Full wwPDB X-ray Structure Validation Report (i)

Apr 20, 2024 – 01:03 pm BST

PDB ID	:	5LSE
Title	:	PHOTOSYNTHETIC REACTION CENTER MUTANT WITH Glu L212 replaced with Ala (CHAIN L, EL212W), Asp L213 replaced with ALA (Chain L, DL213A) AND LEU M215 REPLACED WITH ALA (CHAIN M, LM215A)
Authors	:	Fyfe, P.K.; Jones, M.R.
Deposited on	:	2016-08-25
Resolution	:	2.50 Å(reported)

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

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

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

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

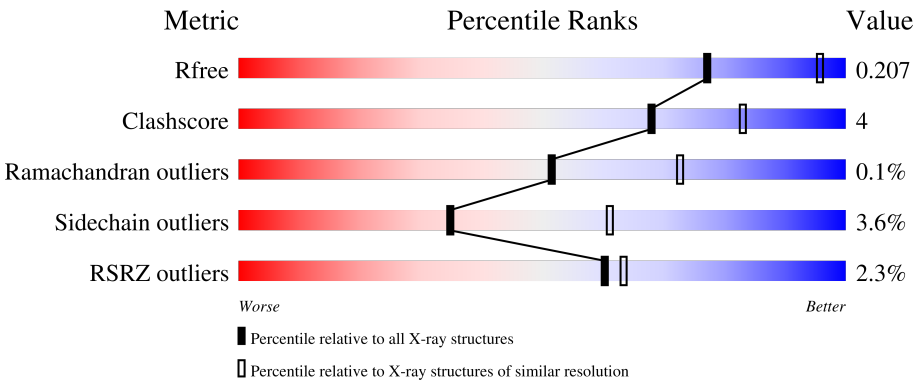
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	L	281	2% 93% 6%
2	M	307	% 87% 9% • •
3	H	260	3% 83% 8% • 8%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	D12	H	305	-	-	-	X

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 7439 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 L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	281	2225	1504	355	358	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	212	ALA	GLU	engineered mutation	UNP P0C0Y8
L	213	ALA	ASP	engineered mutation	UNP P0C0Y8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	300	2397	1599	395	393	10	0	1	0

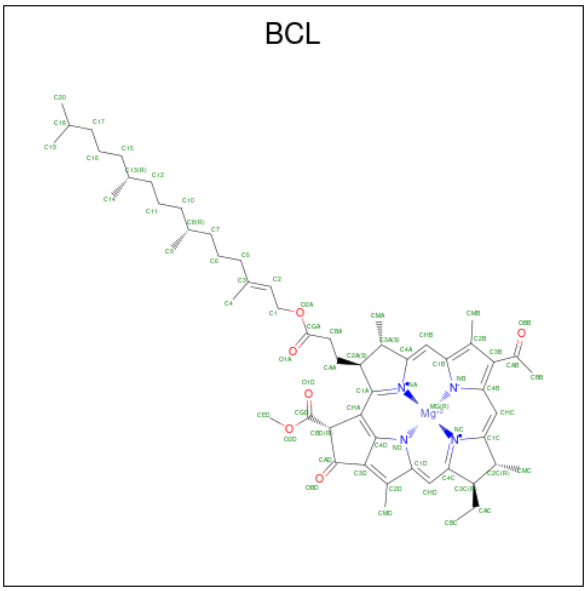
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	215	ALA	LEU	engineered mutation	UNP P0C0Y9

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

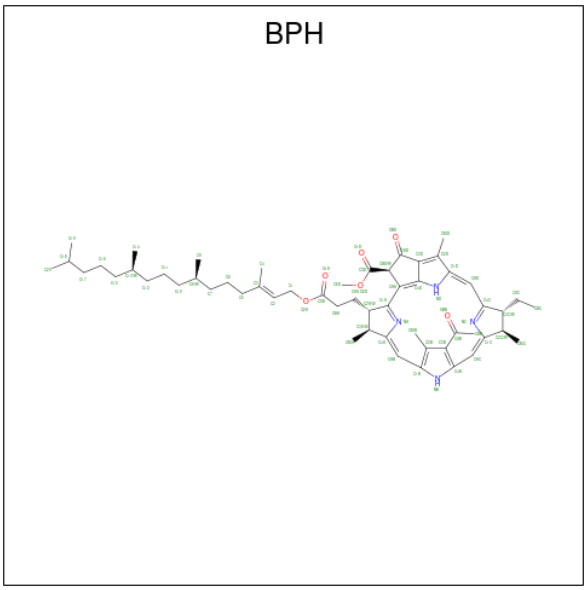
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	240	1837	1173	316	339	9	0	1	0

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



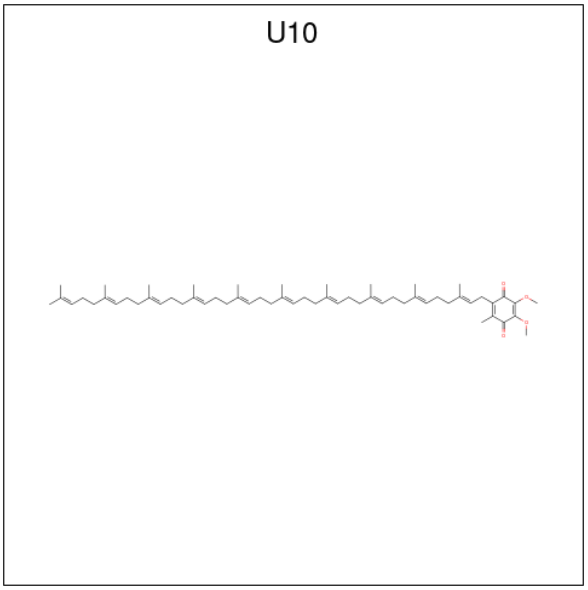
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
4	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
4	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
4	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
4	M	1	66	55	1	4	6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



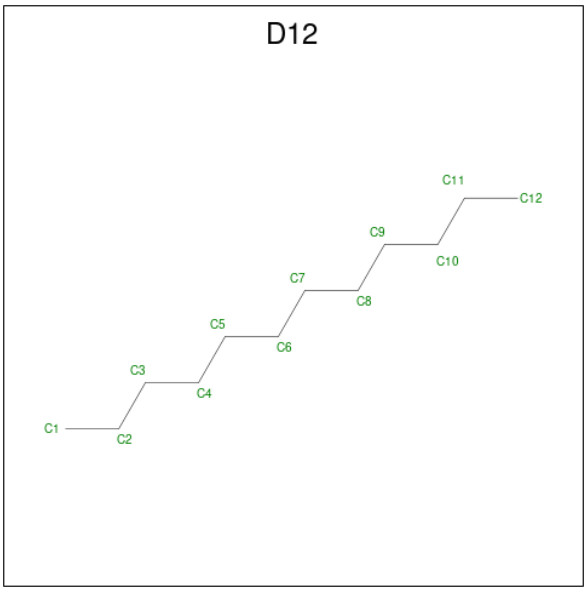
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	L	1	65	55	4	6	0	0
5	M	1	65	55	4	6	0	0

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



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

- Molecule 7 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).

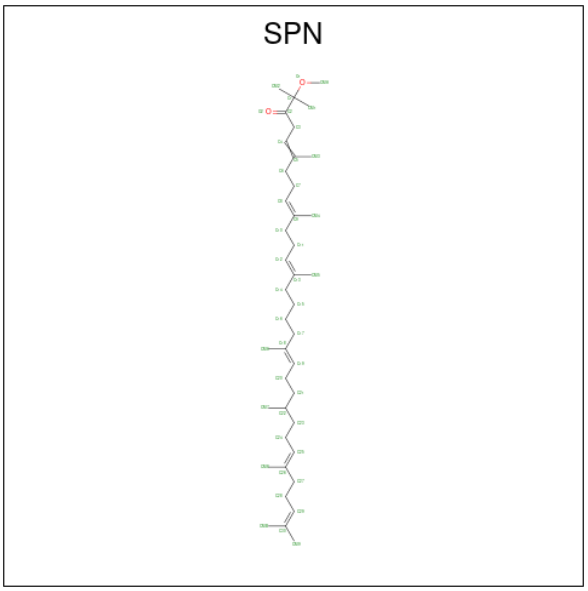


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C 8 8	0	0
7	H	1	Total C 12 12	0	0
7	H	1	Total C 9 9	0	0
7	H	1	Total C 8 8	0	0
7	H	1	Total C 8 8	0	0

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

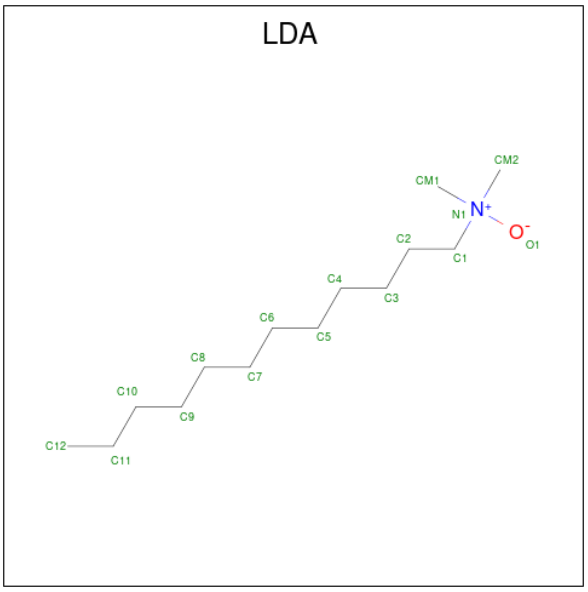
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total Fe 1 1	0	0

- Molecule 9 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$).



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

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

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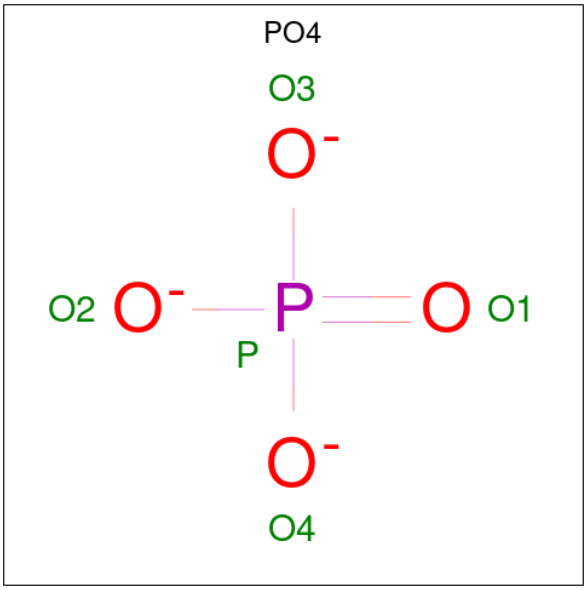
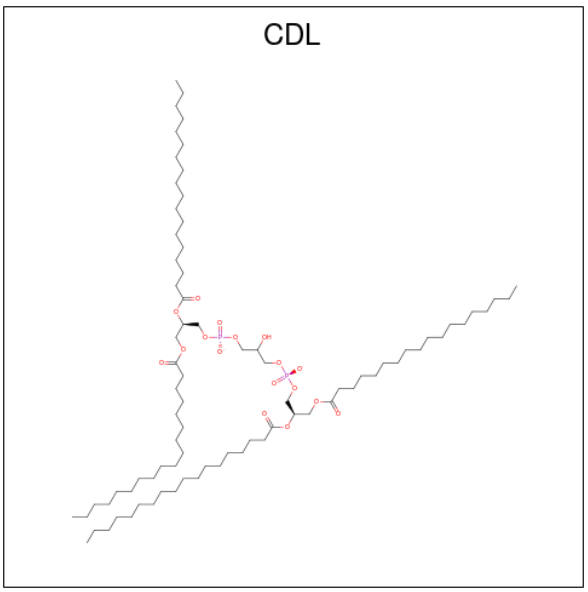
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	H	1	16	14	1	1	0	0

- Molecule 11 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 12 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		
12	M	1	78	59	17	2	0	0

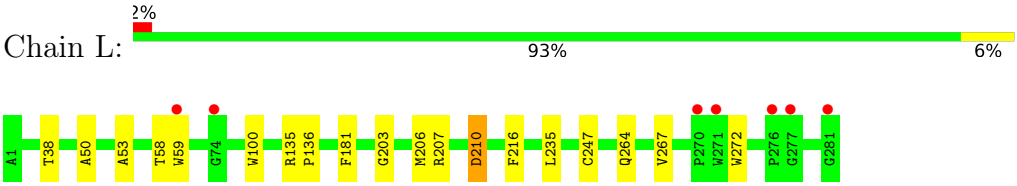
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	L	72	72	72	0	0
			Total	O		
13	M	83	83	83	0	0
			Total	O		
13	H	115	115	115	0	0

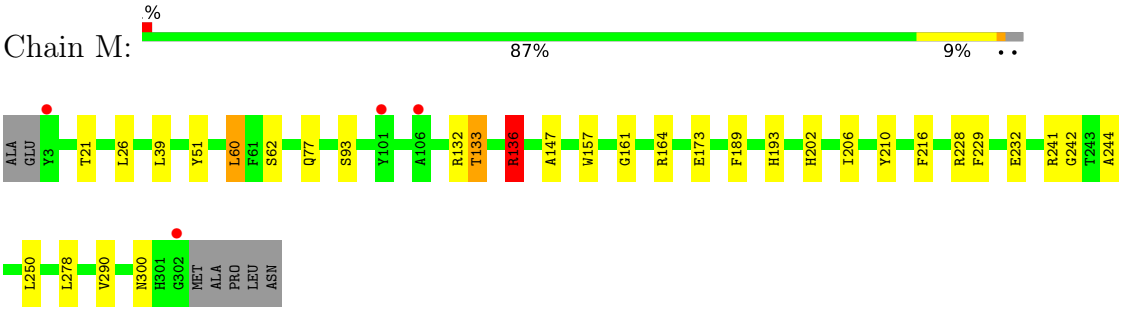
3 Residue-property plots (i)

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.

