Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2026 – 07:17 am BST

PDB ID	:	1E6D / pdb_00001e6d
Title	:	PHOTOSYNTHETIC REACTION CENTER MUTANT WITH TRP M115 REPLACED WITH PHE (CHAIN M, WM115F) PHE M197 REPLACED WITH ARG (CHAIN M, FM197R)
Authors	:	Ridge, J.P.; Fyfe, P.K.; McAuley, K.E.; Van Brederode, M.E.; Robert, B.; Van Grondelle, R.; Isaacs, N.W.; Cogdell, R.J.; Jones, M.R.
Deposited on	:	2000-08-11
Resolution	:	2.30 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 (1)) were used in the production of this report:

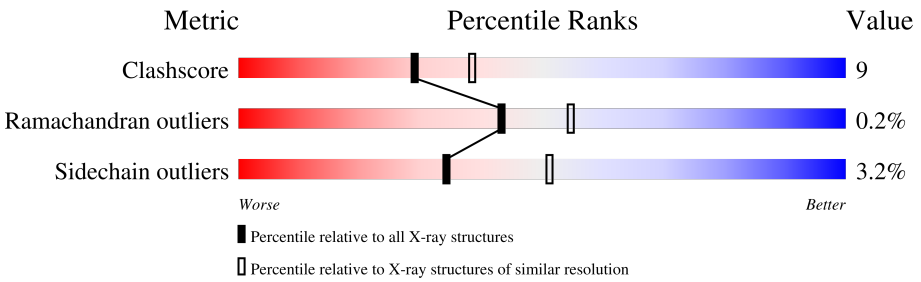
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	260	77% 13% • 8%
2	L	281	80% 17% •
3	M	307	77% 20% • •

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	PO4	M	1800	-	X	-	-
10	PO4	M	1801	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BCL	L	1304	X	-	-	-
5	BCL	M	1301	X	-	-	-
6	BPH	M	1401	X	-	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 7334 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 PHOTOSYNTHETIC REACTION CENTER H SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	240	1829	1169	314	337	9	0	0	0

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER L SUBUNIT.

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

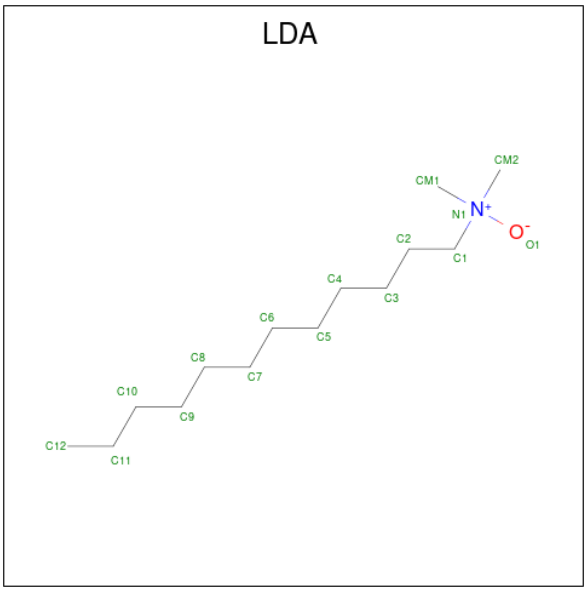
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER M SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	302	2405	1602	396	397	10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

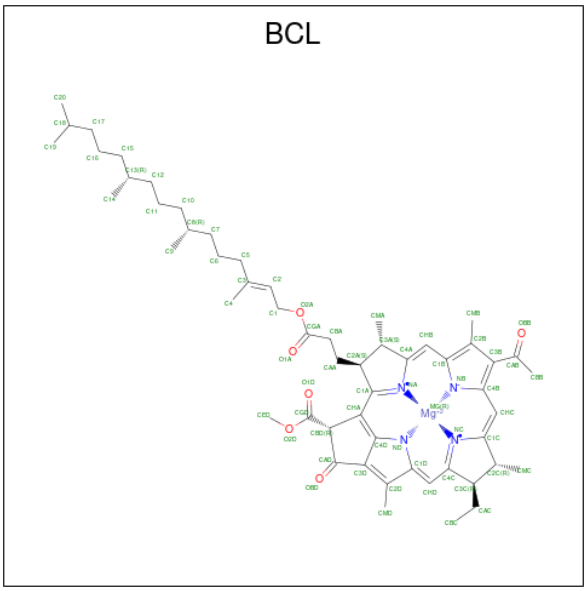
Chain	Residue	Modelled	Actual	Comment	Reference
M	197	ARG	PHE	engineered mutation	UNP P02953
M	115	PHE	TRP	engineered mutation	UNP P02953

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



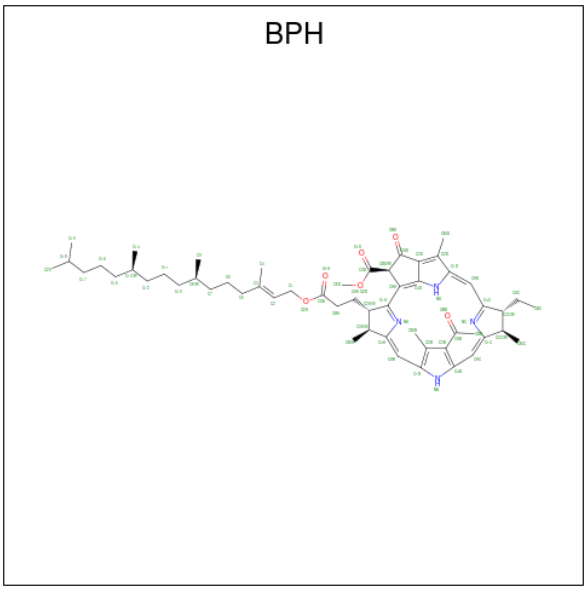
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	H	1	16	14	1	1	0	0
			Total	C	N	O		
4	H	1	16	14	1	1	0	0
			Total	C	N	O		
4	M	1	16	14	1	1	0	0
			Total	C	N	O		
4	M	1	16	14	1	1	0	0
			Total	C	N	O		
4	M	1	16	14	1	1	0	0
			Total	C	N	O		
4	M	1	16	14	1	1	0	0
			Total	C	N	O		
4	M	1	16	14	1	1	0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

- Molecule 5 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



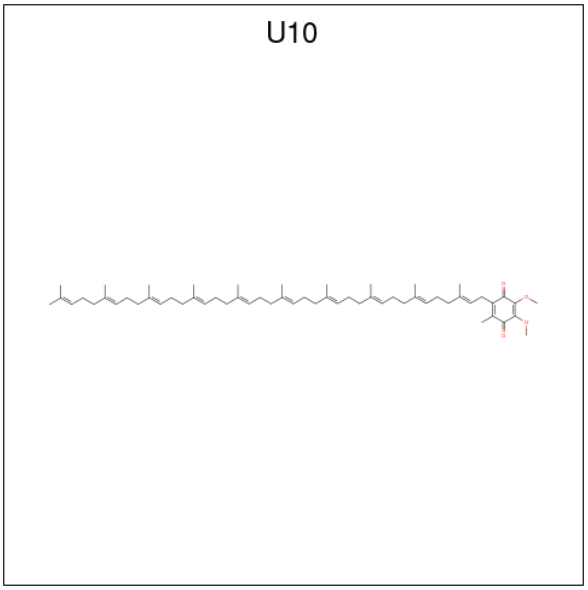
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
5	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	M	1	66	55	1	4	6	0	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

- Molecule 7 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).

