Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2026 – 07:54 am BST

PDB ID	:	8C5X / pdb_00008c5x
Title	:	Double mutant A(L37)C/S(L99)C structure of Photosynthetic Reaction Center From Cereibacter sphaeroides strain RV
Authors	:	Gabdulkhakov, A.; Selikhanov, G.; Fufina, T.; Vasilieva, L.; Atamas, A.; Uhimchuk, D.
Deposited on	:	2023-01-10
Resolution	:	2.60 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

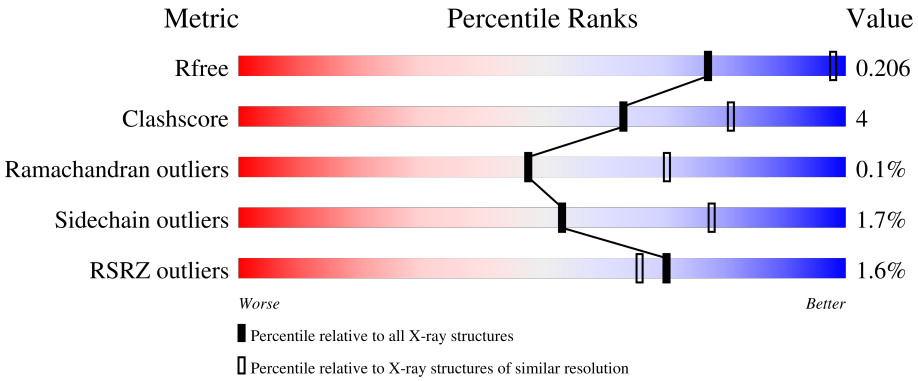
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	89% 10%
2	L	281	2% 93% 6%
3	M	303	2% 91% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	LDA	M	412	-	-	-	X
5	UNL	H	303	-	-	-	X
5	UNL	L	306	-	-	-	X

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 7547 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	240	Total	C	N	O	S	0	3	0
			1848	1183	317	339	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	2	0
			2245	1516	356	363	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	37	CYS	ALA	engineered mutation	UNP P0C0Y8
L	99	CYS	SER	engineered mutation	UNP P0C0Y8
L	178	THR	SER	conflict	UNP P0C0Y8

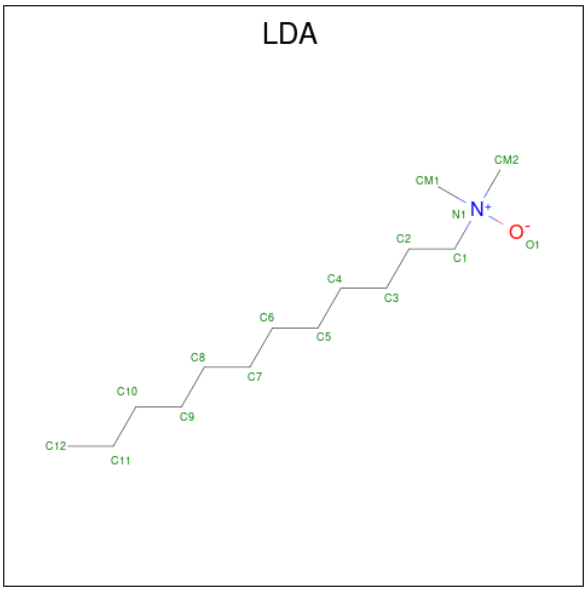
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	2	0
			2425	1621	397	397	10			

There is a discrepancy between the modelled and reference sequences:

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

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

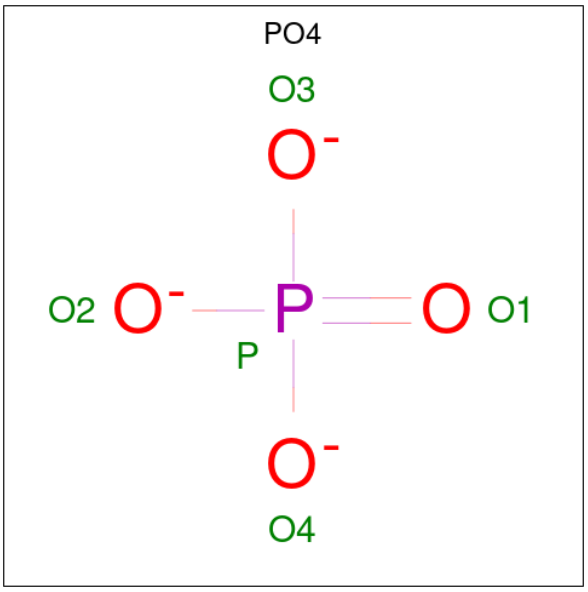


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0

- Molecule 5 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

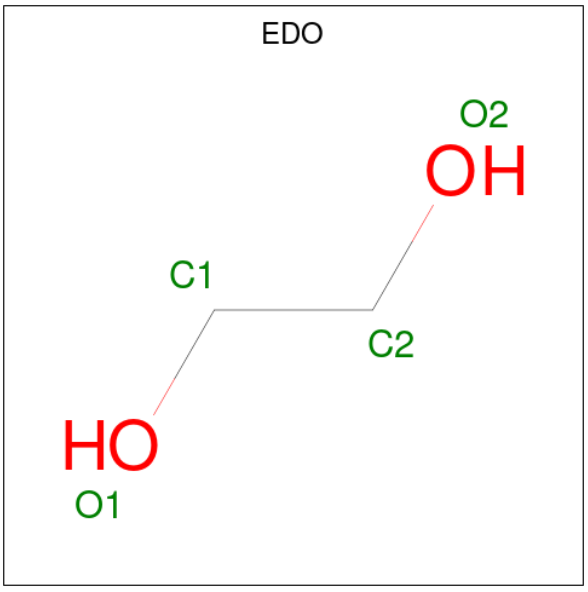
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	4	Total C 51 51	0	0
5	L	3	Total C 37 37	0	0
5	M	3	Total C 39 39	0	0

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total O P 5 4 1	0	0
6	L	1	Total O P 5 4 1	0	0
6	M	1	Total O P 5 4 1	0	0
6	M	1	Total O P 5 4 1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

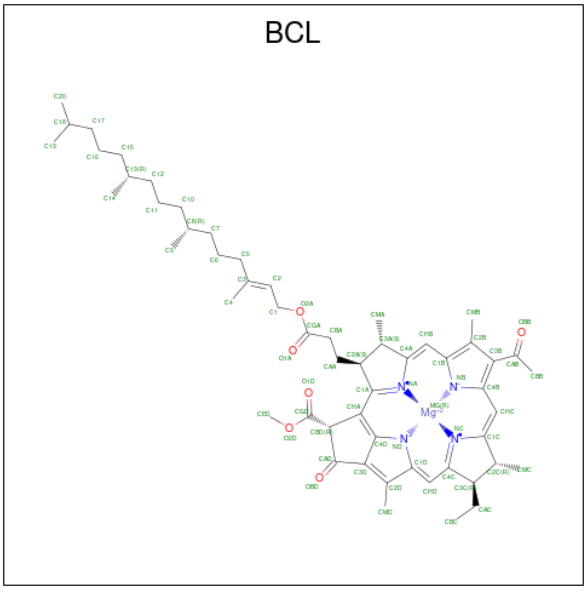


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total C O 4 2 2	0	0
7	H	1	Total C O 4 2 2	0	0
7	H	1	Total C O 4 2 2	0	0
7	L	1	Total C O 4 2 2	0	0
7	L	1	Total C O 4 2 2	0	0
7	L	1	Total C O 4 2 2	0	0
7	M	1	Total C O 4 2 2	0	0
7	M	1	Total C O 4 2 2	0	0

- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K).

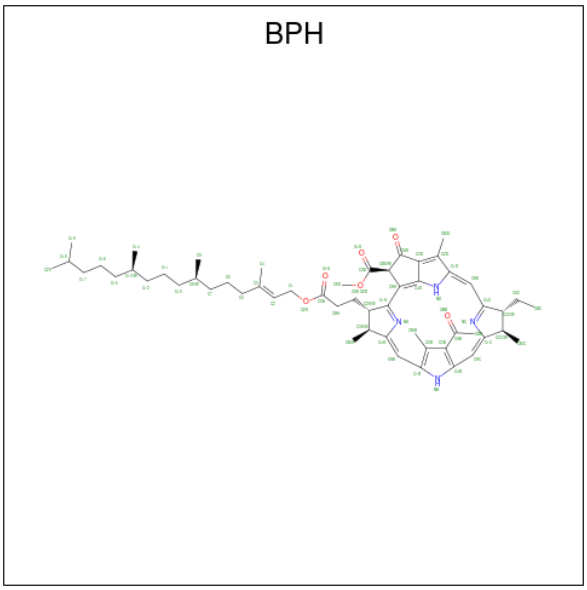
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total K 1 1	0	0

- Molecule 9 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



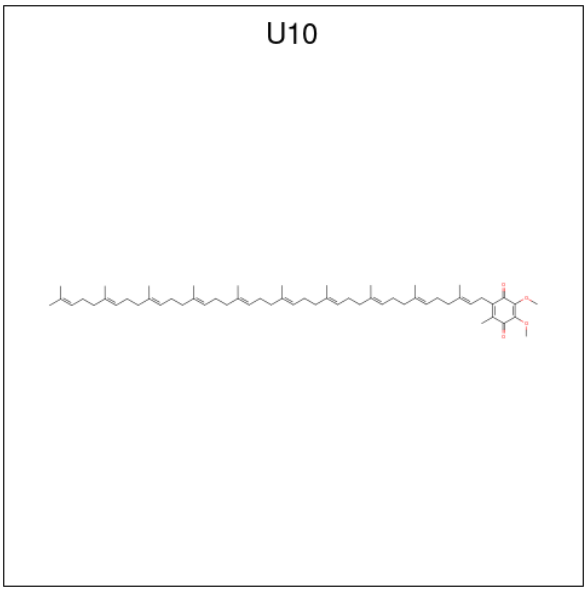
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 10 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



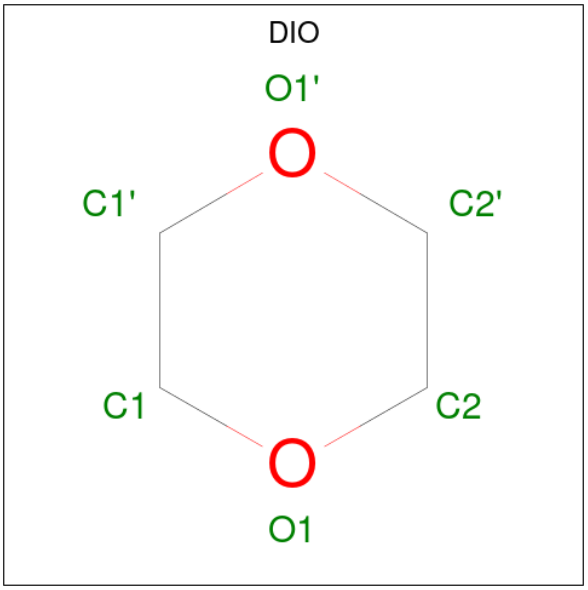
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	N	O	0	0
			65	55	4	6		
10	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 11 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



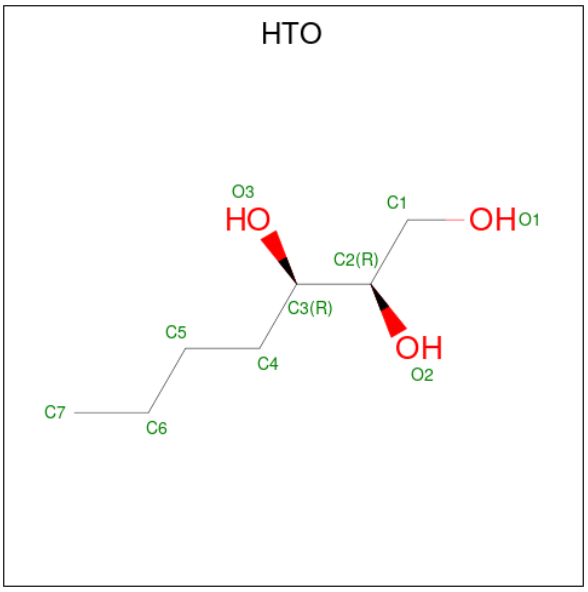
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	1	Total C O 48 44 4	0	0
11	M	1	Total C O 48 44 4	0	0

- Molecule 12 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: $C_4H_8O_2$).



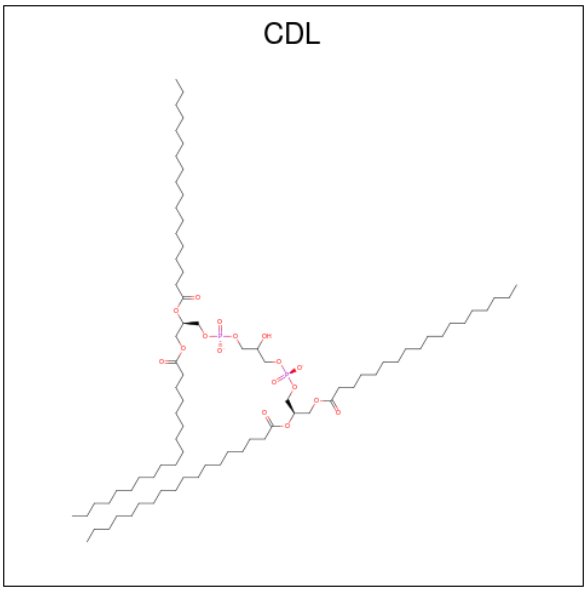
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	L	1	Total C O 6 4 2	0	0

- Molecule 13 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: $C_7H_{16}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	L	1	Total C O 10 7 3	0	0

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

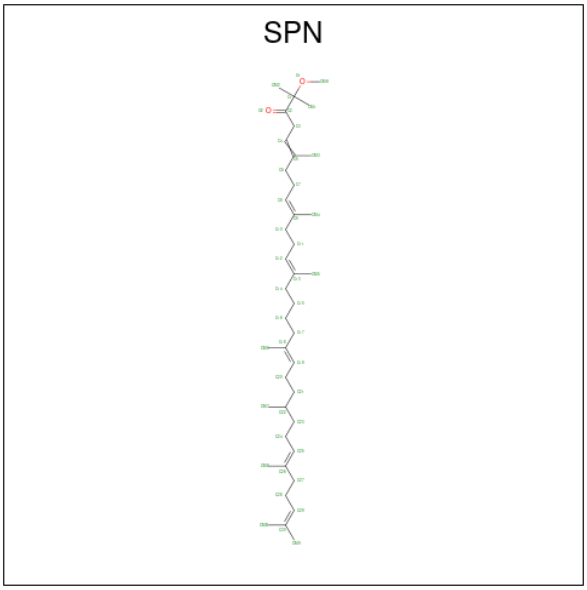


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	M	1	Total C O P 81 62 17 2	0	0

- Molecule 15 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 16 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$) (labeled as "Ligand of Interest" by depositor).



