Full wwPDB X-ray Structure Validation Report

Nov 23, 2020 – 09:19 am GMT

PDB ID	:	6Z27
Title	:	Photosynthetic Reaction Center From Rhodobacter Sphaeroides strain RV LCP crystallization
Authors	:	Gabdulkhakov, A.G.; Fufina, T.Y.; Vasilieva, L.G.; Betzel, C.; Selikhanov, G.K.
Deposited on	:	2020-05-15
Resolution	:	2.10 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:

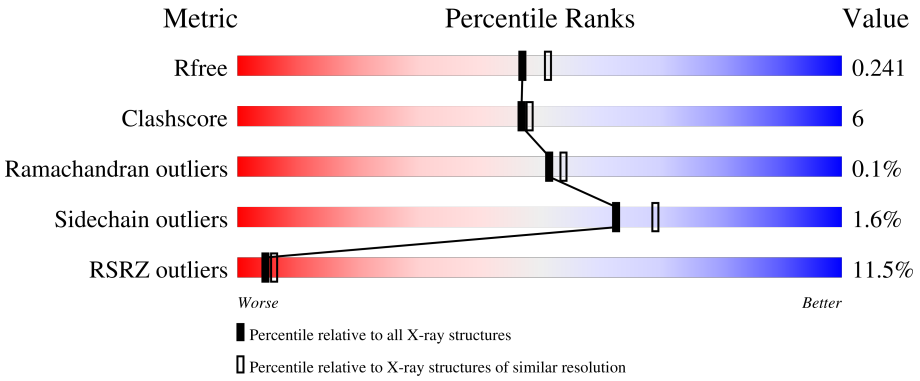
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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	250	9% 82% 13%
2	L	281	12% 81% 15%
3	M	302	12% 90% 10%

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

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7219 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	0	0
			1833	1173	314	337	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	270	Total	C	N	O	S	0	0	0
			2148	1452	340	348	8			

There is a discrepancy between the modelled and reference sequences:

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

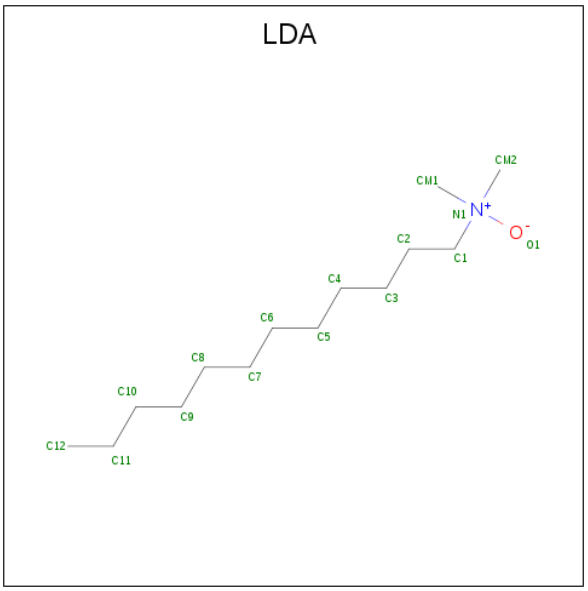
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	2	0
			2428	1622	398	398	10			

There is a discrepancy between the modelled and reference sequences:

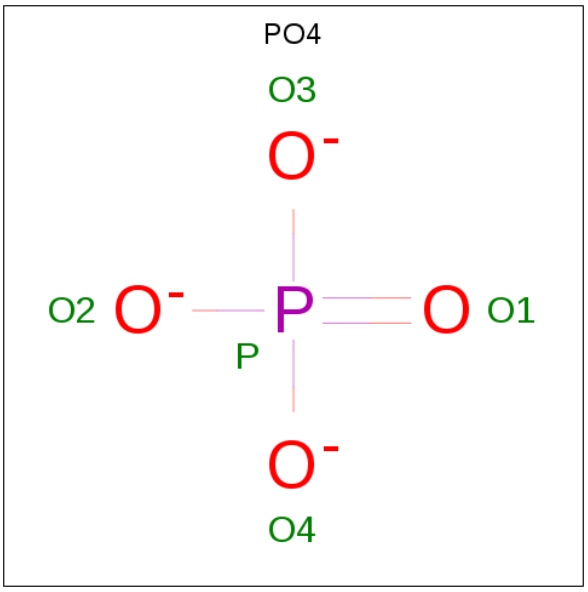
Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	engineered mutation	UNP P0C0Y9

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



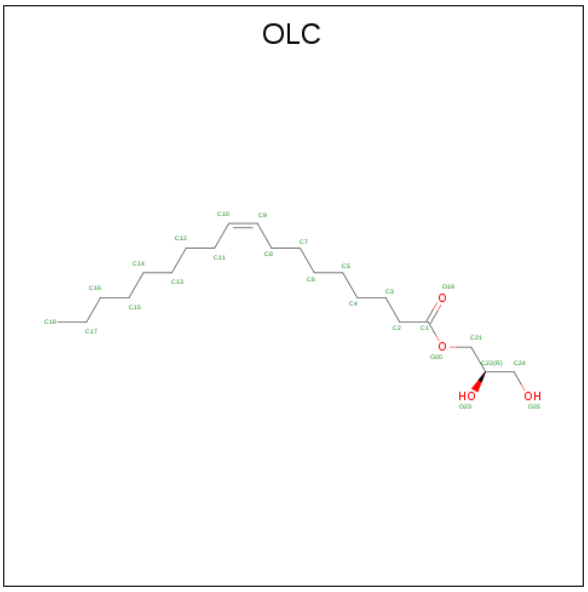
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	L	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



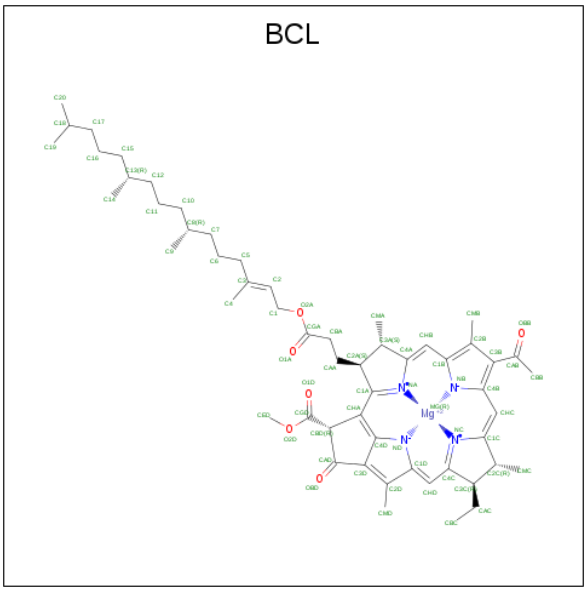
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total O P 5 4 1	0	0
5	H	1	Total O P 5 4 1	0	0
5	H	1	Total O P 5 4 1	0	0
5	M	1	Total O P 5 4 1	0	0
5	M	1	Total O P 5 4 1	0	0
5	M	1	Total O P 5 4 1	0	0
5	M	1	Total O P 5 4 1	0	0
5	M	1	Total O P 5 4 1	0	0

- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



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

- Molecule 7 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
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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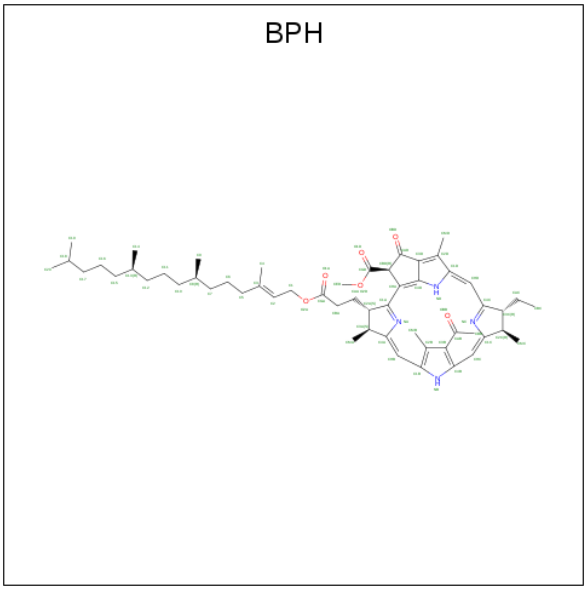
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).

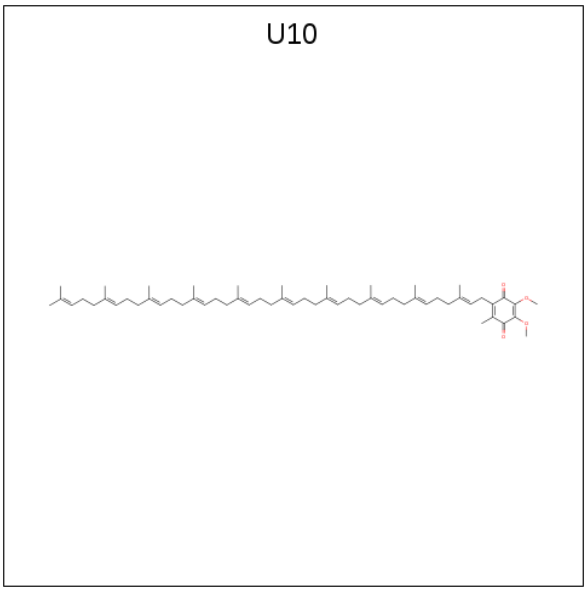


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	0	0
			65	55	4	6		
8	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 9 is FE (III) ION (three-letter code: FE) (formula: Fe).

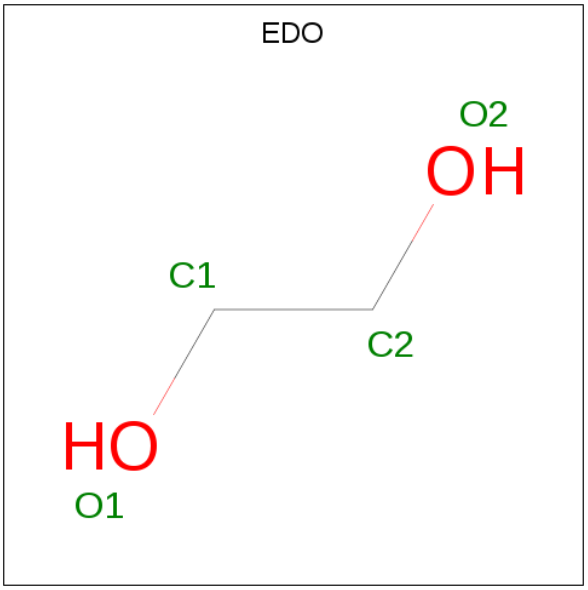
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total	Fe	0	0
			1	1		

- Molecule 10 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
10	M	1	Total C O 48 44 4	0	0

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

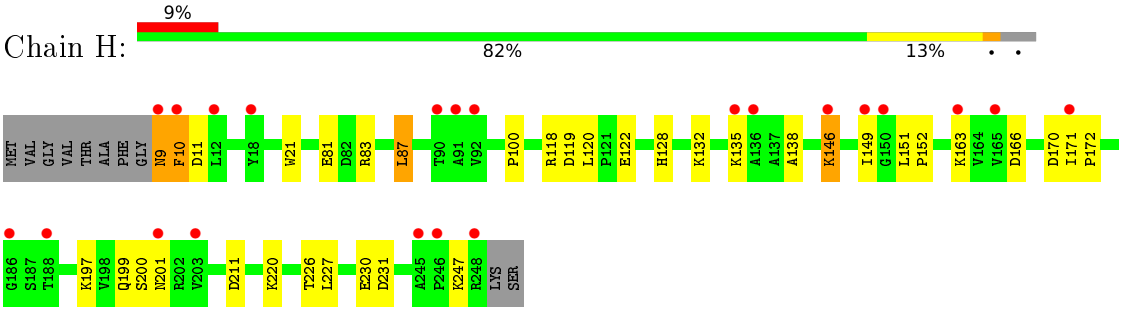
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	H	67	Total O 67 67	0	0
12	L	47	Total O 47 47	0	0
12	M	47	Total O 47 47	0	0

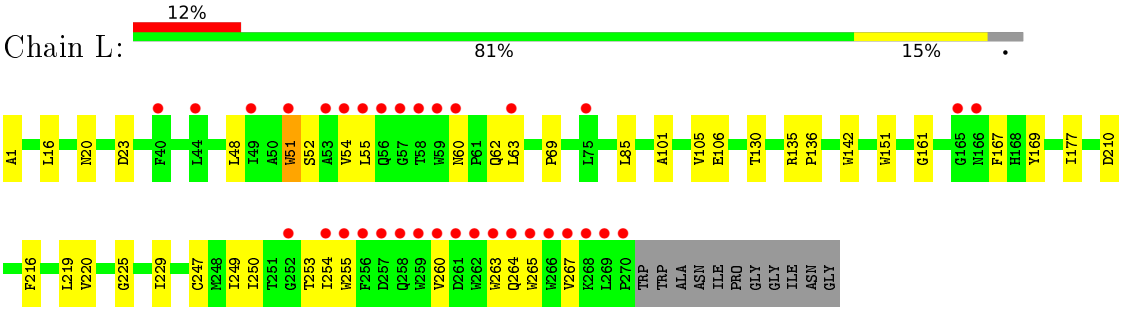
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