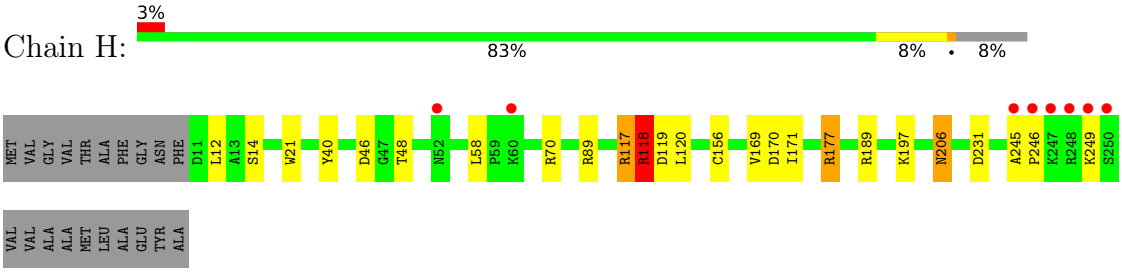
• Molecule 1: Reaction center protein L chain



• Molecule 2: Reaction center protein M chain



• Molecule 3: Reaction center protein H 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	138.99Å 138.99Å 184.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.90 – 2.50 27.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (23.90-2.50) 98.9 (27.05-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.168 , 0.201 0.175 , 0.207	Depositor DCC
R_{free} test set	3515 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 59.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7439	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, U10, FE, D12, SPN, CDL, LDA, BPH, BCL

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	L	0.77	0/2313	0.77	3/3166 (0.1%)
2	M	0.76	0/2494	0.82	5/3404 (0.1%)
3	H	0.79	0/1885	0.94	9/2564 (0.4%)
All	All	0.77	0/6692	0.84	17/9134 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
2	M	0	1
All	All	0	2

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	241	ARG	NE-CZ-NH1	9.11	124.86	120.30
2	M	241	ARG	NE-CZ-NH2	-8.28	116.16	120.30
3	H	117	ARG	NE-CZ-NH2	-8.12	116.24	120.30
3	H	117	ARG	NE-CZ-NH1	7.65	124.13	120.30
3	H	177	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	L	210	ASP	CB-CG-OD1	6.54	124.19	118.30
3	H	189	ARG	NE-CZ-NH2	-6.47	117.07	120.30
2	M	136	ARG	NE-CZ-NH2	-6.40	117.10	120.30
3	H	89	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	M	136	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	L	207	ARG	NE-CZ-NH2	-6.14	117.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	177	ARG	NE-CZ-NH2	-5.95	117.33	120.30
3	H	119	ASP	CB-CG-OD1	5.51	123.26	118.30
3	H	170	ASP	CB-CG-OD1	5.31	123.08	118.30
3	H	118	ARG	NE-CZ-NH2	5.29	122.94	120.30
2	M	228	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	L	207	ARG	NE-CZ-NH1	5.09	122.85	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	203	GLY	Peptide
2	M	300	ASN	Peptide

5.2 Too-close contacts (i)

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	L	2225	0	2187	6	0
2	M	2397	0	2310	20	0
3	H	1837	0	1841	12	0
4	L	132	0	148	6	0
4	M	132	0	148	7	0
5	L	65	0	75	4	0
5	M	65	0	76	9	0
6	L	48	0	63	1	0
6	M	48	0	63	0	0
7	H	37	0	73	0	0
7	L	8	0	15	0	0
8	L	1	0	0	0	0
9	M	43	0	69	5	0
10	H	16	0	31	1	0
10	M	32	0	62	3	0
11	M	5	0	0	0	0
12	M	78	0	100	0	0
13	H	115	0	0	0	0
13	L	72	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	83	0	0	0	0
All	All	7439	0	7261	55	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 (55) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:303:BPH:HBB3	5:L:303:BPH:HHC	1.60	0.84
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.73	0.71
3:H:46:ASP:OD1	3:H:48:THR:HB	1.94	0.67
4:M:401:BCL:HMB1	4:M:401:BCL:HBB2	1.78	0.65
4:L:302:BCL:HMB1	4:L:302:BCL:HBB2	1.80	0.63
5:L:303:BPH:HBB2	2:M:210:TYR:HB3	1.83	0.60
1:L:181:PHE:CD2	5:M:403:BPH:HBB1	2.37	0.59
4:M:401:BCL:HMB1	4:M:401:BCL:CBB	2.32	0.59
5:L:303:BPH:HHC	5:L:303:BPH:CBB	2.31	0.59
5:M:403:BPH:HHC	5:M:403:BPH:HBB3	1.83	0.59
4:L:302:BCL:O1D	10:M:406:LDA:HM22	2.04	0.58
2:M:232:GLU:OE2	3:H:177:ARG:NH2	2.37	0.57
4:M:401:BCL:CAB	9:M:405:SPN:H162	2.36	0.56
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.88	0.55
6:L:304:U10:H28	6:L:304:U10:H251	1.89	0.54
3:H:118:ARG:HD3	3:H:120:LEU:HD12	1.90	0.53
4:L:301:BCL:HMB1	4:L:301:BCL:CBB	2.39	0.53
2:M:77:GLN:HE22	2:M:93:SER:H	1.57	0.53
2:M:242:GLY:CA	3:H:117:ARG:HD3	2.38	0.53
2:M:161:GLY:HA3	9:M:405:SPN:H201	1.90	0.52
2:M:189:PHE:O	2:M:193:HIS:HD2	1.94	0.51
4:M:402:BCL:CBB	4:M:402:BCL:HMB1	2.41	0.51
2:M:157:TRP:CD1	9:M:405:SPN:H202	2.45	0.51
1:L:181:PHE:HB3	5:M:403:BPH:CBB	2.40	0.50
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.94	0.50
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.48	0.49
4:L:302:BCL:HMB1	4:L:302:BCL:CBB	2.43	0.49
3:H:169:VAL:HG23	3:H:171:ILE:HD13	1.95	0.48
2:M:51:TYR:O	2:M:132:ARG:NH2	2.39	0.47
2:M:21:THR:CG2	2:M:26:LEU:HD11	2.44	0.46
3:H:70:ARG:O	3:H:118:ARG:NH1	2.48	0.46
5:M:403:BPH:H7C2	5:M:403:BPH:H142	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:136:ARG:NE	2:M:136:ARG:HA	2.31	0.45
2:M:242:GLY:HA2	3:H:117:ARG:HD3	1.99	0.45
4:M:401:BCL:H92	5:M:403:BPH:HMB1	1.97	0.45
2:M:164:ARG:HH12	2:M:173:GLU:HG3	1.82	0.45
5:M:403:BPH:HHD	5:M:403:BPH:HBC3	1.97	0.45
1:L:181:PHE:HB3	5:M:403:BPH:HBB2	1.99	0.45
2:M:157:TRP:NE1	9:M:405:SPN:H202	2.32	0.45
4:M:401:BCL:H93	4:M:402:BCL:H172	2.00	0.44
5:M:403:BPH:H6C1	5:M:403:BPH:H4C1	1.70	0.44
3:H:40:TYR:HB3	3:H:58:LEU:HD21	2.00	0.44
4:M:401:BCL:C3B	9:M:405:SPN:H152	2.47	0.44
10:M:406:LDA:H92	10:H:301:LDA:H122	1.99	0.44
5:L:303:BPH:HBB1	2:M:210:TYR:CD2	2.52	0.44
2:M:60:LEU:HD21	5:M:403:BPH:H192	1.98	0.44
4:L:301:BCL:HMB1	4:L:301:BCL:HBB3	1.99	0.44
2:M:133:THR:CG2	2:M:147:ALA:HA	2.48	0.44
4:L:301:BCL:CGA	4:L:302:BCL:HBC1	2.48	0.43
1:L:38:THR:HG21	1:L:100:TRP:HE3	1.83	0.43
1:L:50:ALA:O	1:L:53:ALA:HB3	2.19	0.43
3:H:156:CYS:HB3	3:H:206:ASN:O	2.19	0.42
2:M:290:VAL:HG21	3:H:12:LEU:HD23	2.02	0.42
3:H:245:ALA:N	3:H:246:PRO:CD	2.83	0.42
10:M:406:LDA:HM13	3:H:21:TRP:HZ2	1.85	0.41

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	L	279/281 (99%)	271 (97%)	7 (2%)	1 (0%)	34 54
2	M	299/307 (97%)	285 (95%)	14 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	239/260 (92%)	236 (99%)	3 (1%)	0	100	100
All	All	817/848 (96%)	792 (97%)	24 (3%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	58	THR

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	L	218/218 (100%)	209 (96%)	9 (4%)	30	55
2	M	235/239 (98%)	227 (97%)	8 (3%)	37	63
3	H	196/208 (94%)	190 (97%)	6 (3%)	40	67
All	All	649/665 (98%)	626 (96%)	23 (4%)	35	62

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

Mol	Chain	Res	Type
1	L	59	TRP
1	L	206	MET
1	L	210	ASP
1	L	216	PHE
1	L	235	LEU
1	L	247	CYS
1	L	264	GLN
1	L	267	VAL
1	L	272	TRP
2	M	39	LEU
2	M	60	LEU
2	M	62	SER
2	M	133	THR
2	M	136	ARG

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Mol	Chain	Res	Type
2	M	216	PHE
2	M	250	LEU
2	M	278	LEU
3	H	14	SER
3	H	118	ARG
3	H	197	LYS
3	H	206	ASN
3	H	231	ASP
3	H	249	LYS

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

Mol	Chain	Res	Type
2	M	44	ASN
2	M	77	GLN
2	M	193	HIS
3	H	44	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	D12	H	302	-	11,11,11	0.38	0	10,10,10	0.27	0
10	LDA	H	301	-	12,15,15	2.23	1 (8%)	14,17,17	2.73	3 (21%)
4	BCL	L	302	-	64,74,74	1.06	4 (6%)	78,115,115	1.52	15 (19%)
5	BPH	L	303	-	51,70,70	0.71	1 (1%)	52,101,101	1.48	9 (17%)
4	BCL	L	301	-	64,74,74	1.01	4 (6%)	78,115,115	1.42	14 (17%)
9	SPN	M	405	-	40,42,42	3.63	17 (42%)	50,52,52	2.35	19 (38%)
10	LDA	M	407	-	12,15,15	2.44	1 (8%)	14,17,17	2.15	3 (21%)
6	U10	L	304	-	48,48,63	1.83	5 (10%)	58,61,79	1.66	12 (20%)
6	U10	M	404	-	48,48,63	1.71	3 (6%)	58,61,79	1.41	6 (10%)
10	LDA	M	406	-	12,15,15	2.47	1 (8%)	14,17,17	1.69	3 (21%)
12	CDL	M	409	-	77,77,99	1.20	4 (5%)	83,89,111	1.09	7 (8%)
7	D12	H	305	-	7,7,11	0.51	0	6,6,10	0.17	0
7	D12	H	304	-	7,7,11	0.45	0	6,6,10	0.43	0
11	PO4	M	408	-	4,4,4	0.92	0	6,6,6	0.55	0
7	D12	L	305	-	7,7,11	0.48	0	6,6,10	0.30	0
4	BCL	M	401	-	64,74,74	1.10	4 (6%)	78,115,115	1.64	15 (19%)
7	D12	H	303	-	8,8,11	0.44	0	7,7,10	0.25	0
4	BCL	M	402	-	64,74,74	1.36	4 (6%)	78,115,115	1.48	17 (21%)
5	BPH	M	403	-	51,70,70	0.72	0	52,101,101	1.68	12 (23%)

