wwPDB X-ray Structure Validation Summary Report (i)

Nov 23, 2020 – 09:30 am GMT

PDB ID	:	6Z02
Title	:	Photosynthetic Reaction Center From Rhodobacter Sphaeroides strain RV in surfo crystallization
Authors	:	Gabdulkhakov, A.G.; Selikhanov, G.K.; Fufina, T.Y.; Vasilieva, L.G.; Betzel, C.
Deposited on	:	2020-05-07
Resolution	:	2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

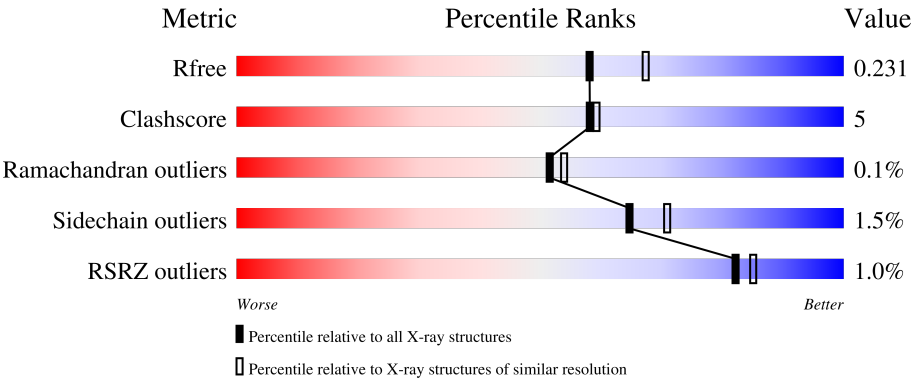
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	H	241	90% 9%
2	L	281	89% 10%
3	M	302	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	409	-	-	-	X
5	D12	H	704	-	-	-	X

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 7930 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
			2244	1516	356	364	8			

There is a discrepancy between the modelled and reference sequences:

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

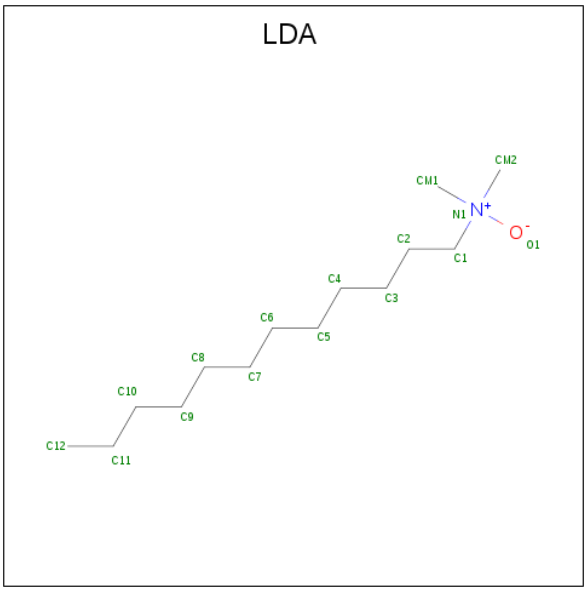
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	4	0
			2436	1630	397	399	10			

There is a discrepancy between the modelled and reference sequences:

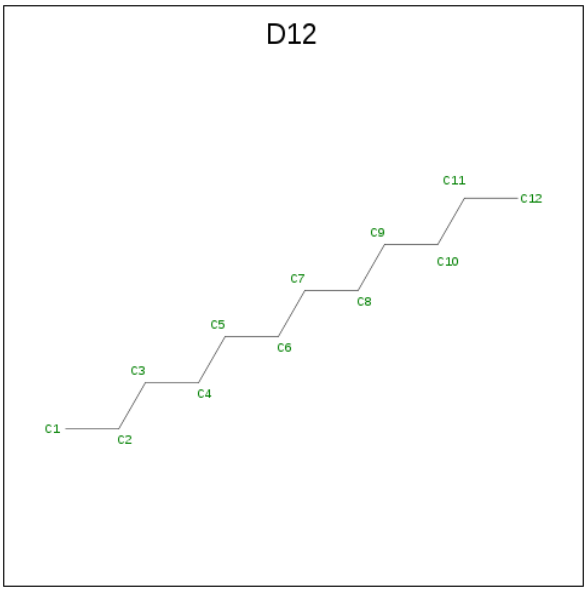
Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	conflict	UNP P0C0Y9

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



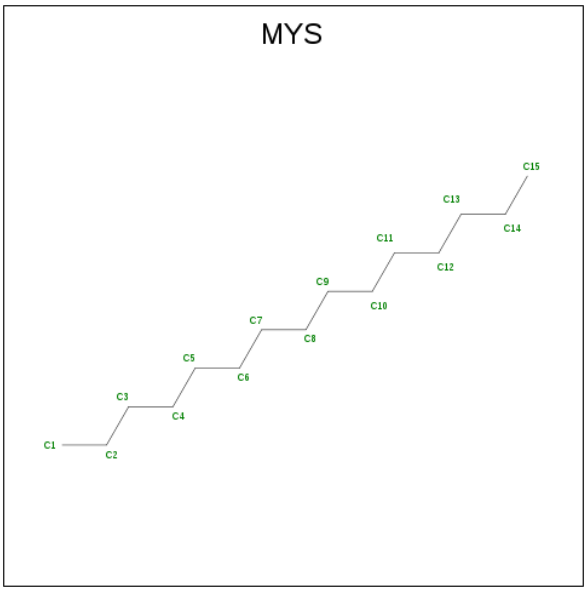
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	L	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



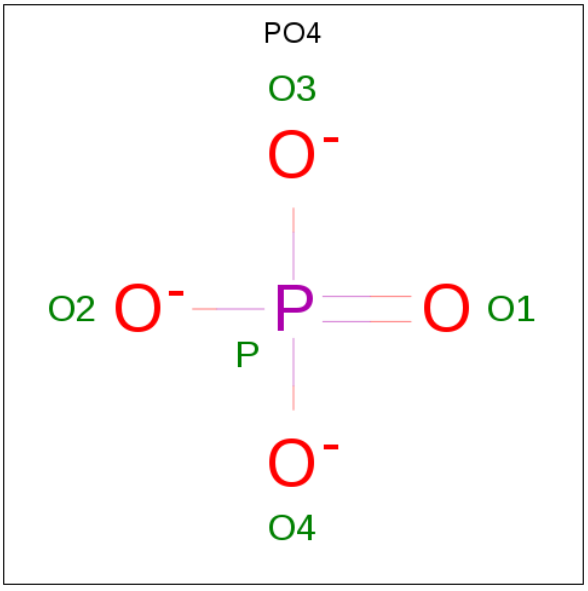
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C 12 12	0	0
5	H	1	Total C 12 12	0	0
5	H	1	Total C 12 12	0	0
5	L	1	Total C 12 12	0	0
5	M	1	Total C 12 12	0	0
5	M	1	Total C 12 12	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	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 PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total O P 5 4 1	0	0

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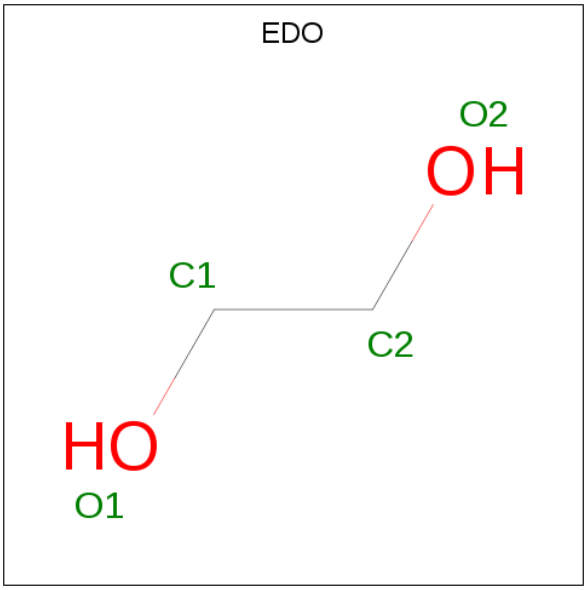
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	M	1	Total O P 5 4 1	0	0
7	M	1	Total O P 5 4 1	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

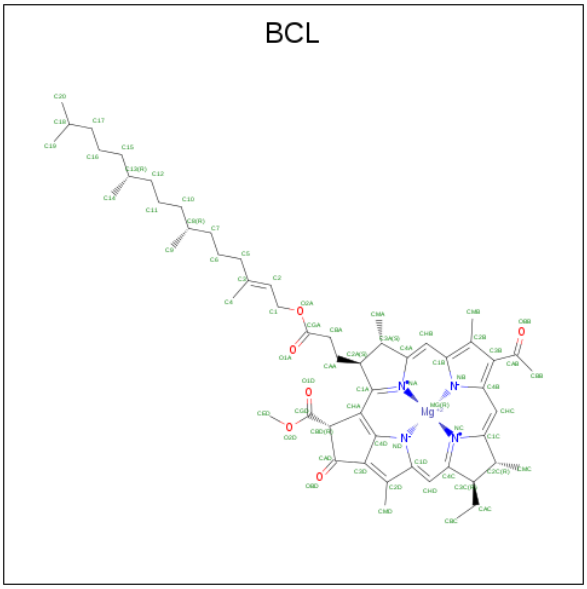
- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	H	1	Total Na 1 1	0	0

- Molecule 10 is POTASSIUM ION (three-letter code: K) (formula: K).

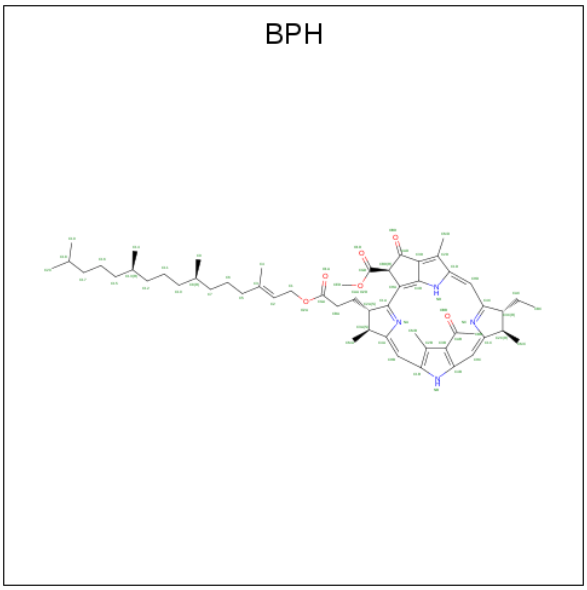
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	H	1	Total K 1 1	0	0

- Molecule 11 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by author).



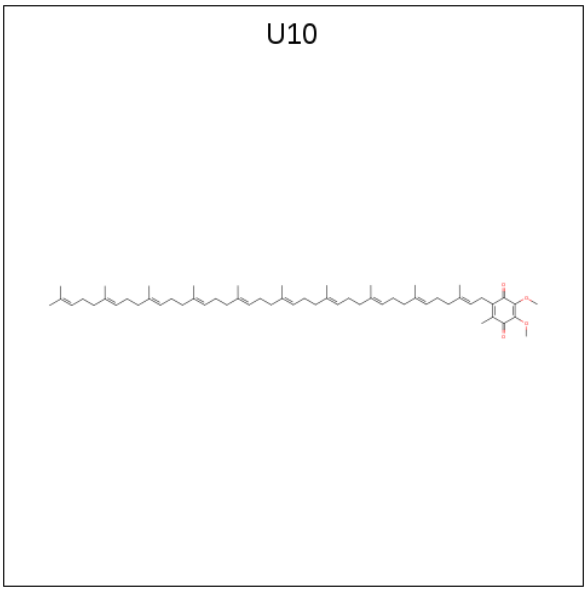
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 12 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by author).



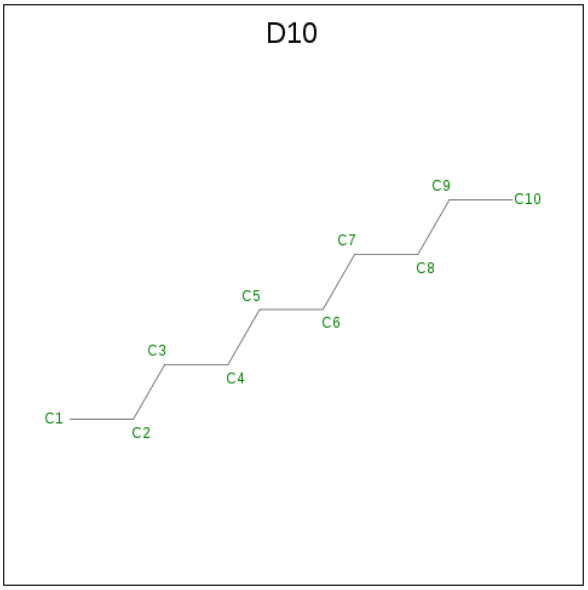
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	N	O	0	0
			65	55	4	6		
12	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 13 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by author).