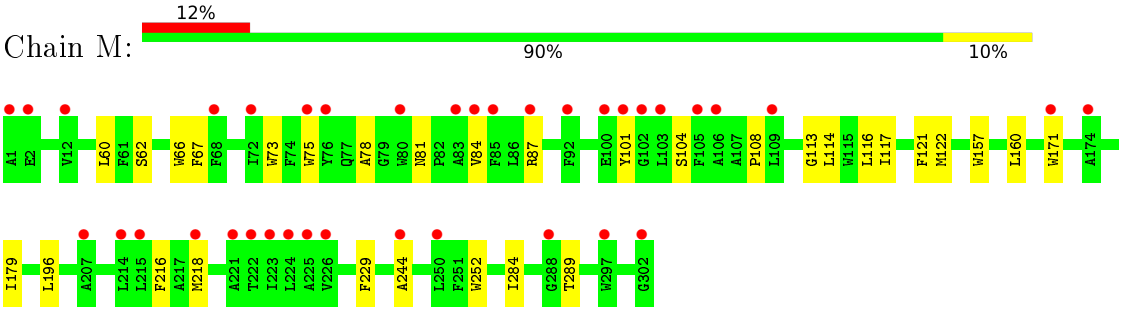
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	99.91Å 99.91Å 234.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.86 – 2.10 48.86 – 1.97	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.86-2.10) 99.9 (48.86-1.97)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 1.97Å)	Xtriage
Refinement program	REFMAC 1.18_3861, PHENIX 1.18_3861	Depositor
R, R_{free}	0.209 , 0.236 0.217 , 0.241	Depositor DCC
R_{free} test set	2100 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å^2)	52.1	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 66.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7219	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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, OLC, BPH, PO4, EDO, FE, 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	0.50	1/1882 (0.1%)	0.62	1/2561 (0.0%)
2	L	0.42	0/2231	0.51	0/3053
3	M	0.42	0/2524	0.50	0/3445
All	All	0.44	1/6637 (0.0%)	0.54	1/9059 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	230	GLU	CD-OE1	-5.22	1.20	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	87	LEU	CA-CB-CG	5.29	127.46	115.30

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	1833	0	1833	23	0
2	L	2148	0	2114	29	0
3	M	2428	0	2344	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	32	0	62	3	0
4	L	16	0	31	1	0
4	M	64	0	124	1	0
5	H	15	0	0	1	0
5	M	25	0	0	0	0
6	L	25	0	40	5	0
6	M	25	0	40	4	0
7	L	66	0	74	2	0
7	M	198	0	222	11	0
8	L	65	0	76	0	0
8	M	65	0	76	6	0
9	M	1	0	0	0	0
10	M	48	0	63	1	0
11	M	4	0	6	0	0
12	H	67	0	0	2	0
12	L	47	0	0	1	0
12	M	47	0	0	0	0
All	All	7219	0	7105	88	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 6.

All (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:171:ILE:HG13	1:H:172:PRO:HD3	1.49	0.94
1:H:9:ASN:ND2	1:H:9:ASN:O	2.18	0.77
1:H:146:LYS:HE3	1:H:200:SER:HA	1.66	0.75
1:H:128:HIS:ND1	12:H:801:HOH:O	2.24	0.71
1:H:171:ILE:HG13	1:H:172:PRO:CD	2.25	0.65
6:L:301:OLC:H18B	7:M:404:BCL:H201	1.80	0.63
2:L:250:ILE:HB	2:L:254:ILE:HD11	1.81	0.61
6:M:401:OLC:H11	7:M:403:BCL:H193	1.82	0.61
7:M:403:BCL:H62	7:M:404:BCL:H192	1.81	0.61
7:M:404:BCL:H203	8:M:406:BPH:H5C1	1.81	0.61
3:M:289:THR:HB	4:M:402:LDA:H91	1.82	0.59
3:M:67[A]:PHE:CE1	6:M:401:OLC:H12A	2.39	0.58
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.86	0.58
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.39	0.57
3:M:179:ILE:HD11	7:M:403:BCL:H192	1.87	0.57
1:H:172:PRO:HB2	2:L:210:ASP:OD1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:264:GLN:HA	2:L:267:VAL:HG12	1.87	0.56
3:M:73:TRP:HB2	3:M:114:LEU:HD23	1.89	0.55
4:H:701:LDA:H82	4:H:702:LDA:H121	1.88	0.55
2:L:169:TYR:O	2:L:263:TRP:NE1	2.36	0.55
1:H:87:LEU:HD23	1:H:100:PRO:HA	1.89	0.55
3:M:78:ALA:HB1	3:M:84:VAL:HG13	1.89	0.55
2:L:51:TRP:HA	2:L:54:VAL:HG22	1.90	0.54
2:L:52:SER:HB2	2:L:85:LEU:HD13	1.89	0.53
3:M:157:TRP:CD1	7:M:403:BCL:HBB1	2.44	0.53
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.91	0.53
2:L:253:THR:OG1	2:L:254:ILE:N	2.43	0.52
2:L:229:ILE:HB	6:L:301:OLC:H21	1.92	0.52
2:L:225:GLY:H	6:L:301:OLC:H22	1.73	0.52
7:M:404:BCL:HBB3	7:M:405:BCL:HMD2	1.92	0.52
3:M:101:TYR:O	3:M:104:SER:HB3	2.10	0.51
2:L:177:ILE:HG12	7:L:303:BCL:HMB3	1.92	0.51
2:L:161:GLY:HA2	2:L:167:PHE:CD1	2.46	0.51
2:L:161:GLY:HA2	2:L:167:PHE:CE1	2.45	0.51
1:H:118:ARG:HD2	12:H:803:HOH:O	2.12	0.50
3:M:75:TRP:HE1	6:M:401:OLC:H18	1.76	0.50
3:M:60:LEU:HA	8:M:406:BPH:H4C2	1.94	0.49
1:H:119:ASP:OD1	1:H:220:LYS:HE2	2.12	0.48
2:L:62:GLN:OE1	2:L:151:TRP:NE1	2.45	0.47
3:M:101:TYR:CE1	3:M:108:PRO:HD3	2.50	0.46
1:H:152:PRO:HA	1:H:163:LYS:HD3	1.97	0.46
7:M:405:BCL:HBB2	7:M:405:BCL:HMB1	1.97	0.46
7:M:403:BCL:HMB1	7:M:403:BCL:HBB3	1.97	0.45
1:H:132:LYS:NZ	5:H:703:PO4:O4	2.47	0.45
6:L:301:OLC:H17A	8:M:406:BPH:HMA1	1.99	0.45
3:M:218:MET:HG2	3:M:252:TRP:CH2	2.51	0.45
1:H:146:LYS:HE2	1:H:146:LYS:HB2	1.50	0.45
1:H:197:LYS:NZ	1:H:199:GLN:HG3	2.31	0.45
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.99	0.45
1:H:170:ASP:OD1	1:H:172:PRO:HD2	2.17	0.45
2:L:254:ILE:HG13	2:L:255:TRP:N	2.31	0.45
2:L:249:ILE:HA	2:L:249:ILE:HD12	1.90	0.44
3:M:113:GLY:O	3:M:117:ILE:HG12	2.17	0.44
7:L:303:BCL:HMB1	7:L:303:BCL:HBB3	1.99	0.44
3:M:160:LEU:HD23	3:M:284:ILE:HG21	2.00	0.44
2:L:250:ILE:HA	2:L:254:ILE:HG12	2.00	0.44
3:M:81:ASN:ND2	3:M:84:VAL:HG12	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:211:ASP:OD2	1:H:247:LYS:NZ	2.50	0.43
1:H:135:LYS:HG2	1:H:166:ASP:OD2	2.18	0.43
4:H:702:LDA:H22	4:H:702:LDA:HM11	1.48	0.43
2:L:225:GLY:N	6:L:301:OLC:H22	2.33	0.43
3:M:62:SER:OG	3:M:121:PHE:O	2.36	0.43
3:M:116:LEU:HD21	3:M:171:TRP:CD1	2.54	0.43
4:L:302:LDA:HM22	4:L:302:LDA:H22	1.70	0.42
3:M:196:LEU:HD23	3:M:196:LEU:HA	1.87	0.42
2:L:130:THR:HG23	2:L:249:ILE:HD13	2.01	0.42
1:H:149:ILE:HD13	1:H:166:ASP:HA	2.01	0.42
2:L:101:ALA:O	2:L:105:VAL:HG23	2.19	0.42
2:L:169:TYR:CD2	2:L:260:VAL:HG22	2.54	0.42
2:L:20:ASN:HA	2:L:23:ASP:HB2	2.01	0.42
1:H:10:PHE:HB3	1:H:11:ASP:H	1.37	0.42
1:H:151:LEU:HD23	1:H:201:ASN:C	2.40	0.42
2:L:1:ALA:N	12:L:403:HOH:O	2.53	0.42
2:L:219:LEU:HG	2:L:220:VAL:HG13	2.02	0.41
3:M:114:LEU:HA	3:M:114:LEU:HD12	1.90	0.41
8:M:406:BPH:H4C1	8:M:406:BPH:H7C2	2.02	0.41
1:H:81:GLU:O	1:H:83:ARG:HG2	2.20	0.41
8:M:406:BPH:C7	8:M:406:BPH:H4C1	2.50	0.41
2:L:16:LEU:HG	2:L:106:GLU:HG2	2.03	0.41
2:L:48:LEU:HB3	2:L:85:LEU:HD22	2.02	0.41
6:M:401:OLC:C11	7:M:403:BCL:H193	2.48	0.41
1:H:120:LEU:N	1:H:226:THR:HB	2.36	0.41
2:L:60:ASN:HB3	2:L:63:LEU:HD12	2.03	0.41
7:M:404:BCL:H202	8:M:406:BPH:H8	2.03	0.41
2:L:51:TRP:O	2:L:55:LEU:HG	2.20	0.40
10:M:408:U10:H28	10:M:408:U10:H322	1.51	0.40
1:H:21:TRP:HZ2	4:H:701:LDA:HM13	1.85	0.40
2:L:135:ARG:HB3	2:L:136:PRO:HD3	2.03	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	238/250 (95%)	230 (97%)	7 (3%)	1 (0%)	34 32
2	L	268/281 (95%)	259 (97%)	9 (3%)	0	100 100
3	M	302/302 (100%)	292 (97%)	10 (3%)	0	100 100
All	All	808/833 (97%)	781 (97%)	26 (3%)	1 (0%)	51 54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	138	ALA

5.3.2 Protein sidechains

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	195/202 (96%)	191 (98%)	4 (2%)	53 59
2	L	213/220 (97%)	209 (98%)	4 (2%)	57 63
3	M	238/236 (101%)	236 (99%)	2 (1%)	81 86
All	All	646/658 (98%)	636 (98%)	10 (2%)	62 71

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	9	ASN
1	H	10	PHE
1	H	146	LYS
1	H	231	ASP
2	L	51	TRP
2	L	216	PHE
2	L	247	CYS
2	L	265	TRP
3	M	87	ARG
3	M	216	PHE

