W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 01:34 pm BST

PDB ID	:	5M7K
Title	:	Blastochloris viridis photosynthetic reaction center - RC_vir_xfel
Authors	:	Sharma, A.S.; Johansson, L.; Dunevall, E.; Wahlgren, W.Y.; Neutze, R.; Katona, G.
Deposited on	:	2016-10-28
Resolution	:	3.50 Å(reported)

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

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 3.50 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.
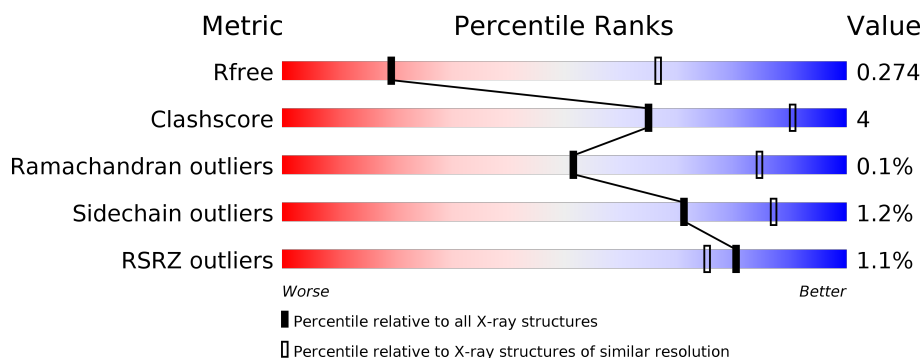
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on 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	A	356	83% 10% 7%
2	B	274	85% 15%
3	C	324	% 93% 6% ·
4	D	258	3% 88% 6% 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	MPG	B	306	-	-	-	X
9	MPG	C	407	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 9890 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2598	1637	465	478	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	273	Total	C	N	O	S	0	2	0
			2170	1458	350	355	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	323	Total	C	N	O	S	0	0	0
			2546	1696	417	422	11			

- Molecule 4 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	243	Total	C	N	O	S	0	0	0
			1771	1140	297	332	2			

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).
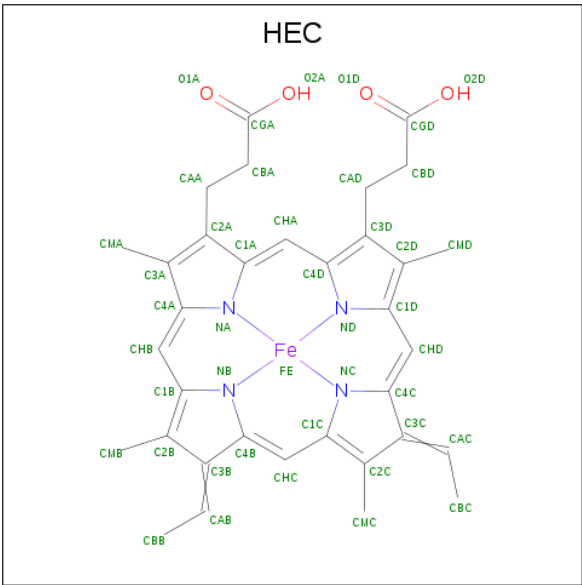
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

• Molecule 6 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).
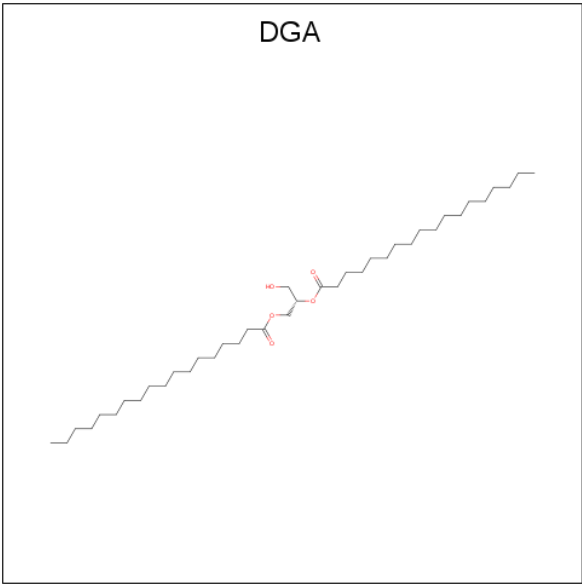
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 37	C 33	O 4	5	0

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).

BCL
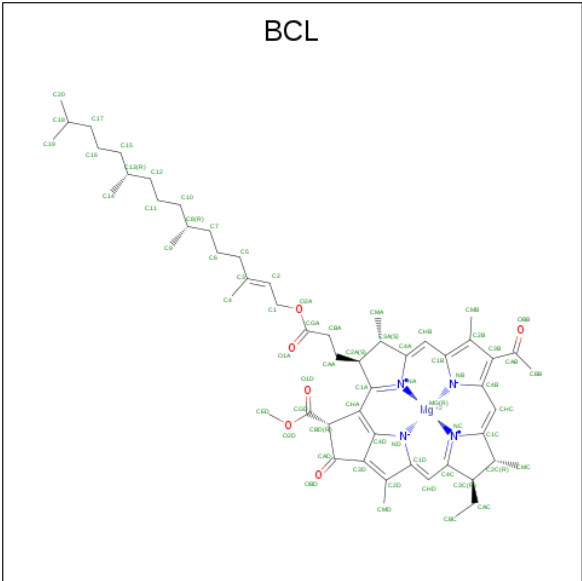
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total 65	C 54	Mg 1	N 4	O 6	15	0
7	B	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	B	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	C	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 8 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).

BPB
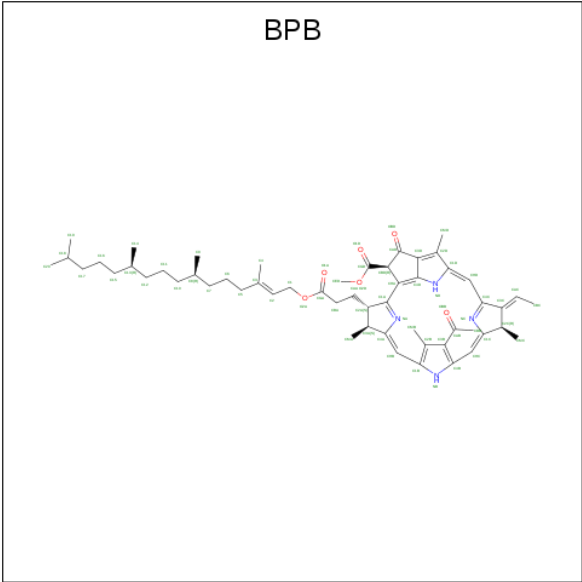
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			65	55	4	6		
8	C	1	Total	C	N	O	0	0
			61	51	4	6		

• Molecule 9 is [(Z)-octadec-9-enyl] (2R)-2,3-bis(oxidanyl)propanoate (three-letter code: MPG) (formula: $C_{21}H_{40}O_4$).