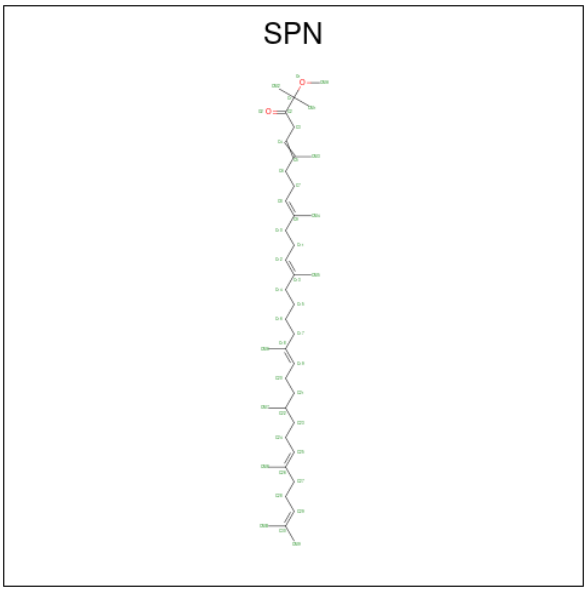


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	L	1	48	44	4	0	0
7	M	1	48	44	4	0	0

- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

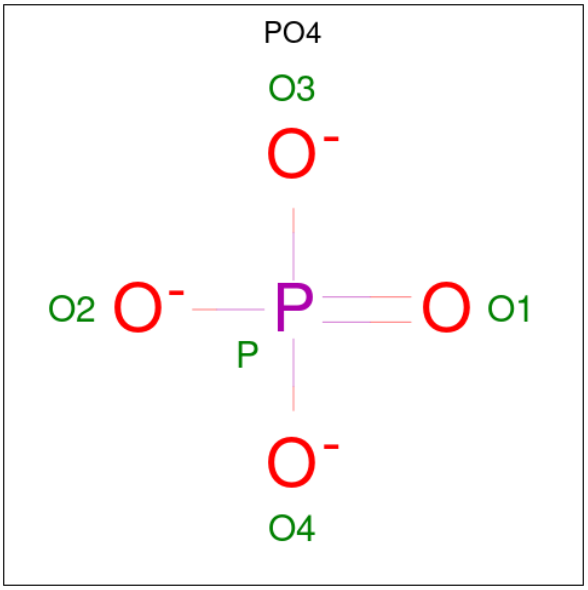
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
8	M	1	1	1	0	0

- Molecule 9 is SPEROIDENONE (CCD ID: 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 PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	H	1	1	1	0	0
			Total	O		
11	H	94	94	94	0	0
			Total	O		
11	L	1	1	1	0	0
			Total	O		
11	L	1	1	1	0	0
			Total	O		
11	L	47	47	47	0	0
			Total	O		
11	M	2	2	2	0	0
			Total	O		
11	M	1	1	1	0	0
			Total	O		
11	M	65	65	65	0	0

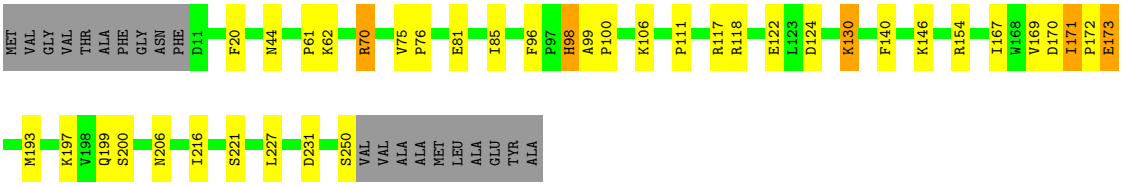
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

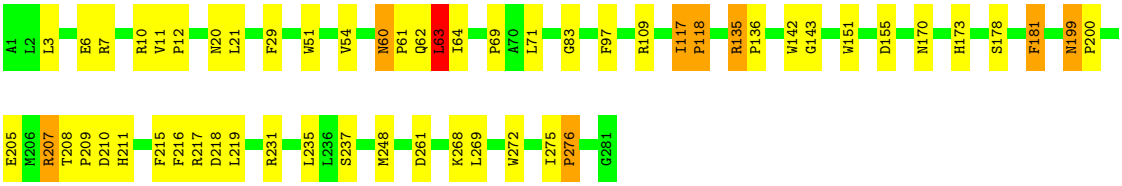
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER H SUBUNIT

Chain H:



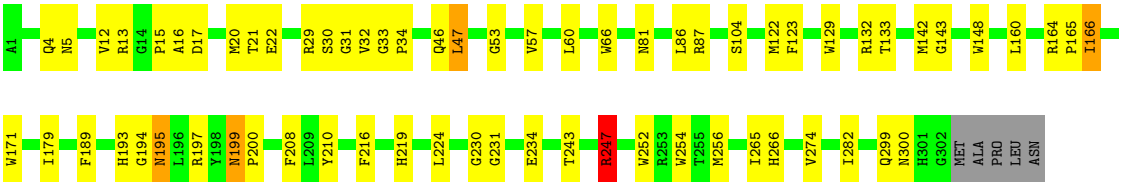
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER L SUBUNIT

Chain L:



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER M SUBUNIT

Chain M:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.20Å 141.20Å 187.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.40 – 2.30	Depositor
% Data completeness (in resolution range)	94.5 (26.40-2.30)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.200	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7334	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

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, U10, BCL, BPH, LDA, SPN, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	H	0.93	0/1877	1.63	19/2553 (0.7%)
2	L	0.97	1/2320 (0.0%)	1.52	23/3175 (0.7%)
3	M	0.88	3/2495 (0.1%)	1.48	21/3404 (0.6%)
All	All	0.93	4/6692 (0.1%)	1.54	63/9132 (0.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	254	TRP	NE1-CE2	-5.23	1.31	1.37
2	L	29	PHE	N-CA	-5.16	1.39	1.46
3	M	252	TRP	NE1-CE2	-5.09	1.31	1.37
3	M	219	HIS	CE1-NE2	-5.00	1.27	1.32

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	70	ARG	CD-NE-CZ	18.28	149.99	124.40
2	L	237	SER	CA-CB-OG	-7.96	95.19	111.10
1	H	98	HIS	CA-CB-CG	-7.27	106.53	113.80
1	H	173	GLU	CB-CG-CD	6.96	124.43	112.60
1	H	96	PHE	CA-CB-CG	-6.92	106.88	113.80
3	M	166	ILE	CB-CA-C	-6.88	103.16	111.97
2	L	6	GLU	N-CA-C	6.79	120.78	112.23
2	L	269	LEU	N-CA-C	-6.70	101.62	109.93
3	M	219	HIS	CA-CB-CG	-6.61	107.19	113.80
2	L	181	PHE	CA-CB-CG	6.49	120.29	113.80
2	L	63	LEU	N-CA-C	-6.47	106.01	114.04
2	L	135	ARG	CD-NE-CZ	6.36	133.30	124.40
3	M	234	GLU	N-CA-C	6.04	117.86	111.28
3	M	208	PHE	CA-CB-CG	-5.98	107.82	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	130	LYS	CB-CG-CD	5.95	124.99	111.30
3	M	231	GLY	N-CA-C	5.92	120.05	112.83
2	L	117	ILE	CA-C-N	5.86	125.55	119.05
2	L	117	ILE	C-N-CA	5.86	125.55	119.05
2	L	60	ASN	CA-C-N	5.79	125.47	119.05
2	L	60	ASN	C-N-CA	5.79	125.47	119.05
2	L	118	PRO	N-CA-CB	5.76	109.66	103.33
1	H	20	PHE	CA-CB-CG	-5.75	108.05	113.80
1	H	206	ASN	CA-CB-CG	-5.71	106.89	112.60
3	M	282	ILE	CA-C-N	5.63	126.23	119.98
3	M	282	ILE	C-N-CA	5.63	126.23	119.98
2	L	170	ASN	CA-C-N	5.55	125.38	119.28
2	L	170	ASN	C-N-CA	5.55	125.38	119.28
3	M	247	ARG	NE-CZ-NH2	5.52	124.17	119.20
3	M	46	GLN	N-CA-C	5.49	118.19	109.96
1	H	124	ASP	CA-CB-CG	5.38	117.98	112.60
2	L	276	PRO	N-CA-CB	5.35	108.01	103.35
1	H	167	ILE	CA-C-O	-5.35	114.69	120.36
2	L	173	HIS	CA-CB-CG	5.35	119.15	113.80
3	M	160	LEU	N-CA-C	5.33	117.08	111.28
2	L	199	ASN	OD1-CG-ND2	-5.31	117.29	122.60
3	M	123	PHE	CA-CB-CG	5.31	119.11	113.80
3	M	15	PRO	N-CA-CB	5.28	107.76	103.32
1	H	44	ASN	CA-C-O	-5.28	115.87	121.94
2	L	20	ASN	CA-C-N	5.25	127.64	120.54
2	L	20	ASN	C-N-CA	5.25	127.64	120.54
1	H	117	ARG	NE-CZ-NH2	5.24	123.91	119.20
3	M	81	ASN	CA-C-N	5.23	124.86	119.05
3	M	81	ASN	C-N-CA	5.23	124.86	119.05
3	M	31	GLY	N-CA-C	-5.23	103.56	112.51
1	H	216	ILE	CA-C-N	5.23	125.23	119.90
1	H	216	ILE	C-N-CA	5.23	125.23	119.90
2	L	29	PHE	N-CA-C	5.22	118.07	109.76
2	L	10	ARG	NE-CZ-NH2	5.21	123.89	119.20
3	M	230	GLY	CA-C-N	5.21	125.86	120.03
3	M	230	GLY	C-N-CA	5.21	125.86	120.03
1	H	206	ASN	OD1-CG-ND2	5.20	127.80	122.60
2	L	3	LEU	N-CA-C	-5.18	103.20	110.50
1	H	154	ARG	NE-CZ-NH2	5.18	123.86	119.20
3	M	132	ARG	NE-CZ-NH2	5.12	123.80	119.20
3	M	266	HIS	CA-CB-CG	-5.11	108.69	113.80
2	L	83	GLY	N-CA-C	5.10	121.78	114.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	70	ARG	CG-CD-NE	5.08	123.17	112.00
1	H	171	ILE	CA-C-N	5.06	125.09	119.32
1	H	171	ILE	C-N-CA	5.06	125.09	119.32
3	M	143	GLY	N-CA-C	-5.04	106.09	112.54
1	H	250	SER	CA-C-O	-5.03	112.25	120.80
3	M	4	GLN	N-CA-C	5.02	119.40	113.28
2	L	109	ARG	NE-CZ-NH2	5.01	123.71	119.20

