Full wwPDB X-ray Structure Validation Report (i)

Apr 21, 2022 – 04:22 am BST

PDB ID	:	7P2C
Title	:	F(M197)H mutant structure of Photosynthetic Reaction Center From Rhodobacter Sphaeroides strain RV by fixed-target serial synchrotron crystallography (room temperature, 26keV)
Authors	:	Gabdulkhakov, A.G.; Selikhanov, G.K.; Guenther, S.; Meents, A.; Fufina, T.Y.; Vasilieva, L.G.
Deposited on	:	2021-07-05
Resolution	:	2.04 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

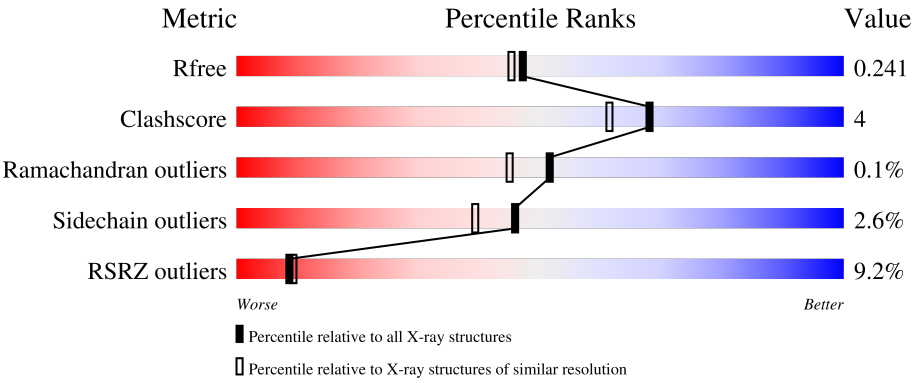
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	242	4% 86% 13%
2	L	281	11% 91% 9%
3	M	303	12% 91% 9%

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 7591 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
			Total	C	N	O	S			
1	H	239	1862	1191	317	344	10	0	5	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	281	2430	1645	387	390	8	0	22	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	engineered mutation	UNP Q3J1A5

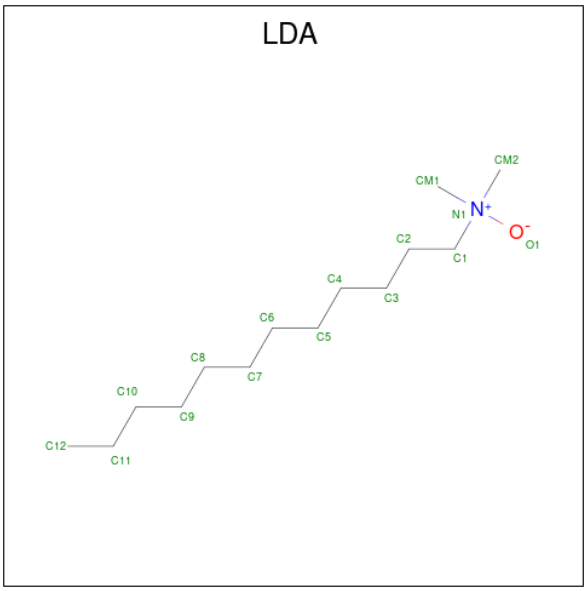
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	302	2455	1636	405	403	11	0	6	0

There are 2 discrepancies between the modelled and reference sequences:

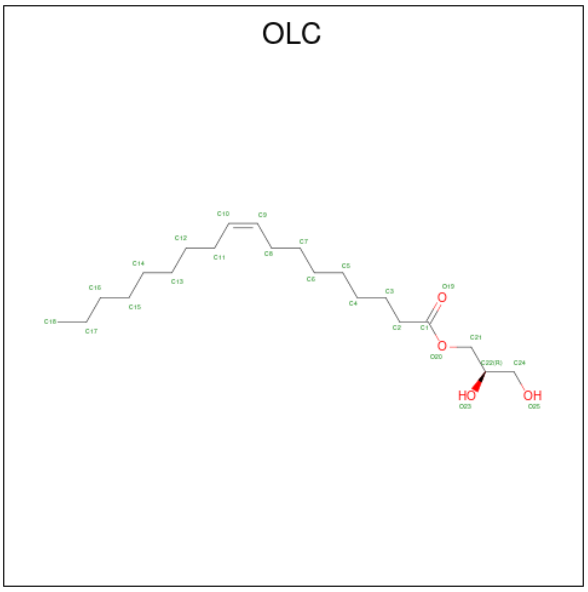
Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	engineered mutation	UNP Q3J1A6
M	197	HIS	PHE	engineered mutation	UNP Q3J1A6

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



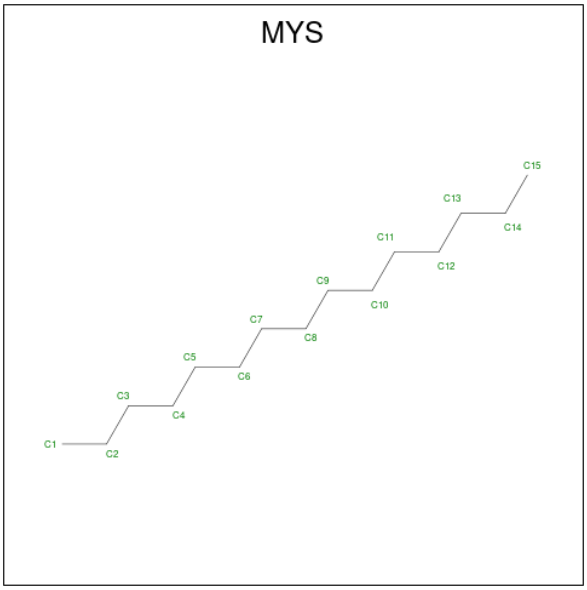
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	H	1	16	14	1	1	0	0
			Total	C	N	O		
4	M	1	16	14	1	1	0	0

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



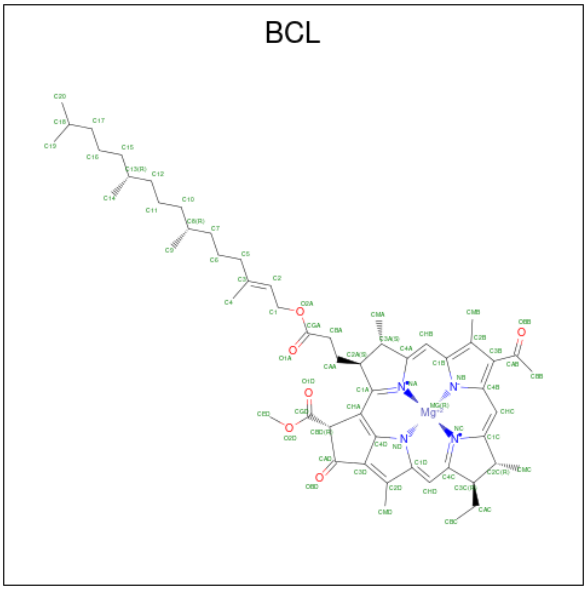
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	L	1	25	21	4	0	0

- Molecule 6 is PENTADECANE (three-letter code: MYS) (formula: $C_{15}H_{32}$).



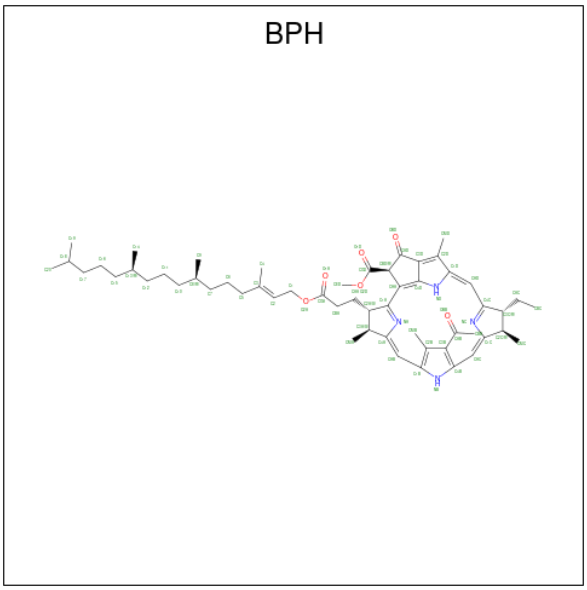
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C 15 15	0	0
6	L	1	Total C 15 15	0	0
6	M	1	Total C 15 15	0	0

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



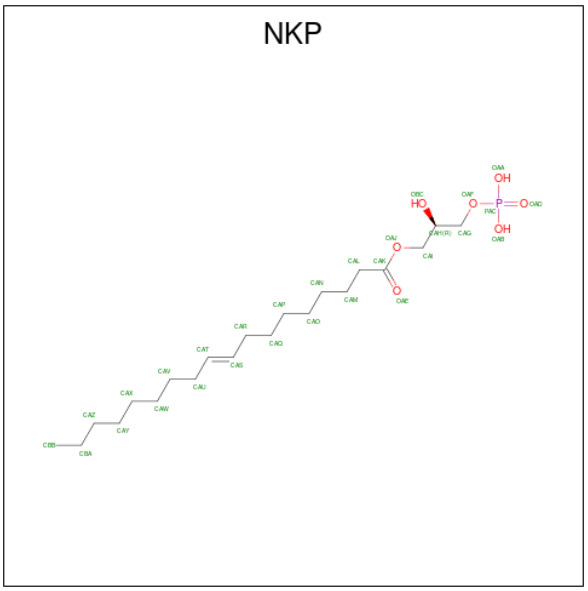
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



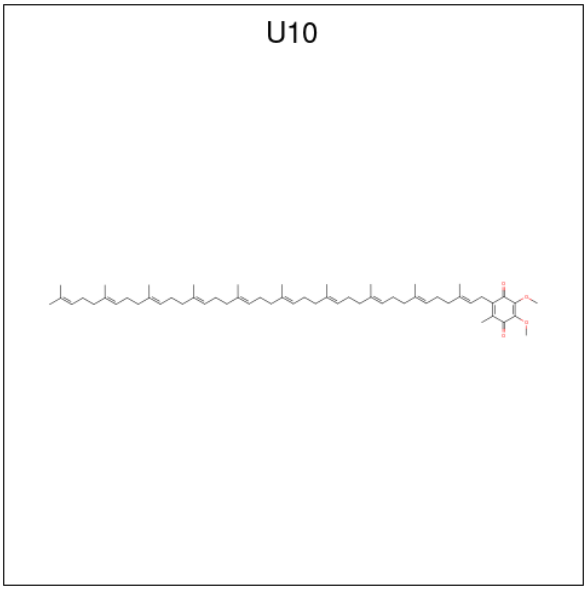
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	0	0
			65	55	4	6		
8	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 9 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
9	M	1	Total C O P 29 21 7 1	0	0
9	M	1	Total C O P 29 21 7 1	0	0

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

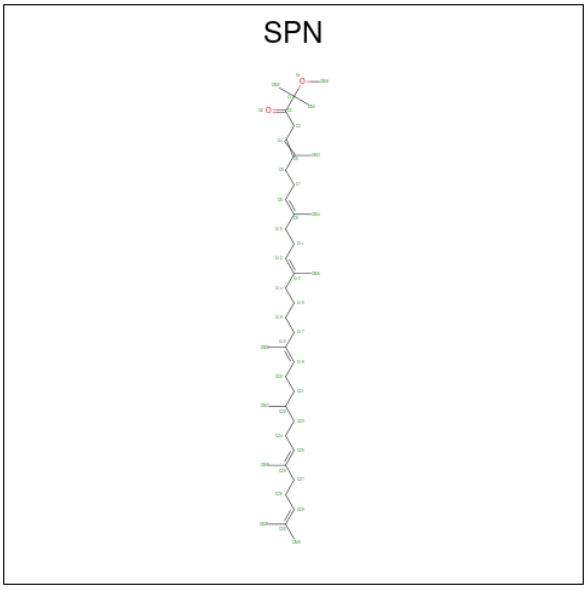


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total C O 63 59 4	0	0

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

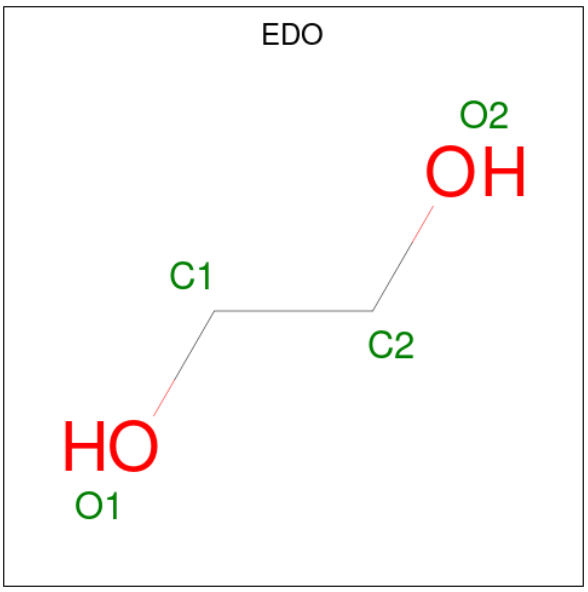
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total Fe 1 1	0	0

- Molecule 12 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$).