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

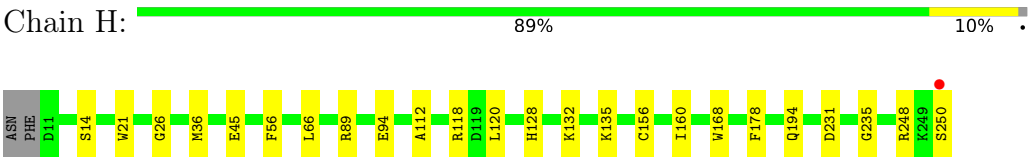
- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	43	Total O 43 43	0	0
17	L	22	Total O 22 22	0	0
17	M	41	Total O 41 41	0	0

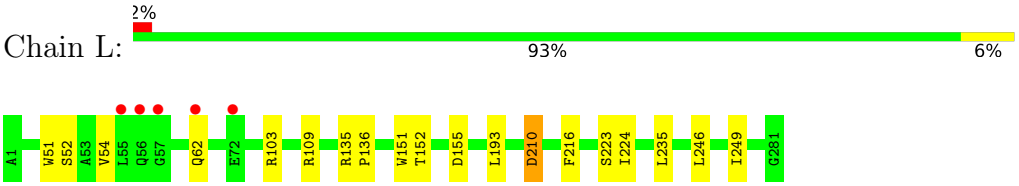
3 Residue-property plots (i)

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.

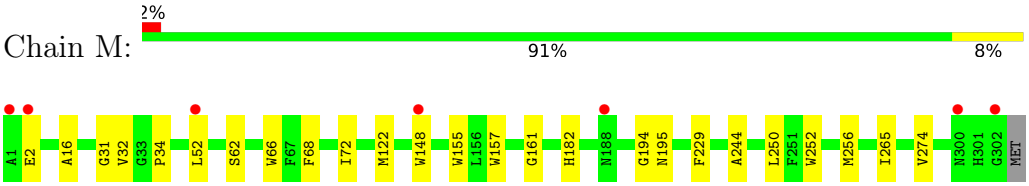
• Molecule 1: Reaction center protein H chain



• 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 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.85Å 139.85Å 186.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.89 – 2.60 29.89 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.89-2.60) 99.9 (29.89-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.186 , 0.207 0.189 , 0.206	Depositor DCC
R_{free} test set	3351 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	52.0	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7547	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: DIO, HTO, U10, BCL, BPH, K, SPN, CDL, PO4, EDO, UNL, LDA, FE

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	0/1905	0.57	0/2590
2	L	0.40	0/2336	0.57	0/3197
3	M	0.38	0/2524	0.54	0/3445
All	All	0.39	0/6765	0.56	0/9232

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	1848	0	1866	17	0
2	L	2245	0	2204	11	0
3	M	2425	0	2345	17	0
4	H	16	0	31	2	0
4	M	96	0	186	6	0
5	H	51	0	0	0	0
5	L	37	0	0	1	0
5	M	39	0	0	0	0
6	H	5	0	0	0	0
6	L	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	10	0	0	0	0
7	H	12	0	18	2	0
7	L	12	0	18	0	0
7	M	8	0	12	0	0
8	H	1	0	0	0	0
9	L	132	0	148	0	0
9	M	132	0	148	3	0
10	L	65	0	76	0	0
10	M	65	0	76	2	0
11	L	48	0	63	3	0
11	M	48	0	63	2	0
12	L	6	0	8	0	0
13	L	10	0	16	0	0
14	M	81	0	106	6	0
15	M	1	0	0	0	0
16	M	43	0	70	7	0
17	H	43	0	0	0	0
17	L	22	0	0	1	0
17	M	41	0	0	0	0
All	All	7547	0	7454	59	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:301:LDA:H121	4:M:408:LDA:H91	1.63	0.78
3:M:34:PRO:HA	4:M:412:LDA:H101	1.75	0.68
2:L:62:GLN:OE1	2:L:151:TRP:NE1	2.28	0.66
3:M:161:GLY:HA3	16:M:407:SPN:H201	1.78	0.65
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.80	0.63
1:H:118[A]:ARG:HD2	1:H:120:LEU:HD12	1.82	0.59
3:M:252:TRP:CE3	3:M:256:MET:HE2	2.39	0.57
2:L:223:SER:HA	11:L:304:U10:H103	1.86	0.55
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.42	0.54
1:H:26:GLY:HA3	14:M:401:CDL:H171	1.90	0.54
3:M:155:TRP:CD2	14:M:401:CDL:H812	2.43	0.53
1:H:45:GLU:HG3	1:H:94[A]:GLU:CD	2.33	0.53
1:H:194:GLN:H	1:H:194:GLN:CD	2.15	0.53
3:M:31:GLY:H	4:M:410:LDA:HM11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:51:TRP:O	2:L:54:VAL:N	2.37	0.53
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.91	0.52
11:M:406:U10:H23	4:M:420:LDA:H62	1.91	0.52
3:M:157:TRP:CE2	16:M:407:SPN:HM73	2.45	0.51
2:L:152:THR:O	2:L:155:ASP:HB2	2.10	0.51
2:L:224:ILE:H	11:L:304:U10:H103	1.74	0.51
3:M:52:LEU:HD12	3:M:52:LEU:O	2.10	0.51
9:M:402:BCL:CAB	16:M:407:SPN:H162	2.41	0.51
1:H:45:GLU:HG3	1:H:94[A]:GLU:OE2	2.11	0.50
1:H:128:HIS:ND1	7:H:307:EDO:H12	2.26	0.50
1:H:21:TRP:HZ2	4:M:408:LDA:HM11	1.77	0.50
2:L:109:ARG:HH12	5:L:306:UNL:C14	2.26	0.49
11:M:406:U10:H28	11:M:406:U10:H322	1.42	0.48
3:M:66:TRP:CZ2	3:M:122:MET:HE3	2.49	0.48
4:M:412:LDA:H21	4:M:412:LDA:HM23	1.57	0.48
1:H:156:CYS:HB2	1:H:248:ARG:HG3	1.95	0.47
16:M:407:SPN:H152	16:M:407:SPN:HM51	1.78	0.47
1:H:132:LYS:NZ	7:H:307:EDO:H11	2.30	0.46
1:H:36:MET:HE1	1:H:56:PHE:O	2.15	0.46
10:M:404:BPH:H9C1	10:M:404:BPH:H111	1.84	0.46
16:M:407:SPN:H71	16:M:407:SPN:HM31	1.84	0.45
1:H:66:LEU:HD13	1:H:118[B]:ARG:HH21	1.82	0.45
1:H:56:PHE:HE2	4:H:301:LDA:H42	1.82	0.45
16:M:407:SPN:H111	16:M:407:SPN:HM41	1.64	0.44
3:M:250:LEU:HD23	3:M:250:LEU:HA	1.85	0.43
9:M:403:BCL:HHC	9:M:403:BCL:OBB	2.17	0.43
2:L:210:ASP:N	2:L:210:ASP:OD1	2.50	0.43
3:M:148:TRP:CE2	14:M:401:CDL:H511	2.53	0.43
10:M:404:BPH:HBC3	10:M:404:BPH:HHD	2.02	0.42
2:L:135:ARG:HB3	2:L:136:PRO:HD3	2.02	0.42
1:H:112:ALA:HA	1:H:235:GLY:O	2.19	0.42
2:L:103:ARG:NH1	17:L:402:HOH:O	2.41	0.42
14:M:401:CDL:HB61	14:M:401:CDL:OA8	2.20	0.42
1:H:160:ILE:HD13	1:H:160:ILE:HA	1.87	0.41
3:M:157:TRP:CZ2	16:M:407:SPN:HM73	2.56	0.41
14:M:401:CDL:H522	14:M:401:CDL:H312	2.01	0.41
3:M:16:ALA:HB1	3:M:32:VAL:HG21	2.01	0.41
3:M:68[B]:PHE:CZ	3:M:72:ILE:HD11	2.56	0.41
1:H:135:LYS:HB3	1:H:135:LYS:HE2	1.88	0.41
1:H:89:ARG:NH2	1:H:94[A]:GLU:HG2	2.36	0.40
9:M:402:BCL:OBB	9:M:402:BCL:HHC	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:148:TRP:NE1	14:M:401:CDL:H511	2.36	0.40
2:L:193:LEU:HD23	11:L:304:U10:C2	2.52	0.40
2:L:246:LEU:HA	2:L:249:ILE:HG22	2.04	0.40
3:M:194:GLY:O	3:M:195:ASN:HB3	2.21	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	241/242 (100%)	238 (99%)	3 (1%)	0	100 100
2	L	281/281 (100%)	268 (95%)	12 (4%)	1 (0%)	30 51
3	M	302/303 (100%)	291 (96%)	11 (4%)	0	100 100
All	All	824/826 (100%)	797 (97%)	26 (3%)	1 (0%)	48 70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	52	SER

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	198/197 (100%)	195 (98%)	3 (2%)	57 80
2	L	223/221 (101%)	220 (99%)	3 (1%)	61 82
3	M	238/237 (100%)	233 (98%)	5 (2%)	47 73
All	All	659/655 (101%)	648 (98%)	11 (2%)	53 78

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	14	SER
1	H	231	ASP
1	H	250	SER
2	L	210	ASP
2	L	216	PHE
2	L	235	LEU
3	M	2	GLU
3	M	62	SER
3	M	182	HIS
3	M	265	ILE
3	M	274	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	129	ASN
2	L	258	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 43 ligands modelled in this entry, 10 are unknown and 2 are monoatomic - leaving 31 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	EDO	H	308	-	3,3,3	0.60	0	2,2,2	0.13	0
4	LDA	M	420	-	12,15,15	2.07	1 (8%)	14,17,17	0.54	0
7	EDO	M	419	-	3,3,3	0.55	0	2,2,2	0.28	0
13	HTO	L	312	-	9,9,9	0.47	0	10,10,10	1.11	1 (10%)
7	EDO	L	309	-	3,3,3	0.52	0	2,2,2	0.30	0
16	SPN	M	407	-	40,42,42	0.38	0	50,52,52	0.70	0
6	PO4	H	306	-	4,4,4	0.86	0	6,6,6	0.49	0
14	CDL	M	401	-	80,80,99	0.47	1 (1%)	86,92,111	0.37	0
6	PO4	M	416	-	4,4,4	0.98	0	6,6,6	0.47	0
9	BCL	M	402	3	69,74,74	1.28	8 (11%)	83,115,115	1.57	15 (18%)
7	EDO	L	310	-	3,3,3	0.43	0	2,2,2	0.50	0
10	BPH	M	404	-	59,70,70	1.24	5 (8%)	61,101,101	2.10	13 (21%)
12	DIO	L	308	-	6,6,6	0.50	0	6,6,6	0.08	0
7	EDO	L	311	-	3,3,3	0.48	0	2,2,2	0.64	0
7	EDO	H	309	-	3,3,3	0.50	0	2,2,2	0.32	0
9	BCL	L	302	2	69,74,74	1.34	10 (14%)	83,115,115	1.46	12 (14%)
4	LDA	M	408	-	12,15,15	2.14	1 (8%)	14,17,17	0.44	0
9	BCL	L	301	2	69,74,74	1.35	8 (11%)	83,115,115	1.42	11 (13%)
4	LDA	H	301	-	12,15,15	1.94	1 (8%)	14,17,17	0.54	0
11	U10	L	304	-	48,48,63	2.58	12 (25%)	58,61,79	2.10	22 (37%)
9	BCL	M	403	3	69,74,74	1.34	8 (11%)	83,115,115	1.40	8 (9%)
4	LDA	M	412	-	12,15,15	2.01	1 (8%)	14,17,17	0.44	0
6	PO4	M	417	-	4,4,4	0.70	0	6,6,6	0.50	0
7	EDO	H	307	-	3,3,3	0.61	0	2,2,2	0.24	0
7	EDO	M	418	-	3,3,3	0.52	0	2,2,2	0.61	0
11	U10	M	406	-	48,48,63	2.66	13 (27%)	58,61,79	1.80	16 (27%)
6	PO4	L	313	-	4,4,4	0.72	0	6,6,6	0.57	0
4	LDA	M	410	-	12,15,15	2.11	1 (8%)	14,17,17	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	LDA	M	411	-	12,15,15	2.08	1 (8%)	14,17,17	0.50	0
10	BPH	L	303	-	59,70,70	1.32	8 (13%)	61,101,101	2.12	10 (16%)
4	LDA	M	409	-	12,15,15	1.98	1 (8%)	14,17,17	0.48	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
7	EDO	H	308	-	-	0/1/1/1	-
4	LDA	M	420	-	-	10/13/13/13	-
7	EDO	M	419	-	-	0/1/1/1	-
13	HTO	L	312	-	-	4/10/10/10	-
7	EDO	L	309	-	-	0/1/1/1	-
16	SPN	M	407	-	-	13/50/51/51	-
14	CDL	M	401	-	-	34/91/91/110	-
9	BCL	M	402	3	-	7/41/137/137	-
7	EDO	L	310	-	-	0/1/1/1	-
10	BPH	M	404	-	-	9/37/105/105	0/5/6/6
12	DIO	L	308	-	-	-	0/1/1/1
7	EDO	L	311	-	-	1/1/1/1	-
7	EDO	H	309	-	-	0/1/1/1	-
9	BCL	L	302	2	-	1/41/137/137	-
4	LDA	M	408	-	-	4/13/13/13	-
9	BCL	L	301	2	-	2/41/137/137	-
4	LDA	H	301	-	-	8/13/13/13	-
11	U10	L	304	-	-	16/45/69/87	0/1/1/1
9	BCL	M	403	3	-	2/41/137/137	-
4	LDA	M	412	-	-	4/13/13/13	-
7	EDO	H	307	-	-	0/1/1/1	-
7	EDO	M	418	-	-	0/1/1/1	-
11	U10	M	406	-	-	10/45/69/87	0/1/1/1
4	LDA	M	410	-	-	4/13/13/13	-
4	LDA	M	411	-	-	6/13/13/13	-
10	BPH	L	303	-	-	3/37/105/105	0/5/6/6
4	LDA	M	409	-	-	5/13/13/13	-