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
10	LDA	M	406	-	-	2/13/13/13	-
12	CDL	M	409	-	-	36/88/88/110	-
7	D12	H	305	-	-	1/5/5/9	-
6	U10	L	304	-	-	17/45/69/87	0/1/1/1
7	D12	H	302	-	-	3/9/9/9	-
7	D12	H	303	-	-	1/6/6/9	-
7	D12	H	304	-	-	1/5/5/9	-
4	BCL	L	302	-	-	4/37/137/137	-
5	BPH	L	303	-	-	3/37/105/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	U10	M	404	-	-	14/45/69/87	0/1/1/1
4	BCL	M	402	-	-	3/37/137/137	-
9	SPN	M	405	-	-	21/50/51/51	-
4	BCL	L	301	-	-	2/37/137/137	-
10	LDA	H	301	-	-	7/13/13/13	-
7	D12	L	305	-	-	2/5/5/9	-
5	BPH	M	403	-	-	14/37/105/105	0/5/6/6
10	LDA	M	407	-	-	5/13/13/13	-
4	BCL	M	401	-	-	9/37/137/137	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	405	SPN	C3-C4	-9.33	1.37	1.50
10	M	407	LDA	O1-N1	-8.26	1.22	1.42
10	M	406	LDA	O1-N1	-8.24	1.22	1.42
6	L	304	U10	C6-C1	7.96	1.49	1.35
10	H	301	LDA	O1-N1	-7.63	1.24	1.42
6	M	404	U10	C6-C1	7.54	1.49	1.35
4	M	402	BCL	MG-NA	7.40	2.23	2.06
9	M	405	SPN	C10-C9	-7.18	1.36	1.51
9	M	405	SPN	C17-C18	-6.95	1.36	1.51
9	M	405	SPN	C6-C5	-6.79	1.37	1.51
9	M	405	SPN	C14-C13	-6.66	1.37	1.51
6	L	304	U10	C36-C34	-6.26	1.38	1.51
6	M	404	U10	C36-C34	-6.15	1.38	1.51
9	M	405	SPN	C4-C5	6.13	1.47	1.33
9	M	405	SPN	C19-C18	6.11	1.47	1.33
9	M	405	SPN	C8-C9	5.81	1.46	1.33
9	M	405	SPN	C12-C13	5.77	1.46	1.33
12	M	409	CDL	OB6-CB5	4.76	1.47	1.34
12	M	409	CDL	OA8-CA7	4.76	1.47	1.33
12	M	409	CDL	OA6-CA5	4.71	1.47	1.34
4	L	301	BCL	MG-NA	4.67	2.17	2.06
9	M	405	SPN	C11-C12	-4.59	1.35	1.50
4	M	401	BCL	MG-NA	4.57	2.17	2.06
9	M	405	SPN	C20-C19	-4.43	1.36	1.50
9	M	405	SPN	C7-C8	-4.35	1.36	1.50
12	M	409	CDL	OB8-CB7	3.81	1.44	1.33
9	M	405	SPN	C21-C22	-3.41	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	402	BCL	C1B-NB	3.31	1.38	1.35
6	L	304	U10	C4-C3	3.30	1.49	1.36
4	M	402	BCL	C4B-NB	3.18	1.38	1.35
4	L	302	BCL	MG-ND	-3.16	1.99	2.05
6	M	404	U10	C4-C3	3.16	1.49	1.36
4	L	302	BCL	C4B-NB	3.00	1.37	1.35
4	M	401	BCL	C1B-NB	2.98	1.37	1.35
5	L	303	BPH	C3A-C2A	-2.89	1.52	1.54
9	M	405	SPN	C16-C15	-2.80	1.35	1.51
4	L	302	BCL	C4D-ND	-2.77	1.33	1.37
9	M	405	SPN	C1-C2	-2.72	1.51	1.53
4	L	301	BCL	C1B-NB	2.55	1.37	1.35
4	L	302	BCL	C3C-C4C	-2.34	1.48	1.51
4	L	301	BCL	C4B-NB	2.22	1.37	1.35
4	L	301	BCL	C4D-ND	-2.14	1.34	1.37
9	M	405	SPN	C21-C20	-2.07	1.46	1.53
6	L	304	U10	C38-C39	2.05	1.38	1.32
9	M	405	SPN	C6-C7	-2.05	1.46	1.53
4	M	402	BCL	C3C-C4C	-2.05	1.49	1.51
6	L	304	U10	C28-C29	2.04	1.37	1.33
4	M	401	BCL	MG-ND	-2.02	2.01	2.05
4	M	401	BCL	C1D-ND	2.01	1.40	1.37

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	H	301	LDA	O1-N1-C1	-6.58	93.13	109.27
10	M	407	LDA	O1-N1-C1	-5.70	95.29	109.27
9	M	405	SPN	CM5-C13-C14	5.54	124.59	115.27
9	M	405	SPN	CM3-C5-C6	5.48	124.50	115.27
10	H	301	LDA	CM1-N1-C1	-5.35	98.99	110.23
10	H	301	LDA	CM2-N1-C1	-5.27	99.15	110.23
4	M	401	BCL	CMB-C2B-C1B	-5.02	120.75	128.46
12	M	409	CDL	OB6-CB5-C51	4.87	122.01	111.50
5	M	403	BPH	O2D-CGD-CBD	4.75	117.02	111.00
6	M	404	U10	C37-C36-C34	4.56	127.99	112.98
10	M	406	LDA	O1-N1-C1	-4.42	98.44	109.27
10	M	407	LDA	CM1-N1-C1	-4.36	101.07	110.23
6	L	304	U10	C37-C36-C34	4.32	127.19	112.98
4	L	302	BCL	CMB-C2B-C1B	-4.28	121.89	128.46
9	M	405	SPN	CM4-C9-C10	4.27	122.46	115.27
9	M	405	SPN	CM6-C18-C17	4.13	122.22	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	402	BCL	C4D-CHA-C1A	4.11	126.25	121.25
4	M	401	BCL	C1-O2A-CGA	3.97	126.85	116.44
5	M	403	BPH	C1-O2A-CGA	3.96	126.82	116.44
4	M	401	BCL	C4D-CHA-C1A	3.96	126.06	121.25
9	M	405	SPN	C11-C10-C9	3.87	125.70	112.98
4	L	302	BCL	CHD-C1D-ND	-3.85	120.92	124.45
9	M	405	SPN	C16-C17-C18	3.81	123.44	113.45
9	M	405	SPN	C16-C15-C14	3.76	126.72	113.19
6	M	404	U10	C30-C29-C31	3.75	121.57	115.27
4	M	402	BCL	CMB-C2B-C1B	-3.74	122.72	128.46
5	L	303	BPH	C4-C3-C5	-3.71	109.03	115.27
9	M	405	SPN	C15-C14-C13	3.62	122.96	113.45
4	M	401	BCL	CMB-C2B-C3B	3.59	131.39	124.68
6	L	304	U10	C30-C29-C31	3.55	121.24	115.27
9	M	405	SPN	C7-C6-C5	3.54	124.63	112.98
4	L	301	BCL	C4D-CHA-C1A	3.51	125.52	121.25
12	M	409	CDL	OA6-CA5-C11	3.42	118.87	111.50
5	M	403	BPH	OBD-CAD-CBD	-3.41	120.81	125.82
10	M	406	LDA	CM1-N1-C1	-3.39	103.11	110.23
6	L	304	U10	C35-C34-C33	-3.36	115.07	123.68
10	M	407	LDA	CM2-N1-C1	-3.34	103.21	110.23
4	L	301	BCL	CMB-C2B-C1B	-3.34	123.33	128.46
9	M	405	SPN	C15-C16-C17	3.31	125.09	113.19
5	M	403	BPH	CMA-C3A-C4A	-3.31	107.14	114.38
4	M	401	BCL	CAA-C2A-C3A	-3.30	103.75	112.78
4	M	402	BCL	C1D-ND-C4D	3.29	108.67	106.33
5	L	303	BPH	CAC-C3C-C2C	3.27	122.44	114.26
4	L	302	BCL	OBB-CAB-C3B	3.27	125.79	119.99
6	L	304	U10	C32-C33-C34	-3.26	119.81	127.66
4	M	402	BCL	CHA-C1A-NA	-3.23	119.01	126.40
6	L	304	U10	C15-C14-C16	3.19	120.63	115.27
4	M	401	BCL	CHA-C1A-NA	-3.18	119.13	126.40
5	M	403	BPH	C1-C2-C3	-3.17	120.55	126.04
4	M	401	BCL	C7-C6-C5	3.17	121.96	113.36
5	L	303	BPH	C4B-NB-C1B	3.17	113.59	107.09
6	L	304	U10	C7-C8-C9	-3.15	121.55	126.79
6	L	304	U10	C36-C34-C33	3.15	127.49	121.12
12	M	409	CDL	OA8-CA7-C31	3.13	121.73	111.91
4	L	302	BCL	CAA-C2A-C3A	-3.11	104.27	112.78
4	M	402	BCL	C2D-C1D-ND	-3.07	107.84	110.10
4	L	301	BCL	C1D-ND-C4D	3.02	108.48	106.33
4	L	301	BCL	C1C-NC-C4C	3.02	108.06	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	302	BCL	CMB-C2B-C3B	3.01	130.31	124.68
4	M	402	BCL	C4A-NA-C1A	2.99	108.05	106.71
6	L	304	U10	C25-C24-C26	2.99	120.30	115.27
4	M	401	BCL	CHD-C1D-ND	-2.98	121.71	124.45
4	L	301	BCL	CAA-C2A-C3A	-2.96	104.68	112.78
4	L	302	BCL	CAC-C3C-C2C	-2.91	106.98	114.26
4	L	301	BCL	CHD-C1D-ND	-2.89	121.80	124.45
5	M	403	BPH	CAC-C3C-C4C	2.83	120.07	113.73
5	M	403	BPH	CED-O2D-CGD	2.80	122.28	115.94
5	L	303	BPH	C1-C2-C3	-2.78	121.23	126.04
4	L	301	BCL	CHA-C1A-NA	-2.76	120.07	126.40
9	M	405	SPN	CM7-C22-C21	2.76	121.30	111.29
4	M	401	BCL	C4-C3-C2	-2.74	116.65	123.68
12	M	409	CDL	OB8-CB7-OB9	-2.72	116.73	123.59
4	M	401	BCL	OBB-CAB-C3B	2.71	124.81	119.99
4	M	402	BCL	CAC-C3C-C4C	-2.71	106.56	112.58
6	M	404	U10	C15-C14-C16	2.68	119.78	115.27
4	M	402	BCL	CAC-C3C-C2C	-2.67	107.58	114.26
5	M	403	BPH	C4B-NB-C1B	2.63	112.49	107.09
6	M	404	U10	C31-C29-C28	-2.62	115.82	121.12
4	L	302	BCL	O2D-CGD-CBD	2.60	115.89	111.27
5	L	303	BPH	CMA-C3A-C4A	-2.60	108.69	114.38
4	M	401	BCL	CMA-C3A-C2A	-2.59	103.38	113.83
4	M	402	BCL	OBB-CAB-CBB	-2.57	114.40	120.17
5	L	303	BPH	O2D-CGD-CBD	2.56	114.25	111.00
4	L	301	BCL	C2D-C1D-ND	-2.55	108.22	110.10
4	M	402	BCL	CHD-C1D-ND	-2.55	122.11	124.45
10	M	406	LDA	CM2-N1-C1	-2.54	104.89	110.23
9	M	405	SPN	C6-C7-C8	2.52	120.17	111.88
4	L	302	BCL	CAA-CBA-CGA	2.52	120.63	113.25
6	L	304	U10	C30-C29-C28	-2.51	117.24	123.68
5	M	403	BPH	CAA-C2A-C3A	-2.51	105.91	112.78
9	M	405	SPN	C17-C18-C19	-2.49	116.08	121.12
4	L	301	BCL	C4B-C3B-CAB	-2.48	122.33	127.13
9	M	405	SPN	CM8-C26-C27	2.48	119.44	115.27
9	M	405	SPN	C20-C21-C22	2.47	124.29	115.76
6	M	404	U10	C32-C33-C34	-2.45	121.75	127.66
4	M	402	BCL	C1-O2A-CGA	2.41	122.76	116.44
4	L	302	BCL	C4D-CHA-C1A	2.40	124.16	121.25
4	M	402	BCL	CED-O2D-CGD	2.38	121.32	115.94
12	M	409	CDL	OB8-CB7-C71	2.36	119.32	111.91
4	L	301	BCL	OBB-CAB-CBB	-2.35	114.89	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	401	BCL	C5-C3-C2	2.34	125.85	121.12
4	L	302	BCL	C1-O2A-CGA	2.32	122.53	116.44
6	L	304	U10	C3M-O3-C3	2.31	124.67	116.47
9	M	405	SPN	C6-C5-C4	-2.31	116.43	121.12
4	M	402	BCL	O2A-C1-C2	2.31	114.72	108.64
4	M	402	BCL	C4B-C3B-CAB	-2.30	122.69	127.13
6	M	404	U10	C17-C18-C19	-2.29	122.14	127.66
4	M	401	BCL	CAA-CBA-CGA	2.27	119.90	113.25
4	L	302	BCL	C4B-C3B-CAB	-2.27	122.74	127.13
4	M	402	BCL	C2A-C1A-CHA	2.26	127.81	123.86
5	M	403	BPH	C6-C7-C8	2.24	123.17	115.92
9	M	405	SPN	CM7-C22-C23	2.23	119.35	111.29
4	L	302	BCL	CHA-C1A-NA	-2.21	121.33	126.40
9	M	405	SPN	CM5-C13-C12	-2.21	118.01	123.68
5	L	303	BPH	CMB-C2B-C3B	2.19	128.78	124.68
4	L	301	BCL	CMB-C2B-C3B	2.19	128.78	124.68
12	M	409	CDL	OB6-CB5-OB7	-2.19	118.41	123.70
4	M	401	BCL	C4B-C3B-CAB	-2.19	122.90	127.13
4	M	402	BCL	CHD-C1D-C2D	2.18	130.04	125.48
4	L	301	BCL	CED-O2D-CGD	2.17	120.84	115.94
5	M	403	BPH	CAC-C3C-C2C	-2.16	108.85	114.26
5	M	403	BPH	CAA-CBA-CGA	2.16	119.58	113.25
4	L	302	BCL	O1D-CGD-CBD	-2.16	120.06	124.48
6	L	304	U10	C20-C19-C21	2.16	118.90	115.27
4	M	401	BCL	C1C-NC-C4C	2.15	107.67	106.71
4	L	301	BCL	CHD-C1D-C2D	2.14	129.97	125.48
12	M	409	CDL	OA8-CA7-OA9	-2.12	118.24	123.59
4	L	302	BCL	C5-C3-C2	-2.09	116.88	121.12
4	M	402	BCL	CMB-C2B-C3B	2.08	128.58	124.68
9	M	405	SPN	C7-C8-C9	-2.06	122.69	127.66
4	L	301	BCL	CAA-C2A-C1A	-2.03	105.33	111.97
5	L	303	BPH	C4C-C3C-C2C	-2.02	100.92	102.84
5	L	303	BPH	CAA-C2A-C3A	-2.01	107.26	112.78
4	L	302	BCL	CED-O2D-CGD	2.01	120.49	115.94
6	L	304	U10	C1M-C1-C6	-2.00	121.13	124.40

There are no chirality outliers.