There are no chirality outliers.

There are no planarity outliers.

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	H	1829	0	1836	18	0
2	L	2232	0	2187	38	0
3	M	2405	0	2324	47	0
4	H	32	0	62	0	0
4	M	80	0	155	11	0
5	L	132	0	148	5	0
5	M	132	0	148	12	0
6	L	65	0	75	6	0
6	M	65	0	76	10	0
7	L	48	0	63	8	0
7	M	48	0	63	3	0
8	M	1	0	0	0	0
9	M	43	0	69	2	0
10	M	10	0	0	3	0
11	H	95	0	0	1	0
11	L	49	0	0	8	0
11	M	68	0	0	1	0
All	All	7334	0	7206	125	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 9.

All (125) 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)
2:L:215:PHE:HB2	3:M:142:MET:HE1	1.38	1.06
3:M:243:THR:O	3:M:247:ARG:HG2	1.58	1.02
5:M:1303:BCL:H191	4:M:1706:LDA:H121	1.47	0.97
6:L:1402:BPH:HHC	6:L:1402:BPH:HBB3	1.51	0.93
4:M:1701:LDA:H91	4:M:1702:LDA:H121	1.54	0.88
7:L:1502:U10:H4M1	11:L:3004:HOH:O	1.75	0.85
1:H:171:ILE:HB	1:H:172:PRO:HD3	1.59	0.83
5:M:1303:BCL:C19	4:M:1706:LDA:H121	2.14	0.77
3:M:243:THR:OG1	3:M:247:ARG:HD3	1.85	0.76
2:L:215:PHE:CB	3:M:142:MET:HE1	2.14	0.76
2:L:261:ASP:OD2	11:L:2047:HOH:O	2.05	0.73
2:L:231:ARG:HD3	3:M:5:ASN:O	1.89	0.72
3:M:199:ASN:HD22	3:M:199:ASN:C	1.98	0.71
3:M:189:PHE:O	3:M:193:HIS:HD2	1.73	0.71
1:H:197:LYS:HE2	1:H:199:GLN:HE21	1.55	0.70
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.72	0.70
4:M:1701:LDA:H91	4:M:1702:LDA:C12	2.21	0.70
3:M:148:TRP:CD1	4:M:1703:LDA:HM22	2.27	0.70
2:L:217:ARG:NH1	11:L:2037:HOH:O	2.24	0.70
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.28	0.68
7:L:1502:U10:H3M3	11:L:2041:HOH:O	1.96	0.66
6:L:1402:BPH:HBB3	6:L:1402:BPH:CHC	2.26	0.65
6:M:1401:BPH:HHC	6:M:1401:BPH:HBB3	1.80	0.64
5:M:1301:BCL:H141	9:M:1600:SPN:H101	1.79	0.64
1:H:146:LYS:NZ	1:H:200:SER:O	2.31	0.63
6:L:1402:BPH:HBB2	3:M:210:TYR:HB3	1.81	0.62
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.81	0.62
3:M:243:THR:O	3:M:247:ARG:CG	2.43	0.61
2:L:208:THR:HB	2:L:209:PRO:HD2	1.81	0.61
2:L:215:PHE:HB2	3:M:142:MET:CE	2.25	0.60
3:M:60:LEU:HA	6:M:1401:BPH:H4C2	1.84	0.60
4:M:1703:LDA:CM2	10:M:1801:PO4:O3	2.50	0.59
3:M:148:TRP:HD1	4:M:1703:LDA:HM22	1.65	0.59
2:L:71:LEU:HD23	2:L:143:GLY:HA3	1.85	0.58
5:L:1302:BCL:CBB	5:L:1302:BCL:HMB3	2.35	0.57
2:L:60:ASN:O	2:L:64:ILE:HG13	2.05	0.56
7:L:1502:U10:H3M1	11:L:2036:HOH:O	2.05	0.56
5:L:1302:BCL:HMB3	5:L:1302:BCL:HBB2	1.89	0.55
6:L:1402:BPH:HHC	6:L:1402:BPH:CBB	2.32	0.54
2:L:218:ASP:OD1	3:M:29:ARG:HD3	2.07	0.54
2:L:231:ARG:HG2	3:M:224:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:265:ILE:HG21	7:M:1501:U10:H3M2	1.90	0.54
1:H:118:ARG:HD2	11:H:2055:HOH:O	2.08	0.53
3:M:189:PHE:O	3:M:193:HIS:CD2	2.59	0.53
4:M:1703:LDA:HM11	10:M:1800:PO4:O4	2.10	0.52
2:L:60:ASN:OD1	2:L:61:PRO:HD2	2.10	0.52
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.91	0.52
3:M:32:VAL:HG12	3:M:33:GLY:O	2.09	0.52
2:L:181:PHE:CD2	6:M:1401:BPH:HBB1	2.45	0.52
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.46	0.51
2:L:215:PHE:CG	3:M:142:MET:HE1	2.46	0.50
2:L:207:ARG:HD2	2:L:207:ARG:N	2.26	0.50
3:M:194:GLY:O	3:M:195:ASN:HB3	2.10	0.50
5:M:1301:BCL:H102	5:M:1303:BCL:H202	1.93	0.50
7:L:1502:U10:C3M	11:L:2041:HOH:O	2.56	0.50
6:M:1401:BPH:HHD	6:M:1401:BPH:HBC3	1.93	0.50
7:L:1502:U10:H202	5:M:1301:BCL:H43	1.94	0.49
2:L:135:ARG:HD2	2:L:248:MET:O	2.12	0.49
1:H:173:GLU:HG2	11:L:2042:HOH:O	2.11	0.49
1:H:169:VAL:HG23	1:H:171:ILE:HD13	1.93	0.49
3:M:66:TRP:CZ2	3:M:122:MET:HE3	2.47	0.49
1:H:171:ILE:HB	1:H:172:PRO:CD	2.37	0.49
5:L:1304:BCL:OBB	5:L:1304:BCL:HHC	2.13	0.49
2:L:219:LEU:HD11	3:M:133:THR:HG22	1.95	0.49
3:M:129:TRP:CH2	4:M:1706:LDA:H102	2.49	0.48
5:M:1301:BCL:C3B	9:M:1600:SPN:H152	2.43	0.48
2:L:272:TRP:NE1	3:M:87:ARG:HG3	2.29	0.48
2:L:181:PHE:HB3	6:M:1401:BPH:CBB	2.44	0.47
1:H:111:PRO:O	3:M:247:ARG:NH2	2.44	0.47
7:L:1502:U10:H322	7:L:1502:U10:H301	1.41	0.47
2:L:200:PRO:HB3	2:L:207:ARG:HD3	1.97	0.47
2:L:178:SER:HB3	7:L:1502:U10:H222	1.97	0.47
1:H:62:LYS:NZ	2:L:199:ASN:HD21	2.14	0.46
3:M:129:TRP:O	3:M:133:THR:HG23	2.16	0.46
6:L:1402:BPH:CHC	6:L:1402:BPH:CBB	2.91	0.46
1:H:140:PHE:HA	3:M:13:ARG:O	2.16	0.46
3:M:21:THR:O	3:M:22:GLU:C	2.57	0.46
6:M:1401:BPH:HBB3	6:M:1401:BPH:CHC	2.45	0.46
3:M:166:ILE:HD11	3:M:171:TRP:CH2	2.51	0.45
2:L:117:ILE:HB	2:L:118:PRO:HD3	1.98	0.45
6:M:1401:BPH:H192	6:M:1401:BPH:H161	1.61	0.45
5:M:1301:BCL:H152	5:M:1301:BCL:H111	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:1706:LDA:H123	4:M:1706:LDA:H92	1.52	0.45
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.65	0.45
2:L:97:PHE:CE1	5:L:1302:BCL:H121	2.51	0.45
1:H:61:PRO:HA	1:H:76:PRO:HD2	2.00	0.44
5:M:1301:BCL:CBB	5:M:1301:BCL:HMB1	2.48	0.44