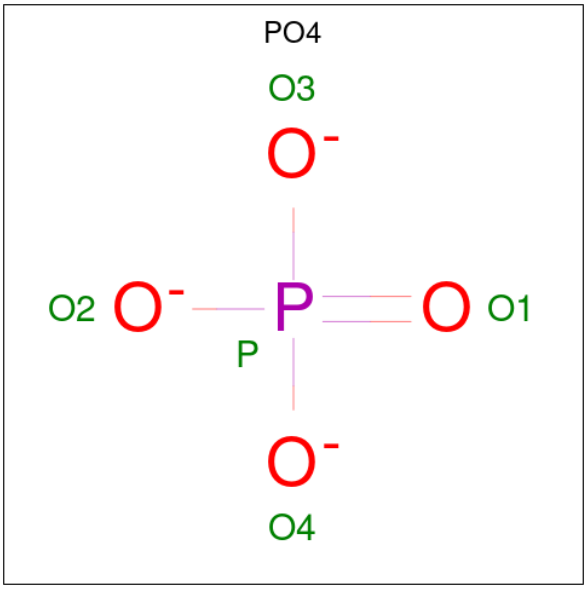
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total C O 43 41 2	0	0

- Molecule 13 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total C O 4 2 2	0	0

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



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

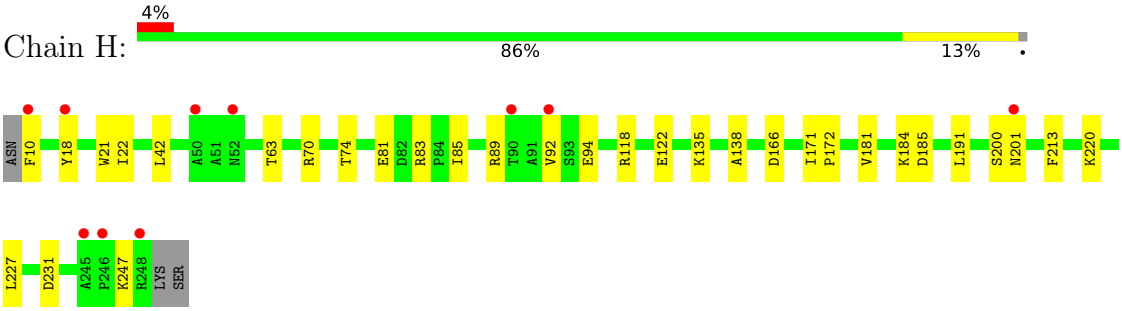
- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	78	Total O 78 78	0	0
15	L	53	Total O 53 53	0	0
15	M	43	Total O 43 43	0	0

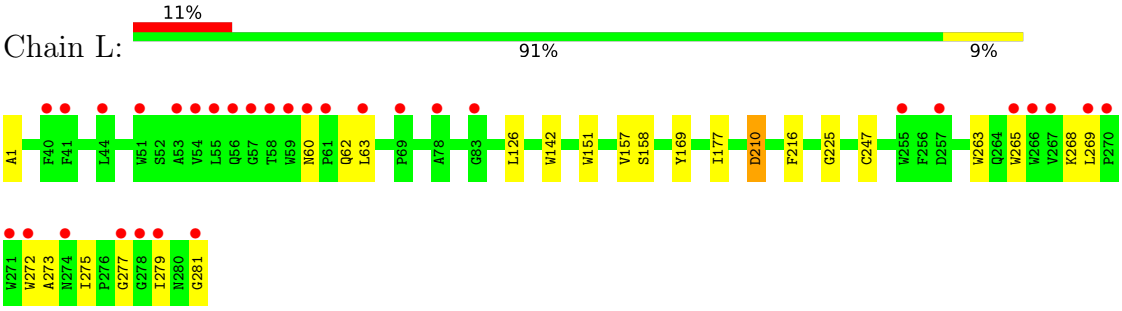
3 Residue-property plots (i)

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

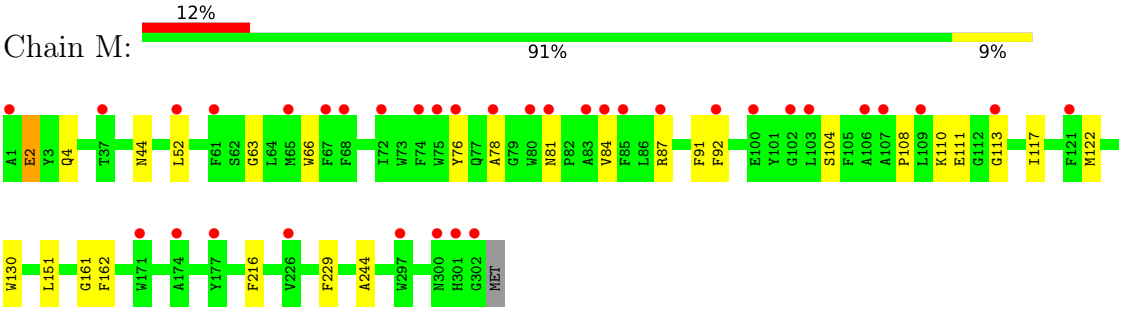
• Molecule 1: Reaction center protein H chain



• Molecule 2: Reaction center protein L chain



• Molecule 3: Reaction center protein M chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	102.50Å 102.50Å 237.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.05 – 2.04 47.05 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.05-2.04) 100.0 (47.05-2.04)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.201 , 0.229 0.211 , 0.241	Depositor DCC
R_{free} test set	4082 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	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	7591	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: BCL, LDA, MYS, U10, EDO, PO4, FE, SPN, NKP, OLC, BPH

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	0.39	0/1911	0.60	0/2601
2	L	0.39	0/2531	0.52	0/3468
3	M	0.40	0/2547	0.53	0/3476
All	All	0.39	0/6989	0.55	0/9545

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	1862	0	1859	16	0
2	L	2430	0	2366	15	0
3	M	2455	0	2374	16	0
4	H	16	0	31	2	0
4	M	16	0	31	2	0
5	L	25	0	40	1	0
6	L	30	0	64	1	0
6	M	15	0	32	0	0
7	L	132	0	148	4	0
7	M	132	0	148	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	65	0	76	1	0
8	M	65	0	76	4	0
9	M	58	0	78	0	0
10	M	63	0	90	2	0
11	M	1	0	0	0	0
12	M	43	0	70	4	0
13	M	4	0	6	0	0
14	M	5	0	0	0	0
15	H	78	0	0	2	0
15	L	53	0	0	0	0
15	M	43	0	0	0	0
All	All	7591	0	7489	57	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.

All (57) 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)
7:M:405:BCL:H203	8:M:406:BPH:H8	1.69	0.74
3:M:108:PRO:HG2	3:M:111:GLU:HB2	1.76	0.67
1:H:135:LYS:HG2	1:H:166:ASP:OD2	1.98	0.64
1:H:247:LYS:NZ	15:H:402:HOH:O	2.33	0.61
1:H:18:TYR:O	1:H:22:ILE:HD12	2.03	0.58
3:M:161:GLY:HA3	12:M:408:SPN:H201	1.85	0.57
2:L:62:GLN:OE1	2:L:151:TRP:NE1	2.36	0.55
3:M:44:ASN:HD22	3:M:44:ASN:N	2.05	0.53
2:L:177:ILE:HG12	7:L:304:BCL:HMB3	1.92	0.51
7:L:305:BCL:HBB2	7:L:305:BCL:HMB1	1.91	0.51
2:L:169:TYR:O	2:L:263[B]:TRP:NE1	2.37	0.51
3:M:63:GLY:HA3	8:M:406:BPH:H5C1	1.92	0.51
3:M:81:ASN:OD1	3:M:84:VAL:HG23	2.12	0.50
4:H:301:LDA:H121	4:M:409:LDA:H91	1.93	0.50
8:M:406:BPH:HBC3	8:M:406:BPH:HHD	1.93	0.50
2:L:277[B]:GLY:O	3:M:87:ARG:NH2	2.45	0.49
3:M:2:GLU:O	3:M:4:GLN:NE2	2.36	0.49
1:H:89:ARG:NH2	1:H:94:GLU:HG2	2.28	0.49
3:M:162:PHE:HB2	12:M:408:SPN:HM71	1.93	0.49
4:H:301:LDA:HM11	4:H:301:LDA:H22	1.66	0.47
1:H:81:GLU:HG3	1:H:85[B]:ILE:HD11	1.98	0.46
1:H:191:LEU:HD11	1:H:213:PHE:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:404:BCL:H202	12:M:408:SPN:H61	1.96	0.46
1:H:171:ILE:HB	1:H:172:PRO:HD3	1.97	0.45
1:H:21:TRP:HZ2	4:M:409:LDA:HM13	1.80	0.45
7:L:304:BCL:H192	7:L:304:BCL:H161	1.71	0.45
7:M:405:BCL:H172	8:M:406:BPH:H9C2	1.99	0.45
2:L:275[A]:ILE:O	2:L:281[A]:GLY:HA3	2.17	0.44
1:H:201:ASN:OD1	1:H:201:ASN:N	2.50	0.44
2:L:157:VAL:HG12	7:L:304:BCL:HBC2	2.00	0.44
2:L:268[A]:LYS:HD3	2:L:268[A]:LYS:HA	1.75	0.44
2:L:142:TRP:CH2	6:L:302:MYS:H71	2.53	0.44
10:M:402:U10:H371	10:M:402:U10:H412	1.84	0.43
1:H:42:LEU:HB3	2:L:1:ALA:HB1	2.01	0.43
3:M:113:GLY:O	3:M:117:ILE:HD12	2.18	0.43
1:H:181:VAL:HG21	1:H:191:LEU:HD12	2.00	0.42
2:L:60:ASN:OD1	2:L:63:LEU:HG	2.20	0.42
2:L:225:GLY:H	5:L:301:OLC:H22	1.84	0.42
3:M:78:ALA:HB2	3:M:92:PHE:CZ	2.55	0.42
1:H:122:GLU:HB2	1:H:227:LEU:HD21	2.00	0.42
7:M:405:BCL:HMB1	7:M:405:BCL:HBB3	2.02	0.42
1:H:184:LYS:HG3	1:H:185:ASP:N	2.35	0.42
8:L:306:BPH:HHB	8:L:306:BPH:HMB1	1.94	0.42
3:M:130:TRP:NE1	3:M:151[B]:LEU:HG	2.35	0.42
1:H:118:ARG:HD2	15:H:420:HOH:O	2.20	0.41
2:L:279[A]:ILE:HG21	3:M:91:PHE:HB3	2.01	0.41
3:M:76:TYR:OH	3:M:110:LYS:HD3	2.19	0.41
3:M:130:TRP:HE1	3:M:151[B]:LEU:HG	1.84	0.41
7:M:404:BCL:CAB	12:M:408:SPN:H162	2.49	0.41
2:L:268[A]:LYS:HA	2:L:273[A]:ALA:HB2	2.03	0.41
2:L:210:ASP:N	2:L:210:ASP:OD2	2.54	0.41
3:M:229:PHE:HB2	3:M:244:ALA:HB2	2.03	0.41
10:M:402:U10:H471	10:M:402:U10:H451	1.85	0.41
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.56	0.41
1:H:83:ARG:HE	1:H:83:ARG:HB2	1.73	0.40
1:H:63[B]:THR:HG22	1:H:74:THR:OG1	2.21	0.40
2:L:126:LEU:HD23	2:L:126:LEU:HA	1.97	0.40

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	H	242/242 (100%)	238 (98%)	3 (1%)	1 (0%)	34 24
2	L	300/281 (107%)	287 (96%)	13 (4%)	0	100 100
3	M	306/303 (101%)	296 (97%)	10 (3%)	0	100 100
All	All	848/826 (103%)	821 (97%)	26 (3%)	1 (0%)	51 45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	138	ALA

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	H	199/197 (101%)	193 (97%)	6 (3%)	41 34
2	L	238/220 (108%)	228 (96%)	10 (4%)	30 22
3	M	241/237 (102%)	236 (98%)	5 (2%)	53 48
All	All	678/654 (104%)	657 (97%)	21 (3%)	46 33