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	410	LDA	O1-N1	-7.25	1.25	1.42
4	M	408	LDA	O1-N1	-7.21	1.25	1.42
4	M	411	LDA	O1-N1	-7.14	1.25	1.42
4	M	420	LDA	O1-N1	-7.09	1.25	1.42
4	M	412	LDA	O1-N1	-6.86	1.26	1.42
4	M	409	LDA	O1-N1	-6.72	1.26	1.42
4	H	301	LDA	O1-N1	-6.66	1.26	1.42
11	M	406	U10	C13-C14	6.57	1.48	1.33
11	M	406	U10	C8-C9	6.23	1.47	1.33
11	L	304	U10	C8-C9	6.20	1.47	1.33
11	M	406	U10	C18-C19	6.20	1.47	1.33
11	L	304	U10	C23-C24	6.19	1.47	1.33
11	L	304	U10	C13-C14	6.16	1.47	1.33
11	M	406	U10	C28-C29	6.12	1.47	1.33
11	L	304	U10	C18-C19	6.11	1.47	1.33
11	M	406	U10	C33-C34	6.08	1.47	1.33
11	M	406	U10	C23-C24	5.87	1.47	1.33
11	L	304	U10	C28-C29	5.84	1.47	1.33
11	L	304	U10	C33-C34	5.80	1.46	1.33
11	L	304	U10	C38-C39	5.78	1.49	1.32
10	M	404	BPH	C1D-C2D	5.73	1.45	1.39
11	M	406	U10	C38-C39	5.64	1.48	1.32
9	M	403	BCL	MG-NA	5.38	2.19	2.06
9	L	301	BCL	MG-NA	5.36	2.19	2.06
10	L	303	BPH	CBD-CGD	-4.80	1.46	1.52
9	L	302	BCL	MG-NA	4.58	2.17	2.06
11	L	304	U10	O4-C4	-4.50	1.25	1.36
9	M	403	BCL	MG-NC	4.24	2.16	2.06
11	M	406	U10	O3-C3	-4.21	1.26	1.36
9	L	301	BCL	MG-NC	4.16	2.16	2.06
11	M	406	U10	O4-C4	-4.08	1.26	1.36
9	M	402	BCL	MG-NA	3.87	2.15	2.06
11	L	304	U10	O3-C3	-3.82	1.27	1.36
9	L	302	BCL	MG-NC	3.71	2.15	2.06
9	L	302	BCL	C3B-C4B	3.58	1.47	1.41
9	M	402	BCL	C3B-C4B	3.54	1.47	1.41
9	M	402	BCL	MG-NC	3.17	2.13	2.06
9	L	302	BCL	O1A-CGA	-3.15	1.13	1.22
9	L	301	BCL	C3B-C4B	3.14	1.46	1.41
10	M	404	BPH	C3B-C4B	3.12	1.46	1.41
9	M	403	BCL	CHD-C1D	3.02	1.44	1.38
9	L	301	BCL	C5-C3	2.98	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	403	BCL	C1D-ND	2.85	1.41	1.37
9	M	403	BCL	C3B-C4B	2.83	1.46	1.41
11	M	406	U10	C3-C2	-2.83	1.40	1.48
10	L	303	BPH	C3D-CAD	-2.80	1.41	1.47
11	M	406	U10	C6-C1	2.79	1.40	1.35
10	M	404	BPH	CBD-CGD	-2.79	1.48	1.52
9	M	402	BCL	C1D-ND	2.78	1.41	1.37
11	M	406	U10	C4-C5	-2.68	1.41	1.48
11	L	304	U10	C3-C2	-2.66	1.41	1.48
10	L	303	BPH	C1D-C2D	2.64	1.42	1.39
9	M	403	BCL	C5-C3	2.60	1.56	1.51
9	M	402	BCL	C1B-NB	2.56	1.40	1.37
10	M	404	BPH	CHA-CBD	2.56	1.54	1.51
9	L	302	BCL	OBD-CAD	2.50	1.26	1.22
9	L	302	BCL	CHD-C1D	2.45	1.43	1.38
9	L	302	BCL	C1B-NB	2.43	1.40	1.37
9	L	302	BCL	C1D-ND	2.41	1.40	1.37
10	L	303	BPH	C1-C2	2.37	1.56	1.49
11	L	304	U10	C4-C5	-2.37	1.42	1.48
9	M	402	BCL	CHD-C1D	2.30	1.42	1.38
10	M	404	BPH	C3D-CAD	-2.24	1.42	1.47
11	M	406	U10	C6-C5	-2.24	1.40	1.46
9	L	301	BCL	CHD-C1D	2.21	1.42	1.38
11	L	304	U10	C6-C1	2.21	1.39	1.35
9	L	302	BCL	C1D-C2D	-2.18	1.41	1.45
9	M	402	BCL	OBD-CAD	2.17	1.26	1.22
9	L	301	BCL	O1A-CGA	-2.17	1.16	1.22
9	M	402	BCL	CMD-C2D	2.14	1.55	1.50
10	L	303	BPH	C2C-C3C	2.12	1.56	1.54
10	L	303	BPH	C3B-C4B	2.12	1.45	1.41
9	M	403	BCL	OBD-CAD	2.10	1.26	1.22
14	M	401	CDL	PA1-OA4	-2.10	1.45	1.55
9	L	301	BCL	C1D-ND	2.10	1.40	1.37
10	L	303	BPH	C4D-CHA	2.09	1.42	1.39
10	L	303	BPH	C5-C3	2.07	1.55	1.51
9	L	302	BCL	CHC-C1C	2.07	1.42	1.37
9	L	301	BCL	C3D-C4D	-2.05	1.39	1.44
9	M	403	BCL	C1B-NB	2.02	1.40	1.37

All (108) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	303	BPH	C4D-CHA-CBD	-12.35	102.93	108.52
10	M	404	BPH	C4D-CHA-CBD	-10.34	103.84	108.52
9	M	402	BCL	CHD-C1D-ND	-5.55	119.35	124.45
11	L	304	U10	C1M-C1-C6	-5.38	115.62	124.40
9	L	301	BCL	CHD-C1D-ND	-5.06	119.80	124.45
9	L	302	BCL	CHD-C1D-ND	-5.01	119.85	124.45
9	M	402	BCL	C4D-CHA-C1A	4.99	127.32	121.25
9	L	302	BCL	C4D-CHA-C1A	4.97	127.30	121.25
10	L	303	BPH	C4D-ND-C1D	-4.97	103.77	108.83
9	M	403	BCL	C4D-CHA-C1A	4.88	127.19	121.25
9	M	403	BCL	CHD-C1D-ND	-4.83	120.02	124.45
10	M	404	BPH	C4D-ND-C1D	-4.72	104.03	108.83
9	L	301	BCL	C4D-CHA-C1A	4.54	126.78	121.25
11	L	304	U10	C32-C33-C34	-4.31	117.29	127.66
10	M	404	BPH	O2D-CGD-CBD	4.26	116.39	111.00
9	M	402	BCL	C1D-ND-C4D	-4.15	103.39	106.33
11	L	304	U10	C25-C24-C26	4.12	122.20	115.27
11	M	406	U10	C35-C34-C36	4.08	122.14	115.27
11	M	406	U10	C17-C18-C19	-3.96	118.12	127.66
11	L	304	U10	C17-C18-C19	-3.94	118.17	127.66
11	L	304	U10	C27-C28-C29	-3.93	118.19	127.66
9	L	302	BCL	C1D-ND-C4D	-3.90	103.57	106.33
11	M	406	U10	C32-C33-C34	-3.89	118.30	127.66
11	M	406	U10	C22-C23-C24	-3.83	118.45	127.66
11	L	304	U10	C12-C13-C14	-3.80	118.51	127.66
11	M	406	U10	C30-C29-C31	3.79	121.65	115.27
10	M	404	BPH	C3D-C4D-ND	3.70	112.76	107.72
10	M	404	BPH	C1-C2-C3	-3.68	119.68	126.04
9	L	301	BCL	C1D-ND-C4D	-3.65	103.74	106.33
10	M	404	BPH	OBD-CAD-CBD	-3.55	120.61	125.82
10	M	404	BPH	CAC-C3C-C4C	3.48	121.52	113.73
9	M	403	BCL	CHA-C1A-NA	-3.45	118.49	126.40
11	M	406	U10	C15-C14-C16	3.45	121.08	115.27
9	M	403	BCL	C1D-ND-C4D	-3.43	103.90	106.33
11	L	304	U10	C7-C8-C9	-3.39	121.15	126.79
11	L	304	U10	C20-C19-C21	3.28	120.80	115.27
10	L	303	BPH	C3D-C4D-ND	3.26	112.16	107.72
10	L	303	BPH	OBD-CAD-CBD	-3.20	121.12	125.82
11	L	304	U10	C30-C29-C31	3.14	120.55	115.27
11	L	304	U10	C3M-O3-C3	3.11	127.50	116.47
9	L	302	BCL	CHA-C1A-NA	-3.01	119.51	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	402	BCL	C2A-C1A-CHA	2.95	129.02	123.86
9	L	301	BCL	CHA-C1A-NA	-2.88	119.80	126.40
9	L	302	BCL	O2D-CGD-CBD	2.87	116.36	111.27
11	M	406	U10	C10-C9-C11	2.82	120.01	115.27
9	M	402	BCL	CAB-C3B-C2B	2.81	132.56	128.34
11	L	304	U10	C6-C1-C2	2.80	121.40	119.18
11	L	304	U10	C22-C23-C24	-2.78	120.96	127.66
9	M	402	BCL	CHA-C1A-NA	-2.78	120.04	126.40
9	L	301	BCL	C2A-C1A-CHA	2.78	128.71	123.86
10	L	303	BPH	CMB-C2B-C3B	2.74	129.80	124.68
11	M	406	U10	C25-C24-C26	2.66	119.75	115.27
9	M	402	BCL	C2D-C1D-ND	2.60	112.02	110.10
11	M	406	U10	C26-C27-C28	-2.59	103.37	111.88
9	L	302	BCL	C2A-C1A-CHA	2.56	128.34	123.86
11	L	304	U10	C4M-O4-C4	2.54	125.48	116.47
9	M	403	BCL	C4A-NA-C1A	2.54	107.85	106.71
9	M	403	BCL	CAB-C3B-C2B	2.51	132.11	128.34
9	M	402	BCL	O2A-C1-C2	-2.51	102.03	108.64
10	L	303	BPH	C2D-C1D-ND	2.50	111.25	109.53
9	L	301	BCL	CHC-C4B-NB	-2.49	121.62	124.26
9	L	302	BCL	O2A-C1-C2	-2.48	102.12	108.64
10	M	404	BPH	C11-C12-C13	-2.46	107.97	115.92
10	M	404	BPH	O2A-C1-C2	-2.46	102.18	108.64
11	L	304	U10	C35-C34-C36	2.44	119.38	115.27
11	M	406	U10	C20-C19-C21	2.44	119.37	115.27
10	M	404	BPH	O2D-CGD-O1D	-2.42	119.12	123.84
10	L	303	BPH	C4C-C3C-C2C	-2.41	100.55	102.84
9	L	302	BCL	C2D-C1D-ND	2.40	111.87	110.10
11	M	406	U10	C1M-C1-C6	-2.40	120.49	124.40
13	L	312	HTO	O1-C1-C2	-2.39	105.87	111.07
11	L	304	U10	C7-C6-C5	2.39	121.35	118.48
11	L	304	U10	C35-C34-C33	-2.36	117.62	123.68
11	L	304	U10	C10-C9-C11	2.33	119.19	115.27
9	L	301	BCL	CAB-C3B-C2B	2.32	131.82	128.34
11	M	406	U10	C35-C34-C33	-2.32	117.72	123.68
9	L	301	BCL	C1-O2A-CGA	2.31	122.51	116.44
11	L	304	U10	C10-C9-C8	-2.30	117.77	123.68
9	M	403	BCL	C2A-C1A-CHA	2.29	127.86	123.86
10	M	404	BPH	CMB-C2B-C3B	2.29	128.96	124.68
9	M	402	BCL	C16-C15-C13	2.28	123.30	115.92
10	M	404	BPH	CAC-C3C-C2C	-2.28	108.56	114.26
10	L	303	BPH	C1-C2-C3	-2.27	122.11	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	301	BCL	OBB-CAB-CBB	-2.27	114.70	119.73
9	M	402	BCL	OBB-CAB-CBB	-2.24	114.77	119.73
11	L	304	U10	C41-C39-C40	2.22	119.52	114.60
11	M	406	U10	C37-C38-C39	-2.22	120.16	127.75
9	L	301	BCL	C16-C15-C13	2.21	123.05	115.92
9	M	402	BCL	C4A-NA-C1A	2.20	107.69	106.71
9	L	302	BCL	C4B-C3B-C2B	-2.18	104.86	108.36
9	L	301	BCL	C4B-C3B-C2B	-2.17	104.86	108.36
9	L	302	BCL	CHC-C4B-NB	-2.17	121.97	124.26
9	L	302	BCL	C11-C12-C13	-2.16	108.92	115.92
9	M	402	BCL	C19-C18-C17	-2.15	98.25	111.54
10	L	303	BPH	CMD-C2D-C3D	2.15	128.70	124.68
11	L	304	U10	C30-C29-C28	-2.15	118.17	123.68
9	M	402	BCL	C4B-C3B-C2B	-2.14	104.91	108.36
10	L	303	BPH	C11-C10-C8	-2.14	109.00	115.92
11	M	406	U10	O5-C5-C6	-2.14	117.81	121.55
9	M	402	BCL	C1-O2A-CGA	2.14	122.05	116.44
9	M	403	BCL	CHC-C4B-NB	-2.11	122.02	124.26
9	M	402	BCL	CHC-C4B-NB	-2.10	122.03	124.26
11	L	304	U10	C15-C14-C16	2.09	118.79	115.27
10	M	404	BPH	CMD-C2D-C3D	2.07	128.56	124.68
11	L	304	U10	C25-C24-C23	-2.07	118.38	123.68
11	M	406	U10	C31-C29-C28	-2.04	116.99	121.12
9	L	302	BCL	C1-O2A-CGA	2.03	121.76	116.44
11	M	406	U10	C4M-O4-C4	2.00	123.57	116.47

There are no chirality outliers.