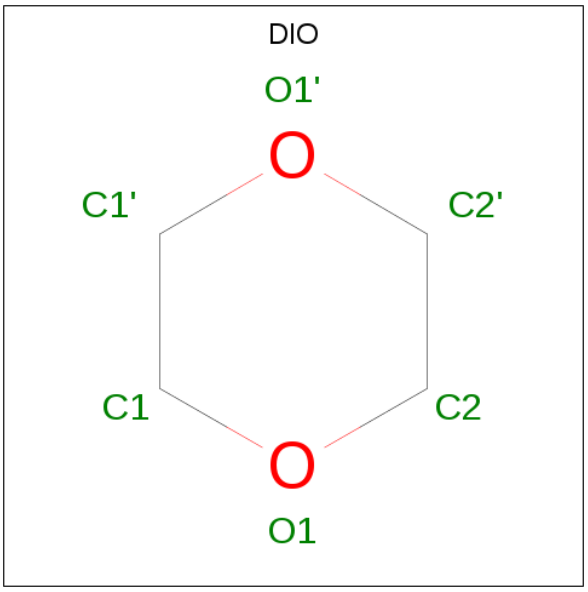
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	L	1	Total C O 48 44 4	0	0
13	M	1	Total C O 48 44 4	0	0

- Molecule 14 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



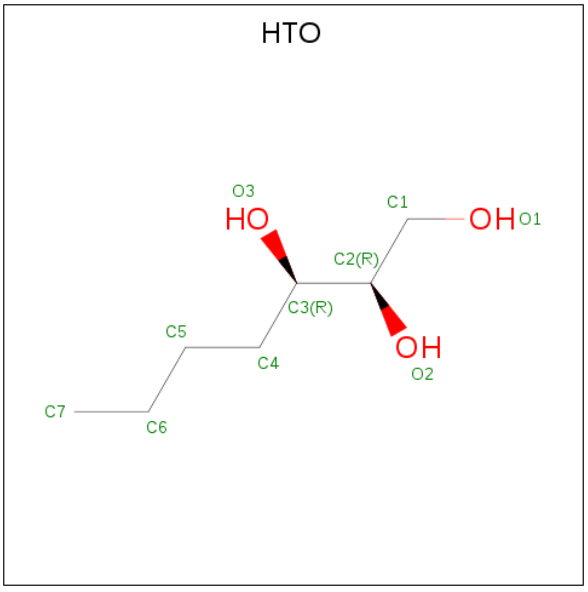
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	L	1	Total C 10 10	0	0

- Molecule 15 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



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

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

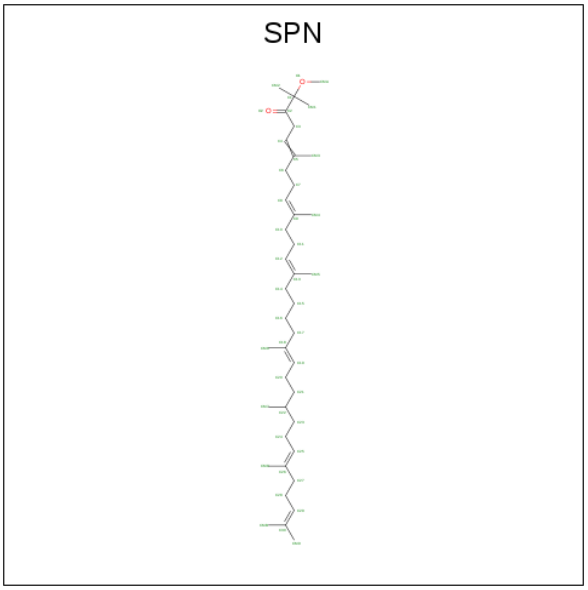


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	L	1	Total	C	O	0	0
			10	7	3		
16	L	1	Total	C	O	0	0
			10	7	3		
16	L	1	Total	C	O	0	0
			9	6	3		

- Molecule 17 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by author).

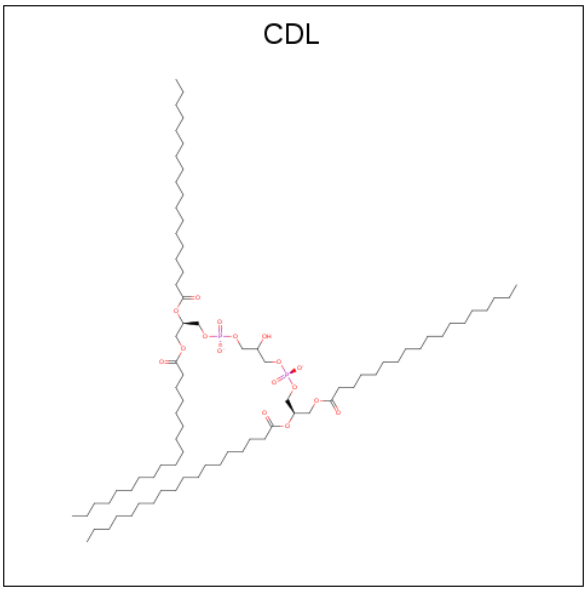
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	M	1	Total Fe 1 1	0	0

- Molecule 18 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$) (labeled as "Ligand of Interest" by author).



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

- Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by author).



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

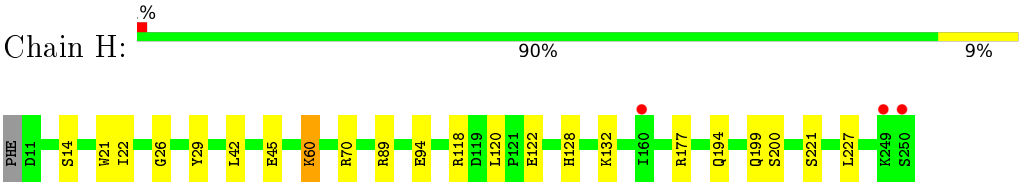
- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	H	217	Total	O	0	0
			217	217		
20	L	107	Total	O	0	0
			107	107		
20	M	120	Total	O	0	0
			120	120		

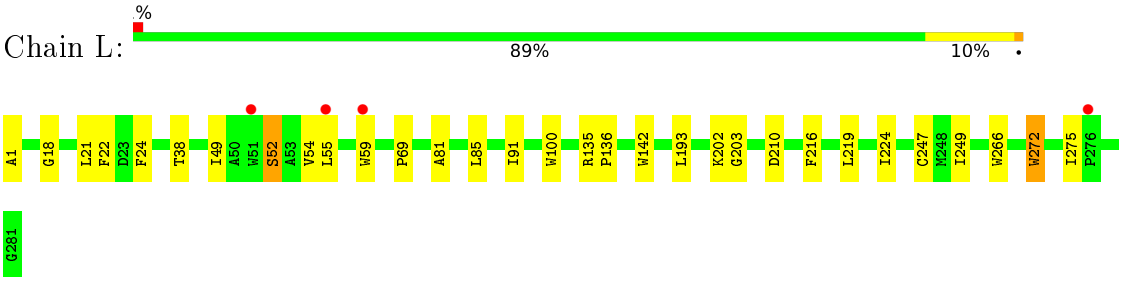
3 Residue-property plots (i)

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.

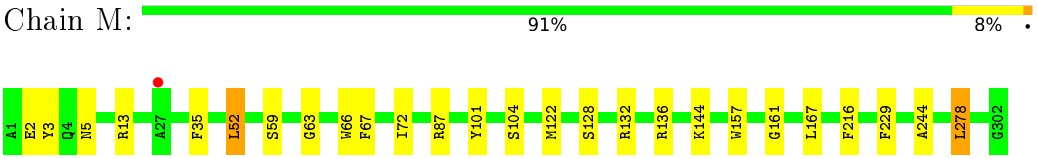
- Molecule 1: Reaction center protein H chain



- 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 185.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.20 – 2.10 43.28 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.20-2.10) 99.6 (43.28-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.201 , 0.226 0.205 , 0.231	Depositor DCC
R_{free} test set	6085 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.1	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7930	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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, DIO, D10, D12, CDL, BPH, MYS, EDO, PO4, HTO, FE, SPN, NA, U10, K

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	0.41	0/1905	0.57	0/2590
2	L	0.38	0/2335	0.50	0/3196
3	M	0.38	0/2541	0.50	0/3468
All	All	0.39	0/6781	0.52	0/9254

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	18	0
2	L	2244	0	2204	21	0
3	M	2436	0	2362	21	0
4	H	32	0	62	4	0
4	L	16	0	31	0	0
4	M	64	0	124	7	0
5	H	36	0	78	5	0
5	L	12	0	26	1	0
5	M	24	0	52	2	0
6	H	15	0	32	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	15	0	32	0	0
6	M	15	0	32	1	0
7	H	5	0	0	0	0
7	M	10	0	0	0	0
8	H	20	0	30	5	0
8	L	20	0	30	0	0
8	M	12	0	18	2	0
9	H	1	0	0	0	0
10	H	1	0	0	0	0
11	L	66	0	74	0	0
11	M	198	0	222	4	0
12	L	65	0	76	0	0
12	M	65	0	76	1	0
13	L	48	0	63	2	0
13	M	48	0	63	0	0
14	L	10	0	22	0	0
15	L	6	0	8	2	0
16	L	29	0	43	3	0
17	M	1	0	0	0	0
18	M	43	0	70	5	0
19	M	81	0	106	6	0
20	H	217	0	0	1	0
20	L	107	0	0	0	0
20	M	120	0	0	1	0
All	All	7930	0	7802	74	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 5.

The worst 5 of 74 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)
5:H:705:D12:H11	4:M:420:LDA:H121	1.42	0.99
5:H:703:D12:H61	5:H:704:D12:H62	1.68	0.76
1:H:26:GLY:HA3	19:M:414:CDL:H192	1.73	0.70
2:L:49:ILE:HG21	16:L:315:HTO:H11	1.73	0.69
1:H:200:SER:H	8:H:710:EDO:H22	1.60	0.67

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	241/241 (100%)	239 (99%)	2 (1%)	0	100 100
2	L	281/281 (100%)	274 (98%)	6 (2%)	1 (0%)	34 32
3	M	304/302 (101%)	292 (96%)	12 (4%)	0	100 100
All	All	826/824 (100%)	805 (98%)	20 (2%)	1 (0%)	51 54

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	198/196 (101%)	195 (98%)	3 (2%)	65 71
2	L	222/220 (101%)	218 (98%)	4 (2%)	59 65
3	M	240/236 (102%)	236 (98%)	4 (2%)	60 67
All	All	660/652 (101%)	649 (98%)	11 (2%)	65 67

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

Mol	Chain	Res	Type
2	L	216	PHE
2	L	247	CYS

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Mol	Chain	Res	Type
3	M	52[B]	LEU
2	L	210	ASP
3	M	52[A]	LEU

