Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 06:34 AM EDT

PDB ID	:	4IN5
Title	:	(M)L214G mutant of the Rhodobacter sphaeroides Reaction Center
Authors	:	Saer, R.G.; Hardjasa, A.; Murphy, M.E.; Beatty, J.T.
Deposited on	:	2013-01-04
Resolution	:	2.20 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:

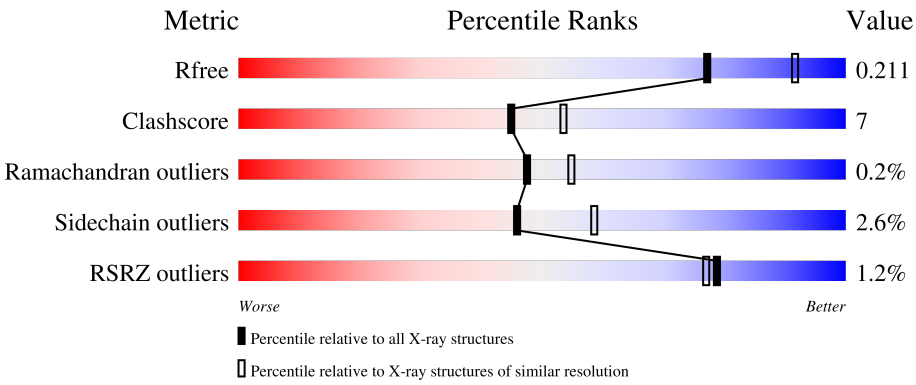
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	282	.% 93% 6% •
2	M	307	2% 88% 10% • •
3	H	266	.% 80% 9% • 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
10	GOL	H	301	-	-	X	-
10	GOL	L	314	-	-	X	-
13	PC1	M	408	-	-	-	X
4	LDA	L	302	-	-	-	X
8	PO4	M	411	-	-	X	-
9	HTO	L	307	-	-	-	X

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 7489 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	2242	1515	356	363	8	0	2	0

- 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	302	2407	1604	395	398	10	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	214	GLY	LEU	engineered mutation	UNP P0C0Y9

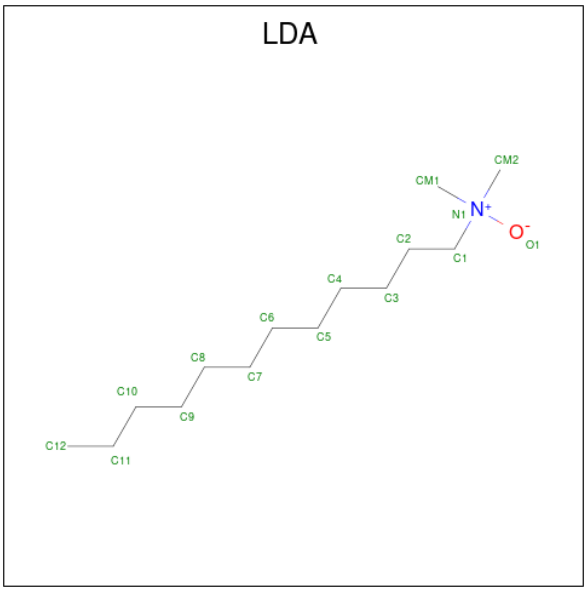
- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	240	1850	1184	320	337	9	0	5	0

There are 6 discrepancies between the modelled and reference sequences:

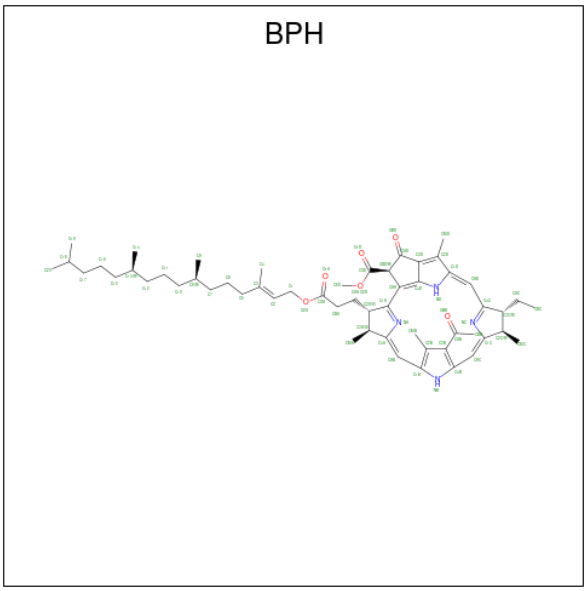
Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	HIS	-	expression tag	UNP P0C0Y7
H	-4	HIS	-	expression tag	UNP P0C0Y7
H	-3	HIS	-	expression tag	UNP P0C0Y7
H	-2	HIS	-	expression tag	UNP P0C0Y7
H	-1	HIS	-	expression tag	UNP P0C0Y7
H	0	HIS	-	expression tag	UNP P0C0Y7

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



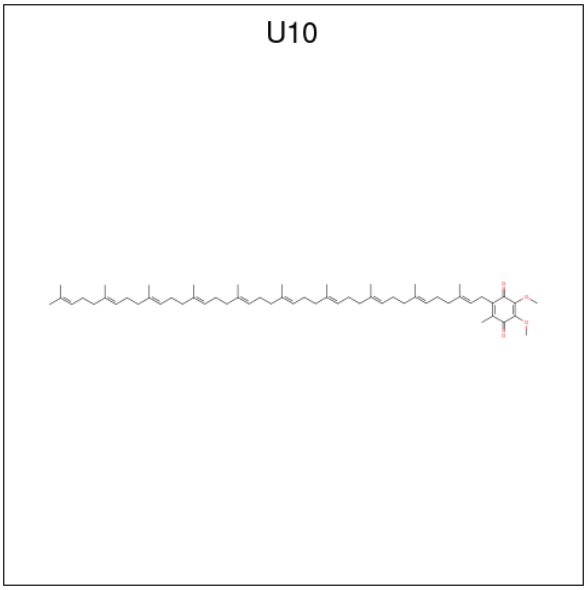
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	L	1	16	14	1	1	0	0
			Total	C	N	O		
4	L	1	16	14	1	1	0	0
			Total	C	N	O		
4	M	1	16	14	1	1	0	0
			Total	C	N	O		
4	M	1	16	14	1	1	0	0
			Total	C	N	O		
4	H	1	16	14	1	1	0	0
			Total	C	N	O		
4	H	1	16	14	1	1	0	0

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



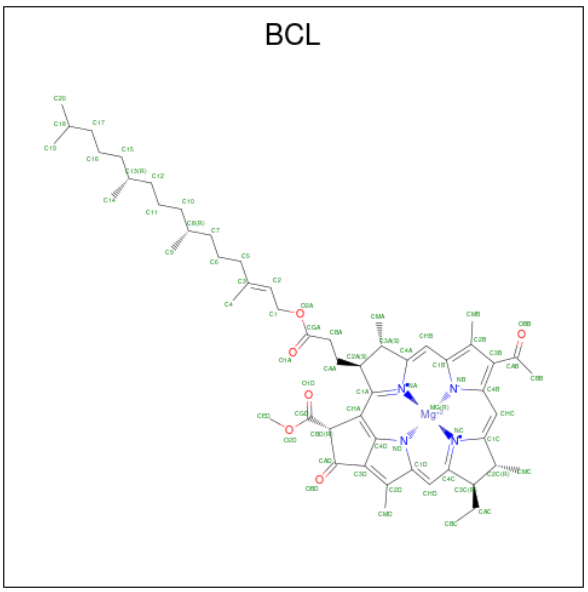
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	L	1	65	55	4	6	0	0
			Total	C	N	O		
5	L	1	65	55	4	6	0	0

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



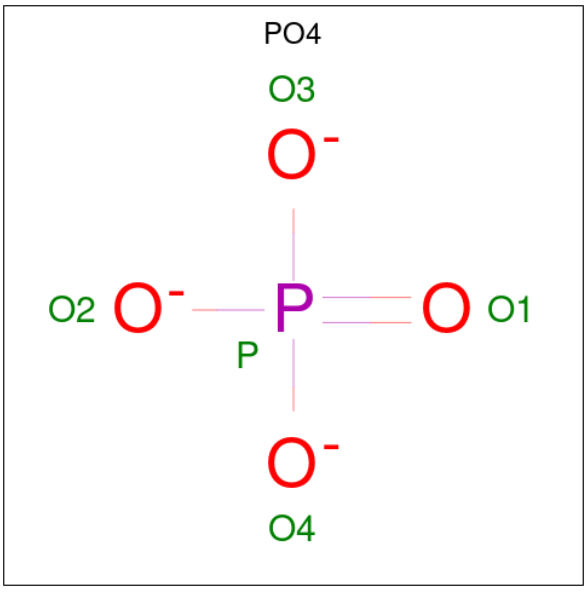
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	L	1	46	38	8	0	1
			Total	C	O		
6	M	1	48	44	4	0	0

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



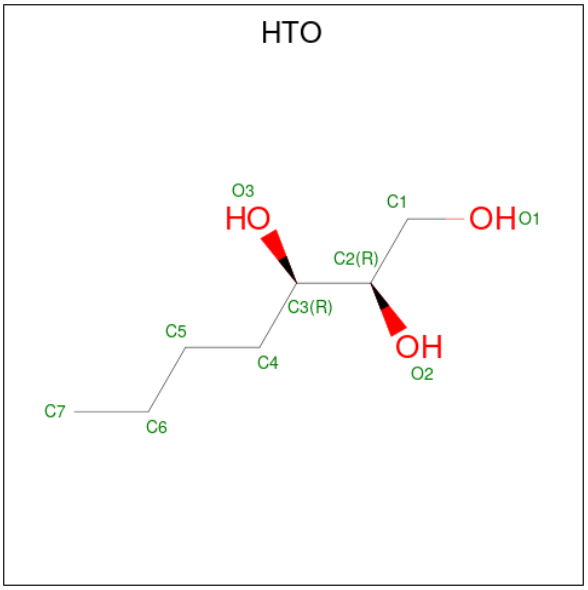
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
7	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
7	M	1	86	75	1	4	6	0	1
			Total	C	Mg	N	O		
7	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
7	M	1	66	55	1	4	6	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



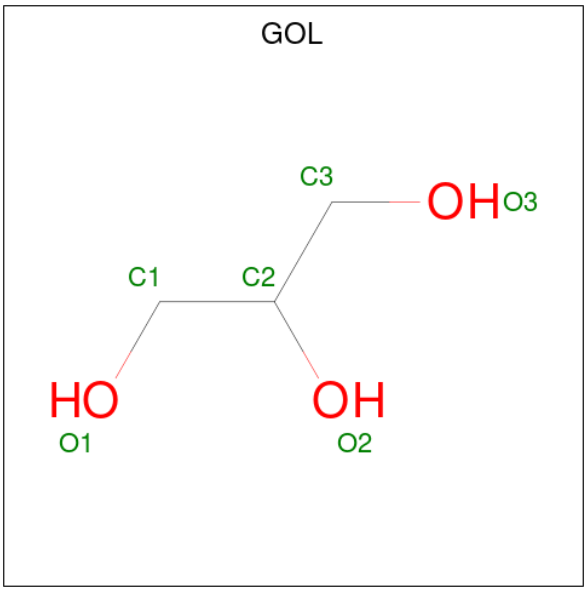
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
8	L	1	5	4	1	0	0
			Total	O	P		
8	M	1	5	4	1	0	0
			Total	O	P		
8	M	1	5	4	1	0	0

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



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

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

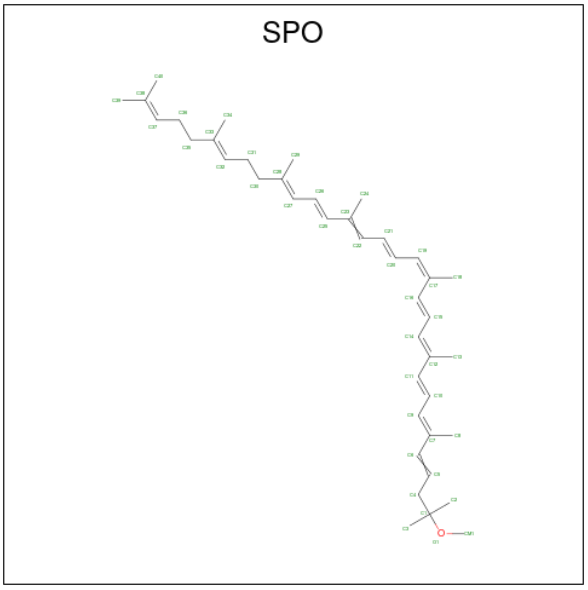


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	L	1	6	3	3	0	0
10	L	1	6	3	3	0	0
10	L	1	6	3	3	0	0
10	L	1	6	3	3	0	0
10	L	1	6	3	3	0	0
10	L	1	6	3	3	0	0
10	M	1	6	3	3	0	0
10	H	1	6	3	3	0	0
10	H	1	6	3	3	0	0
10	H	1	6	3	3	0	0
10	H	1	6	3	3	0	0
10	H	1	6	3	3	0	0

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

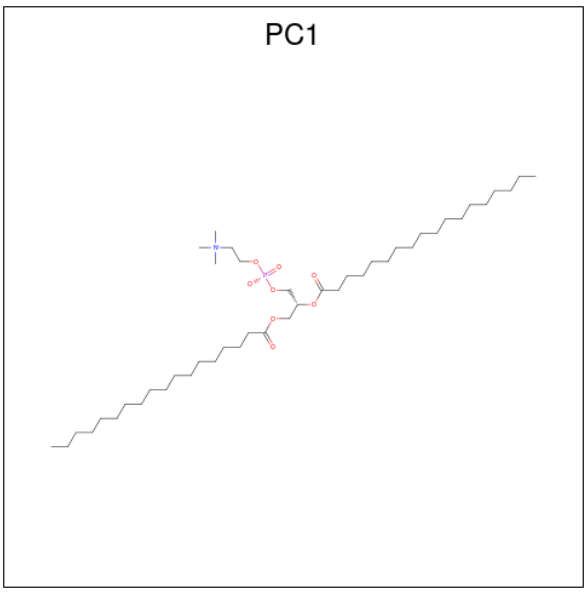
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
11	M	1	1	1	0	0

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 13 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
13	M	1	43	33	1	8	1	0	0

- Molecule 14 is POTASSIUM ION (three-letter code: K) (formula: K).