MPG
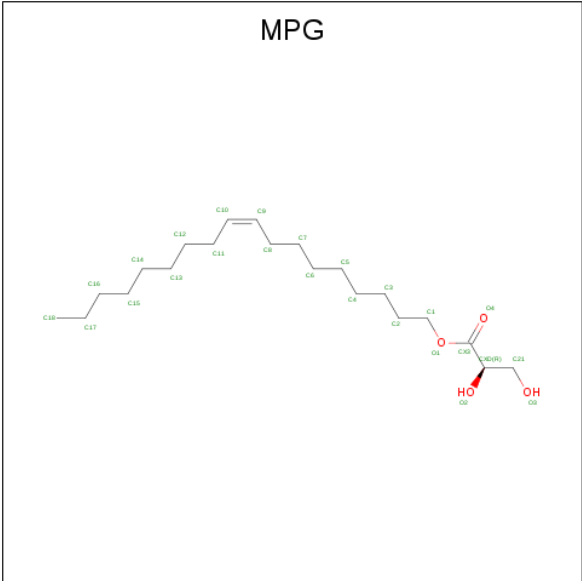
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	22	0
			25	21	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total 25	C 21	O 4	3	0
9	C	1	Total 17	C 17		8	0

- Molecule 10 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	1	Total 1	Fe 1	0	0

- Molecule 11 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).
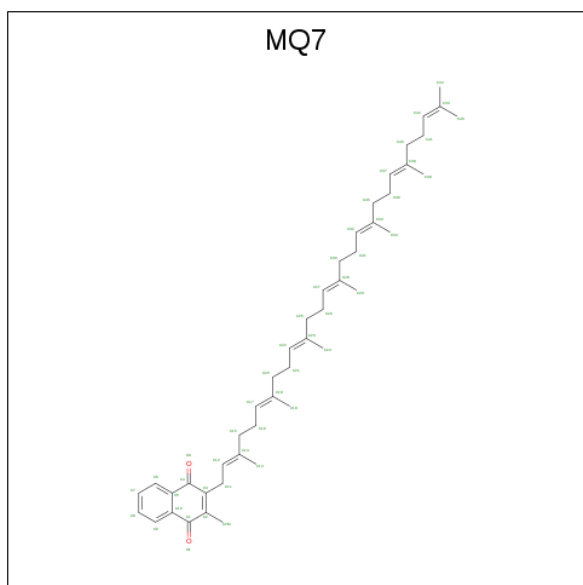
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total 48	C 46	O 2	0	0

- Molecule 12 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: $C_{40}H_{60}$).

NS5
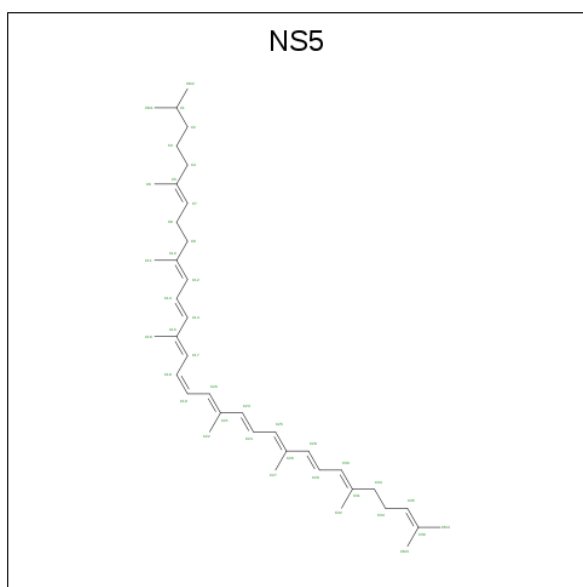
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	1	Total C 40 40		9	0

- Molecule 13 is (2E,6E,10E,14E,18E,22E,26E)-3,7,11,15,19,23,27,31-OCTAMETHYLD OTRIACONTA-2,6,10,14,18,22,26,30-OCTAENYL TRIHYDROGEN DIPHOSPHATE (three-letter code: OTP) (formula: $C_{40}H_{68}O_7P_2$).

OTP
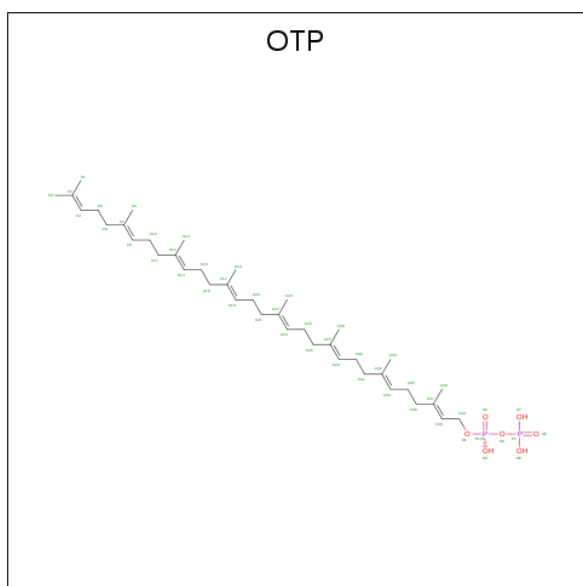
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total C O 41 40 1			0	0

- Molecule 14 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O⁻

O2 O⁻ — P = O   O1

P

O⁻

O4
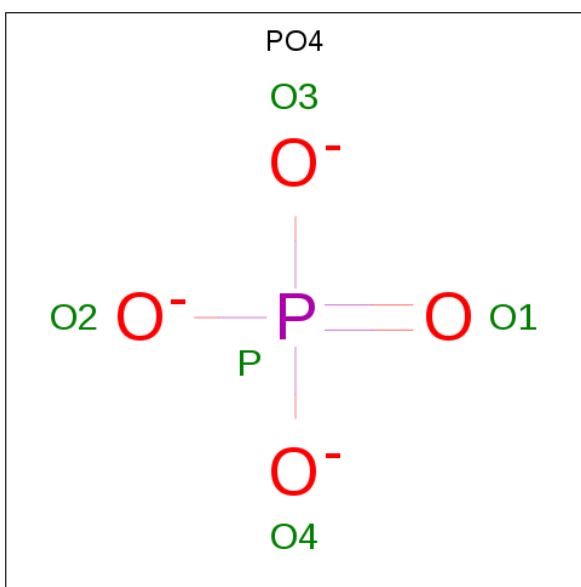
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total 5	O 4	P 1	5	0
14	C	1	Total 5	O 4	P 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
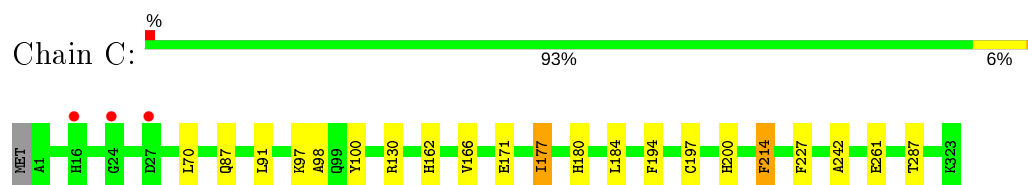
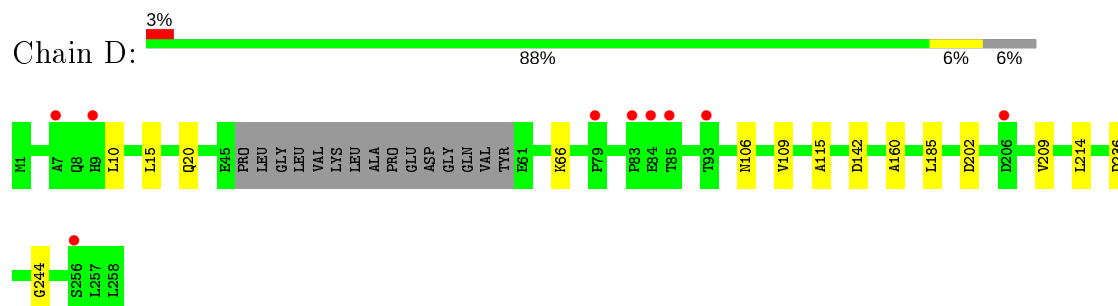- Molecule 1: Photosynthetic reaction center cytochrome c subunit
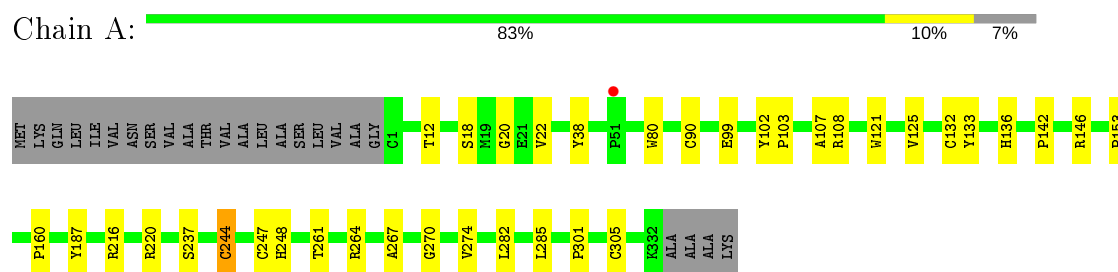
- Molecule 2: Reaction center protein L chain
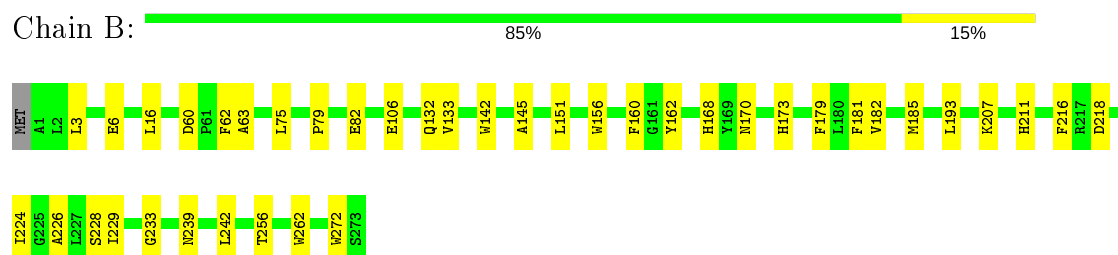
- Molecule 3: Reaction center protein M chain

