W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 15, 2024 – 12:19 pm GMT

PDB ID	:	6Z1J
Title	:	Photosynthetic Reaction Center From Rhodobacter Sphaeroides strain RV LSP co-crystallization with spheroidene
Authors	:	Gabdulkhakov, A.G.; Fufina, T.Y.; Vasilieva, L.G.; Betzel, C.; Selikhanov, G.K.
Deposited on	:	2020-05-13
Resolution	:	2.10 Å(reported)

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

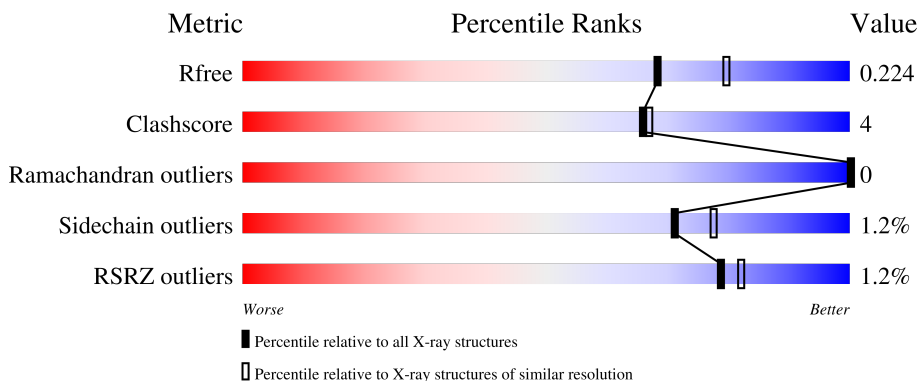|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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		0.224
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		1.2%
RSRZ outliers		1.2%

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	H	241	% 90% 10%
2	L	281	2% 91% 8% •
3	M	302	91% 8%

---

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 7643 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 H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	0	7	0
			1894	1210	324	350	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	21	0
			2422	1639	386	389	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	conflict	UNP P0C0Y8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	301	Total	C	N	O	S	0	5	0
			2441	1631	398	401	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	conflict	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

LDA

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

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).


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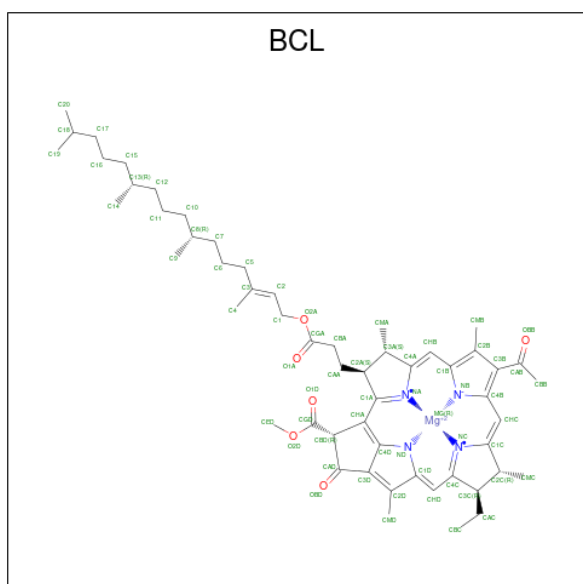
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).

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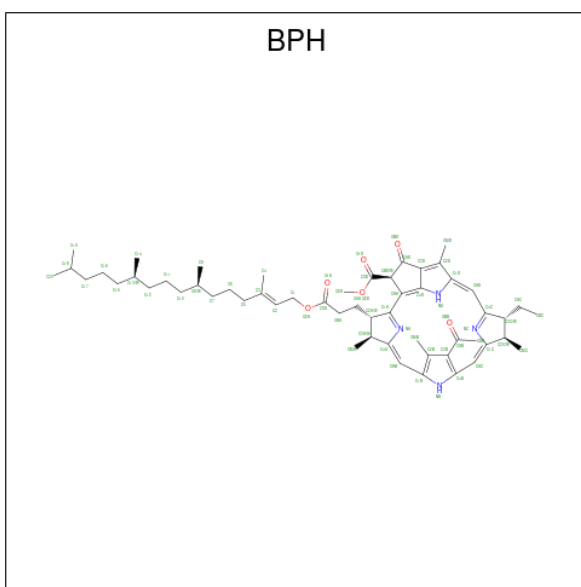
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total 65	C 55	N 4	O 6	0	0
6	M	1	Total 65	C 55	N 4	O 6	0	0

- Molecule 7 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	2	Total 27	C 27	0	0
7	M	3	Total 36	C 36	0	0

- Molecule 8 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC)

(formula: $C_{21}H_{40}O_4$).
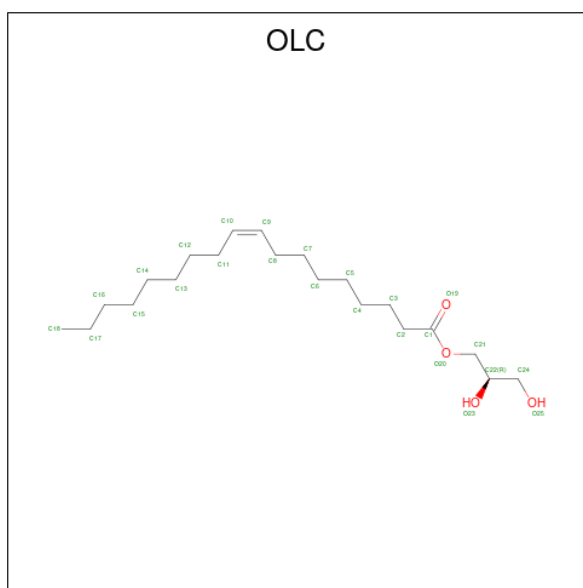
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			25	21	4		