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

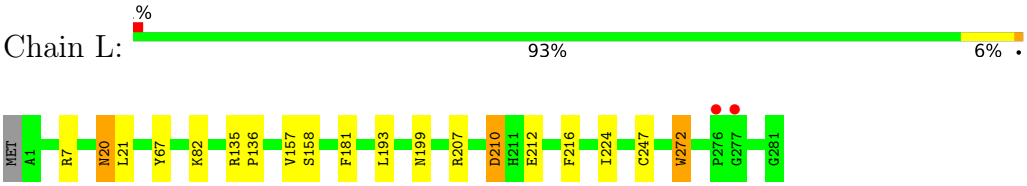
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
15	L	56	56	56	0	0
			Total	O		
15	M	53	53	53	0	0
			Total	O		
15	H	83	83	83	0	0

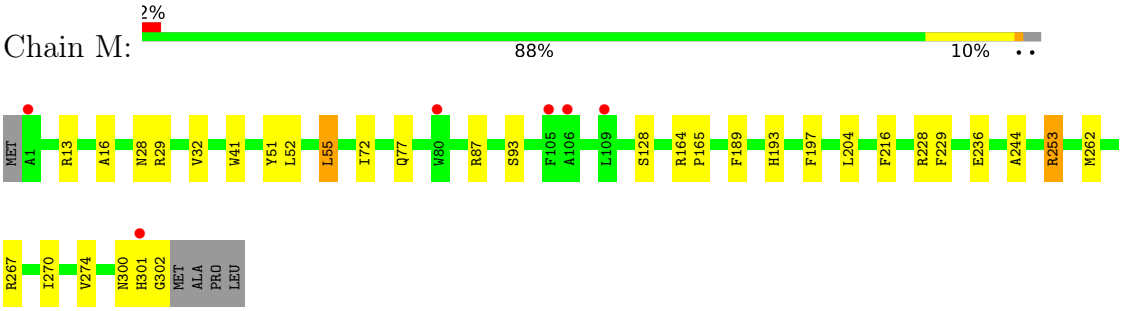
3 Residue-property plots (i)

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.

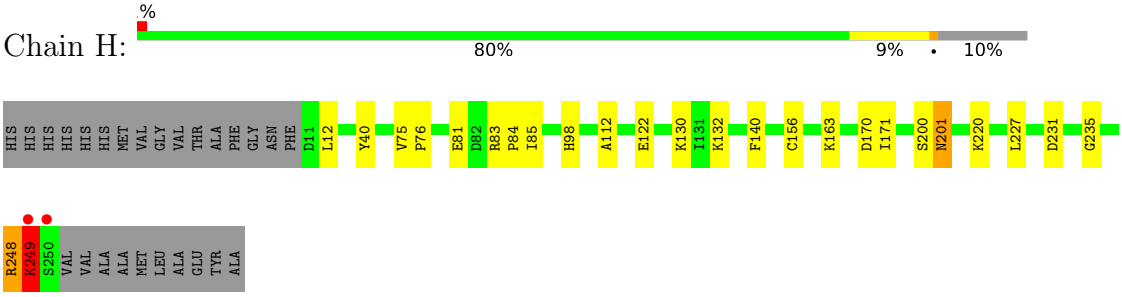
• Molecule 1: Reaction center protein L chain



• 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	139.11Å 139.11Å 184.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.62 – 2.20 55.56 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (55.62-2.20) 99.9 (55.56-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.181 , 0.206 0.188 , 0.211	Depositor DCC
R_{free} test set	5239 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.0	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	0.95	EDS
Total number of atoms	7489	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: FE, K, PC1, U10, SPO, LDA, BCL, PO4, GOL, HTO, BPH

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	0.89	1/2342 (0.0%)	0.76	1/3206 (0.0%)
2	M	0.82	1/2504 (0.0%)	0.82	8/3418 (0.2%)
3	H	0.85	0/1923	0.87	2/2611 (0.1%)
All	All	0.85	2/6769 (0.0%)	0.81	11/9235 (0.1%)

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
3	H	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	67	TYR	CB-CG	5.65	1.60	1.51
2	M	41	TRP	CB-CG	-5.04	1.41	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	83	ARG	NE-CZ-NH2	-8.13	116.23	120.30
3	H	83	ARG	NE-CZ-NH1	7.88	124.24	120.30
2	M	228	ARG	NE-CZ-NH2	-7.79	116.41	120.30
2	M	29	ARG	NE-CZ-NH1	-7.01	116.79	120.30
2	M	253	ARG	NE-CZ-NH2	6.99	123.80	120.30
2	M	262	MET	CG-SD-CE	6.72	110.95	100.20
2	M	228	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	L	210	ASP	CB-CG-OD1	5.89	123.60	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	29	ARG	NE-CZ-NH2	5.41	123.00	120.30
2	M	253	ARG	NE-CZ-NH1	-5.16	117.72	120.30
2	M	267	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	248	ARG	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	2242	0	2194	15	0
2	M	2407	0	2315	19	0
3	H	1850	0	1875	21	0
4	H	32	0	62	3	0
4	L	32	0	62	1	0
4	M	32	0	62	3	0
5	L	130	0	152	9	0
6	L	46	0	46	11	0
6	M	48	0	63	2	0
7	L	66	0	74	2	0
7	M	218	0	226	19	0
8	L	5	0	0	1	0
8	M	10	0	0	3	0
9	H	10	0	16	1	0
9	L	10	0	16	0	0
10	H	30	0	40	5	0
10	L	36	0	48	7	0
10	M	6	0	8	0	0
11	M	1	0	0	0	0
12	M	42	0	60	1	0
13	M	43	0	60	0	0
14	H	1	0	0	0	0
15	H	83	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	L	56	0	0	3	0
15	M	53	0	0	2	0
All	All	7489	0	7379	94	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 7.

All (94) 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)
6:L:304[B]:U10:H1M1	6:L:304[B]:U10:C8	1.67	1.23
6:L:304[B]:U10:H1M1	6:L:304[B]:U10:H8	1.54	0.88
5:L:313:BPH:HBB3	5:L:313:BPH:HHC	1.60	0.84
5:L:303:BPH:HBB3	5:L:303:BPH:HHC	1.60	0.83
10:L:314:GOL:O1	15:L:454:HOH:O	2.00	0.80
6:L:304[B]:U10:C8	6:L:304[B]:U10:C1M	2.54	0.76
10:L:314:GOL:C1	15:L:454:HOH:O	2.34	0.75
6:L:304[B]:U10:H3M2	6:L:304[B]:U10:H4M2	1.69	0.75
2:M:253:ARG:HD2	15:M:546:HOH:O	1.87	0.73
6:L:304[B]:U10:H4M2	6:L:304[B]:U10:C3M	2.19	0.72
2:M:197:PHE:CZ	7:M:403:BCL:HBB2	2.26	0.71
1:L:181:PHE:CD2	5:L:313:BPH:HBB1	2.28	0.69
10:L:314:GOL:H12	15:L:454:HOH:O	1.90	0.68
1:L:224:ILE:HB	6:L:304[A]:U10:H103	1.77	0.67
6:L:304[B]:U10:H1M1	6:L:304[B]:U10:C9	2.25	0.65
7:M:403:BCL:HBB3	7:M:403:BCL:HHC	1.78	0.65
7:M:403:BCL:HHC	7:M:403:BCL:CBB	2.26	0.65
2:M:197:PHE:HZ	7:M:403:BCL:HBB2	1.61	0.64
3:H:201:ASN:H	3:H:201:ASN:HD22	1.44	0.64
10:H:301:GOL:C3	15:H:451:HOH:O	2.48	0.61
5:L:313:BPH:HHD	5:L:313:BPH:HBC3	1.83	0.61
2:M:55:LEU:HD22	2:M:128:SER:HB2	1.82	0.61
10:H:301:GOL:H31	15:H:451:HOH:O	2.00	0.61
3:H:200:SER:H	9:H:308:HTO:H73	1.65	0.60
3:H:248:ARG:HA	3:H:249[A]:LYS:HB2	1.83	0.60
2:M:189:PHE:O	2:M:193:HIS:HD2	1.86	0.58
1:L:181:PHE:HB3	5:L:313:BPH:HBB2	1.85	0.58
2:M:270:ILE:O	2:M:274:VAL:HG13	2.05	0.56
1:L:7:ARG:HH21	3:H:98:HIS:CD2	2.24	0.56
2:M:300:ASN:O	2:M:302:GLY:N	2.40	0.55
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:304:LDA:H123	10:H:307:GOL:H11	1.89	0.54
1:L:20:ASN:HD22	1:L:21:LEU:N	2.06	0.54
1:L:224:ILE:H	6:L:304[A]:U10:H8	1.72	0.54
7:L:305:BCL:CBB	7:L:305:BCL:HMB1	2.39	0.53
1:L:7:ARG:HH21	3:H:98:HIS:HD2	1.57	0.52
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.90	0.52
1:L:181:PHE:HB3	5:L:313:BPH:CBB	2.39	0.52
3:H:40:TYR:OH	4:H:304:LDA:HM12	2.10	0.52
7:M:402:BCL:HBB3	7:M:403:BCL:H41	1.90	0.52
7:M:403:BCL:HAA2	7:M:403:BCL:HBD	1.91	0.51
7:M:402:BCL:HMB1	7:M:402:BCL:OBB	2.10	0.51
5:L:313:BPH:HBB3	5:L:313:BPH:CHC	2.38	0.50
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.94	0.49
7:M:402:BCL:HHC	7:M:402:BCL:HBB2	1.94	0.49
10:L:314:GOL:H31	3:H:85[B]:ILE:CD1	2.43	0.49
1:L:272:TRP:CD1	2:M:87:ARG:HG3	2.48	0.49
1:L:20:ASN:HD22	1:L:20:ASN:C	2.16	0.48
2:M:13:ARG:O	3:H:140:PHE:HA	2.13	0.48
3:H:248:ARG:HA	3:H:249[B]:LYS:HB2	1.95	0.47
2:M:77:GLN:HE22	2:M:93:SER:H	1.60	0.47
7:M:402:BCL:HHC	7:M:402:BCL:CBB	2.45	0.47
3:H:40:TYR:OH	4:H:304:LDA:CM1	2.62	0.47
7:M:401[B]:BCL:H61	7:M:401[B]:BCL:H92	1.60	0.47
3:H:81:GLU:HG3	3:H:85[B]:ILE:HD11	1.97	0.47
3:H:84:PRO:O	3:H:85[A]:ILE:HD13	2.15	0.47
8:M:411:PO4:O3	10:H:301:GOL:O1	2.21	0.46
10:L:314:GOL:H31	3:H:85[B]:ILE:HD13	1.98	0.46
7:M:403:BCL:CBB	7:M:403:BCL:CHC	2.94	0.45
7:L:305:BCL:HMB1	7:L:305:BCL:HBB3	1.98	0.45
2:M:204:LEU:HG	7:M:401[B]:BCL:H192	1.99	0.45
7:M:402:BCL:HBB2	12:M:407:SPO:H243	1.99	0.45
3:H:130:LYS:HE3	3:H:170:ASP:OD2	2.17	0.44
10:L:312:GOL:H12	2:M:236:GLU:OE1	2.18	0.44
7:M:401[A]:BCL:H62	7:M:401[A]:BCL:H2	1.30	0.44
5:L:303:BPH:HHC	5:L:303:BPH:CBB	2.41	0.44
8:M:411:PO4:P	4:M:412:LDA:HM22	2.58	0.44
7:M:401[B]:BCL:H111	7:M:401[B]:BCL:H142	1.52	0.44
6:M:406:U10:H322	6:M:406:U10:H301	1.76	0.44
2:M:197:PHE:CE1	7:M:403:BCL:HBB2	2.53	0.43
8:M:411:PO4:O2	4:M:412:LDA:HM22	2.18	0.43
1:L:135:ARG:HB3	1:L:136:PRO:HD3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:156:CYS:SG	3:H:248:ARG:HB2	2.59	0.43
10:H:301:GOL:H32	15:H:451:HOH:O	2.17	0.42
6:L:304[A]:U10:H71	6:L:304[A]:U10:H1M1	1.67	0.42
2:M:197:PHE:HZ	7:M:403:BCL:CBB	2.31	0.42
4:L:302:LDA:H123	6:L:304[B]:U10:H102	2.01	0.42
6:L:304[B]:U10:H8	6:L:304[B]:U10:C1M	2.37	0.42
4:M:412:LDA:HM23	4:M:412:LDA:H21	1.83	0.42
1:L:82:LYS:HE3	8:L:306:PO4:O2	2.19	0.42
7:M:402:BCL:H71	7:M:403:BCL:H192	2.01	0.41
2:M:164:ARG:HB3	2:M:165:PRO:HD3	2.01	0.41
1:L:157:VAL:HG11	7:M:403:BCL:HBB1	2.02	0.41
1:L:199:ASN:HA	10:L:308:GOL:H31	2.03	0.41
2:M:28:ASN:HB2	2:M:51:TYR:CE2	2.56	0.41
3:H:75:VAL:HA	3:H:76:PRO:C	2.41	0.41
3:H:112:ALA:HA	3:H:235:GLY:O	2.21	0.41
3:H:201:ASN:H	3:H:201:ASN:ND2	2.16	0.41
3:H:132:LYS:HB2	3:H:171:ILE:HD11	2.04	0.40
1:L:193:LEU:HD21	1:L:212:GLU:HB3	2.03	0.40
6:M:406:U10:H303	6:M:406:U10:H261	2.03	0.40
2:M:253:ARG:NH1	15:M:509:HOH:O	2.39	0.40
3:H:248:ARG:CA	3:H:249[A]:LYS:HB2	2.50	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	L	281/282 (100%)	276 (98%)	5 (2%)	0	100	100
2	M	301/307 (98%)	290 (96%)	10 (3%)	1 (0%)	41	46
3	H	243/266 (91%)	240 (99%)	1 (0%)	2 (1%)	19	19
All	All	825/855 (96%)	806 (98%)	16 (2%)	3 (0%)	47	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	249[A]	LYS
3	H	249[B]	LYS
2	M	301	HIS

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	222/221 (100%)	215 (97%)	7 (3%)	39	50
2	M	236/239 (99%)	232 (98%)	4 (2%)	60	74
3	H	200/214 (94%)	191 (96%)	9 (4%)	27	34
All	All	658/674 (98%)	638 (97%)	20 (3%)	46	53