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

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 50 ligands modelled in this entry, 3 are monoatomic - leaving 47 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	EDO	M	419	-	3,3,3	0.40	0	2,2,2	0.59	0
18	SPN	M	407	-	40,42,42	0.60	1 (2%)	50,52,52	1.71	12 (24%)
6	MYS	H	706	-	14,14,14	0.27	0	13,13,13	0.55	0
15	DIO	L	308	-	6,6,6	0.56	0	6,6,6	0.44	0
5	D12	M	413	-	11,11,11	0.27	0	10,10,10	0.55	0
4	LDA	M	409	-	12,15,15	2.07	1 (8%)	14,17,17	0.56	0
4	LDA	L	304	-	12,15,15	2.07	1 (8%)	14,17,17	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	D12	L	305	-	11,11,11	0.28	0	10,10,10	0.51	0
5	D12	H	703	-	11,11,11	0.29	0	10,10,10	0.51	0
16	HTO	L	315	-	9,9,9	0.23	0	10,10,10	1.26	1 (10%)
11	BCL	M	401	-	58,74,74	1.34	4 (6%)	69,115,115	1.56	13 (18%)
8	EDO	L	310	-	3,3,3	0.47	0	2,2,2	0.30	0
4	LDA	M	410	-	12,15,15	2.01	1 (8%)	14,17,17	0.61	0
4	LDA	H	702	-	12,15,15	1.99	1 (8%)	14,17,17	0.47	0
7	PO4	H	707	-	4,4,4	0.84	0	6,6,6	0.39	0
7	PO4	M	415	-	4,4,4	0.86	0	6,6,6	0.43	0
11	BCL	M	403	-	58,74,74	1.30	5 (8%)	69,115,115	1.32	10 (14%)
5	D12	H	704	-	11,11,11	0.33	0	10,10,10	0.40	0
8	EDO	L	311	-	3,3,3	0.53	0	2,2,2	0.17	0
16	HTO	L	314	-	9,9,9	0.26	0	10,10,10	0.87	0
16	HTO	L	316	-	8,8,9	0.56	0	9,9,10	0.82	0
8	EDO	H	708	-	3,3,3	0.52	0	2,2,2	0.25	0
8	EDO	H	710	-	3,3,3	0.52	0	2,2,2	0.37	0
8	EDO	H	712	-	3,3,3	0.49	0	2,2,2	0.44	0
8	EDO	L	313	-	3,3,3	0.51	0	2,2,2	0.24	0
19	CDL	M	414	-	80,80,99	1.06	4 (5%)	86,92,111	1.17	7 (8%)
13	U10	L	303	-	48,48,63	2.61	13 (27%)	58,61,79	1.80	16 (27%)
6	MYS	M	411	-	14,14,14	0.28	0	13,13,13	0.51	0
4	LDA	M	408	-	12,15,15	1.99	1 (8%)	14,17,17	0.56	0
12	BPH	L	302	-	64,70,70	1.03	7 (10%)	76,101,101	1.08	5 (6%)
8	EDO	H	711	-	3,3,3	0.48	0	2,2,2	0.41	0
11	BCL	M	402	-	58,74,74	1.42	4 (6%)	69,115,115	1.45	11 (15%)
8	EDO	L	309	-	3,3,3	0.46	0	2,2,2	0.42	0
8	EDO	M	417	-	3,3,3	0.43	0	2,2,2	0.73	0
14	D10	L	307	-	9,9,9	0.27	0	8,8,8	0.55	0
8	EDO	M	418	-	3,3,3	0.63	0	2,2,2	0.15	0
4	LDA	H	701	-	12,15,15	2.05	1 (8%)	14,17,17	0.74	0
6	MYS	L	306	-	14,14,14	0.31	0	13,13,13	0.41	0
7	PO4	M	416	-	4,4,4	0.81	0	6,6,6	0.57	0
5	D12	H	705	-	11,11,11	0.23	0	10,10,10	0.70	0
11	BCL	L	301	-	58,74,74	1.42	5 (8%)	69,115,115	1.30	8 (11%)
12	BPH	M	404	-	64,70,70	0.93	3 (4%)	76,101,101	1.50	17 (22%)
8	EDO	H	709	-	3,3,3	0.52	0	2,2,2	0.32	0
13	U10	M	406	-	48,48,63	2.60	13 (27%)	58,61,79	1.68	13 (22%)
8	EDO	L	312	-	3,3,3	0.42	0	2,2,2	0.50	0
5	D12	M	412	-	11,11,11	0.28	0	10,10,10	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	LDA	M	420	-	12,15,15	2.01	1 (8%)	14,17,17	0.72	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
8	EDO	M	419	-	-	0/1/1/1	-
18	SPN	M	407	-	-	18/50/51/51	-
6	MYS	H	706	-	-	2/12/12/12	-
15	DIO	L	308	-	-	-	0/1/1/1
5	D12	M	413	-	-	6/9/9/9	-
4	LDA	M	409	-	-	10/13/13/13	-
4	LDA	L	304	-	-	2/13/13/13	-
5	D12	L	305	-	-	2/9/9/9	-
5	D12	H	703	-	-	2/9/9/9	-
16	HTO	L	315	-	-	3/10/10/10	-
11	BCL	M	401	-	-	6/37/137/137	-
4	LDA	M	408	-	-	4/13/13/13	-
4	LDA	M	410	-	-	10/13/13/13	-
4	LDA	H	702	-	-	4/13/13/13	-
8	EDO	H	712	-	-	0/1/1/1	-
11	BCL	M	403	-	-	0/37/137/137	-
5	D12	H	704	-	-	0/9/9/9	-
8	EDO	L	311	-	-	0/1/1/1	-
16	HTO	L	314	-	-	2/10/10/10	-
16	HTO	L	316	-	-	5/9/9/10	-
8	EDO	L	310	-	-	0/1/1/1	-
8	EDO	H	708	-	-	0/1/1/1	-
8	EDO	H	710	-	-	0/1/1/1	-
8	EDO	L	313	-	-	0/1/1/1	-
19	CDL	M	414	-	-	27/91/91/110	-
13	U10	L	303	-	-	18/45/69/87	0/1/1/1
6	MYS	M	411	-	-	5/12/12/12	-
12	BPH	L	302	-	-	5/54/105/105	0/5/6/6
8	EDO	H	711	-	-	0/1/1/1	-
11	BCL	M	402	-	-	1/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	L	309	-	-	1/1/1/1	-
8	EDO	M	417	-	-	0/1/1/1	-
14	D10	L	307	-	-	2/7/7/7	-
8	EDO	M	418	-	-	0/1/1/1	-
4	LDA	H	701	-	-	4/13/13/13	-
6	MYS	L	306	-	-	2/12/12/12	-
5	D12	H	705	-	-	3/9/9/9	-
11	BCL	L	301	-	-	1/37/137/137	-
12	BPH	M	404	-	-	14/54/105/105	0/5/6/6
8	EDO	H	709	-	-	0/1/1/1	-
13	U10	M	406	-	-	13/45/69/87	0/1/1/1
8	EDO	L	312	-	-	1/1/1/1	-
5	D12	M	412	-	-	4/9/9/9	-
4	LDA	M	420	-	-	9/13/13/13	-

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	409	LDA	O1-N1	-7.10	1.25	1.42
4	L	304	LDA	O1-N1	-7.09	1.25	1.42
4	H	701	LDA	O1-N1	-6.96	1.25	1.42
4	M	420	LDA	O1-N1	-6.93	1.25	1.42
4	M	410	LDA	O1-N1	-6.86	1.26	1.42

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	M	414	CDL	OA6-CA5-C11	5.26	122.83	111.50
11	M	401	BCL	CMB-C2B-C1B	-4.34	121.80	128.46
11	M	402	BCL	C4A-NA-C1A	4.32	108.65	106.71
11	L	301	BCL	CMB-C2B-C1B	-4.16	122.07	128.46
11	M	402	BCL	CMB-C2B-C1B	-4.11	122.14	128.46

There are no chirality outliers.

5 of 186 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	M	407	SPN	CM1-C1-O1-CMA
18	M	407	SPN	C2-C1-O1-CMA
18	M	407	SPN	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
18	M	407	SPN	CM5-C13-C14-C15
4	M	409	LDA	C2-C1-N1-O1

There are no ring outliers.

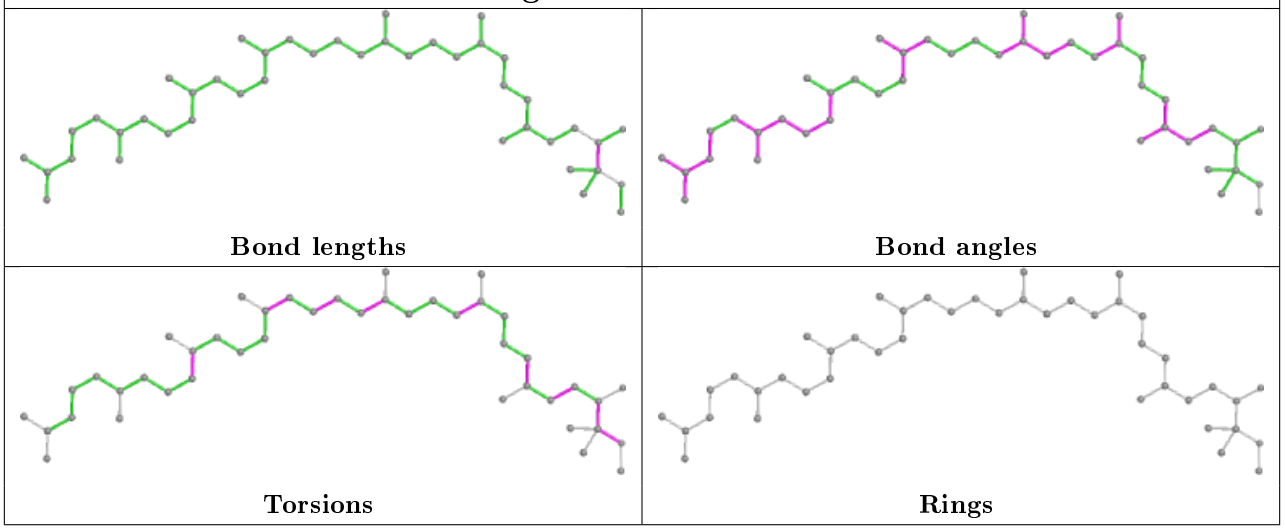
26 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	M	407	SPN	5	0
6	H	706	MYS	1	0
15	L	308	DIO	2	0
5	M	413	D12	1	0
4	M	409	LDA	1	0
5	L	305	D12	1	0
5	H	703	D12	2	0
16	L	315	HTO	2	0
11	M	401	BCL	3	0
4	M	410	LDA	3	0
4	H	702	LDA	2	0
11	M	403	BCL	1	0
5	H	704	D12	2	0
16	L	314	HTO	1	0
8	H	710	EDO	3	0
19	M	414	CDL	6	0
13	L	303	U10	2	0
6	M	411	MYS	1	0
11	M	402	BCL	1	0
8	M	417	EDO	2	0
4	H	701	LDA	2	0
5	H	705	D12	2	0
12	M	404	BPH	1	0
8	H	709	EDO	2	0
5	M	412	D12	1	0
4	M	420	LDA	3	0

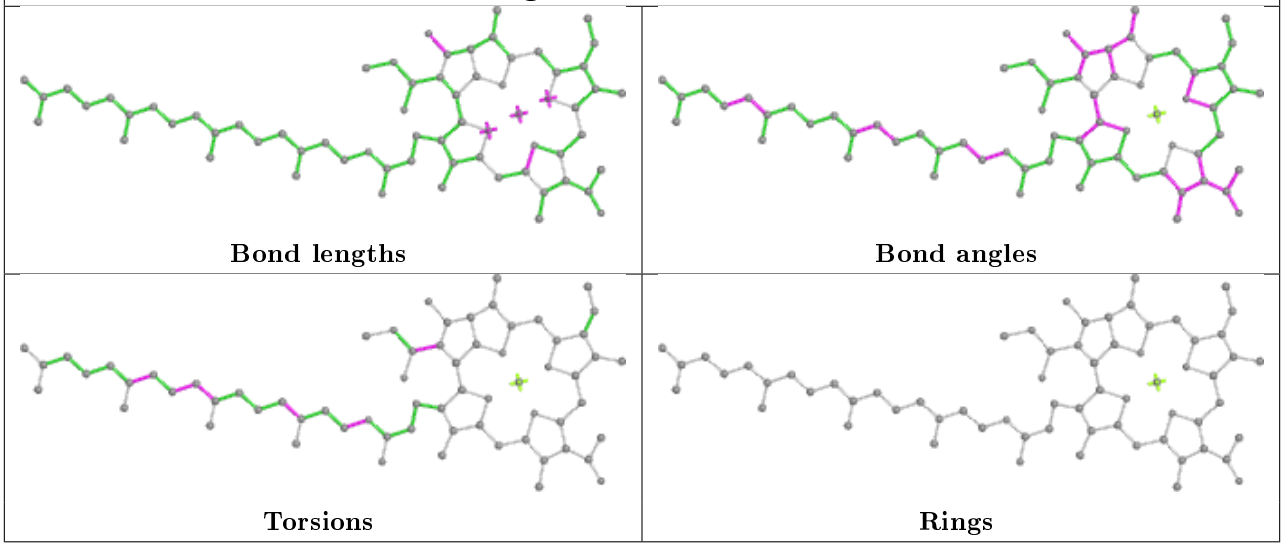
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