All (145) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	401	BCL	C11-C10-C8-C9
5	M	403	BPH	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
5	M	403	BPH	C4-C3-C5-C6
6	L	304	U10	C28-C29-C31-C32
6	L	304	U10	C30-C29-C31-C32
6	M	404	U10	C29-C31-C32-C33
6	M	404	U10	C36-C37-C38-C39
9	M	405	SPN	CM2-C1-C2-O2
9	M	405	SPN	CM2-C1-C2-C3
9	M	405	SPN	C20-C21-C22-CM7
12	M	409	CDL	CA2-OA2-PA1-OA3
12	M	409	CDL	CA2-OA2-PA1-OA4
12	M	409	CDL	CA3-OA5-PA1-OA4
12	M	409	CDL	CB2-OB2-PB2-OB3
12	M	409	CDL	OB9-CB7-OB8-CB6
6	M	404	U10	C37-C38-C39-C40
5	M	403	BPH	C3-C5-C6-C7
12	M	409	CDL	C71-CB7-OB8-CB6
6	L	304	U10	C17-C18-C19-C20
6	L	304	U10	C27-C28-C29-C30
9	M	405	SPN	C11-C12-C13-CM5
6	L	304	U10	C27-C28-C29-C31
9	M	405	SPN	C14-C15-C16-C17
6	M	404	U10	C37-C38-C39-C41
9	M	405	SPN	CM3-C5-C6-C7
9	M	405	SPN	C11-C10-C9-CM4
9	M	405	SPN	CM5-C13-C14-C15
9	M	405	SPN	C16-C17-C18-CM6
9	M	405	SPN	C4-C5-C6-C7
9	M	405	SPN	C11-C10-C9-C8
9	M	405	SPN	C12-C13-C14-C15
9	M	405	SPN	C16-C17-C18-C19
5	M	403	BPH	C6-C7-C8-C9
4	L	301	BCL	C15-C16-C17-C18
5	M	403	BPH	C10-C11-C12-C13
6	M	404	U10	C27-C28-C29-C30
12	M	409	CDL	CA7-C31-C32-C33
12	M	409	CDL	CB5-C51-C52-C53
6	M	404	U10	C34-C36-C37-C38
5	M	403	BPH	C5-C6-C7-C8
6	L	304	U10	C32-C33-C34-C35
5	M	403	BPH	C8-C10-C11-C12
12	M	409	CDL	C78-C79-C80-C81
12	M	409	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
7	H	302	D12	C7-C8-C9-C10
12	M	409	CDL	C72-C73-C74-C75
12	M	409	CDL	C51-CB5-OB6-CB4
12	M	409	CDL	C37-C38-C39-C40
6	L	304	U10	C17-C18-C19-C21
10	M	406	LDA	C2-C3-C4-C5
10	H	301	LDA	C11-C10-C9-C8
12	M	409	CDL	C74-C75-C76-C77
6	L	304	U10	C33-C34-C36-C37
6	M	404	U10	C33-C34-C36-C37
12	M	409	CDL	C11-CA5-OA6-CA4
7	L	305	D12	C2-C3-C4-C5
12	M	409	CDL	OA7-CA5-OA6-CA4
4	M	401	BCL	C2-C1-O2A-CGA
4	M	401	BCL	C11-C10-C8-C7
5	M	403	BPH	C11-C12-C13-C15
9	M	405	SPN	C21-C22-C23-C24
7	H	302	D12	C3-C4-C5-C6
12	M	409	CDL	C11-C12-C13-C14
10	M	407	LDA	C7-C8-C9-C10
6	L	304	U10	C35-C34-C36-C37
6	M	404	U10	C35-C34-C36-C37
5	M	403	BPH	C11-C12-C13-C14
7	H	303	D12	C5-C6-C7-C8
12	M	409	CDL	C31-C32-C33-C34
10	H	301	LDA	C3-C4-C5-C6
12	M	409	CDL	C71-C72-C73-C74
12	M	409	CDL	CA2-OA2-PA1-OA5
12	M	409	CDL	CA3-OA5-PA1-OA2
12	M	409	CDL	OA5-CA3-CA4-CA6
10	H	301	LDA	C5-C6-C7-C8
9	M	405	SPN	C11-C12-C13-C14
5	M	403	BPH	C11-C10-C8-C7
10	H	301	LDA	N1-C1-C2-C3
6	L	304	U10	C32-C33-C34-C36
4	M	401	BCL	C4-C3-C5-C6
10	H	301	LDA	C4-C5-C6-C7
12	M	409	CDL	C18-C19-C20-C21
6	M	404	U10	C27-C28-C29-C31
10	H	301	LDA	C1-C2-C3-C4
6	L	304	U10	C15-C14-C16-C17
4	M	401	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
7	H	305	D12	C2-C3-C4-C5
4	M	402	BCL	C13-C15-C16-C17
5	L	303	BPH	CAD-CBD-CGD-O2D
12	M	409	CDL	OA5-CA3-CA4-OA6
10	M	407	LDA	C5-C6-C7-C8
10	H	301	LDA	C9-C10-C11-C12
12	M	409	CDL	CB2-OB2-PB2-OB5
10	M	406	LDA	C4-C5-C6-C7
12	M	409	CDL	CA3-OA5-PA1-OA3
12	M	409	CDL	CB2-OB2-PB2-OB4
12	M	409	CDL	C19-C20-C21-C22
10	M	407	LDA	C6-C7-C8-C9
6	L	304	U10	C13-C14-C16-C17
4	L	302	BCL	C13-C15-C16-C17
12	M	409	CDL	CB3-CB4-CB6-OB8
5	M	403	BPH	C15-C16-C17-C18
6	M	404	U10	C5-C4-O4-C4M
12	M	409	CDL	C80-C81-C82-C83
5	L	303	BPH	C8-C10-C11-C12
7	H	302	D12	C9-C10-C11-C12
6	L	304	U10	C5-C4-O4-C4M
4	M	402	BCL	C14-C13-C15-C16
12	M	409	CDL	C35-C36-C37-C38
5	L	303	BPH	O2A-C1-C2-C3
4	L	302	BCL	C12-C13-C15-C16
12	M	409	CDL	C17-C18-C19-C20
6	M	404	U10	C30-C29-C31-C32
9	M	405	SPN	CM8-C26-C27-C28
7	H	304	D12	C1-C2-C3-C4
6	M	404	U10	C25-C24-C26-C27
4	M	401	BCL	C15-C16-C17-C18
4	M	401	BCL	C2-C3-C5-C6
6	M	404	U10	C28-C29-C31-C32
9	M	405	SPN	C25-C26-C27-C28
4	L	302	BCL	C14-C13-C15-C16
10	M	407	LDA	C2-C3-C4-C5
4	L	301	BCL	CAD-CBD-CGD-O2D
4	L	302	BCL	CAD-CBD-CGD-O2D
4	M	401	BCL	CAD-CBD-CGD-O2D
5	M	403	BPH	CAD-CBD-CGD-O2D
12	M	409	CDL	C72-C71-CB7-OB8
6	M	404	U10	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
12	M	409	CDL	C52-C51-CB5-OB6
5	M	403	BPH	O2A-C1-C2-C3
4	M	402	BCL	CHA-CBD-CGD-O2D
6	L	304	U10	C3-C4-O4-C4M
9	M	405	SPN	C6-C7-C8-C9
9	M	405	SPN	C10-C11-C12-C13
7	L	305	D12	C5-C6-C7-C8
12	M	409	CDL	C72-C71-CB7-OB9
9	M	405	SPN	C2-C3-C4-C5
10	M	407	LDA	C4-C5-C6-C7
6	L	304	U10	C31-C32-C33-C34
9	M	405	SPN	C18-C19-C20-C21
12	M	409	CDL	C52-C51-CB5-OB7
6	L	304	U10	C29-C31-C32-C33
4	M	401	BCL	C5-C6-C7-C8
5	M	403	BPH	C6-C7-C8-C10
6	L	304	U10	C19-C21-C22-C23

There are no ring outliers.

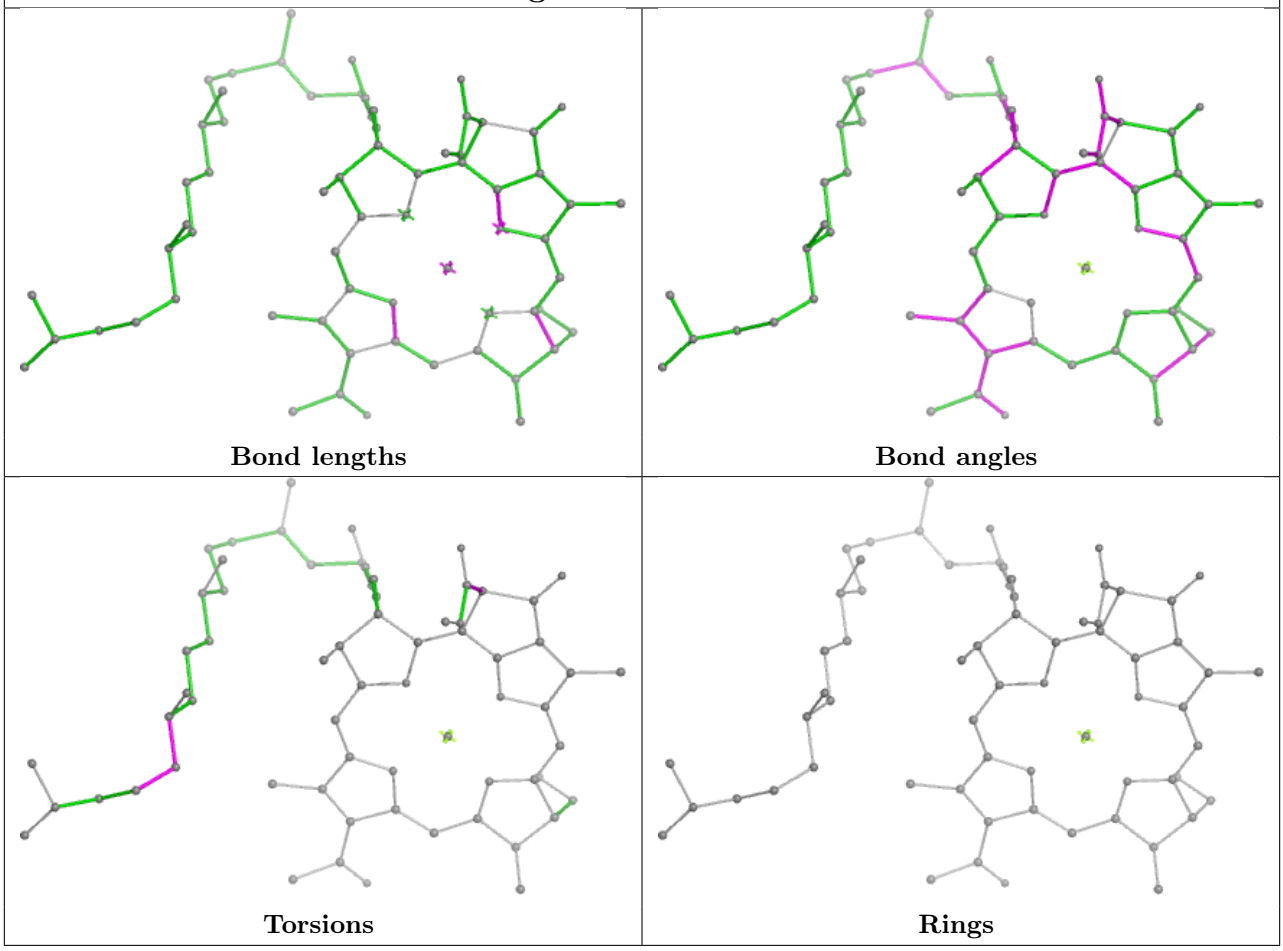
10 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	301	LDA	1	0
4	L	302	BCL	4	0
5	L	303	BPH	4	0
4	L	301	BCL	3	0
9	M	405	SPN	5	0
6	L	304	U10	1	0
10	M	406	LDA	3	0
4	M	401	BCL	6	0
4	M	402	BCL	2	0
5	M	403	BPH	9	0