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	ASN
1	L	158	SER
1	L	207	ARG
1	L	210	ASP
1	L	216	PHE
1	L	247	CYS
1	L	272	TRP
2	M	52	LEU
2	M	55	LEU
2	M	72	ILE
2	M	216	PHE
3	H	12	LEU
3	H	163[A]	LYS
3	H	163[B]	LYS
3	H	201	ASN
3	H	220[A]	LYS
3	H	220[B]	LYS
3	H	231	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	249[A]	LYS
3	H	249[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	20	ASN
1	L	159	ASN
1	L	183	ASN
2	M	77	GLN
2	M	187	ASN
2	M	193	HIS
3	H	98	HIS
3	H	201	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 37 ligands modelled in this entry, 2 are monoatomic - leaving 35 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	$\#\|Z\| > 2$
6	U10	L	304[B]	-	23,23,63	1.98	2 (8%)	28,31,79	1.17	3 (10%)
9	HTO	H	308	-	9,9,9	0.63	0	10,10,10	0.68	0
10	GOL	H	307	-	5,5,5	0.25	0	5,5,5	0.57	0
4	LDA	H	309	-	12,15,15	2.10	1 (8%)	14,17,17	0.27	0
8	PO4	M	411	-	4,4,4	1.95	2 (50%)	6,6,6	1.37	1 (16%)
9	HTO	L	307	-	9,9,9	0.94	0	10,10,10	0.70	0
10	GOL	L	309	-	5,5,5	0.41	0	5,5,5	0.31	0
10	GOL	L	311	-	5,5,5	0.50	0	5,5,5	0.81	0
6	U10	M	406	-	48,48,63	1.32	3 (6%)	58,61,79	1.59	15 (25%)
10	GOL	L	310	-	5,5,5	1.25	0	5,5,5	1.44	1 (20%)
8	PO4	M	409	-	4,4,4	0.60	0	6,6,6	0.77	0
7	BCL	L	305	-	58,74,74	1.41	8 (13%)	69,115,115	1.68	15 (21%)
10	GOL	L	312	-	5,5,5	0.43	0	5,5,5	0.70	0
10	GOL	L	314	-	5,5,5	0.75	0	5,5,5	0.60	0
13	PC1	M	408	-	42,42,53	1.17	2 (4%)	48,50,61	1.48	7 (14%)
4	LDA	L	301	-	12,15,15	2.04	1 (8%)	14,17,17	0.36	0
7	BCL	M	403	-	58,74,74	1.74	9 (15%)	69,115,115	1.64	16 (23%)
5	BPH	L	303	-	51,70,70	1.59	10 (19%)	52,101,101	1.68	9 (17%)
7	BCL	M	402	-	58,74,74	1.53	10 (17%)	69,115,115	2.05	20 (28%)
7	BCL	M	401[A]	-	58,74,74	1.68	10 (17%)	69,115,115	2.26	20 (28%)
4	LDA	M	412	-	12,15,15	1.99	1 (8%)	14,17,17	0.80	0
4	LDA	M	404	-	12,15,15	2.02	1 (8%)	14,17,17	0.67	0
5	BPH	L	313	-	51,70,70	1.58	9 (17%)	52,101,101	1.58	9 (17%)
10	GOL	H	305	-	5,5,5	0.53	0	5,5,5	0.75	0
7	BCL	M	401[B]	-	58,74,74	1.67	10 (17%)	69,115,115	2.11	18 (26%)
10	GOL	H	302	-	5,5,5	0.56	0	5,5,5	0.76	0
10	GOL	H	303	-	5,5,5	0.48	0	5,5,5	0.49	0
12	SPO	M	407	-	40,41,41	0.90	0	47,50,50	1.39	7 (14%)
10	GOL	M	410	-	5,5,5	0.78	0	5,5,5	0.77	0
10	GOL	L	308	-	5,5,5	1.19	0	5,5,5	1.28	0
6	U10	L	304[A]	-	23,23,63	2.02	2 (8%)	28,31,79	2.05	9 (32%)
4	LDA	H	304	-	12,15,15	2.04	1 (8%)	14,17,17	1.16	1 (7%)
4	LDA	L	302	-	12,15,15	2.15	1 (8%)	14,17,17	0.68	0
10	GOL	H	301	-	5,5,5	1.03	0	5,5,5	1.74	2 (40%)
8	PO4	L	306	-	4,4,4	0.69	0	6,6,6	0.98	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
6	U10	L	304[B]	-	-	6/15/39/87	0/1/1/1
9	HTO	H	308	-	-	2/10/10/10	-
10	GOL	H	307	-	-	3/4/4/4	-
4	LDA	H	309	-	-	6/13/13/13	-
9	HTO	L	307	-	-	7/10/10/10	-
10	GOL	L	309	-	-	0/4/4/4	-
10	GOL	L	311	-	-	0/4/4/4	-
6	U10	M	406	-	-	8/45/69/87	0/1/1/1
10	GOL	L	310	-	-	0/4/4/4	-
7	BCL	L	305	-	-	4/37/137/137	-
10	GOL	L	312	-	-	1/4/4/4	-
10	GOL	L	314	-	-	2/4/4/4	-
13	PC1	M	408	-	-	20/46/46/57	-
4	LDA	L	301	-	-	7/13/13/13	-
7	BCL	M	403	-	-	2/37/137/137	-
5	BPH	L	303	-	-	7/37/105/105	0/5/6/6
7	BCL	M	402	-	-	10/37/137/137	-
7	BCL	M	401[A]	-	-	6/37/137/137	-
4	LDA	M	412	-	-	6/13/13/13	-
4	LDA	M	404	-	-	6/13/13/13	-
5	BPH	L	313	-	-	7/37/105/105	0/5/6/6
10	GOL	H	305	-	-	2/4/4/4	-
7	BCL	M	401[B]	-	-	12/37/137/137	-
10	GOL	H	302	-	-	2/4/4/4	-
10	GOL	H	303	-	-	4/4/4/4	-
12	SPO	M	407	-	-	4/47/47/47	-
10	GOL	M	410	-	-	2/4/4/4	-
10	GOL	L	308	-	-	2/4/4/4	-
6	U10	L	304[A]	-	-	1/15/39/87	0/1/1/1
4	LDA	H	304	-	-	4/13/13/13	-
4	LDA	L	302	-	-	7/13/13/13	-
10	GOL	H	301	-	-	1/4/4/4	-

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	304[B]	U10	C6-C1	8.25	1.50	1.35
6	L	304[A]	U10	C6-C1	8.12	1.50	1.35
4	L	302	LDA	O1-N1	-7.32	1.25	1.42
4	H	309	LDA	O1-N1	-7.09	1.25	1.42
4	H	304	LDA	O1-N1	-7.02	1.25	1.42
4	M	404	LDA	O1-N1	-6.85	1.26	1.42
4	L	301	LDA	O1-N1	-6.82	1.26	1.42
4	M	412	LDA	O1-N1	-6.77	1.26	1.42
7	M	403	BCL	OBD-CAD	6.58	1.31	1.22
6	M	406	U10	C6-C1	6.56	1.47	1.35
7	M	403	BCL	O2D-CGD	5.59	1.46	1.33
7	M	402	BCL	C3D-C2D	5.57	1.49	1.39
7	M	401[A]	BCL	O2A-CGA	5.16	1.48	1.33
7	M	401[B]	BCL	O2A-CGA	5.16	1.48	1.33
5	L	303	BPH	C3D-C2D	4.97	1.48	1.39
5	L	313	BPH	C3A-C2A	-4.95	1.50	1.54
7	M	403	BCL	C3D-C2D	4.93	1.48	1.39
13	M	408	PC1	O21-C21	4.86	1.48	1.34
7	M	401[A]	BCL	O2D-CGD	4.73	1.44	1.33
7	M	401[B]	BCL	O2D-CGD	4.73	1.44	1.33
13	M	408	PC1	O31-C31	4.54	1.46	1.33
7	L	305	BCL	C3B-C2B	4.54	1.47	1.39
7	L	305	BCL	OBD-CAD	4.47	1.28	1.22
5	L	303	BPH	OBD-CAD	4.39	1.28	1.22
7	M	401[A]	BCL	C3D-C2D	4.34	1.47	1.39
7	M	401[B]	BCL	C3D-C2D	4.34	1.47	1.39
7	L	305	BCL	C3D-C2D	4.20	1.47	1.39
7	M	401[A]	BCL	OBD-CAD	4.04	1.28	1.22
7	M	401[B]	BCL	OBD-CAD	4.04	1.28	1.22
7	M	401[A]	BCL	MG-NC	-4.03	1.96	2.06
7	M	401[B]	BCL	MG-NC	-4.03	1.96	2.06
7	L	305	BCL	O2A-CGA	4.00	1.45	1.33
7	M	402	BCL	OBD-CAD	3.94	1.27	1.22
7	M	402	BCL	O2A-CGA	3.93	1.44	1.33
5	L	303	BPH	O2D-CGD	3.89	1.42	1.33
5	L	313	BPH	C2C-C3C	-3.61	1.51	1.54
7	M	402	BCL	O2D-CGD	3.52	1.41	1.33
5	L	313	BPH	O2A-CGA	3.48	1.43	1.33
7	M	403	BCL	C3B-C2B	3.44	1.45	1.39
7	M	401[A]	BCL	MG-NA	-3.42	1.98	2.06
7	M	401[B]	BCL	MG-NA	-3.42	1.98	2.06
7	M	403	BCL	O2A-CGA	3.39	1.43	1.33
6	L	304[B]	U10	C4-C3	3.38	1.50	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	313	BPH	C3D-C2D	3.35	1.45	1.39
5	L	313	BPH	O2D-CGD	3.35	1.41	1.33
5	L	303	BPH	C2C-C3C	-3.24	1.51	1.54
6	M	406	U10	C4-C3	3.18	1.49	1.36
5	L	303	BPH	O2A-CGA	3.10	1.42	1.33
7	M	402	BCL	C3B-C2B	2.91	1.44	1.39
7	M	403	BCL	C4B-CHC	2.85	1.48	1.41
5	L	313	BPH	C3B-C2B	2.81	1.44	1.39
5	L	313	BPH	CBD-CGD	-2.66	1.48	1.52
7	L	305	BCL	C4B-CHC	2.65	1.48	1.41
6	L	304[A]	U10	C4-C3	2.62	1.47	1.36
7	M	401[A]	BCL	C3B-C2B	2.57	1.44	1.39
7	M	401[B]	BCL	C3B-C2B	2.57	1.44	1.39
7	M	402	BCL	MG-NA	-2.56	2.00	2.06
6	M	406	U10	O3-C3M	-2.56	1.39	1.45
8	M	411	PO4	P-O4	-2.54	1.47	1.54
7	M	402	BCL	C2D-C1D	2.51	1.48	1.42
5	L	313	BPH	OBD-CAD	2.48	1.25	1.22
5	L	303	BPH	C4B-NB	-2.47	1.30	1.38
7	L	305	BCL	O2D-CGD	2.44	1.39	1.33
5	L	303	BPH	C3B-C2B	2.43	1.43	1.39
7	M	401[A]	BCL	CAA-C2A	2.29	1.58	1.54
7	M	401[B]	BCL	CAA-C2A	2.29	1.58	1.54
7	M	403	BCL	O1D-CGD	2.29	1.27	1.21
7	L	305	BCL	C1B-CHB	2.28	1.47	1.41
5	L	313	BPH	O2D-CED	-2.24	1.40	1.45
8	M	411	PO4	P-O3	-2.22	1.47	1.54
7	M	401[A]	BCL	C4B-NB	-2.21	1.33	1.35
7	M	401[B]	BCL	C4B-NB	-2.21	1.33	1.35
7	M	402	BCL	C4B-CHC	2.21	1.47	1.41
7	M	403	BCL	C2D-C1D	2.18	1.47	1.42
5	L	303	BPH	O2D-CED	-2.18	1.40	1.45
7	M	401[A]	BCL	C3C-C4C	-2.12	1.48	1.51
7	M	401[B]	BCL	C3C-C4C	-2.12	1.48	1.51
5	L	303	BPH	CBD-CGD	-2.11	1.49	1.52
7	M	403	BCL	MG-NA	2.09	2.11	2.06
7	L	305	BCL	C2D-C1D	2.09	1.47	1.42
5	L	303	BPH	OBB-CAB	2.05	1.29	1.22
7	M	402	BCL	CBB-CAB	-2.03	1.43	1.49
7	M	402	BCL	CBD-CGD	-2.01	1.46	1.52