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	10	PHE
1	H	70	ARG

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Mol	Chain	Res	Type
1	H	92	VAL
1	H	200	SER
1	H	220	LYS
1	H	231	ASP
2	L	158	SER
2	L	210	ASP
2	L	216	PHE
2	L	247	CYS
2	L	265[A]	TRP
2	L	265[B]	TRP
2	L	269[A]	LEU
2	L	269[B]	LEU
2	L	272[A]	TRP
2	L	272[B]	TRP
3	M	2	GLU
3	M	52[A]	LEU
3	M	52[B]	LEU
3	M	104	SER
3	M	216	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	M	44	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\#\|Z\| > 2$
8	BPH	L	306	-	64,70,70	1.01	5 (7%)	76,101,101	1.27	9 (11%)
6	MYS	L	303	-	14,14,14	0.28	0	13,13,13	0.51	0
12	SPN	M	408	-	40,42,42	0.58	0	50,52,52	1.44	9 (18%)
9	NKP	M	403	-	28,28,28	0.53	0	31,32,32	0.46	0
4	LDA	M	409	-	12,15,15	2.06	1 (8%)	14,17,17	0.39	0
4	LDA	H	301	-	12,15,15	2.01	1 (8%)	14,17,17	0.61	0
6	MYS	M	410	-	14,14,14	0.25	0	13,13,13	0.62	0
8	BPH	M	406	-	64,70,70	0.94	5 (7%)	76,101,101	1.16	7 (9%)
9	NKP	M	401	-	28,28,28	0.34	0	31,32,32	0.63	1 (3%)
13	EDO	M	411	-	3,3,3	0.35	0	2,2,2	1.29	0
10	U10	M	402	-	63,63,63	2.66	17 (26%)	76,79,79	1.73	22 (28%)
6	MYS	L	302	-	14,14,14	0.26	0	13,13,13	0.56	0
5	OLC	L	301	-	24,24,24	0.95	1 (4%)	25,25,25	0.87	2 (8%)
7	BCL	L	305	-	58,74,74	1.32	3 (5%)	69,115,115	1.37	9 (13%)
7	BCL	M	405	-	58,74,74	1.38	3 (5%)	69,115,115	1.49	11 (15%)
14	PO4	M	412	-	4,4,4	0.92	0	6,6,6	0.34	0
7	BCL	L	304	-	58,74,74	1.45	4 (6%)	69,115,115	1.43	10 (14%)
7	BCL	M	404	-	58,74,74	1.20	4 (6%)	69,115,115	1.54	12 (17%)

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
8	BPH	L	306	-	-	4/54/105/105	0/5/6/6
6	MYS	L	303	-	-	6/12/12/12	-
12	SPN	M	408	-	-	18/50/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NKP	M	403	-	-	10/28/28/28	-
4	LDA	M	409	-	-	3/13/13/13	-
4	LDA	H	301	-	-	5/13/13/13	-
6	MYS	M	410	-	-	2/12/12/12	-
8	BPH	M	406	-	-	9/54/105/105	0/5/6/6
9	NKP	M	401	-	-	7/28/28/28	-
13	EDO	M	411	-	-	1/1/1/1	-
10	U10	M	402	-	-	12/63/87/87	0/1/1/1
6	MYS	L	302	-	-	3/12/12/12	-
5	OLC	L	301	-	-	8/24/24/24	-
7	BCL	L	305	-	-	2/37/137/137	-
7	BCL	M	405	-	-	2/37/137/137	-
7	BCL	L	304	-	-	2/37/137/137	-
7	BCL	M	404	-	-	0/37/137/137	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	409	LDA	O1-N1	-7.02	1.25	1.42
4	H	301	LDA	O1-N1	-6.91	1.26	1.42
10	M	402	U10	C33-C34	6.36	1.48	1.33
10	M	402	U10	C48-C49	6.14	1.47	1.33
10	M	402	U10	C43-C44	6.07	1.47	1.33
10	M	402	U10	C8-C9	6.05	1.47	1.33
10	M	402	U10	C18-C19	5.97	1.47	1.33
10	M	402	U10	C38-C39	5.97	1.47	1.33
10	M	402	U10	C13-C14	5.86	1.47	1.33
10	M	402	U10	C28-C29	5.82	1.46	1.33
7	L	304	BCL	MG-NA	5.76	2.19	2.06
10	M	402	U10	C23-C24	5.75	1.46	1.33
7	M	405	BCL	MG-NA	5.54	2.19	2.06
7	L	305	BCL	MG-NA	5.53	2.19	2.06
7	M	405	BCL	C1B-NB	5.48	1.40	1.35
10	M	402	U10	C53-C54	5.44	1.48	1.32
7	L	305	BCL	C1B-NB	5.43	1.40	1.35
7	L	304	BCL	C1B-NB	5.37	1.40	1.35
10	M	402	U10	O3-C3	-4.86	1.25	1.36
10	M	402	U10	O4-C4	-4.76	1.25	1.36
7	M	404	BCL	MG-NA	4.68	2.17	2.06
7	L	304	BCL	MG-NC	4.31	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	301	OLC	O20-C1	4.14	1.45	1.33
7	M	404	BCL	C1B-NB	3.89	1.38	1.35
7	M	405	BCL	MG-NC	3.71	2.15	2.06
7	M	404	BCL	MG-NC	3.27	2.14	2.06
7	L	305	BCL	MG-NC	3.13	2.13	2.06
10	M	402	U10	C4-C5	-3.02	1.40	1.48
8	L	306	BPH	CAC-C3C	3.00	1.59	1.54
7	L	304	BCL	C4B-NB	2.98	1.37	1.35
8	L	306	BPH	OBD-CAD	2.98	1.26	1.22
10	M	402	U10	C3-C2	-2.93	1.40	1.48
8	M	406	BPH	C3D-CAD	-2.82	1.41	1.47
8	L	306	BPH	C1B-C2B	-2.79	1.39	1.45
10	M	402	U10	C6-C1	2.48	1.39	1.35
7	M	404	BCL	C4B-NB	2.37	1.37	1.35
10	M	402	U10	C6-C5	-2.31	1.40	1.46
10	M	402	U10	C1-C2	-2.29	1.39	1.47
8	L	306	BPH	CHC-C1C	2.29	1.41	1.36
8	L	306	BPH	C3D-CAD	-2.24	1.42	1.47
8	M	406	BPH	C2C-C1C	-2.22	1.48	1.52
8	M	406	BPH	O2A-CGA	-2.11	1.27	1.33
8	M	406	BPH	OBD-CAD	2.07	1.25	1.22
8	M	406	BPH	CHC-C1C	2.06	1.40	1.36

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	405	BCL	CAD-C3D-C4D	-4.60	105.90	108.47
7	L	304	BCL	CMB-C2B-C1B	-4.40	121.70	128.46
7	M	404	BCL	CMB-C2B-C1B	-4.39	121.72	128.46
10	M	402	U10	C22-C23-C24	-4.31	117.29	127.66
7	M	405	BCL	C4A-NA-C1A	4.26	108.62	106.71
8	L	306	BPH	C1C-NC-C4C	-4.15	106.90	110.54
8	L	306	BPH	OBD-CAD-CBD	-3.97	120.22	125.89
7	L	305	BCL	OBD-CAD-CBD	-3.87	120.37	125.89
7	M	405	BCL	CMB-C2B-C1B	-3.82	122.59	128.46
7	L	305	BCL	CAD-C3D-C4D	-3.74	106.38	108.47
7	L	305	BCL	CMB-C2B-C1B	-3.69	122.80	128.46
10	M	402	U10	C17-C18-C19	-3.66	118.84	127.66
12	M	408	SPN	CM5-C13-C14	3.64	121.39	115.27
10	M	402	U10	C47-C48-C49	-3.64	118.90	127.66
7	M	405	BCL	OBD-CAD-CBD	-3.62	120.73	125.89
7	M	404	BCL	C16-C15-C13	3.58	127.48	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	402	U10	C30-C29-C31	3.46	121.09	115.27
10	M	402	U10	C45-C44-C46	3.46	121.09	115.27
7	M	404	BCL	OBD-CAD-CBD	-3.34	121.12	125.89
12	M	408	SPN	CM3-C5-C6	3.29	120.81	115.27
7	L	304	BCL	CMB-C2B-C3B	3.28	130.81	124.68
7	M	404	BCL	C4A-NA-C1A	3.22	108.15	106.71
10	M	402	U10	C40-C39-C41	3.22	120.68	115.27
7	M	405	BCL	CHA-C1A-NA	-3.20	119.08	126.40
7	L	305	BCL	CHA-C1A-NA	-3.18	119.11	126.40
7	M	404	BCL	CMB-C2B-C3B	3.17	130.60	124.68
8	M	406	BPH	OBD-CAD-CBD	-3.16	121.39	125.89
7	M	404	BCL	CAD-C3D-C4D	-3.14	106.72	108.47
7	L	304	BCL	CAD-C3D-C4D	-3.14	106.72	108.47
12	M	408	SPN	CM4-C9-C10	3.12	120.51	115.27
7	L	304	BCL	OBD-CAD-CBD	-2.99	121.62	125.89
10	M	402	U10	C12-C13-C14	-2.98	120.49	127.66
7	M	404	BCL	CHA-C1A-NA	-2.95	119.64	126.40
10	M	402	U10	C25-C24-C26	2.91	120.16	115.27
7	M	405	BCL	CMB-C2B-C3B	2.89	130.08	124.68
12	M	408	SPN	C3-C4-C5	-2.88	121.99	126.79
12	M	408	SPN	CM6-C18-C17	2.88	120.11	115.27
10	M	402	U10	C37-C38-C39	-2.81	120.90	127.66
7	L	305	BCL	CMB-C2B-C3B	2.81	129.93	124.68
7	L	304	BCL	CHA-C1A-NA	-2.79	120.01	126.40
7	M	405	BCL	CMD-C2D-C3D	2.78	129.87	124.68
10	M	402	U10	C42-C43-C44	-2.75	121.04	127.66
10	M	402	U10	C10-C9-C11	2.75	119.89	115.27
10	M	402	U10	C50-C49-C51	2.75	119.89	115.27
8	M	406	BPH	C11-C10-C8	2.73	124.75	115.92
7	M	405	BCL	C2A-C1A-CHA	2.68	128.55	123.86
5	L	301	OLC	O20-C1-C2	2.63	120.17	111.91
5	L	301	OLC	O20-C1-O19	-2.63	116.95	123.59
7	L	305	BCL	CMD-C2D-C3D	2.62	129.58	124.68
12	M	408	SPN	CM8-C26-C27	2.58	119.62	115.27
7	L	304	BCL	C2A-C1A-CHA	2.58	128.36	123.86
10	M	402	U10	C27-C28-C29	-2.57	121.46	127.66
7	M	404	BCL	CMD-C2D-C3D	2.57	129.48	124.68
10	M	402	U10	C15-C14-C16	2.56	119.57	115.27
7	L	305	BCL	C2A-C1A-CHA	2.53	128.29	123.86
7	M	404	BCL	C2A-C1A-CHA	2.47	128.17	123.86
7	L	304	BCL	CMD-C2D-C3D	2.45	129.27	124.68
7	M	404	BCL	OBB-CAB-CBB	-2.45	114.65	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	406	BPH	C1-C2-C3	-2.39	121.91	126.04
7	M	405	BCL	C4B-C3B-CAB	-2.39	122.52	127.13
7	M	404	BCL	CBC-CAC-C3C	-2.38	108.17	113.47
10	M	402	U10	C20-C19-C21	2.38	119.27	115.27
10	M	402	U10	C7-C8-C9	-2.36	122.86	126.79
7	M	405	BCL	O2D-CGD-CBD	2.34	115.43	111.27
7	L	304	BCL	OBB-CAB-CBB	-2.33	114.93	120.17
10	M	402	U10	C35-C34-C36	2.33	119.18	115.27
10	M	402	U10	C56-C54-C55	2.32	119.73	114.60
8	M	406	BPH	CMD-C2D-C3D	2.31	129.00	124.68
8	L	306	BPH	CMD-C2D-C3D	2.29	128.96	124.68
12	M	408	SPN	C7-C8-C9	-2.24	122.26	127.66
7	L	304	BCL	C16-C15-C13	-2.24	108.69	115.92
10	M	402	U10	C4M-O4-C4	2.24	124.39	116.47
9	M	401	NKP	OAB-PAC-OAF	-2.23	100.79	106.73
8	M	406	BPH	CHC-C1C-NC	-2.22	122.56	125.20
8	L	306	BPH	O2D-CGD-CBD	2.20	115.18	111.27
7	L	305	BCL	C11-C10-C8	-2.20	108.81	115.92
8	L	306	BPH	CMB-C2B-C1B	-2.19	121.69	125.06
8	M	406	BPH	CAC-C3C-C4C	2.19	118.29	112.67
12	M	408	SPN	CMB-C30-CM9	2.18	119.43	114.60
10	M	402	U10	C32-C33-C34	-2.16	122.45	127.66
8	L	306	BPH	OBD-CAD-C3D	2.15	131.55	127.98
8	L	306	BPH	O2D-CGD-O1D	-2.15	119.64	123.84
7	M	404	BCL	C1-C2-C3	-2.12	122.37	126.04
12	M	408	SPN	C20-C19-C18	-2.11	122.59	127.66
8	L	306	BPH	O2A-CGA-O1A	-2.08	118.35	123.59
8	M	406	BPH	C1C-NC-C4C	-2.06	108.73	110.54
10	M	402	U10	C26-C27-C28	-2.06	105.13	111.88
7	L	305	BCL	C4A-NA-C1A	2.04	107.62	106.71
7	M	405	BCL	OBD-CAD-C3D	2.03	131.35	127.98
8	L	306	BPH	C3A-C4A-CHB	2.02	125.32	121.83
7	L	304	BCL	CHC-C1C-NC	-2.02	121.72	124.51
10	M	402	U10	C22-C21-C19	-2.01	106.36	112.98