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

Mol	Chain	Res	Type
3	M	188	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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	$\#\|Z\| > 2$
4	LDA	H	701	-	12,15,15	1.97	1 (8%)	14,17,17	0.44	0
4	LDA	M	402	-	12,15,15	2.00	1 (8%)	14,17,17	0.51	0
8	BPH	L	304	-	64,70,70	0.99	5 (7%)	76,101,101	1.27	7 (9%)
5	PO4	H	703	-	4,4,4	0.79	0	6,6,6	0.39	0
5	PO4	M	413	-	4,4,4	0.73	0	6,6,6	0.54	0
7	BCL	M	404	-	58,74,74	1.38	3 (5%)	69,115,115	1.49	10 (14%)
5	PO4	M	416	-	4,4,4	0.82	0	6,6,6	0.37	0
7	BCL	M	403	-	58,74,74	1.25	3 (5%)	69,115,115	1.45	11 (15%)
5	PO4	M	415	-	4,4,4	0.85	0	6,6,6	1.23	1 (16%)
11	EDO	M	417	-	3,3,3	0.37	0	2,2,2	1.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PO4	H	704	-	4,4,4	0.86	0	6,6,6	0.45	0
7	BCL	M	405	-	58,74,74	1.36	6 (10%)	69,115,115	1.28	9 (13%)
6	OLC	L	301	-	24,24,24	0.97	1 (4%)	25,25,25	0.93	1 (4%)
8	BPH	M	406	-	64,70,70	0.94	3 (4%)	76,101,101	1.22	8 (10%)
7	BCL	L	303	-	58,74,74	1.42	4 (6%)	69,115,115	1.29	10 (14%)
4	LDA	M	411	-	12,15,15	2.08	1 (8%)	14,17,17	0.55	0
5	PO4	M	414	-	4,4,4	0.76	0	6,6,6	0.50	0
4	LDA	H	702	-	12,15,15	1.88	1 (8%)	14,17,17	0.57	0
6	OLC	M	401	-	24,24,24	0.92	1 (4%)	25,25,25	0.85	0
4	LDA	M	409	-	12,15,15	2.06	1 (8%)	14,17,17	0.46	0
10	U10	M	408	-	48,48,63	2.66	14 (29%)	58,61,79	1.69	13 (22%)
4	LDA	L	302	-	12,15,15	2.03	1 (8%)	14,17,17	0.47	0
4	LDA	M	410	-	12,15,15	1.94	1 (8%)	14,17,17	0.52	0
5	PO4	M	412	-	4,4,4	1.02	0	6,6,6	0.86	0
5	PO4	H	705	-	4,4,4	0.76	0	6,6,6	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
4	LDA	H	702	-	-	7/13/13/13	-
11	EDO	M	417	-	-	1/1/1/1	-
4	LDA	H	701	-	-	3/13/13/13	-
4	LDA	M	402	-	-	5/13/13/13	-
8	BPH	L	304	-	-	4/54/105/105	0/5/6/6
7	BCL	M	404	-	-	4/37/137/137	-
4	LDA	L	302	-	-	7/13/13/13	-
4	LDA	M	410	-	-	6/13/13/13	-
10	U10	M	408	-	-	10/45/69/87	0/1/1/1
7	BCL	M	405	-	-	3/37/137/137	-
6	OLC	M	401	-	-	13/24/24/24	-
4	LDA	M	409	-	-	4/13/13/13	-
4	LDA	M	411	-	-	8/13/13/13	-
7	BCL	M	403	-	-	6/37/137/137	-
6	OLC	L	301	-	-	12/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BPH	M	406	-	-	21/54/105/105	0/5/6/6
7	BCL	L	303	-	-	1/37/137/137	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	411	LDA	O1-N1	-7.14	1.25	1.42
4	M	409	LDA	O1-N1	-7.04	1.25	1.42
4	L	302	LDA	O1-N1	-6.90	1.26	1.42
4	M	402	LDA	O1-N1	-6.85	1.26	1.42
4	H	701	LDA	O1-N1	-6.70	1.26	1.42
4	M	410	LDA	O1-N1	-6.58	1.26	1.42
4	H	702	LDA	O1-N1	-6.45	1.27	1.42
10	M	408	U10	C8-C9	6.32	1.48	1.33
10	M	408	U10	C28-C29	6.19	1.47	1.33
10	M	408	U10	C33-C34	6.16	1.47	1.33
10	M	408	U10	C13-C14	6.06	1.47	1.33
7	M	404	BCL	MG-NA	6.04	2.20	2.06
10	M	408	U10	C23-C24	5.94	1.47	1.33
7	M	405	BCL	C1B-NB	5.70	1.40	1.35
10	M	408	U10	C18-C19	5.66	1.46	1.33
7	M	404	BCL	C1B-NB	5.56	1.40	1.35
7	L	303	BCL	MG-NA	5.44	2.19	2.06
7	L	303	BCL	C1B-NB	5.42	1.40	1.35
10	M	408	U10	C38-C39	5.21	1.47	1.32
10	M	408	U10	O4-C4	-4.88	1.24	1.36
10	M	408	U10	O3-C3	-4.84	1.25	1.36
7	M	405	BCL	MG-NA	4.78	2.17	2.06
7	M	403	BCL	C1B-NB	4.73	1.39	1.35
7	L	303	BCL	MG-NC	4.28	2.16	2.06
7	M	403	BCL	MG-NA	4.26	2.16	2.06
6	L	301	OLC	O20-C1	4.16	1.45	1.33
6	M	401	OLC	O20-C1	3.97	1.44	1.33
7	M	404	BCL	MG-NC	3.73	2.15	2.06
10	M	408	U10	C3-C2	-3.32	1.39	1.48
8	M	406	BPH	C3D-CAD	-3.06	1.41	1.47
8	L	304	BPH	C3D-CAD	-2.99	1.41	1.47
7	M	403	BCL	MG-NC	2.90	2.13	2.06
8	L	304	BPH	C1B-C2B	-2.80	1.39	1.45
10	M	408	U10	C4-C5	-2.79	1.40	1.48
7	M	405	BCL	OBD-CAD	2.76	1.26	1.22
8	L	304	BPH	CHC-C1C	2.72	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	408	U10	C6-C5	-2.71	1.39	1.46
8	L	304	BPH	OBD-CAD	2.62	1.26	1.22
7	L	303	BCL	C4B-NB	2.57	1.37	1.35
10	M	408	U10	C6-C1	2.54	1.39	1.35
7	M	405	BCL	MG-NC	2.36	2.11	2.06
8	L	304	BPH	C4A-NA	2.28	1.40	1.35
8	M	406	BPH	C1B-C2B	-2.27	1.40	1.45
7	M	405	BCL	O1A-CGA	-2.26	1.15	1.22
7	M	405	BCL	C4B-NB	2.19	1.37	1.35
8	M	406	BPH	CHC-C1C	2.14	1.41	1.36
10	M	408	U10	C1-C2	-2.05	1.39	1.47

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	404	BCL	C4D-C3D-CAD	-4.24	106.10	108.47
7	M	403	BCL	CMB-C2B-C1B	-4.22	121.98	128.46
7	M	404	BCL	C4A-NA-C1A	4.10	108.55	106.71
10	M	408	U10	C32-C33-C34	-4.09	117.81	127.66
7	M	404	BCL	CMB-C2B-C1B	-3.84	122.57	128.46
7	M	403	BCL	OBD-CAD-CBD	-3.81	120.46	125.89
10	M	408	U10	C22-C23-C24	-3.78	118.55	127.66
7	L	303	BCL	CMB-C2B-C1B	-3.73	122.72	128.46
8	L	304	BPH	C1C-NC-C4C	-3.73	107.26	110.54
7	M	405	BCL	CMB-C2B-C1B	-3.67	122.82	128.46
10	M	408	U10	C30-C29-C31	3.59	121.31	115.27
7	M	405	BCL	OBD-CAD-CBD	-3.53	120.85	125.89
8	M	406	BPH	C17-C16-C15	3.48	129.25	113.24
7	M	404	BCL	OBD-CAD-CBD	-3.46	120.95	125.89
7	M	403	BCL	C4D-C3D-CAD	-3.45	106.55	108.47
7	L	303	BCL	OBD-CAD-CBD	-3.38	121.06	125.89
8	L	304	BPH	OBD-CAD-CBD	-3.31	121.17	125.89
10	M	408	U10	C17-C18-C19	-3.26	119.81	127.66
7	M	403	BCL	C6-C7-C8	3.23	126.38	115.92
7	M	404	BCL	CHA-C1A-NA	-3.22	119.03	126.40
8	L	304	BPH	C1-C2-C3	-3.21	120.49	126.04
8	M	406	BPH	O2A-C1-C2	-3.12	100.45	108.64
7	M	403	BCL	CMD-C2D-C3D	3.09	130.46	124.68
7	M	405	BCL	CHA-C1A-NA	-3.08	119.35	126.40
7	M	403	BCL	CMB-C2B-C3B	3.07	130.41	124.68
7	M	403	BCL	CHA-C1A-NA	-2.97	119.60	126.40
10	M	408	U10	C20-C19-C21	2.94	120.21	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	408	U10	C25-C24-C26	2.89	120.14	115.27
7	M	404	BCL	CMB-C2B-C3B	2.86	130.03	124.68
8	M	406	BPH	OBD-CAD-CBD	-2.85	121.83	125.89
7	M	405	BCL	CMB-C2B-C3B	2.83	129.97	124.68
7	L	303	BCL	C4D-C3D-CAD	-2.80	106.91	108.47
10	M	408	U10	C12-C13-C14	-2.77	120.98	127.66
7	L	303	BCL	CHA-C1A-NA	-2.77	120.05	126.40
7	L	303	BCL	CMB-C2B-C3B	2.77	129.86	124.68
10	M	408	U10	C35-C34-C36	2.75	119.89	115.27
8	L	304	BPH	CMD-C2D-C3D	2.74	129.81	124.68
7	M	404	BCL	C2A-C1A-CHA	2.74	128.65	123.86
10	M	408	U10	C27-C28-C29	-2.69	121.19	127.66
7	M	405	BCL	CMD-C2D-C3D	2.57	129.48	124.68
10	M	408	U10	C37-C38-C39	-2.55	119.04	127.75
7	L	303	BCL	C2A-C1A-CHA	2.53	128.28	123.86
7	M	405	BCL	C2A-C1A-CHA	2.50	128.23	123.86
7	M	405	BCL	C4D-C3D-CAD	-2.49	107.08	108.47
7	M	404	BCL	CMD-C2D-C3D	2.43	129.22	124.68
7	L	303	BCL	C1C-NC-C4C	2.42	107.79	106.71
10	M	408	U10	C41-C39-C40	2.38	119.87	114.60
5	M	415	PO4	O2-P-O1	-2.36	102.27	110.89
7	L	303	BCL	OBB-CAB-CBB	-2.32	114.94	120.17
8	L	304	BPH	C11-C10-C8	-2.32	108.42	115.92
8	M	406	BPH	CHC-C1C-NC	-2.31	122.46	125.20
6	L	301	OLC	C3-C2-C1	-2.30	105.27	113.62
10	M	408	U10	C15-C14-C16	2.28	119.10	115.27
7	M	404	BCL	CED-O2D-CGD	2.26	121.04	115.94
8	M	406	BPH	C1C-NC-C4C	-2.26	108.56	110.54
8	L	304	BPH	CHC-C1C-NC	-2.25	122.52	125.20
8	M	406	BPH	C6-C5-C3	2.25	119.35	113.45
7	M	403	BCL	C16-C15-C13	2.25	123.18	115.92
8	M	406	BPH	C15-C13-C12	-2.23	100.38	112.13
8	L	304	BPH	O2D-CGD-O1D	-2.20	119.55	123.84
7	L	303	BCL	CMD-C2D-C3D	2.20	128.78	124.68
8	M	406	BPH	C16-C15-C13	2.18	122.96	115.92
7	M	403	BCL	C1C-NC-C4C	2.17	107.68	106.71
7	M	403	BCL	C2A-C1A-CHA	2.16	127.64	123.86
7	M	404	BCL	OBB-CAB-CBB	-2.14	115.36	120.17
10	M	408	U10	C22-C21-C19	-2.13	105.95	112.98
7	L	303	BCL	C16-C15-C13	-2.08	109.18	115.92
7	M	405	BCL	C4B-C3B-CAB	-2.06	123.15	127.13
7	M	405	BCL	CAA-CBA-CGA	2.04	119.21	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	403	BCL	OBB-CAB-CBB	-2.01	115.64	120.17

There are no chirality outliers.