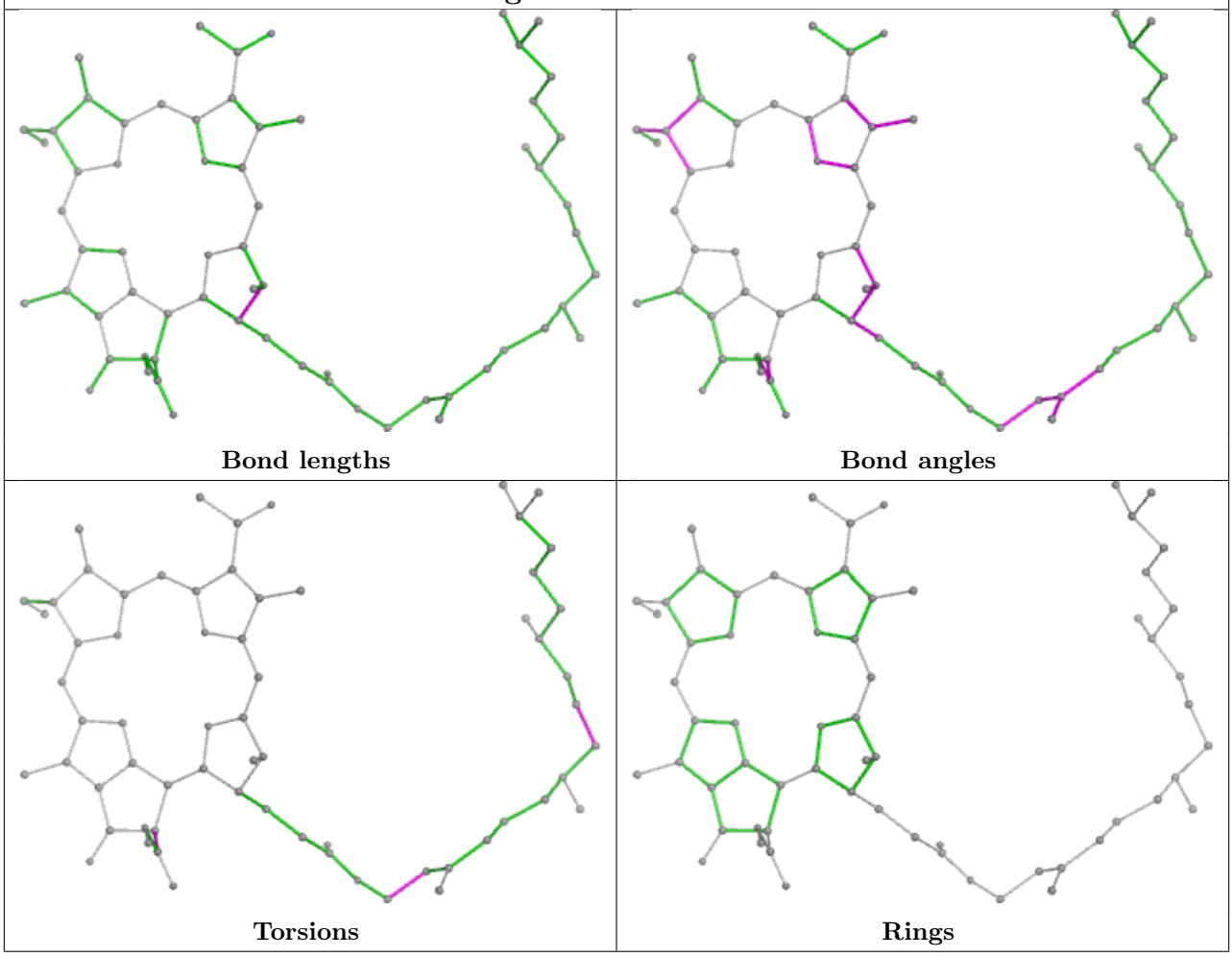
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

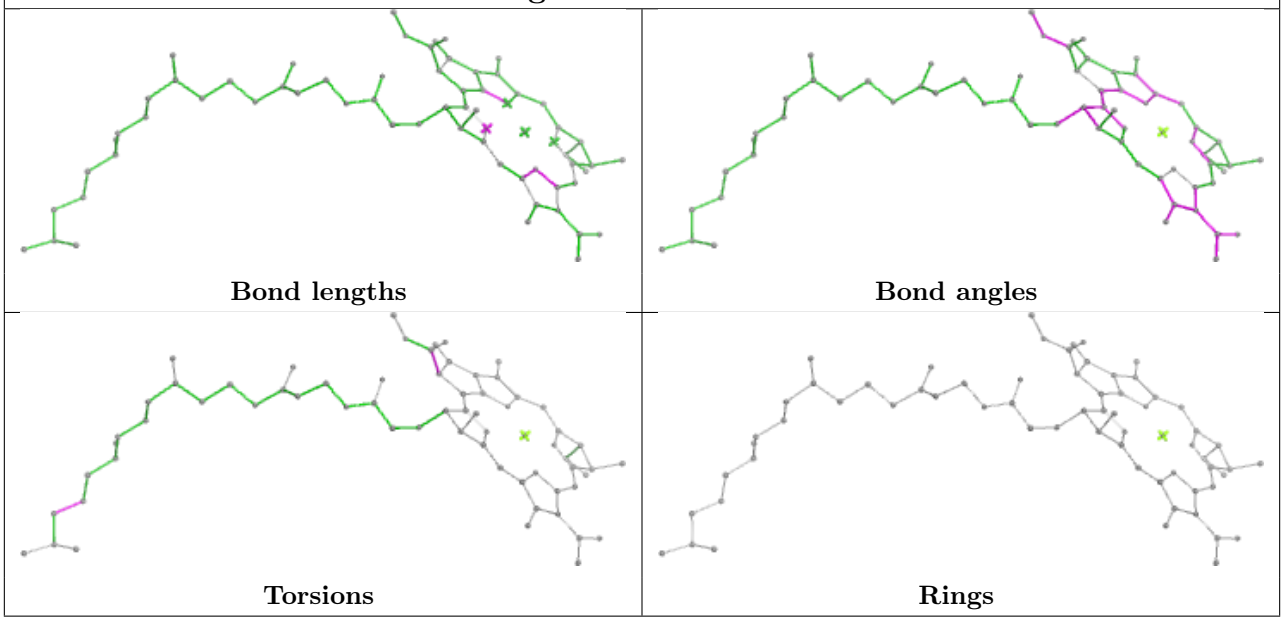
Ligand BCL L 302



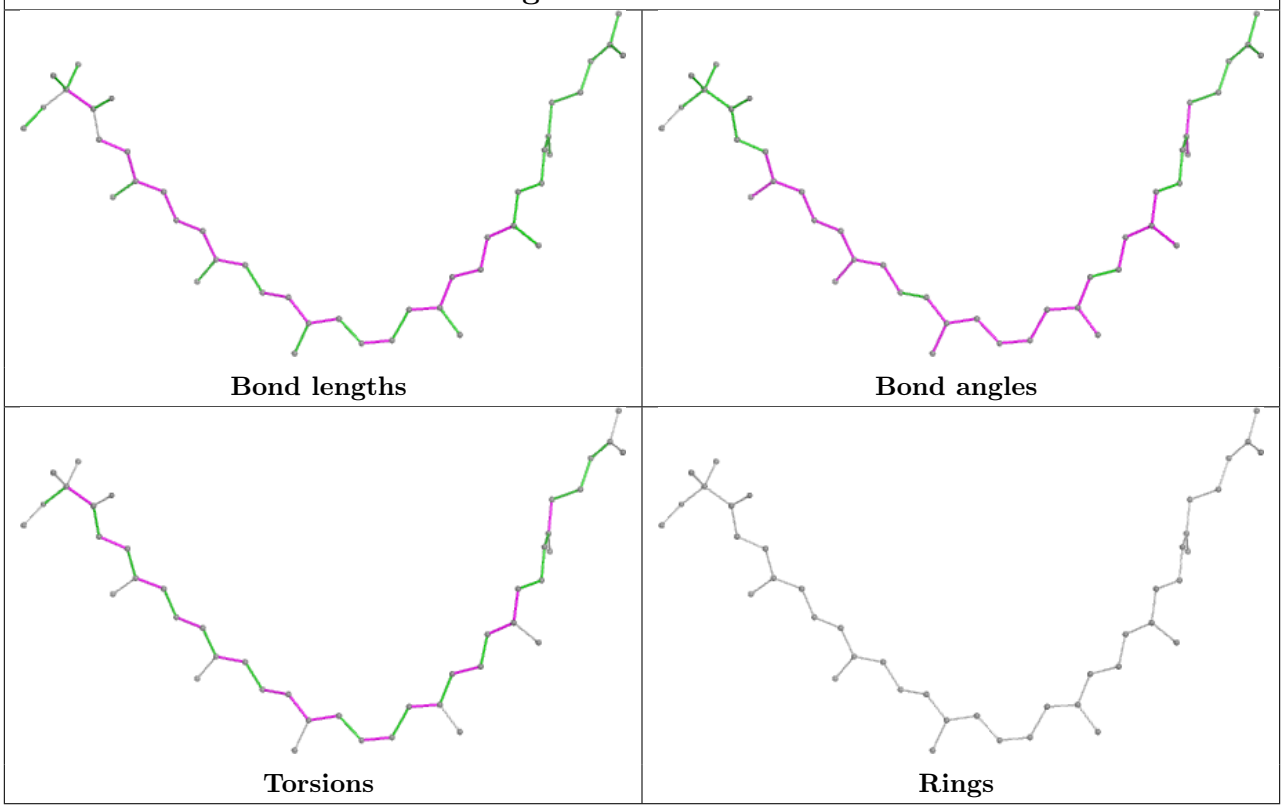
Ligand BPH L 303



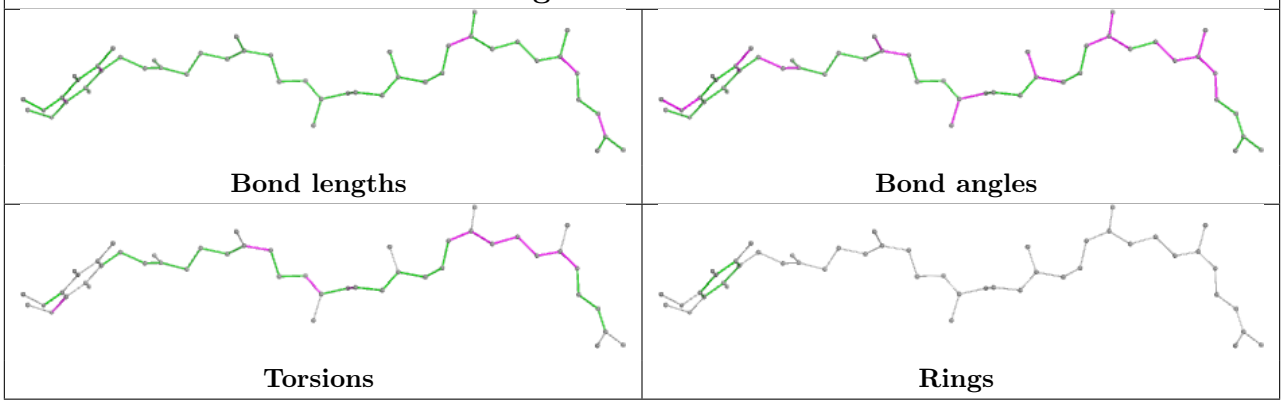
Ligand BCL L 301



Ligand SPN M 405



Ligand U10 L 304



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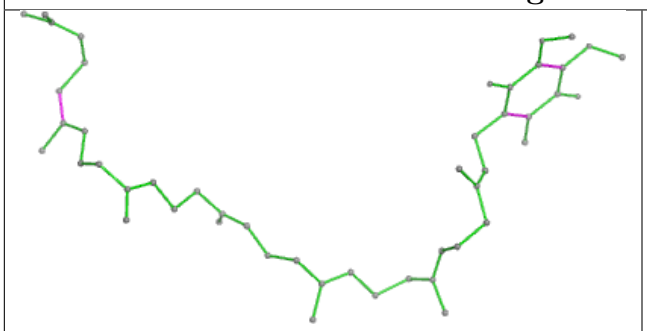
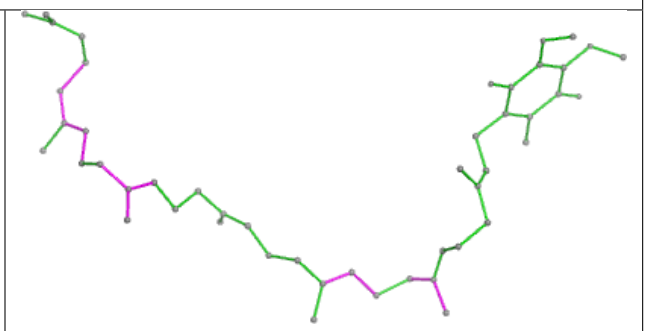
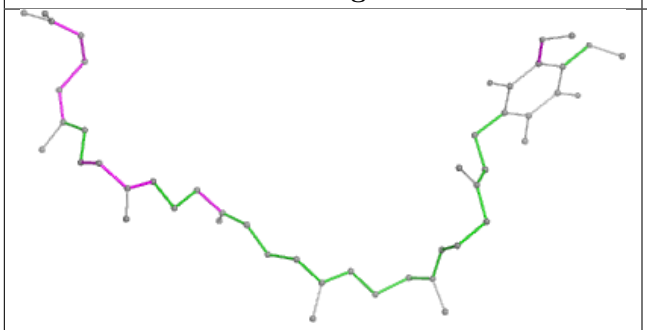