1:H:81:GLU:HG3	1:H:85:ILE:HD11	1.99	0.44
2:L:62:GLN:HB2	2:L:151:TRP:CD1	2.52	0.44
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.53	0.44
3:M:256:MET:CE	7:M:1501:U10:H102	2.47	0.44
2:L:211:HIS:CE1	3:M:20:MET:HE2	2.52	0.43
3:M:247:ARG:HG2	3:M:247:ARG:H	1.54	0.43
1:H:122:GLU:HB2	1:H:227:LEU:HD21	2.01	0.43
3:M:265:ILE:HD12	3:M:265:ILE:HA	1.85	0.43
3:M:300:ASN:N	3:M:300:ASN:OD1	2.50	0.43
1:H:130:LYS:HE3	1:H:170:ASP:OD1	2.19	0.43
6:L:1402:BPH:HBA2	6:L:1402:BPH:H3A	1.85	0.43
6:M:1401:BPH:HHD	6:M:1401:BPH:CBC	2.49	0.43
3:M:34:PRO:O	3:M:47:LEU:HB2	2.18	0.43
1:H:75:VAL:HA	1:H:76:PRO:C	2.43	0.43
7:L:1502:U10:H272	7:L:1502:U10:H251	1.43	0.42
5:L:1302:BCL:CBB	5:L:1302:BCL:CMB	2.97	0.42
3:M:199:ASN:HD22	3:M:200:PRO:N	2.15	0.42
2:L:155:ASP:OD1	3:M:197:ARG:NH1	2.37	0.42
2:L:51:TRP:O	2:L:54:VAL:HG22	2.20	0.42
3:M:53:GLY:O	3:M:57:VAL:HG23	2.20	0.42
7:M:1501:U10:H28	7:M:1501:U10:H322	1.73	0.41
2:L:205:GLU:OE2	11:L:2032:HOH:O	2.21	0.41
5:M:1301:BCL:H141	5:M:1301:BCL:H162	1.84	0.41
2:L:275:ILE:HA	2:L:276:PRO:HD3	1.91	0.41
4:M:1703:LDA:HM23	10:M:1801:PO4:P	2.61	0.41
3:M:17:ASP:OD2	11:M:2016:HOH:O	2.22	0.41
3:M:179:ILE:HG23	5:M:1301:BCL:HED1	2.01	0.41
3:M:16:ALA:HB1	3:M:32:VAL:HG21	2.03	0.41
3:M:164:ARG:N	3:M:165:PRO:HD2	2.35	0.41
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.38	0.41
2:L:11:VAL:HB	2:L:12:PRO:HD2	2.02	0.41
2:L:181:PHE:HB3	6:M:1401:BPH:HBB2	2.03	0.41
6:M:1401:BPH:HBC3	6:M:1401:BPH:CHD	2.50	0.41
5:M:1301:BCL:H101	5:M:1301:BCL:H61	1.68	0.41
2:L:63:LEU:HD12	2:L:63:LEU:HA	1.88	0.40
1:H:99:ALA:HA	1:H:100:PRO:HD3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:194:GLY:O	3:M:195:ASN:CB	2.69	0.40
5:M:1301:BCL:H3A	5:M:1301:BCL:HBA1	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	238/260 (92%)	233 (98%)	5 (2%)	0	100	100
2	L	279/281 (99%)	271 (97%)	8 (3%)	0	100	100
3	M	300/307 (98%)	290 (97%)	8 (3%)	2 (1%)	18	23
All	All	817/848 (96%)	794 (97%)	21 (3%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	30	SER
3	M	195	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/208 (94%)	190 (97%)	5 (3%)	40	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	220/220 (100%)	213 (97%)	7 (3%)	34	51
3	M	236/240 (98%)	227 (96%)	9 (4%)	29	44
All	All	651/668 (98%)	630 (97%)	21 (3%)	34	51

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	70	ARG
1	H	106	LYS
1	H	193	MET
1	H	221	SER
1	H	231	ASP
2	L	21	LEU
2	L	63	LEU
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	235	LEU
2	L	268	LYS
3	M	12	VAL
3	M	47	LEU
3	M	86	LEU
3	M	104	SER
3	M	199	ASN
3	M	216	PHE
3	M	247	ARG
3	M	274	VAL
3	M	299	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
1	H	206	ASN
2	L	183	ASN
2	L	199	ASN
2	L	280	ASN
3	M	28	ASN
3	M	187	ASN
3	M	193	HIS

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Mol	Chain	Res	Type
3	M	199	ASN
3	M	299	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\#\|Z\| > 2$
5	BCL	M	1301	3	69,74,74	1.47	9 (13%)	83,115,115	2.20	22 (26%)
4	LDA	M	1705	-	12,15,15	2.24	1 (8%)	14,17,17	0.70	0
5	BCL	M	1303	3	69,74,74	1.44	10 (14%)	83,115,115	2.32	19 (22%)
7	U10	L	1502	-	48,48,63	2.05	16 (33%)	58,61,79	1.67	10 (17%)
4	LDA	M	1701	-	12,15,15	2.26	1 (8%)	14,17,17	0.64	0
6	BPH	M	1401	-	59,70,70	1.99	14 (23%)	61,101,101	2.78	19 (31%)
4	LDA	H	1707	-	12,15,15	2.27	1 (8%)	14,17,17	0.75	0
9	SPN	M	1600	-	40,42,42	3.80	17 (42%)	50,52,52	2.40	19 (38%)
5	BCL	L	1304	2	69,74,74	1.47	10 (14%)	83,115,115	2.33	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	PO4	M	1801	-	4,4,4	2.21	1 (25%)	6,6,6	1.29	0
10	PO4	M	1800	-	4,4,4	3.26	2 (50%)	6,6,6	1.88	2 (33%)
7	U10	M	1501	-	48,48,63	1.89	15 (31%)	58,61,79	1.53	10 (17%)
4	LDA	M	1703	-	12,15,15	2.27	1 (8%)	14,17,17	0.67	0
6	BPH	L	1402	-	59,70,70	2.13	14 (23%)	61,101,101	2.58	19 (31%)
5	BCL	L	1302	2	69,74,74	1.46	9 (13%)	83,115,115	2.38	23 (27%)
4	LDA	M	1706	-	12,15,15	2.46	1 (8%)	14,17,17	0.86	0
4	LDA	M	1702	-	12,15,15	2.50	1 (8%)	14,17,17	0.64	0
4	LDA	H	1704	-	12,15,15	2.25	1 (8%)	14,17,17	0.43	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
5	BCL	M	1301	3	1/1/21/25	14/41/137/137	-
4	LDA	M	1705	-	-	7/13/13/13	-
5	BCL	M	1303	3	-	5/41/137/137	-
7	U10	L	1502	-	-	18/45/69/87	0/1/1/1
4	LDA	M	1701	-	-	2/13/13/13	-
6	BPH	M	1401	-	1/1/18/22	15/37/105/105	0/5/6/6
4	LDA	H	1707	-	-	4/13/13/13	-
9	SPN	M	1600	-	-	21/50/51/51	-
5	BCL	L	1304	2	1/1/21/25	6/41/137/137	-
7	U10	M	1501	-	-	8/45/69/87	0/1/1/1
4	LDA	M	1703	-	-	7/13/13/13	-
6	BPH	L	1402	-	-	5/37/105/105	0/5/6/6
5	BCL	L	1302	2	-	1/41/137/137	-
4	LDA	M	1706	-	-	9/13/13/13	-
4	LDA	M	1702	-	-	6/13/13/13	-
4	LDA	H	1704	-	-	8/13/13/13	-