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	301	OLC	O20-C21-C22-O23
8	M	406	BPH	C4B-C3B-CAB-CBB
8	M	406	BPH	C4B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
8	M	406	BPH	C2B-C3B-CAB-CBB
8	M	406	BPH	C2B-C3B-CAB-OBB
10	M	402	U10	C32-C33-C34-C35
10	M	402	U10	C32-C33-C34-C36
10	M	402	U10	C43-C44-C46-C47
10	M	402	U10	C45-C44-C46-C47
12	M	408	SPN	CM2-C1-C2-O2
12	M	408	SPN	CM2-C1-C2-C3
12	M	408	SPN	C11-C10-C9-CM4
12	M	408	SPN	C12-C13-C14-C15
12	M	408	SPN	CM5-C13-C14-C15
12	M	408	SPN	C26-C27-C28-C29
9	M	403	NKP	OAE-CAK-OAJ-CAI
9	M	403	NKP	CAL-CAK-OAJ-CAI
12	M	408	SPN	C16-C17-C18-CM6
12	M	408	SPN	C11-C10-C9-C8
12	M	408	SPN	C16-C17-C18-C19
10	M	402	U10	C24-C26-C27-C28
12	M	408	SPN	C14-C15-C16-C17
10	M	402	U10	C42-C43-C44-C45
9	M	403	NKP	CAT-CAU-CAV-CAW
5	L	301	OLC	O20-C21-C22-C24
5	L	301	OLC	C3-C4-C5-C6
6	L	303	MYS	C5-C6-C7-C8
9	M	403	NKP	CAN-CAO-CAP-CAQ
8	L	306	BPH	C4-C3-C5-C6
6	L	302	MYS	C6-C7-C8-C9
6	L	303	MYS	C7-C8-C9-C10
4	H	301	LDA	C1-C2-C3-C4
8	L	306	BPH	C2-C3-C5-C6
6	L	302	MYS	C5-C6-C7-C8
8	M	406	BPH	C13-C15-C16-C17
9	M	403	NKP	CAP-CAQ-CAR-CAS
4	H	301	LDA	C7-C8-C9-C10
9	M	403	NKP	CAY-CAZ-CBA-CBB
8	M	406	BPH	C4-C3-C5-C6
12	M	408	SPN	CM3-C5-C6-C7
9	M	403	NKP	CAW-CAX-CAY-CAZ
4	H	301	LDA	C9-C10-C11-C12
9	M	401	NKP	CAL-CAM-CAN-CAO
5	L	301	OLC	C4-C5-C6-C7
6	L	303	MYS	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
8	M	406	BPH	C2-C3-C5-C6
10	M	402	U10	C29-C31-C32-C33
12	M	408	SPN	C4-C5-C6-C7
6	L	303	MYS	C11-C12-C13-C14
7	L	304	BCL	C15-C16-C17-C18
4	M	409	LDA	C9-C10-C11-C12
6	L	303	MYS	C11-C10-C9-C8
9	M	401	NKP	CAT-CAU-CAV-CAW
12	M	408	SPN	C21-C22-C23-C24
8	L	306	BPH	CAD-CBD-CGD-O2D
8	M	406	BPH	CAD-CBD-CGD-O2D
6	M	410	MYS	C11-C10-C9-C8
12	M	408	SPN	CM1-C1-O1-CMA
12	M	408	SPN	CM2-C1-O1-CMA
4	M	409	LDA	C1-C2-C3-C4
9	M	401	NKP	CAS-CAT-CAU-CAV
9	M	401	NKP	CAU-CAV-CAW-CAX
10	M	402	U10	C14-C16-C17-C18
9	M	401	NKP	CAQ-CAR-CAS-CAT
9	M	401	NKP	CAG-OAF-PAC-OAD
13	M	411	EDO	O1-C1-C2-O2
6	M	410	MYS	C9-C10-C11-C12
7	L	305	BCL	C12-C13-C15-C16
12	M	408	SPN	CM7-C22-C23-C24
10	M	402	U10	C5-C4-O4-C4M
4	M	409	LDA	C7-C8-C9-C10
9	M	403	NKP	CAQ-CAR-CAS-CAT
9	M	403	NKP	CAG-CAH-CAI-OAJ
9	M	403	NKP	CAR-CAS-CAT-CAU
5	L	301	OLC	C2-C3-C4-C5
7	L	305	BCL	C14-C13-C15-C16
4	H	301	LDA	C5-C6-C7-C8
12	M	408	SPN	C9-C10-C11-C12
5	L	301	OLC	O20-C1-C2-C3
10	M	402	U10	C25-C24-C26-C27
10	M	402	U10	C42-C43-C44-C46
5	L	301	OLC	C9-C10-C11-C12
10	M	402	U10	C23-C24-C26-C27
7	L	304	BCL	CAD-CBD-CGD-O2D
7	M	405	BCL	CAD-CBD-CGD-O2D
8	L	306	BPH	O2A-C1-C2-C3
8	M	406	BPH	O2A-C1-C2-C3

Continued on next page...

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Mol	Chain	Res	Type	Atoms
12	M	408	SPN	C2-C1-O1-CMA
6	L	303	MYS	C4-C5-C6-C7
4	H	301	LDA	C2-C1-N1-O1
9	M	401	NKP	OAF-CAG-CAH-OBC
6	L	302	MYS	C11-C12-C13-C14
7	M	405	BCL	CAA-CBA-CGA-O2A
5	L	301	OLC	C1-C2-C3-C4

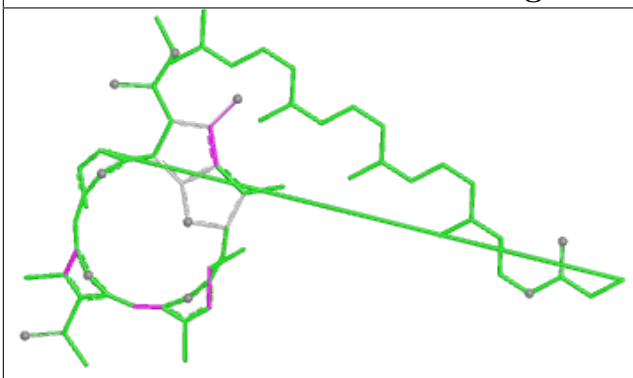
There are no ring outliers.

12 monomers are involved in 21 short contacts:

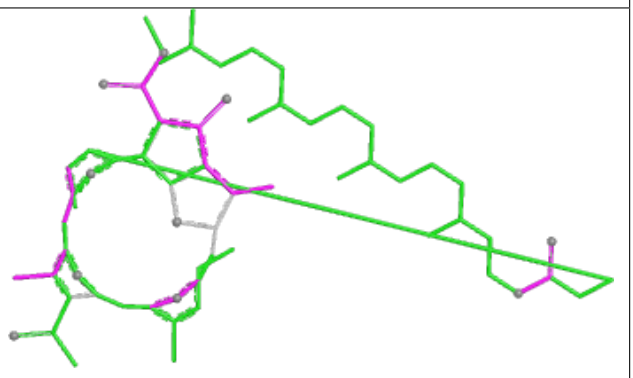
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	306	BPH	1	0
12	M	408	SPN	4	0
4	M	409	LDA	2	0
4	H	301	LDA	2	0
8	M	406	BPH	4	0
10	M	402	U10	2	0
6	L	302	MYS	1	0
5	L	301	OLC	1	0
7	L	305	BCL	1	0
7	M	405	BCL	3	0
7	L	304	BCL	3	0
7	M	404	BCL	2	0

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.