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	301	OLC	O23-C22-C24-O25
8	M	406	BPH	C4C-C3C-CAC-CBC
8	M	406	BPH	C2C-C3C-CAC-CBC
8	M	406	BPH	C4B-C3B-CAB-CBB
4	M	411	LDA	C2-C1-N1-CM1
4	M	411	LDA	C2-C1-N1-CM2
4	H	702	LDA	C2-C1-N1-O1
4	H	702	LDA	C2-C1-N1-CM1
10	M	408	U10	C27-C28-C29-C30
10	M	408	U10	C27-C28-C29-C31
8	M	406	BPH	C4-C3-C5-C6
4	L	302	LDA	C7-C8-C9-C10
6	L	301	OLC	C12-C13-C14-C15
6	M	401	OLC	C3-C4-C5-C6
8	M	406	BPH	C2-C3-C5-C6
7	M	404	BCL	C14-C13-C15-C16
8	M	406	BPH	C6-C7-C8-C9
8	M	406	BPH	C11-C12-C13-C14
8	M	406	BPH	C14-C13-C15-C16
10	M	408	U10	C24-C26-C27-C28
10	M	408	U10	C29-C31-C32-C33
8	M	406	BPH	C5-C6-C7-C8
6	M	401	OLC	C14-C15-C16-C17
6	L	301	OLC	C2-C1-O20-C21
6	M	401	OLC	C4-C5-C6-C7
4	M	411	LDA	C7-C8-C9-C10
6	L	301	OLC	C21-C22-C24-O25
6	M	401	OLC	C21-C22-C24-O25
4	M	411	LDA	C6-C7-C8-C9
4	M	402	LDA	C4-C5-C6-C7
8	L	304	BPH	C2-C3-C5-C6
6	M	401	OLC	C6-C7-C8-C9
4	M	402	LDA	C1-C2-C3-C4
4	H	702	LDA	C1-C2-C3-C4
4	M	409	LDA	C7-C8-C9-C10
8	L	304	BPH	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
6	L	301	OLC	O19-C1-O20-C21
7	M	404	BCL	C15-C16-C17-C18
4	M	409	LDA	C4-C5-C6-C7
4	M	410	LDA	C11-C10-C9-C8
6	L	301	OLC	C6-C7-C8-C9
4	H	701	LDA	C1-C2-C3-C4
4	L	302	LDA	C1-C2-C3-C4
4	M	411	LDA	C9-C10-C11-C12
6	M	401	OLC	O23-C22-C24-O25
6	M	401	OLC	C15-C16-C17-C18
8	M	406	BPH	C2B-C3B-CAB-CBB
8	M	406	BPH	C8-C10-C11-C12
4	H	702	LDA	C9-C10-C11-C12
4	M	410	LDA	C1-C2-C3-C4
7	M	404	BCL	C12-C13-C15-C16
7	M	403	BCL	C11-C12-C13-C15
8	M	406	BPH	C11-C12-C13-C15
7	M	403	BCL	C11-C12-C13-C14
4	M	410	LDA	C9-C10-C11-C12
4	H	702	LDA	N1-C1-C2-C3
10	M	408	U10	C25-C24-C26-C27
4	M	409	LDA	C11-C10-C9-C8
4	L	302	LDA	C2-C3-C4-C5
4	M	410	LDA	C6-C7-C8-C9
4	H	701	LDA	C7-C8-C9-C10
10	M	408	U10	C23-C24-C26-C27
4	L	302	LDA	C5-C6-C7-C8
4	M	409	LDA	C1-C2-C3-C4
4	H	702	LDA	C7-C8-C9-C10
4	L	302	LDA	C4-C5-C6-C7
4	M	402	LDA	C9-C10-C11-C12
8	M	406	BPH	C11-C10-C8-C9
8	M	406	BPH	C4B-C3B-CAB-OBB
8	M	406	BPH	C2B-C3B-CAB-OBB
7	L	303	BCL	CAD-CBD-CGD-O2D
4	M	402	LDA	C2-C1-N1-CM2
6	L	301	OLC	C3-C4-C5-C6
4	H	701	LDA	C9-C10-C11-C12
4	H	702	LDA	C5-C6-C7-C8
8	M	406	BPH	C13-C15-C16-C17
4	M	402	LDA	C7-C8-C9-C10
4	L	302	LDA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
8	M	406	BPH	C10-C11-C12-C13
8	M	406	BPH	C15-C16-C17-C18
6	M	401	OLC	O20-C21-C22-C24
6	M	401	OLC	O19-C1-O20-C21
6	L	301	OLC	O20-C1-C2-C3
6	L	301	OLC	C1-C2-C3-C4
11	M	417	EDO	O1-C1-C2-O2
7	M	405	BCL	C15-C16-C17-C18
6	M	401	OLC	C7-C8-C9-C10
4	M	410	LDA	C4-C5-C6-C7
6	M	401	OLC	C2-C1-O20-C21
10	M	408	U10	C5-C4-O4-C4M
6	M	401	OLC	C11-C12-C13-C14
4	M	410	LDA	C7-C8-C9-C10
8	M	406	BPH	C12-C13-C15-C16
7	M	405	BCL	C14-C13-C15-C16
6	L	301	OLC	C11-C12-C13-C14
7	M	403	BCL	C4-C3-C5-C6
4	M	411	LDA	C3-C4-C5-C6
8	L	304	BPH	CAD-CBD-CGD-O2D
7	M	403	BCL	CAD-CBD-CGD-O2D
8	M	406	BPH	CAD-CBD-CGD-O2D
8	L	304	BPH	O2A-C1-C2-C3
4	L	302	LDA	C3-C4-C5-C6
6	L	301	OLC	O20-C21-C22-O23
7	M	404	BCL	CAA-CBA-CGA-O2A
6	M	401	OLC	C9-C10-C11-C12
7	M	403	BCL	C2-C3-C5-C6
6	L	301	OLC	C5-C6-C7-C8
4	M	411	LDA	C2-C1-N1-O1
7	M	403	BCL	C16-C17-C18-C19
7	M	405	BCL	C12-C13-C15-C16
10	M	408	U10	C28-C29-C31-C32
10	M	408	U10	C3-C4-O4-C4M
4	M	411	LDA	C1-C2-C3-C4
8	M	406	BPH	C2A-CAA-CBA-CGA
10	M	408	U10	C30-C29-C31-C32

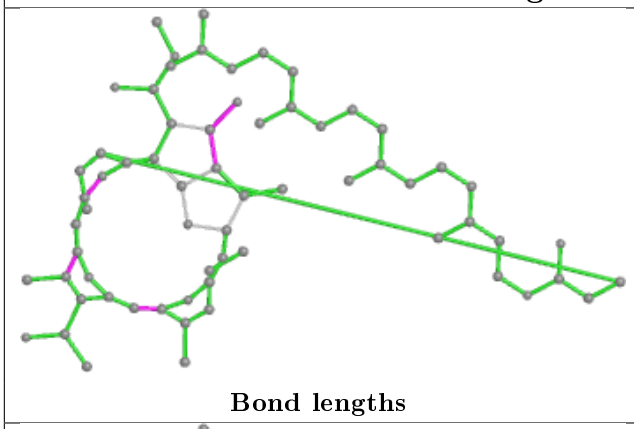
There are no ring outliers.

13 monomers are involved in 29 short contacts:

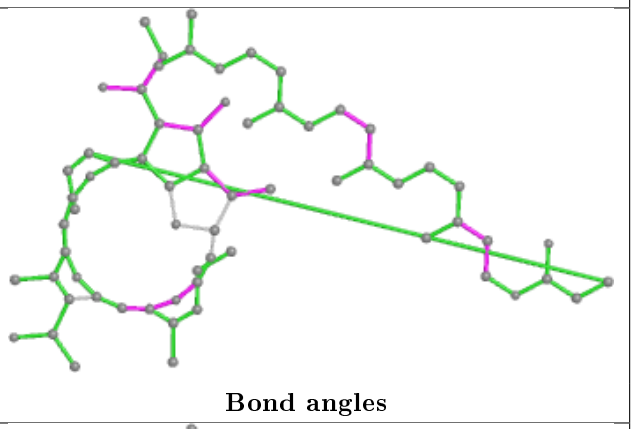
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	701	LDA	2	0
4	M	402	LDA	1	0
5	H	703	PO4	1	0
7	M	404	BCL	5	0
7	M	403	BCL	6	0
7	M	405	BCL	2	0
6	L	301	OLC	5	0
8	M	406	BPH	6	0
7	L	303	BCL	2	0
4	H	702	LDA	2	0
6	M	401	OLC	4	0
10	M	408	U10	1	0
4	L	302	LDA	1	0

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.