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1600	SPN	C8-C9	9.65	1.56	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1600	SPN	C4-C5	8.95	1.54	1.33
4	M	1702	LDA	O1-N1	-8.62	1.22	1.42
9	M	1600	SPN	C12-C13	8.45	1.53	1.33
4	M	1706	LDA	O1-N1	-8.42	1.22	1.42
9	M	1600	SPN	C19-C18	8.03	1.52	1.33
4	M	1703	LDA	O1-N1	-7.82	1.23	1.42
4	H	1707	LDA	O1-N1	-7.81	1.23	1.42
4	M	1701	LDA	O1-N1	-7.79	1.23	1.42
4	H	1704	LDA	O1-N1	-7.75	1.24	1.42
4	M	1705	LDA	O1-N1	-7.69	1.24	1.42
6	M	1401	BPH	C2C-C3C	-7.57	1.47	1.54
6	L	1402	BPH	C2C-C3C	-7.22	1.48	1.54
9	M	1600	SPN	C3-C4	-6.21	1.41	1.50
9	M	1600	SPN	C10-C9	-6.18	1.38	1.51
7	L	1502	U10	C7-C8	-6.13	1.41	1.50
10	M	1800	PO4	P-O1	6.06	1.65	1.50
6	L	1402	BPH	C3A-C2A	-5.95	1.49	1.54
5	L	1302	BCL	MG-NA	5.95	2.20	2.06
6	M	1401	BPH	C1D-C2D	5.70	1.45	1.39
9	M	1600	SPN	C14-C13	-5.55	1.39	1.51
6	L	1402	BPH	O2D-CGD	5.50	1.46	1.33
9	M	1600	SPN	C6-C5	-5.38	1.40	1.51
5	M	1303	BCL	O2D-CGD	5.37	1.46	1.33
5	M	1303	BCL	MG-NA	5.36	2.19	2.06
5	L	1304	BCL	O2D-CGD	5.27	1.46	1.33
9	M	1600	SPN	C17-C18	-5.19	1.40	1.51
5	M	1301	BCL	O2D-CGD	5.17	1.45	1.33
5	L	1302	BCL	O2D-CGD	4.97	1.45	1.33
7	M	1501	U10	O3-C3	4.66	1.48	1.36
6	M	1401	BPH	C1B-C2B	4.57	1.44	1.39
5	M	1301	BCL	MG-NA	4.43	2.16	2.06
6	L	1402	BPH	C1D-C2D	4.35	1.44	1.39
6	L	1402	BPH	C1B-C2B	4.34	1.44	1.39
10	M	1801	PO4	P-O1	4.26	1.60	1.50
6	M	1401	BPH	O2D-CGD	4.09	1.43	1.33
7	M	1501	U10	C33-C34	4.07	1.42	1.33
5	L	1304	BCL	MG-NA	4.01	2.15	2.06
7	L	1502	U10	O3-C3	3.77	1.46	1.36
7	L	1502	U10	O4-C4M	-3.72	1.36	1.45
7	M	1501	U10	C23-C24	3.69	1.41	1.33
9	M	1600	SPN	C25-C26	3.67	1.41	1.33
7	L	1502	U10	O4-C4	3.66	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1301	BCL	O2A-CGA	3.65	1.44	1.33
6	L	1402	BPH	O2A-CGA	3.53	1.43	1.33
5	L	1304	BCL	C2-C3	3.52	1.41	1.33
9	M	1600	SPN	O1-CMA	3.51	1.54	1.43
5	M	1301	BCL	CMA-C3A	3.48	1.60	1.53
5	M	1301	BCL	CAA-C2A	3.41	1.60	1.54
7	M	1501	U10	C7-C8	-3.39	1.45	1.50
6	L	1402	BPH	CBD-CGD	-3.36	1.47	1.52
6	L	1402	BPH	CMA-C3A	3.32	1.59	1.53
7	M	1501	U10	O4-C4	3.31	1.45	1.36
6	L	1402	BPH	O2D-CED	-3.30	1.37	1.45
7	L	1502	U10	C8-C9	3.30	1.40	1.33
6	L	1402	BPH	CHA-CBD	3.28	1.55	1.51
6	M	1401	BPH	O2D-CED	-3.22	1.37	1.45
6	M	1401	BPH	O2A-CGA	3.16	1.42	1.33
7	M	1501	U10	O3-C3M	-3.14	1.37	1.45
7	L	1502	U10	C18-C19	3.13	1.40	1.33
7	L	1502	U10	C28-C29	3.11	1.40	1.33
9	M	1600	SPN	C29-C30	3.04	1.41	1.32
5	L	1304	BCL	C3B-C4B	3.03	1.46	1.41
9	M	1600	SPN	C20-C19	-2.99	1.40	1.50
5	M	1301	BCL	C2-C3	2.98	1.40	1.33
9	M	1600	SPN	C11-C12	-2.97	1.40	1.50
9	M	1600	SPN	C7-C8	-2.96	1.40	1.50
5	L	1302	BCL	C2-C3	2.95	1.40	1.33
5	M	1303	BCL	O2A-CGA	2.91	1.41	1.33
7	M	1501	U10	C13-C14	2.83	1.39	1.33
7	L	1502	U10	C38-C39	2.80	1.40	1.32
7	M	1501	U10	C38-C39	2.78	1.40	1.32
6	M	1401	BPH	CBD-CGD	-2.76	1.48	1.52
7	L	1502	U10	C33-C34	2.75	1.39	1.33
7	M	1501	U10	C31-C29	2.75	1.57	1.51
5	M	1303	BCL	C2-C3	2.75	1.39	1.33
5	M	1301	BCL	C2C-C3C	-2.73	1.46	1.54
7	M	1501	U10	C8-C9	2.72	1.39	1.33
6	M	1401	BPH	CHA-CBD	2.71	1.54	1.51
7	L	1502	U10	O3-C3M	-2.65	1.39	1.45
5	L	1304	BCL	CAA-C2A	2.64	1.59	1.54
5	M	1303	BCL	O2D-CED	-2.61	1.39	1.45
9	M	1600	SPN	C21-C22	-2.60	1.38	1.52
6	L	1402	BPH	C2-C3	2.59	1.39	1.33
5	M	1303	BCL	C2C-C3C	-2.50	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1302	BCL	CBB-CAB	2.48	1.55	1.50
6	M	1401	BPH	CMA-C3A	2.48	1.58	1.53
6	L	1402	BPH	C3B-C2B	-2.48	1.35	1.39
5	M	1301	BCL	C3B-C4B	2.47	1.45	1.41
5	L	1304	BCL	C3B-C2B	-2.43	1.34	1.42
5	L	1302	BCL	C2C-C3C	-2.40	1.47	1.54
5	M	1303	BCL	MG-NC	2.39	2.11	2.06
6	L	1402	BPH	CAC-C3C	-2.38	1.48	1.53
5	L	1302	BCL	MG-ND	-2.38	2.01	2.05
7	M	1501	U10	C18-C19	2.36	1.38	1.33
5	L	1302	BCL	O2A-CGA	2.36	1.40	1.33
10	M	1800	PO4	P-O3	-2.33	1.47	1.54
5	L	1304	BCL	O2A-CGA	2.32	1.40	1.33
9	M	1600	SPN	C16-C15	-2.30	1.38	1.51
7	L	1502	U10	C13-C14	2.29	1.38	1.33
5	M	1303	BCL	C4-C3	2.28	1.56	1.50
5	M	1303	BCL	C3B-C4B	2.27	1.45	1.41
7	M	1501	U10	C20-C19	2.25	1.56	1.50
6	M	1401	BPH	C3D-C4D	2.23	1.44	1.41
5	L	1304	BCL	O1D-CGD	2.23	1.26	1.21
7	L	1502	U10	C36-C34	2.20	1.55	1.51
7	L	1502	U10	C25-C24	2.20	1.56	1.50
6	M	1401	BPH	C4D-ND	-2.17	1.35	1.38
6	M	1401	BPH	O1D-CGD	2.17	1.26	1.21
7	M	1501	U10	O4-C4M	-2.17	1.40	1.45
5	L	1304	BCL	CAC-C3C	2.13	1.58	1.54
6	L	1402	BPH	CAA-C2A	2.12	1.58	1.54
5	L	1302	BCL	O2D-CED	-2.11	1.40	1.45
7	L	1502	U10	C16-C14	2.10	1.55	1.51
7	L	1502	U10	C23-C24	2.10	1.38	1.33
7	M	1501	U10	C7-C6	2.10	1.54	1.51
6	M	1401	BPH	C2-C3	2.09	1.38	1.33
5	L	1302	BCL	C4-C3	2.09	1.56	1.50
5	M	1303	BCL	O1D-CGD	2.08	1.26	1.21
7	L	1502	U10	C15-C14	2.06	1.56	1.50
6	M	1401	BPH	CMC-C2C	-2.06	1.49	1.53
7	M	1501	U10	C35-C34	2.01	1.55	1.50
5	M	1301	BCL	CMB-C2B	2.00	1.55	1.50
5	L	1304	BCL	MG-ND	-2.00	2.01	2.05

