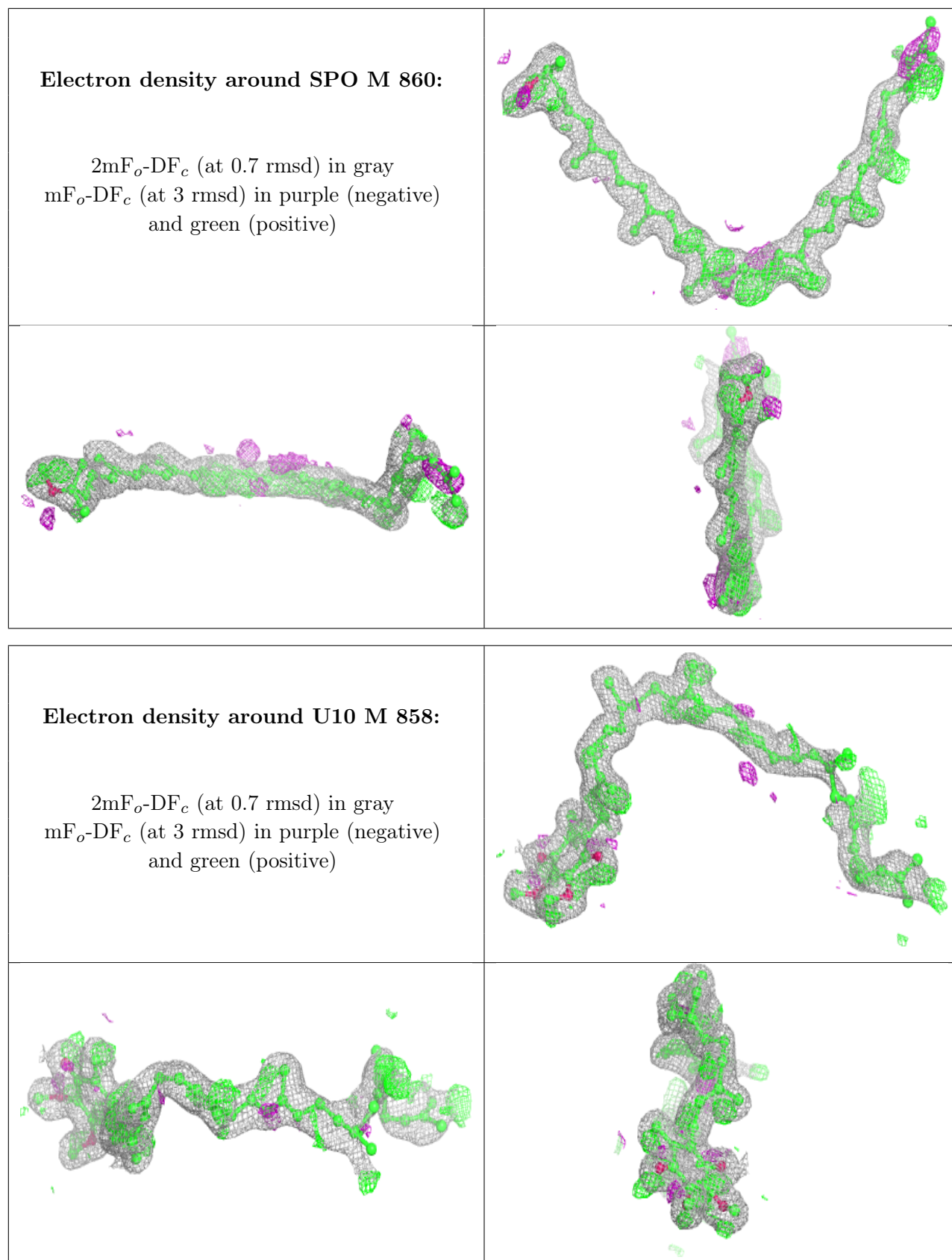
Electron density around BCL M 851:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