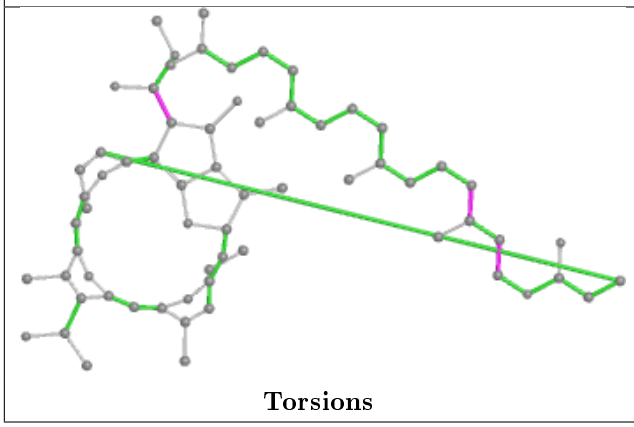
Ligand BPH L 304



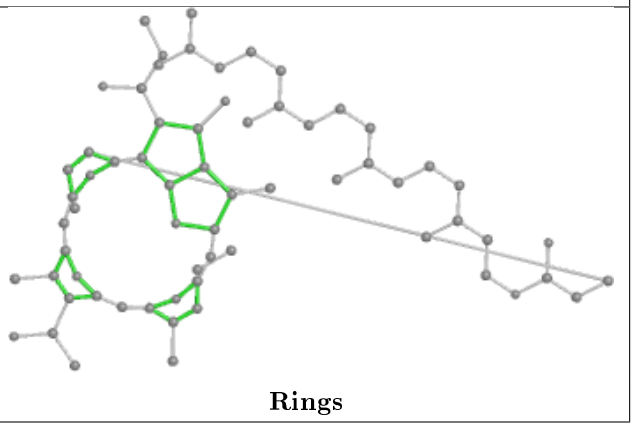
Bond lengths



Bond angles

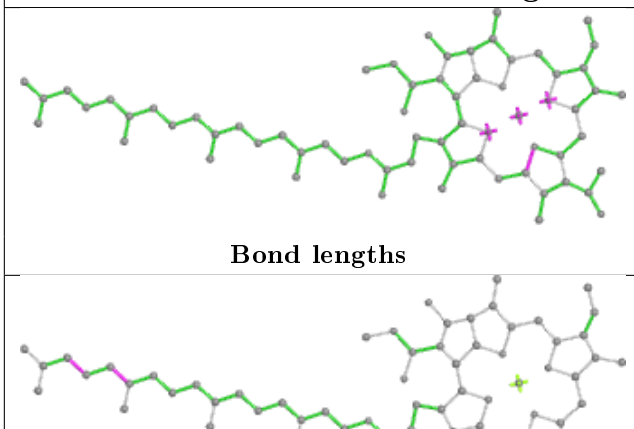


Torsions

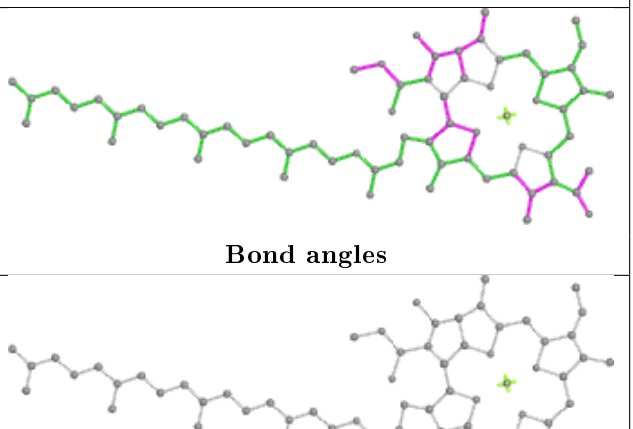


Rings

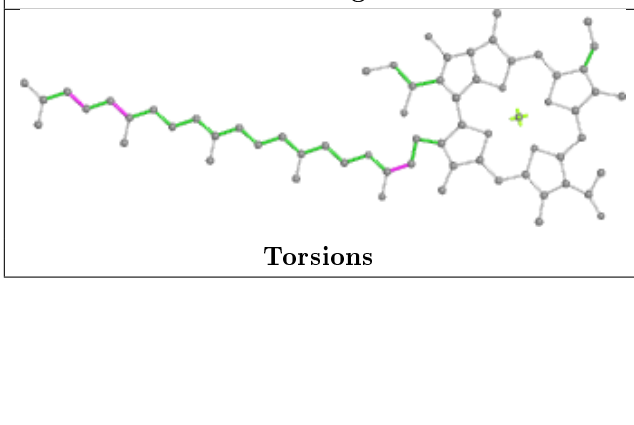
Ligand BCL M 404



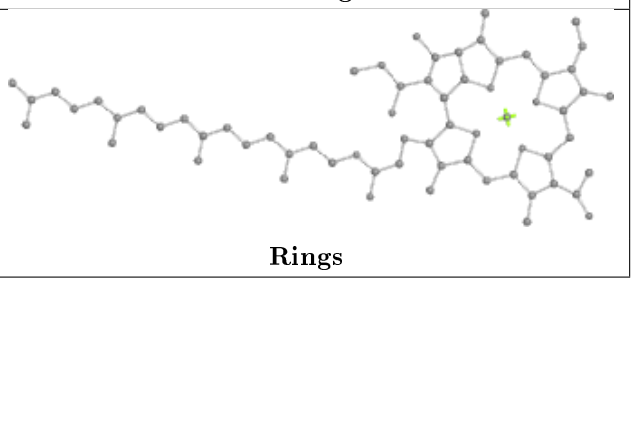
Bond lengths



Bond angles

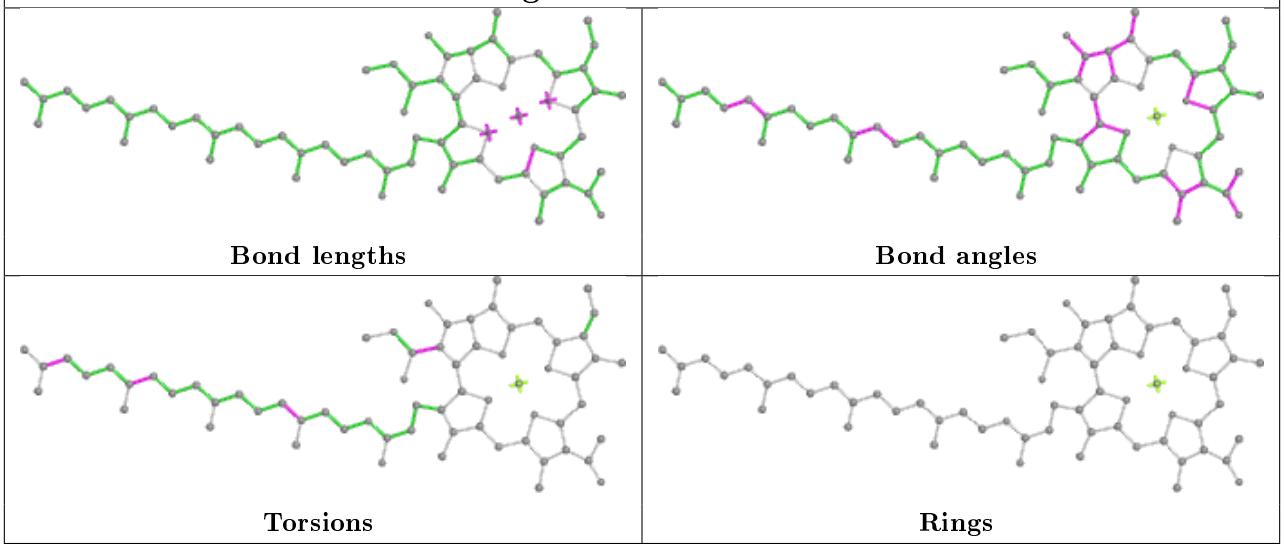


Torsions

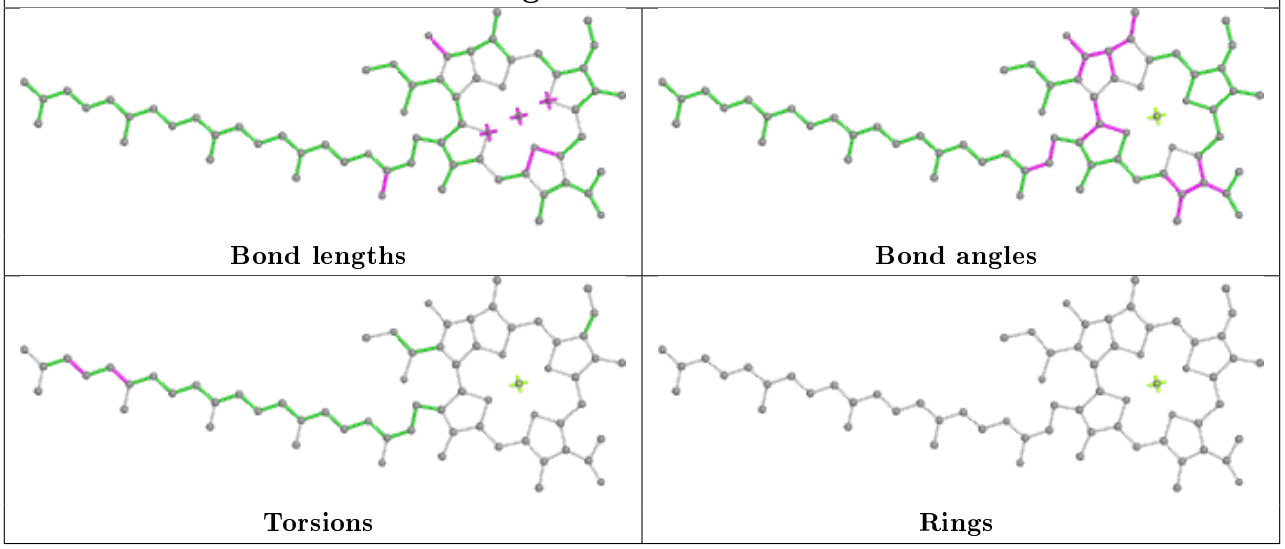


Rings

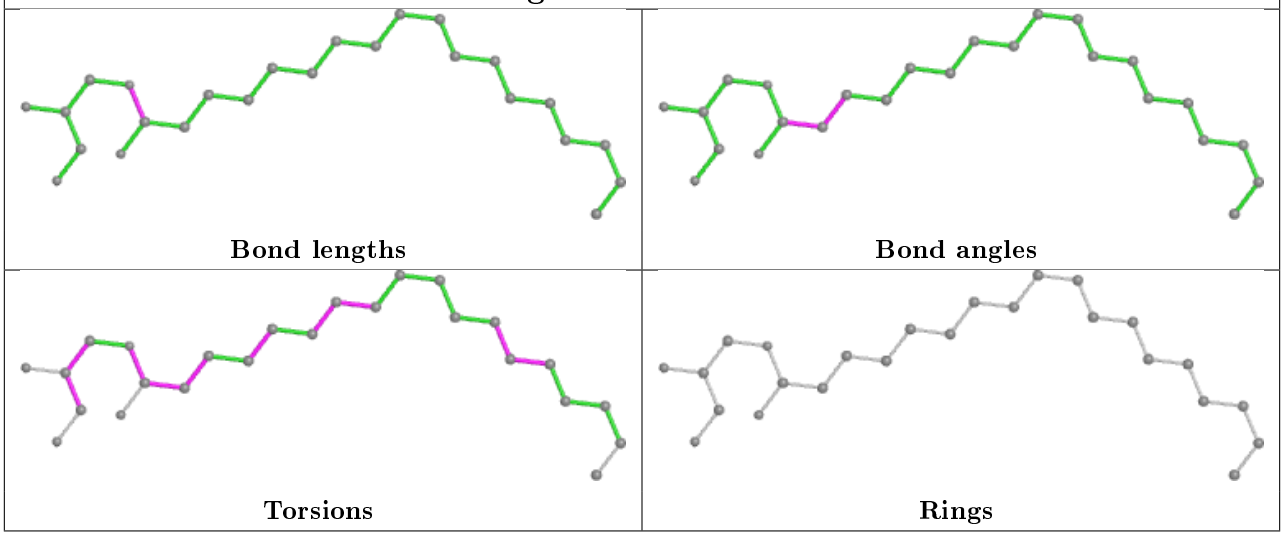
Ligand BCL M 403



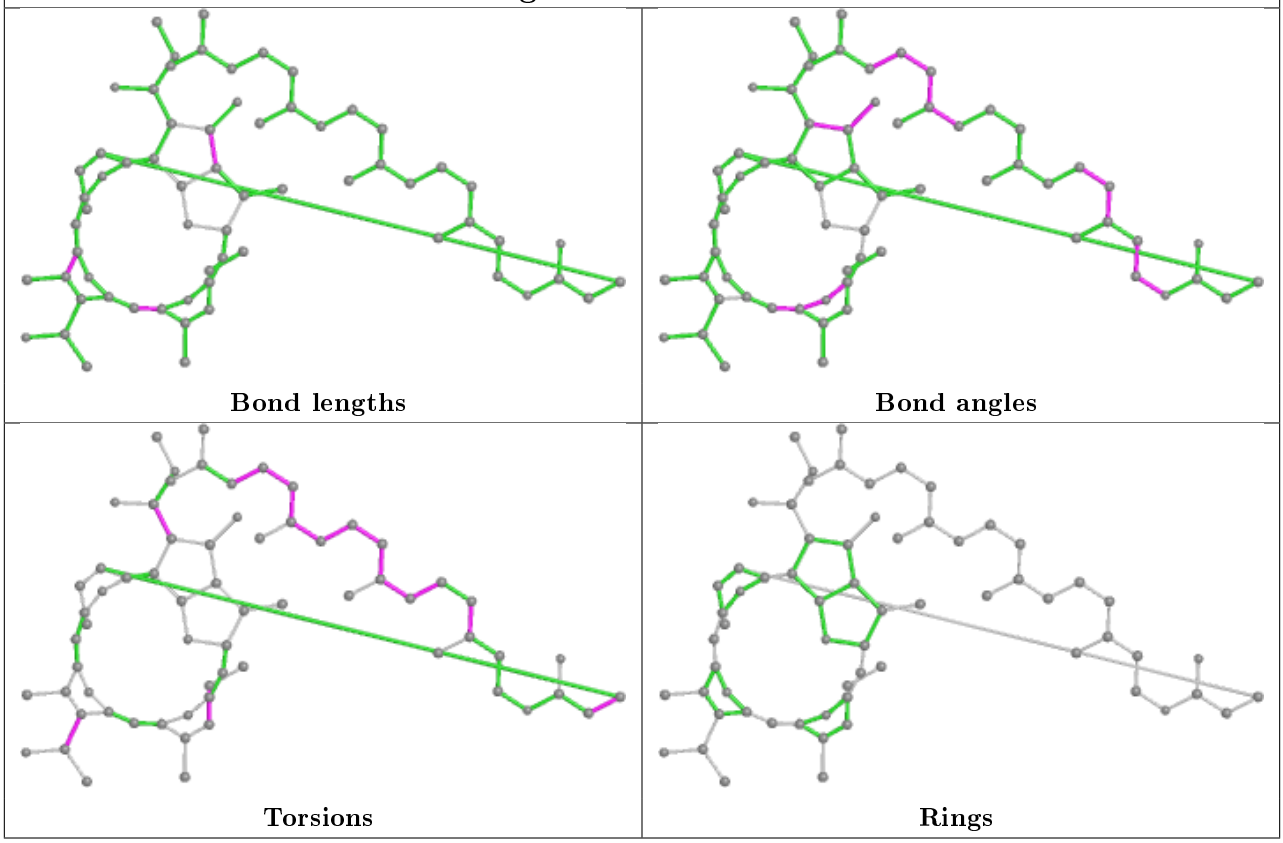
Ligand BCL M 405



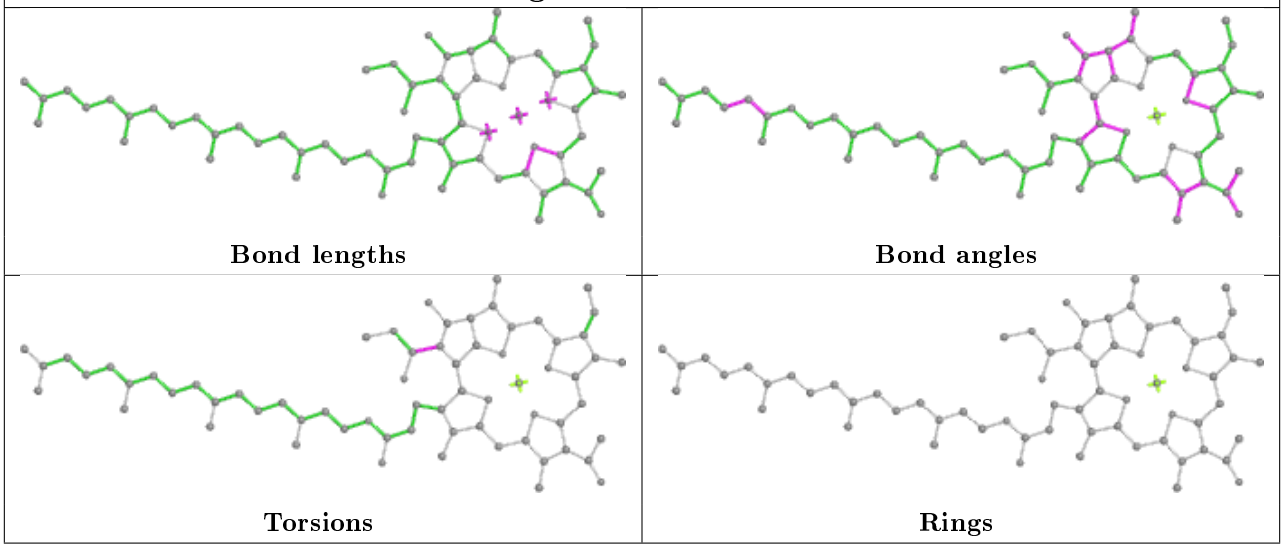
Ligand OLC L 301

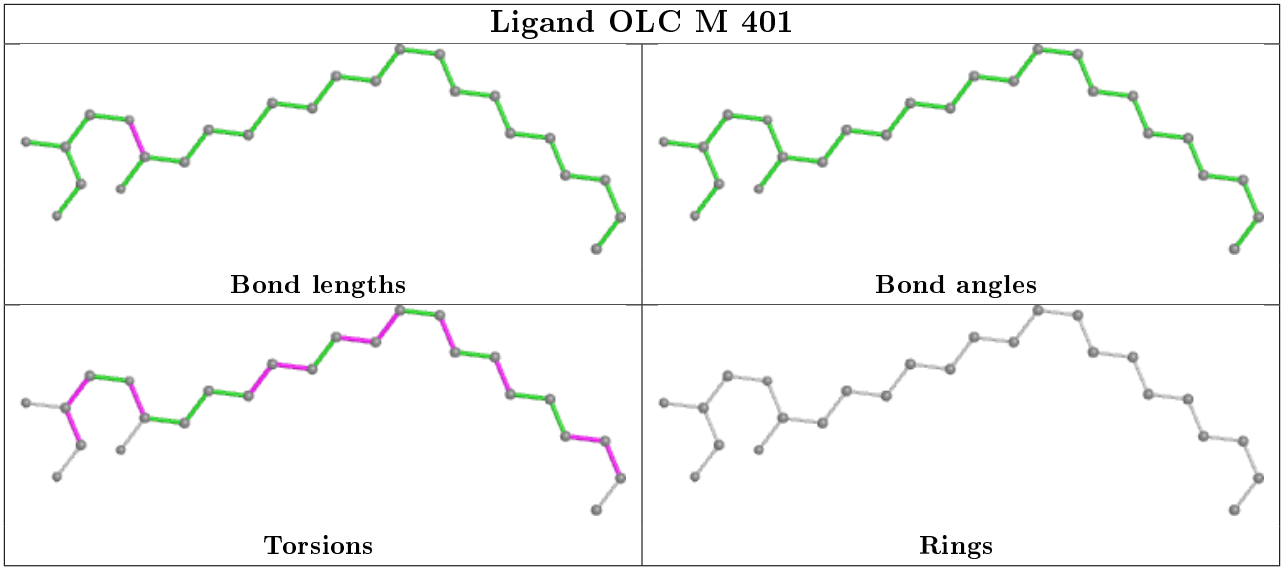


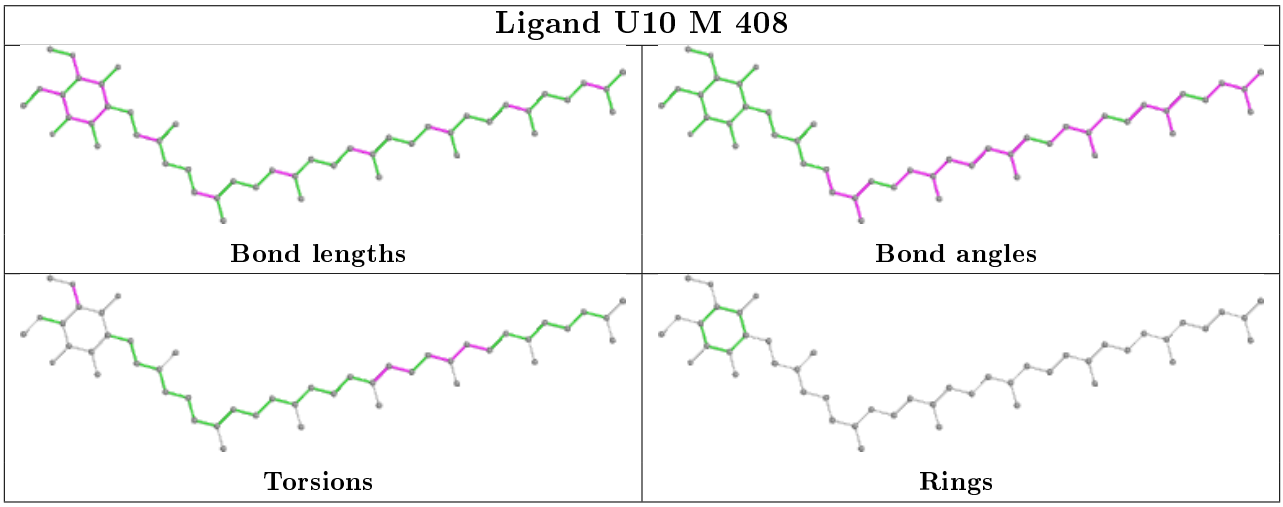
Ligand BPH M 406



Ligand BCL L 303







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	240/250 (96%)	0.49	22 (9%) 9 11	40, 58, 79, 109	0
2	L	270/281 (96%)	0.71	34 (12%) 3 5	37, 56, 102, 127	0
3	M	302/302 (100%)	0.70	37 (12%) 4 5	37, 56, 90, 116	0
All	All	812/833 (97%)	0.64	93 (11%) 4 6	37, 57, 90, 127	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	51	TRP	9.1
2	L	255	TRP	9.0
3	M	1	ALA	8.7
2	L	266	TRP	8.1
1	H	9	ASN	7.7
1	H	246	PRO	7.3
1	H	92	VAL	7.0
2	L	263	TRP	7.0
2	L	257	ASP	6.9
2	L	59	TRP	6.9
2	L	267	VAL	6.8
1	H	165	VAL	6.6
2	L	268	LYS	6.3
2	L	265	TRP	5.9
2	L	270	PRO	5.8
3	M	68	PHE	5.1
2	L	258	GLN	4.9
2	L	269	LEU	4.9
1	H	248	ARG	4.8
2	L	264	GLN	4.7
2	L	165	GLY	4.6
2	L	254	ILE	4.6
3	M	72	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
2	L	262	TRP	4.5
3	M	83	ALA	4.4
3	M	302	GLY	4.1
2	L	259	TRP	4.0
3	M	103	LEU	4.0
1	H	90	THR	3.9
1	H	18	TYR	3.7
2	L	260	VAL	3.6
1	H	91	ALA	3.6
1	H	245	ALA	3.6
2	L	55	LEU	3.6
2	L	261	ASP	3.6
3	M	106	ALA	3.5
1	H	150	GLY	3.5
3	M	105	PHE	3.5
2	L	40	PHE	3.5
2	L	256	PHE	3.4
3	M	2	GLU	3.4
2	L	58	THR	3.3
2	L	252	GLY	3.3
1	H	149	ILE	3.3
2	L	57	GLY	3.2
3	M	92	PHE	3.1
2	L	166	ASN	3.1
3	M	100	GLU	3.0
3	M	80	TRP	3.0
3	M	297	TRP	3.0
3	M	85	PHE	2.9
3	M	76	TYR	2.9
1	H	10	PHE	2.9
2	L	54	VAL	2.8
1	H	12	LEU	2.8
3	M	288	GLY	2.7
3	M	171	TRP	2.7
3	M	214	LEU	2.7
1	H	188	THR	2.7