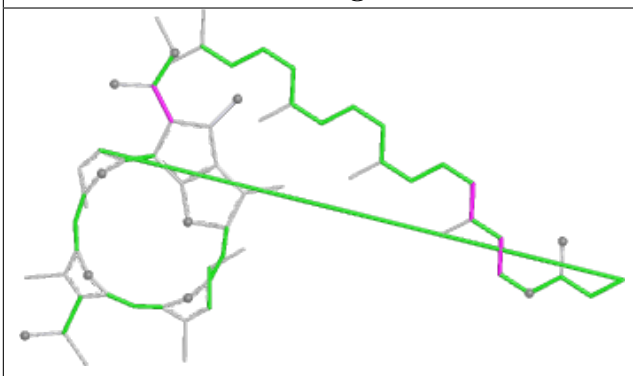
Ligand BPH L 306



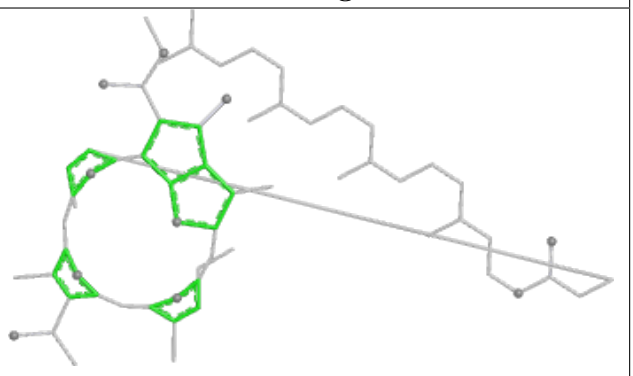
Bond lengths



Bond angles

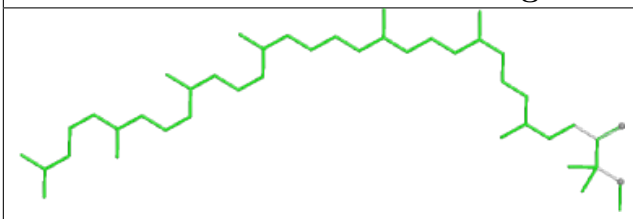


Torsions

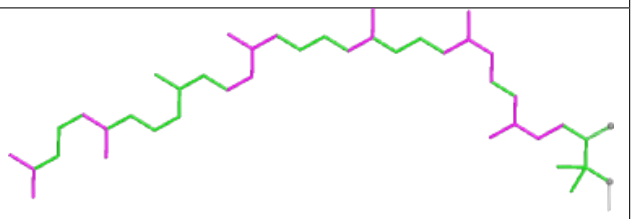


Rings

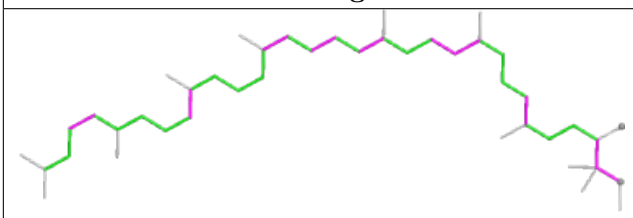
Ligand SPN M 408



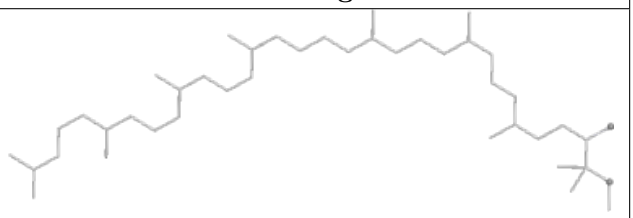
Bond lengths



Bond angles

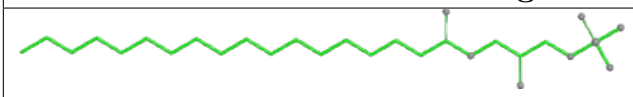


Torsions



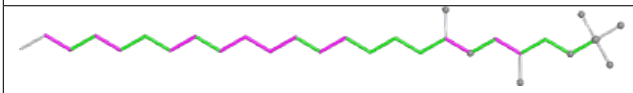
Rings

Ligand NKP M 403

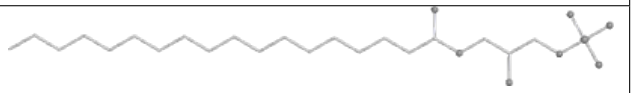


Bond lengths

Bond angles

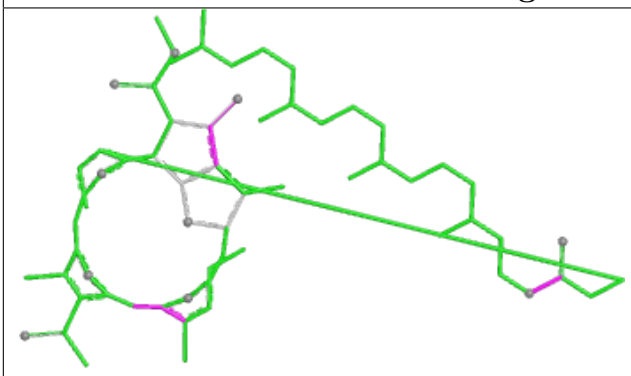


Torsions

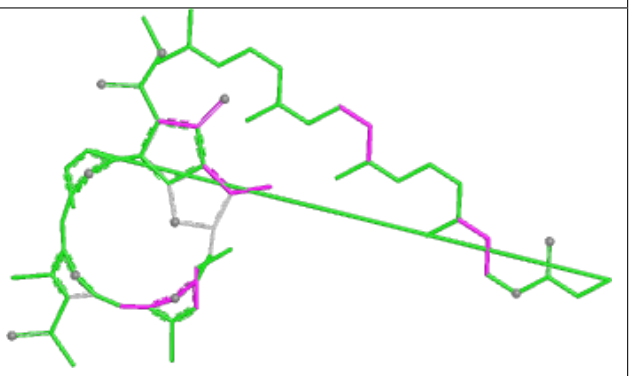


Rings

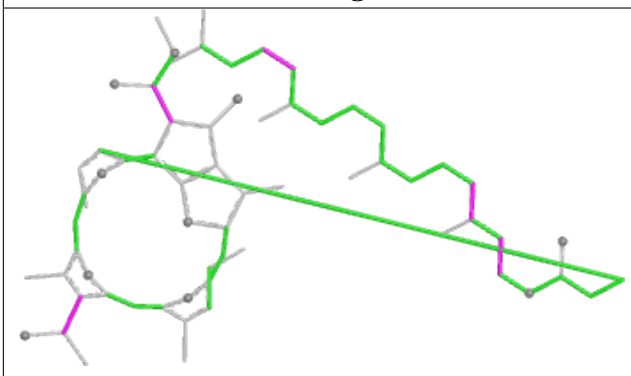
Ligand BPH M 406



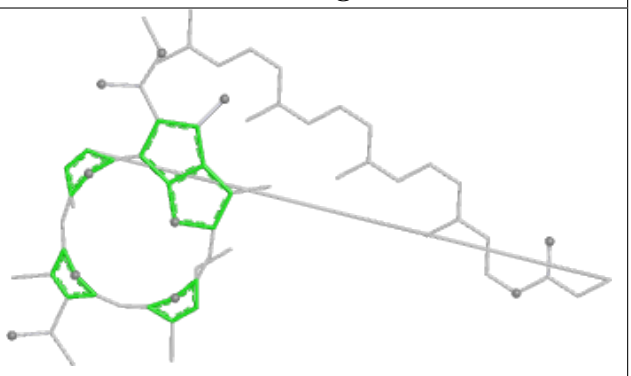
Bond lengths



Bond angles

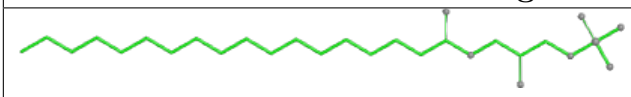


Torsions

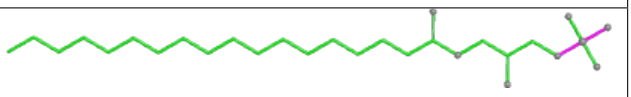


Rings

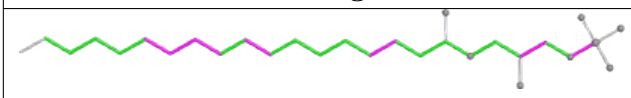
Ligand NKP M 401



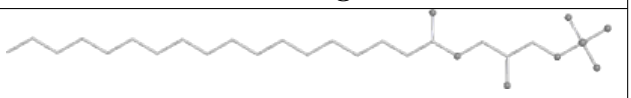
Bond lengths



Bond angles

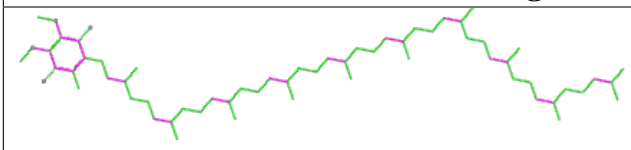


Torsions

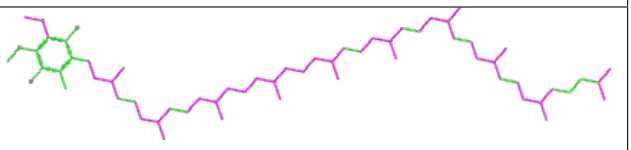


Rings

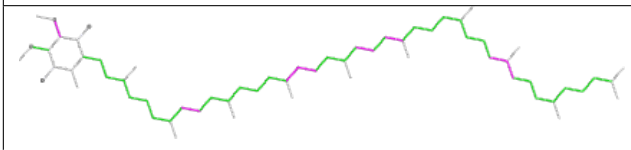
Ligand U10 M 402



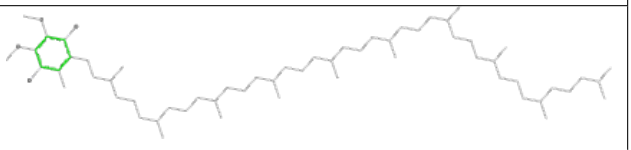
Bond lengths



Bond angles

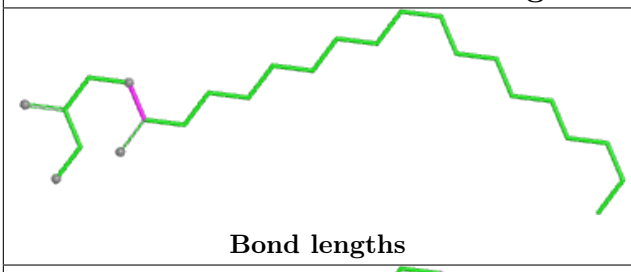


Torsions

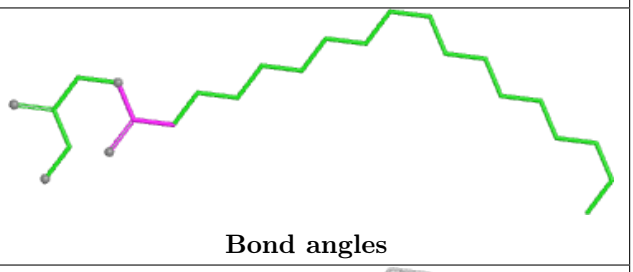


Rings

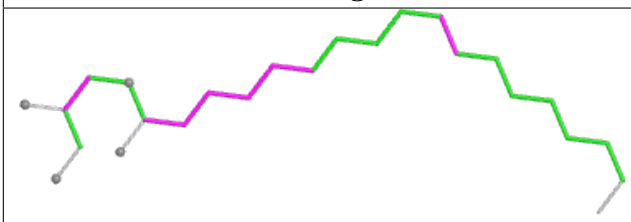
Ligand OLC L 301



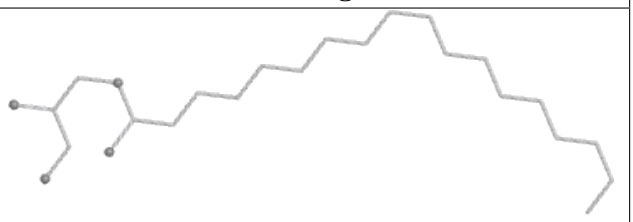
Bond lengths



Bond angles

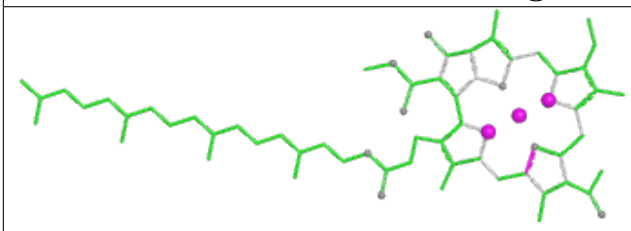


Torsions

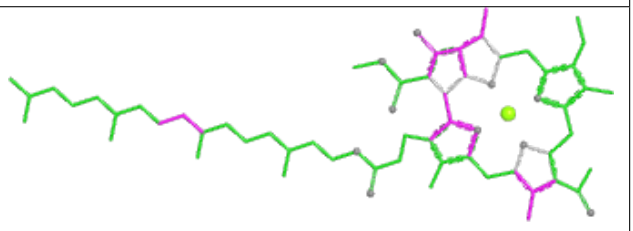


Rings

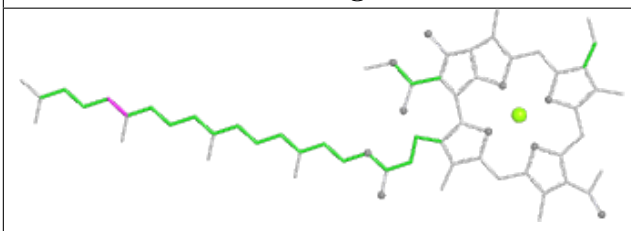
Ligand BCL L 305



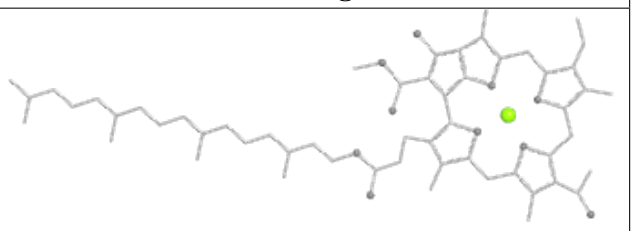
Bond lengths



Bond angles

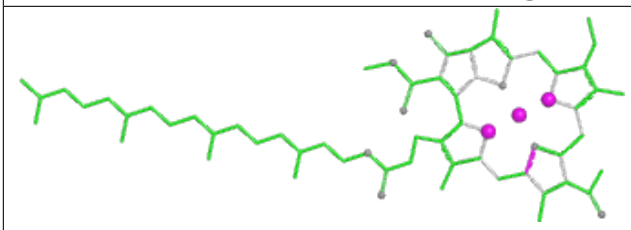


Torsions

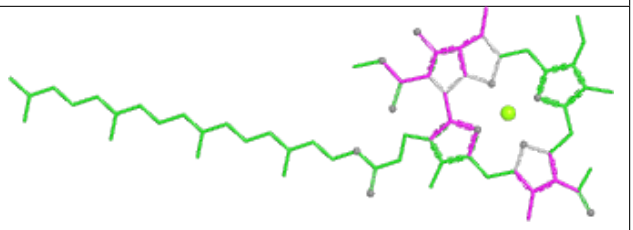


Rings

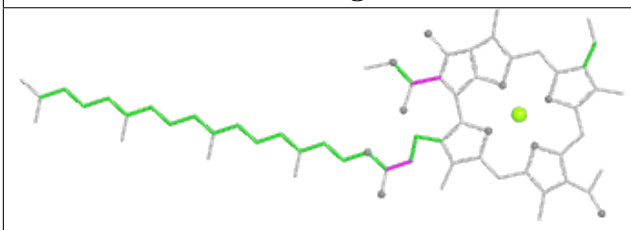
Ligand BCL M 405



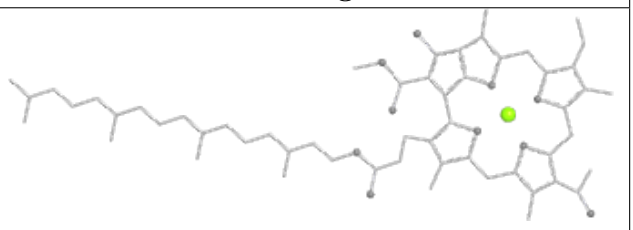
Bond lengths



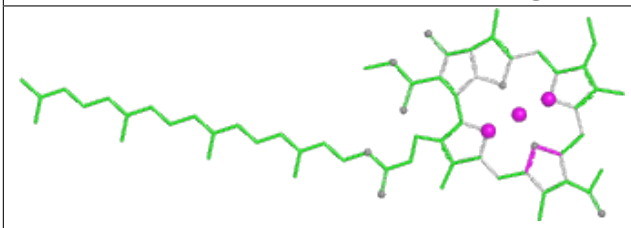
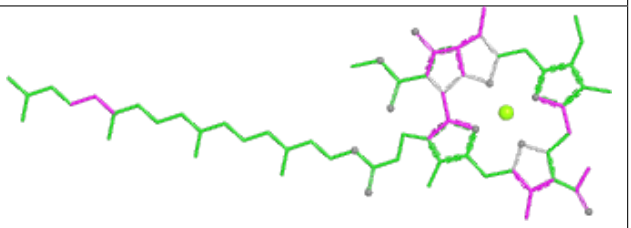
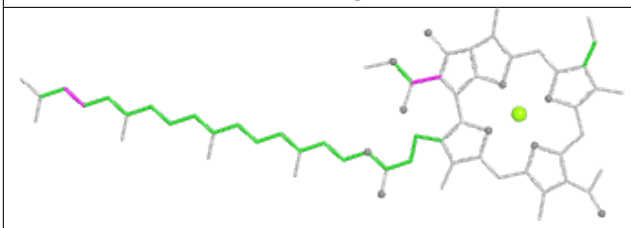
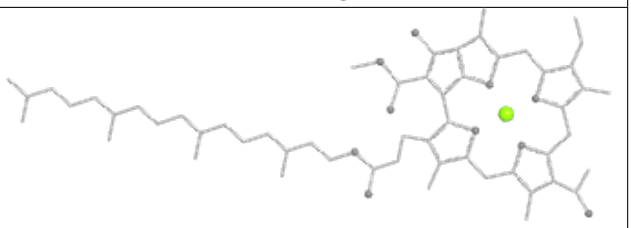
Bond angles