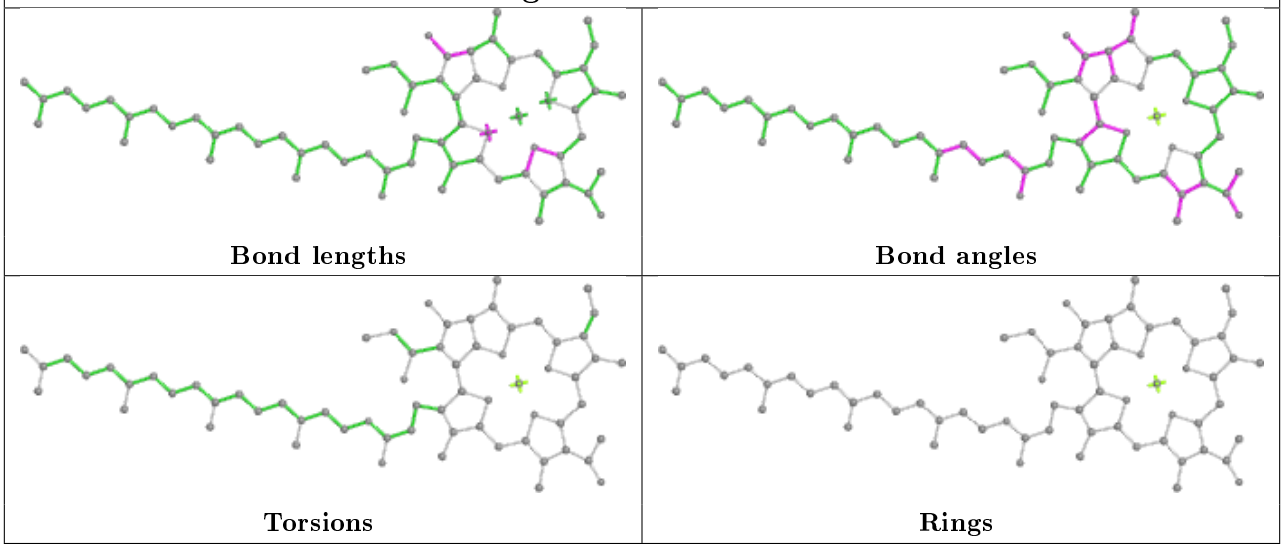
Ligand SPN M 407



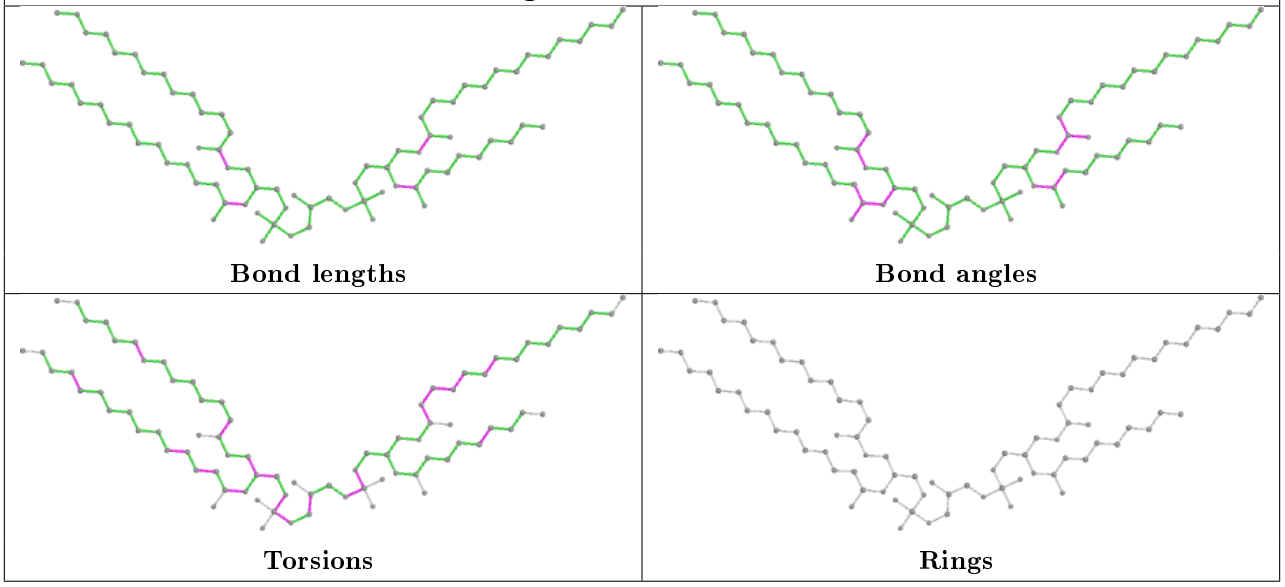
Ligand BCL M 401



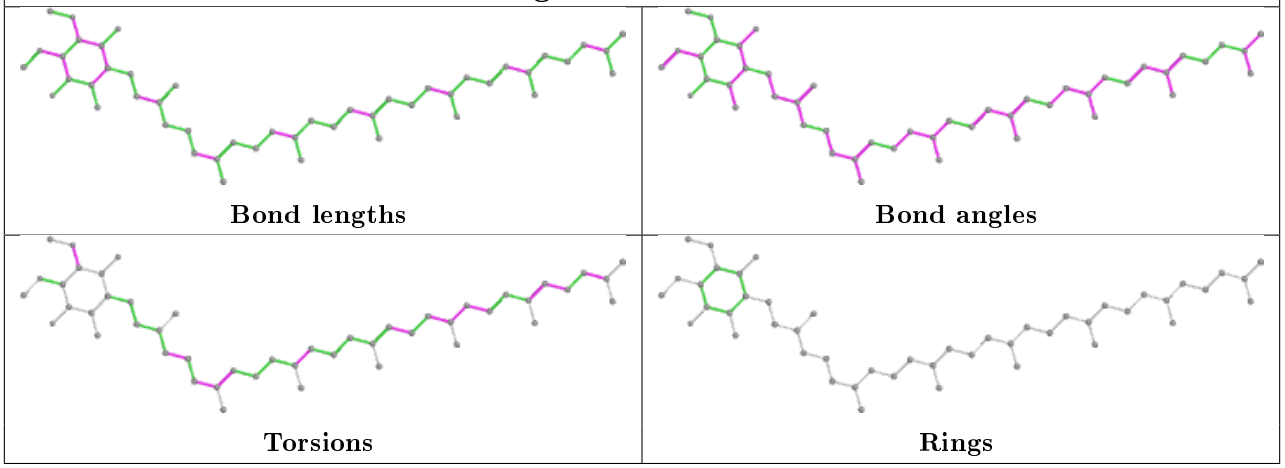
Ligand BCL M 403



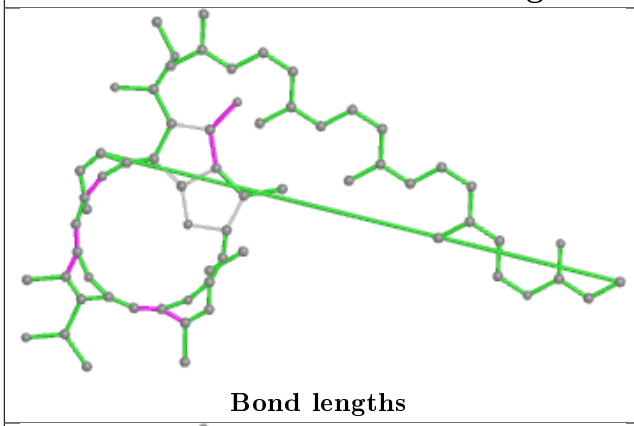
Ligand CDL M 414



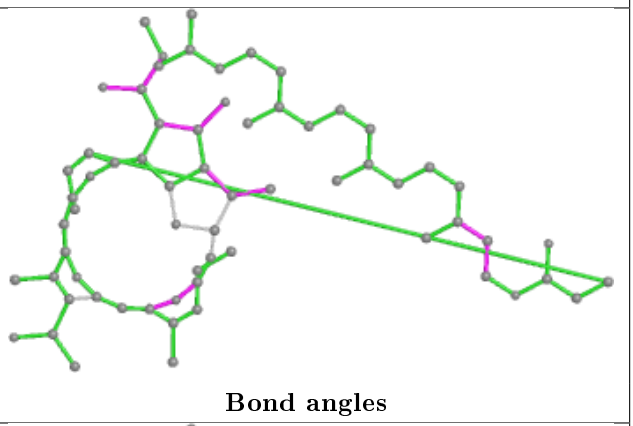
Ligand U10 L 303



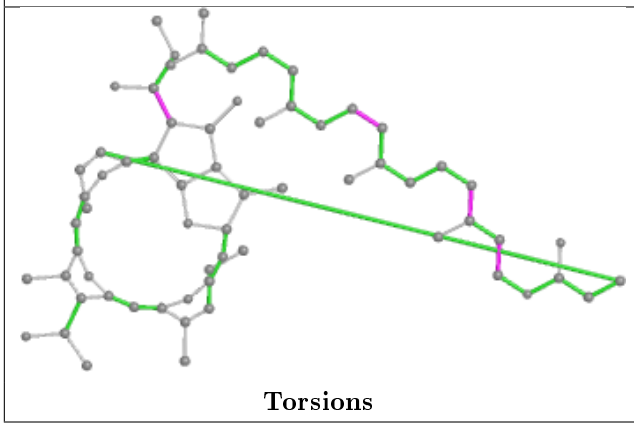
Ligand BPH L 302



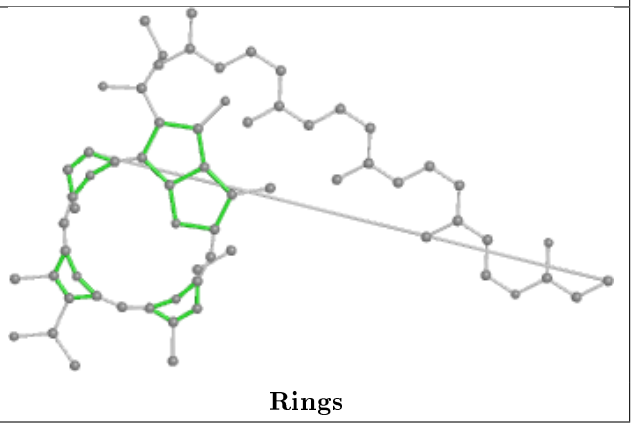
Bond lengths



Bond angles

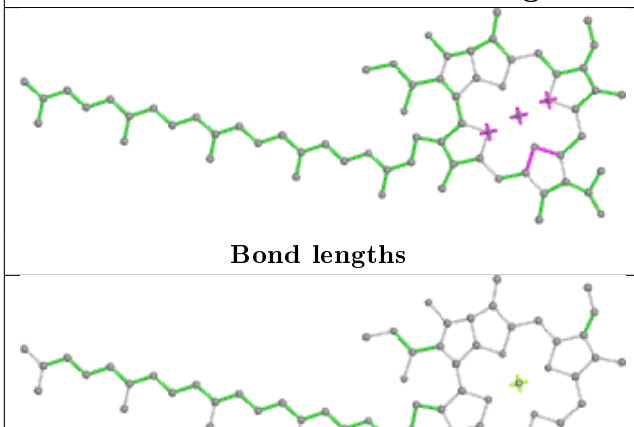


Torsions

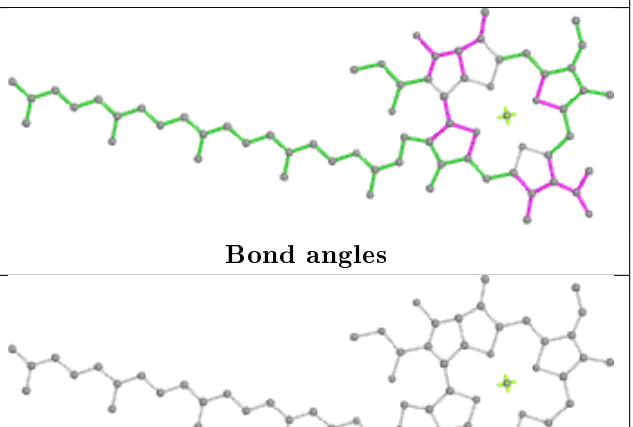


Rings

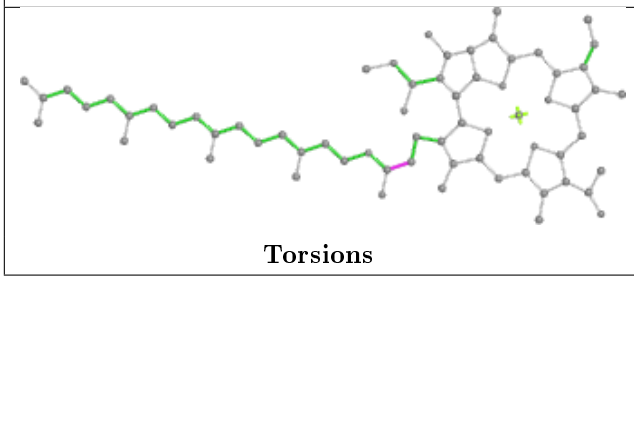
Ligand BCL M 402



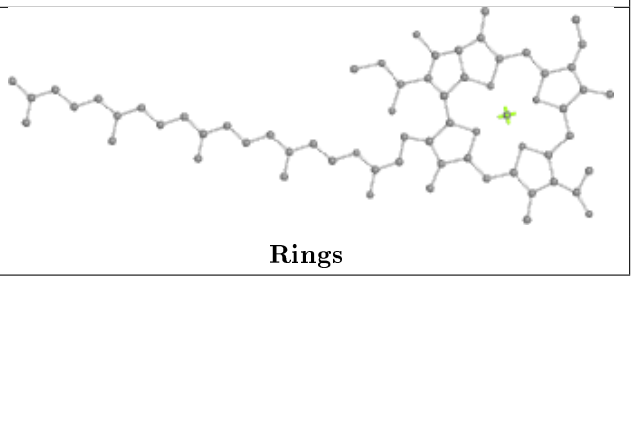
Bond lengths



Bond angles

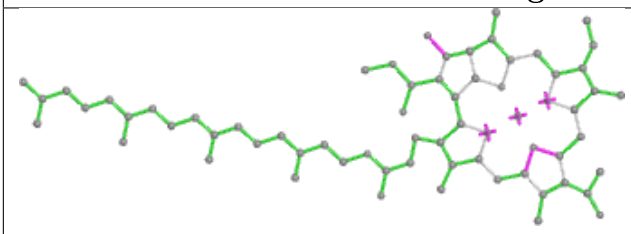


Torsions

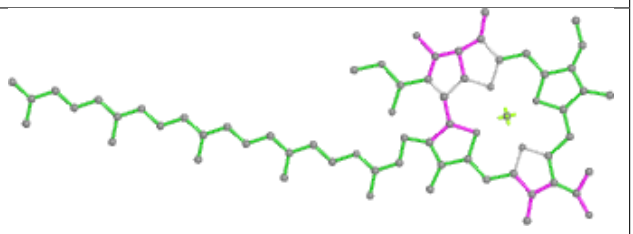


Rings

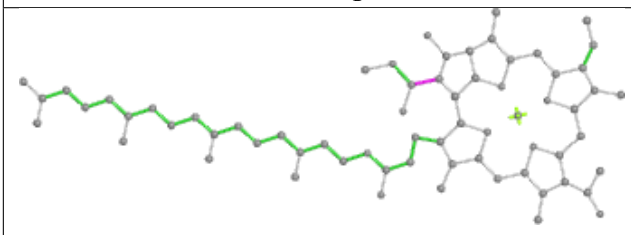
Ligand BCL L 301



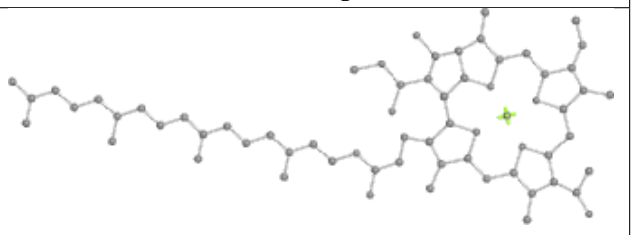
Bond lengths



Bond angles

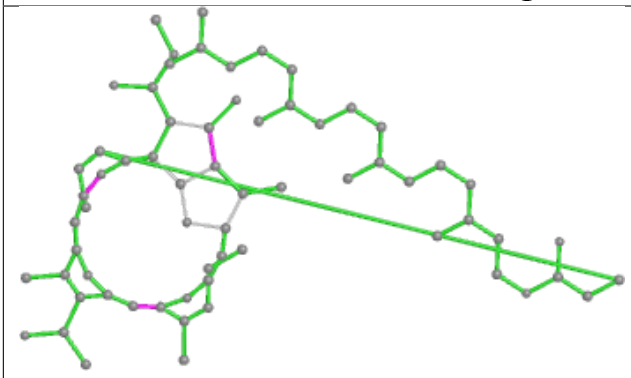


Torsions

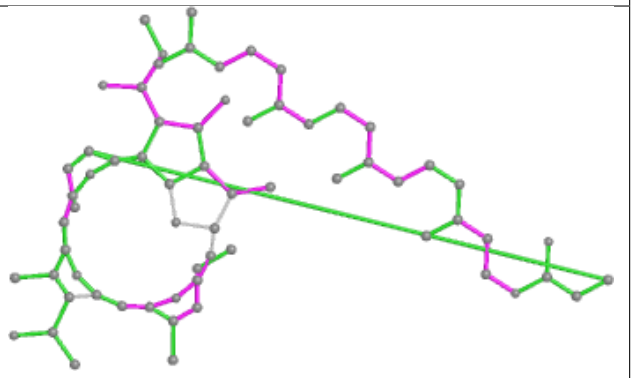


Rings

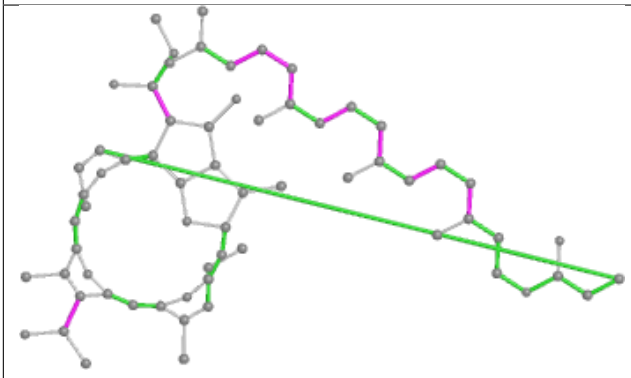
Ligand BPH M 404



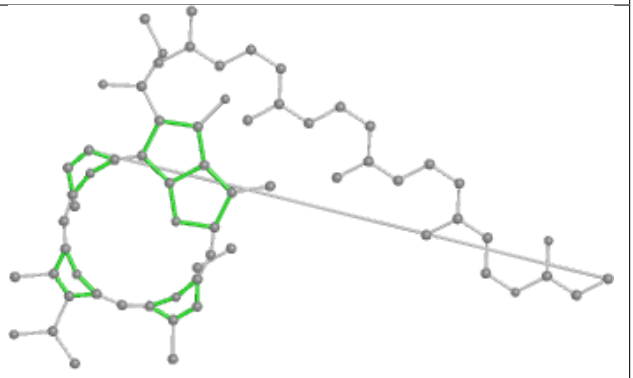
Bond lengths



Bond angles

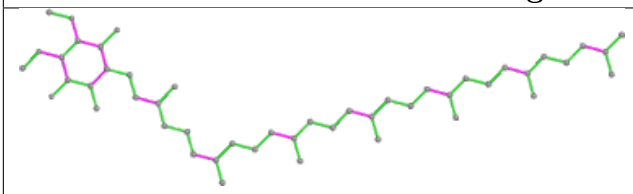


Torsions

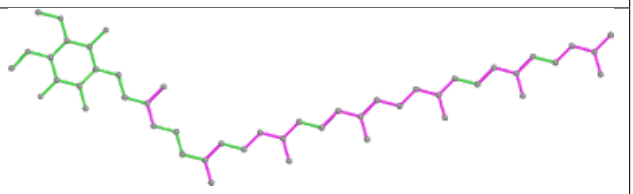


Rings

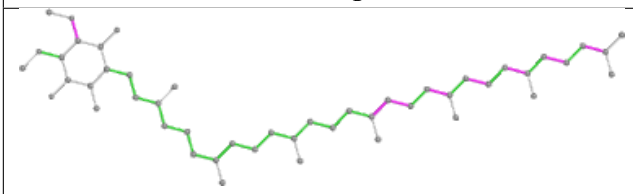
Ligand U10 M 406



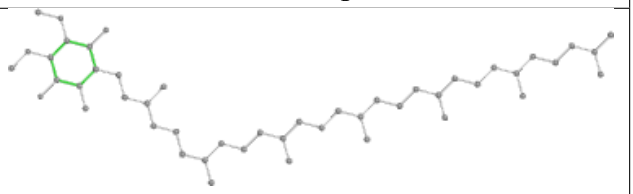
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	240/241 (99%)	-0.55	3 (1%)	77	80	26, 36, 49, 81	0
2	L	281/281 (100%)	-0.24	4 (1%)	75	78	24, 36, 64, 94	0
3	M	302/302 (100%)	-0.27	1 (0%)	94	94	22, 37, 58, 77	0
All	All	823/824 (99%)	-0.34	8 (0%)	82	85	22, 36, 59, 94	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	59	TRP	4.0
2	L	55	LEU	3.6
1	H	250	SER	3.3
2	L	276	PRO	3.1
1	H	249	LYS	2.5

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