2	L	56	GLN	2.7
3	M	215	LEU	2.7
1	H	171	ILE	2.7
3	M	75	TRP	2.6
2	L	44	LEU	2.6
3	M	221	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	M	244	ALA	2.5
3	M	207	ALA	2.5
1	H	201	ASN	2.5
3	M	109	LEU	2.5
3	M	222	THR	2.5
3	M	223	ILE	2.4
3	M	84	VAL	2.4
1	H	135	LYS	2.4
2	L	63	LEU	2.4
3	M	218	MET	2.4
1	H	136	ALA	2.4
3	M	224	LEU	2.3
2	L	49	ILE	2.3
3	M	101	TYR	2.3
2	L	75	LEU	2.3
3	M	102	GLY	2.3
1	H	146	LYS	2.3
3	M	174	ALA	2.3
2	L	60	ASN	2.3
3	M	87	ARG	2.3
2	L	53	ALA	2.3
3	M	12	VAL	2.2
1	H	186	GLY	2.2
3	M	225	ALA	2.2
1	H	203	VAL	2.1
1	H	163	LYS	2.1
3	M	250	LEU	2.1
3	M	226	VAL	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

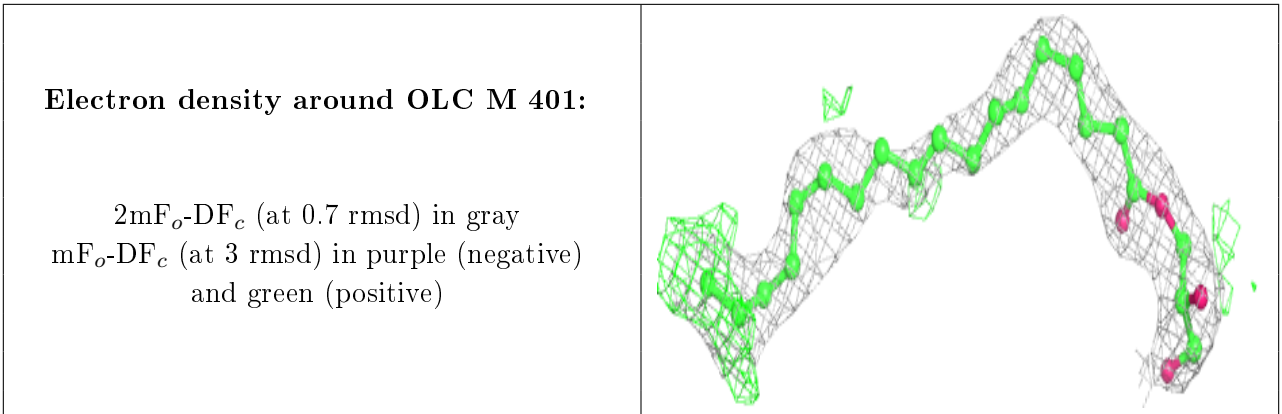
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

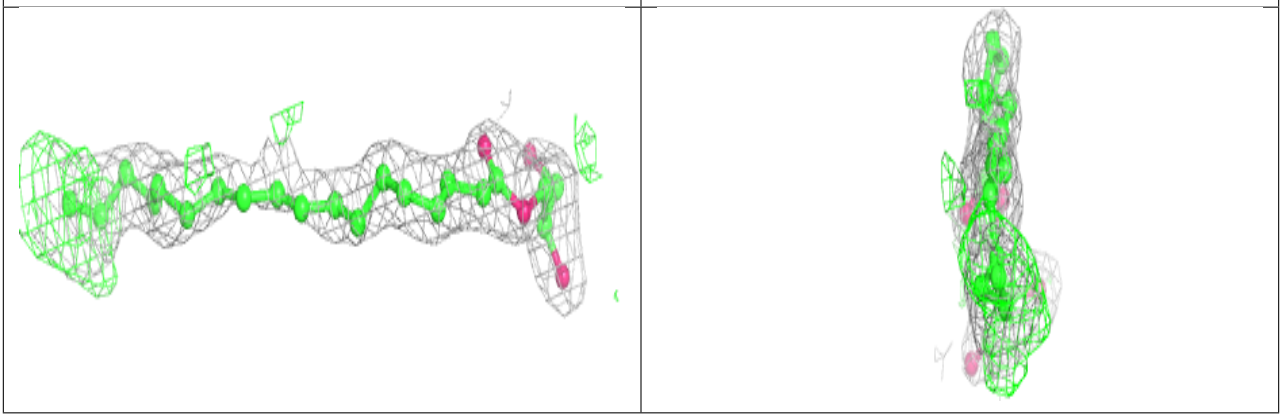
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	LDA	L	302	16/16	0.56	0.26	63,76,87,88	0
4	LDA	M	402	16/16	0.60	0.33	65,80,93,94	0
4	LDA	M	410	16/16	0.62	0.36	64,72,84,89	0
4	LDA	H	701	16/16	0.71	0.26	47,69,76,81	0
4	LDA	M	411	16/16	0.76	0.24	64,69,75,75	0
4	LDA	M	409	16/16	0.77	0.41	71,83,100,100	0
6	OLC	M	401	25/25	0.83	0.21	57,70,86,88	0
5	PO4	H	705	5/5	0.84	0.39	76,77,101,107	0
5	PO4	M	413	5/5	0.85	0.14	71,72,92,101	0
5	PO4	M	416	5/5	0.86	0.15	76,85,89,93	5
6	OLC	L	301	25/25	0.86	0.24	49,61,77,79	0
5	PO4	H	703	5/5	0.88	0.30	74,80,98,101	0
10	U10	M	408	48/63	0.89	0.21	37,53,70,72	0
7	BCL	L	303	66/66	0.89	0.14	44,54,62,66	0
8	BPH	M	406	65/65	0.90	0.17	40,50,114,123	0
5	PO4	M	414	5/5	0.90	0.30	82,87,99,103	0
4	LDA	H	702	16/16	0.90	0.19	49,59,74,78	0
7	BCL	M	404	66/66	0.91	0.13	42,52,70,81	0
7	BCL	M	403	66/66	0.92	0.21	47,55,87,90	0
11	EDO	M	417	4/4	0.92	0.16	56,59,60,64	0
5	PO4	H	704	5/5	0.92	0.37	81,91,95,96	0
8	BPH	L	304	65/65	0.95	0.18	39,46,58,63	0
5	PO4	M	415	5/5	0.95	0.17	48,64,67,75	5
7	BCL	M	405	66/66	0.95	0.17	44,51,59,71	0
5	PO4	M	412	5/5	0.99	0.11	48,50,57,70	0
9	FE	M	407	1/1	0.99	0.15	40,40,40,40	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 OLC M 401:

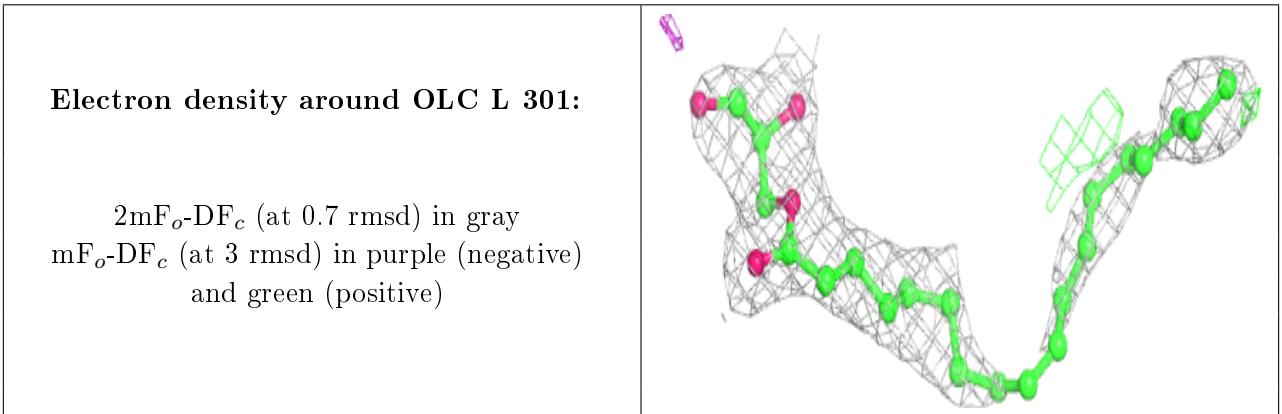
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