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	401[A]	BCL	C1C-NC-C4C	-8.04	103.09	106.71
7	M	401[B]	BCL	C1C-NC-C4C	-8.04	103.09	106.71
7	M	402	BCL	C1C-NC-C4C	-7.18	103.48	106.71
13	M	408	PC1	O21-C21-C22	6.57	125.65	111.50
5	L	303	BPH	O2D-CGD-CBD	6.36	119.06	111.00
7	M	402	BCL	C1-O2A-CGA	5.76	131.55	116.44
7	M	401[A]	BCL	C4C-CHD-C1D	-5.62	117.58	125.88
7	M	401[B]	BCL	C4C-CHD-C1D	-5.62	117.58	125.88
7	M	401[A]	BCL	C3C-C4C-CHD	-5.26	112.15	123.39
7	M	401[B]	BCL	C3C-C4C-CHD	-5.26	112.15	123.39
5	L	313	BPH	O2D-CGD-CBD	5.24	117.63	111.00
7	M	401[A]	BCL	CHD-C4C-NC	5.13	130.77	125.08
7	M	401[B]	BCL	CHD-C4C-NC	5.13	130.77	125.08
7	M	402	BCL	CAD-C3D-C4D	-4.90	105.74	108.47
7	L	305	BCL	C4A-NA-C1A	-4.88	104.51	106.71
7	M	401[A]	BCL	C4-C3-C5	4.85	123.44	115.27
7	M	401[A]	BCL	C5-C3-C2	-4.44	112.12	121.12
6	L	304[A]	U10	C1M-C1-C6	-4.37	117.26	124.40
7	M	403	BCL	C3C-C4C-CHD	-4.28	114.24	123.39
7	L	305	BCL	O1D-CGD-CBD	4.25	133.19	124.48
7	L	305	BCL	O2D-CGD-O1D	-4.17	115.68	123.84
6	L	304[A]	U10	C8-C7-C6	4.09	123.07	112.05
7	L	305	BCL	C3C-C4C-CHD	-4.08	114.67	123.39
7	M	403	BCL	O2D-CGD-O1D	-4.00	116.02	123.84
7	M	402	BCL	C3C-C4C-CHD	-3.99	114.88	123.39
5	L	303	BPH	C4C-C3C-C2C	-3.90	99.13	102.84
5	L	303	BPH	O2D-CGD-O1D	-3.73	116.55	123.84
6	M	406	U10	C32-C33-C34	-3.69	118.78	127.66
7	L	305	BCL	C1C-NC-C4C	-3.62	105.08	106.71
7	M	402	BCL	C4B-CHC-C1C	-3.59	123.00	130.12
5	L	313	BPH	C3D-CAD-CBD	3.58	112.33	107.61
7	M	403	BCL	CHD-C4C-NC	3.49	128.96	125.08
7	M	401[A]	BCL	C16-C15-C13	-3.43	104.85	115.92
7	L	305	BCL	C2A-C1A-CHA	-3.36	117.98	123.86
6	M	406	U10	C1M-C1-C6	-3.33	118.96	124.40
7	M	403	BCL	O2A-CGA-O1A	-3.26	115.36	123.59
7	M	401[A]	BCL	C1-O2A-CGA	3.25	124.97	116.44
7	M	403	BCL	OBB-CAB-C3B	3.23	125.72	119.99
5	L	313	BPH	C1-O2A-CGA	3.22	124.89	116.44
13	M	408	PC1	O31-C31-C32	3.21	121.97	111.91
6	L	304[A]	U10	C3M-O3-C3	3.20	127.80	116.47
5	L	313	BPH	O2D-CGD-O1D	-3.19	117.60	123.84
7	M	402	BCL	O2D-CGD-CBD	3.18	116.93	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	401[A]	BCL	O2D-CGD-CBD	3.18	116.92	111.27
7	M	401[B]	BCL	O2D-CGD-CBD	3.18	116.92	111.27
13	M	408	PC1	O21-C21-O22	-3.16	116.06	123.70
7	M	401[A]	BCL	C3A-C2A-C1A	-3.16	96.61	101.34
7	M	401[B]	BCL	C3A-C2A-C1A	-3.16	96.61	101.34
6	M	406	U10	C30-C29-C31	3.15	120.56	115.27
7	M	402	BCL	O2A-C1-C2	3.14	116.89	108.64
7	M	401[A]	BCL	OBB-CAB-C3B	3.12	125.53	119.99
7	M	401[B]	BCL	OBB-CAB-C3B	3.12	125.53	119.99
6	L	304[A]	U10	C1-C6-C5	-3.12	116.65	119.58
7	L	305	BCL	CAD-C3D-C4D	-3.10	106.74	108.47
7	M	401[A]	BCL	C4B-CHC-C1C	-3.10	123.98	130.12
7	M	401[B]	BCL	C4B-CHC-C1C	-3.10	123.98	130.12
13	M	408	PC1	C2-O21-C21	3.08	125.38	117.79
7	M	401[A]	BCL	O2A-CGA-CBA	3.05	121.48	111.91
7	M	401[B]	BCL	O2A-CGA-CBA	3.05	121.48	111.91
6	L	304[A]	U10	O2-C2-C3	-3.02	114.52	120.93
7	L	305	BCL	C4C-CHD-C1D	-3.02	121.43	125.88
7	M	403	BCL	C2A-C1A-CHA	-3.00	118.61	123.86
7	M	402	BCL	CED-O2D-CGD	-2.99	109.17	115.94
6	M	406	U10	C6-C1-C2	2.99	121.55	119.18
7	M	402	BCL	C4-C3-C2	-2.98	116.03	123.68
7	M	401[A]	BCL	C2A-C1A-CHA	-2.95	118.71	123.86
7	M	401[B]	BCL	C2A-C1A-CHA	-2.95	118.71	123.86
7	L	305	BCL	CHD-C4C-NC	2.94	128.34	125.08
7	M	401[A]	BCL	OBD-CAD-C3D	-2.92	123.13	127.98
7	M	401[B]	BCL	OBD-CAD-C3D	-2.92	123.13	127.98
6	L	304[A]	U10	C7-C6-C5	2.92	121.99	118.48
13	M	408	PC1	O31-C31-O32	-2.92	116.23	123.59
6	M	406	U10	C27-C28-C29	-2.88	120.73	127.66
7	M	403	BCL	C1-C2-C3	-2.88	121.07	126.04
12	M	407	SPO	C40-C38-C39	2.87	120.94	114.60
12	M	407	SPO	C24-C23-C22	2.87	126.94	122.92
5	L	303	BPH	O2A-CGA-O1A	-2.83	116.44	123.59
12	M	407	SPO	C3-C1-C4	-2.83	106.51	110.86
7	M	403	BCL	O2A-CGA-CBA	2.80	120.69	111.91
7	M	403	BCL	C1C-NC-C4C	-2.78	105.45	106.71
5	L	303	BPH	CMB-C2B-C3B	2.77	129.86	124.68
5	L	303	BPH	CED-O2D-CGD	2.69	122.03	115.94
7	M	403	BCL	CBB-CAB-C3B	-2.68	112.37	120.34
7	M	402	BCL	O2D-CGD-O1D	-2.68	118.60	123.84
12	M	407	SPO	C20-C19-C17	-2.68	123.49	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	402	BCL	C4B-C3B-CAB	2.67	132.29	127.13
7	M	402	BCL	C3D-CAD-CBD	2.66	111.11	107.61
7	M	401[A]	BCL	CHC-C1C-NC	2.66	128.19	124.51
7	M	401[B]	BCL	CHC-C1C-NC	2.66	128.19	124.51
6	M	406	U10	C17-C18-C19	-2.64	121.29	127.66
7	M	402	BCL	O2A-CGA-CBA	2.63	120.15	111.91
5	L	303	BPH	C1-C2-C3	-2.59	121.57	126.04
5	L	303	BPH	CBC-CAC-C3C	2.57	118.94	113.77
7	M	402	BCL	C3A-C2A-C1A	-2.56	97.50	101.34
7	L	305	BCL	C3A-C2A-C1A	-2.56	97.50	101.34
6	M	406	U10	C31-C29-C28	-2.54	115.97	121.12
6	M	406	U10	C4M-O4-C4	2.52	125.40	116.47
5	L	313	BPH	CAC-C3C-C2C	-2.51	108.00	114.26
6	L	304[B]	U10	C1M-C1-C6	-2.49	120.34	124.40
13	M	408	PC1	O21-C2-C3	2.48	117.38	108.40
7	L	305	BCL	C1-O2A-CGA	2.46	122.91	116.44
6	M	406	U10	C26-C27-C28	-2.46	103.81	111.88
6	M	406	U10	C41-C39-C40	2.45	120.02	114.60
7	M	402	BCL	CHB-C4A-NA	2.44	127.88	124.51
10	H	301	GOL	C3-C2-C1	2.42	121.09	111.70
7	M	402	BCL	CHD-C4C-NC	2.41	127.75	125.08
6	M	406	U10	C22-C21-C19	-2.39	105.12	112.98
6	M	406	U10	C3M-O3-C3	2.37	124.86	116.47
7	M	402	BCL	C5-C3-C2	2.36	125.89	121.12
7	M	401[B]	BCL	C4-C3-C2	-2.34	117.67	123.68
4	H	304	LDA	CM1-N1-C1	-2.33	105.33	110.23
5	L	313	BPH	CBA-CAA-C2A	-2.32	107.02	113.81
6	M	406	U10	C25-C24-C26	2.31	119.16	115.27
7	M	402	BCL	O2A-CGA-O1A	-2.30	117.79	123.59
7	M	401[A]	BCL	C16-C17-C18	-2.29	105.18	115.98
6	L	304[A]	U10	O4-C4-C3	-2.29	115.00	123.64
10	L	310	GOL	O3-C3-C2	2.28	121.13	110.20
6	L	304[A]	U10	C4-C3-C2	-2.28	116.21	120.68
7	L	305	BCL	O2A-CGA-O1A	-2.27	117.86	123.59
7	M	401[B]	BCL	C4-C3-C5	2.27	119.09	115.27
5	L	313	BPH	C4-C3-C2	-2.27	117.86	123.68
7	M	402	BCL	CHC-C1C-NC	2.25	127.63	124.51
6	M	406	U10	C35-C34-C36	2.24	119.05	115.27
10	H	301	GOL	O3-C3-C2	2.20	120.74	110.20
12	M	407	SPO	C35-C36-C37	-2.20	104.66	111.88
12	M	407	SPO	C21-C20-C19	2.19	127.96	123.47
7	M	401[A]	BCL	CMB-C2B-C3B	2.17	128.74	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	401[B]	BCL	CMB-C2B-C3B	2.17	128.74	124.68
5	L	313	BPH	CMA-C3A-C4A	-2.16	109.64	114.38
7	M	401[B]	BCL	C1-C2-C3	-2.15	122.33	126.04
7	M	403	BCL	O2D-CGD-CBD	2.14	115.06	111.27
6	M	406	U10	C15-C14-C16	2.13	118.86	115.27
7	M	403	BCL	O1D-CGD-CBD	2.13	128.84	124.48
7	L	305	BCL	OBD-CAD-C3D	-2.11	124.48	127.98
13	M	408	PC1	C3-C2-C1	-2.11	106.81	111.79
7	L	305	BCL	C4-C3-C5	2.10	118.81	115.27
7	M	401[A]	BCL	CHB-C4A-NA	2.10	127.41	124.51
7	M	401[B]	BCL	CHB-C4A-NA	2.10	127.41	124.51
6	L	304[B]	U10	C7-C8-C9	-2.09	123.31	126.79
7	M	403	BCL	OBD-CAD-C3D	-2.09	124.51	127.98
6	L	304[A]	U10	O3-C3-C2	2.08	123.59	116.56
7	M	403	BCL	CMD-C2D-C3D	-2.07	120.81	124.68
7	M	403	BCL	CHB-C4A-NA	2.07	127.37	124.51
7	L	305	BCL	CMB-C2B-C3B	2.05	128.52	124.68
6	L	304[B]	U10	C12-C13-C14	-2.05	120.75	127.75
7	M	401[A]	BCL	CAD-C3D-C4D	-2.05	107.33	108.47
7	M	401[B]	BCL	CAD-C3D-C4D	-2.05	107.33	108.47
5	L	313	BPH	CMB-C2B-C3B	2.03	128.48	124.68
5	L	303	BPH	C3D-CAD-CBD	2.03	110.27	107.61
7	M	403	BCL	CAD-C3D-C4D	-2.03	107.34	108.47
12	M	407	SPO	C15-C14-C12	-2.02	124.42	127.31
8	M	411	PO4	O4-P-O2	2.02	114.45	107.97
7	M	402	BCL	OBD-CAD-C3D	-2.01	124.65	127.98

There are no chirality outliers.

All (151) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	404	LDA	C2-C1-N1-O1
4	M	404	LDA	C2-C1-N1-CM2
6	L	304[B]	U10	C1-C6-C7-C8
6	L	304[B]	U10	C5-C6-C7-C8
7	M	401[B]	BCL	C4-C3-C5-C6
7	M	402	BCL	C2-C1-O2A-CGA
9	L	307	HTO	C1-C2-C3-O3
9	L	307	HTO	C1-C2-C3-C4
9	L	307	HTO	O2-C2-C3-O3
9	L	307	HTO	O2-C2-C3-C4
10	L	308	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	L	314	GOL	O1-C1-C2-C3
10	M	410	GOL	O1-C1-C2-C3
10	H	302	GOL	C1-C2-C3-O3
10	H	303	GOL	C1-C2-C3-O3
10	H	307	GOL	O1-C1-C2-C3
12	M	407	SPO	O1-C1-C4-C5
12	M	407	SPO	C2-C1-C4-C5
12	M	407	SPO	C3-C1-C4-C5
13	M	408	PC1	C11-O13-P-O14
13	M	408	PC1	C11-O13-P-O11
13	M	408	PC1	O22-C21-O21-C2
13	M	408	PC1	C2-C3-O31-C31
13	M	408	PC1	O32-C31-O31-C3
13	M	408	PC1	C32-C31-O31-C3
13	M	408	PC1	C22-C21-O21-C2
6	L	304[B]	U10	C12-C11-C9-C10
6	M	406	U10	C30-C29-C31-C32
6	L	304[B]	U10	C12-C11-C9-C8
6	M	406	U10	C28-C29-C31-C32
7	M	401[B]	BCL	C2-C3-C5-C6
6	L	304[B]	U10	C9-C11-C12-C13
7	M	401[B]	BCL	C11-C12-C13-C14
5	L	313	BPH	C5-C6-C7-C8
7	L	305	BCL	C15-C16-C17-C18
7	M	401[B]	BCL	C10-C11-C12-C13
7	M	402	BCL	C8-C10-C11-C12
7	M	401[B]	BCL	C12-C13-C15-C16
7	M	402	BCL	C6-C7-C8-C10
7	M	401[A]	BCL	C13-C15-C16-C17
6	L	304[A]	U10	C9-C11-C12-C13
6	M	406	U10	C29-C31-C32-C33
7	M	401[A]	BCL	C3-C5-C6-C7
7	M	401[B]	BCL	C15-C16-C17-C18
7	M	401[B]	BCL	C5-C6-C7-C8
4	L	302	LDA	C2-C3-C4-C5
4	L	301	LDA	C7-C8-C9-C10
13	M	408	PC1	C3-C2-O21-C21
13	M	408	PC1	C29-C2A-C2B-C2C
7	M	401[A]	BCL	C16-C17-C18-C19
4	L	302	LDA	C3-C4-C5-C6
10	L	312	GOL	C1-C2-C3-O3
10	H	305	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	H	304	LDA	C7-C8-C9-C10
4	H	304	LDA	C11-C10-C9-C8
13	M	408	PC1	C25-C26-C27-C28
4	L	302	LDA	C7-C8-C9-C10
13	M	408	PC1	C26-C27-C28-C29
7	M	402	BCL	CBA-CGA-O2A-C1
5	L	303	BPH	C2-C3-C5-C6
10	L	314	GOL	O1-C1-C2-O2
10	M	410	GOL	O1-C1-C2-O2
10	H	305	GOL	O1-C1-C2-O2
7	M	402	BCL	O1A-CGA-O2A-C1
4	M	412	LDA	C1-C2-C3-C4
4	H	309	LDA	C3-C4-C5-C6
5	L	313	BPH	C15-C16-C17-C18
7	M	401[B]	BCL	C8-C10-C11-C12
4	L	301	LDA	C3-C4-C5-C6
7	M	401[A]	BCL	C16-C17-C18-C20
5	L	313	BPH	C8-C10-C11-C12
5	L	303	BPH	C4-C3-C5-C6
7	M	401[B]	BCL	C14-C13-C15-C16
4	H	309	LDA	C1-C2-C3-C4
4	H	309	LDA	C11-C10-C9-C8
5	L	313	BPH	C16-C17-C18-C19
12	M	407	SPO	C1-C4-C5-C6
4	H	309	LDA	C7-C8-C9-C10
4	L	301	LDA	C6-C7-C8-C9
10	H	302	GOL	O2-C2-C3-O3
10	H	303	GOL	O2-C2-C3-O3
4	H	309	LDA	C9-C10-C11-C12
4	L	301	LDA	C2-C3-C4-C5
4	L	302	LDA	C5-C6-C7-C8
4	M	412	LDA	C7-C8-C9-C10
7	M	402	BCL	C11-C10-C8-C7
4	M	412	LDA	N1-C1-C2-C3
4	H	309	LDA	C5-C6-C7-C8
13	M	408	PC1	C22-C23-C24-C25
5	L	313	BPH	C16-C17-C18-C20
4	M	412	LDA	C3-C4-C5-C6
10	L	308	GOL	O2-C2-C3-O3
4	M	404	LDA	C1-C2-C3-C4
7	M	401[A]	BCL	C6-C7-C8-C9
7	M	402	BCL	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	M	408	PC1	C23-C24-C25-C26
4	L	301	LDA	C11-C10-C9-C8
4	H	304	LDA	C1-C2-C3-C4
7	M	401[B]	BCL	C3-C5-C6-C7
5	L	313	BPH	CAD-CBD-CGD-O2D
4	M	412	LDA	C6-C7-C8-C9
4	M	404	LDA	C2-C1-N1-CM1
4	M	404	LDA	C3-C4-C5-C6
10	H	307	GOL	O1-C1-C2-O2
4	L	302	LDA	C1-C2-C3-C4
5	L	303	BPH	C8-C10-C11-C12
4	L	301	LDA	C1-C2-C3-C4
4	M	404	LDA	C5-C6-C7-C8
13	M	408	PC1	O13-C11-C12-N
7	L	305	BCL	C16-C17-C18-C20
4	L	301	LDA	C4-C5-C6-C7
7	L	305	BCL	C2-C1-O2A-CGA
13	M	408	PC1	C1-O11-P-O13
4	L	302	LDA	C11-C10-C9-C8
7	M	403	BCL	C15-C16-C17-C18
9	L	307	HTO	C4-C5-C6-C7
13	M	408	PC1	C2-C1-O11-P
6	M	406	U10	C5-C4-O4-C4M
9	L	307	HTO	C3-C4-C5-C6
5	L	303	BPH	C14-C13-C15-C16
7	M	401[B]	BCL	C6-C7-C8-C9
7	M	402	BCL	C11-C10-C8-C9
13	M	408	PC1	C31-C32-C33-C34
5	L	303	BPH	O2A-C1-C2-C3
6	M	406	U10	C35-C34-C36-C37
9	H	308	HTO	C4-C5-C6-C7
13	M	408	PC1	C27-C28-C29-C2A
6	M	406	U10	C33-C34-C36-C37
7	M	403	BCL	CAA-CBA-CGA-O2A
9	L	307	HTO	O3-C3-C4-C5
9	H	308	HTO	O3-C3-C4-C5
10	H	303	GOL	O1-C1-C2-C3
7	M	402	BCL	C4C-C3C-CAC-CBC
6	M	406	U10	C25-C24-C26-C27
4	L	302	LDA	C9-C10-C11-C12
7	L	305	BCL	CAD-CBD-CGD-O2D
7	M	401[A]	BCL	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	M	401[B]	BCL	CAD-CBD-CGD-O2D
7	M	402	BCL	CAD-CBD-CGD-O2D
6	M	406	U10	C23-C24-C26-C27
6	L	304[B]	U10	C2-C3-O3-C3M
5	L	313	BPH	O2A-C1-C2-C3
4	H	304	LDA	C6-C7-C8-C9
5	L	303	BPH	C16-C17-C18-C20
13	M	408	PC1	O31-C31-C32-C33
10	H	303	GOL	O1-C1-C2-O2
10	H	301	GOL	O1-C1-C2-C3
4	M	412	LDA	C5-C6-C7-C8
13	M	408	PC1	O32-C31-C32-C33
10	H	307	GOL	O2-C2-C3-O3
5	L	303	BPH	C13-C15-C16-C17

