Full wwPDB X-ray Structure Validation Report ⓘ

Dec 23, 2021 – 12:05 PM EST

PDB ID	:	7MH5
Title	:	Crystal structure of R. sphaeroides Photosynthetic Reaction Center variant; Y(M210)3-iodotyrosine
Authors	:	Mathews, I.; Weaver, J.; Boxer, S.G.
Deposited on	:	2021-04-14
Resolution	:	2.85 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 following versions of software and data (see references ⓘ) were used in the production of this report:

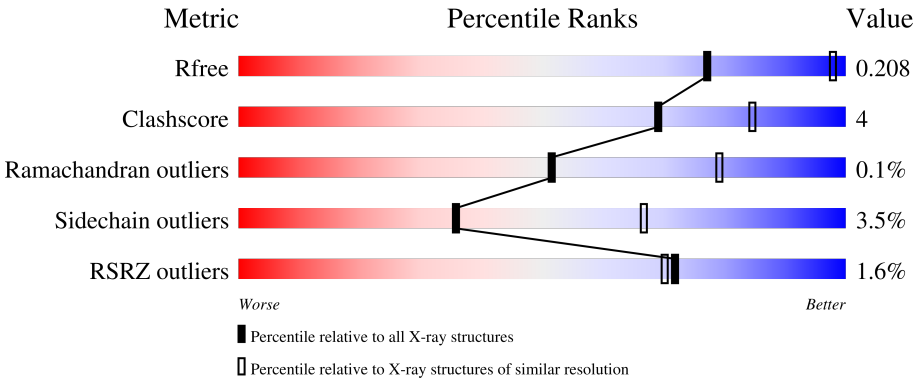
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.25
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.25

1 Overall quality at a glance (i)

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

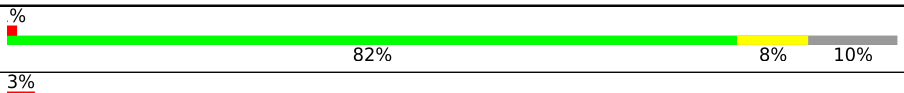
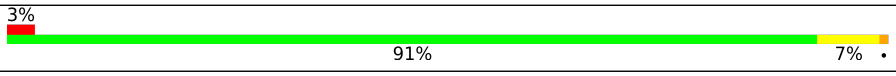
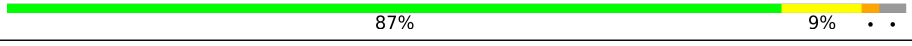
The reported resolution of this entry is 2.85 Å.

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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	266	
2	L	282	
3	M	308	

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
5	BPH	M	409	X	-	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 7273 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	239	Total	C	N	O	S	0	2	0
			1844	1180	315	340	9			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	260	VAL	-	expression tag	UNP P0C0Y7
H	261	HIS	-	expression tag	UNP P0C0Y7
H	262	HIS	-	expression tag	UNP P0C0Y7
H	263	HIS	-	expression tag	UNP P0C0Y7
H	264	HIS	-	expression tag	UNP P0C0Y7
H	265	HIS	-	expression tag	UNP P0C0Y7
H	266	HIS	-	expression tag	UNP P0C0Y7

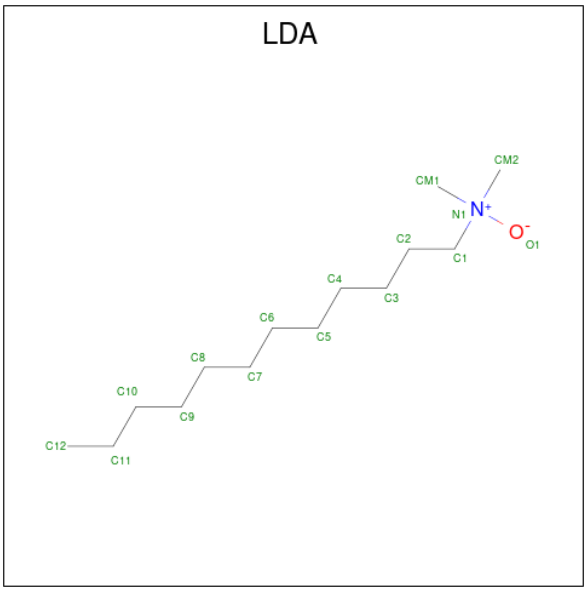
- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

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

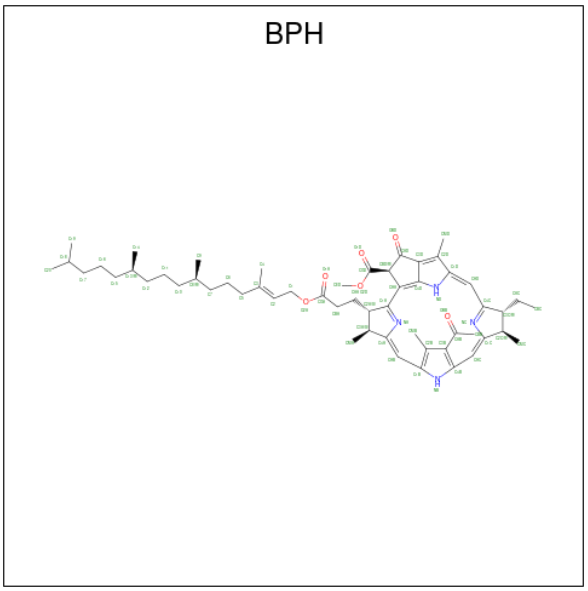
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	M	300	Total	C	I	N	O	S	0	0	0
			2396	1599	2	392	393	10			

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



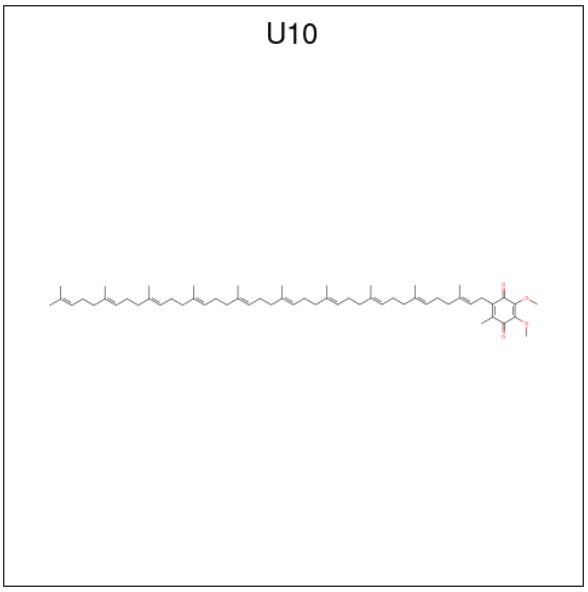
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			55	45	4	6		

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			18	14	4		

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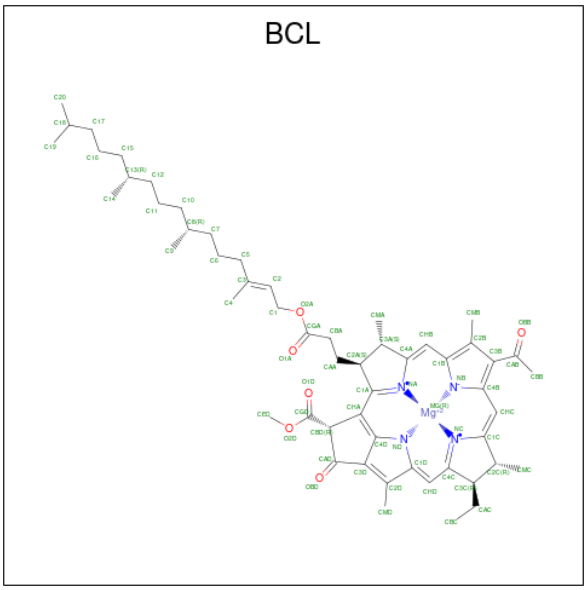
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	C	O	0	0
			38	34	4		

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

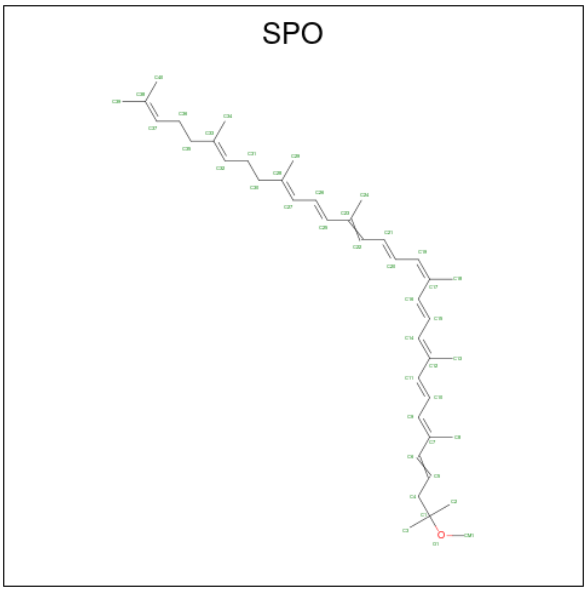


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

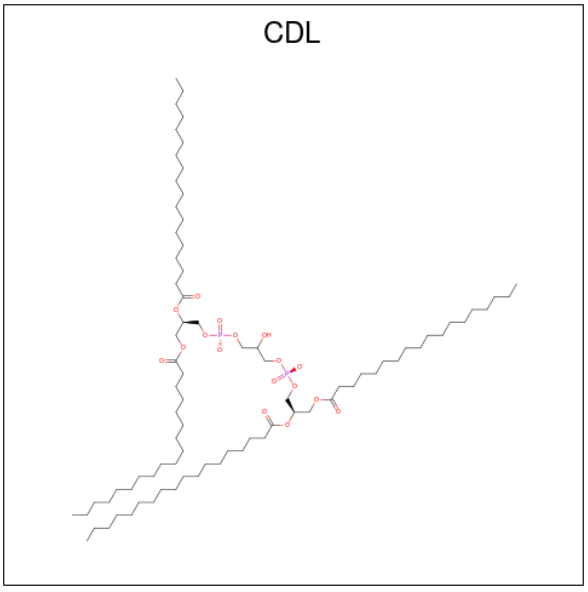
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	M	1	42	41	1	0	0

- Molecule 10 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
10	M	1	69	50	17	2	0	0

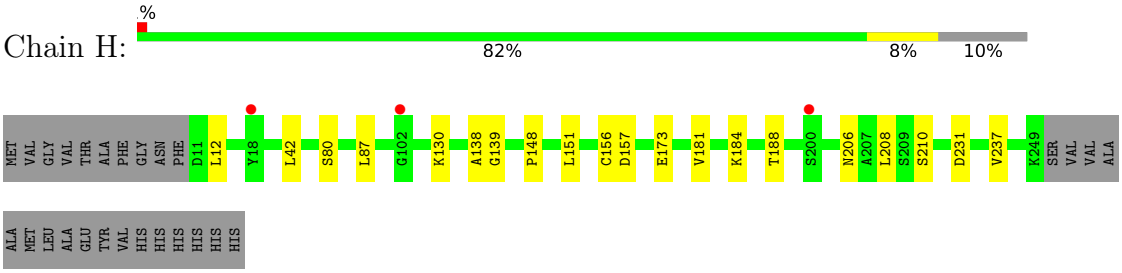
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	H	82	Total O 82 82	0	0
11	L	45	Total O 45 45	0	0
11	M	57	Total O 57 57	0	0

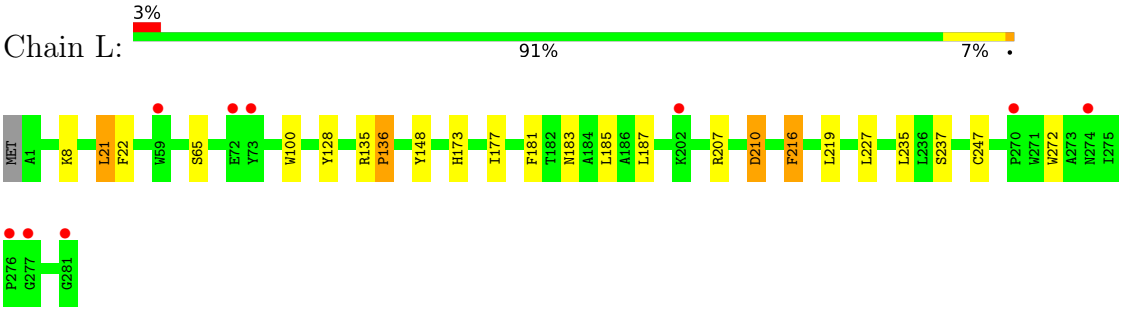
3 Residue-property plots (i)

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.