- Molecule 9 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 10 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).
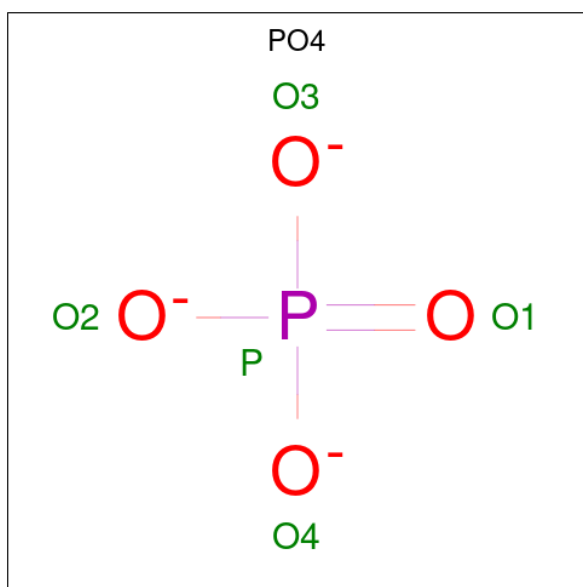
U10
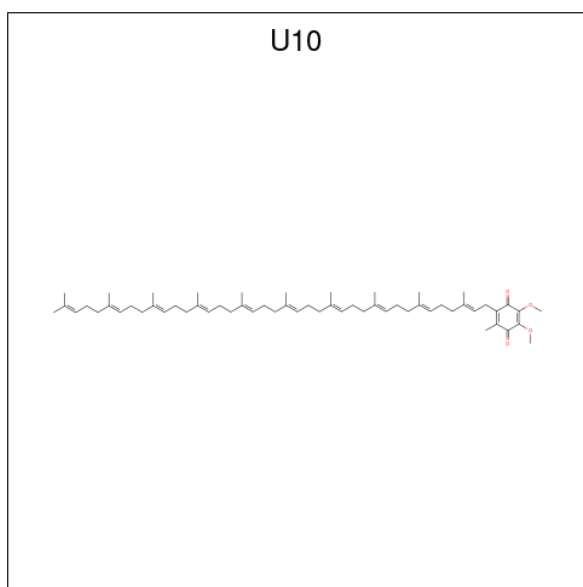
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	M	1	48	44	4	0	0

- Molecule 11 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$) (labeled as "Ligand of Interest" by depositor).
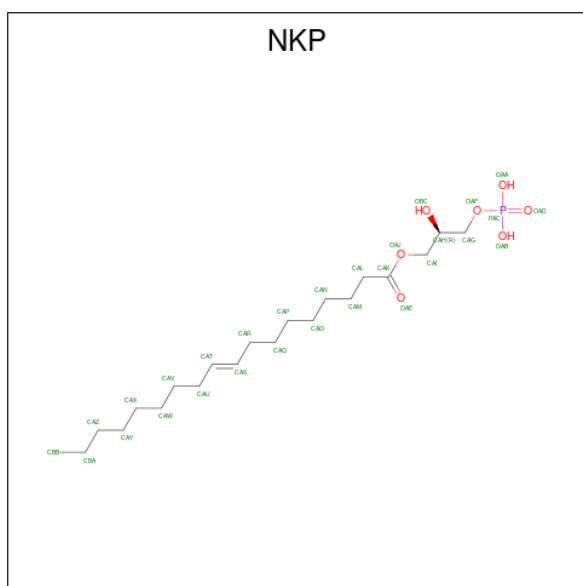
SPN
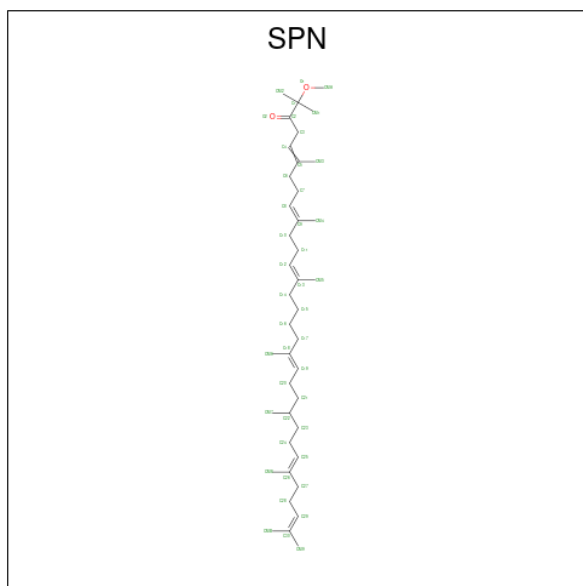
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	M	1	43	41	2	0	0

- Molecule 12 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

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

- Molecule 13 is (2R)-2-hydroxy-3-(phosphonooxy)propyl (9E)-octadec-9-enoate (three-letter code: NKP) (formula: $C_{21}H_{41}O_7P$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total 29	C 21	O 7	P 1	0	0
13	M	1	Total 29	C 21	O 7	P 1	0	0

• Molecule 14 is water.

| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	H	78	Total O 78 78	0	0
14	L	50	Total O 50 50	0	0
14	M	57	Total O 57 57	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.
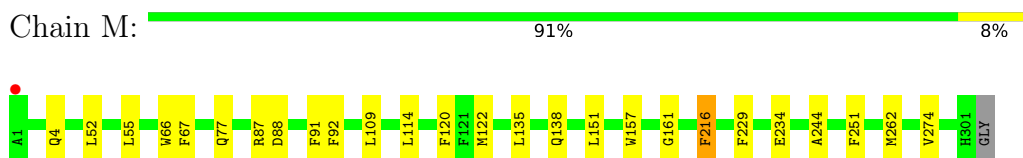
• Molecule 1: Reaction center protein H chain
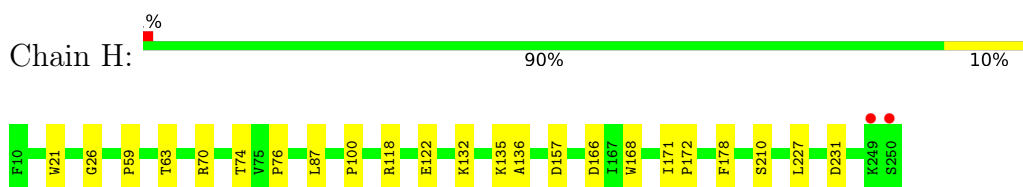
• Molecule 2: Reaction center protein L chain
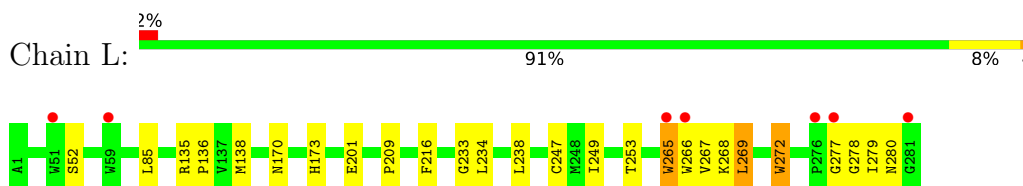
• Molecule 3: Reaction center protein M chain

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	99.89Å 99.89Å 238.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.07 – 2.10 48.88 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.07-2.10) 100.0 (48.88-2.10)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18_3861, PHENIX 1.18_3861	Depositor
R, R_{free}	0.188 , 0.224 0.188 , 0.224	Depositor DCC
R_{free} test set	3567 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.6	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7643	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[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, SPN, FE, OLC, UNL, LDA, PO4, BCL, BPH, NKP

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	H	0.42	0/1946	0.56	0/2646
2	L	0.41	0/2523	0.49	0/3457
3	M	0.41	0/2533	0.50	0/3458
All	All	0.41	0/7002	0.51	0/9561

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	H	1894	0	1895	13	0
2	L	2422	0	2356	17	0
3	M	2441	0	2361	25	0
4	H	16	0	31	1	0
4	M	48	0	93	2	0
5	L	132	0	148	3	0
5	M	132	0	148	2	0
6	L	65	0	76	0	0
6	M	65	0	76	2	0
7	L	27	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	36	0	0	0	0
8	L	25	0	40	0	0
9	M	1	0	0	0	0
10	M	48	0	63	0	0
11	M	43	0	70	10	0
12	M	5	0	0	1	0
13	M	58	0	78	3	0
14	H	78	0	0	0	0
14	L	50	0	0	0	0
14	M	57	0	0	1	0
All	All	7643	0	7435	59	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 4.

The worst 5 of 59 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.74	0.69
2:L:267[A]:VAL:HG13	2:L:280[A]:ASN:HB3	1.76	0.68
2:L:277[B]:GLY:O	3:M:87:ARG:NH2	2.28	0.66
2:L:201:GLU:OE2	3:M:138:GLN:HG3	2.01	0.61
5:L:301:BCL:CAB	11:M:406:SPN:H162	2.32	0.60

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	H	246/241 (102%)	240 (98%)	6 (2%)	0	100	100
2	L	299/281 (106%)	291 (97%)	8 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	304/302 (101%)	294 (97%)	10 (3%)	0	100	100
All	All	849/824 (103%)	825 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	H	203/196 (104%)	202 (100%)	1 (0%)	88	92
2	L	237/220 (108%)	229 (97%)	8 (3%)	37	39
3	M	240/236 (102%)	237 (99%)	3 (1%)	69	75
All	All	680/652 (104%)	668 (98%)	12 (2%)	71	65

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	272[A]	TRP
2	L	272[B]	TRP
3	M	216	PHE
3	M	52[A]	LEU
2	L	265[A]	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 22 ligands modelled in this entry, 5 are unknown and 1 is monoatomic - leaving 16 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	BPH	M	403	-	51,70,70	0.86	2 (3%)	52,101,101	1.10	6 (11%)
6	BPH	L	303	-	51,70,70	1.01	3 (5%)	52,101,101	1.00	3 (5%)
5	BCL	L	301	-	64,74,74	1.35	6 (9%)	78,115,115	1.62	15 (19%)
5	BCL	L	302	-	64,74,74	1.33	7 (10%)	78,115,115	1.45	8 (10%)
10	U10	M	405	-	48,48,63	2.59	13 (27%)	58,61,79	1.77	15 (25%)
11	SPN	M	406	-	40,42,42	0.32	0	50,52,52	0.37	0
5	BCL	M	401	-	64,74,74	1.29	5 (7%)	78,115,115	1.53	10 (12%)
12	PO4	M	413	-	4,4,4	0.95	0	6,6,6	0.30	0
4	LDA	M	407	-	12,15,15	2.00	1 (8%)	14,17,17	0.41	0
4	LDA	M	408	-	12,15,15	2.04	1 (8%)	14,17,17	0.55	0
4	LDA	H	301	-	12,15,15	2.01	1 (8%)	14,17,17	0.60	0
13	NKP	M	414	-	28,28,28	0.37	0	31,32,32	0.40	0
5	BCL	M	402	-	64,74,74	1.24	5 (7%)	78,115,115	1.48	8 (10%)
4	LDA	M	409	-	12,15,15	2.11	1 (8%)	14,17,17	0.62	0
13	NKP	M	415	-	28,28,28	0.35	0	31,32,32	0.47	0
8	OLC	L	306	-	24,24,24	0.95	1 (4%)	25,25,25	0.79	2 (8%)