All (143) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	301	LDA	C2-C1-N1-O1
4	H	301	LDA	C2-C1-N1-CM1
4	M	408	LDA	C2-C1-N1-CM1
4	M	409	LDA	C2-C1-N1-O1
4	M	409	LDA	C2-C1-N1-CM1
4	M	409	LDA	C2-C1-N1-CM2
4	M	420	LDA	N1-C1-C2-C3
11	L	304	U10	C9-C11-C12-C13
11	L	304	U10	C12-C13-C14-C15
11	L	304	U10	C12-C13-C14-C16
11	L	304	U10	C23-C24-C26-C27
11	L	304	U10	C25-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
11	L	304	U10	C29-C31-C32-C33
11	L	304	U10	C34-C36-C37-C38
13	L	312	HTO	O1-C1-C2-O2
13	L	312	HTO	O1-C1-C2-C3
13	L	312	HTO	O3-C3-C4-C5
14	M	401	CDL	CB2-OB2-PB2-OB5
14	M	401	CDL	CB3-OB5-PB2-OB3
16	M	407	SPN	C4-C5-C6-C7
16	M	407	SPN	CM3-C5-C6-C7
16	M	407	SPN	C11-C10-C9-C8
16	M	407	SPN	C11-C10-C9-CM4
16	M	407	SPN	C12-C13-C14-C15
16	M	407	SPN	CM5-C13-C14-C15
11	M	406	U10	C37-C38-C39-C40
11	L	304	U10	C27-C28-C29-C30
11	L	304	U10	C27-C28-C29-C31
16	M	407	SPN	C16-C17-C18-CM6
16	M	407	SPN	C16-C17-C18-C19
11	M	406	U10	C24-C26-C27-C28
11	M	406	U10	C37-C38-C39-C41
14	M	401	CDL	CB2-C1-CA2-OA2
14	M	401	CDL	CA2-C1-CB2-OB2
14	M	401	CDL	O1-C1-CA2-OA2
14	M	401	CDL	O1-C1-CB2-OB2
16	M	407	SPN	C14-C15-C16-C17
7	L	311	EDO	O1-C1-C2-O2
11	M	406	U10	C29-C31-C32-C33
16	M	407	SPN	C26-C27-C28-C29
14	M	401	CDL	CA3-OA5-PA1-OA2
10	M	404	BPH	C10-C11-C12-C13
4	H	301	LDA	C7-C8-C9-C10
4	H	301	LDA	C3-C4-C5-C6
14	M	401	CDL	C71-C72-C73-C74
14	M	401	CDL	C16-C17-C18-C19
14	M	401	CDL	C78-C79-C80-C81
14	M	401	CDL	C11-C12-C13-C14
14	M	401	CDL	C36-C37-C38-C39
10	M	404	BPH	C8-C10-C11-C12
14	M	401	CDL	C39-C40-C41-C42
4	M	409	LDA	C4-C5-C6-C7
4	M	410	LDA	C7-C8-C9-C10
4	M	411	LDA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
14	M	401	CDL	C20-C21-C22-C23
4	M	420	LDA	C4-C5-C6-C7
4	M	412	LDA	C3-C4-C5-C6
4	H	301	LDA	C1-C2-C3-C4
14	M	401	CDL	CA5-C11-C12-C13
4	M	420	LDA	C7-C8-C9-C10
4	M	420	LDA	C11-C10-C9-C8
4	M	412	LDA	C1-C2-C3-C4
14	M	401	CDL	C55-C56-C57-C58
4	M	411	LDA	C1-C2-C3-C4
16	M	407	SPN	CM1-C1-O1-CMA
16	M	407	SPN	CM2-C1-O1-CMA
14	M	401	CDL	C35-C36-C37-C38
11	L	304	U10	C30-C29-C31-C32
13	L	312	HTO	C2-C3-C4-C5
4	M	420	LDA	C1-C2-C3-C4
4	M	420	LDA	C9-C10-C11-C12
11	L	304	U10	C28-C29-C31-C32
4	M	408	LDA	C3-C4-C5-C6
14	M	401	CDL	C17-C18-C19-C20
4	M	411	LDA	C11-C10-C9-C8
14	M	401	CDL	C80-C81-C82-C83
10	L	303	BPH	O2A-C1-C2-C3
4	M	420	LDA	C6-C7-C8-C9
14	M	401	CDL	C31-C32-C33-C34
4	M	408	LDA	C7-C8-C9-C10
14	M	401	CDL	C19-C20-C21-C22
9	L	302	BCL	C15-C16-C17-C18
10	M	404	BPH	C4-C3-C5-C6
9	M	402	BCL	C8-C10-C11-C12
4	M	410	LDA	C4-C5-C6-C7
14	M	401	CDL	C34-C35-C36-C37
10	L	303	BPH	CAD-CBD-CGD-O2D
10	M	404	BPH	CAD-CBD-CGD-O2D
14	M	401	CDL	CA3-CA4-CA6-OA8
4	H	301	LDA	C2-C1-N1-CM2
4	M	411	LDA	C2-C1-N1-CM1
4	M	420	LDA	C2-C1-N1-CM1
4	M	420	LDA	C2-C1-N1-CM2
4	M	410	LDA	C11-C10-C9-C8
4	H	301	LDA	C9-C10-C11-C12
10	M	404	BPH	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	M	401	CDL	CA3-OA5-PA1-OA3
14	M	401	CDL	CB2-OB2-PB2-OB4
4	M	409	LDA	C3-C4-C5-C6
4	M	420	LDA	C2-C1-N1-O1
14	M	401	CDL	CB7-C71-C72-C73
14	M	401	CDL	C79-C80-C81-C82
14	M	401	CDL	C11-CA5-OA6-CA4
4	H	301	LDA	C6-C7-C8-C9
9	M	402	BCL	C2-C1-O2A-CGA
10	M	404	BPH	C16-C17-C18-C20
4	M	408	LDA	C1-C2-C3-C4
4	M	412	LDA	C5-C6-C7-C8
14	M	401	CDL	OA7-CA5-OA6-CA4
9	L	301	BCL	C16-C17-C18-C19
10	M	404	BPH	C16-C17-C18-C19
14	M	401	CDL	C73-C74-C75-C76
11	L	304	U10	C5-C4-O4-C4M
9	M	402	BCL	C11-C10-C8-C9
10	M	404	BPH	C11-C10-C8-C9
11	L	304	U10	C24-C26-C27-C28
9	M	402	BCL	C11-C12-C13-C15
10	M	404	BPH	C5-C6-C7-C8
11	M	406	U10	C5-C4-O4-C4M
16	M	407	SPN	C2-C3-C4-C5
11	M	406	U10	C25-C24-C26-C27
9	M	402	BCL	C4C-C3C-CAC-CBC
14	M	401	CDL	C51-C52-C53-C54
9	M	403	BCL	CAA-CBA-CGA-O2A
9	M	402	BCL	C4-C3-C5-C6
11	L	304	U10	C15-C14-C16-C17
9	L	301	BCL	CAD-CBD-CGD-O2D
9	M	402	BCL	CAD-CBD-CGD-O2D
11	L	304	U10	C22-C23-C24-C25
4	M	411	LDA	C9-C10-C11-C12
14	M	401	CDL	C52-C51-CB5-OB6
9	M	403	BCL	CHA-CBD-CGD-O2D
11	M	406	U10	C23-C24-C26-C27
10	L	303	BPH	CHA-CBD-CGD-O1D
14	M	401	CDL	C21-C22-C23-C24
11	L	304	U10	C20-C19-C21-C22
11	M	406	U10	C28-C29-C31-C32
14	M	401	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
4	M	410	LDA	C9-C10-C11-C12
4	M	412	LDA	C7-C8-C9-C10
4	M	411	LDA	C6-C7-C8-C9
11	M	406	U10	C30-C29-C31-C32
11	M	406	U10	C3-C4-O4-C4M

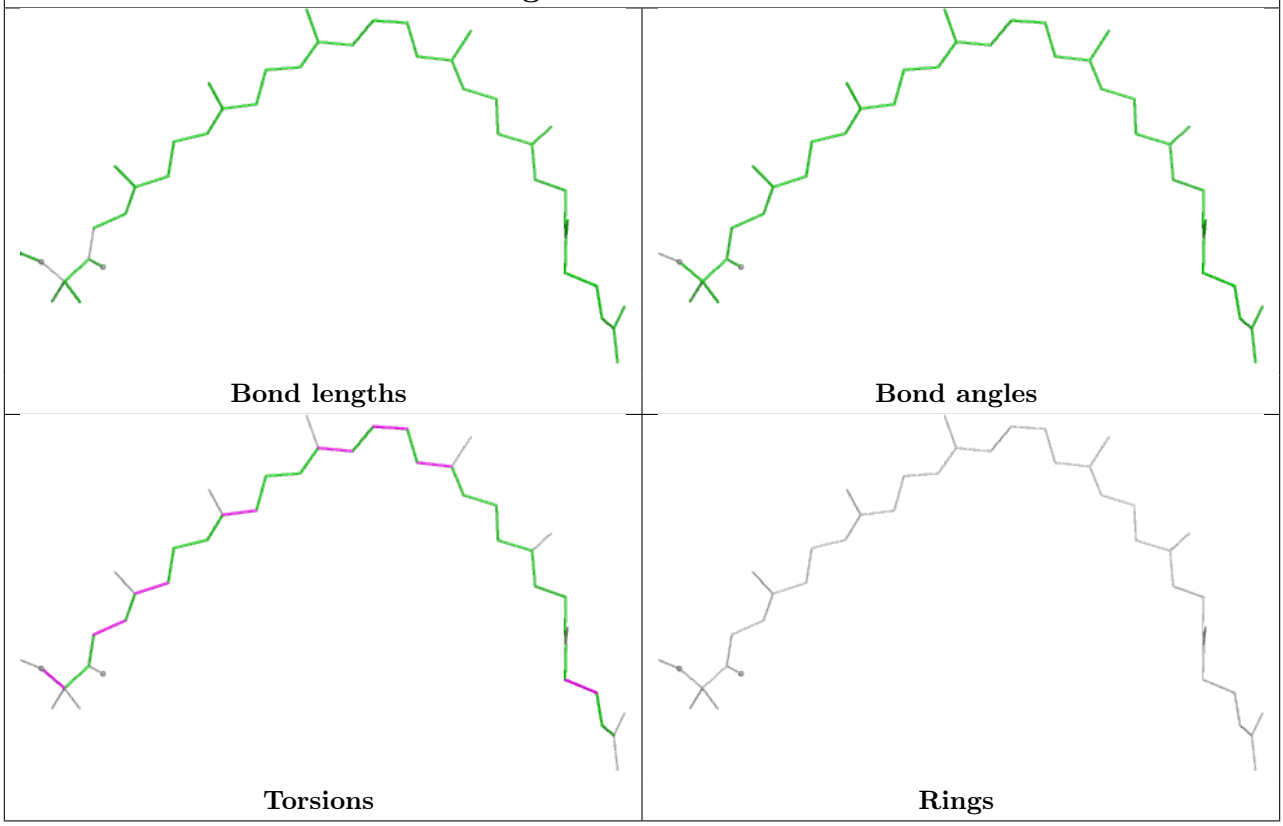
There are no ring outliers.