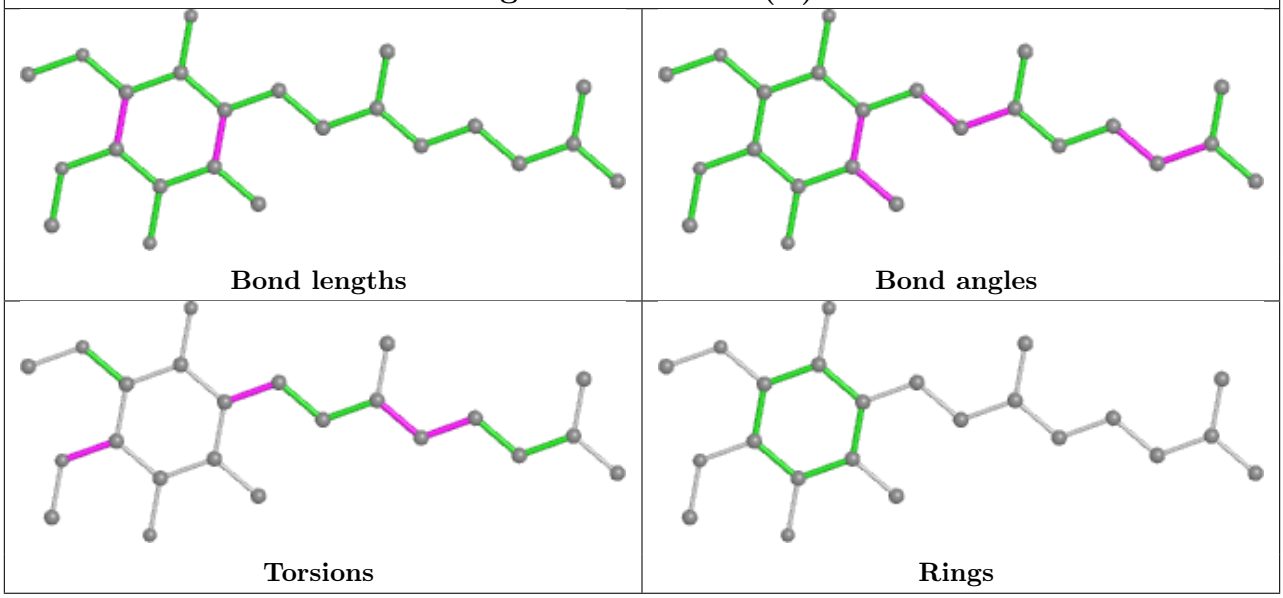
There are no ring outliers.

22 monomers are involved in 62 short contacts:

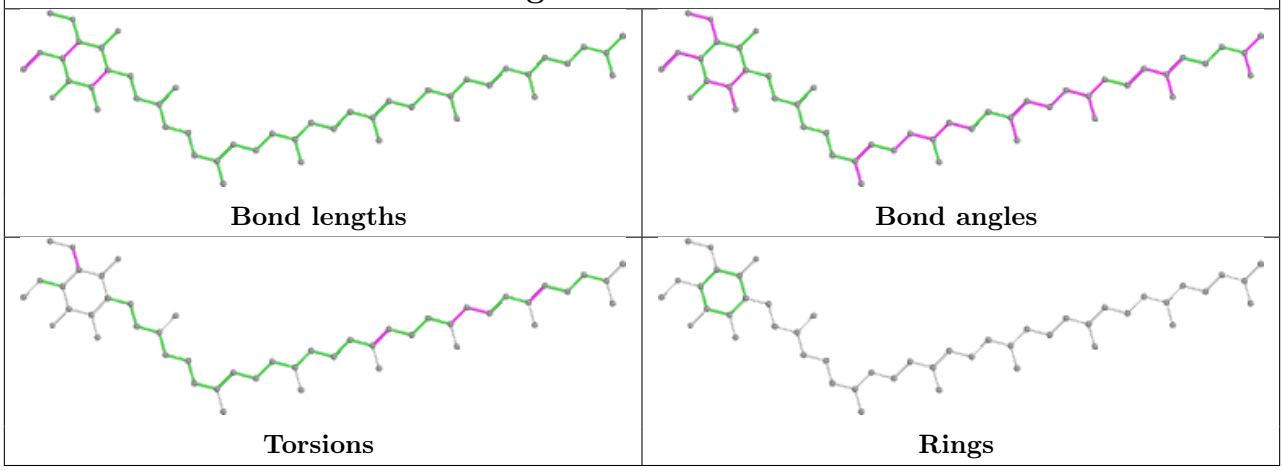
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	304[B]	U10	8	0
9	H	308	HTO	1	0
10	H	307	GOL	1	0
8	M	411	PO4	3	0
6	M	406	U10	2	0
7	L	305	BCL	2	0
10	L	312	GOL	1	0
10	L	314	GOL	5	0
7	M	403	BCL	11	0
5	L	303	BPH	3	0
7	M	402	BCL	6	0
7	M	401[A]	BCL	1	0
4	M	412	LDA	3	0
5	L	313	BPH	6	0
7	M	401[B]	BCL	3	0
12	M	407	SPO	1	0
10	L	308	GOL	1	0
6	L	304[A]	U10	3	0
4	H	304	LDA	3	0
4	L	302	LDA	1	0
10	H	301	GOL	4	0
8	L	306	PO4	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.

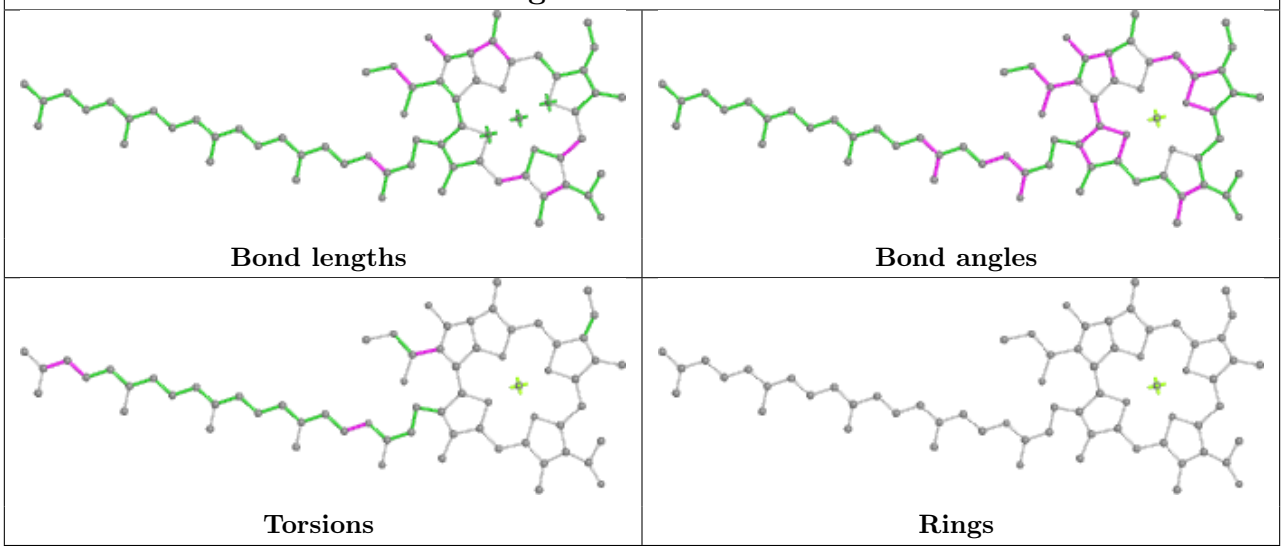
Ligand U10 L 304 (B)