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	BPH	M	403	-	-	9/37/105/105	0/5/6/6
6	BPH	L	303	-	-	2/37/105/105	0/5/6/6
5	BCL	L	301	-	-	1/37/137/137	-
5	BCL	L	302	-	-	1/37/137/137	-
10	U10	M	405	-	-	9/45/69/87	0/1/1/1
11	SPN	M	406	-	-	19/50/51/51	-
5	BCL	M	401	-	-	1/37/137/137	-
4	LDA	M	407	-	-	6/13/13/13	-
4	LDA	M	408	-	-	6/13/13/13	-
4	LDA	H	301	-	-	3/13/13/13	-
13	NKP	M	414	-	-	6/28/28/28	-
5	BCL	M	402	-	-	1/37/137/137	-
4	LDA	M	409	-	-	8/13/13/13	-
13	NKP	M	415	-	-	6/28/28/28	-
8	OLC	L	306	-	-	11/24/24/24	-

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	409	LDA	O1-N1	-7.25	1.25	1.42
4	M	408	LDA	O1-N1	-7.01	1.25	1.42
4	H	301	LDA	O1-N1	-6.89	1.26	1.42
4	M	407	LDA	O1-N1	-6.77	1.26	1.42
10	M	405	U10	C8-C9	6.20	1.47	1.33

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	402	BCL	CHD-C1D-ND	-5.88	119.05	124.45
5	L	301	BCL	CHD-C1D-ND	-5.55	119.36	124.45
5	M	401	BCL	C4D-CHA-C1A	5.44	127.86	121.25
5	L	302	BCL	C4D-CHA-C1A	5.20	127.58	121.25
5	M	401	BCL	CHD-C1D-ND	-5.11	119.76	124.45

There are no chirality outliers.

5 of 89 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	407	LDA	C2-C1-N1-CM1
4	M	407	LDA	C2-C1-N1-CM2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	M	409	LDA	C2-C1-N1-O1
4	M	409	LDA	C2-C1-N1-CM1
4	M	409	LDA	C2-C1-N1-CM2

There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	403	BPH	2	0
5	L	301	BCL	2	0
5	L	302	BCL	1	0
11	M	406	SPN	10	0
5	M	401	BCL	1	0
12	M	413	PO4	1	0
4	M	407	LDA	1	0
4	M	408	LDA	1	0
4	H	301	LDA	1	0
13	M	414	NKP	2	0
5	M	402	BCL	2	0
13	M	415	NKP	1	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 BPH M 403

Bond lengths

Bond angles

Torsions

Rings

Ligand BPH L 303

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL L 301

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL L 302

Bond lengths

Bond angles

Torsions

Rings

Ligand U10 M 405

Bond lengths

Bond angles

Torsions

Rings

Ligand SPN M 406

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL M 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NKP M 414

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL M 402

Bond lengths

Bond angles

Torsions

Rings

Ligand NKP M 415

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC L 306

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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 ⓘ

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	H	241/241 (100%)	-0.37	2 (0%)	86	88	26, 36, 49, 95	0
2	L	281/281 (100%)	-0.34	7 (2%)	57	62	23, 32, 45, 66	0
3	M	301/302 (99%)	-0.30	1 (0%)	94	94	23, 33, 55, 104	0
All	All	823/824 (99%)	-0.33	10 (1%)	79	82	23, 34, 51, 104	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	6.7
1	H	250	SER	5.3
1	H	249	LYS	5.0
2	L	59	TRP	4.2
2	L	266[A]	TRP	3.9