- Molecule 4: Reaction center protein H chain

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.90Å 84.80Å 384.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.44 – 3.50 55.44 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.44-3.50) 100.0 (55.44-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.91 (at 3.49Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.253 , 0.274 0.253 , 0.274	Depositor DCC
R_{free} test set	1294 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	77.1	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 75.2	EDS
L-test for twinning[2]	$<|L|> = 0.34$, $<L^2> = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	9890	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, MPG, BPB, PO4, DGA, FE2, MQ7, HEC, OTP, FME, NS5

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	0.27	0/2665	0.46	0/3633
2	B	0.26	0/2263	0.42	0/3089
3	C	0.26	0/2650	0.40	0/3629
4	D	0.25	0/1804	0.45	0/2485
All	All	0.26	0/9382	0.43	0/12836

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	HIS	Peptide

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	2598	0	2576	31	0
2	B	2170	0	2100	24	0
3	C	2546	0	2430	14	0
4	D	1771	0	1656	7	0
5	A	172	0	128	14	0
6	A	37	0	58	2	0
7	B	197	0	218	8	0
7	C	66	0	74	3	0
8	B	65	0	74	2	0
8	C	61	0	63	1	0
9	B	50	0	80	0	0
9	C	17	0	31	0	0
10	C	1	0	0	0	0
11	C	48	0	64	1	0
12	C	40	0	60	2	0
13	C	41	0	65	2	0
14	C	10	0	0	0	0
All	All	9890	0	9677	80	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 80 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:A:244:CYS:HB3	5:A:403:HEC:C3B	2.28	0.63
1:A:153:PRO:HD3	1:A:160:PRO:HB3	1.81	0.61
1:A:80:TRP:CD1	1:A:133:TYR:HB2	2.36	0.61
1:A:244:CYS:SG	2:B:162:TYR:HB3	2.41	0.60
1:A:99:GLU:OE2	1:A:108:ARG:NH2	2.35	0.59

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	330/356 (93%)	313 (95%)	17 (5%)	0	100	100
2	B	273/274 (100%)	262 (96%)	11 (4%)	0	100	100
3	C	321/324 (99%)	313 (98%)	7 (2%)	1 (0%)	41	75
4	D	239/258 (93%)	234 (98%)	5 (2%)	0	100	100
All	All	1163/1212 (96%)	1122 (96%)	40 (3%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	177	ILE

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	280/297 (94%)	277 (99%)	3 (1%)	73	88
2	B	218/219 (100%)	215 (99%)	3 (1%)	67	85
3	C	247/250 (99%)	245 (99%)	2 (1%)	81	91
4	D	167/212 (79%)	164 (98%)	3 (2%)	59	81
All	All	912/978 (93%)	901 (99%)	11 (1%)	71	87

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

Mol	Chain	Res	Type
2	B	185	MET
2	B	272	TRP
4	D	20	GLN
2	B	160	PHE
3	C	214	PHE

Some 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 ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
4	FME	D	1	4	8,9,10	0.92	0	7,9,11	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	D	1	4	-	4/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	FME	CB-CA-N-CN
4	D	1	FME	C-CA-CB-CG
4	D	1	FME	CA-CB-CG-SD
4	D	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	#$|Z| > 2$
7	BCL	C	401	-	58,74,74	1.24	5 (8%)	69,115,115	1.45	11 (15%)
6	DGA	A	405	-	36,36,43	1.17	3 (8%)	38,38,45	3.13	6 (15%)
7	BCL	B	302	-	58,74,74	1.28	5 (8%)	69,115,115	1.51	12 (17%)
14	PO4	C	408	-	4,4,4	0.92	0	6,6,6	0.43	0
7	BCL	B	301	-	57,73,74	1.29	5 (8%)	67,113,115	1.25	8 (11%)
12	NS5	C	405	-	39,39,39	2.33	18 (46%)	44,46,46	2.07	13 (29%)
5	HEC	A	401	1	26,50,50	2.19	4 (15%)	18,82,82	2.01	7 (38%)
9	MPG	B	305	-	24,24,24	1.24	1 (4%)	24,25,25	1.53	3 (12%)
14	PO4	C	409	-	4,4,4	0.88	0	6,6,6	0.50	0
8	BPB	B	304	-	64,70,70	1.11	5 (7%)	64,101,101	1.19	6 (9%)
7	BCL	B	303	-	58,74,74	1.31	5 (8%)	69,115,115	1.38	11 (15%)
9	MPG	B	306	-	24,24,24	1.26	1 (4%)	24,25,25	1.30	2 (8%)
11	MQ7	C	404	-	49,49,49	1.81	10 (20%)	60,63,63	1.60	15 (25%)
9	MPG	C	407	-	16,16,24	0.79	0	15,15,25	0.75	0
5	HEC	A	402	1	26,50,50	2.14	5 (19%)	18,82,82	2.22	8 (44%)
5	HEC	A	403	1	26,50,50	2.16	4 (15%)	18,82,82	2.03	6 (33%)
8	BPB	C	402	-	60,66,70	1.15	5 (8%)	59,96,101	1.24	6 (10%)
5	HEC	A	404	1	26,50,50	2.21	4 (15%)	18,82,82	1.82	5 (27%)
13	OTP	C	406	-	40,40,48	0.66	0	47,47,61	1.97	16 (34%)