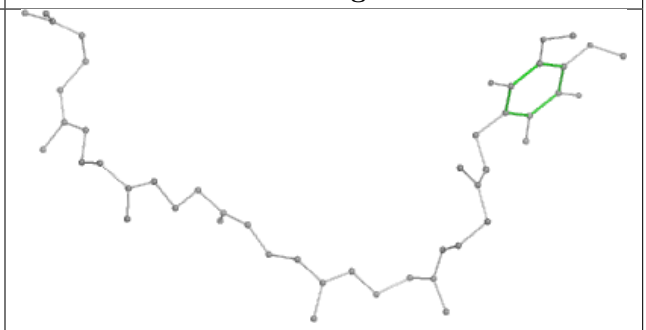
Bond lengths



Bond angles

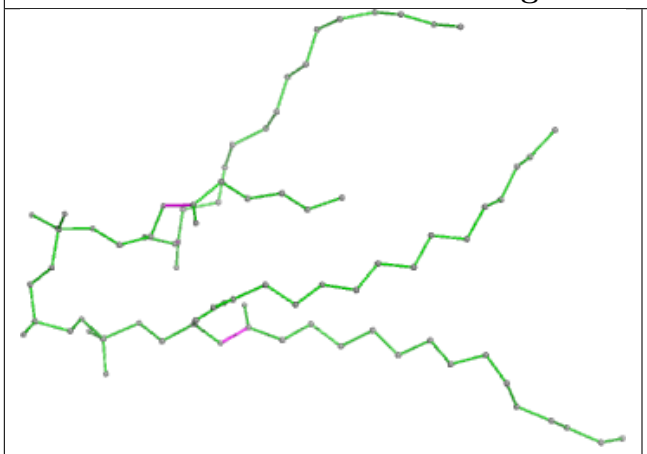


Torsions

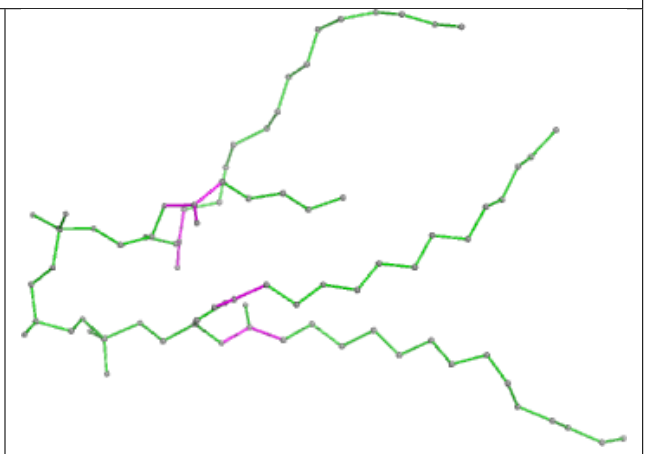


Rings

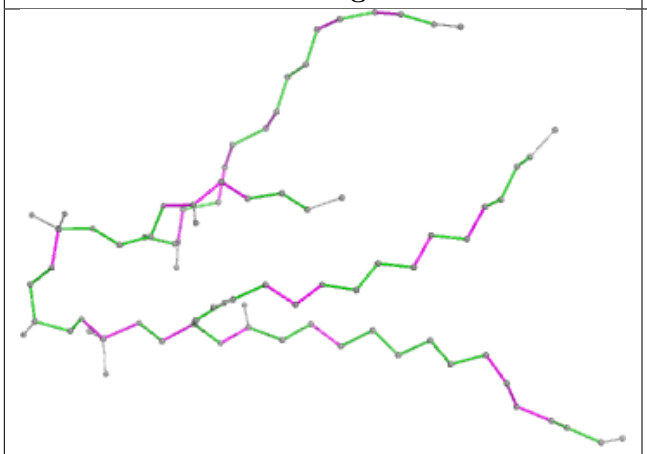
Ligand CDL M 409



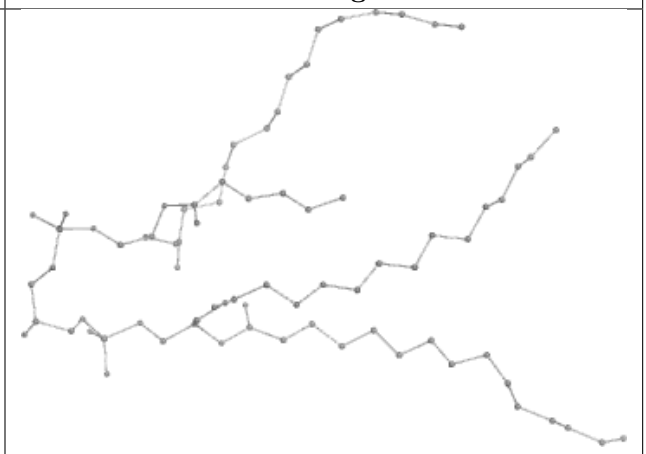
Bond lengths



Bond angles

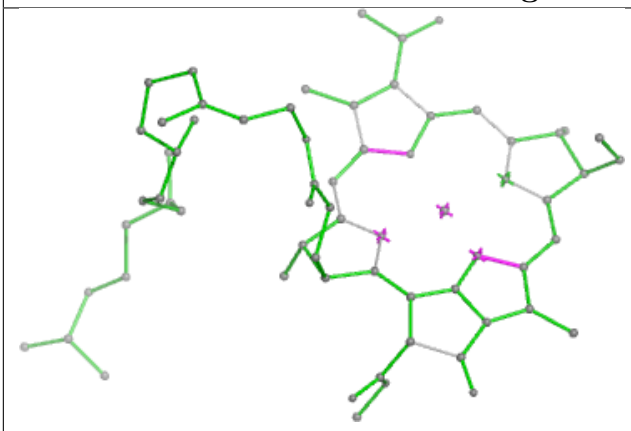


Torsions

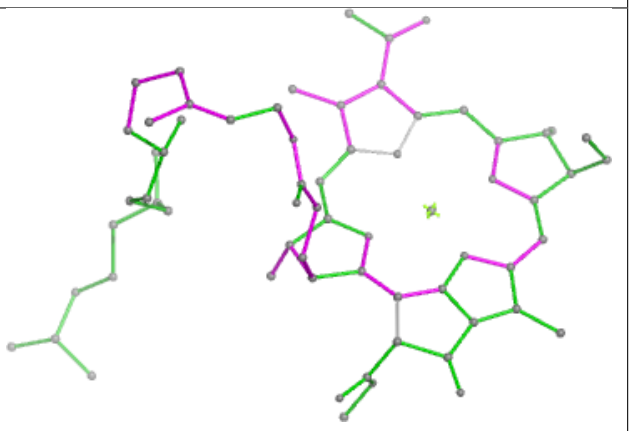


Rings

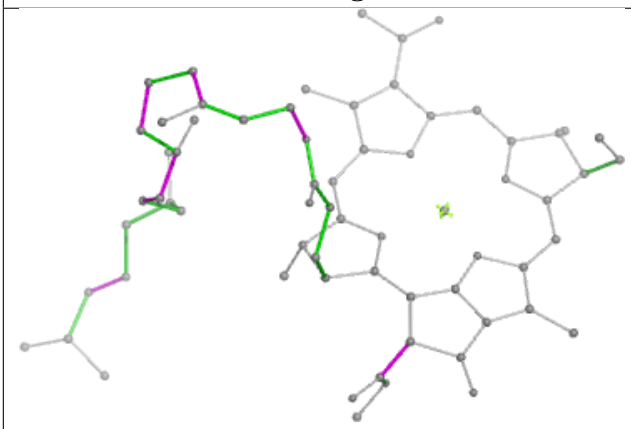
Ligand BCL M 401



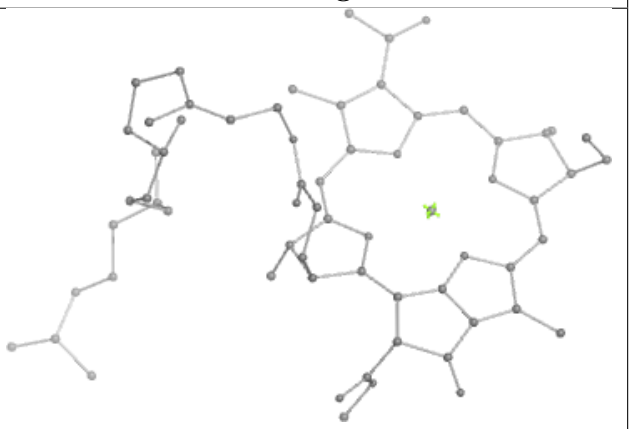
Bond lengths



Bond angles

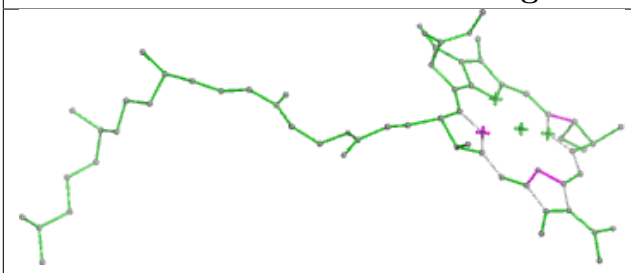


Torsions

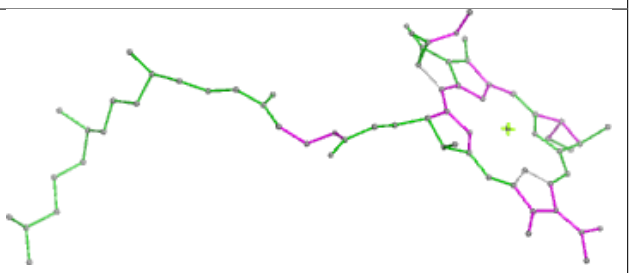


Rings

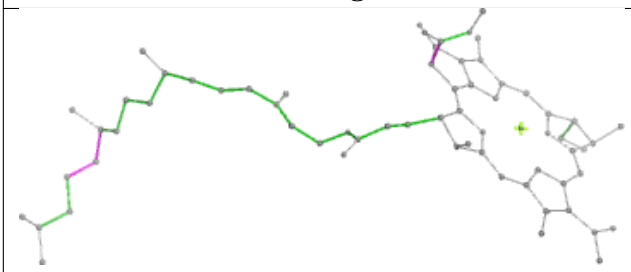
Ligand BCL M 402



Bond lengths

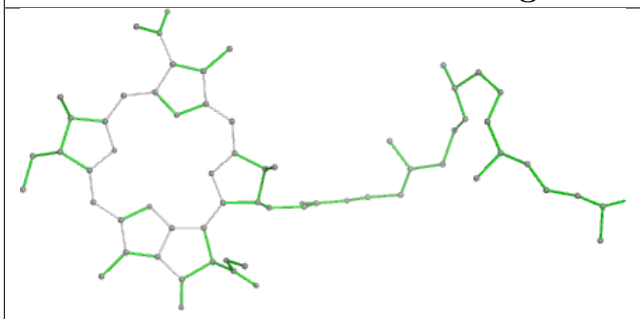
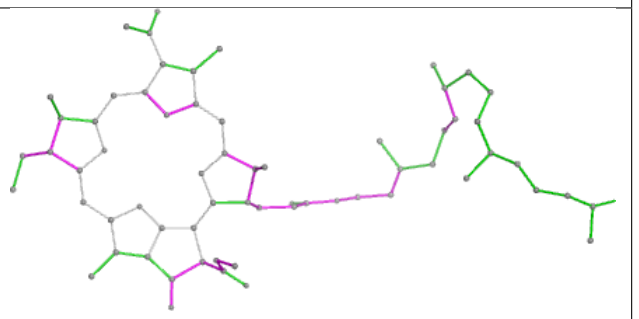
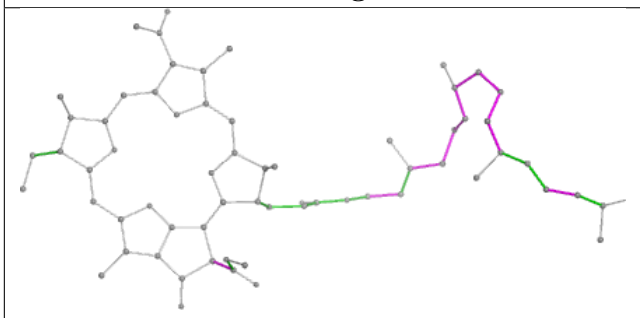
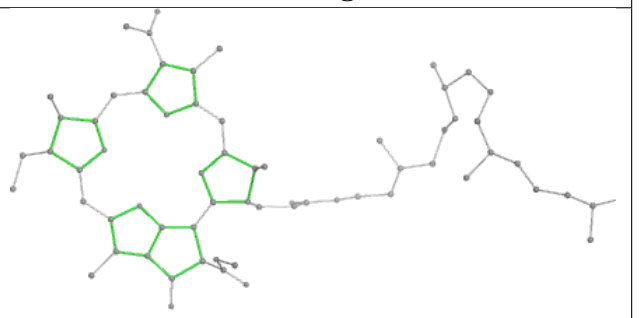