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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	LDA	M	407	16/16	0.62	0.30	27,55,72,79	0
4	LDA	M	409	16/16	0.73	0.34	56,68,95,96	0
7	UNL	M	411	12/-	0.75	0.23	34,50,59,61	0
7	UNL	M	412	12/-	0.75	0.19	55,64,71,77	0
4	LDA	M	408	16/16	0.78	0.26	63,71,87,94	0
8	OLC	L	306	25/25	0.80	0.18	33,44,60,63	0
7	UNL	L	305	15/-	0.82	0.24	43,51,68,74	0
7	UNL	L	304	12/-	0.86	0.11	37,43,63,66	0
13	NKP	M	415	29/29	0.87	0.20	33,56,76,82	0
7	UNL	M	410	12/-	0.89	0.20	37,46,50,51	0
12	PO4	M	413	5/5	0.90	0.28	57,66,79,80	0
11	SPN	M	406	43/43	0.90	0.16	30,41,60,74	0
13	NKP	M	414	29/29	0.91	0.14	29,52,59,75	0
4	LDA	H	301	16/16	0.91	0.16	38,46,58,66	0
10	U10	M	405	48/63	0.92	0.17	21,30,55,60	0
6	BPH	M	403	65/65	0.94	0.12	22,30,81,93	0
5	BCL	M	401	66/66	0.94	0.11	21,29,41,56	0
5	BCL	L	302	66/66	0.95	0.11	21,29,34,38	0
5	BCL	L	301	66/66	0.95	0.10	24,30,59,67	0