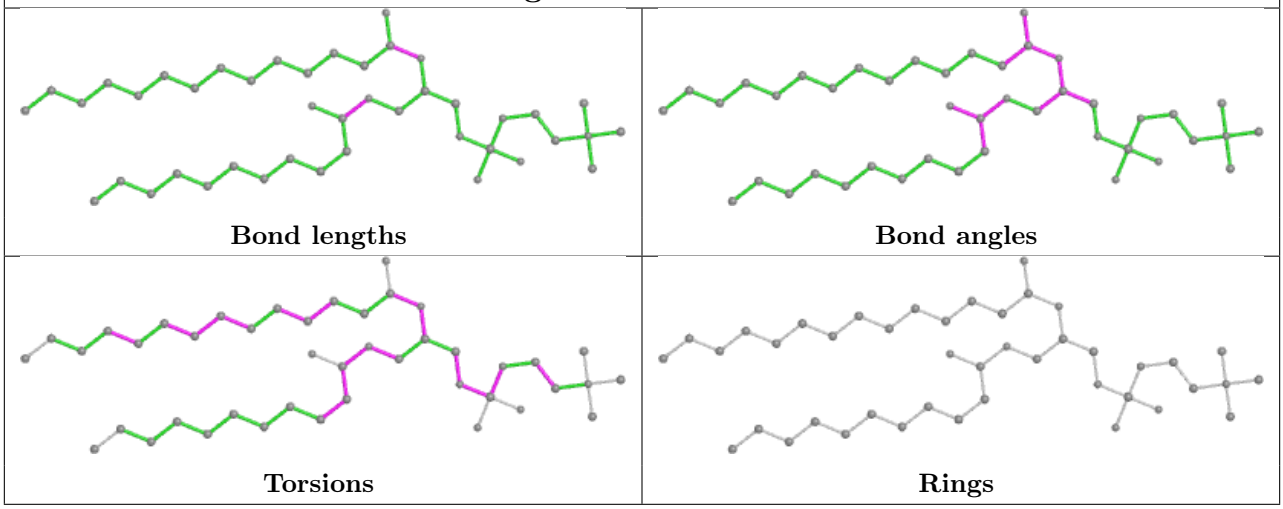
Ligand U10 M 406



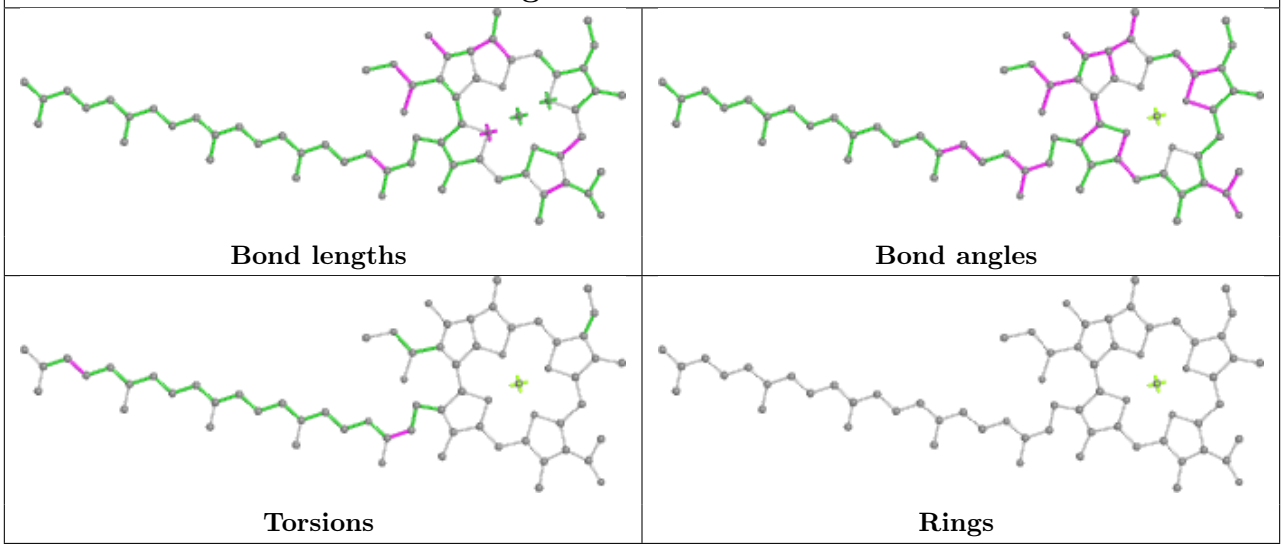
Ligand BCL L 305



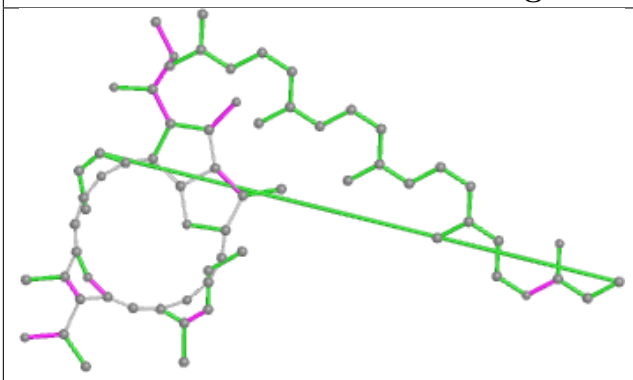
Ligand PC1 M 408



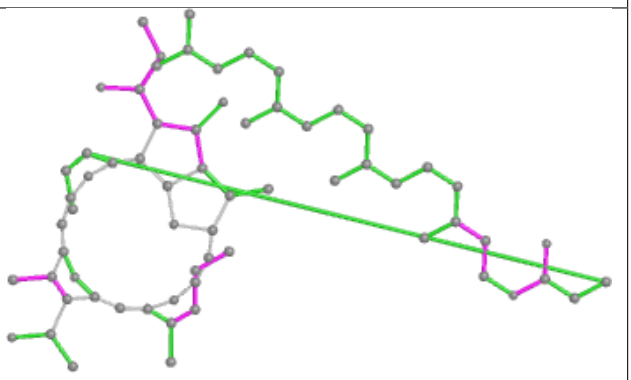
Ligand BCL M 403



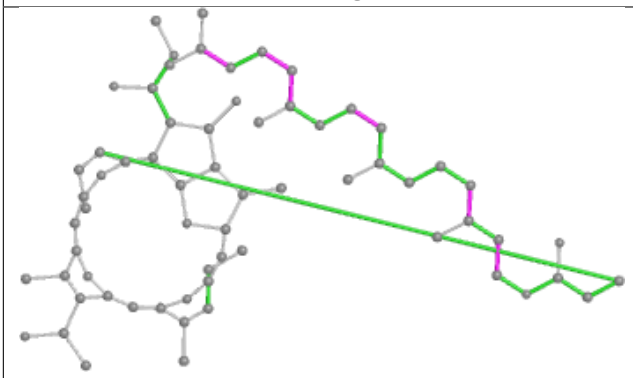
Ligand BPH L 303



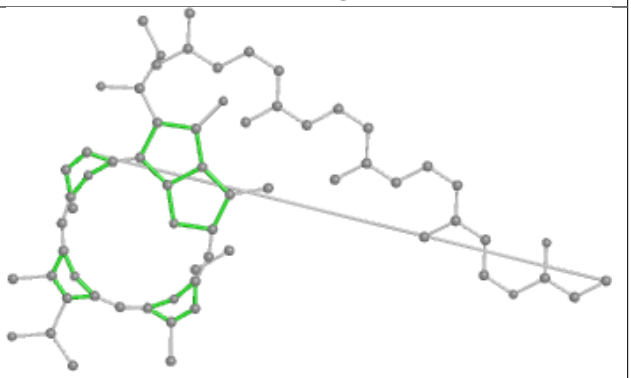
Bond lengths



Bond angles

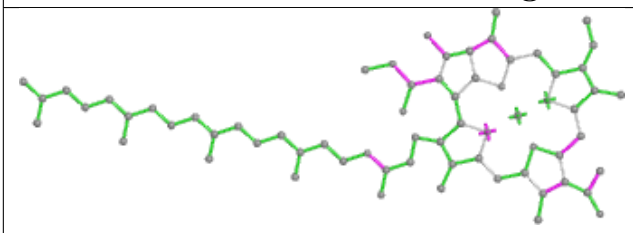


Torsions

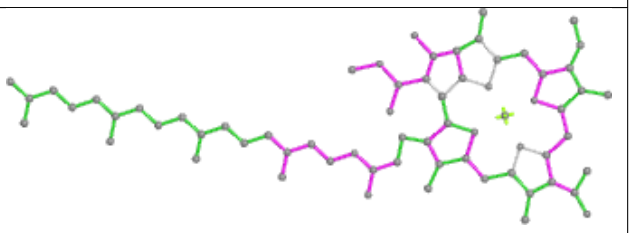


Rings

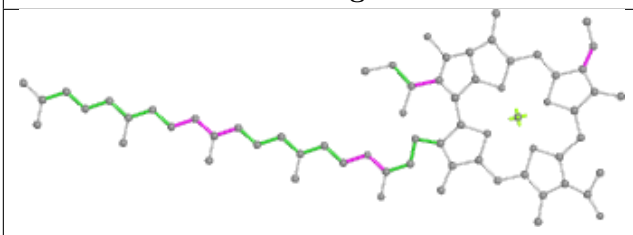
Ligand BCL M 402



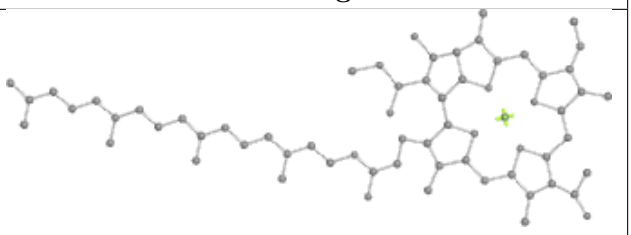
Bond lengths



Bond angles

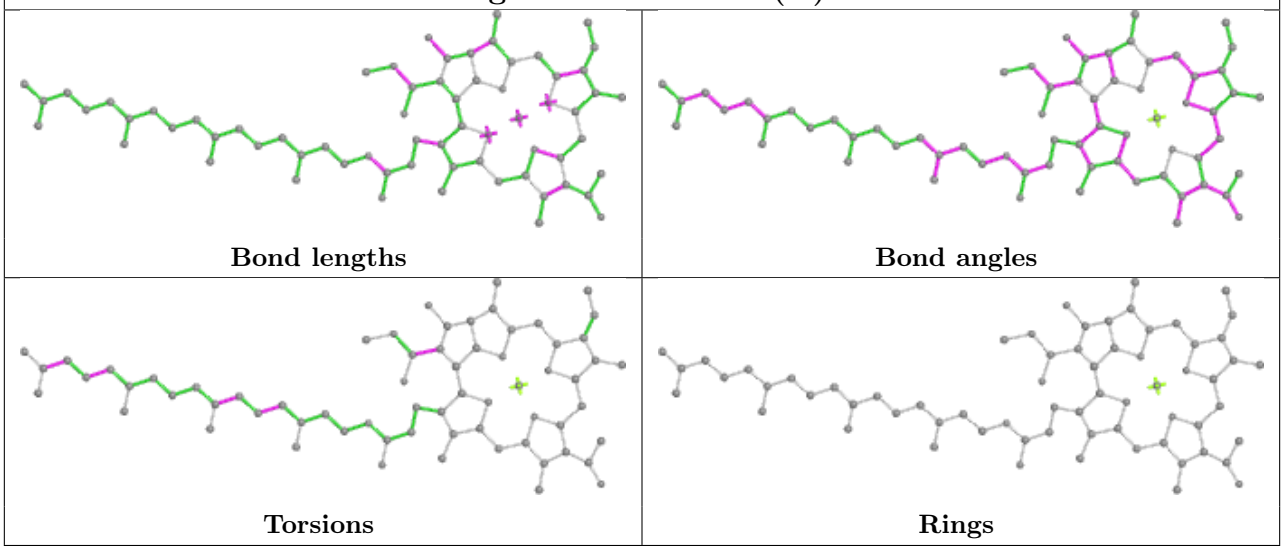


Torsions

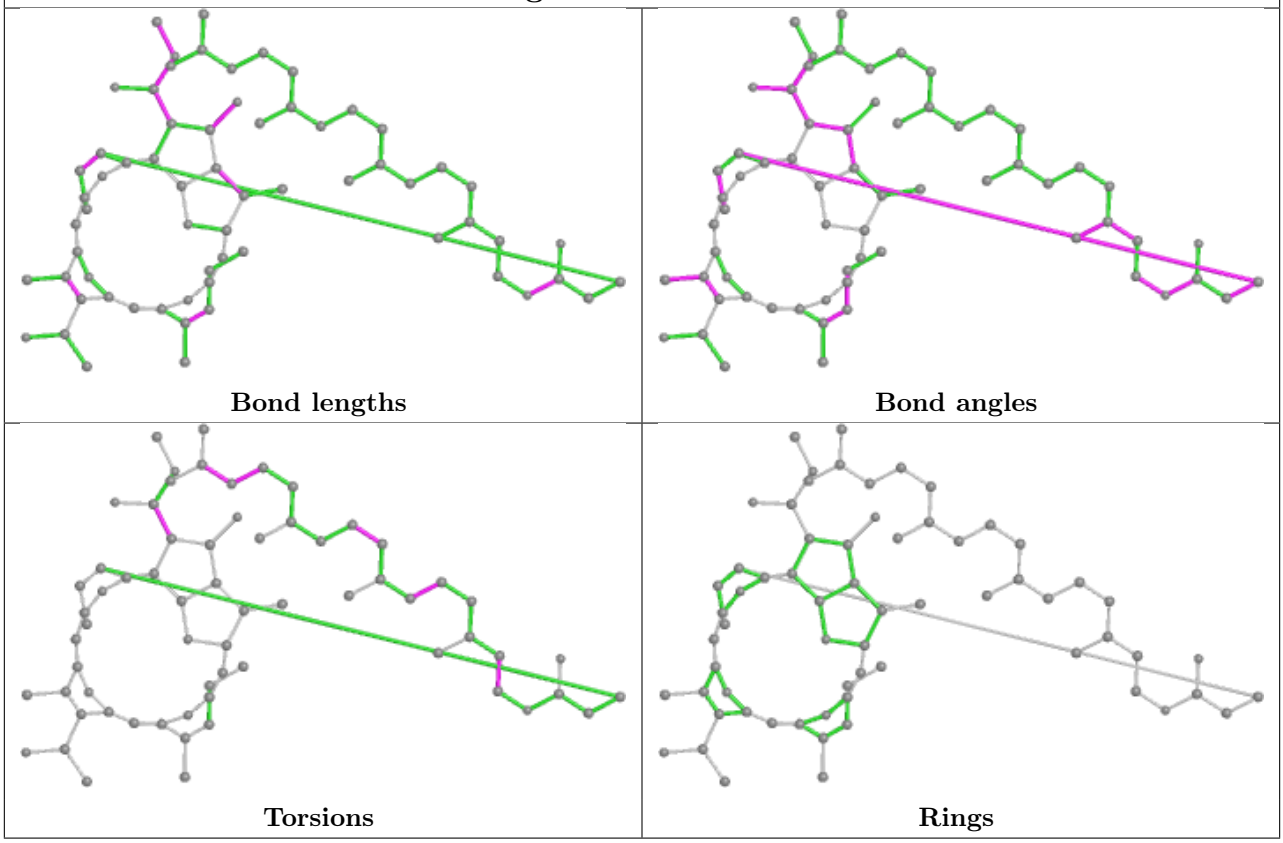


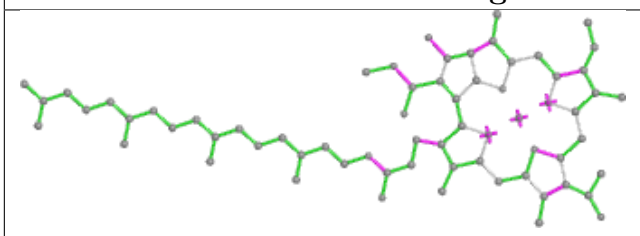
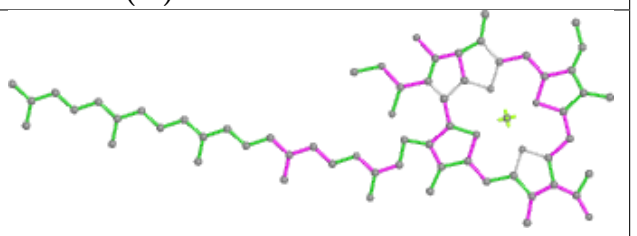
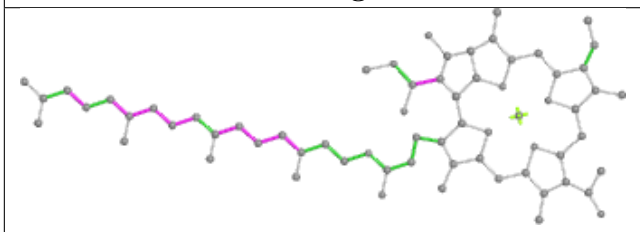
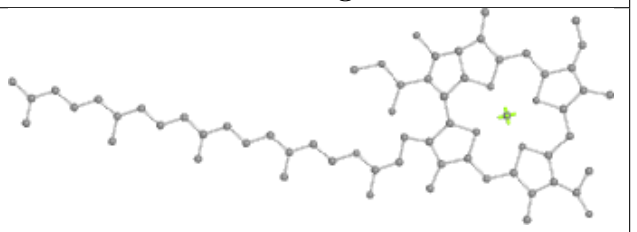
Rings

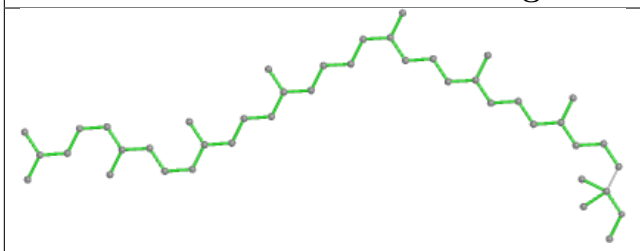
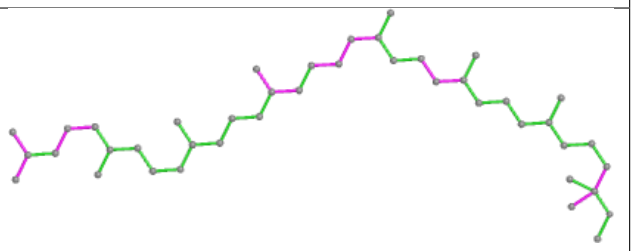
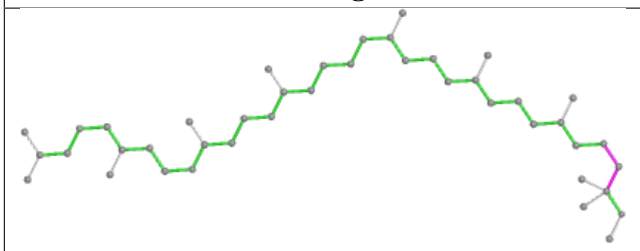
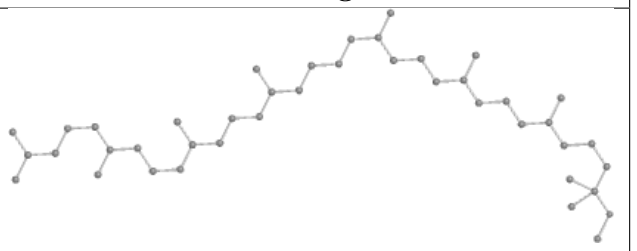
Ligand BCL M 401 (A)