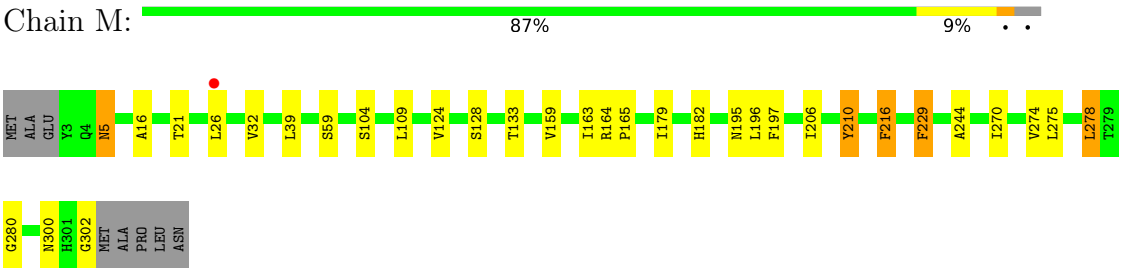
• Molecule 1: Reaction center protein H chain



• 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	141.41Å 141.41Å 186.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.95 – 2.85 38.92 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.95-2.85) 99.9 (38.92-2.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.180 , 0.205 0.187 , 0.208	Depositor DCC
R_{free} test set	2495 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	69.1	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 58.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7273	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: BPH, FE, CDL, LDA, SPO, BCL, TYI, U10

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	0.66	0/1893	0.79	0/2575
2	L	0.67	0/2320	0.75	0/3175
3	M	0.66	0/2472	0.77	0/3373
All	All	0.66	0/6685	0.77	0/9123

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	1844	0	1844	9	0
2	L	2232	0	2187	18	0
3	M	2396	0	2304	20	0
4	H	16	0	31	2	0
4	M	64	0	124	0	0
5	L	65	0	76	1	0
5	M	55	0	53	2	0
6	L	18	0	15	2	0
6	M	38	0	47	2	0
7	L	66	0	74	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	183	0	189	13	0
8	M	1	0	0	0	0
9	M	42	0	60	0	0
10	M	69	0	82	0	0
11	H	82	0	0	1	0
11	L	45	0	0	0	0
11	M	57	0	0	0	0
All	All	7273	0	7086	52	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 (52) 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)
3:M:210:TYI:I2	7:M:401:BCL:C4D	2.77	1.03
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.43	0.96
3:M:210:TYI:I2	7:M:401:BCL:C1D	2.95	0.79
3:M:197:PHE:HZ	7:M:403:BCL:HBB2	1.59	0.67
7:M:402:BCL:HHC	7:M:402:BCL:HBB2	1.76	0.65
5:L:301:BPH:HHC	5:L:301:BPH:HBB3	1.78	0.64
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.77	0.64
3:M:197:PHE:CZ	7:M:403:BCL:HBB2	2.32	0.64
7:M:401:BCL:HBB2	7:M:401:BCL:HHC	1.81	0.61
1:H:156:CYS:HB3	1:H:206:ASN:O	2.01	0.61
3:M:124:VAL:O	3:M:128:SER:OG	2.15	0.59
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.86	0.58
1:H:181:VAL:O	1:H:188:THR:HA	2.05	0.57
7:L:303:BCL:CBB	7:L:303:BCL:HMB1	2.35	0.57
2:L:227:LEU:HD21	3:M:5:ASN:HD21	1.71	0.56
3:M:179:ILE:HG23	7:M:402:BCL:HED1	1.92	0.51
2:L:187:LEU:HD13	3:M:216:PHE:CG	2.45	0.51
2:L:181:PHE:CD2	5:M:409:BPH:HBB1	2.46	0.50
7:M:403:BCL:HAA2	7:M:403:BCL:HBD	1.94	0.49
7:L:303:BCL:HMB1	7:L:303:BCL:HBB3	1.94	0.49
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.95	0.48
1:H:208:LEU:HD11	1:H:237:VAL:HG22	1.96	0.47
3:M:206:ILE:HD13	7:M:401:BCL:HMD1	1.97	0.47
2:L:128:TYR:HD1	7:M:401:BCL:HBB1	1.79	0.47
3:M:270:ILE:O	3:M:274:VAL:HG13	2.15	0.47
2:L:135:ARG:HB3	2:L:136:PRO:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:183:ASN:ND2	2:L:237:SER:HB3	2.30	0.46
1:H:130:LYS:NZ	11:H:405:HOH:O	2.41	0.46
2:L:216:PHE:CZ	6:L:302:U10:H72	2.51	0.46
4:H:301:LDA:H123	6:M:410:U10:H202	1.98	0.46
2:L:21:LEU:HD13	2:L:22:PHE:CE2	2.51	0.45
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.52	0.45
3:M:159:VAL:HA	3:M:163:ILE:HB	1.98	0.45
2:L:100:TRP:CH2	6:M:410:U10:H251	2.51	0.45
1:H:42:LEU:HD11	4:H:301:LDA:HM23	1.99	0.44
2:L:65:SER:HA	2:L:148:TYR:O	2.18	0.44
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.99	0.43
3:M:197:PHE:CE1	7:M:403:BCL:HMC2	2.53	0.43
2:L:210:ASP:N	2:L:210:ASP:OD1	2.52	0.43
2:L:185:LEU:HD12	2:L:185:LEU:O	2.19	0.43
2:L:177:ILE:HG12	7:L:303:BCL:HMB3	2.00	0.42
3:M:300:ASN:C	3:M:302:GLY:H	2.22	0.42
1:H:157:ASP:OD2	1:H:210:SER:OG	2.37	0.42
3:M:275:LEU:HD23	3:M:278:LEU:HD12	2.01	0.41
1:H:138:ALA:HA	1:H:139:GLY:HA2	1.81	0.41
6:L:302:U10:O5	6:L:302:U10:H8	2.19	0.41
2:L:219:LEU:HD11	3:M:133:THR:HG22	2.01	0.41
3:M:280:GLY:HA2	7:M:403:BCL:HED3	2.02	0.41
1:H:87:LEU:HD11	2:L:8:LYS:HA	2.03	0.41
1:H:148:PRO:HA	1:H:151:LEU:HD12	2.03	0.41
2:L:185:LEU:HD13	5:M:409:BPH:C1D	2.50	0.41
7:M:402:BCL:HHC	7:M:402:BCL:CBB	2.46	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	239/266 (90%)	237 (99%)	2 (1%)	0	100	100
2	L	279/282 (99%)	269 (96%)	10 (4%)	0	100	100
3	M	297/308 (96%)	281 (95%)	15 (5%)	1 (0%)	41	68
All	All	815/856 (95%)	787 (97%)	27 (3%)	1 (0%)	51	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	195	ASN

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	196/215 (91%)	191 (97%)	5 (3%)	46	75
2	L	220/221 (100%)	212 (96%)	8 (4%)	35	66
3	M	234/240 (98%)	224 (96%)	10 (4%)	29	59
All	All	650/676 (96%)	627 (96%)	23 (4%)	36	67

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	LEU
1	H	80	SER
1	H	173	GLU
1	H	184	LYS
1	H	231	ASP
2	L	21	LEU
2	L	136	PRO
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	235	LEU
2	L	247	CYS

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Mol	Chain	Res	Type
2	L	272	TRP
3	M	5	ASN
3	M	39	LEU
3	M	59	SER
3	M	104	SER
3	M	109	LEU
3	M	182	HIS
3	M	196	LEU
3	M	216	PHE
3	M	229	PHE
3	M	278	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	183	ASN
2	L	264	GLN
3	M	77	GLN
3	M	202	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TYI	M	210	3	13,14,15	0.89	1 (7%)	16,19,21	2.01	5 (31%)

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
3	TYI	M	210	3	-	2/5/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	210	TYI	CE2-I2	-2.37	2.04	2.10

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	210	TYI	CB-CG-CD1	3.84	127.02	120.44
3	M	210	TYI	CD2-CE2-I2	-3.34	112.44	118.61
3	M	210	TYI	CZ-CE1-I1	3.33	124.55	119.42
3	M	210	TYI	CB-CG-CD2	-2.82	115.59	120.44
3	M	210	TYI	CZ-CE2-I2	2.46	123.22	119.42

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	210	TYI	CA-CB-CG-CD1
3	M	210	TYI	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	210	TYI	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	BCL	M	402	-	43,59,74	1.93	11 (25%)	51,97,115	1.81	15 (29%)
5	BPH	L	301	-	64,70,70	0.58	1 (1%)	76,101,101	0.82	5 (6%)
9	SPO	M	411	-	40,41,41	1.59	8 (20%)	47,50,50	1.19	7 (14%)
4	LDA	M	405	-	12,15,15	0.12	0	14,17,17	0.31	0
4	LDA	H	301	-	12,15,15	0.12	0	14,17,17	0.28	0
5	BPH	M	409	-	54,60,70	0.61	1 (1%)	64,89,101	0.95	3 (4%)
6	U10	M	410	-	38,38,63	0.74	2 (5%)	46,49,79	0.50	0
7	BCL	L	303	-	58,74,74	1.62	7 (12%)	69,115,115	1.62	16 (23%)
4	LDA	M	407	-	12,15,15	0.18	0	14,17,17	0.16	0
4	LDA	M	404	-	12,15,15	0.21	0	14,17,17	0.23	0
7	BCL	M	401	-	58,74,74	1.61	10 (17%)	69,115,115	1.85	18 (26%)
10	CDL	M	412	-	68,68,99	0.34	0	74,80,111	0.45	0
6	U10	L	302	-	18,18,63	0.95	2 (11%)	22,25,79	1.07	2 (9%)
7	BCL	M	403	-	58,74,74	1.64	7 (12%)	69,115,115	1.73	15 (21%)
4	LDA	M	406	-	12,15,15	0.16	0	14,17,17	0.18	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	BCL	M	402	-	-	5/19/119/137	-
5	BPH	L	301	-	-	9/54/105/105	0/5/6/6
9	SPO	M	411	-	-	7/47/47/47	-
4	LDA	M	405	-	-	3/13/13/13	-
5	BPH	M	409	-	1/1/16/22	15/42/93/105	0/5/6/6
4	LDA	H	301	-	-	4/13/13/13	-
6	U10	M	410	-	-	3/33/57/87	0/1/1/1
7	BCL	L	303	-	-	3/37/137/137	-
4	LDA	M	404	-	-	3/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	M	407	-	-	4/13/13/13	-
7	BCL	M	401	-	-	7/37/137/137	-
10	CDL	M	412	-	-	21/79/79/110	-
6	U10	L	302	-	-	6/9/33/87	0/1/1/1
7	BCL	M	403	-	-	10/37/137/137	-
4	LDA	M	406	-	-	3/13/13/13	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	303	BCL	O2D-CGD	5.45	1.46	1.33
7	L	303	BCL	OBD-CAD	5.29	1.29	1.22
7	M	401	BCL	O2D-CGD	5.10	1.45	1.33
7	M	403	BCL	O2D-CGD	4.92	1.45	1.33
7	M	402	BCL	O2D-CGD	4.87	1.45	1.33
7	M	403	BCL	C3B-C2B	4.84	1.48	1.39
7	M	402	BCL	O2A-CGA	4.81	1.47	1.33
7	M	403	BCL	OBD-CAD	4.80	1.29	1.22
7	M	403	BCL	C3D-C2D	4.67	1.47	1.39
7	M	402	BCL	C3D-C2D	4.56	1.47	1.39
7	M	402	BCL	C3B-C2B	4.48	1.47	1.39
7	M	401	BCL	O2A-CGA	4.44	1.46	1.33
7	M	401	BCL	C3B-C2B	4.41	1.47	1.39
7	M	401	BCL	C3D-C2D	4.36	1.47	1.39
7	M	402	BCL	OBD-CAD	4.29	1.28	1.22
7	L	303	BCL	C3D-C2D	4.16	1.46	1.39
7	L	303	BCL	C3B-C2B	4.10	1.46	1.39
7	L	303	BCL	O2A-CGA	4.06	1.45	1.33
9	M	411	SPO	C9-C7	4.01	1.41	1.35
7	M	401	BCL	OBD-CAD	4.00	1.27	1.22
7	M	403	BCL	O2A-CGA	3.97	1.45	1.33
9	M	411	SPO	C14-C12	3.72	1.40	1.35
9	M	411	SPO	C19-C17	3.63	1.40	1.35
7	M	402	BCL	C2D-C1D	3.53	1.50	1.42
9	M	411	SPO	C22-C23	3.43	1.40	1.35
7	M	403	BCL	C2D-C1D	3.43	1.50	1.42
7	L	303	BCL	C2D-C1D	3.16	1.49	1.42
7	M	401	BCL	C2D-C1D	3.07	1.49	1.42
9	M	411	SPO	C16-C17	-2.68	1.40	1.45
9	M	411	SPO	C25-C23	-2.62	1.40	1.45
7	M	401	BCL	C1B-CHB	2.49	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	411	SPO	C11-C12	-2.47	1.40	1.45
7	M	401	BCL	MG-NA	-2.39	2.00	2.06
7	M	402	BCL	C1B-CHB	2.36	1.47	1.41
6	L	302	U10	C3-C2	-2.31	1.42	1.48
6	M	410	U10	C4-C5	-2.23	1.42	1.48
6	M	410	U10	C6-C1	2.22	1.39	1.35
7	L	303	BCL	C4B-CHC	2.22	1.47	1.41
7	M	402	BCL	MG-NA	-2.21	2.01	2.06
7	M	402	BCL	MG-NC	-2.21	2.01	2.06
7	M	401	BCL	MG-NC	-2.19	2.01	2.06
7	M	402	BCL	CHD-C4C	2.16	1.47	1.41
7	M	401	BCL	C4B-CHC	2.14	1.46	1.41
6	L	302	U10	C6-C1	2.13	1.39	1.35
5	L	301	BPH	CHC-C4B	2.08	1.45	1.40
7	M	402	BCL	C4B-CHC	2.07	1.46	1.41
9	M	411	SPO	C6-C7	-2.07	1.41	1.45
5	M	409	BPH	C3D-C2D	2.03	1.43	1.39
7	M	403	BCL	C4B-CHC	2.03	1.46	1.41