6	BPH	L	303	65/65	0.96	0.14	20,26,34,36	0
5	BCL	M	402	66/66	0.97	0.12	20,27,38,49	0
9	FE	M	404	1/1	1.00	0.10	26,26,26,26	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 OLC L 306:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
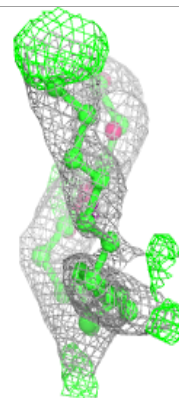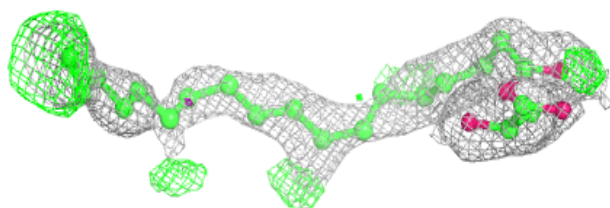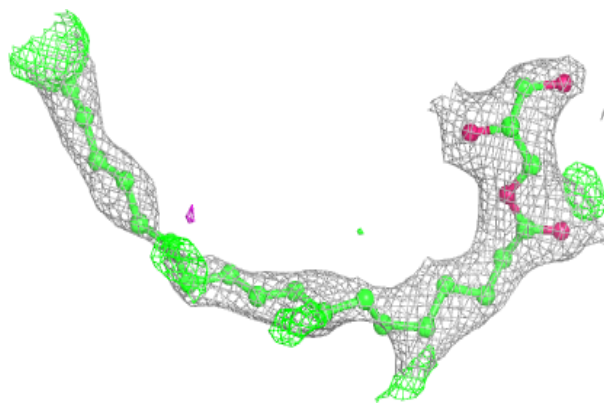
Electron density around NKP M 415:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
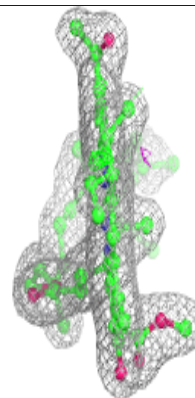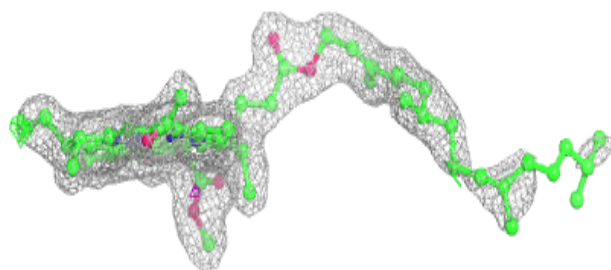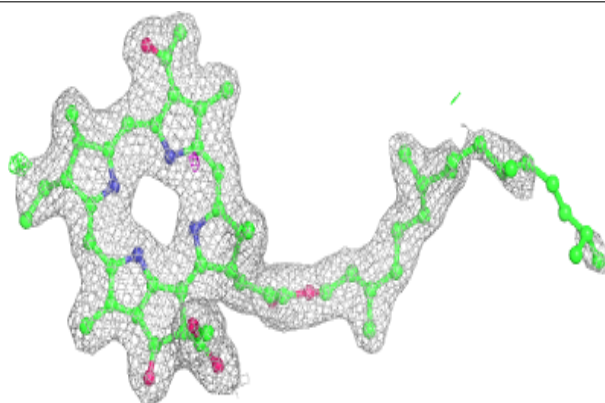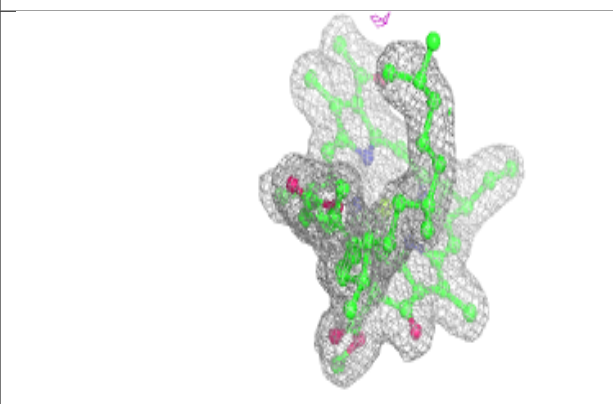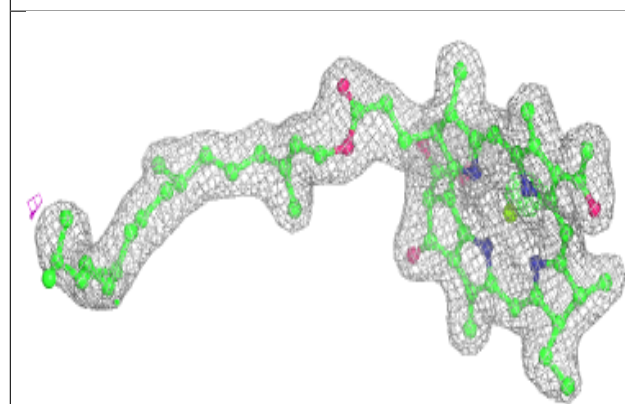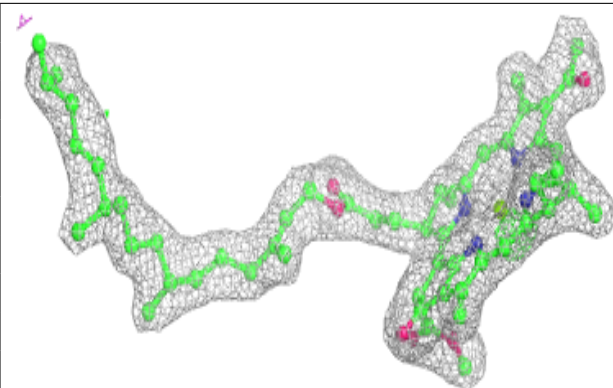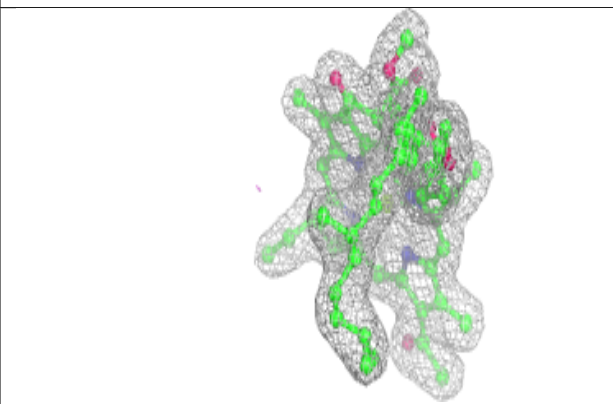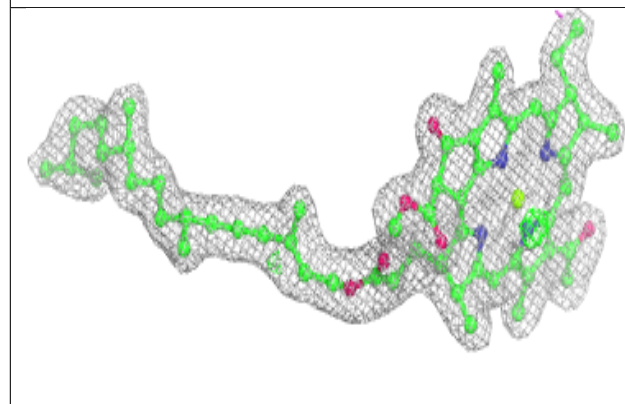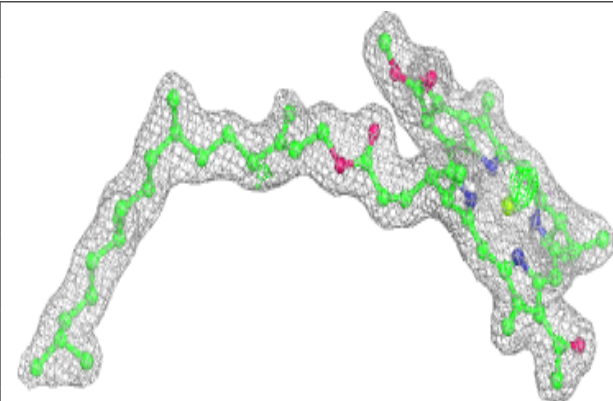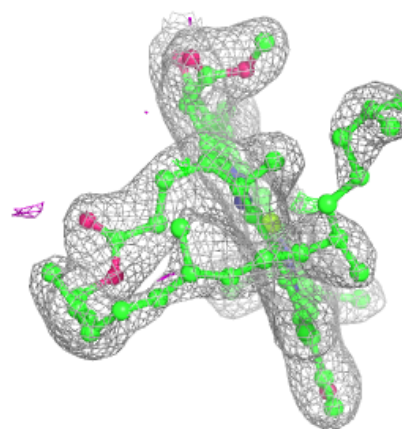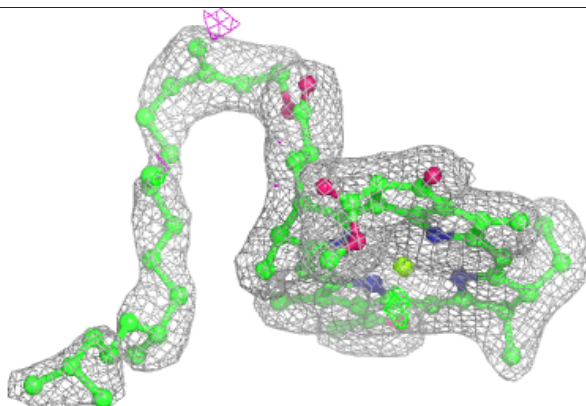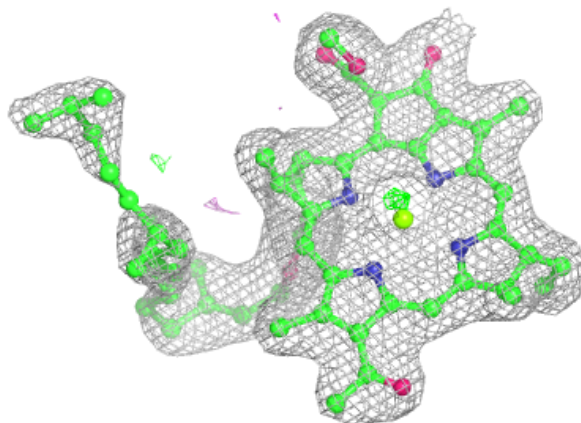mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