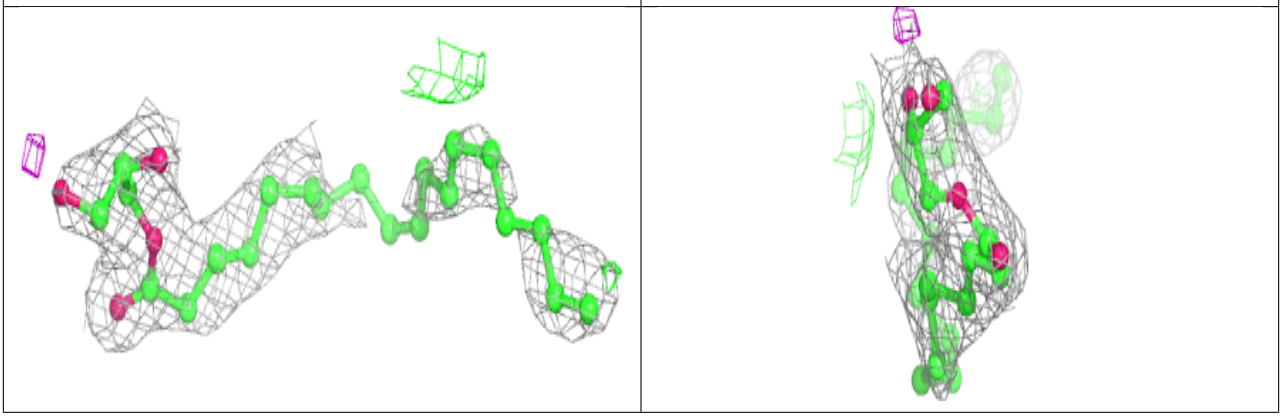




Electron density around OLC L 301:

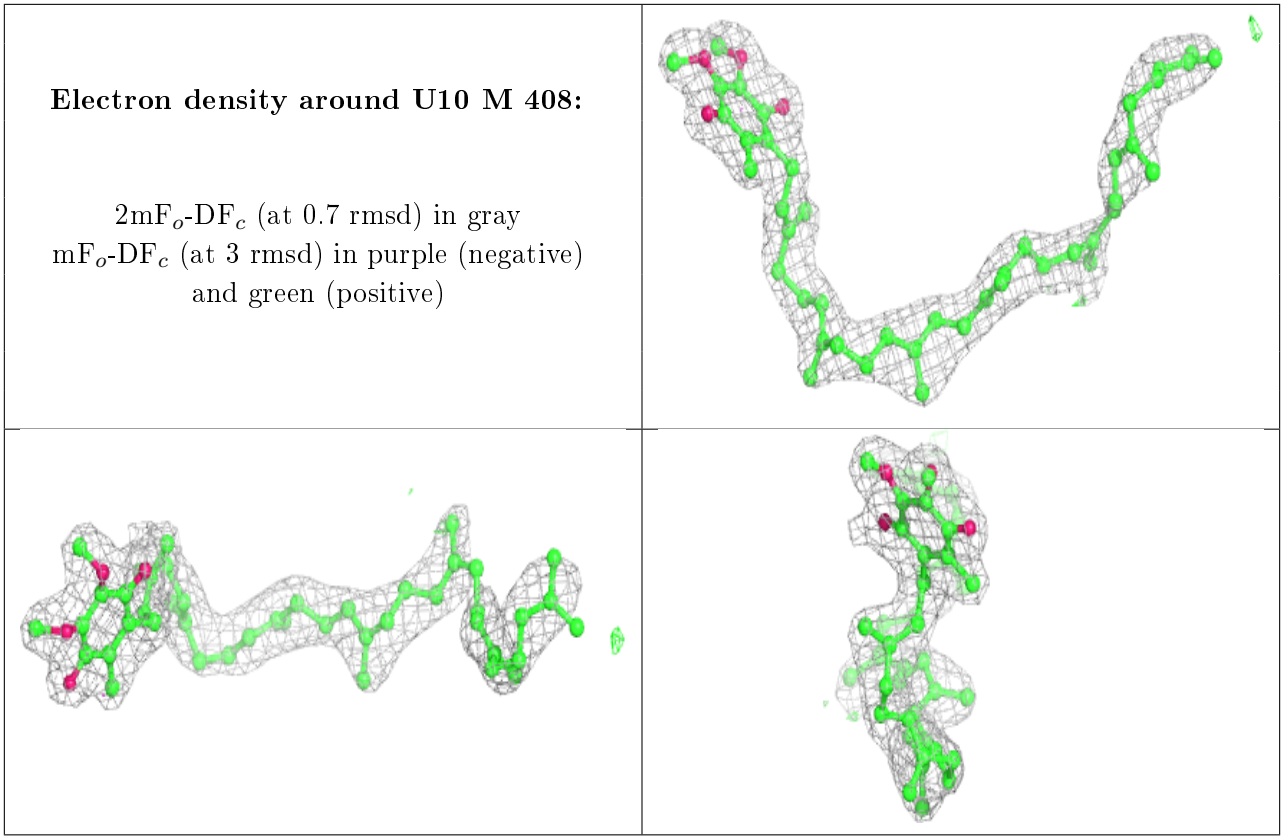
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





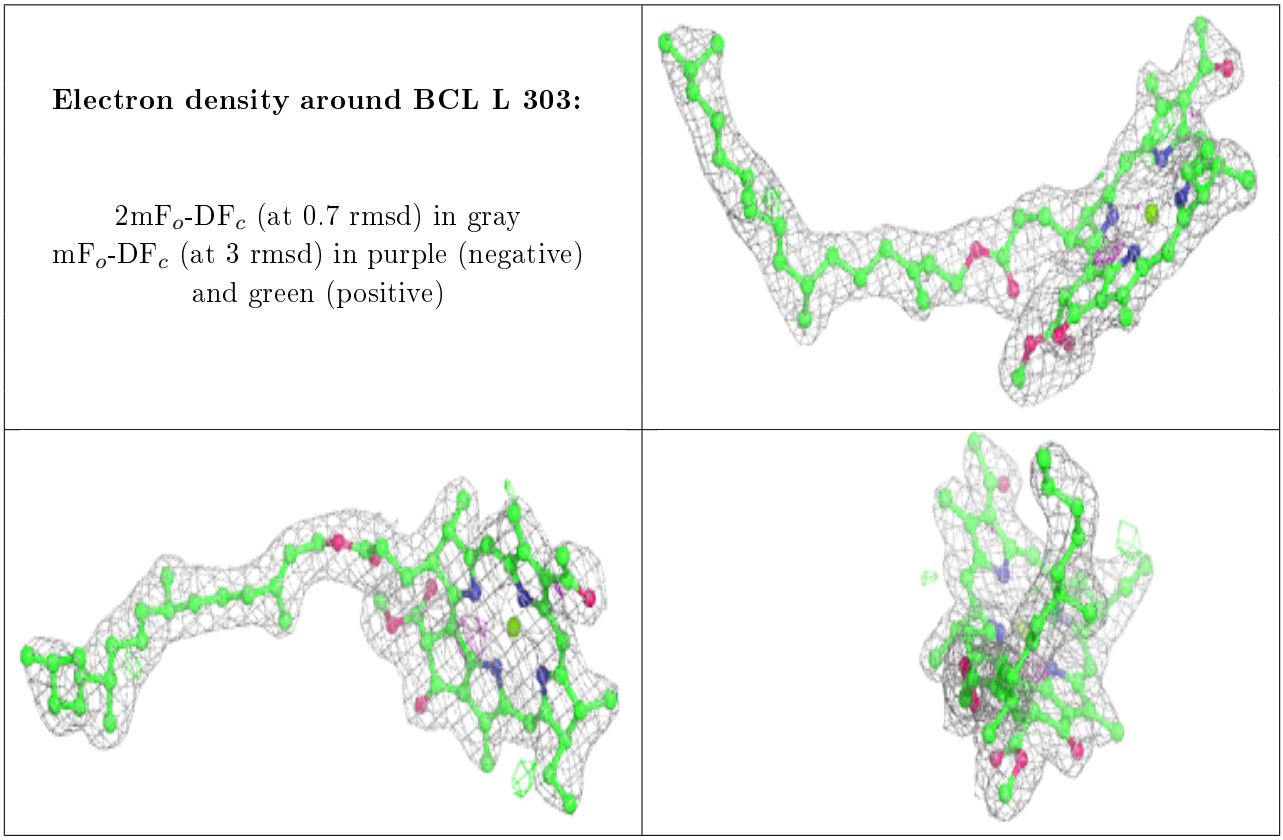
Electron density around U10 M 408:

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



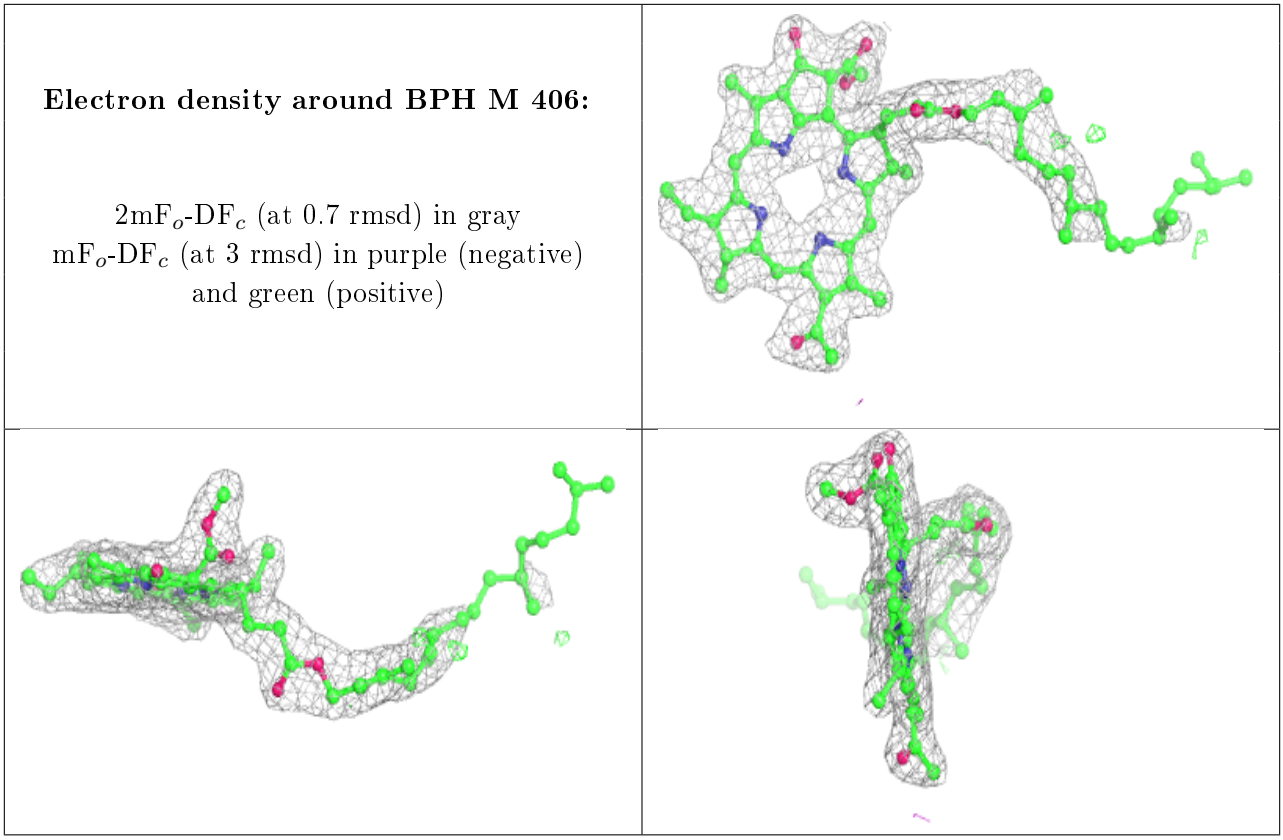
Electron density around BCL L 303:

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



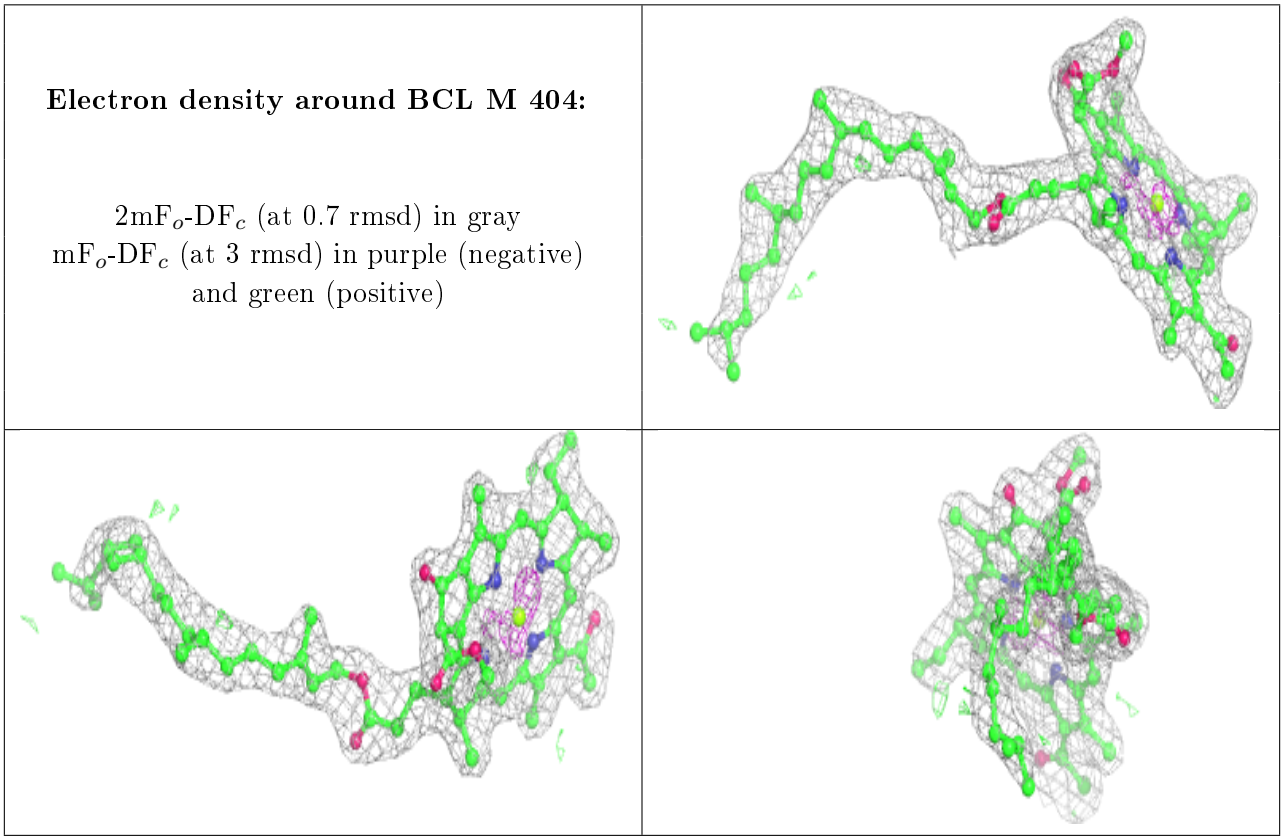
Electron density around BPH M 406:

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



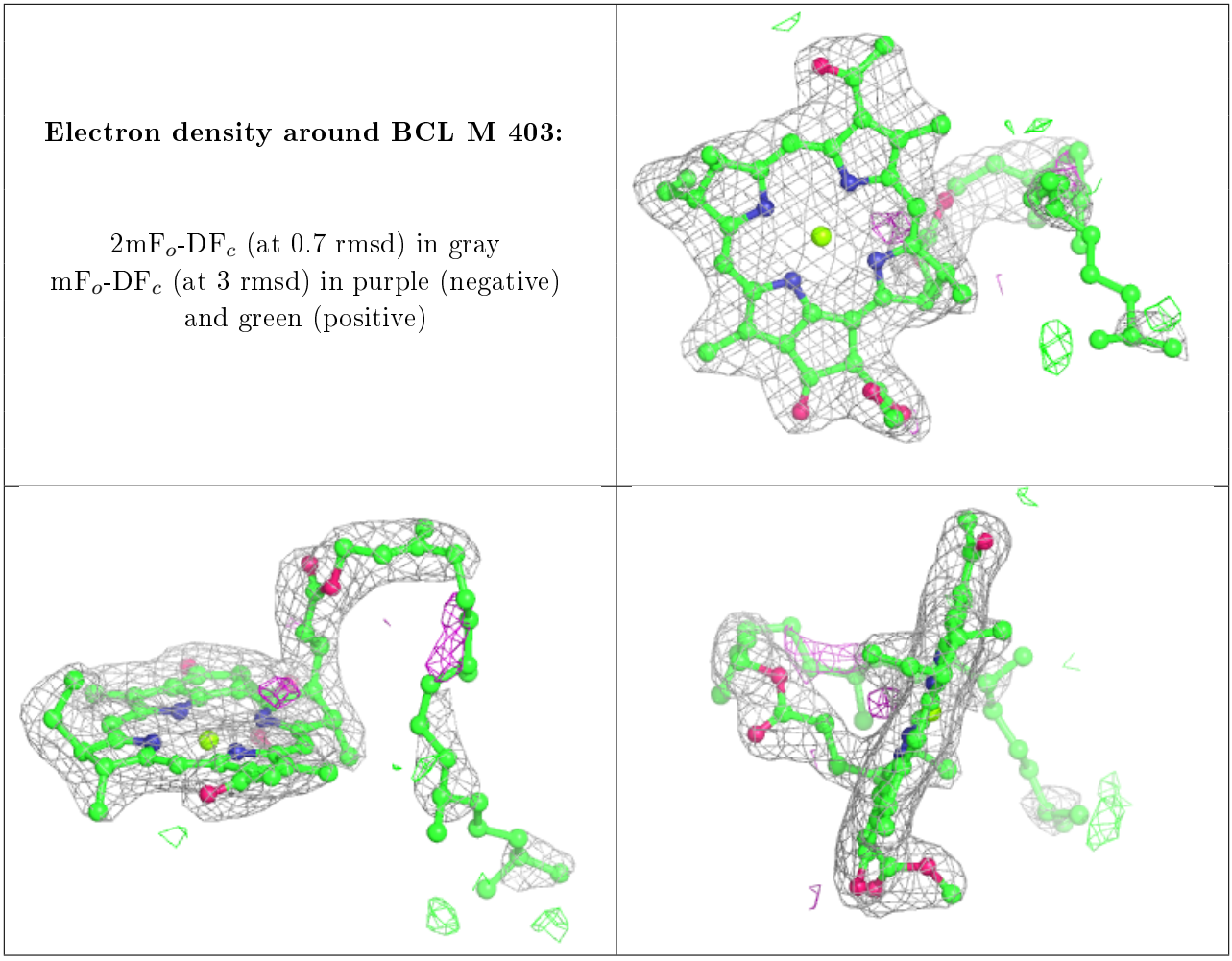
Electron density around BCL M 404:

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



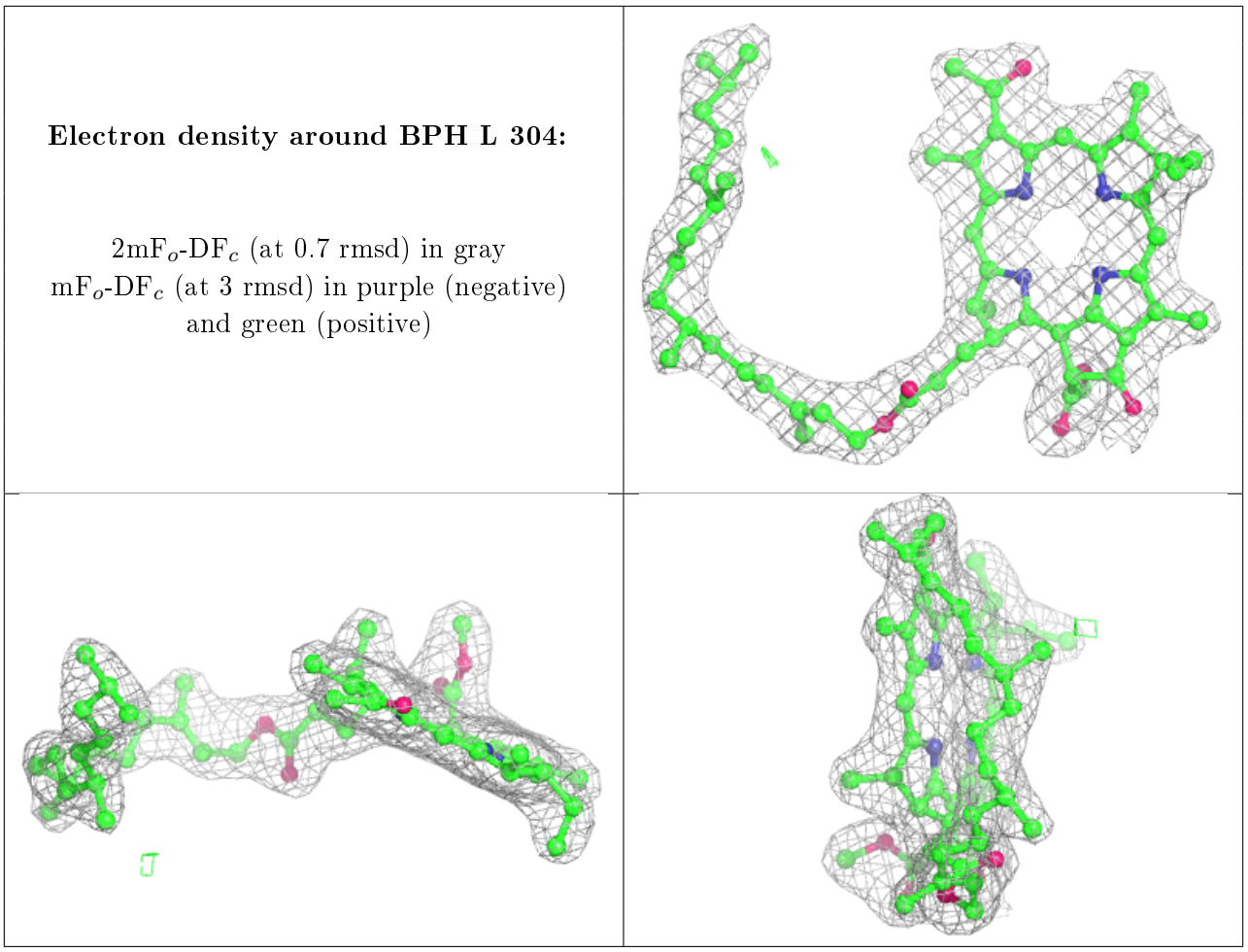
Electron density around BCL M 403:

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



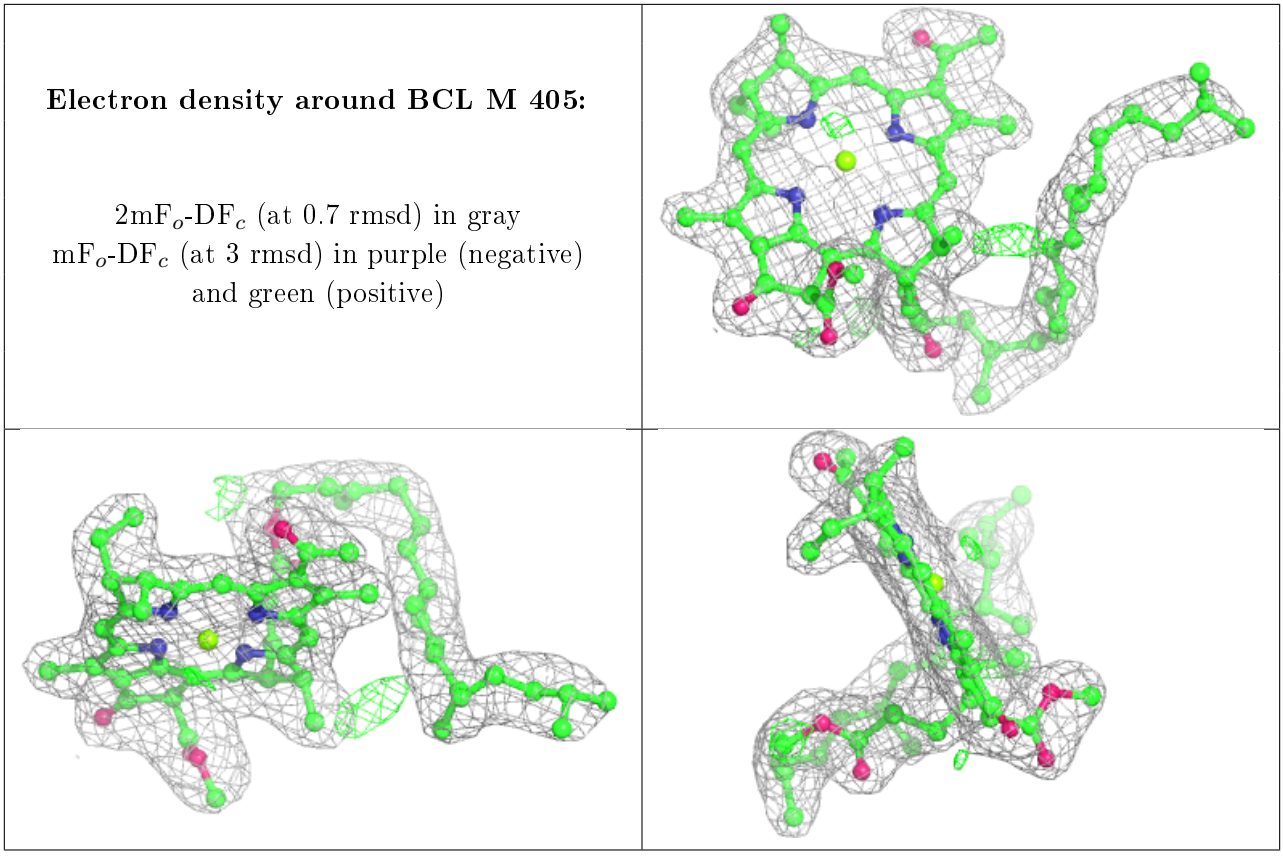
Electron density around BPH L 304:

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



Electron density around BCL M 405:

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



6.5 Other polymers

There are no such residues in this entry.