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	401	BCL	O2D-CGD-CBD	5.49	121.02	111.27
7	M	402	BCL	O2D-CGD-CBD	5.47	120.99	111.27
7	M	401	BCL	CHD-C4C-NC	5.06	130.70	125.08
7	M	403	BCL	O2D-CGD-CBD	4.68	119.58	111.27
7	M	403	BCL	CHD-C4C-NC	4.40	129.96	125.08
7	M	401	BCL	C3C-C4C-CHD	-4.35	114.10	123.39
7	M	401	BCL	C4C-CHD-C1D	-4.31	119.53	125.88
7	L	303	BCL	CHD-C4C-NC	4.20	129.74	125.08
7	L	303	BCL	C4C-CHD-C1D	-4.19	119.69	125.88
7	L	303	BCL	C3C-C4C-CHD	-4.12	114.60	123.39
7	M	403	BCL	C4C-CHD-C1D	-4.03	119.94	125.88
7	M	403	BCL	C3C-C4C-CHD	-4.00	114.86	123.39
7	M	402	BCL	CHD-C4C-NC	3.95	129.46	125.08
7	M	403	BCL	CHC-C1C-NC	3.71	129.64	124.51
7	M	401	BCL	CHC-C1C-NC	3.69	129.61	124.51
7	M	402	BCL	C3C-C4C-CHD	-3.68	115.53	123.39
7	L	303	BCL	CED-O2D-CGD	3.68	124.25	115.94
7	M	403	BCL	CMB-C2B-C3B	3.67	131.54	124.68
7	M	401	BCL	C4A-NA-C1A	3.65	108.35	106.71
7	M	401	BCL	CHB-C4A-NA	3.53	129.40	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	403	BCL	O2D-CGD-O1D	-3.53	116.94	123.84
6	L	302	U10	C7-C6-C5	3.49	122.67	118.48
7	L	303	BCL	CHB-C4A-NA	3.17	128.89	124.51
7	M	403	BCL	CHB-C4A-NA	3.14	128.85	124.51
7	M	401	BCL	C1C-NC-C4C	-3.13	105.30	106.71
5	M	409	BPH	C1C-NC-C4C	-3.10	107.81	110.54
7	M	402	BCL	CHC-C1C-NC	3.06	128.75	124.51
7	M	401	BCL	OBD-CAD-C3D	-3.05	122.92	127.98
7	L	303	BCL	CHC-C1C-NC	3.04	128.71	124.51
7	M	402	BCL	C1-O2A-CGA	3.02	124.36	116.44
7	M	402	BCL	C4C-CHD-C1D	-3.00	121.45	125.88
7	M	401	BCL	C1-O2A-CGA	2.93	124.13	116.44
7	M	402	BCL	CHB-C4A-NA	2.89	128.51	124.51
7	L	303	BCL	O2A-CGA-CBA	2.87	120.90	111.91
7	L	303	BCL	CMB-C2B-C3B	2.85	130.01	124.68
7	L	303	BCL	C4-C3-C5	2.84	120.05	115.27
7	L	303	BCL	CAD-C3D-C4D	2.78	110.02	108.47
7	M	403	BCL	C4-C3-C5	2.66	119.74	115.27
7	M	402	BCL	CMB-C2B-C3B	2.66	129.65	124.68
7	L	303	BCL	C2A-C1A-CHA	-2.59	119.32	123.86
7	M	401	BCL	C4-C3-C5	2.58	119.62	115.27
7	M	403	BCL	O2A-CGA-CBA	2.53	119.86	111.91
7	M	401	BCL	O1D-CGD-CBD	-2.52	119.32	124.48
7	M	402	BCL	O1D-CGD-CBD	-2.51	119.35	124.48
5	L	301	BPH	CHD-C4C-NC	-2.50	122.23	125.20
7	L	303	BCL	O2A-CGA-O1A	-2.50	117.28	123.59
7	L	303	BCL	C1B-CHB-C4A	-2.46	125.24	130.12
7	M	401	BCL	C4B-CHC-C1C	-2.45	125.27	130.12
9	M	411	SPO	C24-C23-C22	-2.42	119.54	122.92
5	L	301	BPH	C4A-NA-C1A	-2.40	106.20	108.14
7	M	403	BCL	C4B-C3B-CAB	2.38	131.71	127.13
7	L	303	BCL	C5-C3-C2	-2.36	116.35	121.12
7	M	401	BCL	C5-C3-C2	-2.34	116.38	121.12
5	L	301	BPH	C1B-NB-C4B	2.31	110.87	106.51
9	M	411	SPO	C10-C9-C7	2.28	130.56	127.31
7	M	403	BCL	CED-O2D-CGD	2.27	121.07	115.94
7	M	402	BCL	C1B-CHB-C4A	-2.24	125.68	130.12
9	M	411	SPO	C18-C17-C19	-2.23	119.80	122.92
9	M	411	SPO	C13-C12-C14	-2.21	119.82	122.92
7	M	403	BCL	C4A-NA-C1A	2.20	107.69	106.71
7	M	402	BCL	O2A-CGA-CBA	2.19	118.77	111.91
7	M	401	BCL	C1B-CHB-C4A	-2.18	125.80	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	402	BCL	C2A-C1A-CHA	-2.17	120.06	123.86
7	M	402	BCL	C4B-CHC-C1C	-2.17	125.82	130.12
9	M	411	SPO	C8-C7-C9	-2.16	119.90	122.92
7	M	403	BCL	C4B-CHC-C1C	-2.15	125.85	130.12
5	L	301	BPH	C1C-NC-C4C	-2.15	108.65	110.54
7	L	303	BCL	C4B-CHC-C1C	-2.15	125.86	130.12
7	M	401	BCL	O2A-CGA-CBA	2.15	118.65	111.91
5	M	409	BPH	C1B-NB-C4B	2.14	110.54	106.51
7	M	401	BCL	O2D-CGD-O1D	-2.14	119.65	123.84
7	M	402	BCL	O2D-CGD-O1D	-2.14	119.65	123.84
7	L	303	BCL	O2D-CGD-CBD	2.14	115.07	111.27
7	M	401	BCL	CMB-C2B-C3B	2.11	128.62	124.68
7	M	402	BCL	C1-C2-C3	-2.11	123.34	126.75
7	M	403	BCL	C1C-NC-C4C	-2.10	105.76	106.71
9	M	411	SPO	C21-C20-C19	2.09	127.76	123.47
5	M	409	BPH	CHD-C4C-NC	-2.08	122.73	125.20
6	L	302	U10	C8-C7-C6	2.07	117.62	112.05
5	L	301	BPH	C2B-C1B-NB	-2.06	106.68	109.79
9	M	411	SPO	C20-C21-C22	2.00	127.58	123.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	409	BPH	C8

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	301	LDA	C2-C1-N1-CM1
4	M	405	LDA	N1-C1-C2-C3
5	M	409	BPH	C4C-C3C-CAC-CBC
5	M	409	BPH	C2C-C3C-CAC-CBC
5	M	409	BPH	C4B-C3B-CAB-CBB
5	M	409	BPH	C4B-C3B-CAB-OBB
6	L	302	U10	C1-C6-C7-C8
6	L	302	U10	C5-C6-C7-C8
7	M	401	BCL	CHA-CBD-CGD-O2D
7	M	403	BCL	CBD-CGD-O2D-CED
9	M	411	SPO	C4-C1-O1-CM1
10	M	412	CDL	CA3-OA5-PA1-OA2
10	M	412	CDL	CA3-OA5-PA1-OA3
10	M	412	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
10	M	412	CDL	CB2-OB2-PB2-OB3
7	M	401	BCL	CBD-CGD-O2D-CED
7	M	403	BCL	O1D-CGD-O2D-CED
7	M	402	BCL	CBD-CGD-O2D-CED
7	M	401	BCL	O1D-CGD-O2D-CED
7	M	402	BCL	O1D-CGD-O2D-CED
10	M	412	CDL	CA7-C31-C32-C33
5	L	301	BPH	C11-C12-C13-C15
6	M	410	U10	C24-C26-C27-C28
6	L	302	U10	C7-C8-C9-C10
5	M	409	BPH	C5-C6-C7-C8
10	M	412	CDL	C33-C34-C35-C36
4	M	404	LDA	C4-C5-C6-C7
4	H	301	LDA	C6-C7-C8-C9
10	M	412	CDL	C13-C14-C15-C16
4	M	405	LDA	C1-C2-C3-C4
4	M	406	LDA	C1-C2-C3-C4
4	M	407	LDA	C1-C2-C3-C4
10	M	412	CDL	C11-CA5-OA6-CA4
6	L	302	U10	C7-C8-C9-C11
7	L	303	BCL	C2A-CAA-CBA-CGA
7	M	401	BCL	C15-C16-C17-C18
4	H	301	LDA	C9-C10-C11-C12
4	M	404	LDA	C1-C2-C3-C4
4	M	406	LDA	C9-C10-C11-C12
4	M	407	LDA	C3-C4-C5-C6
5	L	301	BPH	C13-C15-C16-C17
7	M	403	BCL	C13-C15-C16-C17
10	M	412	CDL	OA5-CA3-CA4-OA6
4	M	407	LDA	C9-C10-C11-C12
9	M	411	SPO	C3-C1-O1-CM1
10	M	412	CDL	OA7-CA5-OA6-CA4
10	M	412	CDL	C39-C40-C41-C42
10	M	412	CDL	C17-C18-C19-C20
10	M	412	CDL	CB2-OB2-PB2-OB5
4	M	405	LDA	C6-C7-C8-C9
7	M	402	BCL	C4C-C3C-CAC-CBC
7	M	403	BCL	C16-C17-C18-C19
5	L	301	BPH	C5-C6-C7-C8
9	M	411	SPO	C18-C17-C19-C20
5	L	301	BPH	CAD-CBD-CGD-O2D
7	M	401	BCL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
7	L	303	BCL	C15-C16-C17-C18
7	M	403	BCL	C6-C7-C8-C9
10	M	412	CDL	CB2-OB2-PB2-OB4
7	M	403	BCL	CAD-CBD-CGD-O1D
5	L	301	BPH	O2A-C1-C2-C3
5	M	409	BPH	O2A-C1-C2-C3
5	L	301	BPH	C11-C12-C13-C14
6	M	410	U10	C14-C16-C17-C18
5	M	409	BPH	C2B-C3B-CAB-OBB
5	L	301	BPH	C4-C3-C5-C6
5	M	409	BPH	C4-C3-C5-C6
10	M	412	CDL	OA5-CA3-CA4-CA6
10	M	412	CDL	C72-C71-CB7-OB8
9	M	411	SPO	C2-C1-O1-CM1
5	M	409	BPH	C6-C7-C8-C10
6	L	302	U10	C5-C4-O4-C4M
4	H	301	LDA	C11-C10-C9-C8
4	M	406	LDA	C2-C3-C4-C5
5	M	409	BPH	C6-C7-C8-C9
10	M	412	CDL	C72-C73-C74-C75
9	M	411	SPO	C34-C33-C35-C36
7	M	401	BCL	C12-C13-C15-C16
7	M	403	BCL	C6-C7-C8-C10
6	L	302	U10	C3-C4-O4-C4M
6	M	410	U10	C3-C4-O4-C4M
5	L	301	BPH	C2-C3-C5-C6
9	M	411	SPO	C32-C33-C35-C36
4	M	404	LDA	C11-C10-C9-C8
10	M	412	CDL	C36-C37-C38-C39
5	M	409	BPH	C2-C3-C5-C6
5	L	301	BPH	C4B-C3B-CAB-OBB
5	M	409	BPH	C2B-C3B-CAB-CBB
5	M	409	BPH	CAD-CBD-CGD-O2D
7	L	303	BCL	CAD-CBD-CGD-O2D
10	M	412	CDL	C71-C72-C73-C74
10	M	412	CDL	C52-C51-CB5-OB6
5	M	409	BPH	CHA-CBD-CGD-O2D
7	M	402	BCL	CHA-CBD-CGD-O1D
7	M	402	BCL	CHA-CBD-CGD-O2D
7	M	403	BCL	CHA-CBD-CGD-O1D
7	M	403	BCL	C16-C17-C18-C20
5	M	409	BPH	NC-C1C-CHC-C4B