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
7	BCL	C	401	-	-	6/37/137/137	-
6	DGA	A	405	-	-	14/37/37/45	-
7	BCL	B	302	-	-	4/37/137/137	-
7	BCL	B	301	-	-	6/36/136/137	-
12	NS5	C	405	-	-	13/43/43/43	-
5	HEC	A	401	1	-	0/6/54/54	-
9	MPG	B	305	-	-	14/25/25/25	-
9	MPG	B	306	-	-	11/25/25/25	-
5	HEC	A	402	1	-	1/6/54/54	-
8	BPB	B	304	-	-	7/47/105/105	0/5/6/6
11	MQ7	C	404	-	-	3/41/61/61	0/2/2/2
9	MPG	C	407	-	-	6/14/14/25	-
7	BCL	B	303	-	-	5/37/137/137	-
5	HEC	A	403	1	-	0/6/54/54	-
8	BPB	C	402	-	-	11/43/101/105	0/5/6/6
5	HEC	A	404	1	-	0/6/54/54	-
13	OTP	C	406	-	-	13/45/45/55	-

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	404	MQ7	C3-C2	7.19	1.48	1.35
5	A	404	HEC	C3B-C2B	-5.62	1.34	1.40
5	A	401	HEC	C3B-C2B	-5.57	1.34	1.40
5	A	404	HEC	C3C-C2C	-5.51	1.35	1.40
5	A	403	HEC	C3C-C2C	-5.29	1.35	1.40

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	405	DGA	OG2-CG2-CG3	-12.84	78.58	107.93
6	A	405	DGA	OG2-CG2-CG1	-10.09	82.77	106.13
6	A	405	DGA	CG3-CG2-CG1	7.00	132.75	112.63
12	C	405	NS5	C18-C17-C15	-6.46	118.10	127.31
12	C	405	NS5	C19-C20-C21	-5.98	118.78	127.31

There are no chirality outliers.

5 of 114 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	401	BCL	CAD-CBD-CGD-O1D
7	C	401	BCL	CAD-CBD-CGD-O2D
6	A	405	DGA	CA2-CA1-OG1-CG1
6	A	405	DGA	OA1-CA1-OG1-CG1
6	A	405	DGA	OG1-CG1-CG2-OG2

There are no ring outliers.

14 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	401	BCL	3	0
6	A	405	DGA	2	0
7	B	302	BCL	3	0
7	B	301	BCL	2	0
12	C	405	NS5	2	0
5	A	401	HEC	2	0
8	B	304	BPB	2	0
7	B	303	BCL	3	0
11	C	404	MQ7	1	0
5	A	402	HEC	3	0
5	A	403	HEC	6	0
8	C	402	BPB	1	0
5	A	404	HEC	3	0
13	C	406	OTP	2	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 C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand DGA A 405

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL B 302

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NS5 C 405

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand MPG B 305

Bond lengths

Bond angles

Torsions

Rings

Ligand BPB B 304

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL B 303

Bond lengths

Bond angles

Torsions

Rings

Ligand MPG B 306

Bond lengths

Bond angles

Torsions

Rings

Ligand MQ7 C 404

Bond lengths

Bond angles

Torsions

Rings

Ligand MPG C 407

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC A 402

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC A 403

Bond lengths

Bond angles

Torsions

Rings

Ligand BPB C 402

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC A 404

Bond lengths

Bond angles

Torsions

Rings

Ligand OTP C 406

Bond lengths

Bond angles

Torsions

Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	A	332/356 (93%)	-0.35	1 (0%)	94	91	30, 44, 65, 82	0
2	B	273/274 (99%)	-0.32	0	100	100	34, 56, 91, 111	0
3	C	323/324 (99%)	-0.20	3 (0%)	84	79	33, 61, 90, 110	0
4	D	242/258 (93%)	0.23	9 (3%)	41	37	53, 96, 116, 147	0
All	All	1170/1212 (96%)	-0.18	13 (1%)	80	75	30, 58, 104, 147	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	85	THR	3.6
4	D	84	GLU	3.1
3	C	24	GLY	3.1
4	D	7	ALA	2.4
4	D	256	SER	2.4