16	HTO	L	316	9/10	0.65	0.20	50,62,68,70	0
16	HTO	L	314	10/10	0.67	0.33	39,49,60,62	10
6	MYS	M	411	15/15	0.72	0.22	57,64,75,77	0
13	U10	L	303	48/63	0.76	0.29	29,49,58,66	48
8	EDO	H	710	4/4	0.77	0.29	54,59,60,72	0
5	D12	H	704	12/12	0.78	0.48	56,65,70,71	0
4	LDA	H	701	16/16	0.79	0.24	36,48,57,61	0
4	LDA	M	409	16/16	0.80	0.45	60,71,94,94	0
5	D12	L	305	12/12	0.82	0.44	56,62,67,67	0
5	D12	H	705	12/12	0.82	0.32	54,58,75,75	0
4	LDA	M	410	16/16	0.83	0.35	55,65,73,75	0
5	D12	H	703	12/12	0.84	0.31	52,56,66,75	0
4	LDA	M	408	16/16	0.85	0.19	43,51,68,72	0
4	LDA	L	304	16/16	0.85	0.19	49,61,79,87	0
15	DIO	L	308	6/6	0.86	0.20	56,59,62,68	0
5	D12	M	412	12/12	0.86	0.30	54,62,66,67	0
19	CDL	M	414	81/100	0.88	0.23	29,52,67,72	81
6	MYS	L	306	15/15	0.88	0.21	41,51,67,68	0
6	MYS	H	706	15/15	0.88	0.18	55,65,72,74	0
8	EDO	H	709	4/4	0.88	0.24	48,55,61,68	0
4	LDA	H	702	16/16	0.88	0.21	45,51,59,65	0
14	D10	L	307	10/10	0.89	0.40	47,62,67,69	0
5	D12	M	413	12/12	0.89	0.25	44,52,65,67	0
4	LDA	M	420	16/16	0.89	0.27	56,64,69,69	0
8	EDO	H	708	4/4	0.90	0.15	60,67,68,73	0
8	EDO	L	313	4/4	0.91	0.12	58,58,68,72	0
7	PO4	M	416	5/5	0.91	0.18	37,43,54,61	5
16	HTO	L	315	10/10	0.91	0.36	56,61,69,72	0
18	SPN	M	407	43/43	0.92	0.15	30,41,58,71	0
8	EDO	L	310	4/4	0.92	0.42	53,54,55,62	0
8	EDO	L	309	4/4	0.93	0.12	49,56,58,60	0
13	U10	M	406	48/63	0.93	0.16	20,31,59,63	0
8	EDO	M	419	4/4	0.93	0.26	48,57,63,81	0
8	EDO	H	712	4/4	0.93	0.13	42,45,47,59	0
8	EDO	M	417	4/4	0.94	0.12	37,39,41,41	0
7	PO4	H	707	5/5	0.94	0.21	69,74,79,80	0
8	EDO	L	312	4/4	0.95	0.31	37,40,45,54	0
8	EDO	H	711	4/4	0.95	0.12	44,45,46,51	0
12	BPH	M	404	65/65	0.95	0.13	28,37,82,91	0
9	NA	H	713	1/1	0.97	0.07	40,40,40,40	0
11	BCL	L	301	66/66	0.97	0.10	22,29,39,47	0
7	PO4	M	415	5/5	0.97	0.12	66,67,69,71	0
11	BCL	M	403	66/66	0.97	0.14	20,29,48,56	0