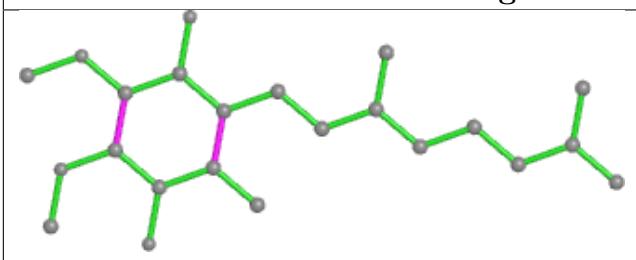
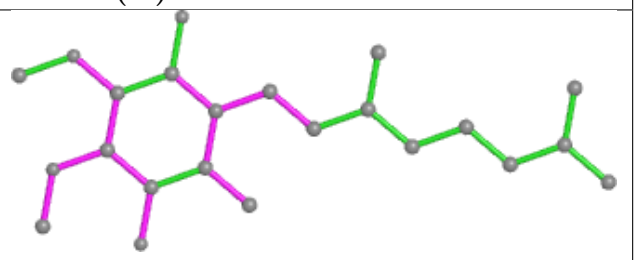
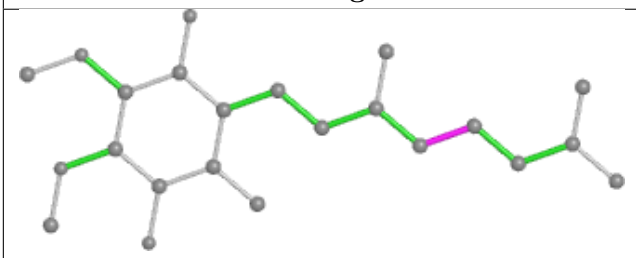
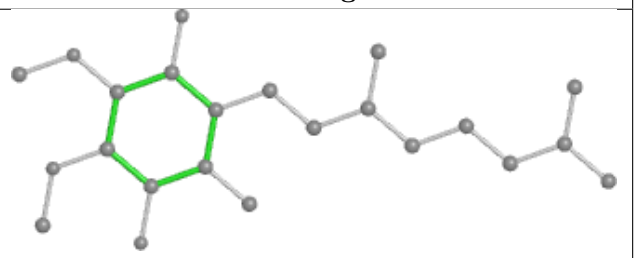


Ligand BPH L 313



Ligand BCL M 401 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPO M 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand U10 L 304 (A)	
 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	281/282 (99%)	-0.46	2 (0%)	87	86	29, 38, 63, 83	0
2	M	302/307 (98%)	-0.48	6 (1%)	65	63	29, 42, 64, 104	6 (1%)
3	H	240/266 (90%)	-0.72	2 (0%)	86	85	30, 41, 56, 106	3 (1%)
All	All	823/855 (96%)	-0.54	10 (1%)	79	77	29, 40, 63, 106	9 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	250	SER	5.8
1	L	277	GLY	3.0
2	M	105	PHE	2.9
2	M	1	ALA	2.7
3	H	249[A]	LYS	2.5
2	M	109	LEU	2.5
1	L	276	PRO	2.3
2	M	301	HIS	2.1
2	M	106	ALA	2.1
2	M	80	TRP	2.0

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)

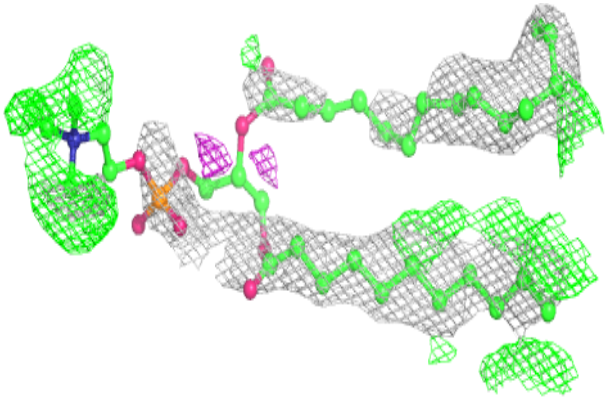
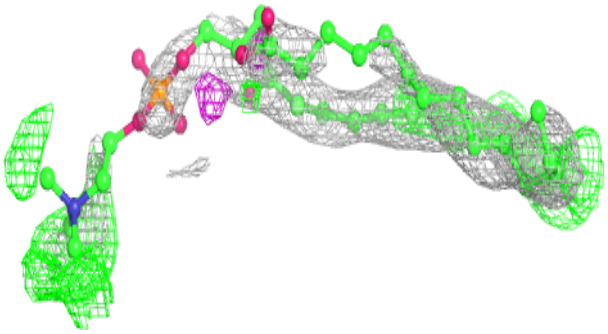
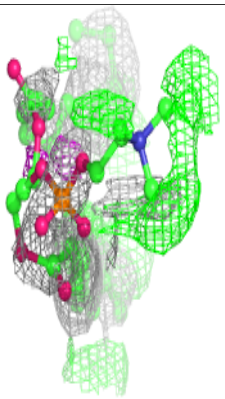
There are no monosaccharides in this entry.

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.

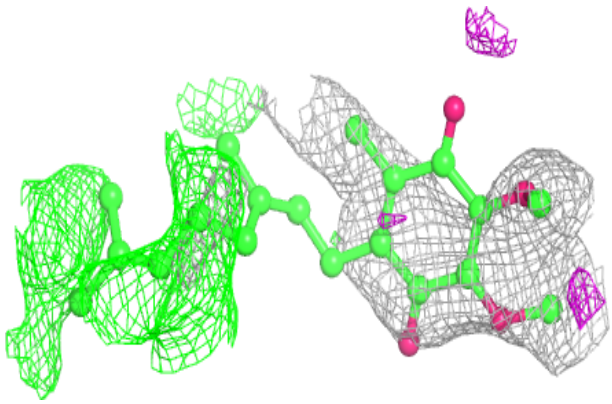
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	PC1	M	408	43/54	0.35	0.45	78,108,166,179	0
4	LDA	H	309	16/16	0.56	0.26	78,89,134,144	0
4	LDA	L	302	16/16	0.57	0.47	91,97,115,118	0
9	HTO	H	308	10/10	0.58	0.31	71,98,111,112	0
4	LDA	L	301	16/16	0.61	0.32	84,96,122,123	0
9	HTO	L	307	10/10	0.67	0.41	75,90,100,103	0
4	LDA	M	404	16/16	0.75	0.25	66,78,98,98	0
10	GOL	L	310	6/6	0.77	0.15	49,64,77,81	0
4	LDA	M	412	16/16	0.77	0.22	66,76,87,101	0
10	GOL	H	302	6/6	0.80	0.35	68,76,78,88	0
10	GOL	H	303	6/6	0.80	0.19	73,80,83,83	0
10	GOL	M	410	6/6	0.80	0.16	61,61,69,69	0
6	U10	L	304[B]	23/63	0.83	0.30	47,64,69,74	23
6	U10	L	304[A]	23/63	0.83	0.30	32,59,75,78	23
10	GOL	H	301	6/6	0.84	0.20	42,59,64,66	0
10	GOL	L	311	6/6	0.84	0.21	54,67,77,82	0
10	GOL	L	309	6/6	0.87	0.26	82,82,88,89	0
4	LDA	H	304	16/16	0.90	0.14	49,66,81,82	0
10	GOL	L	314	6/6	0.91	0.14	58,69,75,77	0
10	GOL	L	308	6/6	0.91	0.14	42,58,66,72	0
6	U10	M	406	48/63	0.93	0.15	30,53,78,90	0
8	PO4	M	409	5/5	0.93	0.13	63,69,76,81	0
7	BCL	M	401[B]	66/66	0.94	0.21	24,35,62,70	20
10	GOL	H	305	6/6	0.94	0.19	41,49,58,68	0
7	BCL	M	401[A]	66/66	0.94	0.21	24,35,53,65	20
10	GOL	H	307	6/6	0.95	0.25	56,73,81,85	0
12	SPO	M	407	42/42	0.95	0.16	34,43,80,96	0
10	GOL	L	312	6/6	0.95	0.20	53,55,60,61	0
5	BPH	L	303	65/65	0.96	0.11	27,34,44,49	0
5	BPH	L	313	65/65	0.96	0.14	31,41,118,122	0
8	PO4	L	306	5/5	0.97	0.10	56,56,61,64	0
7	BCL	L	305	66/66	0.97	0.14	28,35,50,71	0
7	BCL	M	402	66/66	0.97	0.14	29,36,81,84	0
14	K	H	306	1/1	0.97	0.05	46,46,46,46	0
7	BCL	M	403	66/66	0.98	0.12	28,33,55,81	0
8	PO4	M	411	5/5	0.99	0.09	47,48,60,64	0
11	FE	M	405	1/1	1.00	0.12	30,30,30,30	0

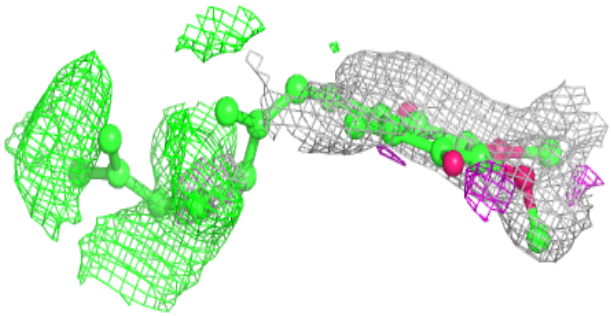
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

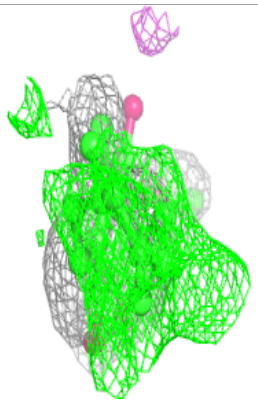
Electron density around PC1 M 408: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around U10 L 304 (B):

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

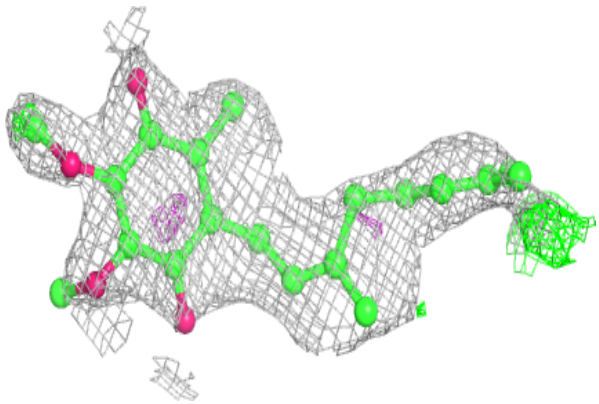


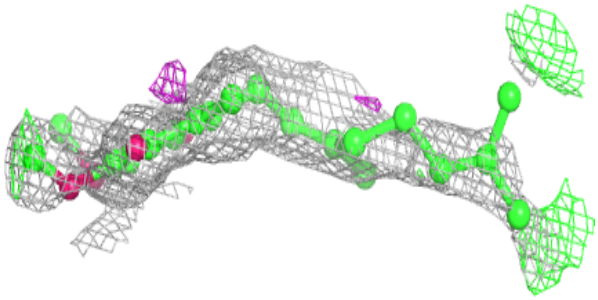


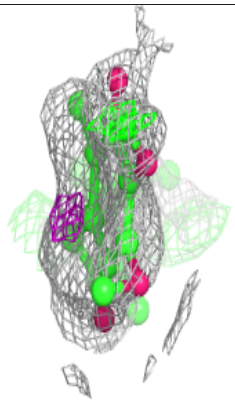


Electron density around U10 L 304 (A):

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

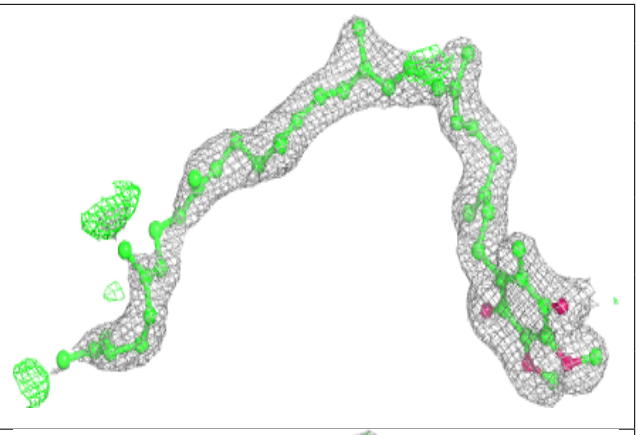


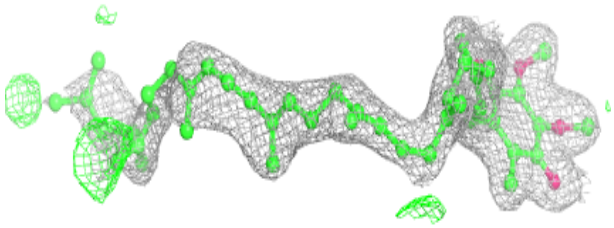


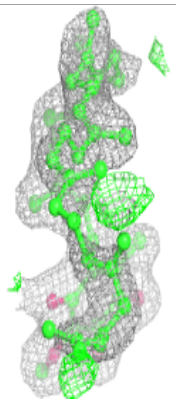


Electron density around U10 M 406:

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

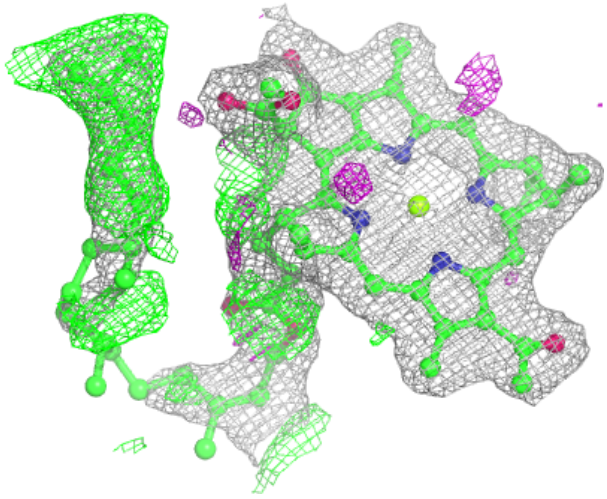


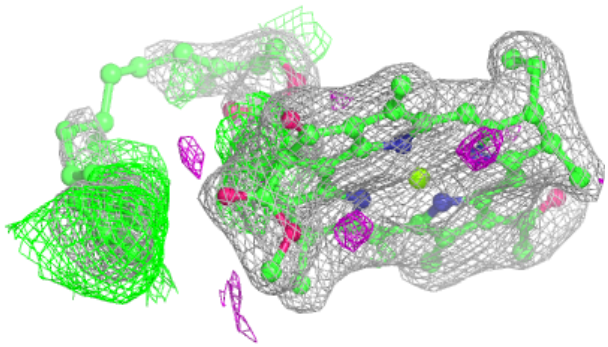


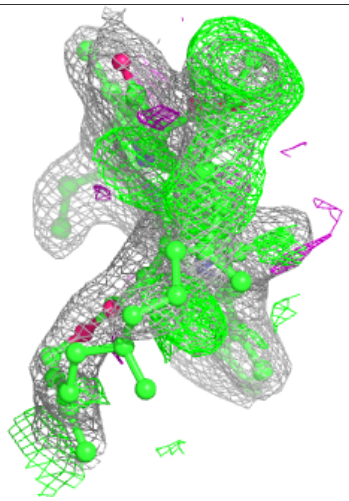


Electron density around BCL M 401 (B):