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	FME	D	1	10/11	0.87	0.46	57,67,76,92	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
9	MPG	B	306	25/25	0.68	0.43	69,82,90,94	3
9	MPG	C	407	17/25	0.71	0.49	73,81,109,112	8
12	NS5	C	405	40/40	0.82	0.36	47,68,89,96	9
13	OTP	C	406	41/49	0.83	0.32	45,67,80,85	0
8	BPB	C	402	61/65	0.91	0.29	52,64,78,80	0
11	MQ7	C	404	48/48	0.91	0.30	43,63,70,72	0
14	PO4	C	409	5/5	0.91	0.25	95,95,101,106	0
9	MPG	B	305	25/25	0.92	0.30	64,91,97,99	22
5	HEC	A	401	43/43	0.94	0.30	42,49,54,57	0
8	BPB	B	304	65/65	0.94	0.22	38,47,56,57	0
10	FE2	C	403	1/1	0.95	0.10	67,67,67,67	0
7	BCL	B	301	65/66	0.95	0.20	42,50,158,164	15
7	BCL	B	303	66/66	0.96	0.20	34,40,47,52	0
5	HEC	A	403	43/43	0.96	0.23	24,35,39,45	0
5	HEC	A	404	43/43	0.96	0.20	36,43,50,53	0
5	HEC	A	402	43/43	0.96	0.27	39,44,48,62	0
14	PO4	C	408	5/5	-	-	81,82,84,85	5
6	DGA	A	405	37/44	0.75	0.39	50,71,91,92	5
7	BCL	B	302	66/66	0.94	0.23	40,45,52,58	0
7	BCL	C	401	66/66	0.94	0.24	41,45,58,60	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 MPG B 306:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
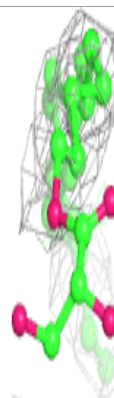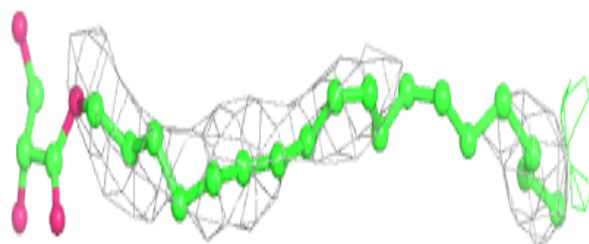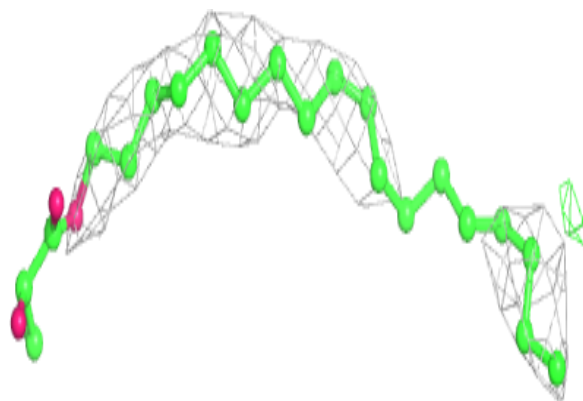
Electron density around MPG C 407:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
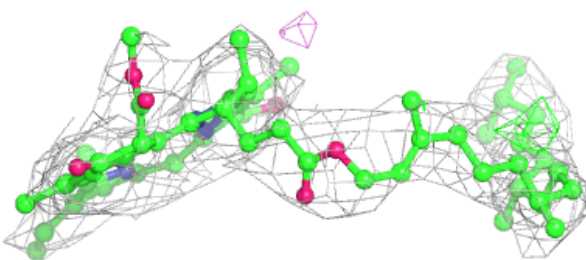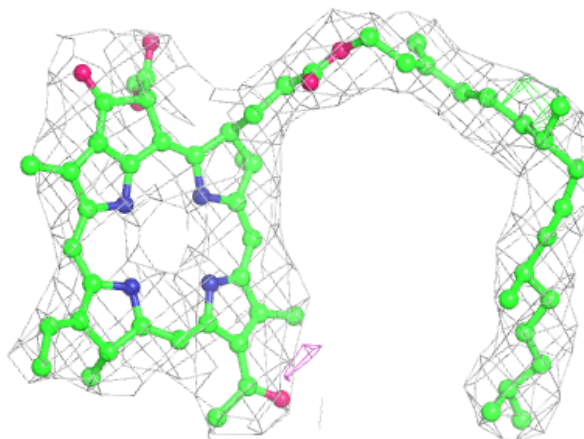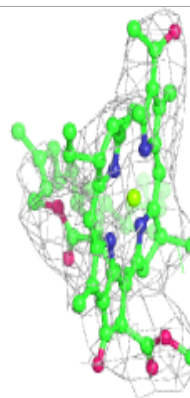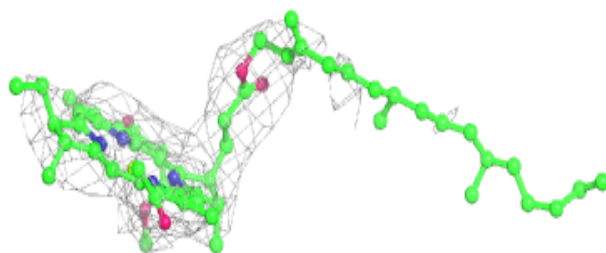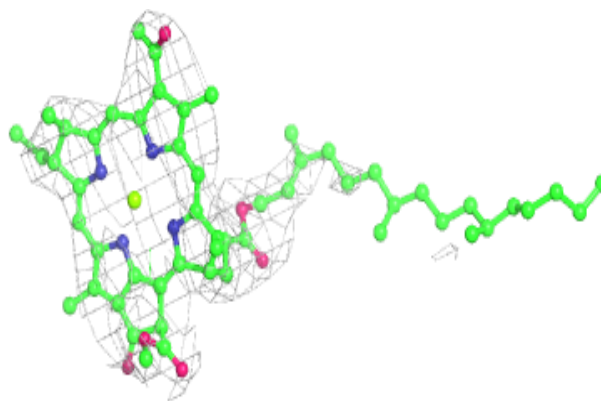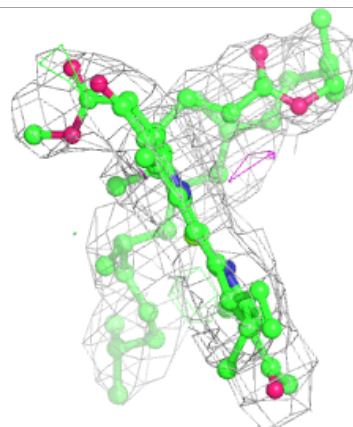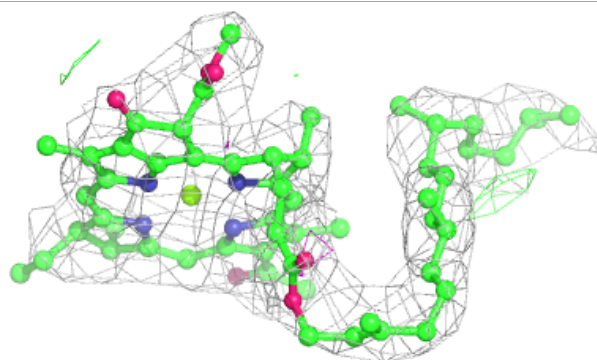