13 monomers are involved in 30 short contacts:

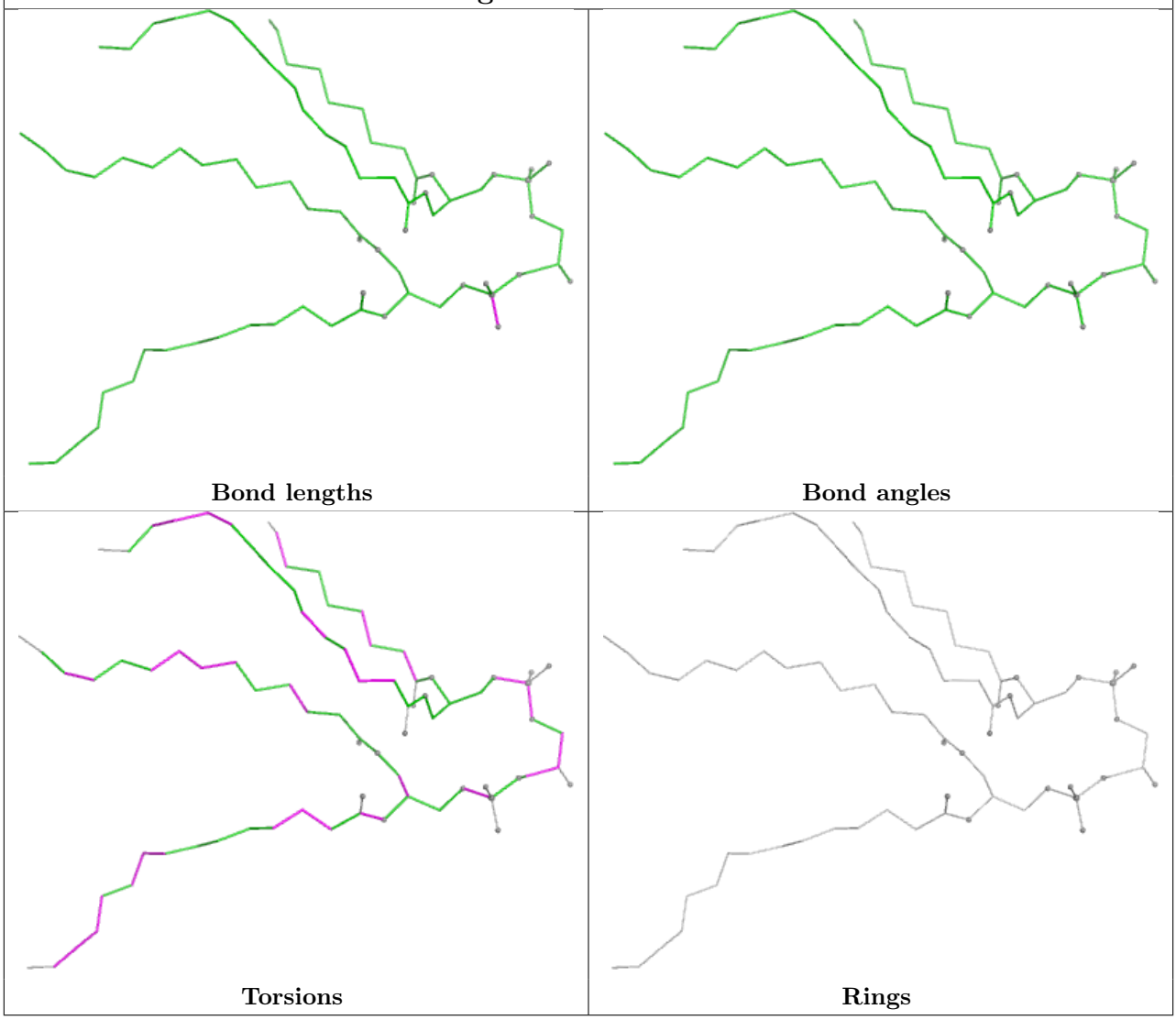
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	420	LDA	1	0
16	M	407	SPN	7	0
14	M	401	CDL	6	0
9	M	402	BCL	2	0
10	M	404	BPH	2	0
4	M	408	LDA	2	0
4	H	301	LDA	2	0
11	L	304	U10	3	0
9	M	403	BCL	1	0
4	M	412	LDA	2	0
7	H	307	EDO	2	0
11	M	406	U10	2	0
4	M	410	LDA	1	0

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

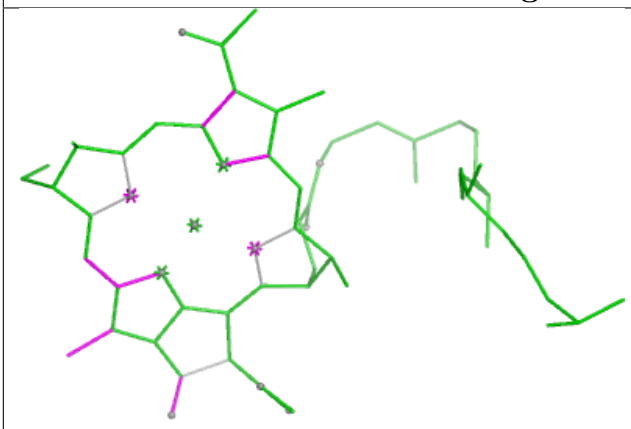
Ligand SPN M 407



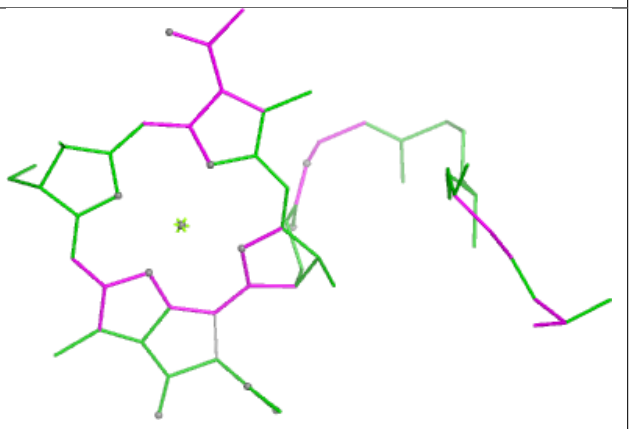
Ligand CDL M 401



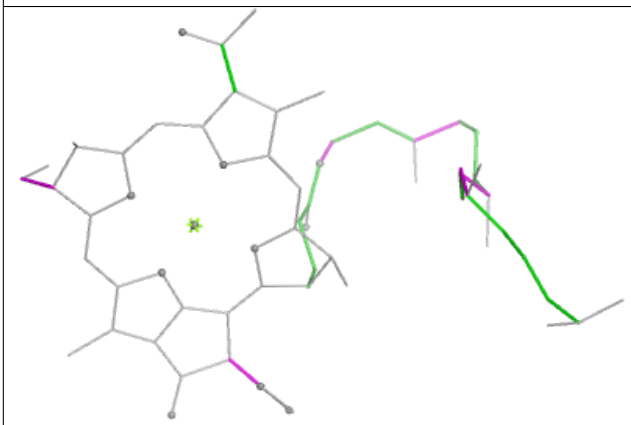
Ligand BCL M 402



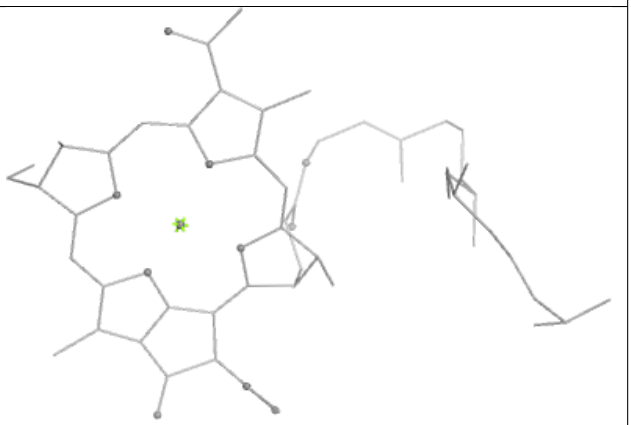
Bond lengths



Bond angles

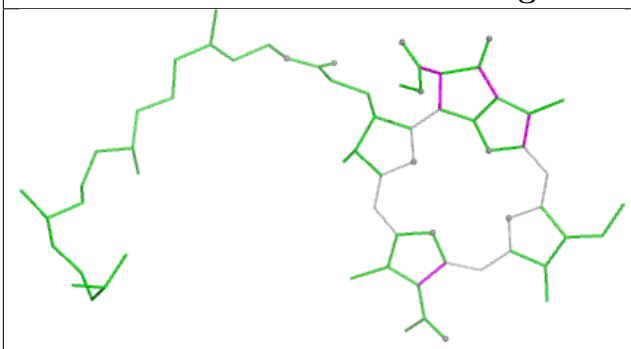


Torsions

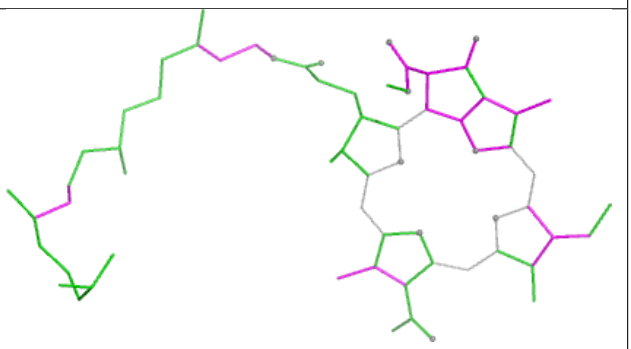


Rings

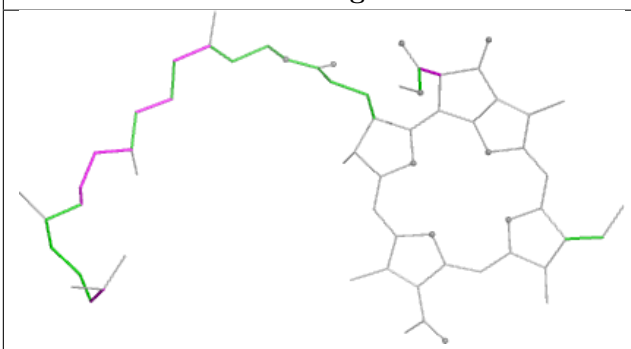
Ligand BPH M 404



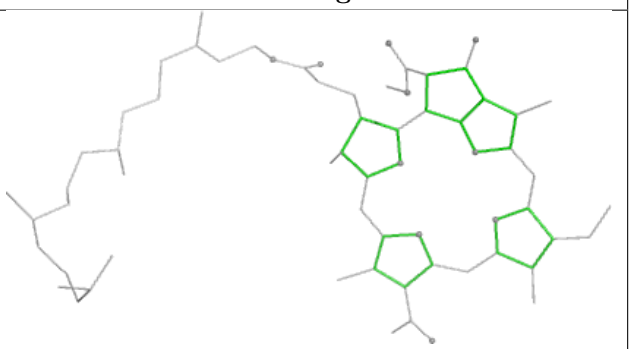
Bond lengths



Bond angles

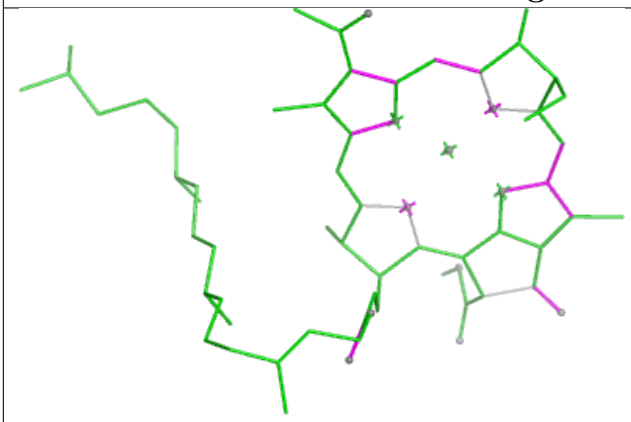


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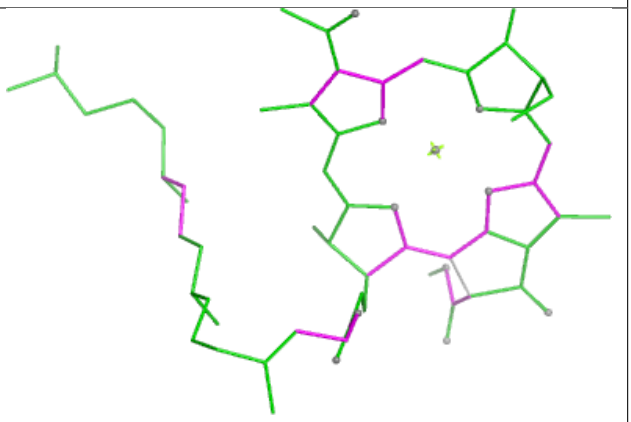