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	1401	BPH	O2D-CGD-CBD	15.11	130.15	111.00
6	L	1402	BPH	O2D-CGD-CBD	12.34	126.63	111.00
5	L	1302	BCL	C4A-NA-C1A	10.95	111.63	106.71
5	M	1303	BCL	C1C-NC-C4C	10.45	111.40	106.71
5	L	1302	BCL	C1C-NC-C4C	9.09	110.79	106.71
5	M	1303	BCL	C4A-NA-C1A	8.79	110.66	106.71
5	L	1304	BCL	O2D-CGD-CBD	8.31	126.04	111.27
5	M	1301	BCL	C1C-NC-C4C	7.85	110.23	106.71
5	M	1301	BCL	C4A-NA-C1A	7.77	110.20	106.71
5	L	1304	BCL	C4A-NA-C1A	7.11	109.90	106.71
5	L	1304	BCL	C1C-NC-C4C	6.56	109.65	106.71
5	M	1301	BCL	O2D-CGD-CBD	6.30	122.46	111.27
6	M	1401	BPH	O1D-CGD-CBD	-6.23	114.37	124.74
7	M	1501	U10	C27-C28-C29	5.98	142.07	127.66
7	L	1502	U10	C4M-O4-C4	5.85	137.21	116.47
5	M	1303	BCL	O2D-CGD-CBD	5.80	121.58	111.27
6	L	1402	BPH	O2D-CGD-O1D	-5.68	112.73	123.84
5	L	1304	BCL	C1-O2A-CGA	5.65	131.27	116.44
5	M	1301	BCL	O2A-CGA-CBA	5.45	129.02	111.91
5	M	1303	BCL	CAC-C3C-C4C	-5.43	100.52	112.58
5	L	1302	BCL	O2D-CGD-CBD	5.34	120.75	111.27
9	M	1600	SPN	C10-C9-C8	-5.30	110.39	121.12
5	L	1304	BCL	CAB-C3B-C2B	5.11	136.00	128.34
6	L	1402	BPH	CMA-C3A-C4A	-5.06	103.30	114.38
9	M	1600	SPN	C7-C8-C9	-5.05	115.50	127.66
6	M	1401	BPH	C4D-CHA-CBD	-4.97	106.27	108.52
9	M	1600	SPN	C3-C4-C5	-4.82	118.78	126.79
9	M	1600	SPN	C6-C5-C4	-4.74	111.52	121.12
9	M	1600	SPN	CM5-C13-C14	4.73	123.22	115.27
6	M	1401	BPH	O2D-CGD-O1D	-4.70	114.65	123.84
5	L	1304	BCL	CHB-C1B-NB	4.66	129.19	124.26
6	L	1402	BPH	CBC-CAC-C3C	4.61	123.05	113.77
5	L	1304	BCL	O1D-CGD-CBD	-4.57	115.13	124.48
7	L	1502	U10	C7-C8-C9	4.33	134.00	126.79
5	L	1302	BCL	CAC-C3C-C4C	-4.32	103.00	112.58
6	M	1401	BPH	C4C-C3C-C2C	4.32	106.94	102.84
9	M	1600	SPN	CM4-C9-C10	4.25	122.43	115.27
5	M	1301	BCL	O2D-CGD-O1D	-4.16	115.70	123.84
7	M	1501	U10	C4M-O4-C4	4.13	131.09	116.47
5	M	1301	BCL	O2A-CGA-O1A	-4.07	113.31	123.59
5	M	1303	BCL	O2A-CGA-CBA	4.02	124.51	111.91
6	L	1402	BPH	O2A-CGA-O1A	-4.00	113.49	123.59
9	M	1600	SPN	C17-C18-C19	-3.97	113.08	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	1304	BCL	CAC-C3C-C4C	-3.90	103.92	112.58
6	L	1402	BPH	O2A-CGA-CBA	3.88	124.09	111.91
5	L	1302	BCL	OBB-CAB-C3B	3.83	127.49	120.41
5	L	1302	BCL	O2A-CGA-CBA	3.80	123.84	111.91
5	M	1301	BCL	CHB-C1B-NB	3.73	128.21	124.26
6	M	1401	BPH	CMA-C3A-C4A	-3.72	106.22	114.38
6	M	1401	BPH	CED-O2D-CGD	3.72	124.36	115.94
9	M	1600	SPN	CM7-C22-C21	3.69	124.65	111.29
5	M	1301	BCL	OBB-CAB-C3B	3.66	127.18	120.41
5	M	1301	BCL	CAA-C2A-C3A	-3.64	102.81	112.78
7	L	1502	U10	C12-C13-C14	3.60	136.34	127.66
6	L	1402	BPH	OBD-CAD-CBD	-3.57	120.58	125.82
9	M	1600	SPN	CM3-C5-C6	3.54	121.22	115.27
5	M	1303	BCL	CHD-C1D-ND	-3.53	121.21	124.45
6	L	1402	BPH	C4D-CHA-CBD	-3.53	106.92	108.52
9	M	1600	SPN	C14-C13-C12	-3.47	114.10	121.12
9	M	1600	SPN	CM6-C18-C17	3.44	121.06	115.27
5	M	1303	BCL	CHB-C1B-NB	3.44	127.90	124.26
7	L	1502	U10	C32-C33-C34	3.41	135.87	127.66
10	M	1800	PO4	O2-P-O1	-3.40	98.47	110.89
5	M	1303	BCL	CMD-C2D-C1D	3.38	130.68	124.71
5	M	1303	BCL	O2D-CGD-O1D	-3.36	117.27	123.84
6	M	1401	BPH	C1C-C2C-C3C	3.33	106.01	102.84
5	L	1304	BCL	C4D-CHA-C1A	3.33	125.30	121.25
9	M	1600	SPN	C20-C19-C18	-3.32	119.66	127.66
5	L	1302	BCL	C1-O2A-CGA	3.32	125.15	116.44
7	L	1502	U10	C8-C7-C6	3.32	120.99	112.05
5	L	1304	BCL	CAA-C2A-C3A	-3.31	103.72	112.78
5	L	1304	BCL	CAC-C3C-C2C	-3.30	106.01	114.26
5	L	1302	BCL	CAA-C2A-C3A	-3.25	103.88	112.78
6	L	1402	BPH	C4C-C3C-C2C	3.24	105.92	102.84
5	L	1304	BCL	O2D-CGD-O1D	-3.21	117.56	123.84
7	L	1502	U10	C22-C23-C24	3.18	135.31	127.66
5	L	1302	BCL	O2A-C1-C2	-3.16	100.32	108.64
9	M	1600	SPN	C11-C12-C13	-3.15	120.06	127.66
6	L	1402	BPH	C4A-C3A-C2A	3.15	105.83	102.84
6	L	1402	BPH	O1D-CGD-CBD	-3.15	119.50	124.74
5	L	1302	BCL	O2D-CGD-O1D	-3.13	117.72	123.84