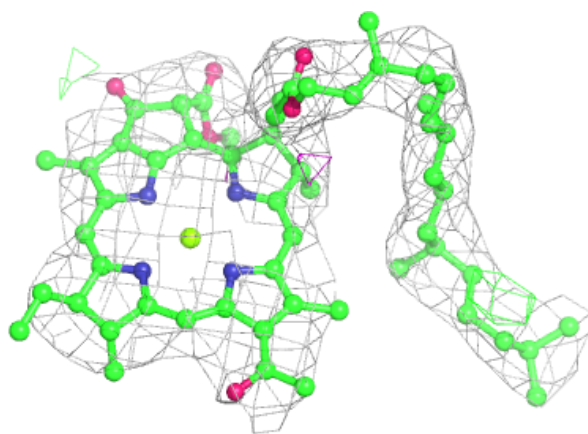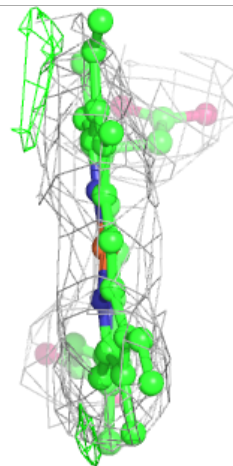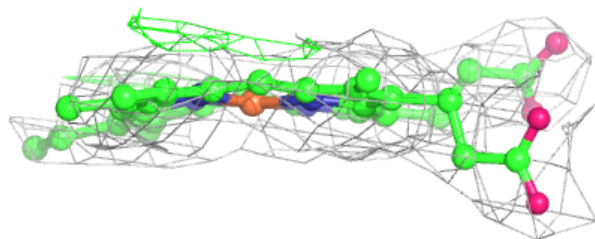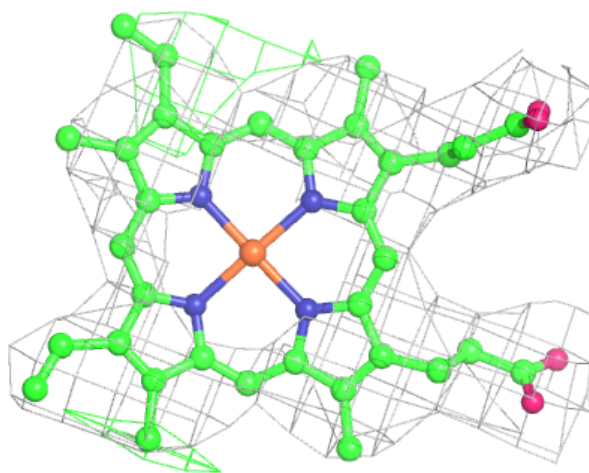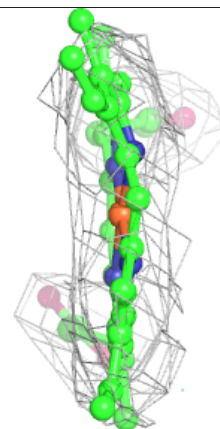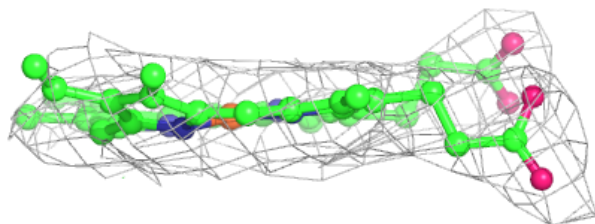$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
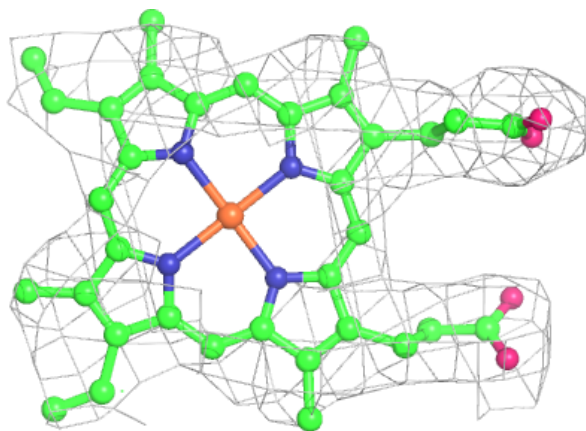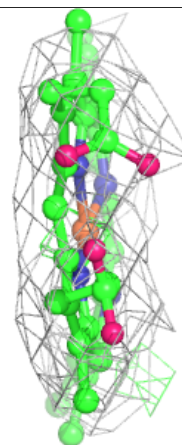and green (positive)
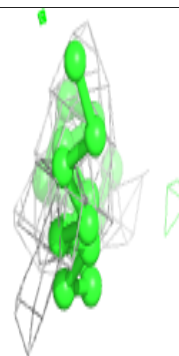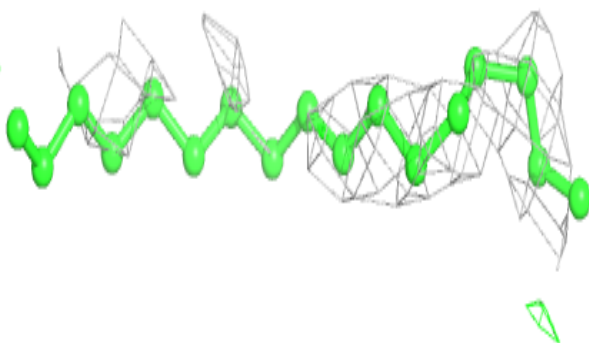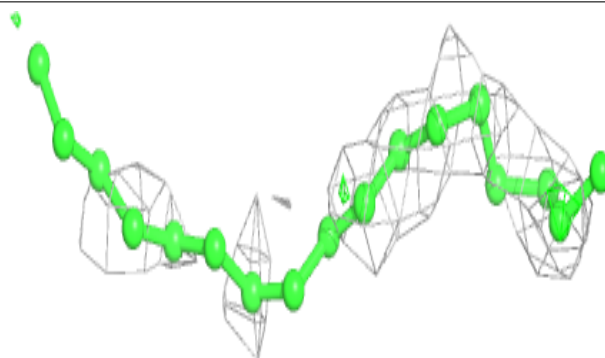
Electron density around NS5 C 405:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
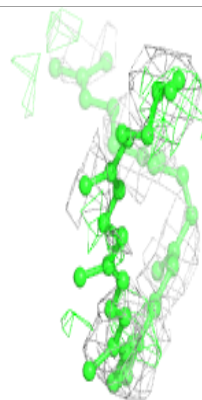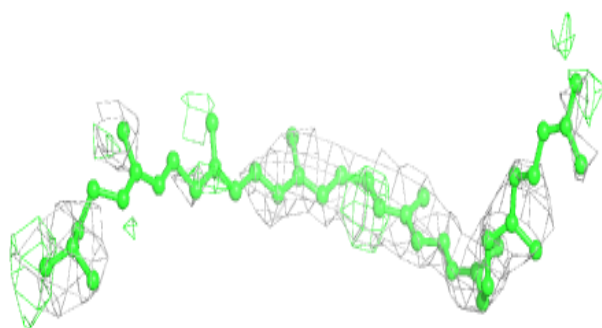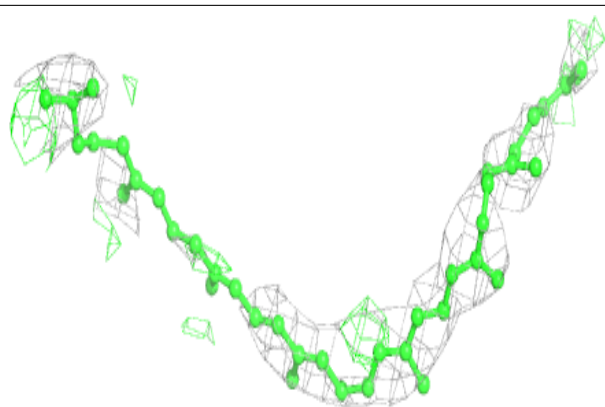
Electron density around OTP C 406:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
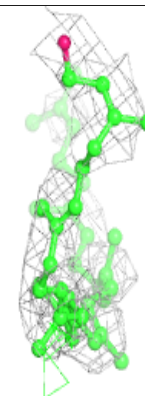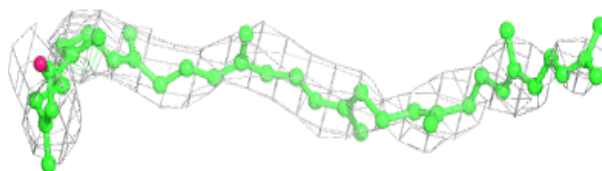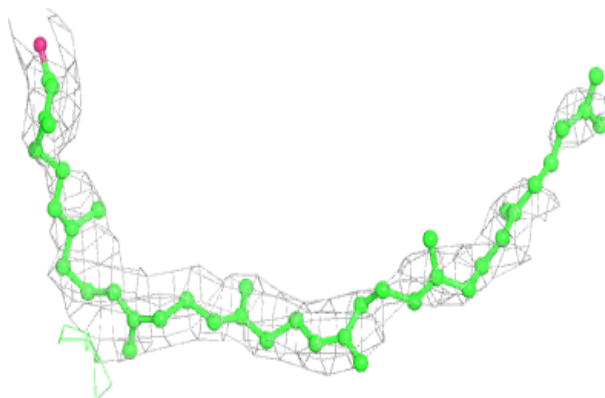
Electron density around BPB C 402:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
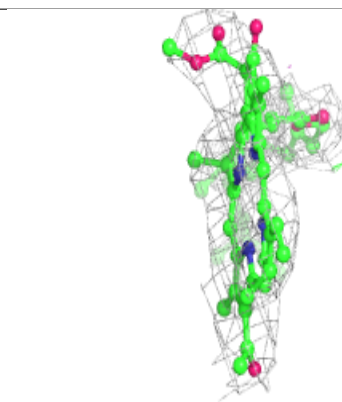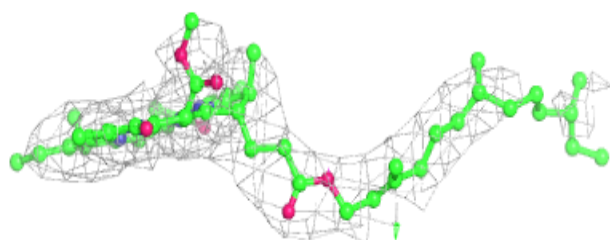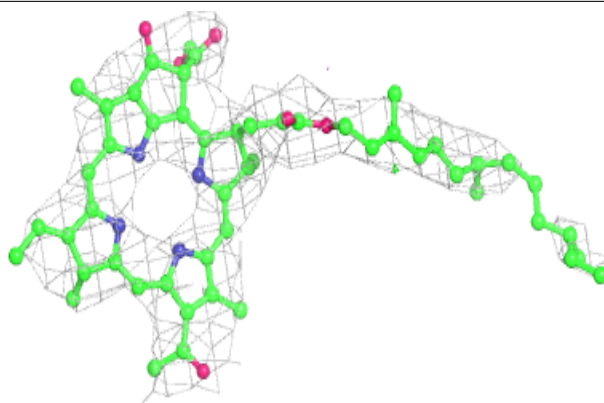
Electron density around MQ7 C 404:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
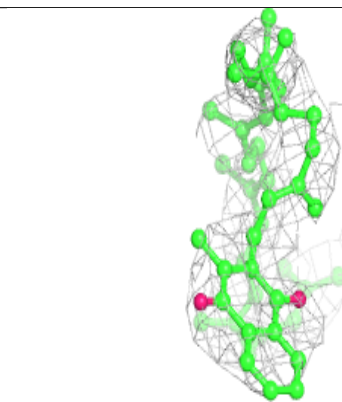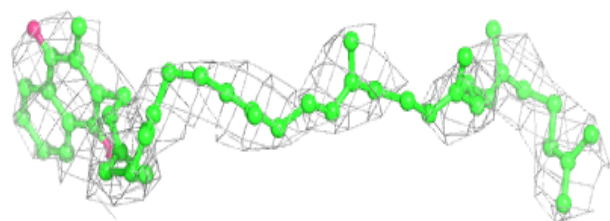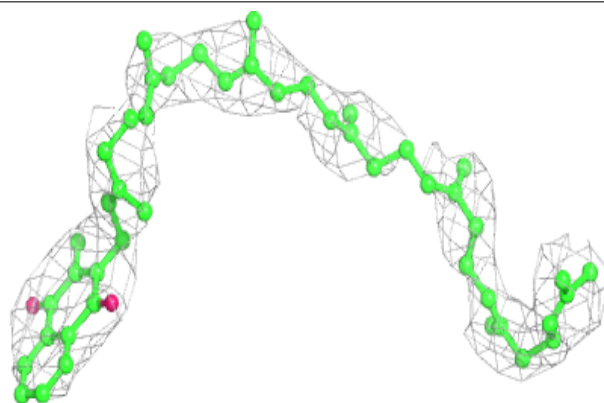
Electron density around MPG B 305:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
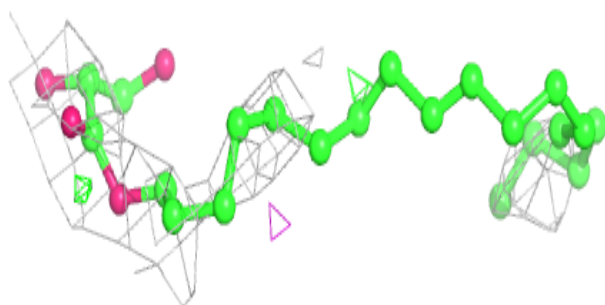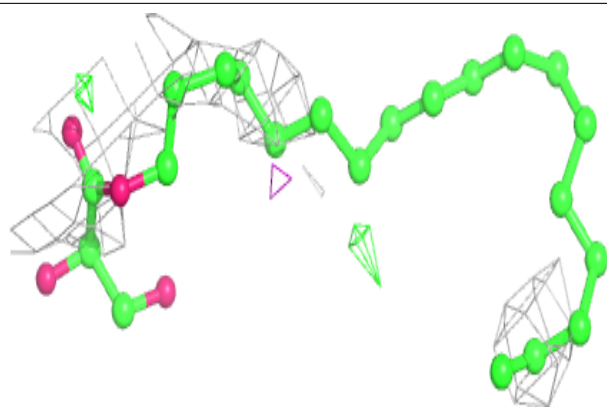
Electron density around HEC A 401:

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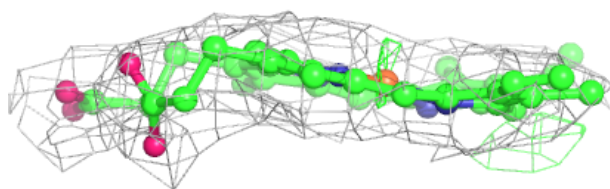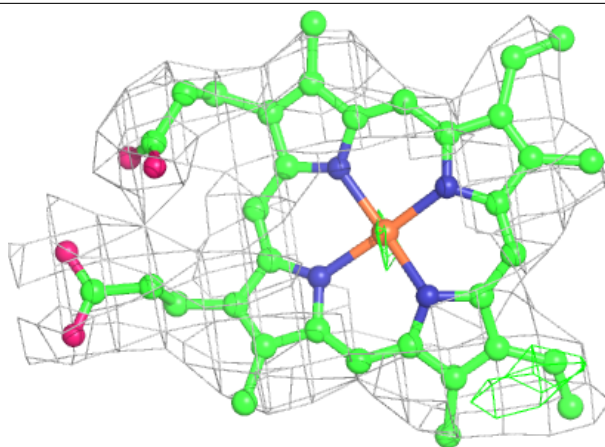$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
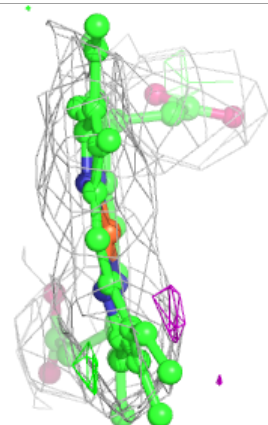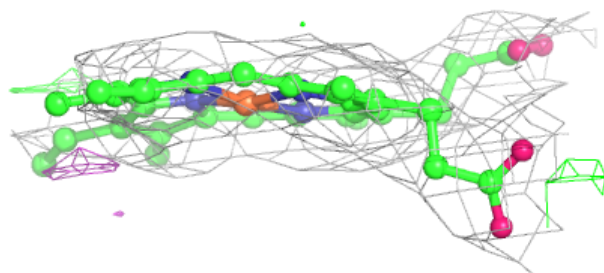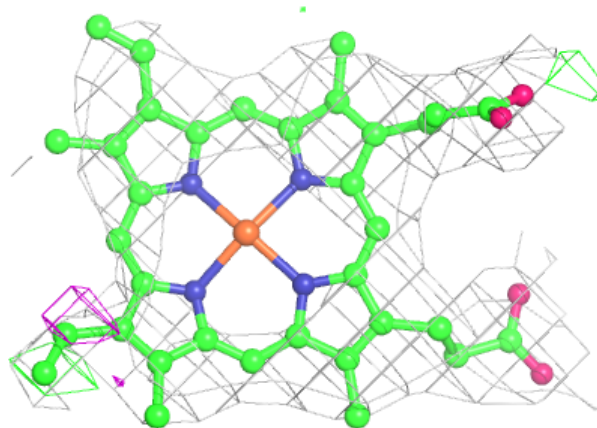
Electron density around BPB B 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
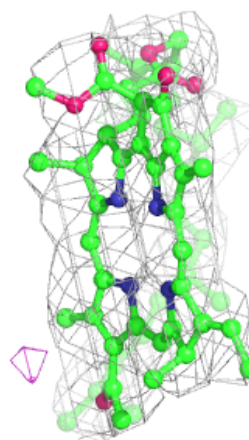
Electron density around BCL B 301:

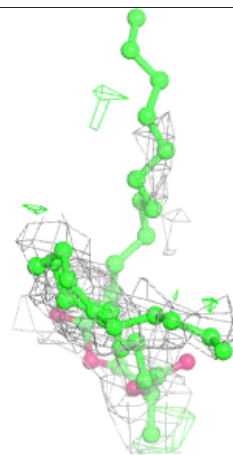$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around BCL B 303:

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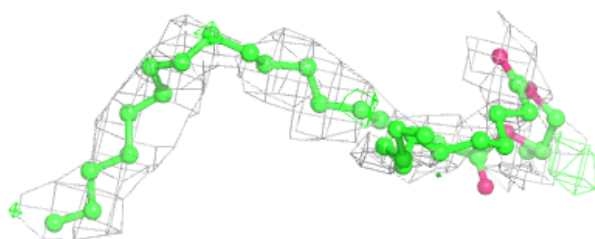and green (positive)

Electron density around HEC A 403:

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

Electron density around HEC A 404:

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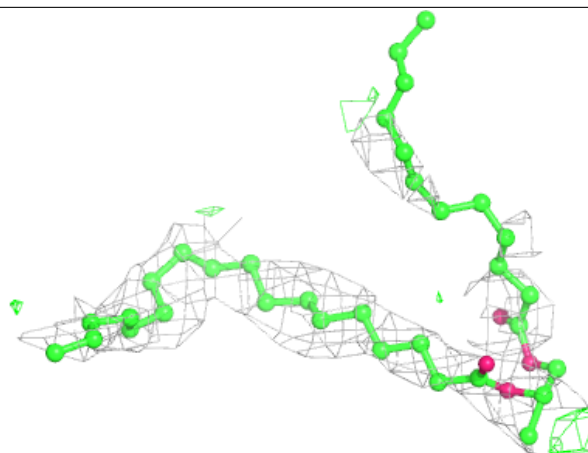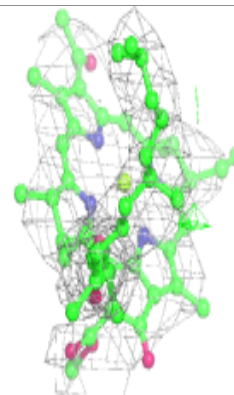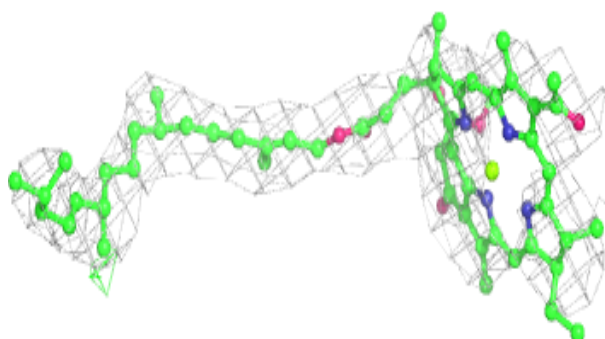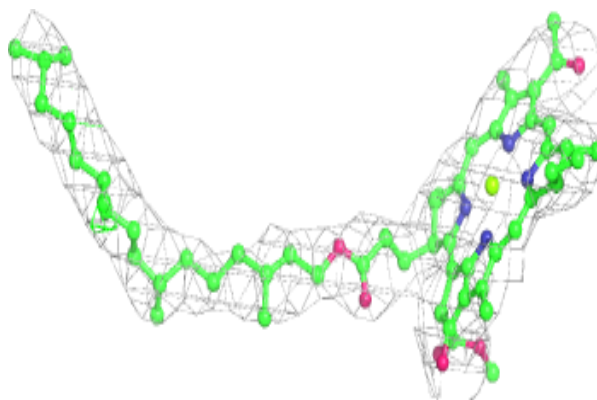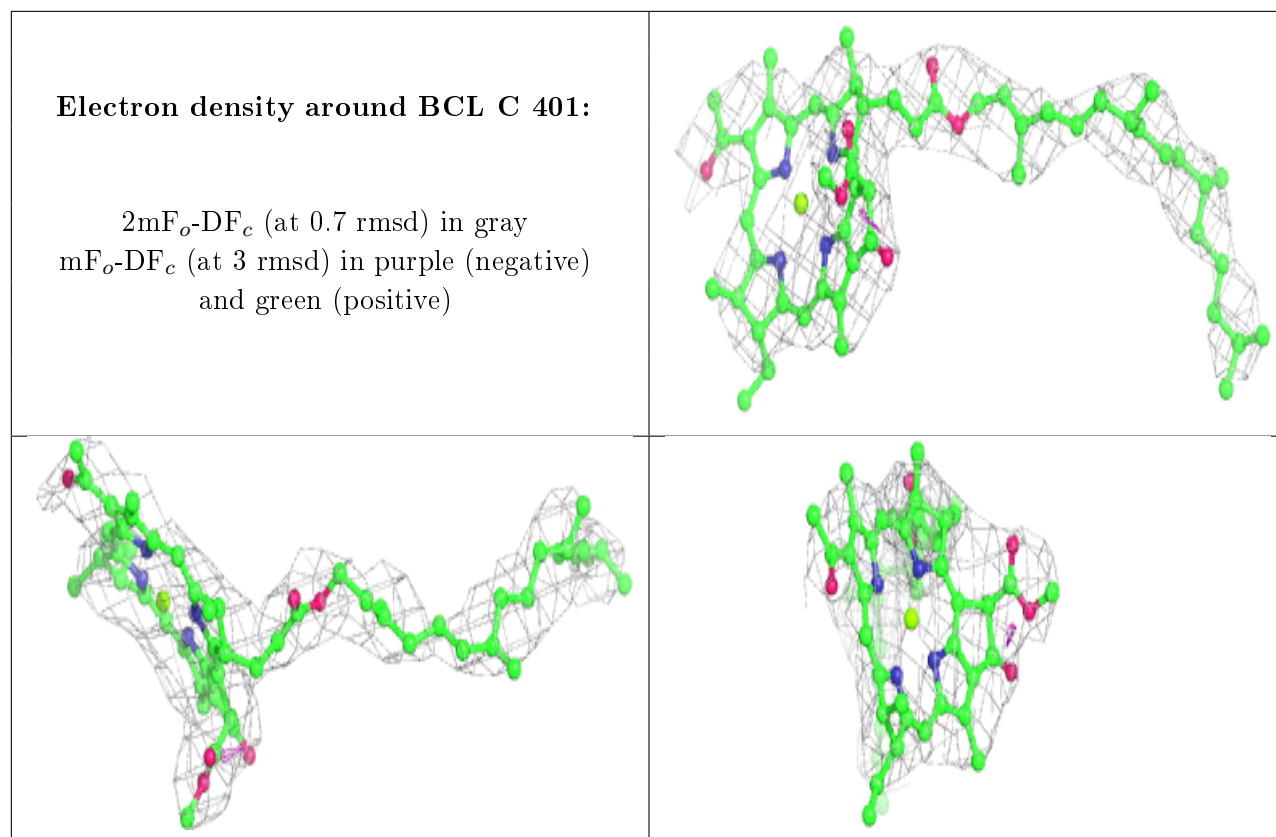and green (positive)

Electron density around HEC A 402:

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

Electron density around DGA A 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 BCL B 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 C 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)

6.5 Other polymers ⓘ

There are no such residues in this entry.