Rings

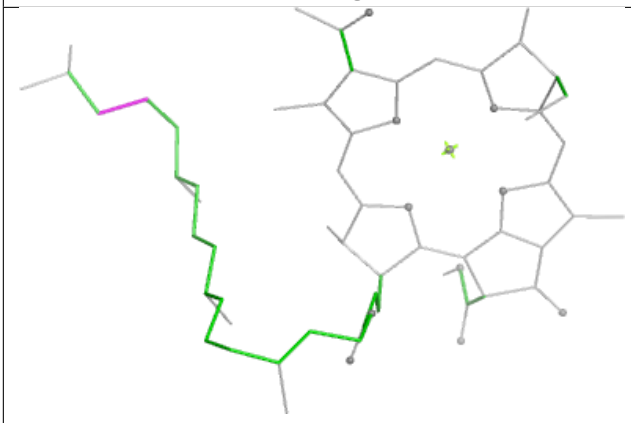
Ligand BCL L 302



Bond lengths



Bond angles

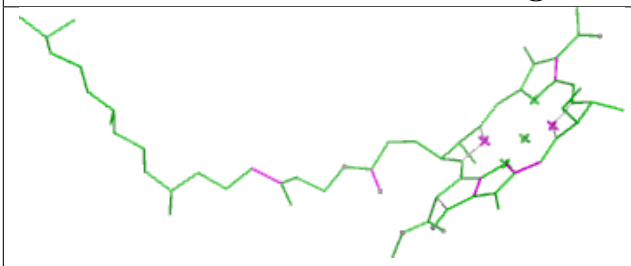


Torsions

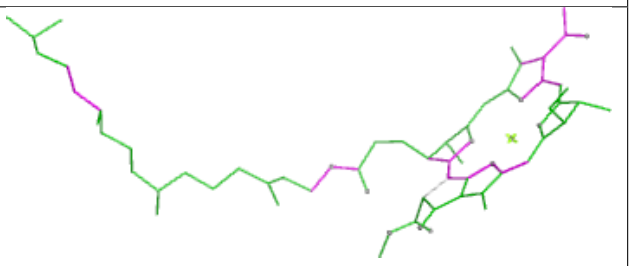


Rings

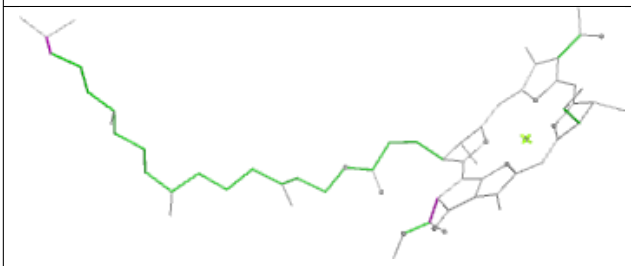
Ligand BCL L 301



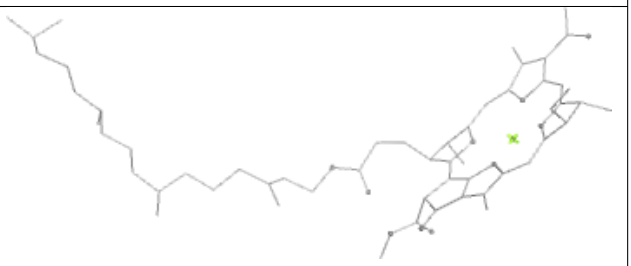
Bond lengths



Bond angles

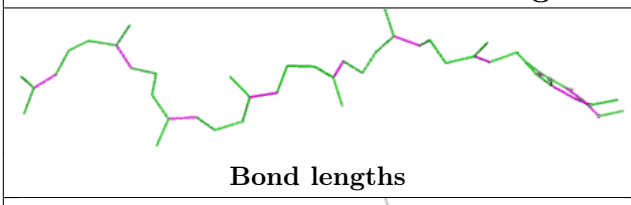


Torsions

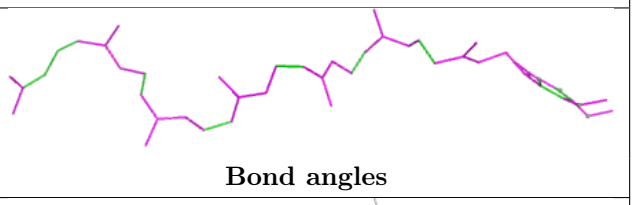


Rings

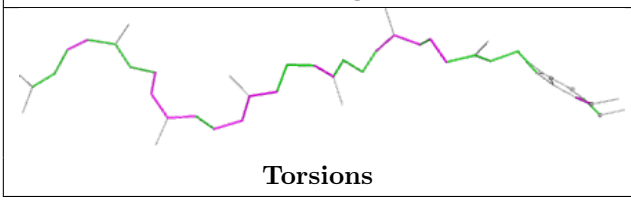
Ligand U10 L 304



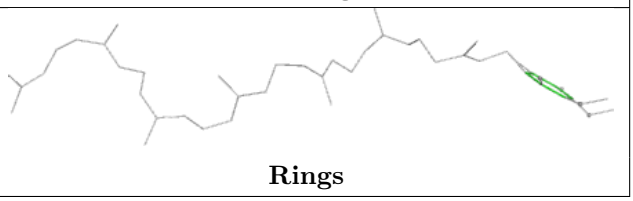
Bond lengths



Bond angles

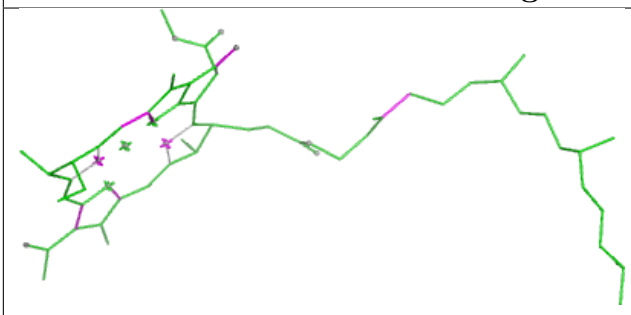


Torsions

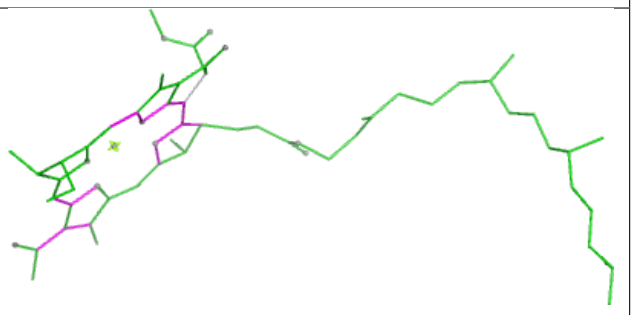


Rings

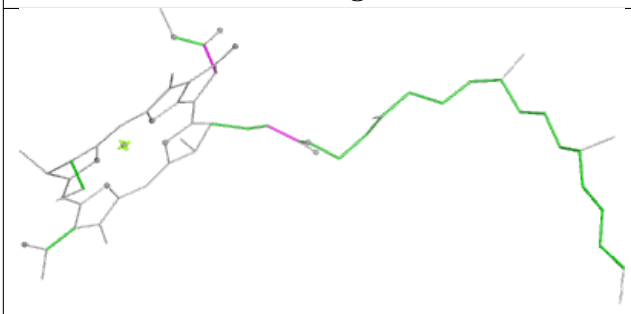
Ligand BCL M 403



Bond lengths



Bond angles

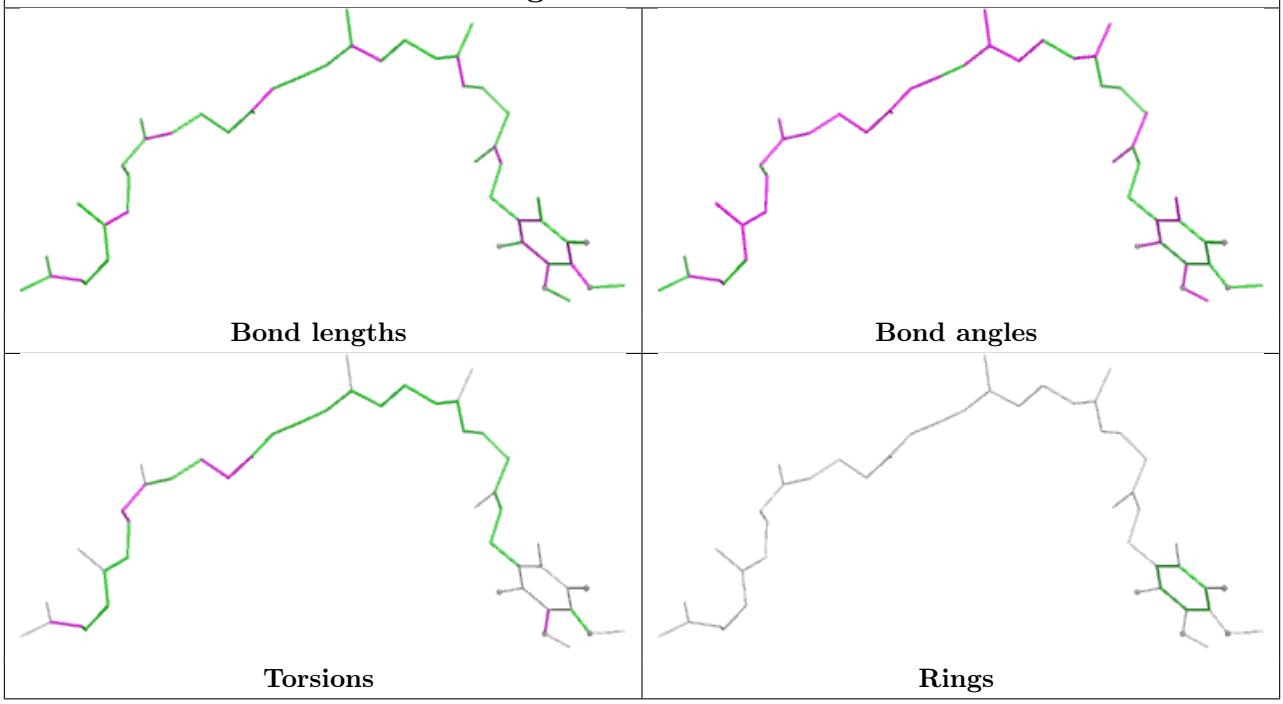


Torsions

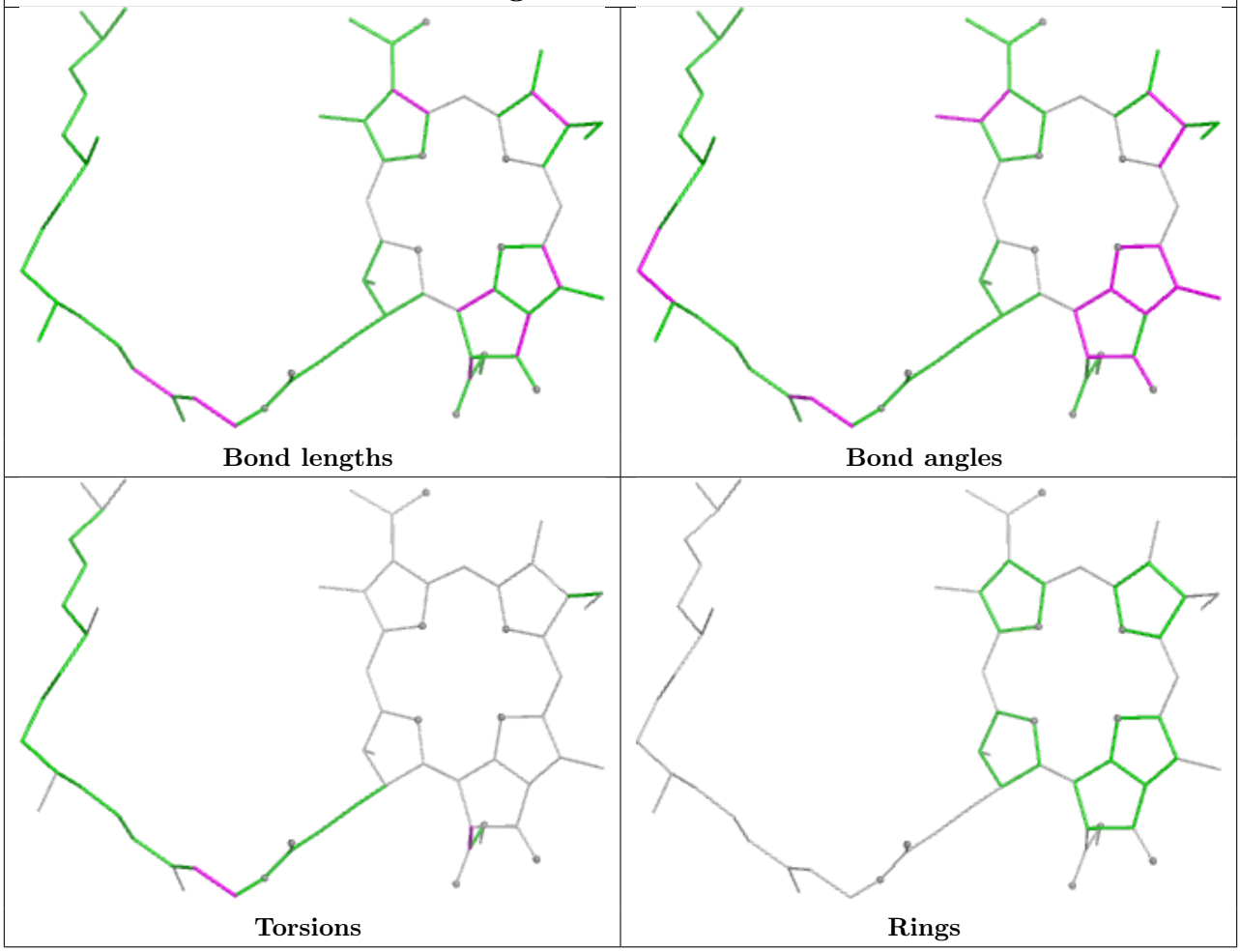


Rings

Ligand U10 M 406



Ligand BPH L 303



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	240/242 (99%)	-0.49	1 (0%)	88	86	26, 47, 61, 87	3 (1%)
2	L	281/281 (100%)	-0.23	5 (1%)	67	63	26, 48, 75, 105	2 (0%)
3	M	302/303 (99%)	-0.31	7 (2%)	61	55	25, 49, 70, 95	2 (0%)
All	All	823/826 (99%)	-0.33	13 (1%)	70	66	25, 48, 70, 105	7 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	188	ASN	3.1
2	L	56	GLN	3.0
3	M	302	GLY	3.0
3	M	1	ALA	3.0
1	H	250	SER	2.9
3	M	148	TRP	2.8
3	M	300	ASN	2.7
3	M	52	LEU	2.6
2	L	57	GLY	2.5
2	L	62	GLN	2.5
2	L	55	LEU	2.1
2	L	72	GLU	2.0
3	M	2	GLU	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides 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	412	16/16	0.44	0.51	81,108,126,131	0
5	UNL	H	303	12/-	0.57	0.40	85,89,96,99	0
5	UNL	L	306	15/-	0.60	0.40	47,64,81,85	0
11	U10	L	304	48/63	0.61	0.37	43,71,109,123	0
5	UNL	H	305	15/-	0.63	0.29	69,73,94,96	0
5	UNL	H	304	12/-	0.68	0.29	76,81,104,105	0
5	UNL	H	302	12/-	0.68	0.29	73,79,86,86	0
4	LDA	M	420	16/16	0.72	0.28	68,77,117,120	0
5	UNL	M	415	12/-	0.74	0.40	58,84,94,94	0
5	UNL	M	413	15/-	0.76	0.35	53,72,87,91	0
4	LDA	M	410	16/16	0.79	0.23	59,69,94,107	0
5	UNL	M	414	12/-	0.81	0.29	62,71,81,83	0
13	HTO	L	312	10/10	0.82	0.21	63,75,86,89	0
12	DIO	L	308	6/6	0.83	0.24	92,94,95,101	0
4	LDA	M	409	16/16	0.84	0.19	60,68,84,86	0
4	LDA	M	411	16/16	0.85	0.24	73,79,95,98	0
7	EDO	H	307	4/4	0.85	0.21	61,67,73,74	0
7	EDO	H	309	4/4	0.85	0.23	61,64,75,83	0
6	PO4	H	306	5/5	0.87	0.17	80,88,92,94	0
6	PO4	M	417	5/5	0.88	0.12	47,47,61,68	5
7	EDO	L	311	4/4	0.89	0.19	53,58,62,64	0
14	CDL	M	401	81/100	0.89	0.21	42,64,80,87	81
4	LDA	M	408	16/16	0.90	0.15	39,60,73,78	0
10	BPH	M	404	65/65	0.90	0.13	38,49,107,122	0
5	UNL	L	305	12/-	0.90	0.17	61,66,73,74	0
5	UNL	L	307	10/-	0.91	0.22	53,74,80,82	0
11	U10	M	406	48/63	0.92	0.12	33,47,68,78	0
6	PO4	L	313	5/5	0.92	0.16	71,84,104,110	0
4	LDA	H	301	16/16	0.92	0.15	66,74,80,82	0
7	EDO	L	309	4/4	0.92	0.17	61,65,70,73	0
7	EDO	H	308	4/4	0.93	0.17	47,48,50,65	0
6	PO4	M	416	5/5	0.93	0.08	77,78,84,89	0
7	EDO	M	418	4/4	0.93	0.15	47,48,51,54	0
16	SPN	M	407	43/43	0.94	0.12	41,56,70,86	0
9	BCL	M	402	66/66	0.95	0.10	35,48,85,95	0
7	EDO	L	310	4/4	0.96	0.15	47,48,52,56	0
10	BPH	L	303	65/65	0.97	0.07	33,41,53,57	0