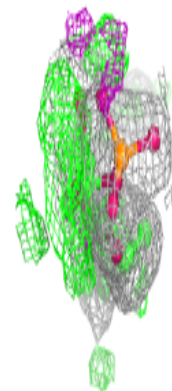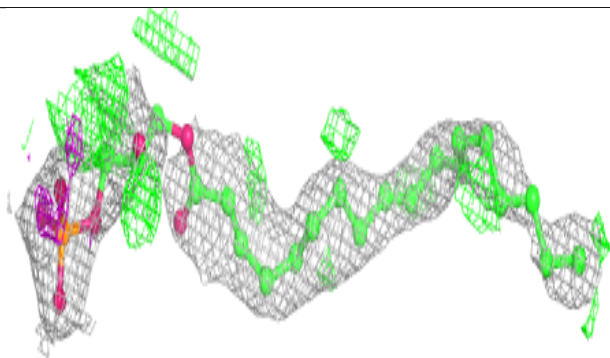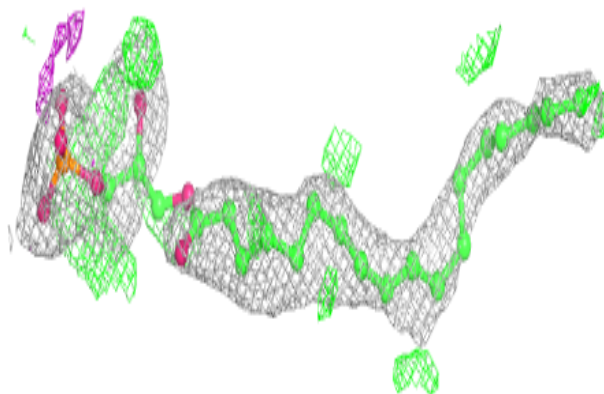
Electron density around SPN M 406:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
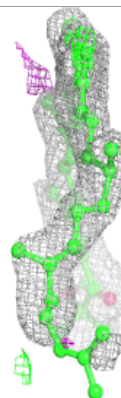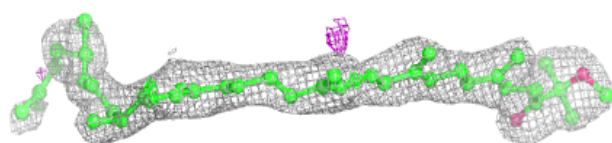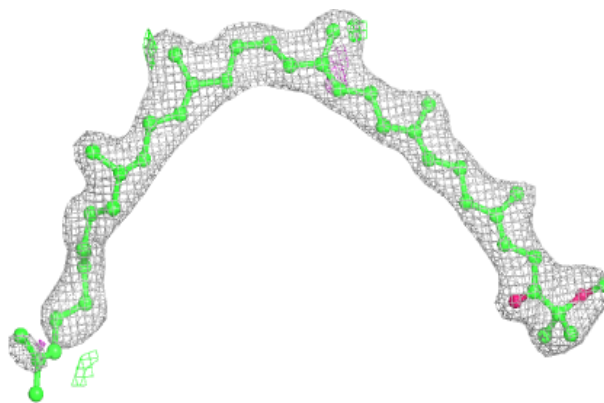
Electron density around NKP M 414:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
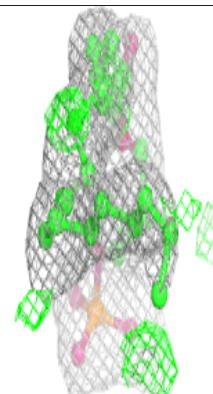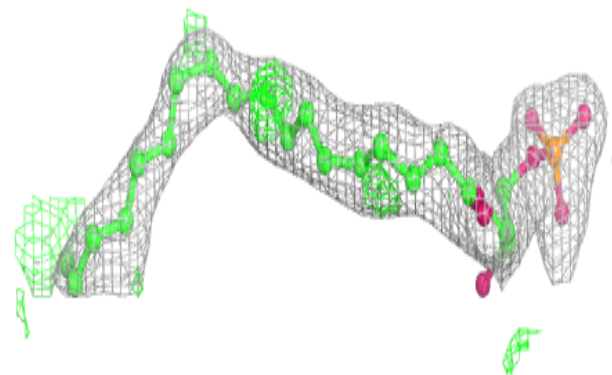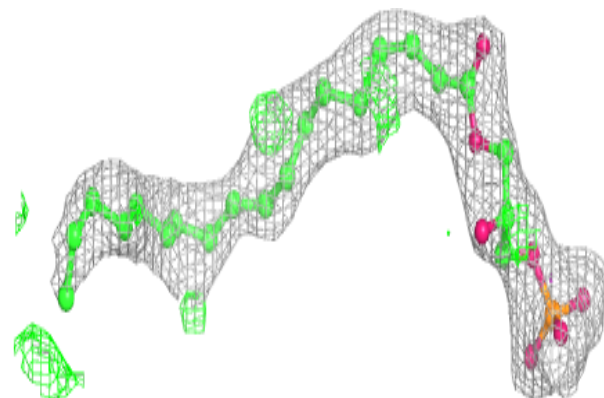
Electron density around U10 M 405:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
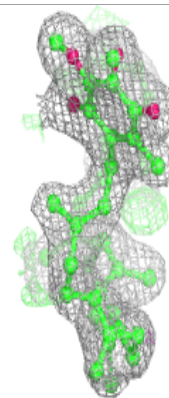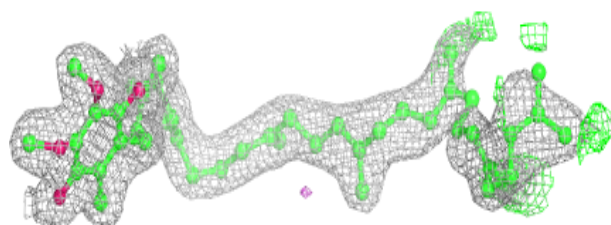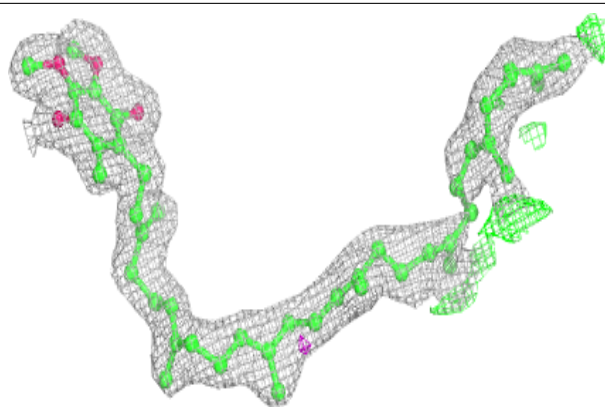
Electron density around BPH M 403:

$2mF_o\text{-}DF_c$ (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 401:

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

Electron density around BCL L 302:

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

Electron density around BCL L 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
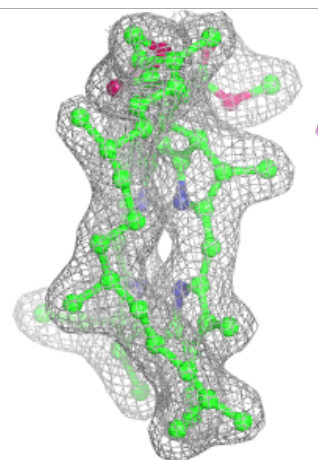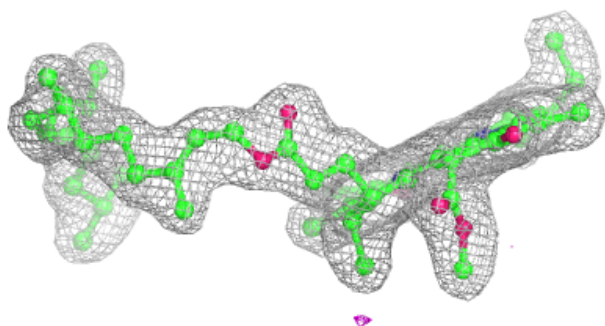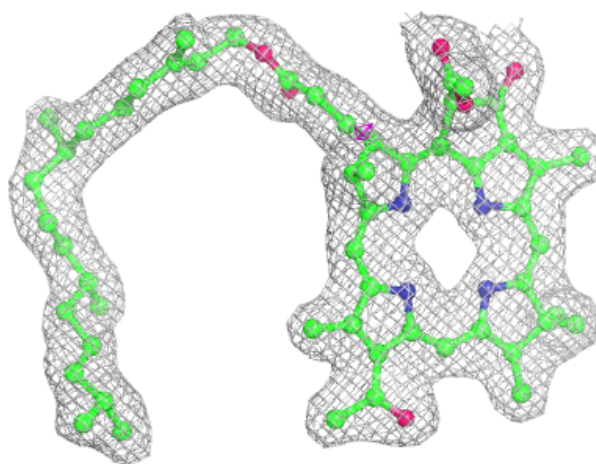mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
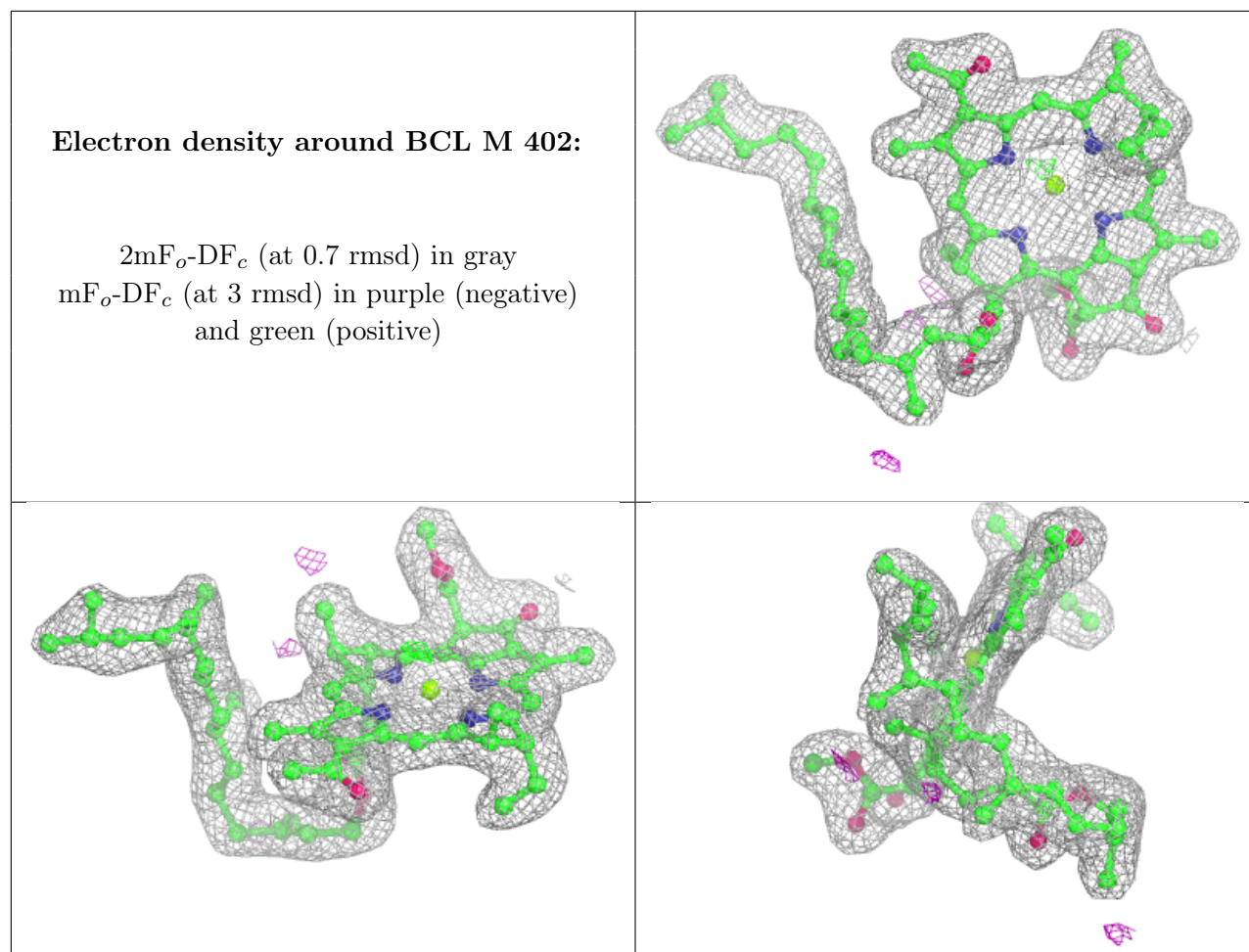
Electron density around BPH L 303:

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

Electron density around BCL M 402:

$2mF_o$-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.