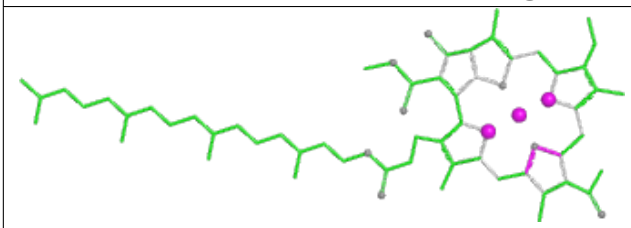
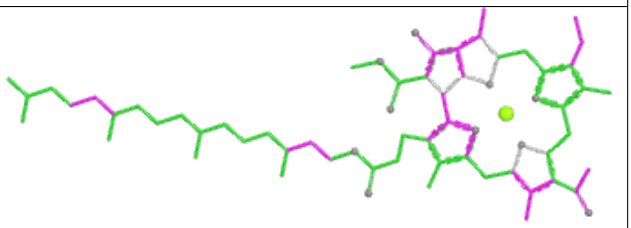
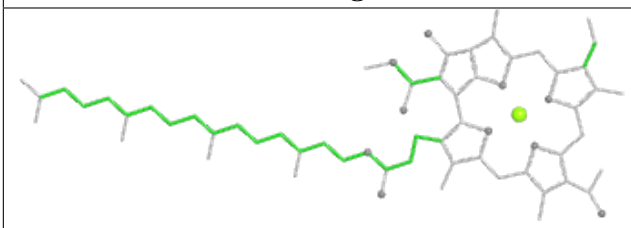
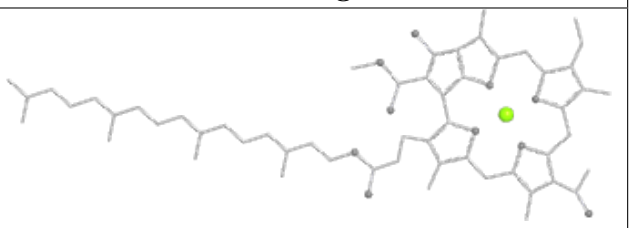


Torsions



Rings

Ligand BCL L 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL M 404	
 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

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, 95^{th} 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	239/242 (98%)	0.07	10 (4%) 36 39	24, 39, 62, 86	0
2	L	281/281 (100%)	0.60	31 (11%) 5 5	21, 38, 65, 118	0
3	M	302/303 (99%)	0.59	35 (11%) 4 4	21, 37, 67, 98	0
All	All	822/826 (99%)	0.44	76 (9%) 9 9	21, 38, 65, 118	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	59	TRP	11.5
3	M	1	ALA	10.2
2	L	63	LEU	7.9
2	L	277[A]	GLY	7.6
2	L	51	TRP	7.0
3	M	301	HIS	6.8
2	L	266[A]	TRP	6.7
2	L	58	THR	6.6
2	L	272[A]	TRP	6.3
3	M	68	PHE	5.8
2	L	267[A]	VAL	5.7
2	L	83	GLY	5.3
2	L	271[A]	TRP	5.3
3	M	106	ALA	4.7
2	L	57	GLY	4.7
1	H	10	PHE	4.6
2	L	265[A]	TRP	4.5
2	L	274[A]	ASN	4.2
3	M	78	ALA	4.2
3	M	297	TRP	4.2
2	L	281[A]	GLY	4.1
3	M	102	GLY	3.9
2	L	269[A]	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	L	60	ASN	3.8
2	L	55	LEU	3.7
1	H	246	PRO	3.6
3	M	75	TRP	3.6
2	L	279[A]	ILE	3.5
3	M	300	ASN	3.5
3	M	84	VAL	3.5
3	M	72	ILE	3.4
2	L	53	ALA	3.4
3	M	85	PHE	3.4
3	M	92	PHE	3.4
1	H	18	TYR	3.3
1	H	50	ALA	3.3
3	M	83	ALA	3.1
3	M	80	TRP	3.1
1	H	245	ALA	3.1
3	M	76	TYR	3.1
3	M	171	TRP	3.1
1	H	90	THR	3.0
3	M	174	ALA	3.0
1	H	52	ASN	2.9
3	M	100	GLU	2.8
2	L	255	TRP	2.7
3	M	61	PHE	2.7
3	M	121	PHE	2.7
2	L	61	PRO	2.7
2	L	41	PHE	2.6
2	L	56	GLN	2.6
3	M	302	GLY	2.6
3	M	177	TYR	2.6
2	L	278[A]	GLY	2.5
3	M	37	THR	2.4
3	M	87	ARG	2.4
3	M	65	MET	2.4
2	L	257	ASP	2.4
3	M	74	PHE	2.3
3	M	52[A]	LEU	2.3
2	L	270[A]	PRO	2.2
3	M	81	ASN	2.2
1	H	92	VAL	2.2
2	L	40	PHE	2.1
3	M	67	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	54	VAL	2.1
3	M	109	LEU	2.1
3	M	103	LEU	2.1
2	L	69	PRO	2.1
1	H	248	ARG	2.0
2	L	78	ALA	2.0
3	M	107	ALA	2.0
2	L	44	LEU	2.0
3	M	113	GLY	2.0
1	H	201	ASN	2.0
3	M	226	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	LDA	M	409	16/16	0.61	0.29	41,62,72,81	0
12	SPN	M	408	43/43	0.74	0.26	40,58,81,96	0
6	MYS	L	303	15/15	0.75	0.22	51,58,64,66	0
5	OLC	L	301	25/25	0.80	0.24	35,51,72,74	0
6	MYS	M	410	15/15	0.81	0.21	46,62,75,77	0
9	NKP	M	403	29/29	0.82	0.24	36,61,75,81	0
6	MYS	L	302	15/15	0.82	0.21	56,62,76,80	0
9	NKP	M	401	29/29	0.86	0.30	34,71,85,96	0
10	U10	M	402	63/63	0.87	0.21	21,48,80,86	0
4	LDA	H	301	16/16	0.88	0.17	34,45,61,70	0
7	BCL	L	304	66/66	0.88	0.16	25,36,50,60	0
13	EDO	M	411	4/4	0.91	0.14	42,46,53,54	0

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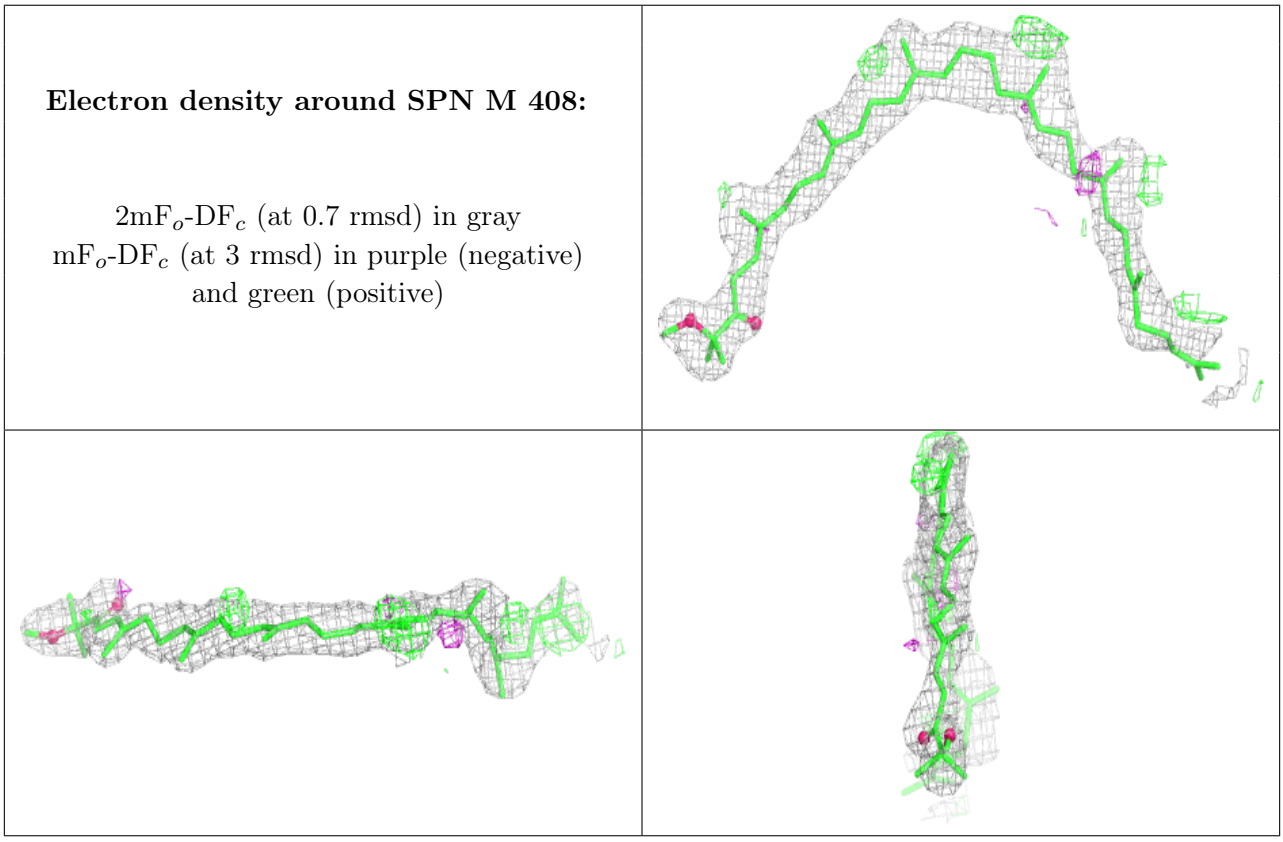
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	PO4	M	412	5/5	0.91	0.19	53,64,72,78	0
7	BCL	M	405	66/66	0.93	0.13	25,33,60,78	0
8	BPH	M	406	65/65	0.93	0.17	23,34,94,106	0
7	BCL	L	305	66/66	0.93	0.16	27,35,58,71	0
7	BCL	M	404	66/66	0.93	0.14	28,37,81,85	0
8	BPH	L	306	65/65	0.95	0.16	22,29,45,55	0
11	FE	M	407	1/1	1.00	0.12	23,23,23,23	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.