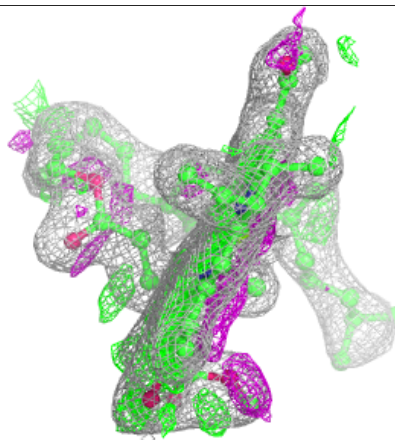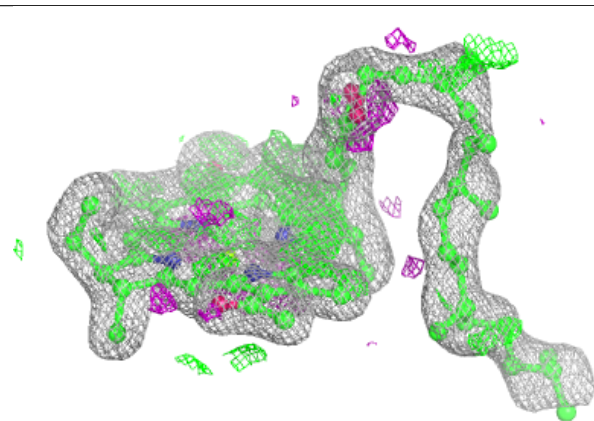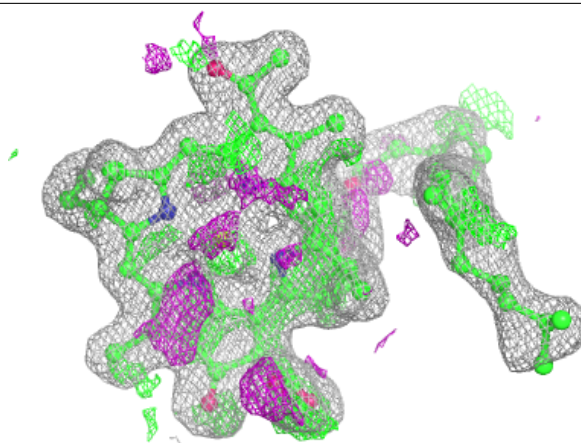
Electron density around BPH L 856:

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

Electron density around BCL M 853:

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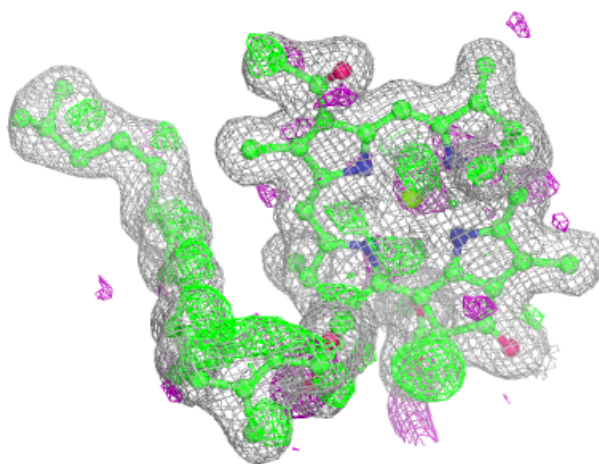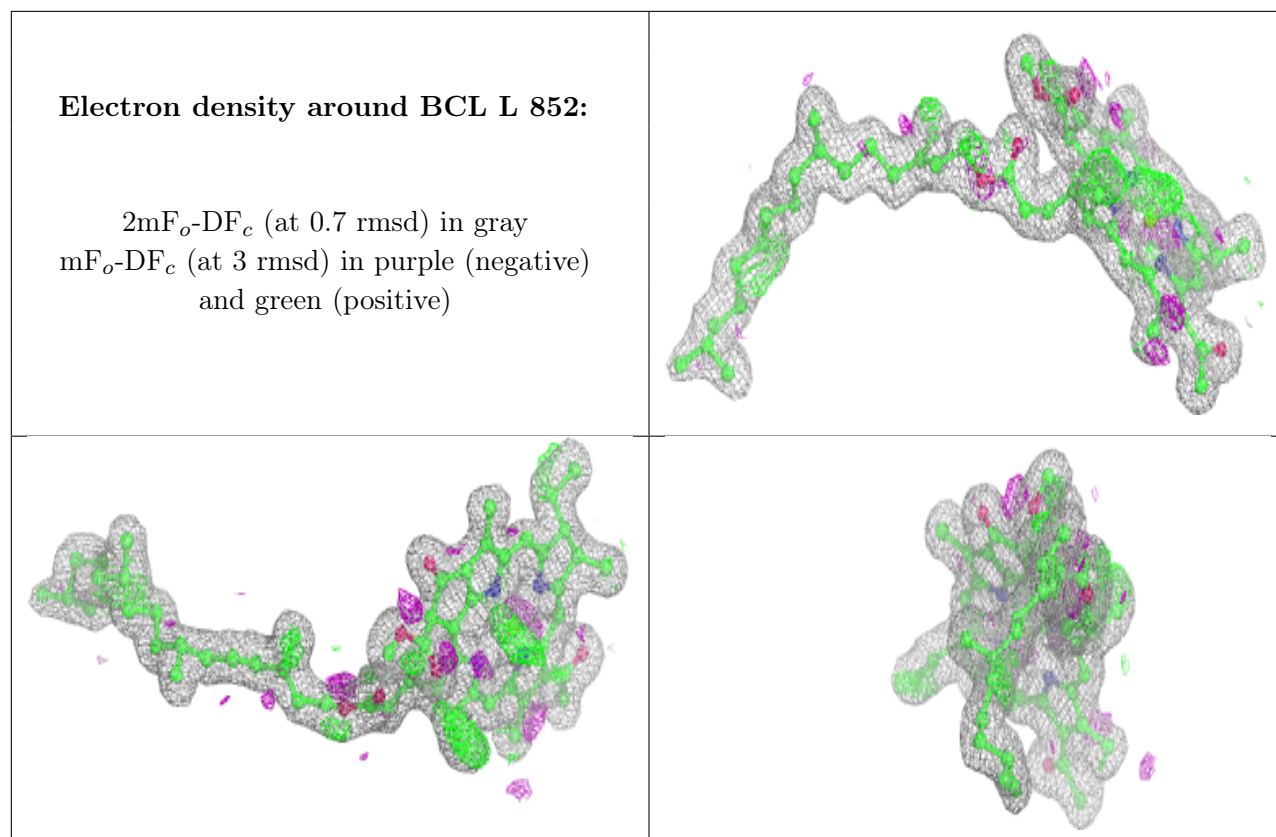and green (positive)

Electron density around BPH M 855:

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

Electron density around BCL L 854:

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

Electron density around BCL L 852:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
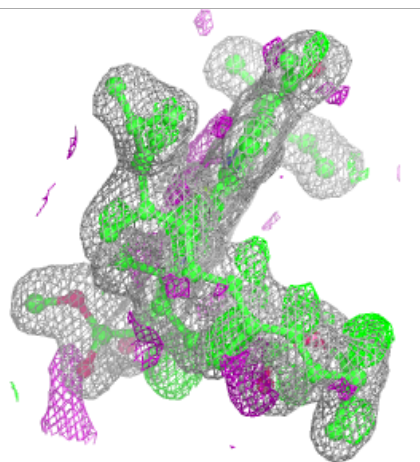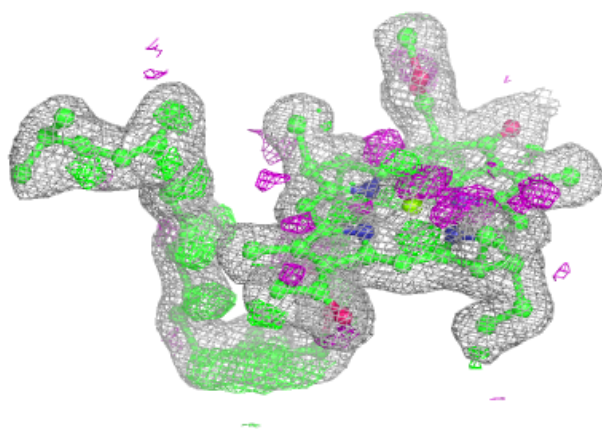
6.5 Other polymers (i)

There are no such residues in this entry.