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Mol	Chain	Res	Type	Atoms
4	M	407	LDA	C6-C7-C8-C9
10	M	412	CDL	C52-C51-CB5-OB7
7	M	401	BCL	C14-C13-C15-C16
9	M	411	SPO	C1-C4-C5-C6
7	M	403	BCL	C11-C12-C13-C15

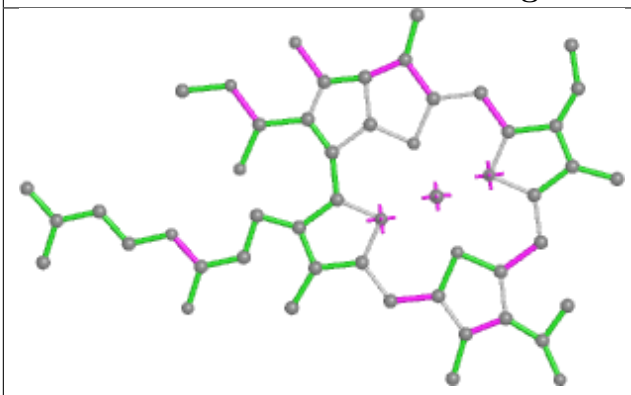
There are no ring outliers.

9 monomers are involved in 24 short contacts:

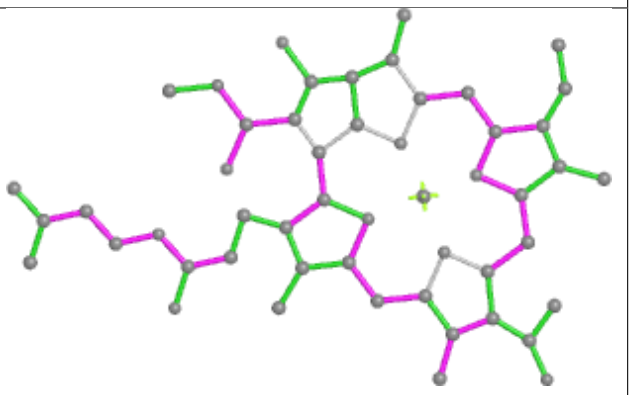
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	402	BCL	3	0
5	L	301	BPH	1	0
4	H	301	LDA	2	0
5	M	409	BPH	2	0
6	M	410	U10	2	0
7	L	303	BCL	3	0
7	M	401	BCL	5	0
6	L	302	U10	2	0
7	M	403	BCL	5	0