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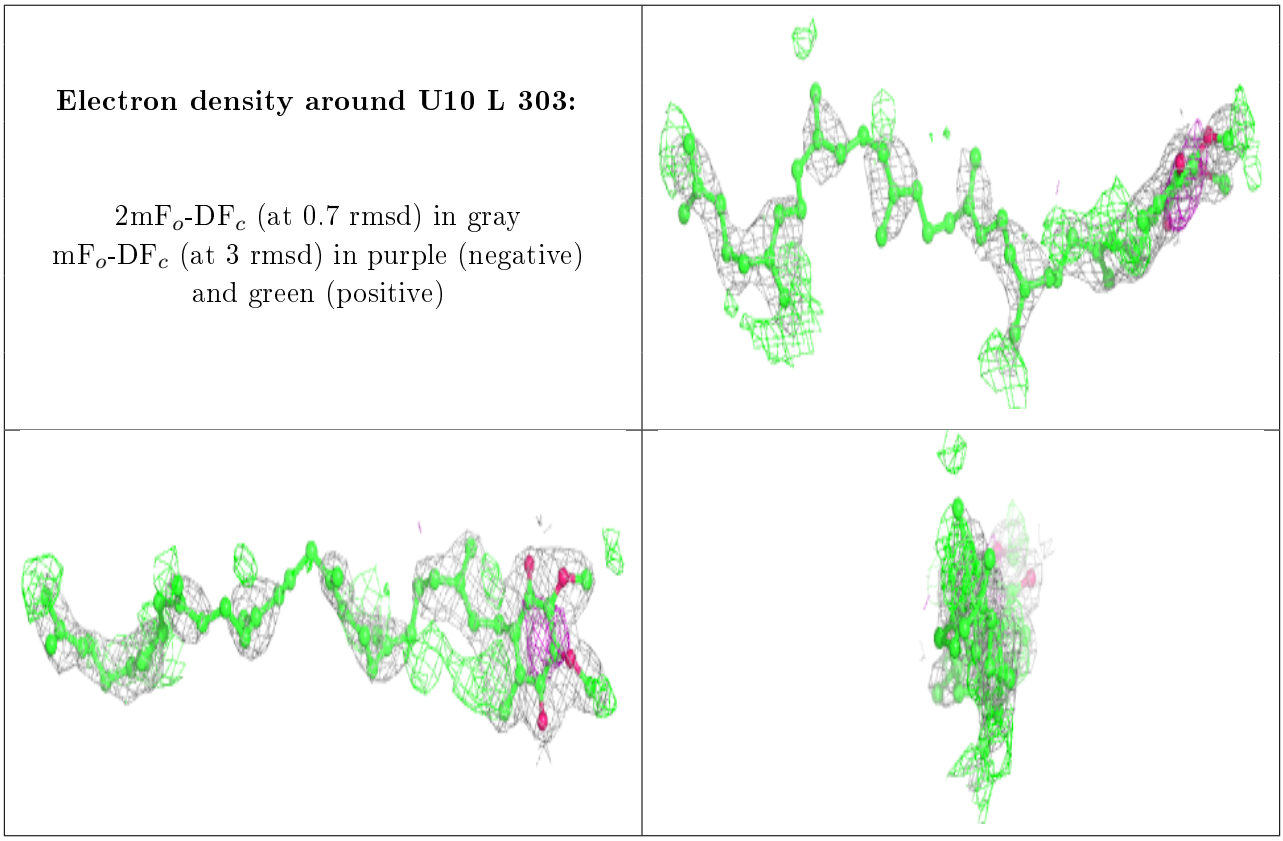
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	EDO	M	418	4/4	0.97	0.07	28,34,36,42	0
12	BPH	L	302	65/65	0.97	0.12	22,29,42,50	0
11	BCL	M	401	66/66	0.97	0.11	22,31,58,64	0
8	EDO	L	311	4/4	0.97	0.09	37,40,42,45	0
10	K	H	714	1/1	0.98	0.06	39,39,39,39	0
11	BCL	M	402	66/66	0.98	0.10	22,28,53,64	0
17	FE	M	405	1/1	1.00	0.11	25,25,25,25	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.

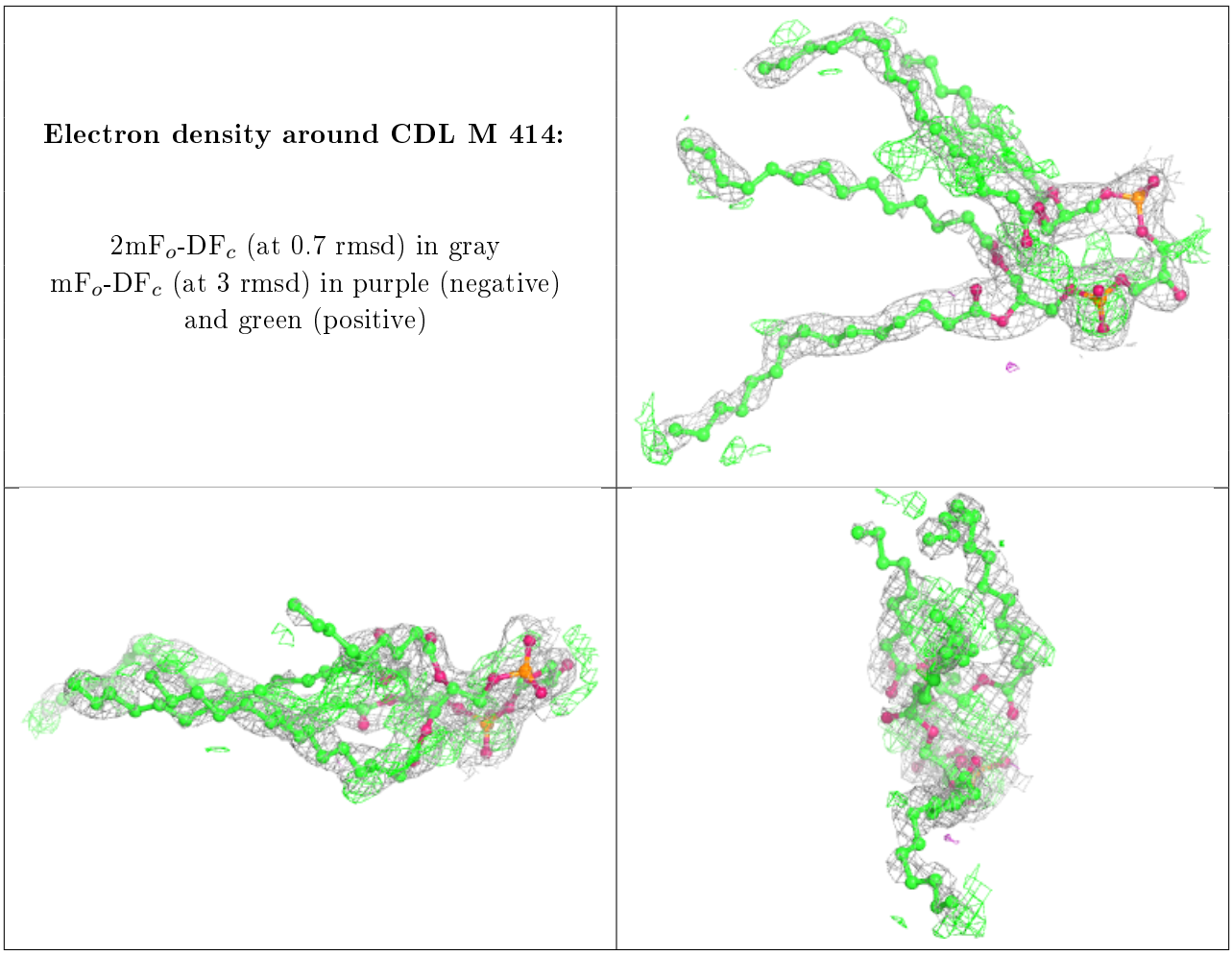
Electron density around U10 L 303:

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



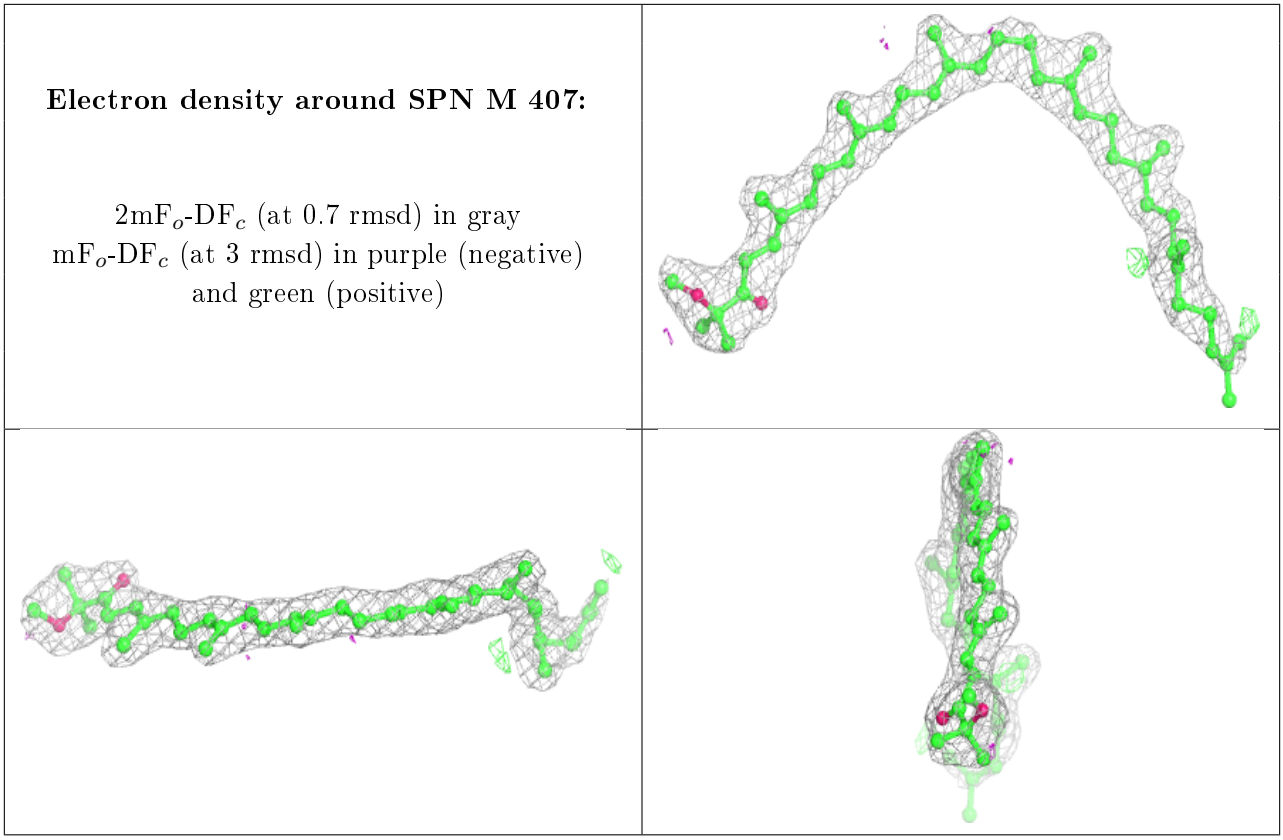
Electron density around CDL M 414:

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



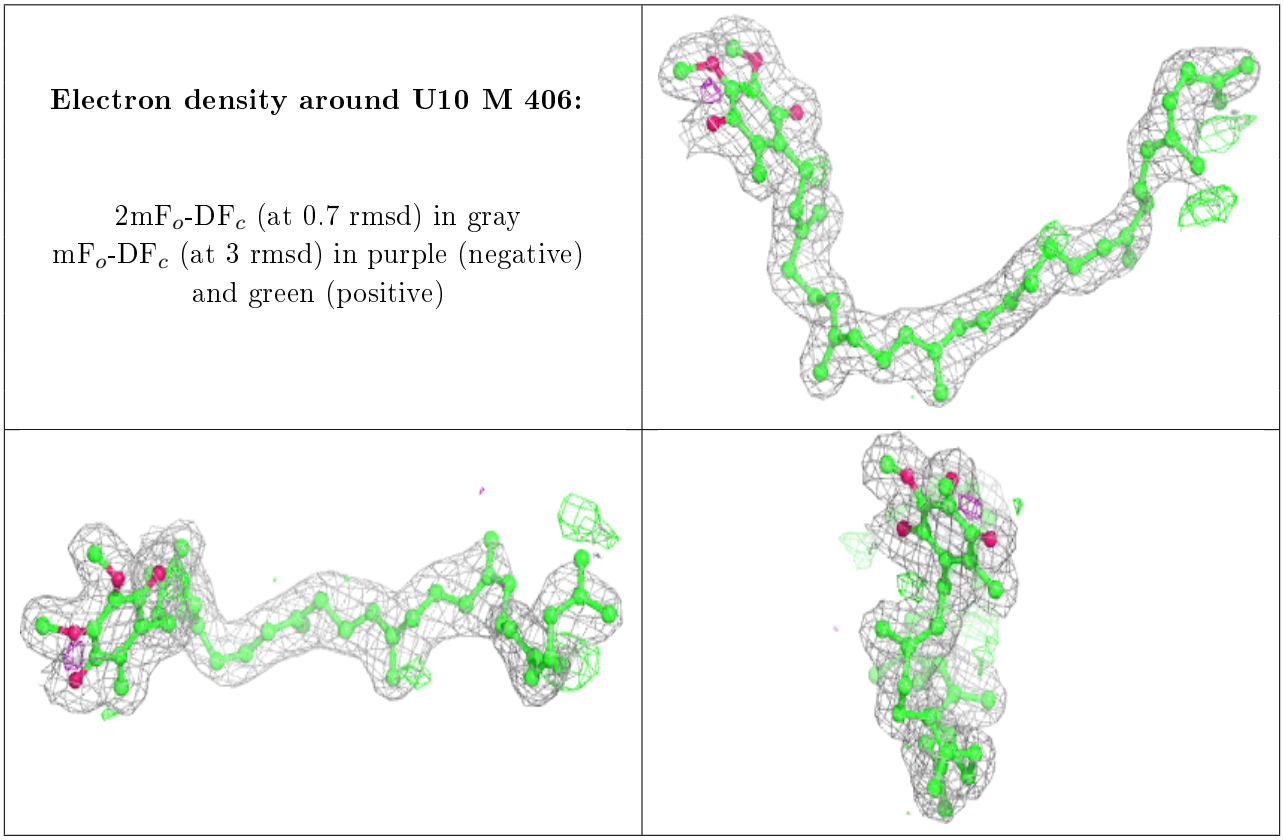
Electron density around SPN M 407:

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



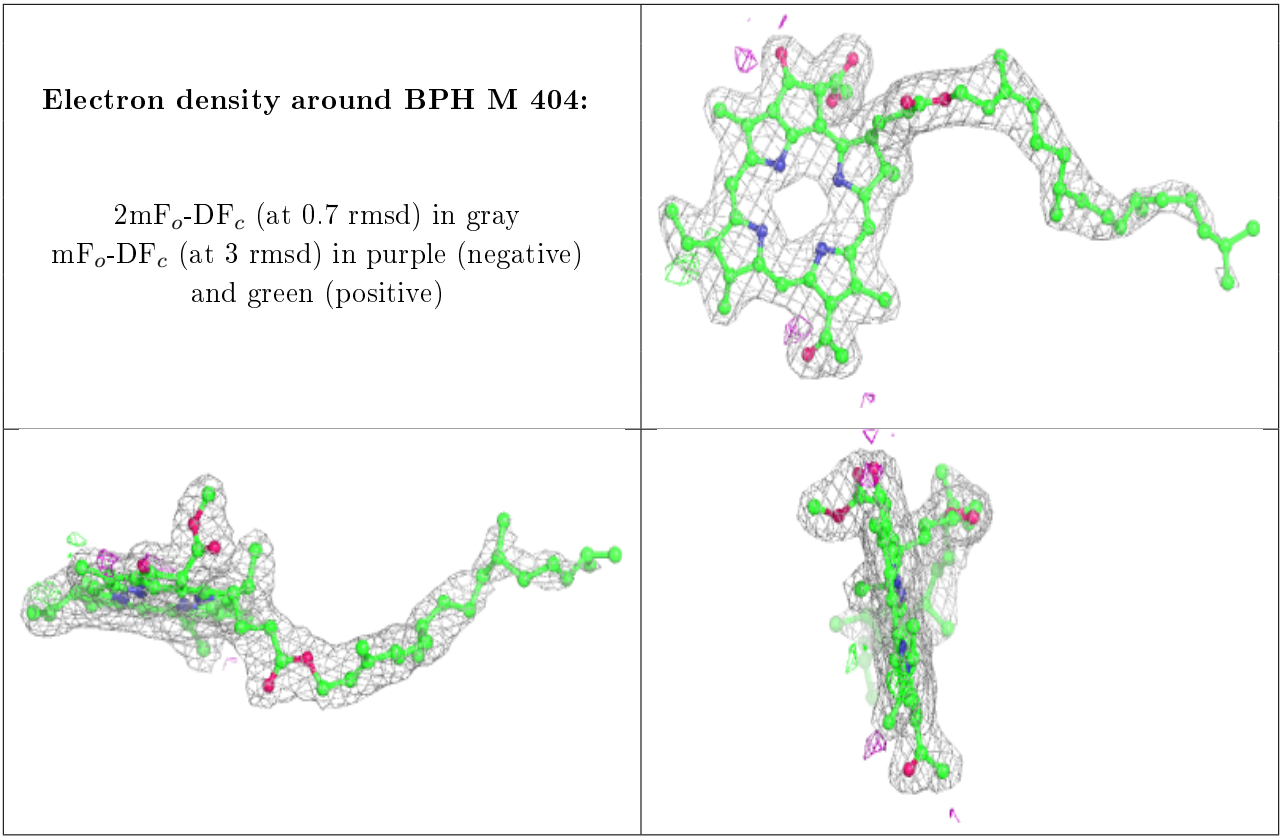
Electron density around U10 M 406:

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



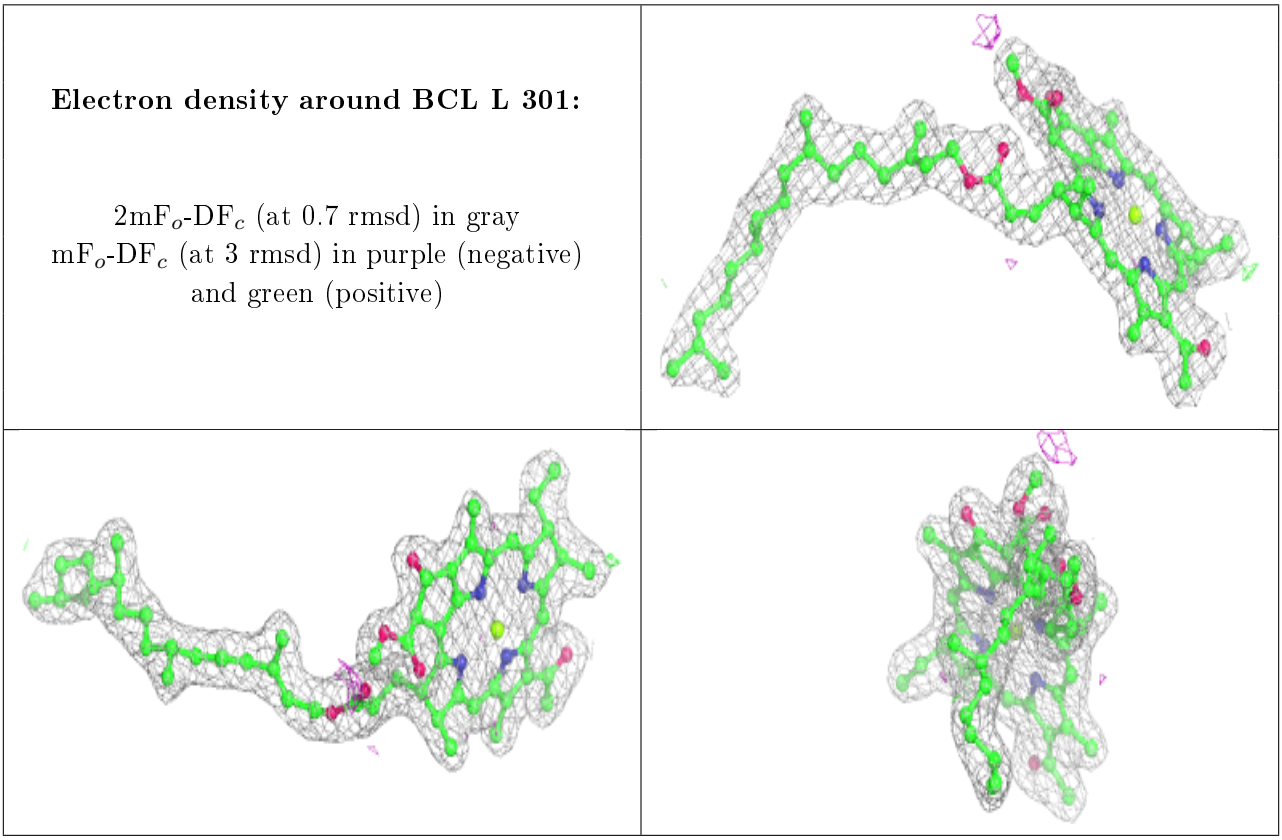
Electron density around BPH M 404:

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



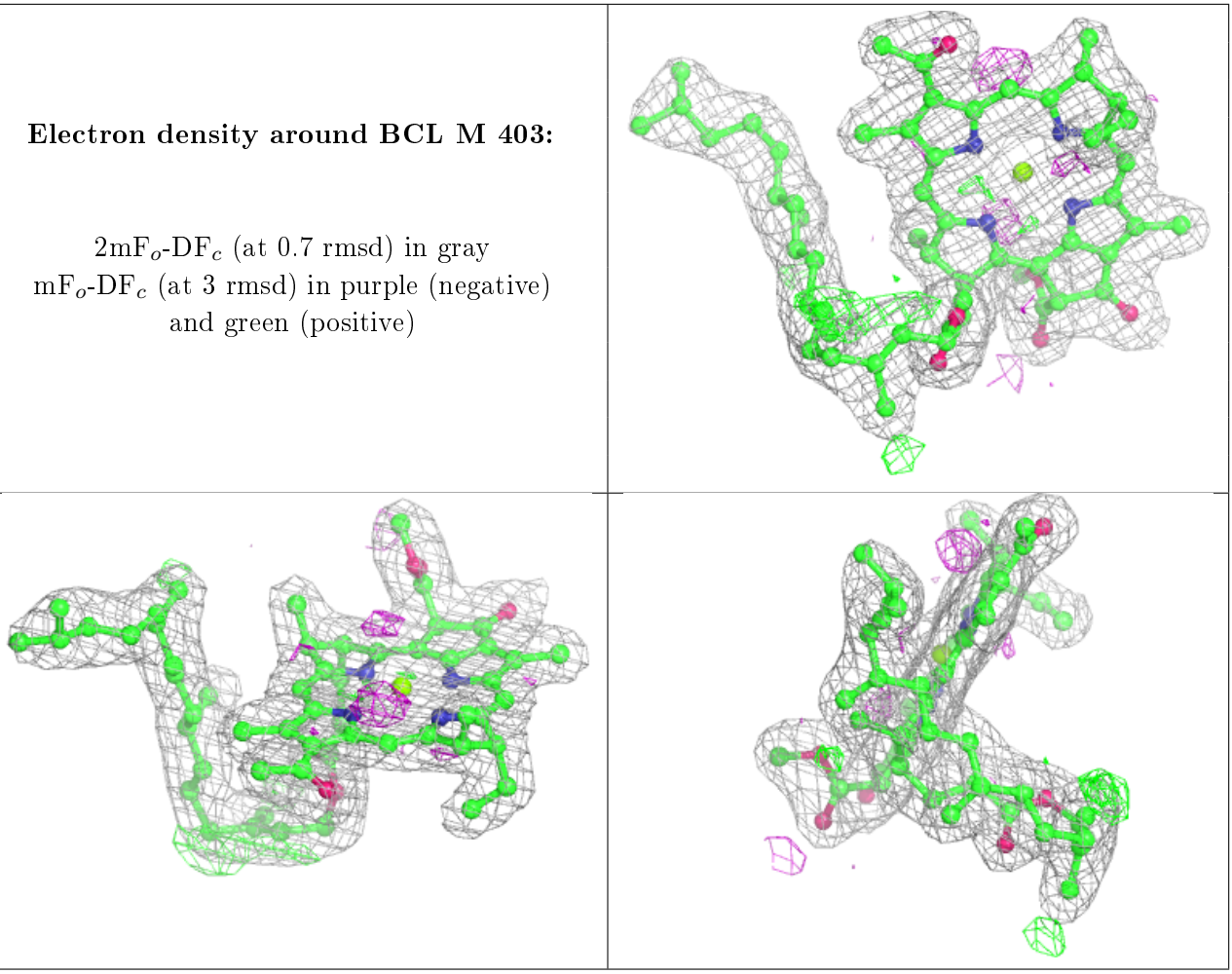
Electron density around BCL L 301:

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



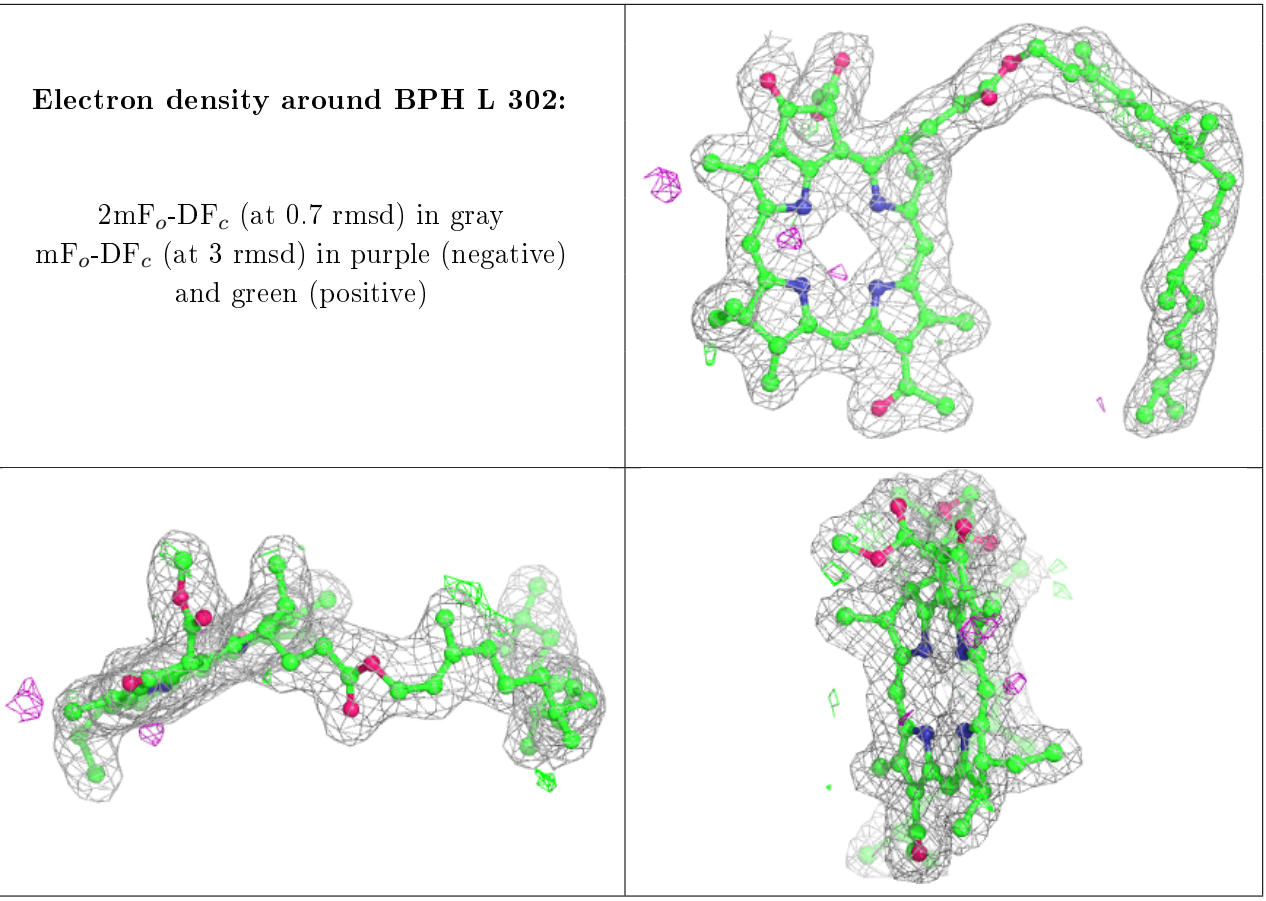
Electron density around BCL M 403:

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



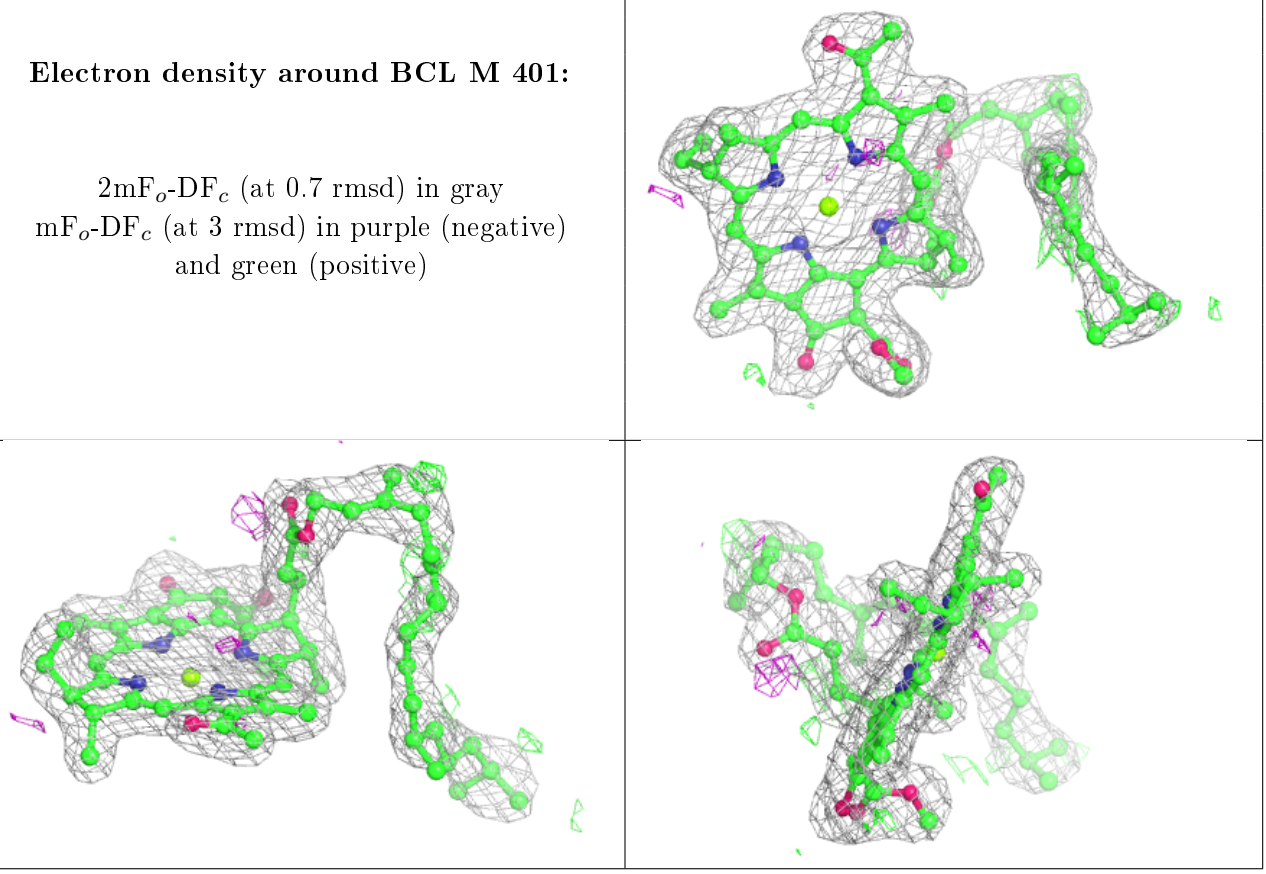
Electron density around BPH L 302:

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



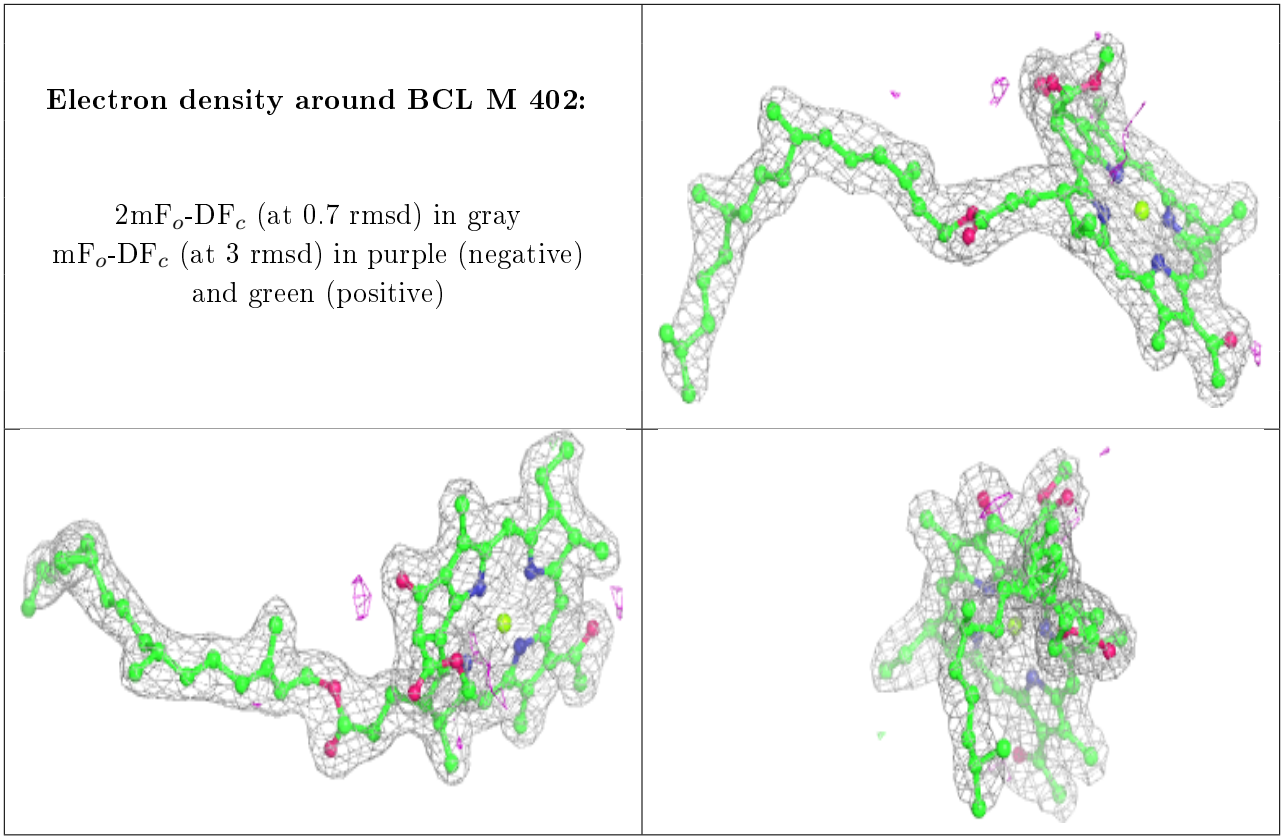
Electron density around BCL M 401:

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



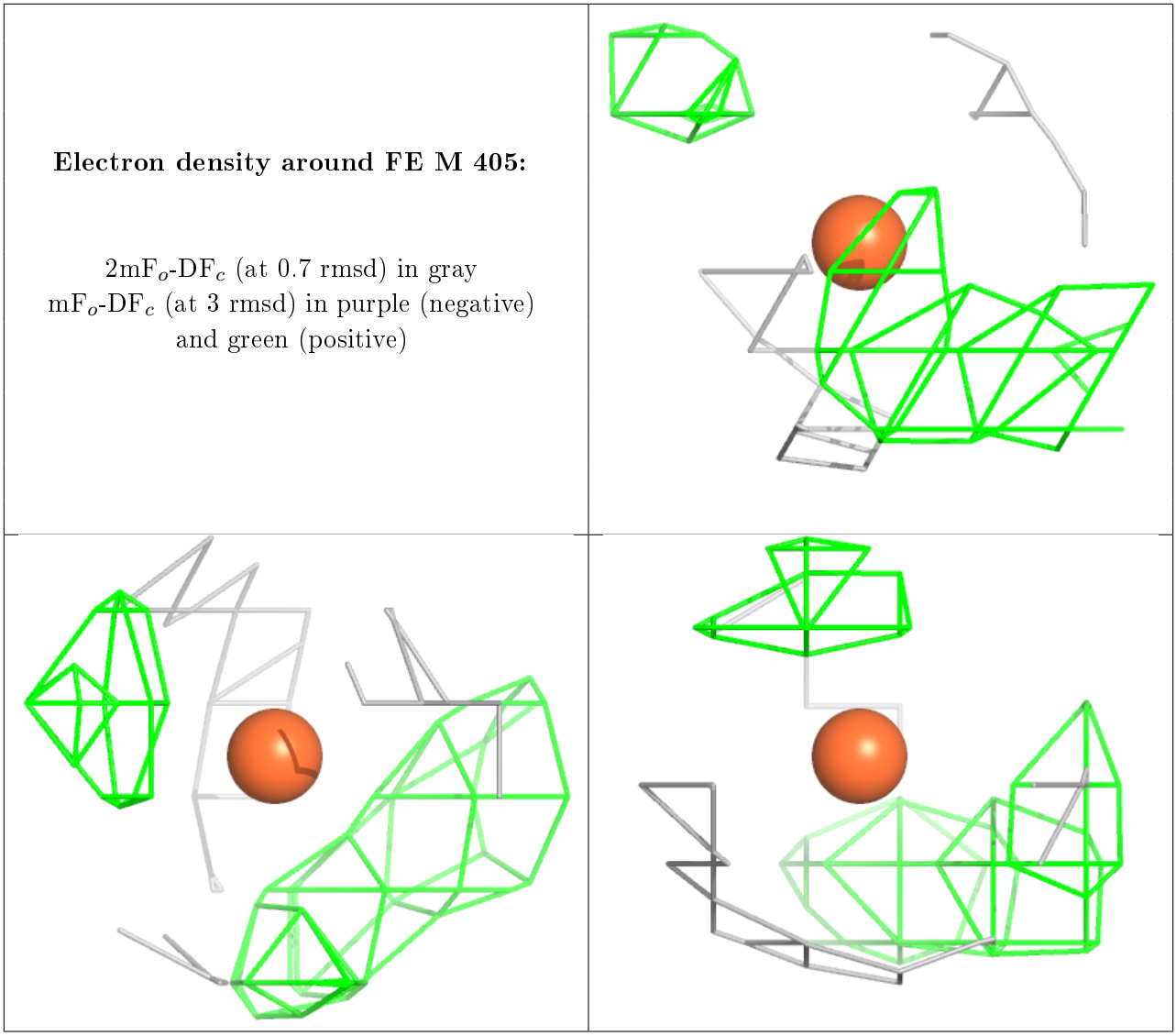
Electron density around BCL M 402:

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



Electron density around 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.