Bond angles



Torsions

Rings

Ligand BPH M 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	L	281/281 (100%)	-0.50	7 (2%)	57	61	33, 43, 76, 118	0
2	M	300/307 (97%)	-0.45	4 (1%)	77	79	32, 47, 74, 108	0
3	H	240/260 (92%)	-0.39	8 (3%)	46	50	37, 46, 66, 146	0
All	All	821/848 (96%)	-0.45	19 (2%)	60	63	32, 46, 74, 146	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	250	SER	7.7
1	L	59	TRP	6.3
3	H	246	PRO	6.2
3	H	249	LYS	6.1
3	H	247	LYS	5.2
2	M	302	GLY	3.9
1	L	270	PRO	3.3
1	L	281	GLY	3.3
2	M	3	TYR	3.2
1	L	271	TRP	2.9
1	L	276	PRO	2.8
3	H	245	ALA	2.7
1	L	277	GLY	2.4
2	M	101	TYR	2.3
3	H	60	LYS	2.2
3	H	52[A]	ASN	2.2
1	L	74	GLY	2.2
2	M	106	ALA	2.2
3	H	248	ARG	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)

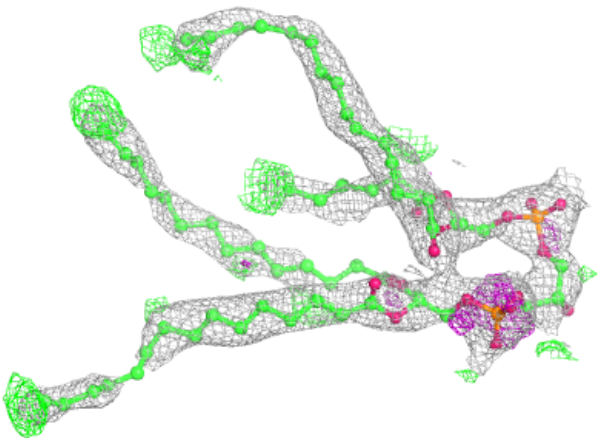
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

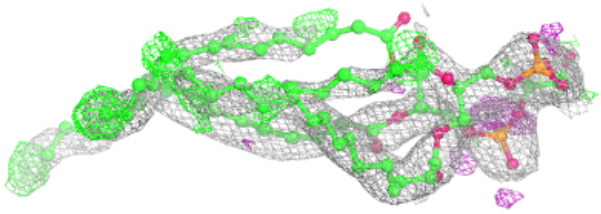
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	D12	H	305	8/12	0.57	0.50	81,85,87,88	0
7	D12	L	305	8/12	0.67	0.23	83,90,93,94	0
10	LDA	M	407	16/16	0.73	0.29	79,92,108,111	0
12	CDL	M	409	78/100	0.78	0.30	50,93,130,139	0
6	U10	L	304	48/63	0.79	0.26	47,68,94,100	0
7	D12	H	304	8/12	0.84	0.20	74,76,86,87	0
10	LDA	M	406	16/16	0.86	0.22	43,62,79,80	0
7	D12	H	303	9/12	0.87	0.23	75,76,81,83	0
7	D12	H	302	12/12	0.88	0.28	75,78,80,81	0
5	BPH	M	403	65/65	0.91	0.16	38,45,97,103	0
6	U10	M	404	48/63	0.91	0.23	34,49,91,103	0
9	SPN	M	405	43/43	0.92	0.18	38,51,90,98	0
10	LDA	H	301	16/16	0.95	0.12	57,65,75,78	0
4	BCL	M	401	66/66	0.96	0.16	32,37,90,93	0
4	BCL	L	301	66/66	0.97	0.16	33,40,50,64	0
4	BCL	M	402	66/66	0.97	0.16	34,40,60,71	0
5	BPH	L	303	65/65	0.97	0.14	30,37,46,48	0
11	PO4	M	408	5/5	0.97	0.20	70,71,78,79	0
4	BCL	L	302	66/66	0.97	0.15	28,34,60,72	0
8	FE	L	306	1/1	0.99	0.12	35,35,35,35	0

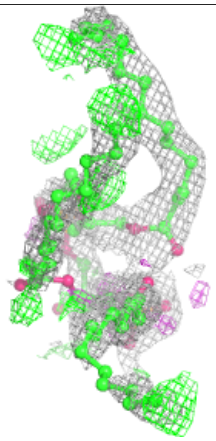
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CDL 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)

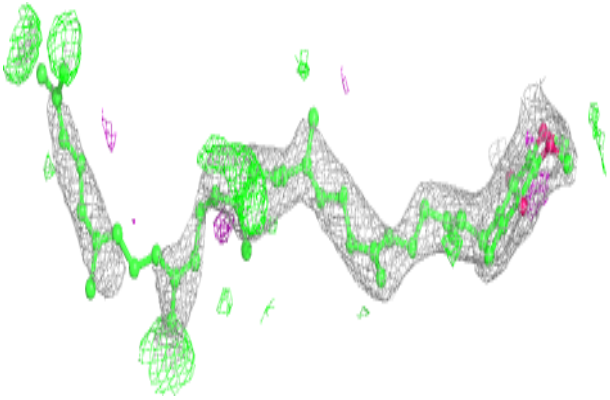


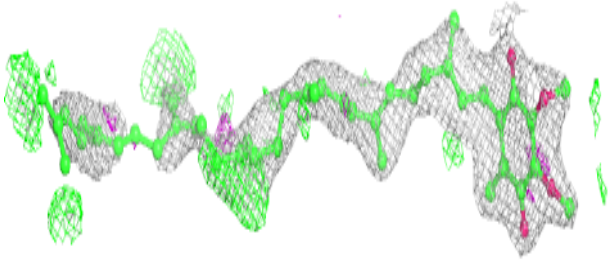


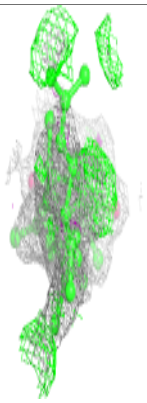


Electron density around U10 L 304:

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

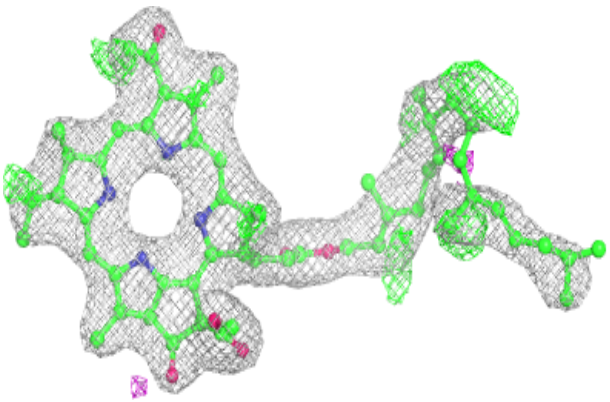


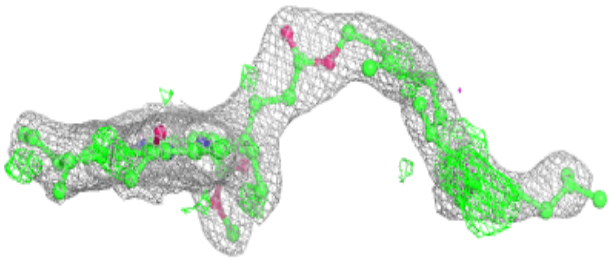


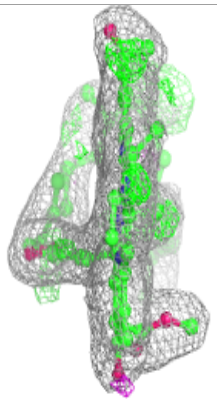


Electron density around BPH M 403:

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

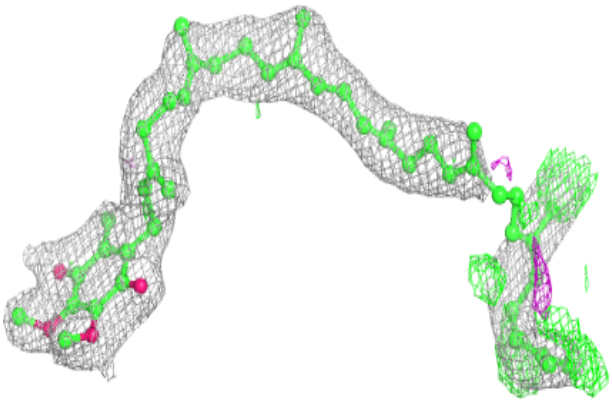


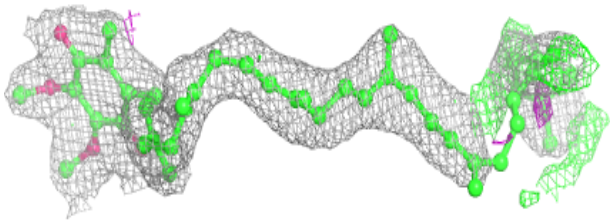


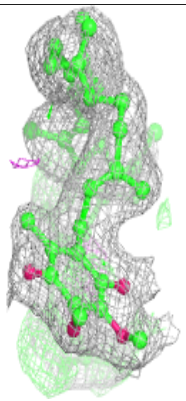


Electron density around U10 M 404:

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

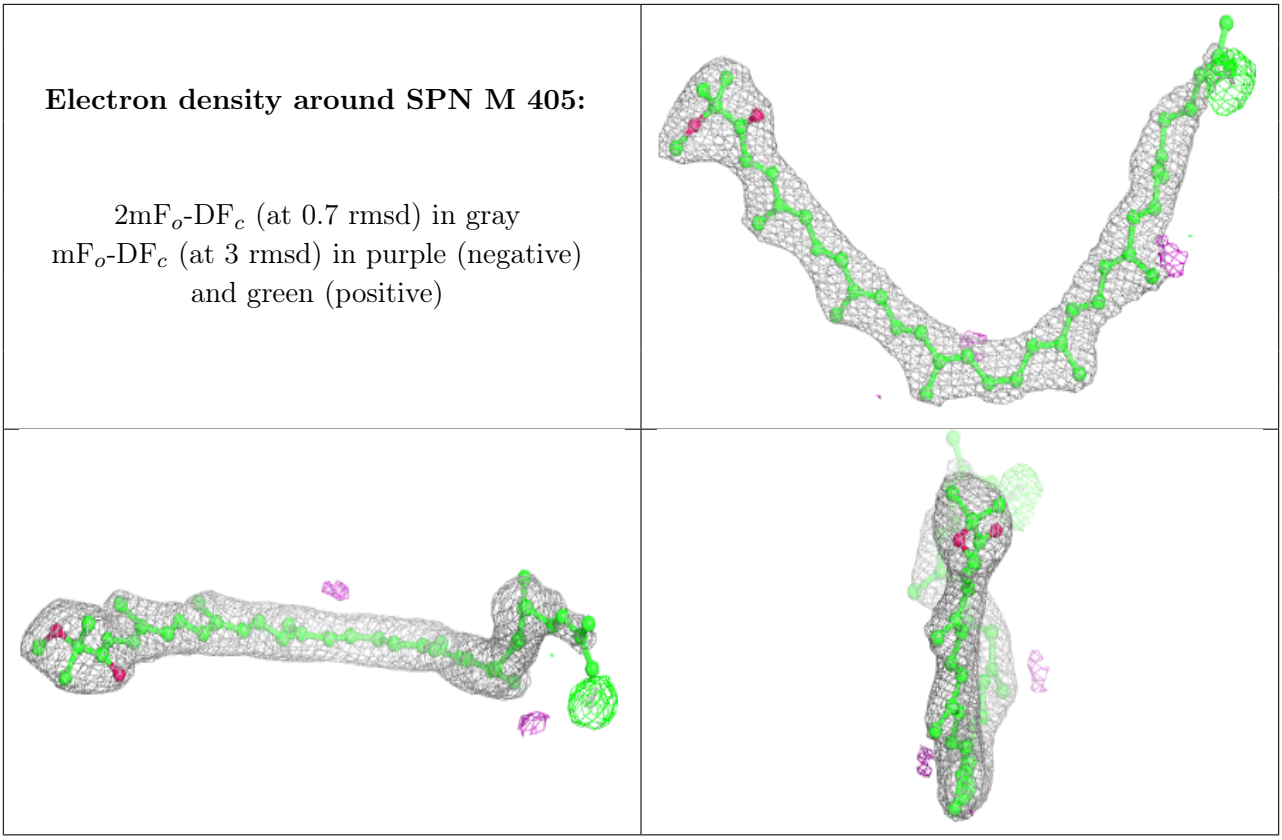






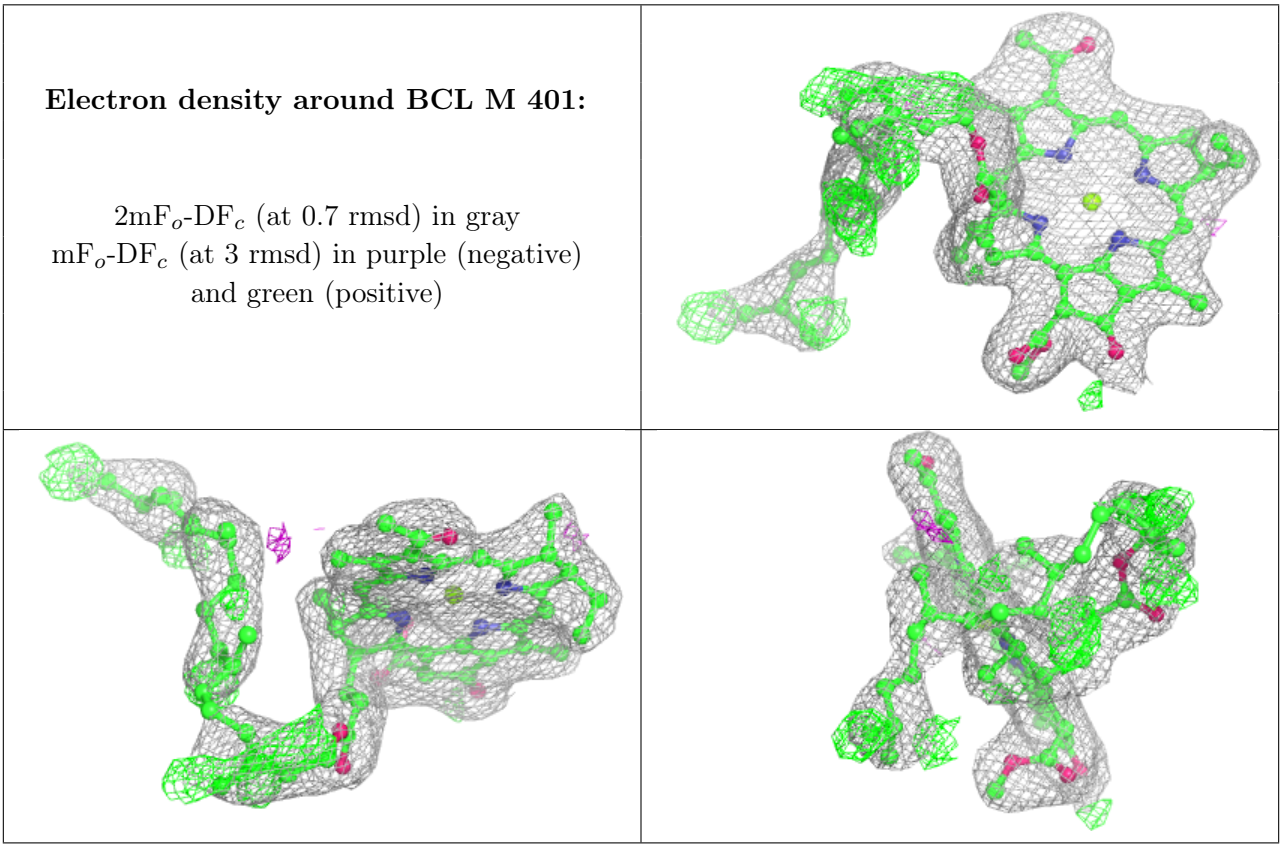
Electron density around SPN M 405:

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



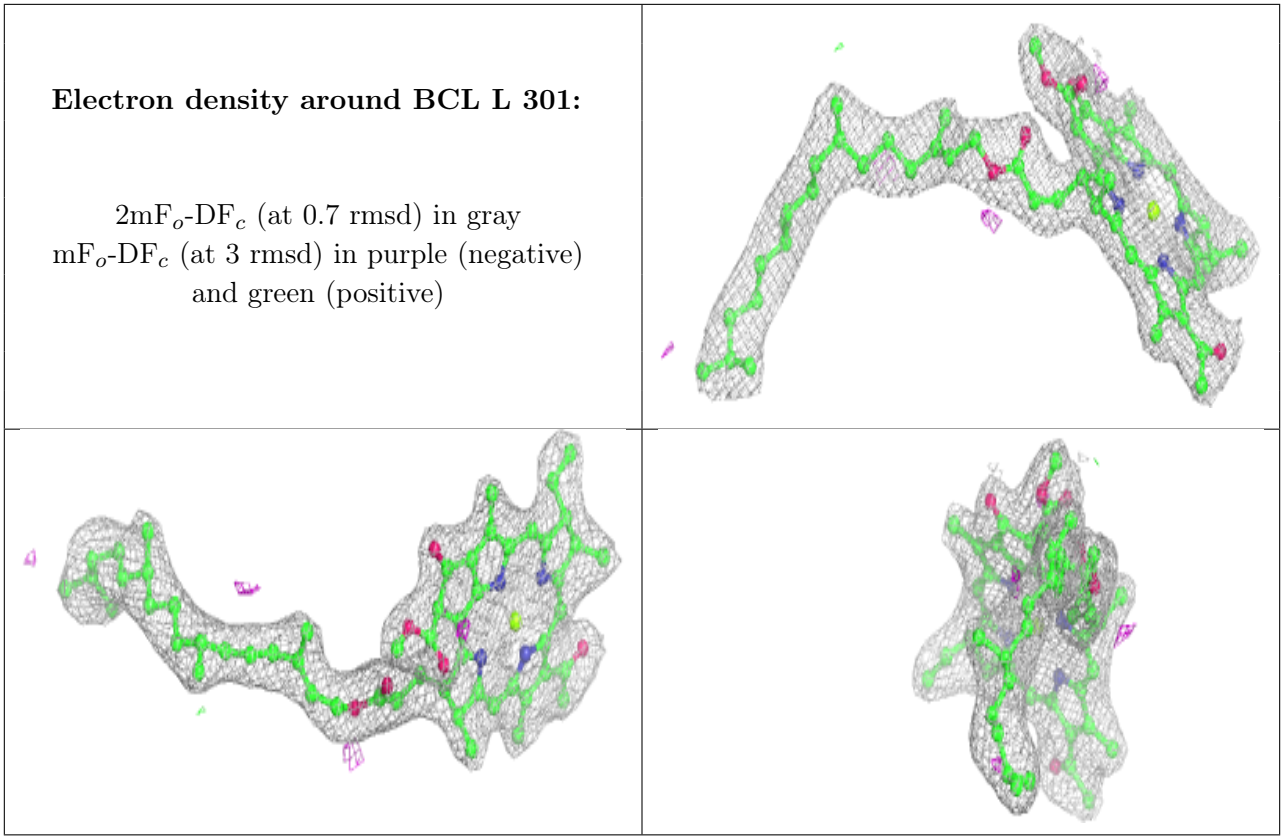
Electron density around BCL M 401:

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



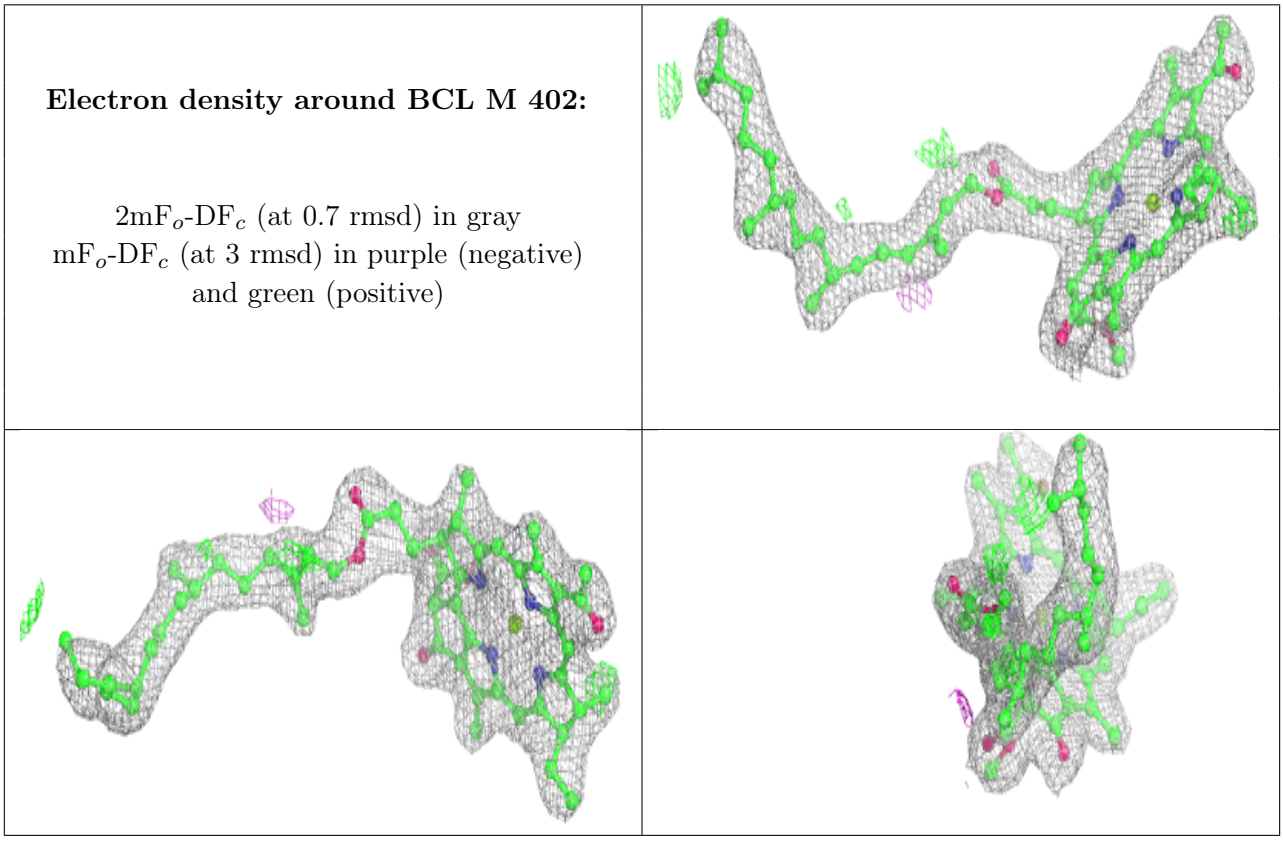
Electron density around BCL L 301:

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



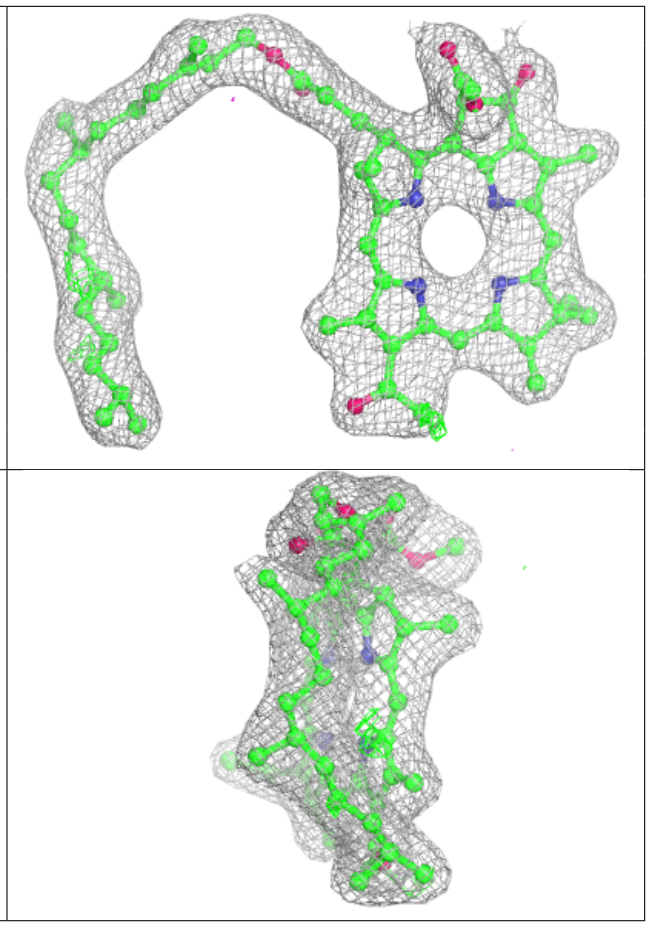
Electron density around BCL M 402:

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



Electron density around BPH L 303:

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



Electron density around BCL L 302:

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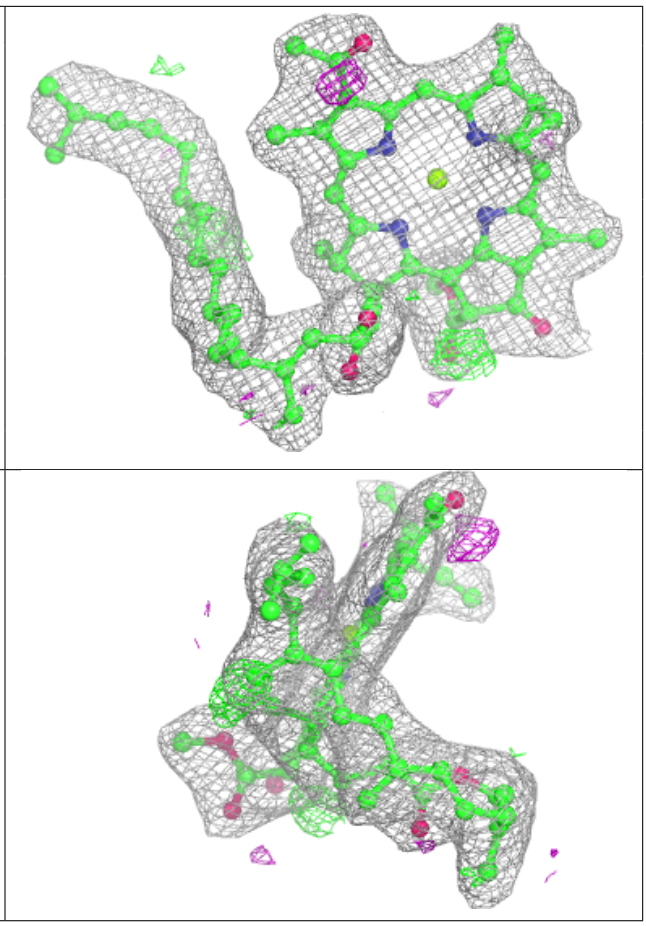
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.