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

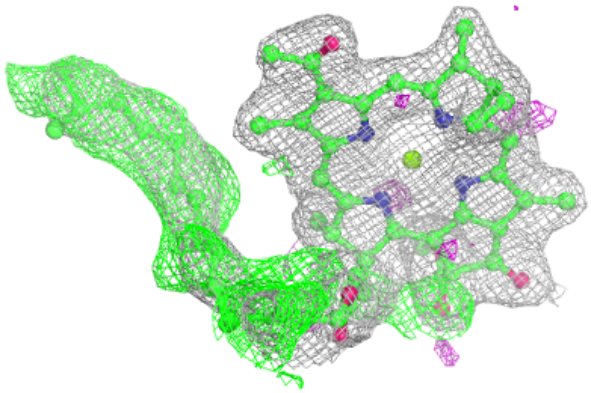


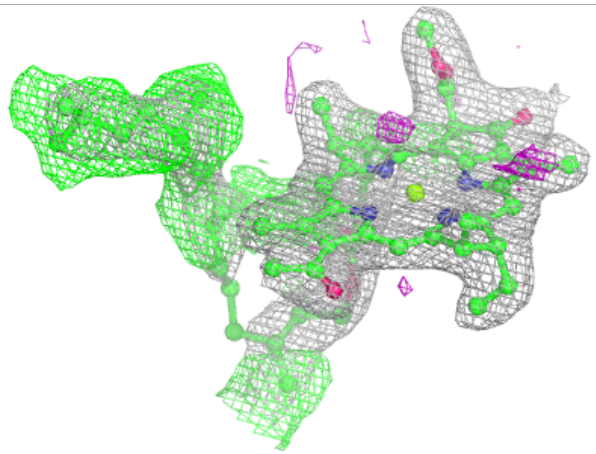


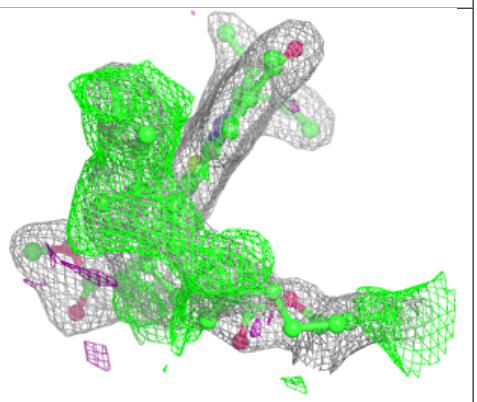


Electron density around BCL M 401 (A):

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

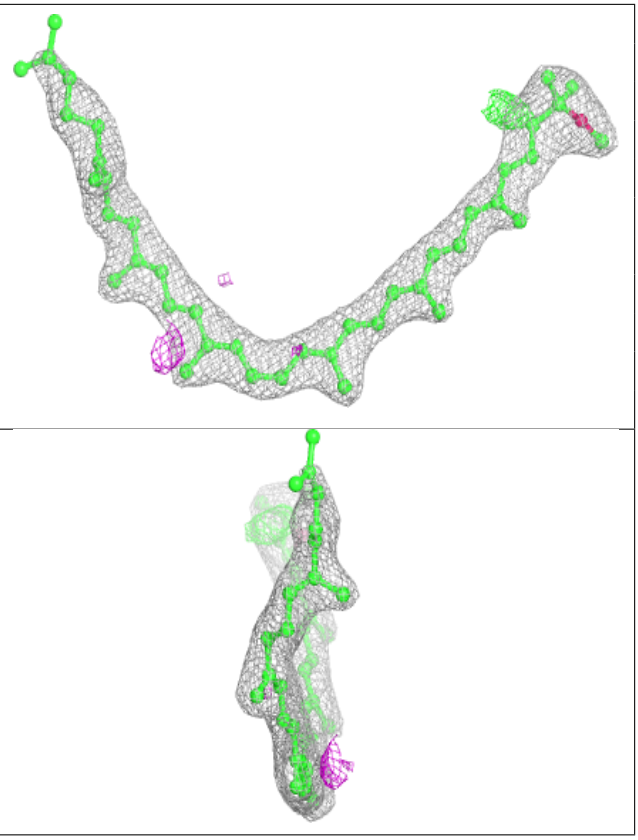


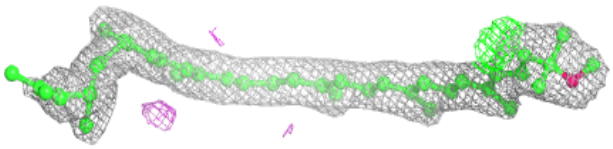




Electron density around SPO M 407:

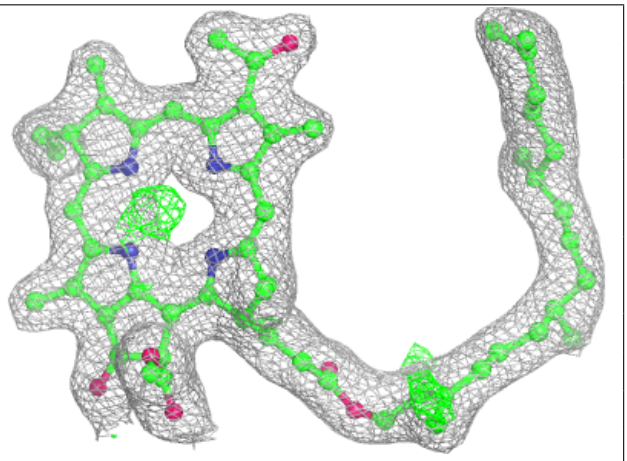
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

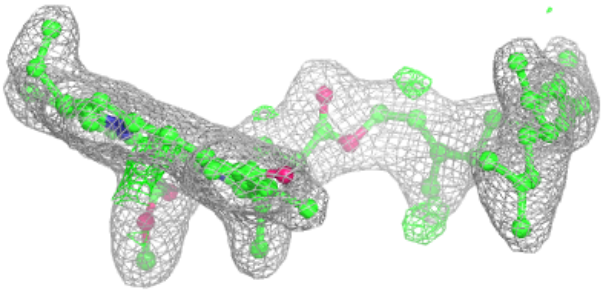


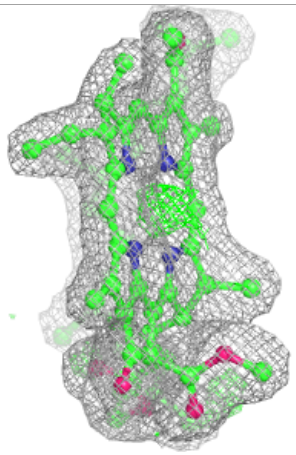


Electron density around BPH L 303:

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

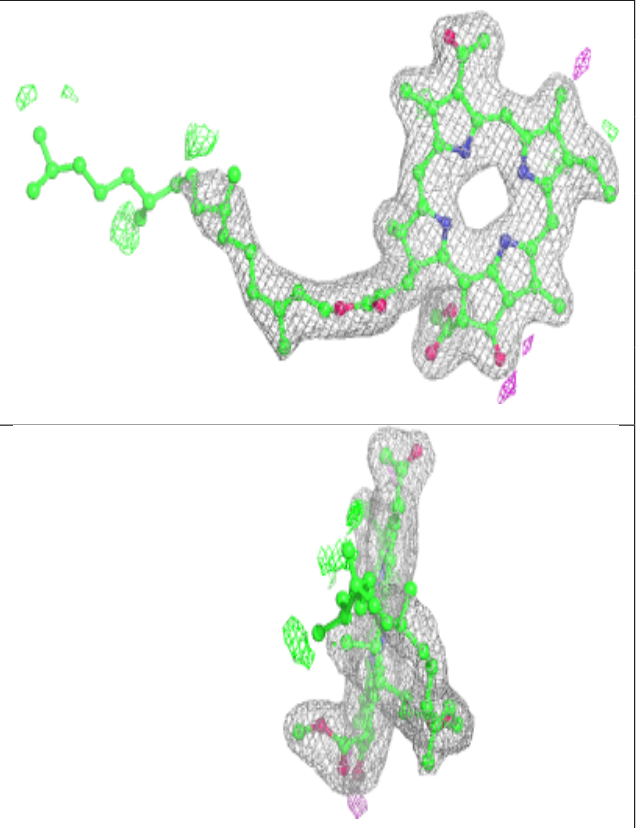


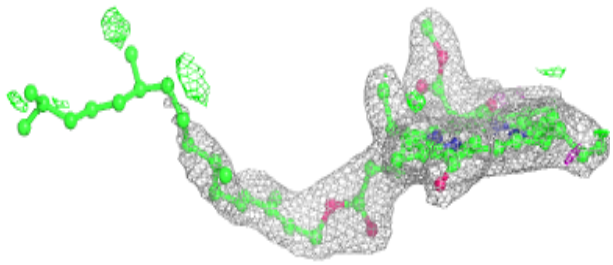




Electron density around BPH L 313:

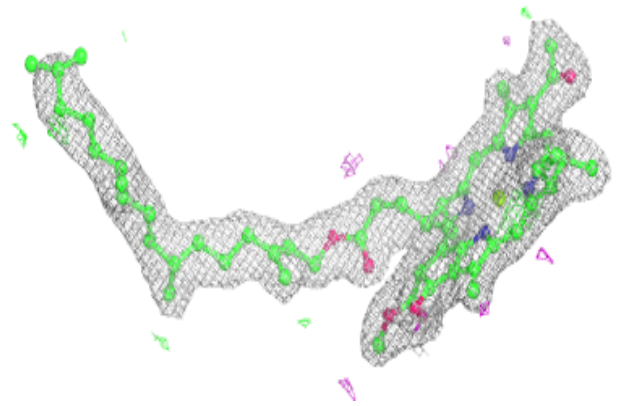
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

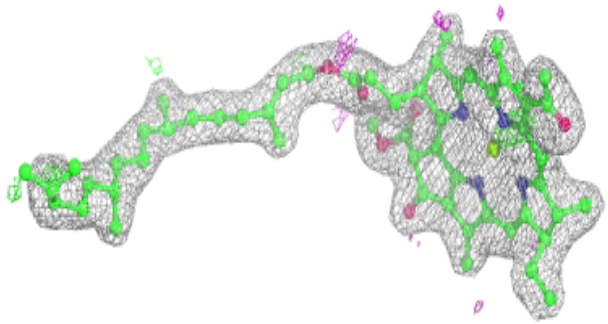


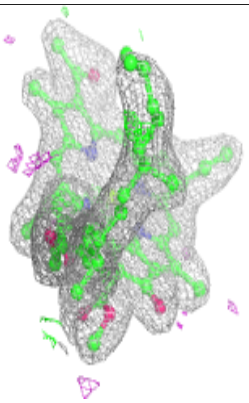


Electron density around BCL L 305:

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

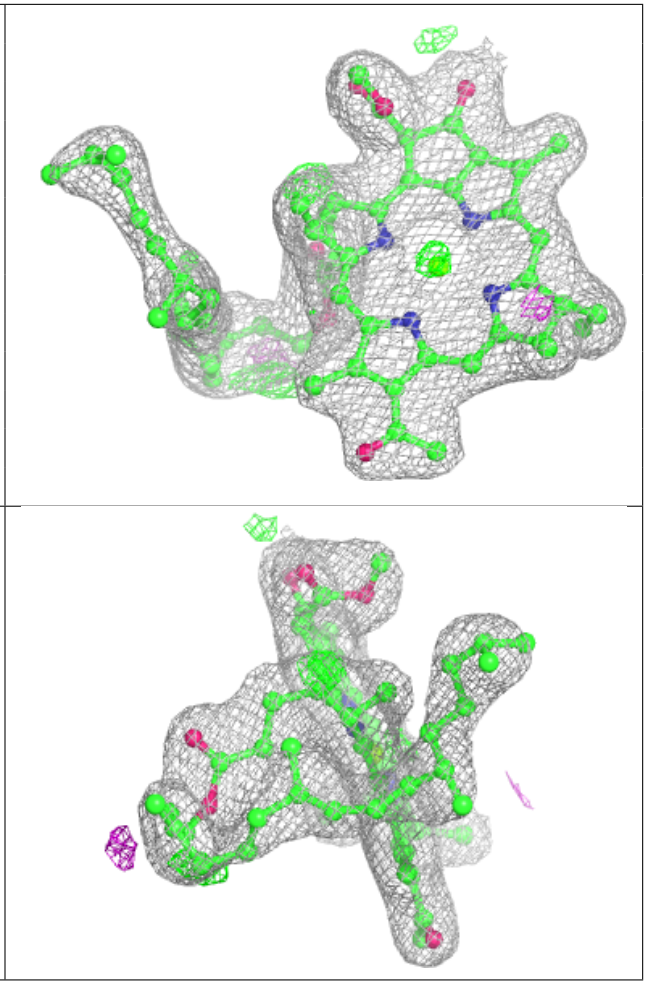






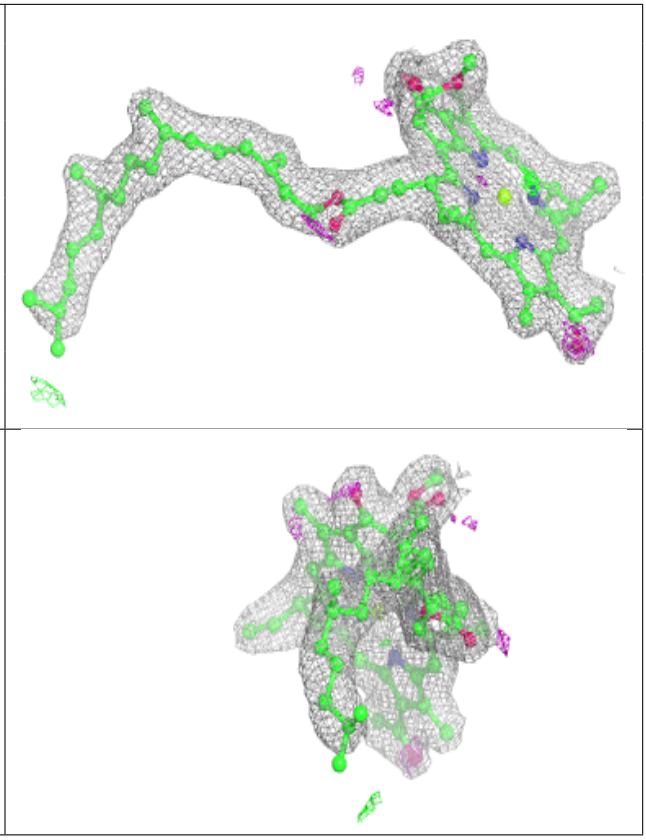
Electron density around BCL M 402:

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



Electron density around 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)



6.5 Other polymers (i)

There are no such residues in this entry.