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

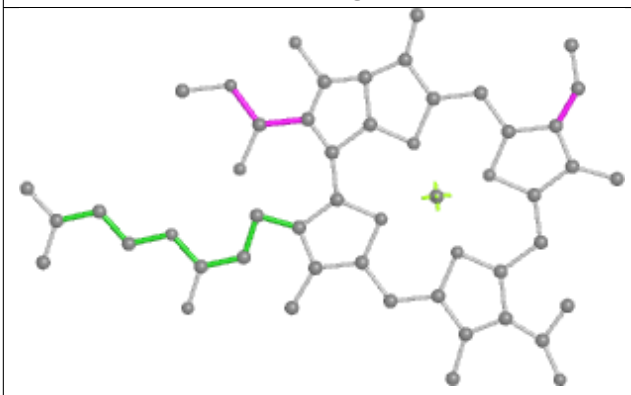
Ligand BCL M 402



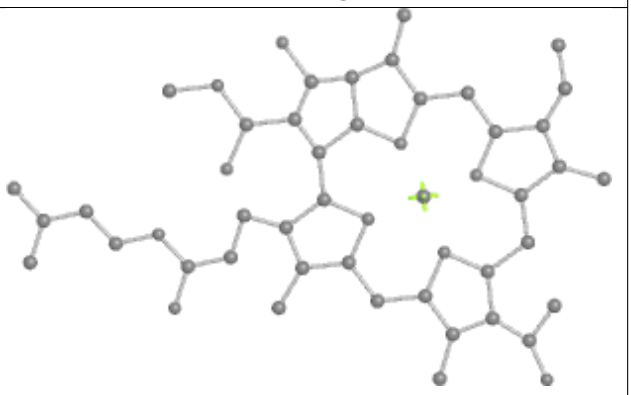
Bond lengths



Bond angles

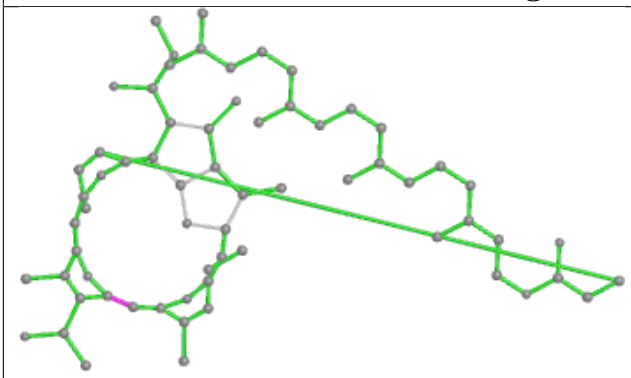


Torsions

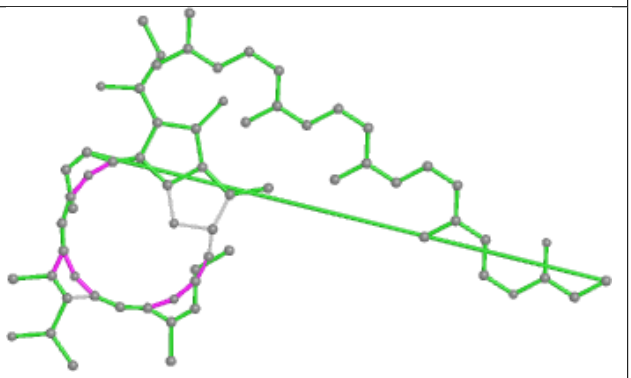


Rings

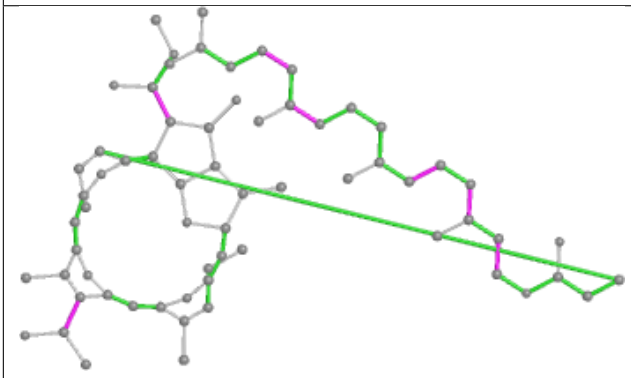
Ligand BPH L 301



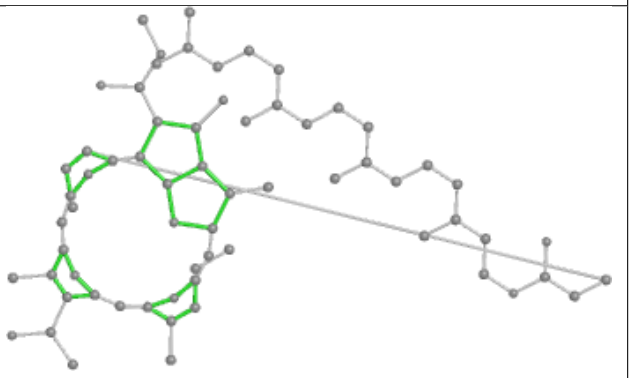
Bond lengths



Bond angles

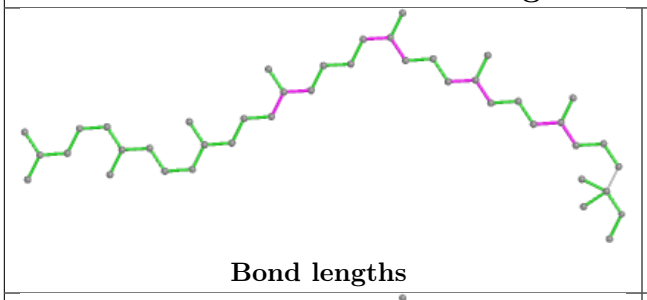


Torsions

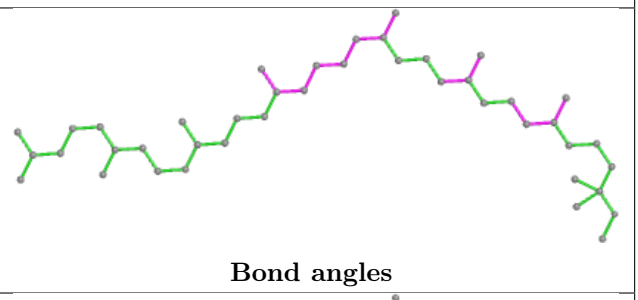


Rings

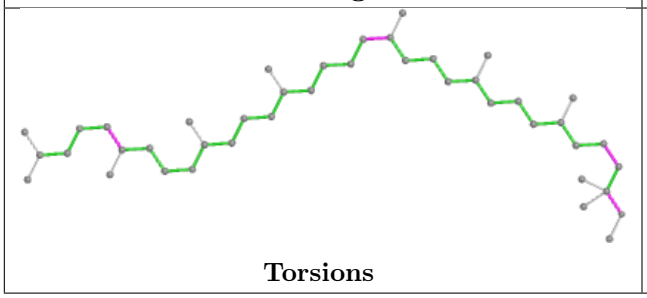
Ligand SPO M 411



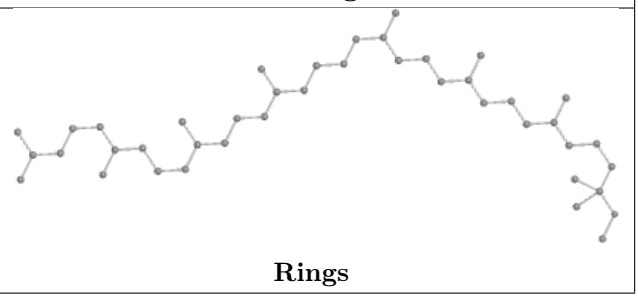
Bond lengths



Bond angles

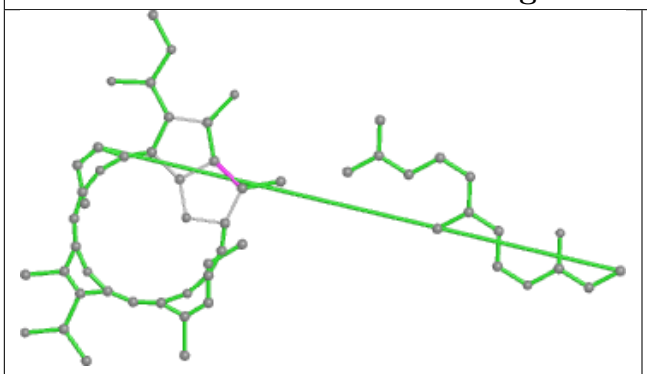


Torsions

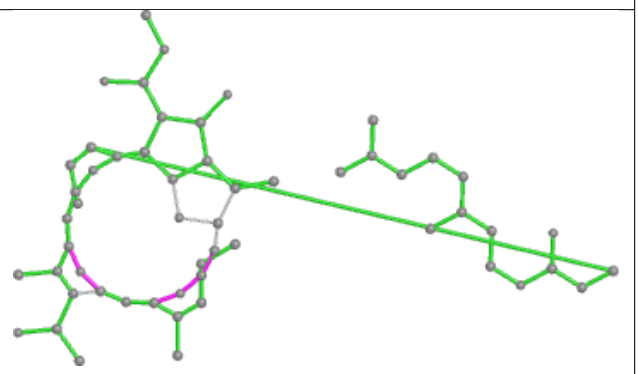


Rings

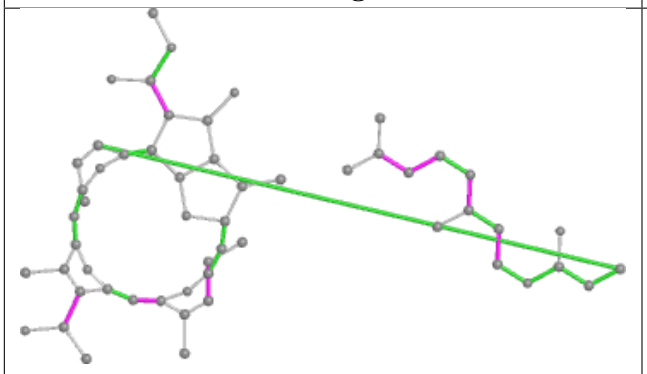
Ligand BPH M 409



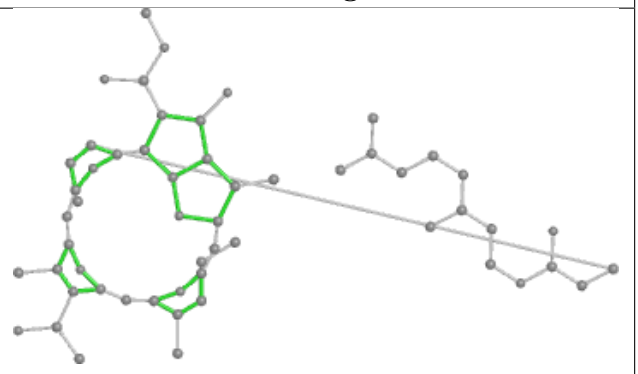
Bond lengths



Bond angles

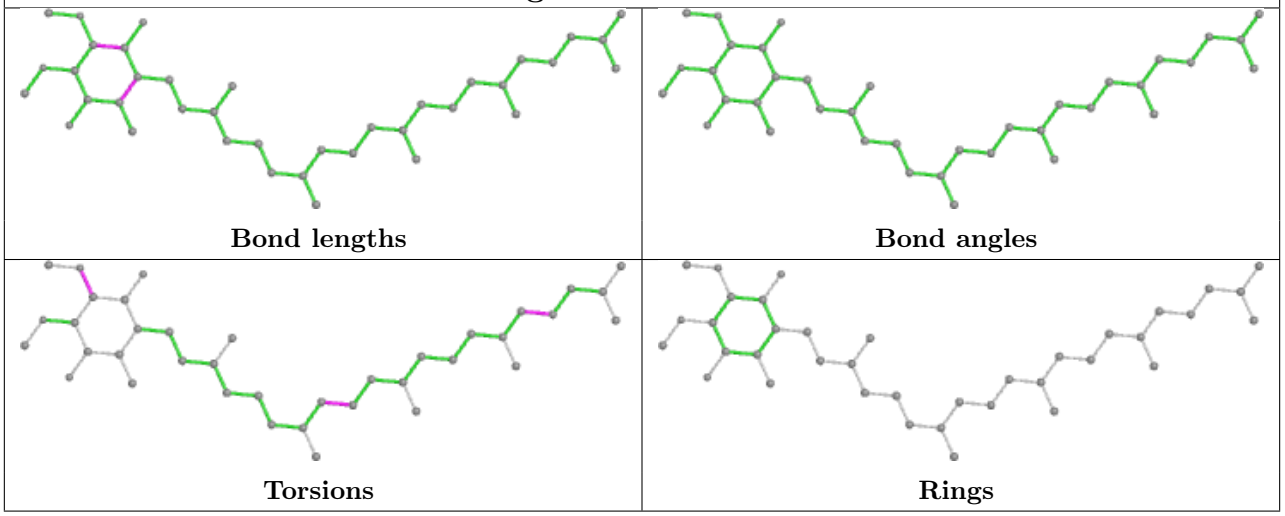


Torsions

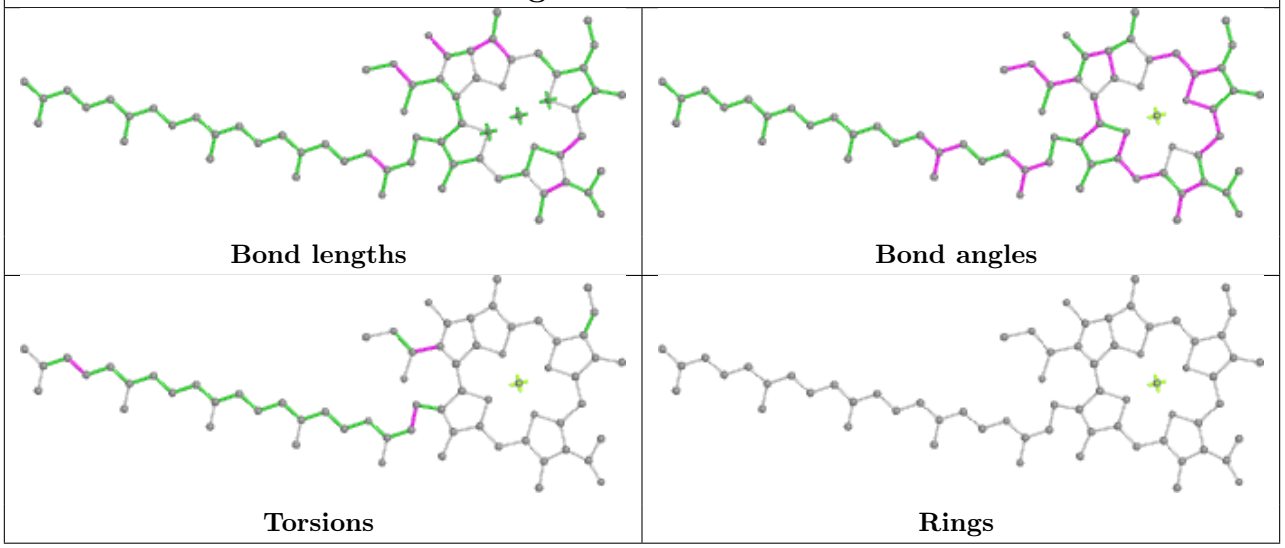


Rings

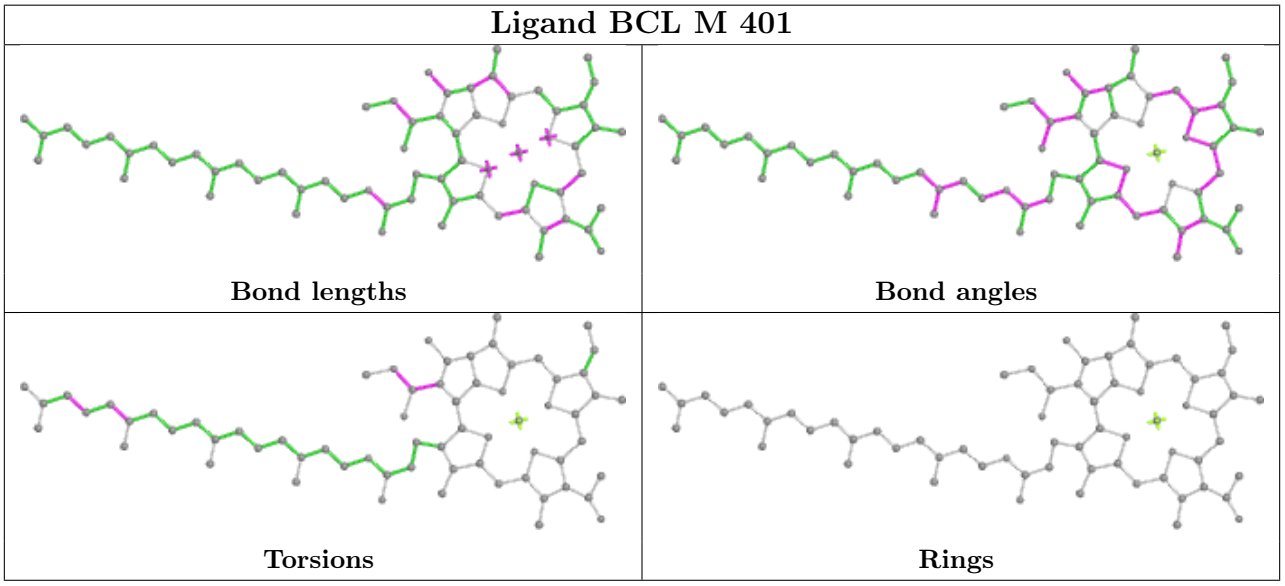
Ligand U10 M 410



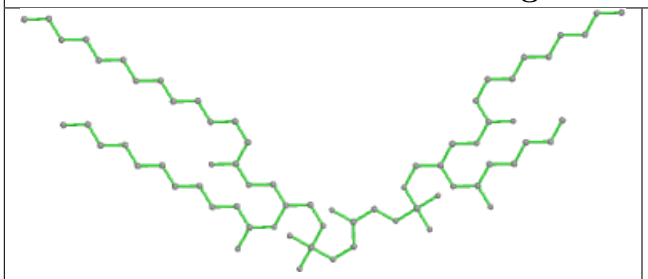
Ligand BCL L 303



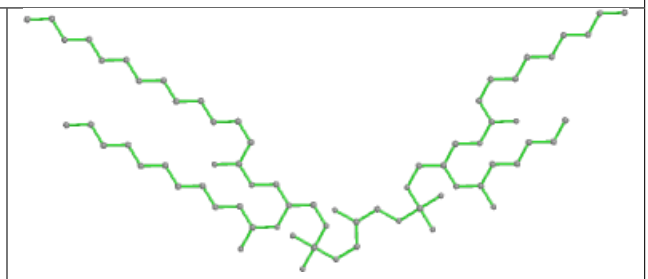
Ligand BCL M 401



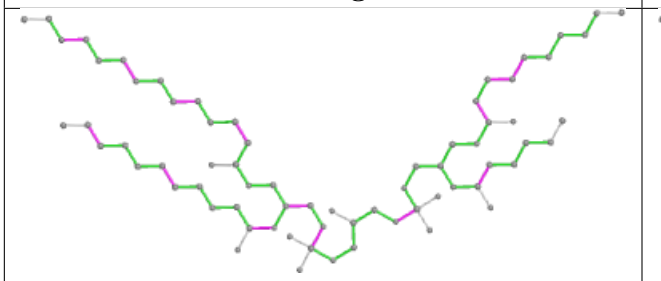
Ligand CDL M 412



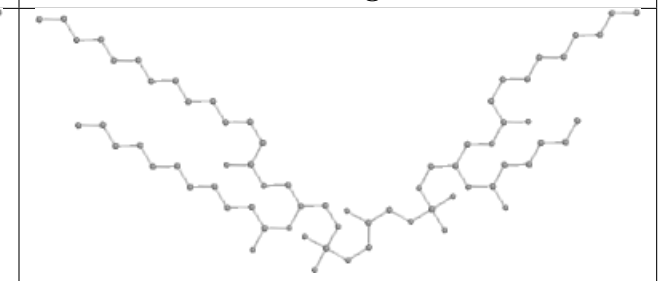
Bond lengths



Bond angles

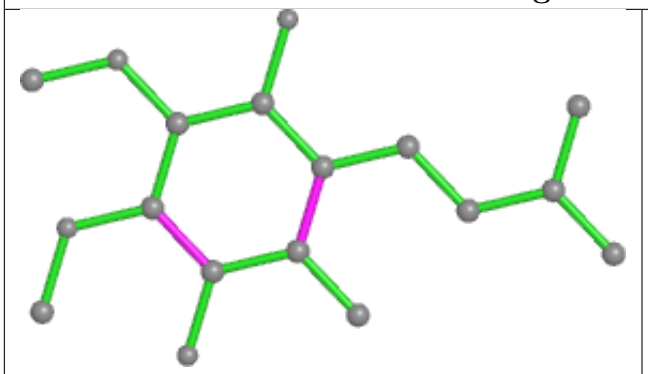


Torsions

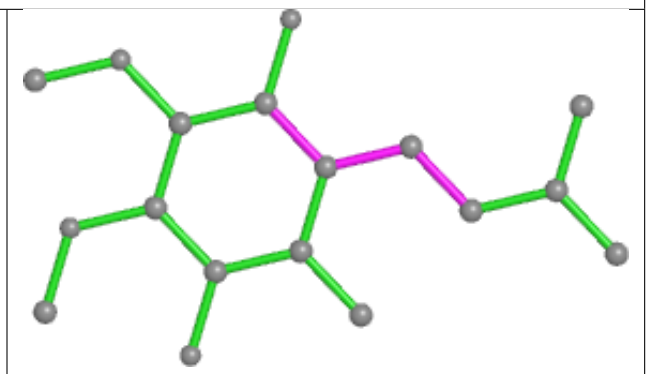


Rings

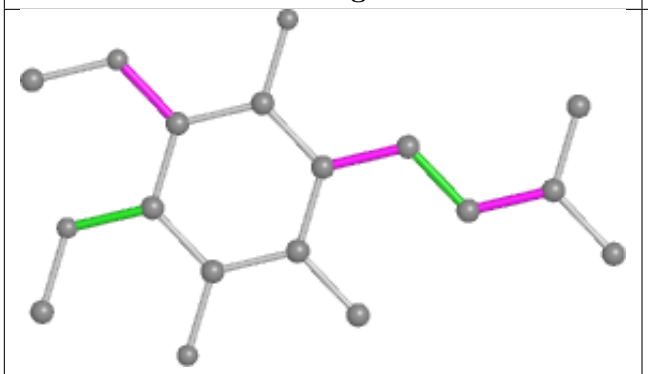
Ligand U10 L 302



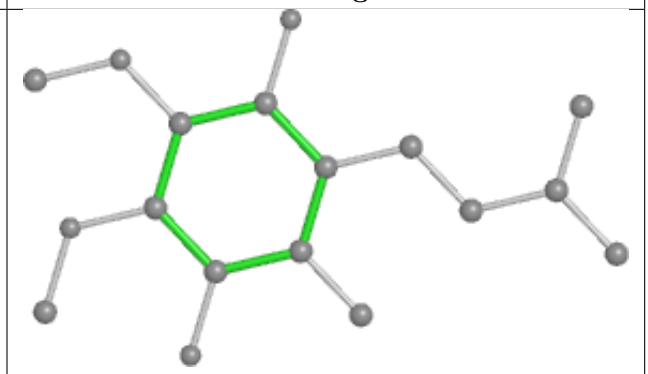
Bond lengths



Bond angles

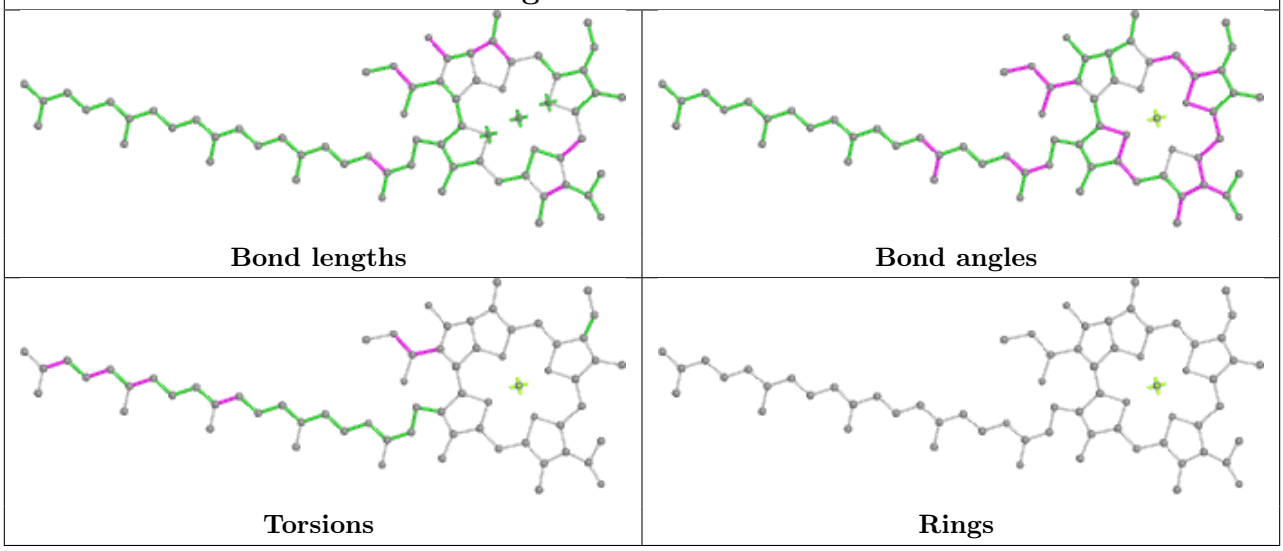


Torsions



Rings