5	L	1302	BCL	C2C-C3C-C4C	3.13	106.03	101.34
6	L	1402	BPH	C1-C2-C3	3.13	131.45	126.04
6	L	1402	BPH	CAC-C3C-C2C	3.12	122.04	114.26
5	M	1303	BCL	CAB-C3B-C2B	3.10	132.98	128.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	1501	U10	C22-C23-C24	-3.06	120.30	127.66
5	M	1301	BCL	CMA-C3A-C2A	-2.98	101.79	113.83
5	M	1303	BCL	O1D-CGD-CBD	-2.97	118.41	124.48
5	M	1301	BCL	C2C-C3C-C4C	2.96	105.77	101.34
5	L	1302	BCL	C1D-ND-C4D	-2.95	104.24	106.33
5	L	1302	BCL	OBB-CAB-CBB	-2.94	113.22	119.73
7	L	1502	U10	C25-C24-C26	-2.83	110.50	115.27
7	L	1502	U10	C35-C34-C36	-2.83	110.51	115.27
7	L	1502	U10	C3M-O3-C3	2.83	126.50	116.47
6	L	1402	BPH	C1C-C2C-C3C	2.83	105.53	102.84
5	L	1302	BCL	O2A-CGA-O1A	-2.82	116.46	123.59
5	L	1304	BCL	C2C-C3C-C4C	2.81	105.55	101.34
9	M	1600	SPN	C16-C15-C14	2.81	123.29	113.19
9	M	1600	SPN	C11-C10-C9	2.80	122.17	112.98
6	M	1401	BPH	CMC-C2C-C1C	2.79	120.47	114.38
5	M	1301	BCL	C3C-C2C-C1C	2.77	106.34	101.87
5	M	1301	BCL	CAC-C3C-C4C	-2.76	106.46	112.58
5	M	1301	BCL	CMB-C2B-C1B	-2.76	121.17	125.37
5	M	1303	BCL	C3C-C2C-C1C	2.71	106.25	101.87
5	L	1302	BCL	CHB-C1B-NB	2.70	127.12	124.26
6	M	1401	BPH	OBD-CAD-CBD	-2.68	121.89	125.82
5	M	1303	BCL	CHD-C4C-NC	2.65	128.02	125.08
6	L	1402	BPH	C1B-NB-C4B	-2.63	104.75	108.83
5	L	1302	BCL	CAC-C3C-C2C	-2.56	107.86	114.26
5	M	1303	BCL	C3A-C2A-C1A	2.54	105.15	101.34
5	L	1304	BCL	O2A-CGA-CBA	2.53	119.86	111.91
5	L	1302	BCL	CHD-C1D-ND	-2.53	122.13	124.45
7	M	1501	U10	C7-C8-C9	2.52	130.99	126.79
5	L	1304	BCL	C2B-C1B-NB	-2.49	108.56	110.23
6	L	1402	BPH	CMA-C3A-C2A	-2.48	104.00	113.99
5	L	1304	BCL	C2A-C1A-CHA	2.48	128.20	123.86
5	L	1304	BCL	CMB-C2B-C1B	-2.48	121.59	125.37
6	M	1401	BPH	CAA-C2A-C3A	-2.47	106.00	112.78
6	M	1401	BPH	CMA-C3A-C2A	-2.47	104.05	113.99
5	L	1302	BCL	CMA-C3A-C2A	-2.46	103.90	113.83
9	M	1600	SPN	C7-C6-C5	2.45	121.03	112.98
5	L	1302	BCL	CED-O2D-CGD	2.44	121.47	115.94
6	M	1401	BPH	O2A-C1-C2	-2.44	102.21	108.64
7	L	1502	U10	C15-C14-C16	-2.42	111.20	115.27
7	M	1501	U10	C3M-O3-C3	2.41	125.02	116.47
5	M	1301	BCL	C2D-C1D-ND	2.40	111.87	110.10
6	L	1402	BPH	C4-C3-C5	-2.40	111.23	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1301	BCL	C1D-ND-C4D	-2.40	104.63	106.33
5	L	1302	BCL	C2D-C1D-ND	2.38	111.86	110.10
5	M	1303	BCL	O2A-CGA-O1A	-2.36	117.64	123.59
5	M	1301	BCL	CHD-C4C-NC	2.36	127.70	125.08
7	M	1501	U10	C15-C14-C16	-2.33	111.35	115.27
7	M	1501	U10	C30-C29-C28	2.33	129.65	123.68
5	M	1301	BCL	OBB-CAB-CBB	-2.32	114.59	119.73
5	M	1303	BCL	CHC-C1C-NC	2.30	127.70	124.51
6	M	1401	BPH	C1-C2-C3	2.29	130.01	126.04
7	M	1501	U10	C30-C29-C31	-2.28	111.43	115.27
9	M	1600	SPN	C15-C14-C13	2.27	119.42	113.45
6	M	1401	BPH	C1-O2A-CGA	2.27	122.41	116.44
5	L	1302	BCL	C3C-C2C-C1C	2.27	105.53	101.87
5	L	1302	BCL	CHC-C1C-NC	2.26	127.64	124.51
5	L	1304	BCL	C2D-C1D-ND	2.26	111.77	110.10
5	M	1301	BCL	CMA-C3A-C4A	-2.26	105.71	111.77
6	M	1401	BPH	O2A-CGA-CBA	2.26	118.98	111.91
6	M	1401	BPH	O2A-CGA-O1A	-2.23	117.95	123.59
6	L	1402	BPH	CAA-C2A-C3A	-2.23	106.67	112.78
6	M	1401	BPH	C1B-NB-C4B	-2.21	105.40	108.83
6	L	1402	BPH	C4D-ND-C1D	-2.20	106.59	108.83
5	M	1303	BCL	C1D-ND-C4D	-2.17	104.79	106.33
5	L	1304	BCL	OBB-CAB-C3B	2.17	124.41	120.41
5	M	1301	BCL	CED-O2D-CGD	-2.16	111.04	115.94
10	M	1800	PO4	O3-P-O2	2.16	114.90	107.97
5	M	1303	BCL	C7-C6-C5	-2.15	107.51	113.36
6	M	1401	BPH	C4-C3-C5	-2.13	111.69	115.27
5	M	1303	BCL	C2C-C3C-C4C	2.11	104.50	101.34
9	M	1600	SPN	CM4-C9-C8	-2.08	118.34	123.68
5	L	1302	BCL	C1-C2-C3	-2.06	122.48	126.04
5	L	1304	BCL	C3A-C2A-C1A	2.06	104.42	101.34
9	M	1600	SPN	C24-C23-C22	-2.05	108.67	115.76
5	M	1301	BCL	C2B-C1B-NB	-2.03	108.87	110.23
7	M	1501	U10	C32-C33-C34	-2.02	122.80	127.66
7	M	1501	U10	C20-C19-C21	-2.01	111.89	115.27
5	M	1301	BCL	CMB-C2B-C3B	2.01	131.35	125.93