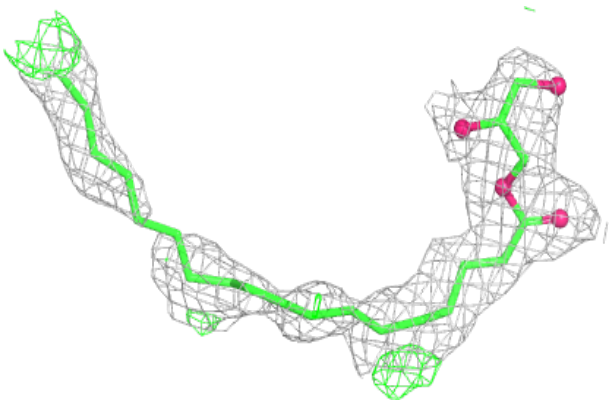
Electron density around SPN M 408:

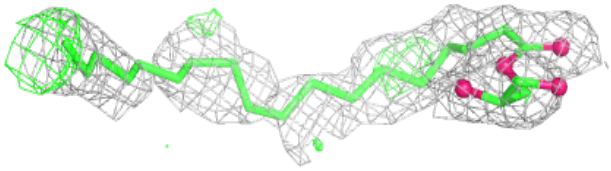
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around OLC L 301:

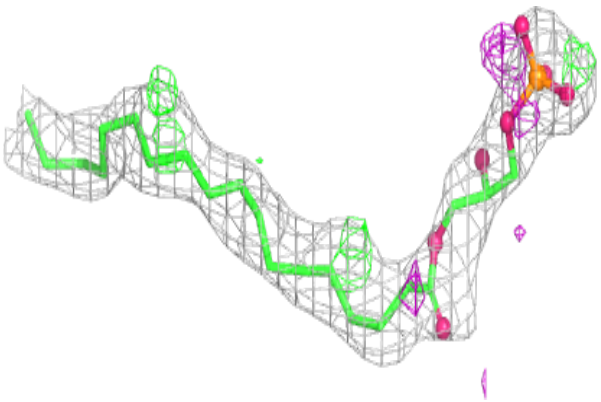
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

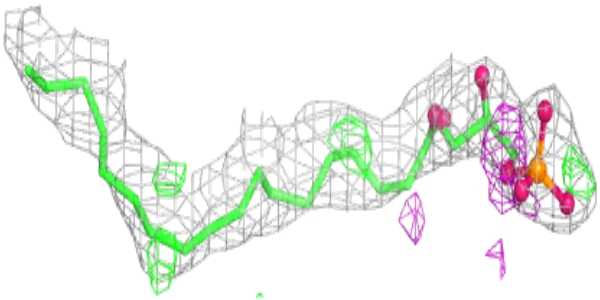


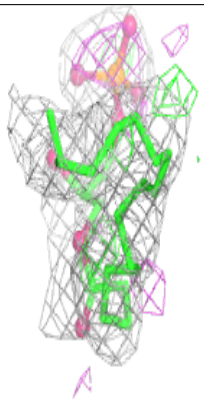


Electron density around NKP M 403:

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

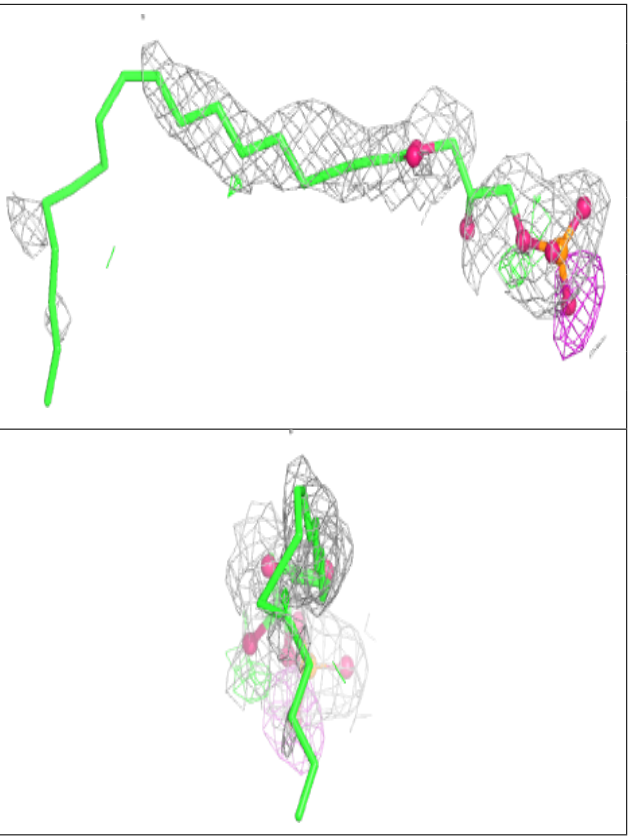






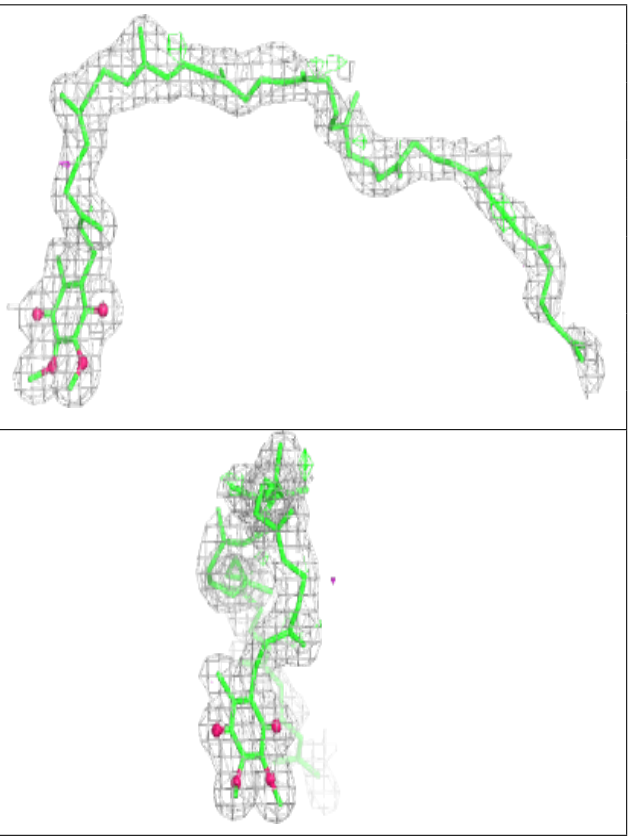
Electron density around NKP M 401:

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



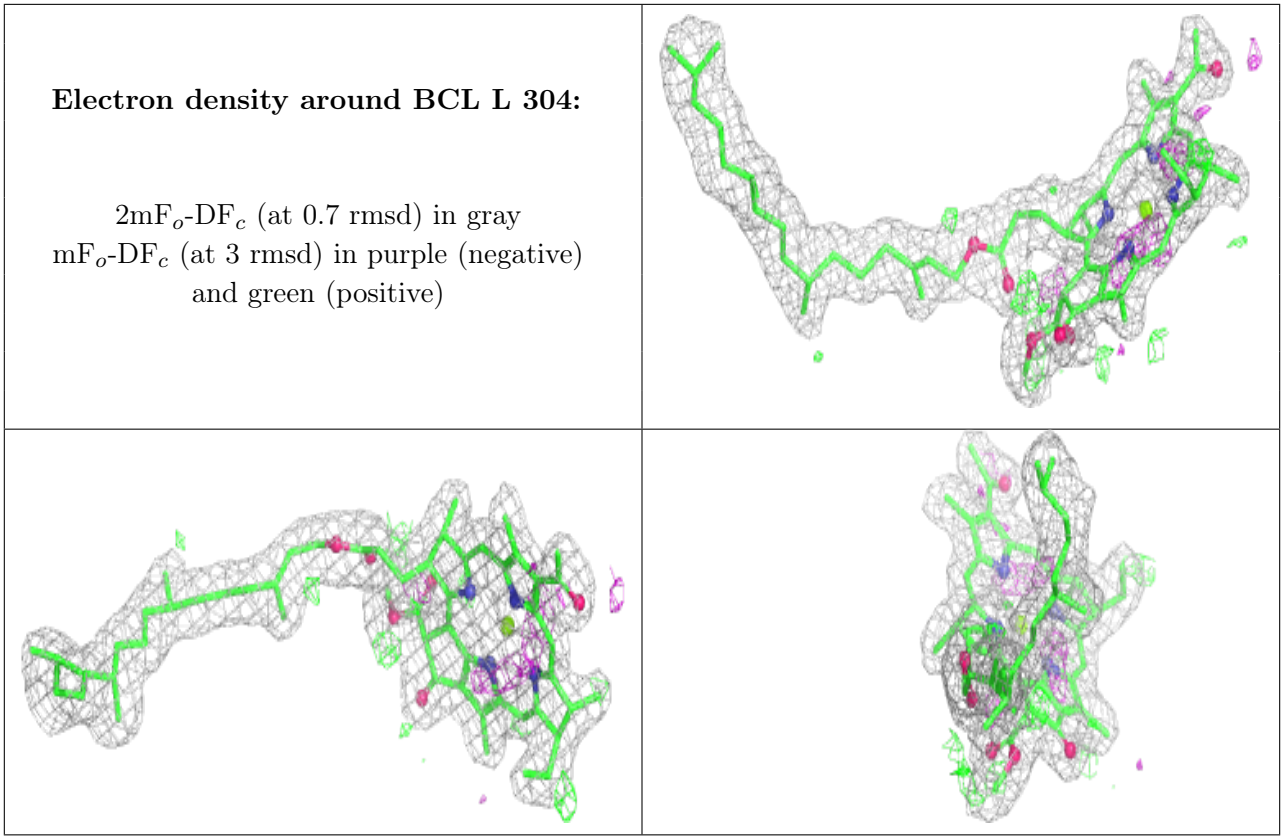
Electron density around U10 M 402:

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



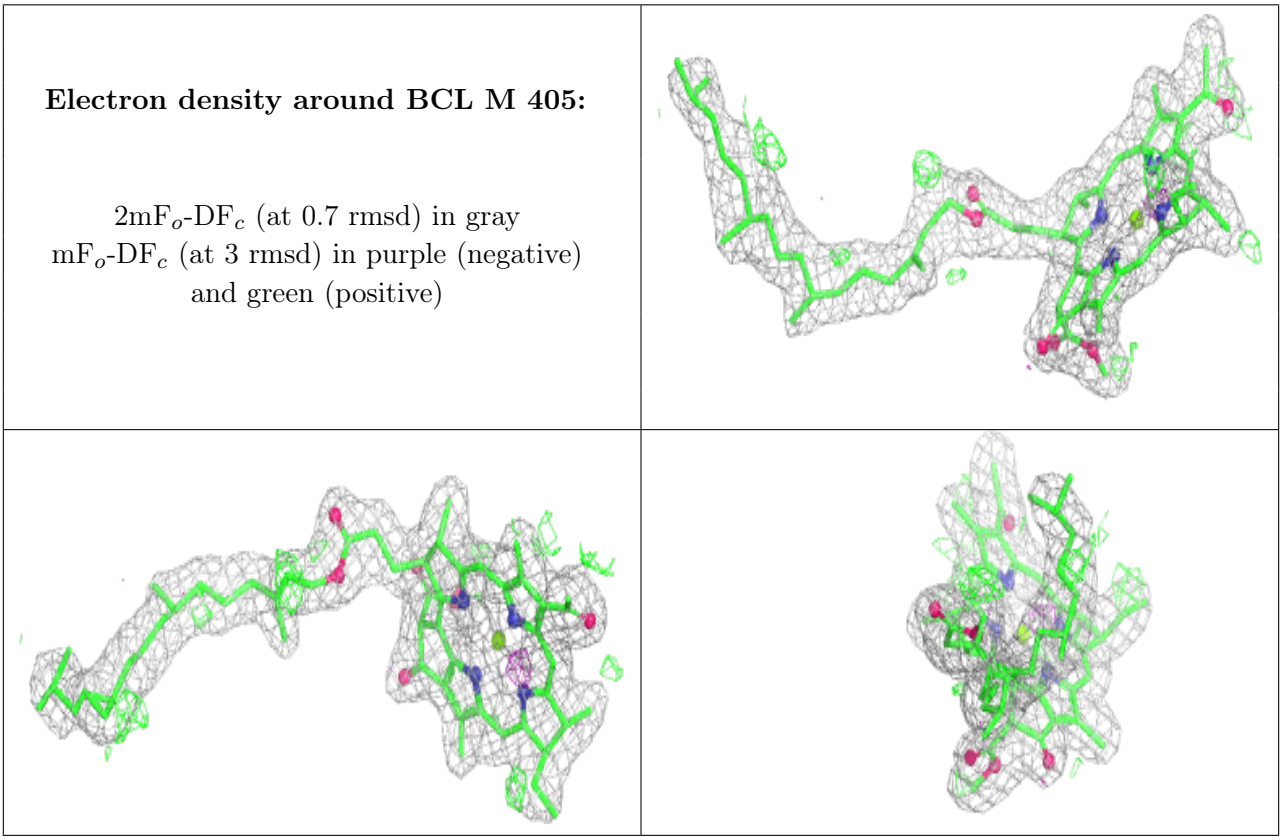
Electron density around BCL L 304:

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



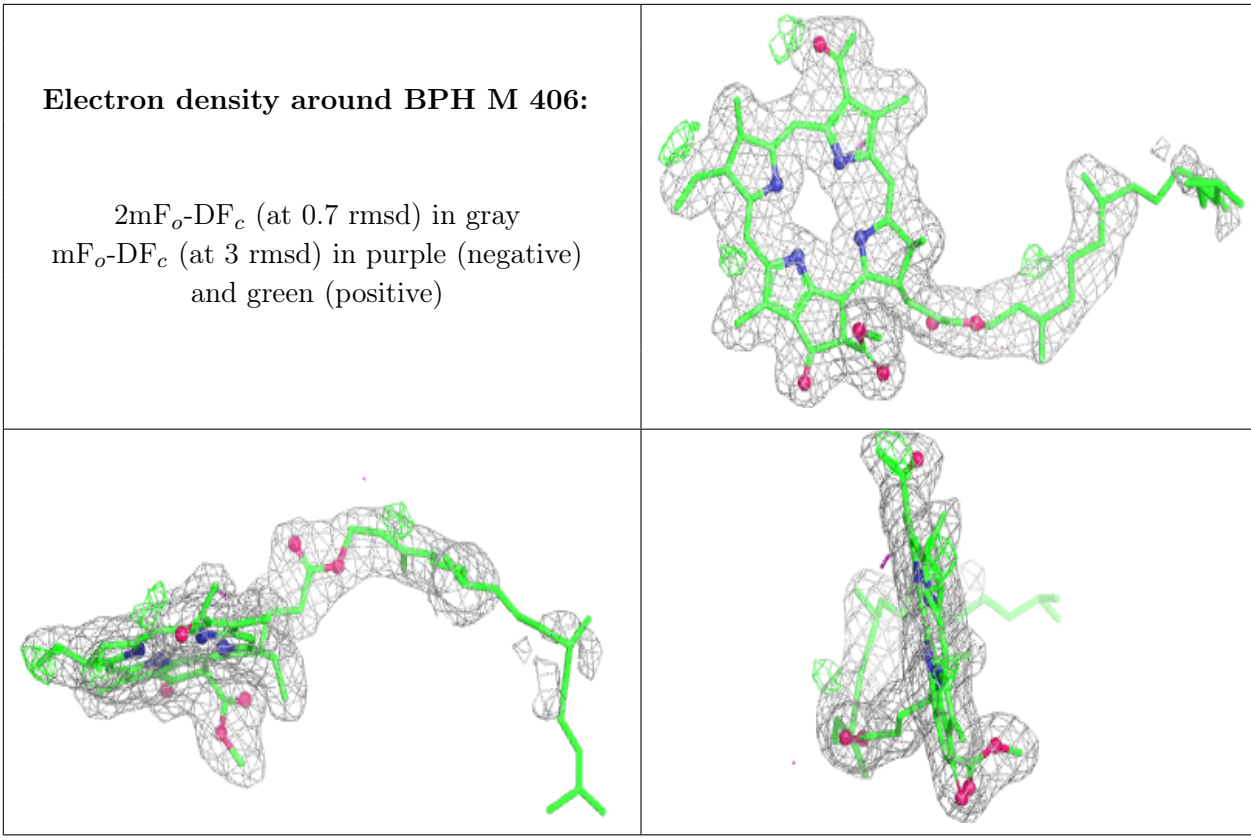
Electron density around BCL M 405:

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



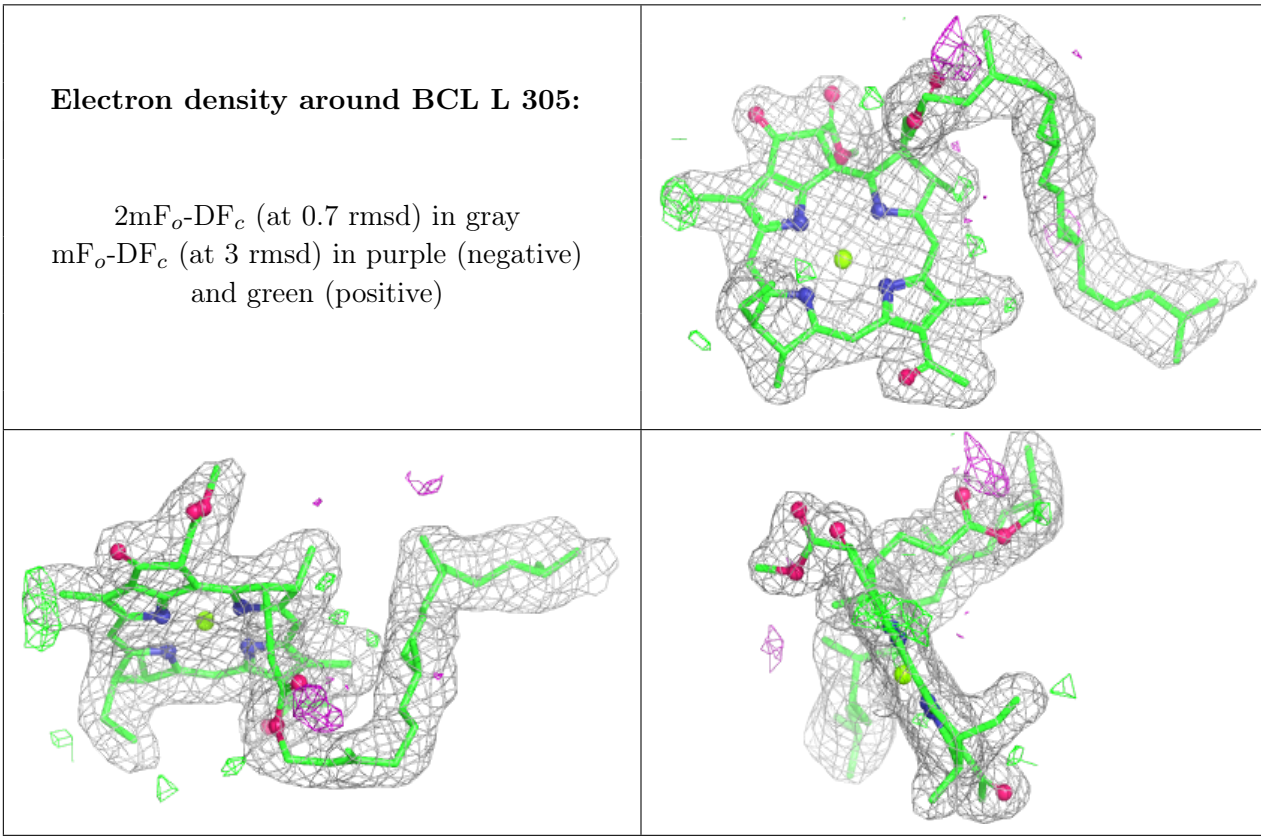
Electron density around BPH M 406:

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



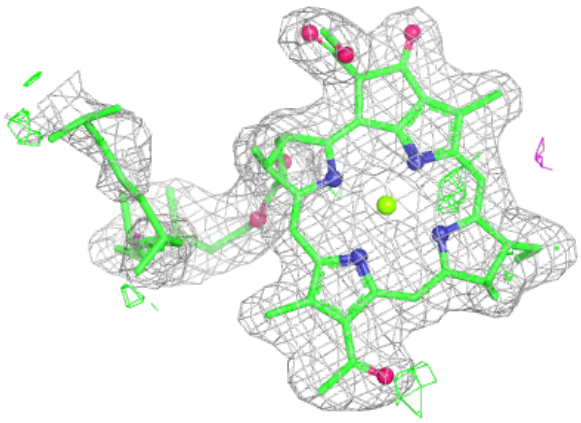
Electron density around BCL L 305:

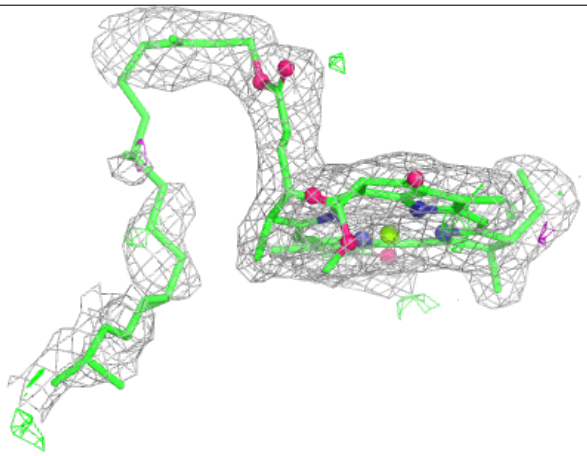
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

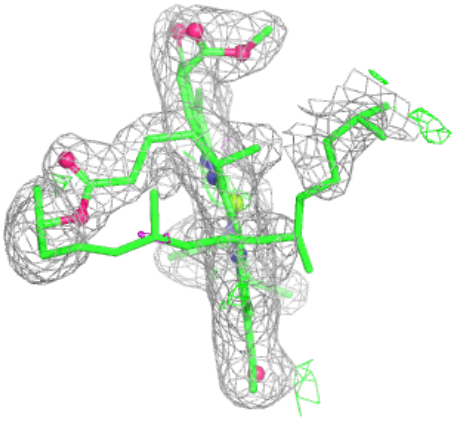


Electron density around BCL M 404:

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

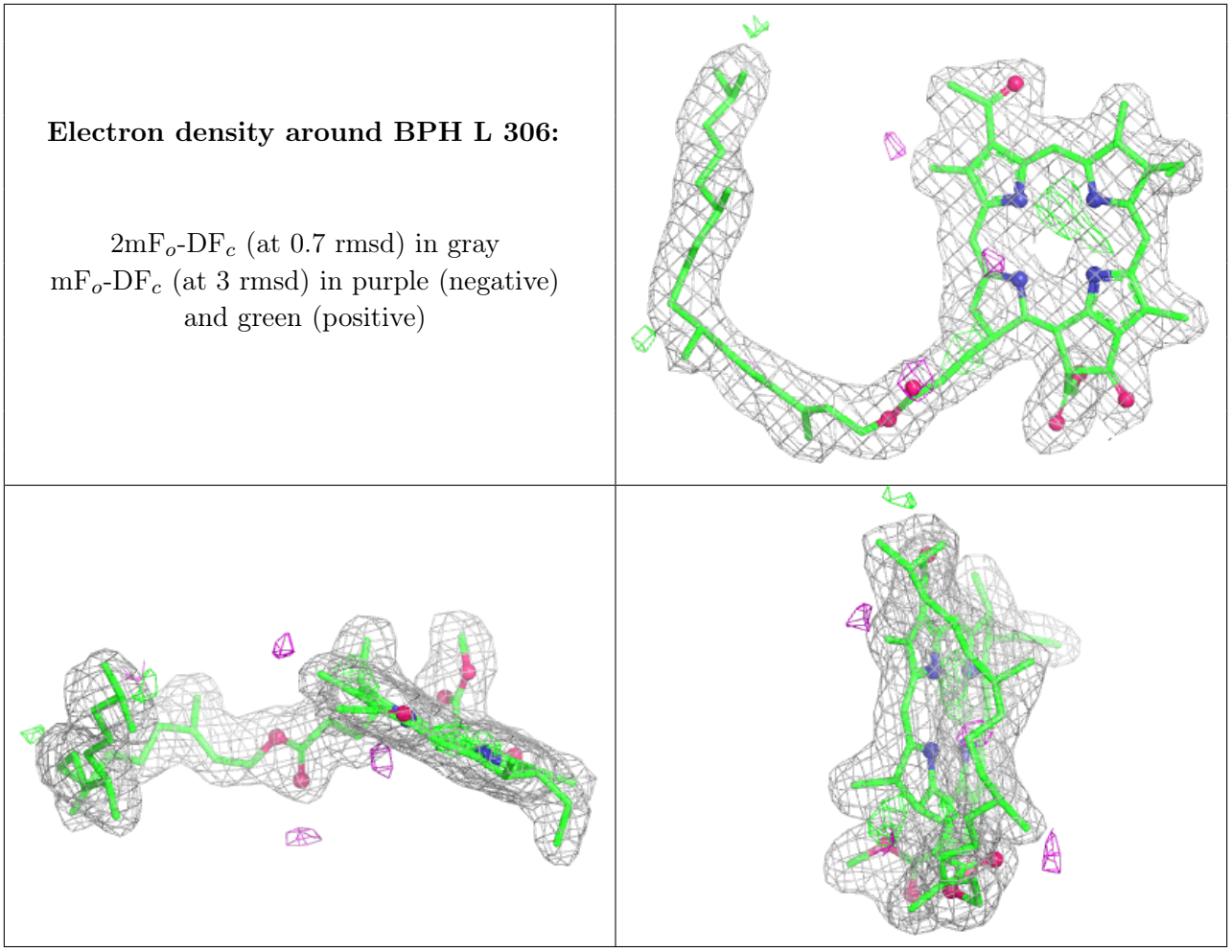






Electron density around BPH L 306:

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



6.5 Other polymers

There are no such residues in this entry.