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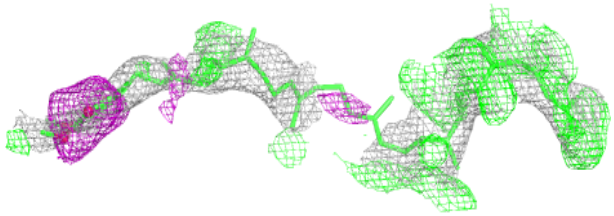
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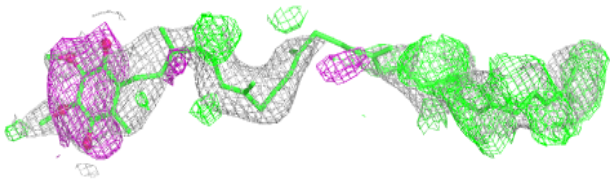
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	BCL	L	302	66/66	0.97	0.07	35,43,56,69	0
7	EDO	M	419	4/4	0.97	0.08	43,46,49,50	0
9	BCL	M	403	66/66	0.97	0.08	36,46,66,80	0
9	BCL	L	301	66/66	0.98	0.07	36,45,52,55	0
8	K	H	310	1/1	0.99	0.06	50,50,50,50	0
15	FE	M	405	1/1	1.00	0.02	39,39,39,39	0

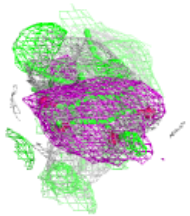
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U10 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)

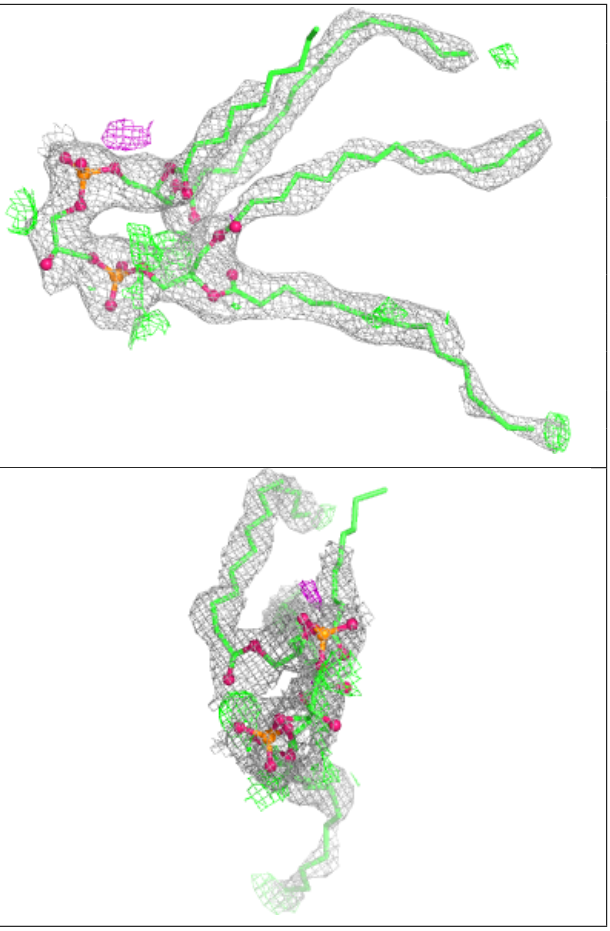






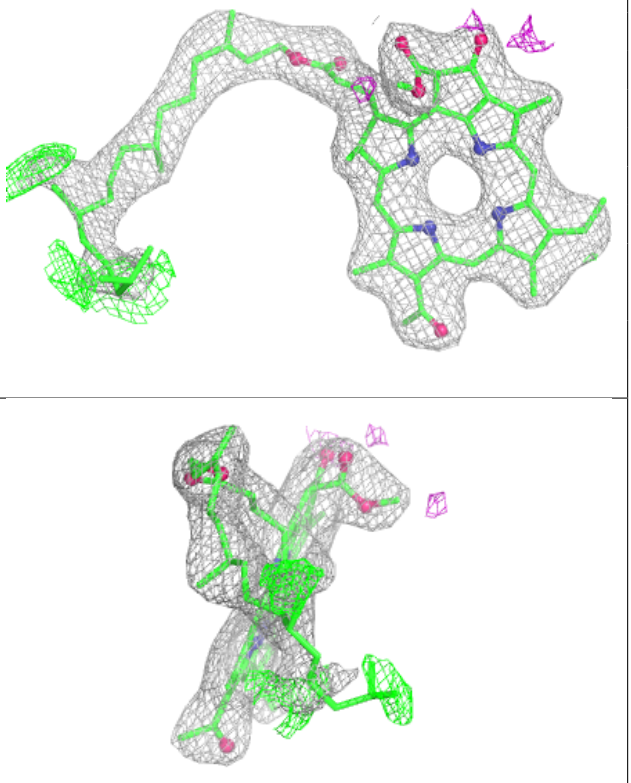
Electron density around CDL M 401:

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



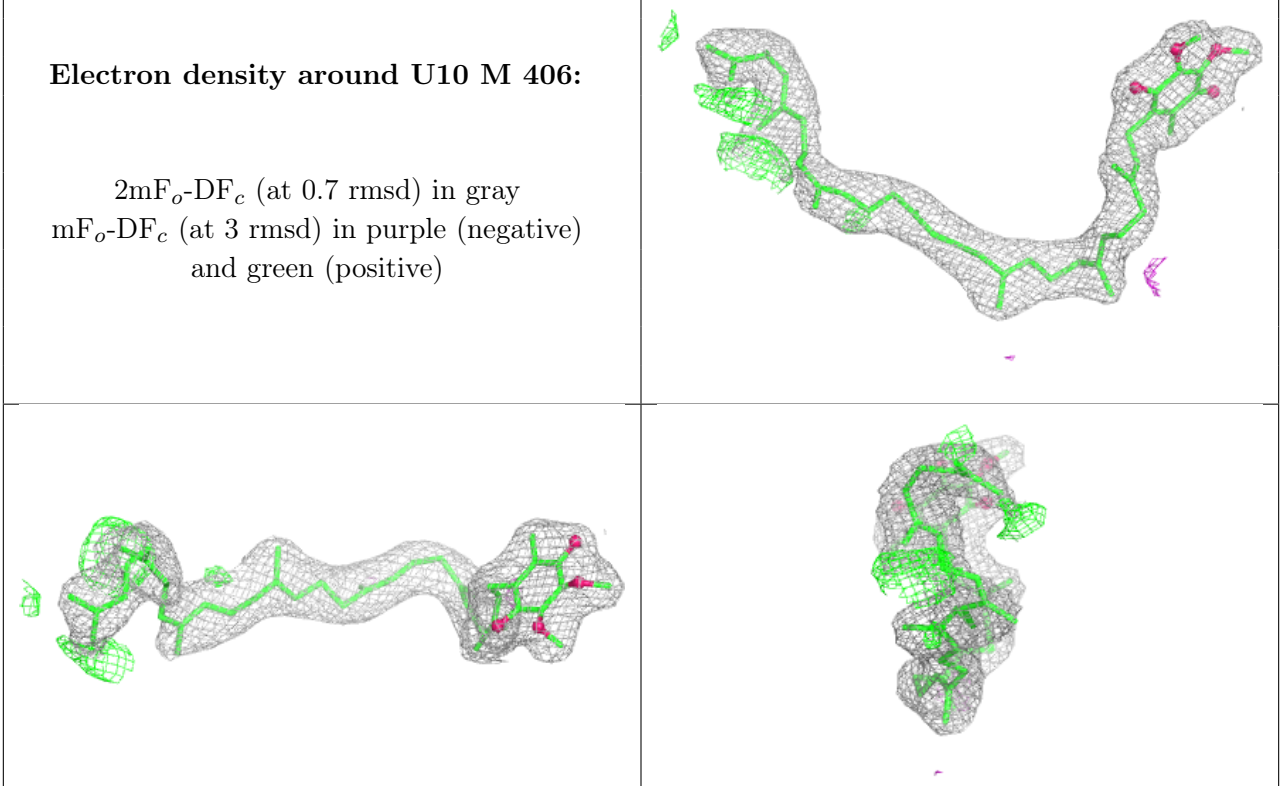
Electron density around BPH M 404:

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



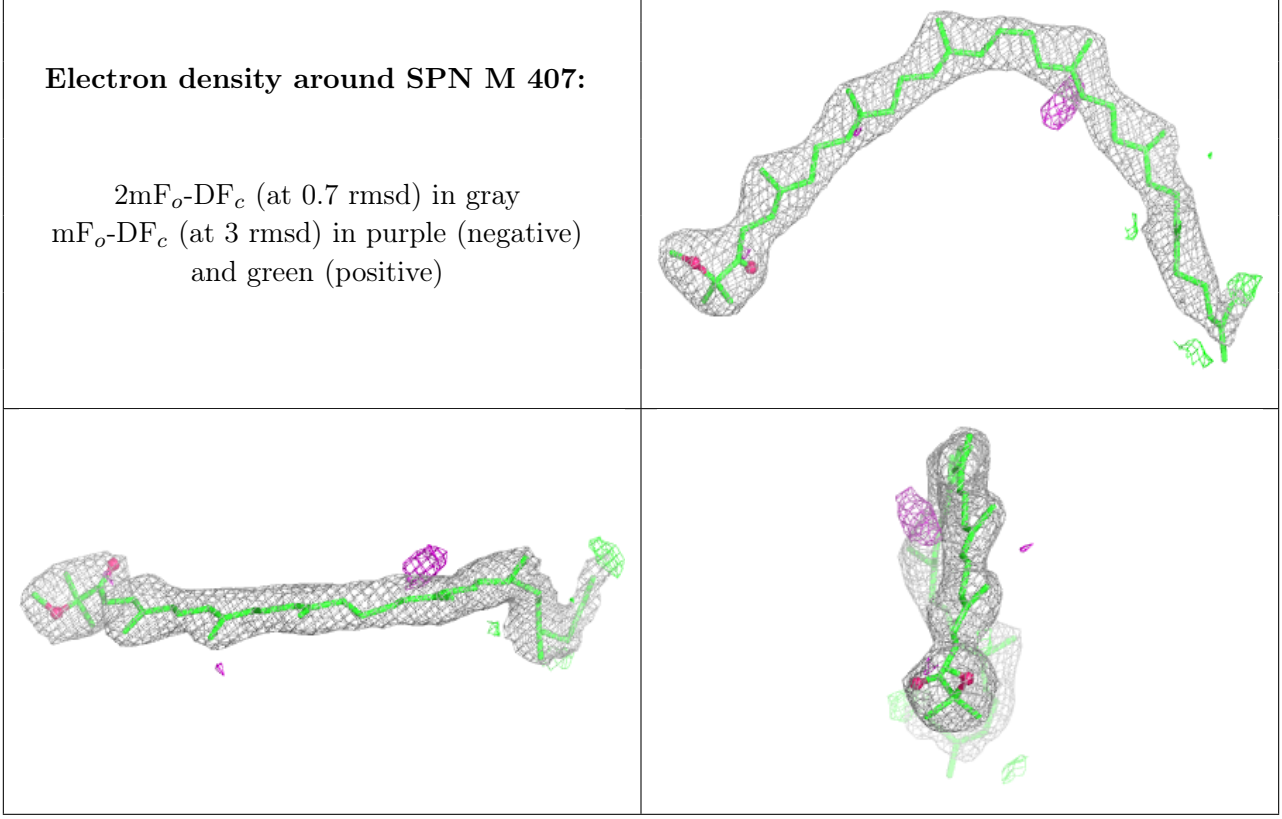
Electron density around U10 M 406:

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



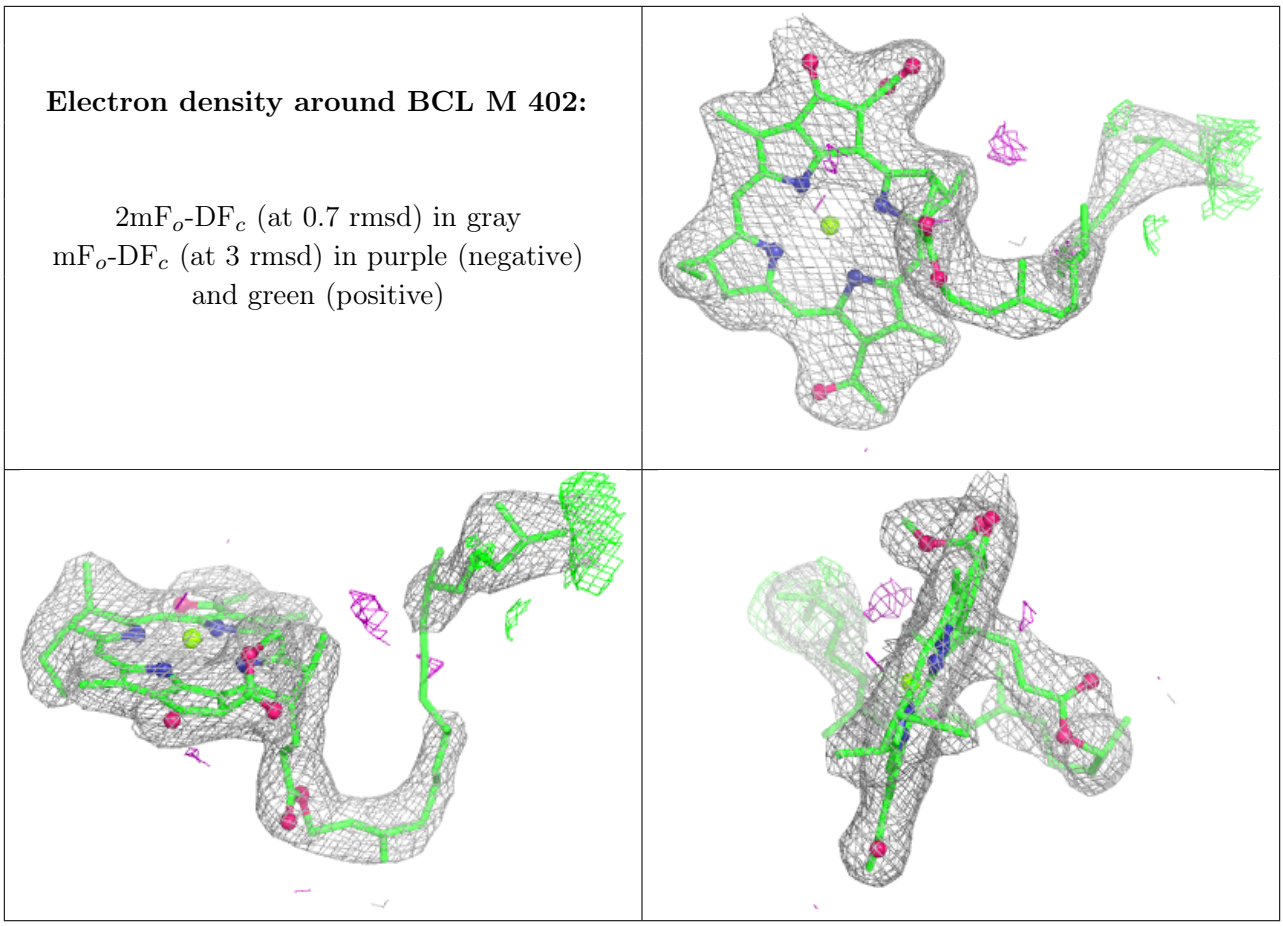
Electron density around SPN M 407:

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



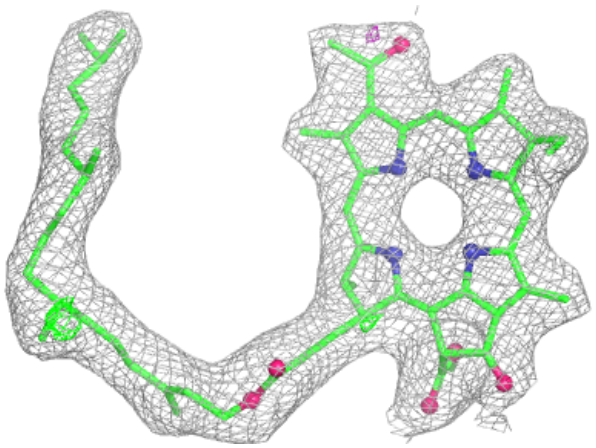
Electron density around BCL M 402:

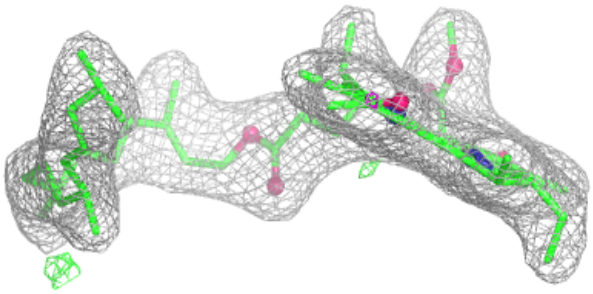
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

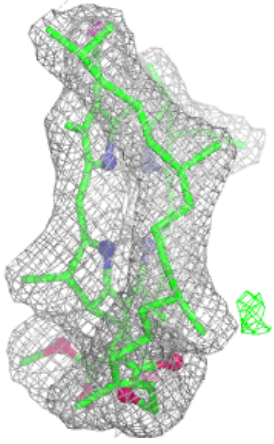


Electron density around BPH L 303:

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

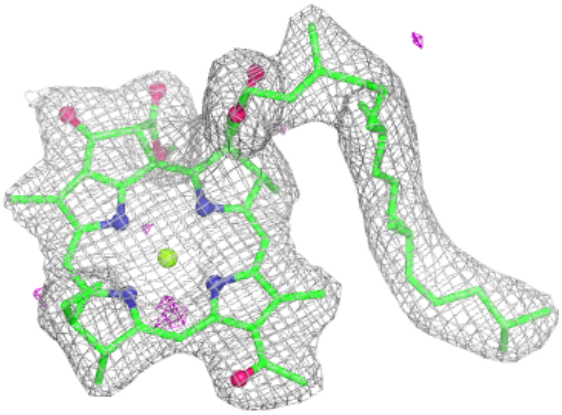


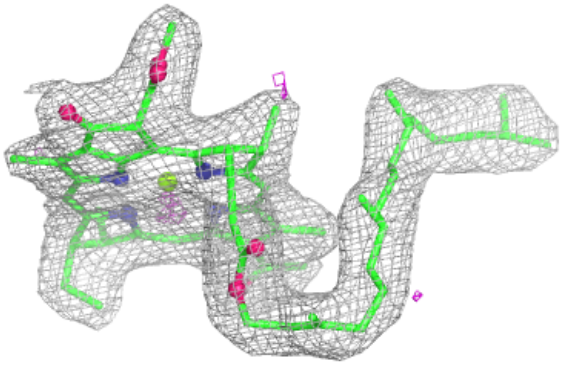


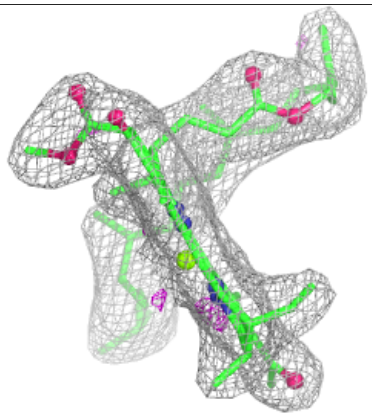


Electron density around BCL L 302:

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

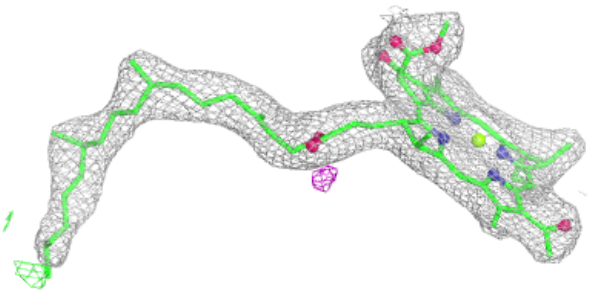


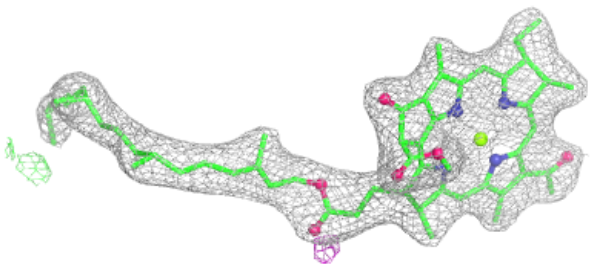


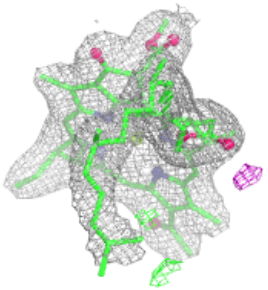


Electron density around BCL M 403:

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

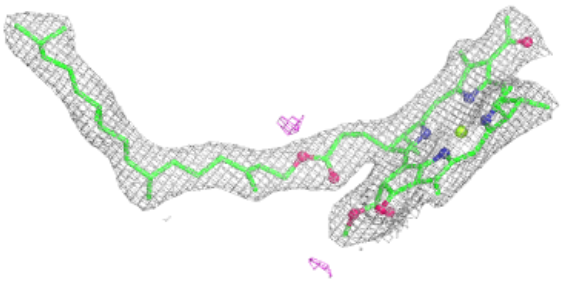


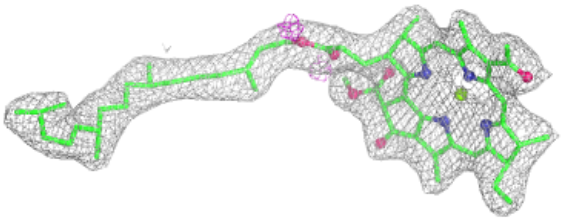


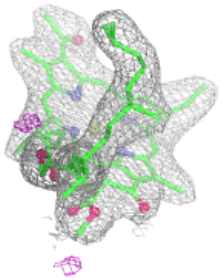


Electron density around BCL L 301:

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

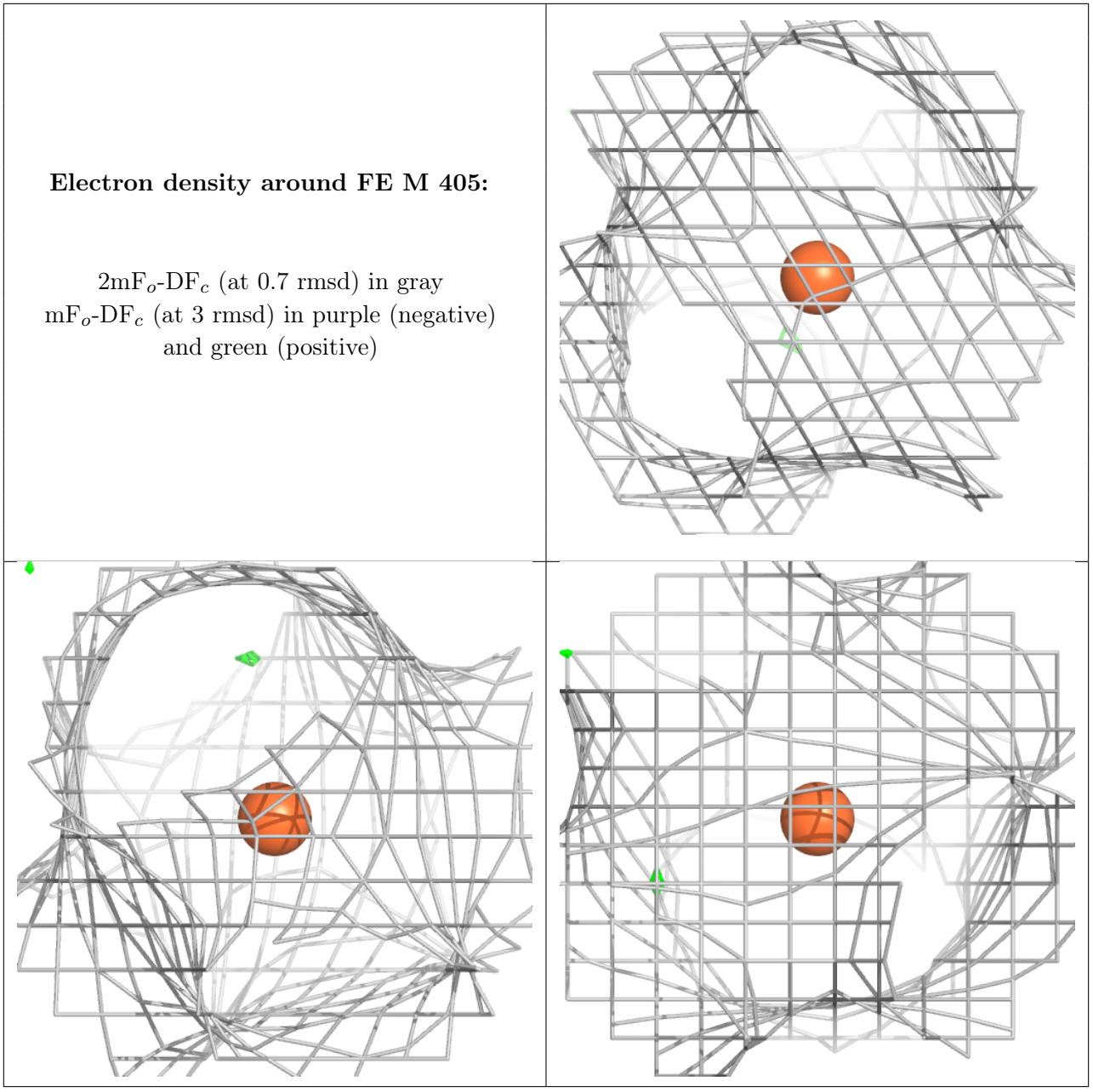






Electron density around FE M 405:

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



6.5 Other polymers

There are no such residues in this entry.