Ligand BCL M 403



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	H	239/266 (89%)	-0.48	3 (1%)	77	76	49, 69, 93, 114	0
2	L	281/282 (99%)	-0.29	9 (3%)	47	42	51, 69, 107, 120	0
3	M	299/308 (97%)	-0.38	1 (0%)	94	94	47, 72, 106, 125	0
All	All	819/856 (95%)	-0.38	13 (1%)	72	70	47, 70, 104, 125	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	270	PRO	4.2
2	L	281	GLY	4.0
2	L	72	GLU	3.4
2	L	274	ASN	2.9
2	L	202	LYS	2.7
1	H	102	GLY	2.7
2	L	73	TYR	2.4
3	M	26	LEU	2.4
1	H	200	SER	2.3
1	H	18[A]	TYR	2.2
2	L	276	PRO	2.1
2	L	277	GLY	2.1
2	L	59	TRP	2.0

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

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
3	TYI	M	210	14/15	0.99	0.15	56,59,62,62	2

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

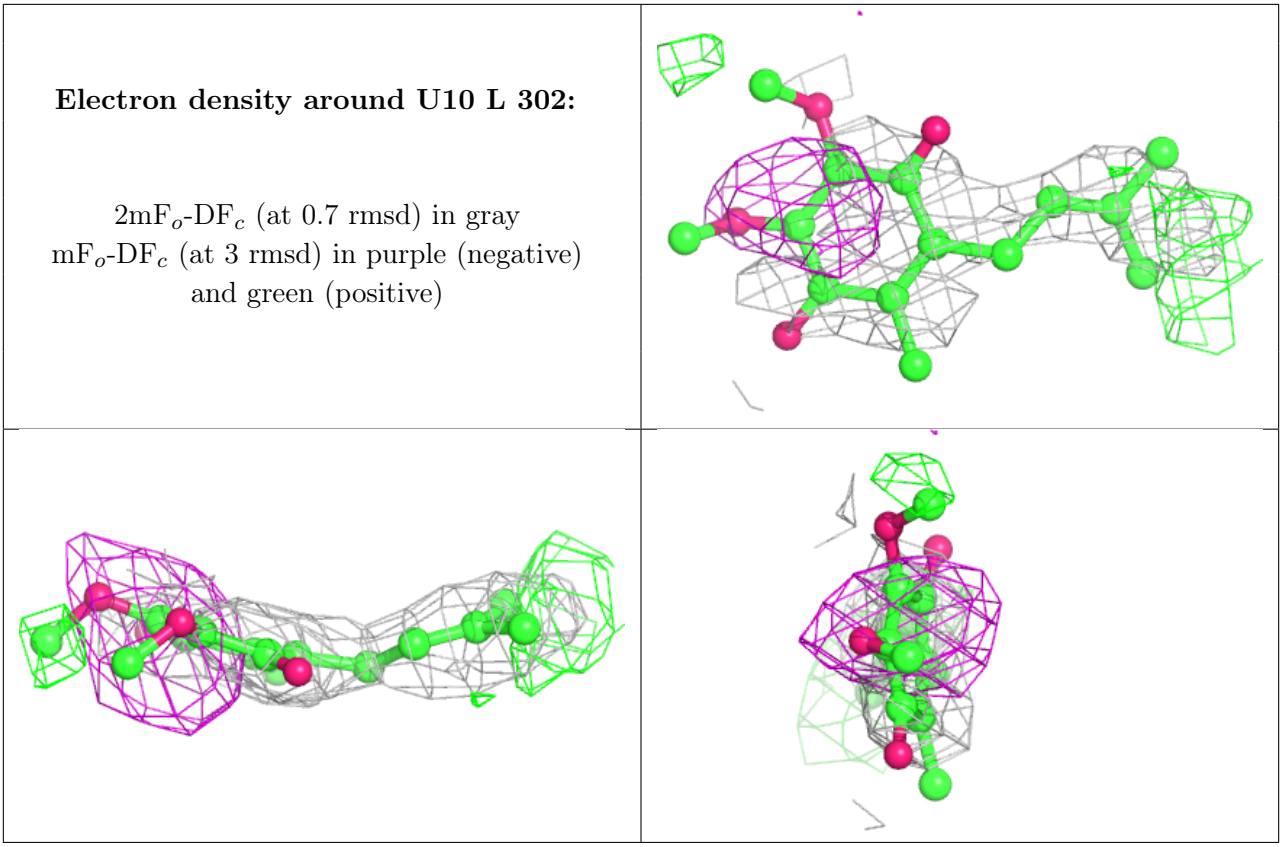
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	LDA	M	407	16/16	0.73	0.26	104,110,135,135	0
6	U10	L	302	18/63	0.77	0.34	105,124,135,138	0
4	LDA	M	406	16/16	0.82	0.31	98,114,125,126	0
4	LDA	M	405	16/16	0.86	0.43	86,93,125,128	0
4	LDA	M	404	16/16	0.90	0.26	83,94,98,101	0
9	SPO	M	411	42/42	0.91	0.23	75,90,111,116	0
10	CDL	M	412	69/100	0.91	0.21	77,99,114,127	0
5	BPH	M	409	55/65	0.94	0.21	65,77,110,114	0
4	LDA	H	301	16/16	0.94	0.19	73,81,105,106	0
7	BCL	L	303	66/66	0.96	0.17	48,58,85,90	0
7	BCL	M	401	66/66	0.96	0.17	49,58,87,91	0
5	BPH	L	301	65/65	0.96	0.18	46,57,84,87	0
6	U10	M	410	38/63	0.96	0.22	51,66,94,100	0
7	BCL	M	403	66/66	0.97	0.18	52,59,95,105	0
7	BCL	M	402	51/66	0.98	0.15	55,60,78,80	0
8	FE	M	408	1/1	0.99	0.15	57,57,57,57	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.

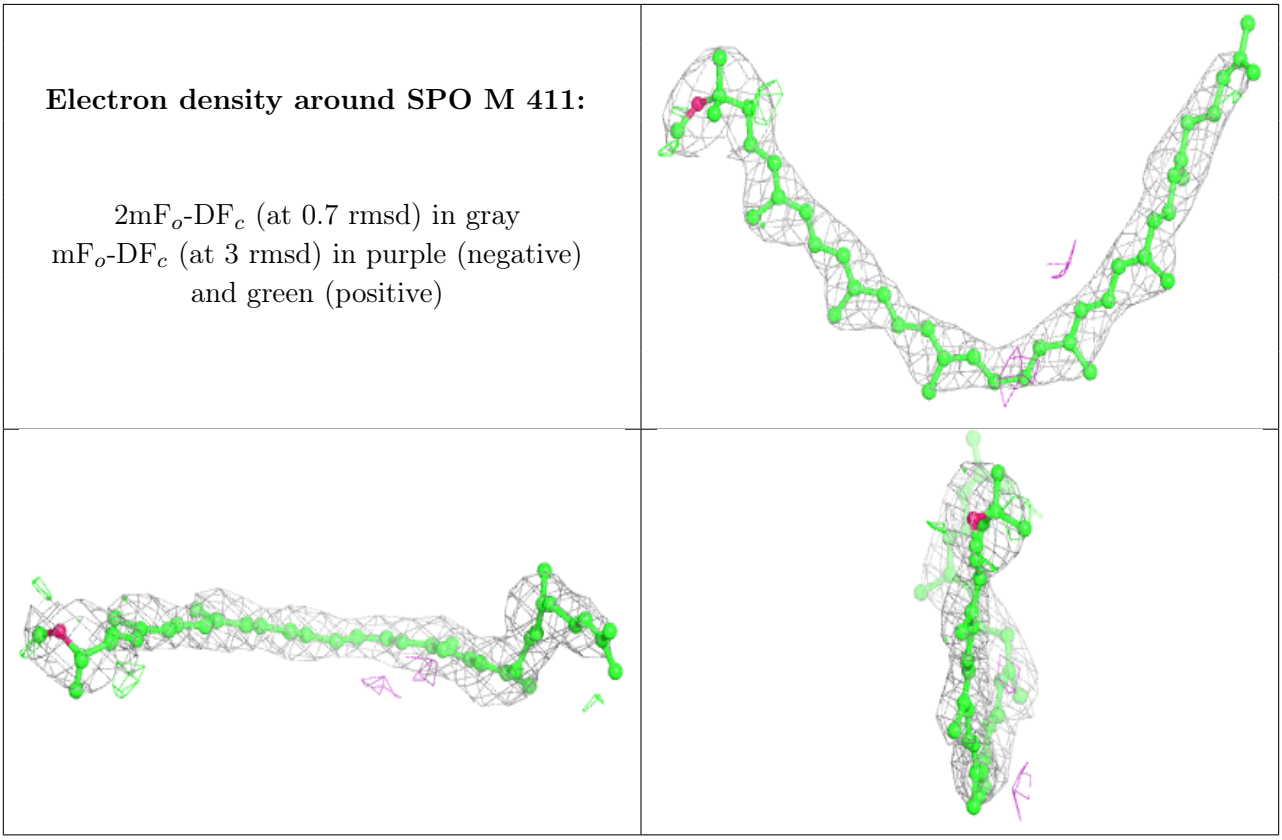
Electron density around U10 L 302:

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



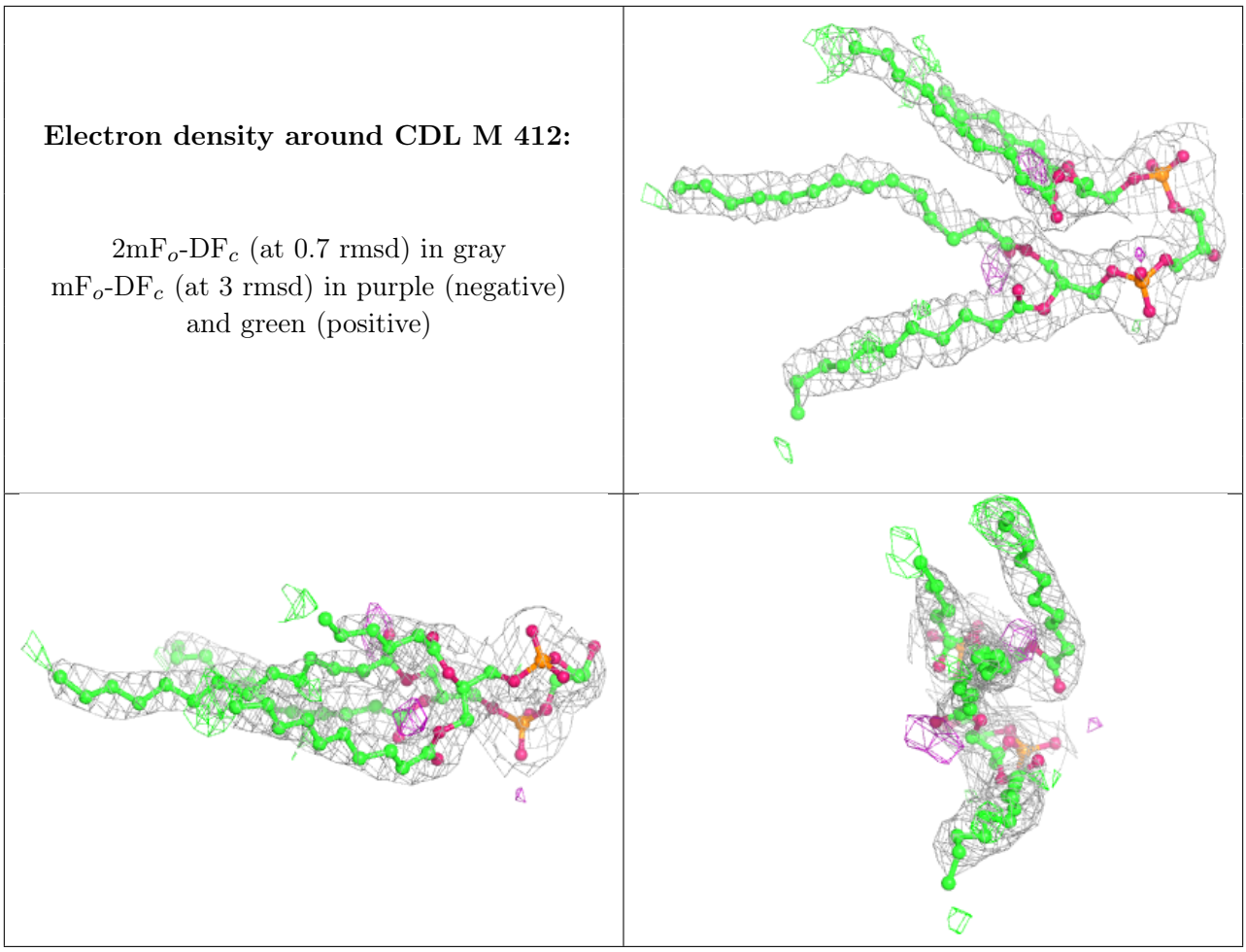
Electron density around SPO M 411:

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



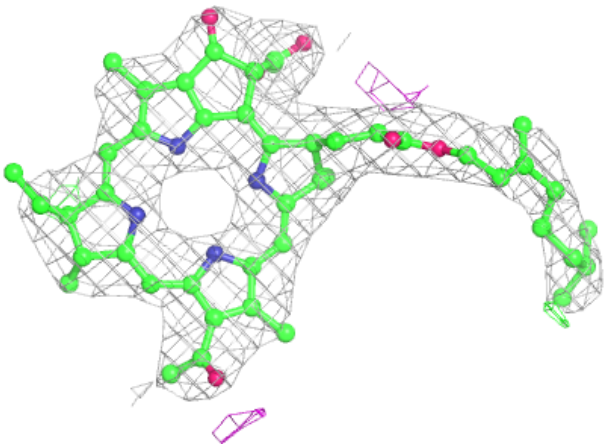
Electron density around CDL M 412:

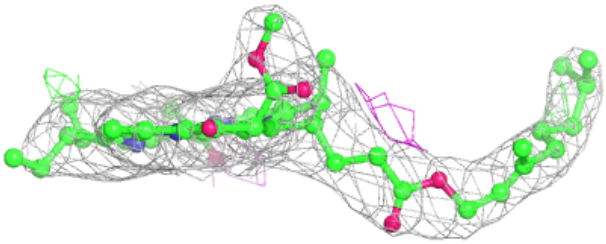
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

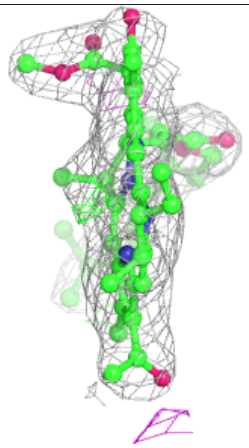


Electron density around BPH M 409:

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

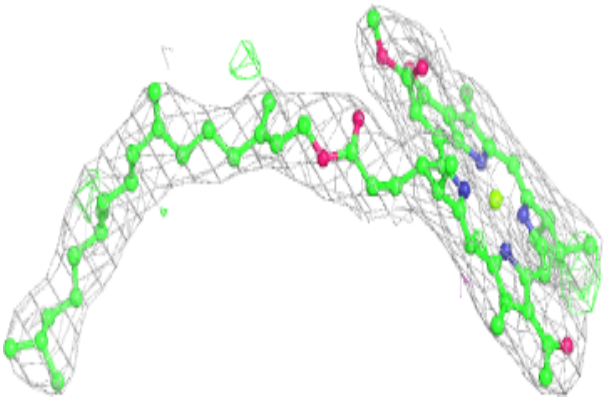


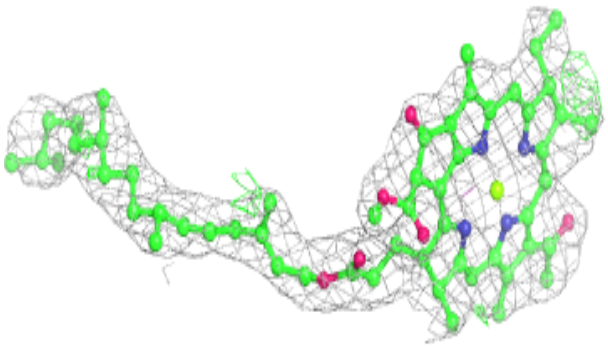


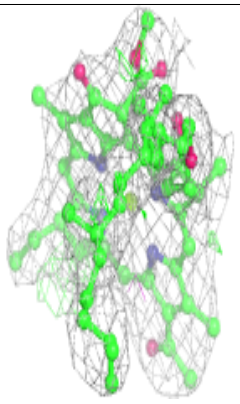


Electron density around BCL L 303:

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

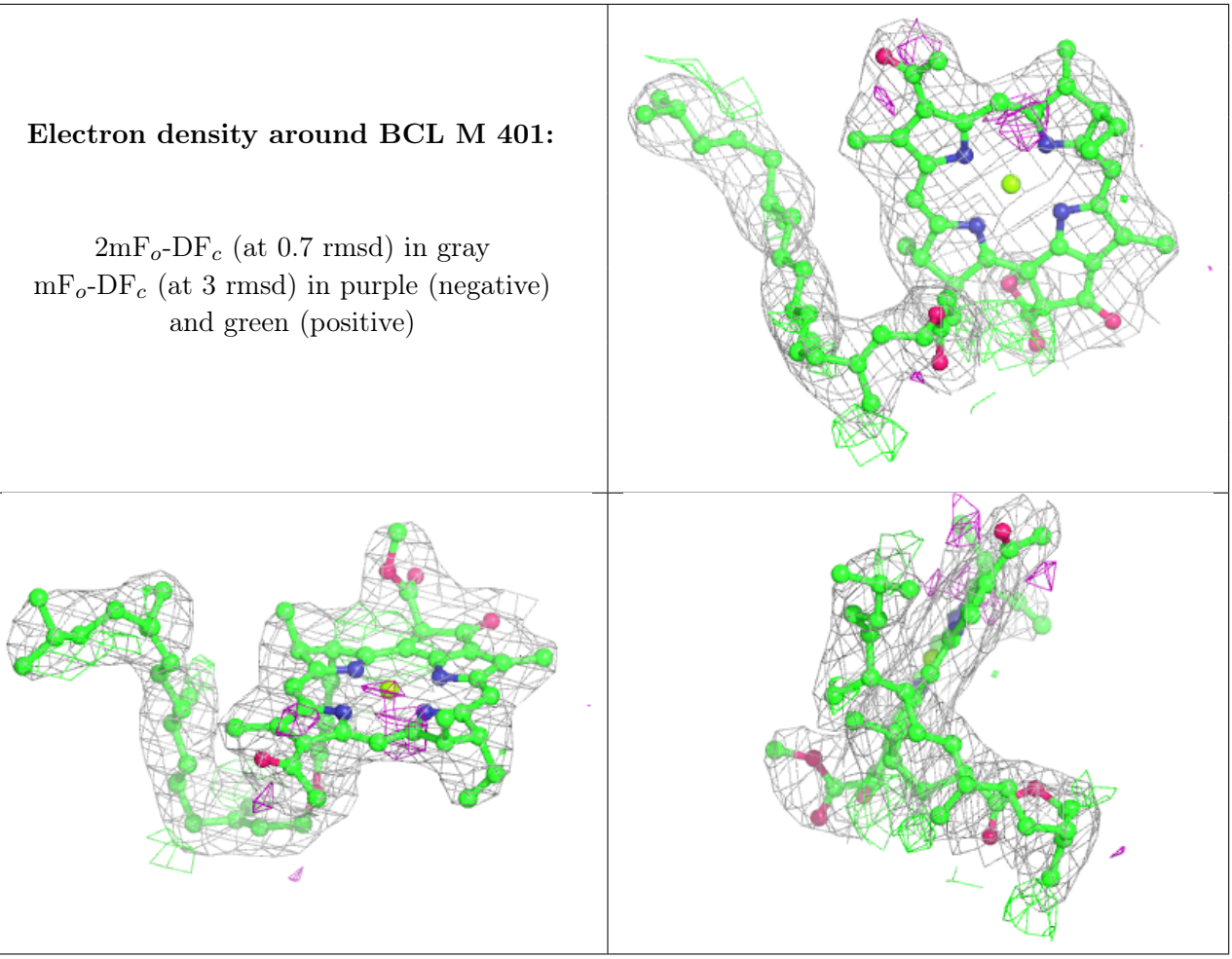






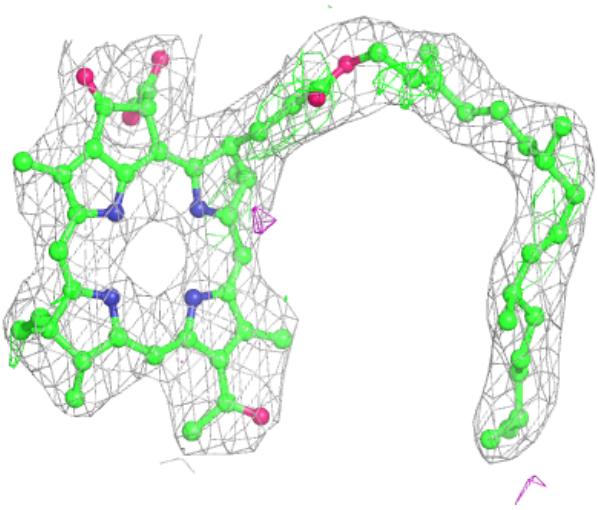
Electron density around BCL M 401:

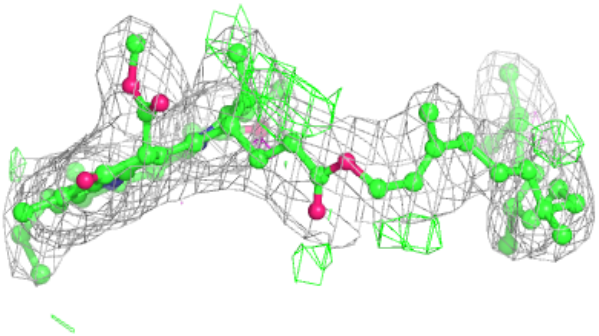
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

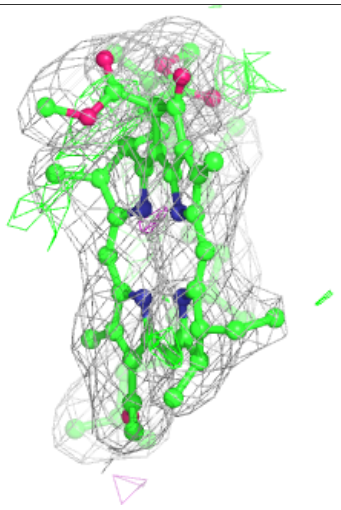


Electron density around BPH L 301:

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

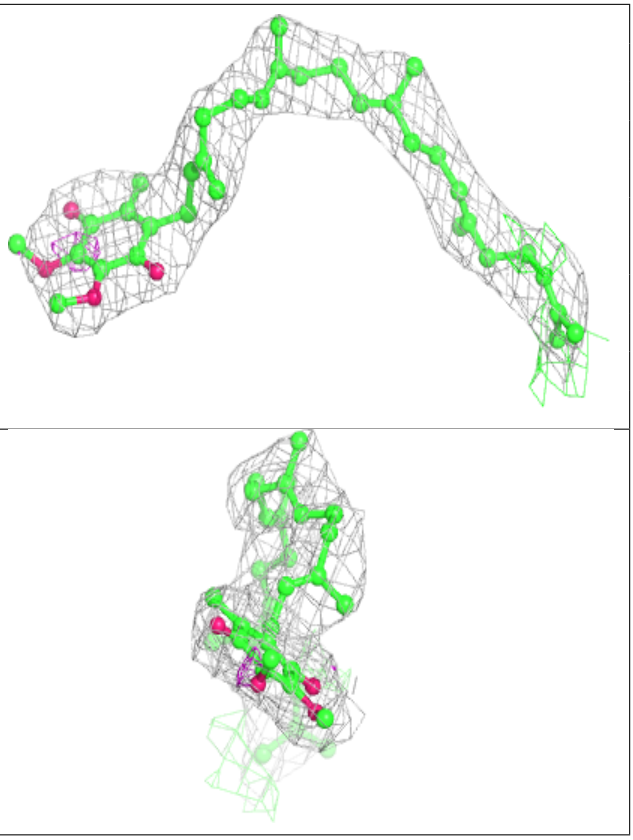






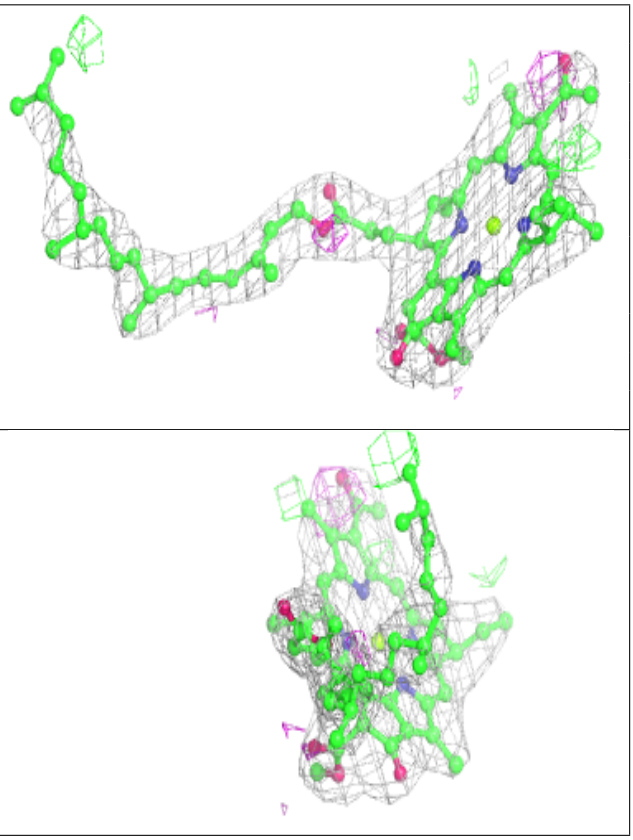
Electron density around U10 M 410:

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



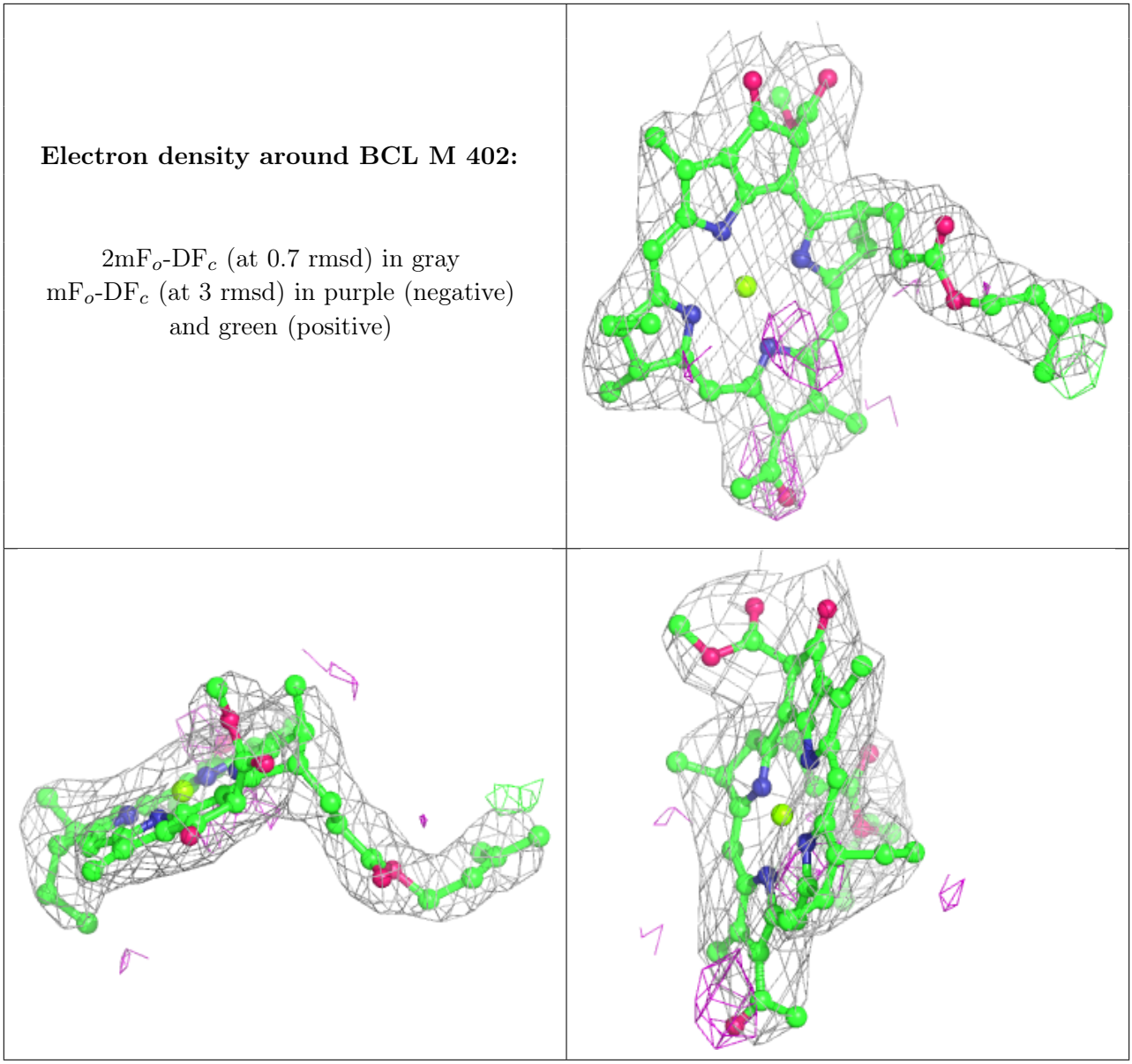
Electron density around BCL M 403:

$2mF_o$-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 M 402:

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



6.5 Other polymers (i)

There are no such residues in this entry.