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1304	BCL	C13
5	M	1301	BCL	C13

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Mol	Chain	Res	Type	Atom
6	M	1401	BPH	C8

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1703	LDA	C2-C1-N1-O1
4	M	1703	LDA	C2-C1-N1-CM1
4	M	1705	LDA	N1-C1-C2-C3
4	M	1706	LDA	C2-C1-N1-O1
4	M	1706	LDA	C2-C1-N1-CM1
6	M	1401	BPH	C1-C2-C3-C4
6	M	1401	BPH	C4-C3-C5-C6
7	L	1502	U10	C23-C24-C26-C27
7	L	1502	U10	C25-C24-C26-C27
7	L	1502	U10	C30-C29-C31-C32
9	M	1600	SPN	CM2-C1-C2-O2
9	M	1600	SPN	CM2-C1-C2-C3
9	M	1600	SPN	C3-C4-C5-CM3
9	M	1600	SPN	CM3-C5-C6-C7
9	M	1600	SPN	CM5-C13-C14-C15
9	M	1600	SPN	C16-C17-C18-CM6
7	L	1502	U10	C12-C11-C9-C10
9	M	1600	SPN	C11-C10-C9-CM4
7	L	1502	U10	C28-C29-C31-C32
9	M	1600	SPN	C14-C15-C16-C17
7	L	1502	U10	C20-C19-C21-C22
6	M	1401	BPH	C2-C3-C5-C6
7	L	1502	U10	C18-C19-C21-C22
9	M	1600	SPN	C4-C5-C6-C7
9	M	1600	SPN	C11-C10-C9-C8
9	M	1600	SPN	C12-C13-C14-C15
9	M	1600	SPN	C16-C17-C18-C19
7	L	1502	U10	C29-C31-C32-C33
7	M	1501	U10	C29-C31-C32-C33
9	M	1600	SPN	C9-C10-C11-C12
6	M	1401	BPH	C1-C2-C3-C5
5	M	1301	BCL	C11-C10-C8-C9
9	M	1600	SPN	C20-C21-C22-CM7
5	L	1304	BCL	C13-C15-C16-C17
5	M	1301	BCL	C10-C11-C12-C13
5	M	1301	BCL	C11-C12-C13-C15
6	M	1401	BPH	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
7	L	1502	U10	C3-C4-O4-C4M
5	M	1301	BCL	C13-C15-C16-C17
6	M	1401	BPH	C15-C16-C17-C18
5	M	1301	BCL	C3-C5-C6-C7
7	L	1502	U10	C12-C11-C9-C8
4	M	1703	LDA	C1-C2-C3-C4
4	H	1704	LDA	C5-C6-C7-C8
4	M	1706	LDA	C7-C8-C9-C10
7	M	1501	U10	C30-C29-C31-C32
9	M	1600	SPN	C24-C25-C26-CM8
7	M	1501	U10	C28-C29-C31-C32
4	H	1707	LDA	C2-C3-C4-C5
4	M	1702	LDA	C5-C6-C7-C8
4	H	1707	LDA	C3-C4-C5-C6
4	M	1701	LDA	C3-C4-C5-C6
4	M	1706	LDA	C11-C10-C9-C8
4	M	1706	LDA	C9-C10-C11-C12
7	M	1501	U10	C25-C24-C26-C27
7	M	1501	U10	C23-C24-C26-C27
4	M	1706	LDA	C6-C7-C8-C9
5	M	1301	BCL	C11-C12-C13-C14
6	L	1402	BPH	C14-C13-C15-C16
6	M	1401	BPH	C6-C7-C8-C9
5	M	1301	BCL	C16-C17-C18-C20
4	H	1704	LDA	C3-C4-C5-C6
6	L	1402	BPH	C8-C10-C11-C12
7	L	1502	U10	C5-C6-C7-C8
4	H	1704	LDA	C1-C2-C3-C4
4	M	1706	LDA	C4-C5-C6-C7
4	M	1706	LDA	C1-C2-C3-C4
4	M	1705	LDA	C2-C3-C4-C5
6	L	1402	BPH	C4-C3-C5-C6
5	M	1301	BCL	C6-C7-C8-C10
6	M	1401	BPH	C12-C13-C15-C16
4	H	1704	LDA	N1-C1-C2-C3
4	M	1706	LDA	N1-C1-C2-C3
6	L	1402	BPH	C2-C3-C5-C6
5	M	1301	BCL	C16-C17-C18-C19
6	M	1401	BPH	C16-C17-C18-C19
6	M	1401	BPH	CBA-CGA-O2A-C1
4	M	1702	LDA	C11-C10-C9-C8
4	H	1707	LDA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
5	L	1304	BCL	C10-C11-C12-C13
4	M	1702	LDA	C4-C5-C6-C7
9	M	1600	SPN	C21-C22-C23-C24
4	M	1703	LDA	C4-C5-C6-C7
4	H	1704	LDA	C11-C10-C9-C8
4	M	1702	LDA	C6-C7-C8-C9
5	M	1301	BCL	CAD-CBD-CGD-O2D
5	M	1303	BCL	CAD-CBD-CGD-O2D
6	M	1401	BPH	CAD-CBD-CGD-O2D
6	M	1401	BPH	C10-C11-C12-C13
7	L	1502	U10	C5-C4-O4-C4M
7	M	1501	U10	C34-C36-C37-C38
6	M	1401	BPH	O1A-CGA-O2A-C1
4	H	1704	LDA	C2-C1-N1-CM1
4	M	1703	LDA	C2-C1-N1-CM2
6	M	1401	BPH	C16-C17-C18-C20
5	L	1304	BCL	O1D-CGD-O2D-CED
4	M	1702	LDA	C3-C4-C5-C6
7	L	1502	U10	C21-C22-C23-C24
5	M	1301	BCL	C11-C10-C8-C7
4	M	1702	LDA	C2-C3-C4-C5
6	L	1402	BPH	O2A-C1-C2-C3
7	L	1502	U10	C1-C6-C7-C8
7	L	1502	U10	C14-C16-C17-C18
5	M	1301	BCL	C2-C1-O2A-CGA
4	H	1707	LDA	C9-C10-C11-C12
5	M	1301	BCL	C14-C13-C15-C16
6	M	1401	BPH	C14-C13-C15-C16
4	M	1705	LDA	C9-C10-C11-C12
4	M	1703	LDA	N1-C1-C2-C3
4	H	1704	LDA	C2-C3-C4-C5
4	M	1703	LDA	C3-C4-C5-C6
5	L	1304	BCL	C12-C13-C15-C16
9	M	1600	SPN	C2-C3-C4-C5
7	M	1501	U10	C14-C16-C17-C18
7	L	1502	U10	C35-C34-C36-C37
9	M	1600	SPN	C25-C26-C27-C28
4	M	1705	LDA	C11-C10-C9-C8
4	M	1705	LDA	C1-C2-C3-C4
7	L	1502	U10	C33-C34-C36-C37
5	M	1301	BCL	C1-C2-C3-C4
5	M	1303	BCL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
7	L	1502	U10	C15-C14-C16-C17
5	L	1304	BCL	C14-C13-C15-C16
5	L	1302	BCL	CAD-CBD-CGD-O2D
4	M	1701	LDA	C1-C2-C3-C4
4	M	1705	LDA	C2-C1-N1-CM1
4	M	1705	LDA	C2-C1-N1-CM2
5	M	1303	BCL	CAA-CBA-CGA-O2A
9	M	1600	SPN	C6-C7-C8-C9
9	M	1600	SPN	C10-C11-C12-C13
9	M	1600	SPN	C18-C19-C20-C21
5	M	1303	BCL	O1D-CGD-O2D-CED
7	M	1501	U10	C26-C27-C28-C29
4	H	1704	LDA	C2-C1-N1-O1
5	M	1303	BCL	CAD-CBD-CGD-O1D
5	L	1304	BCL	C8-C10-C11-C12

There are no ring outliers.

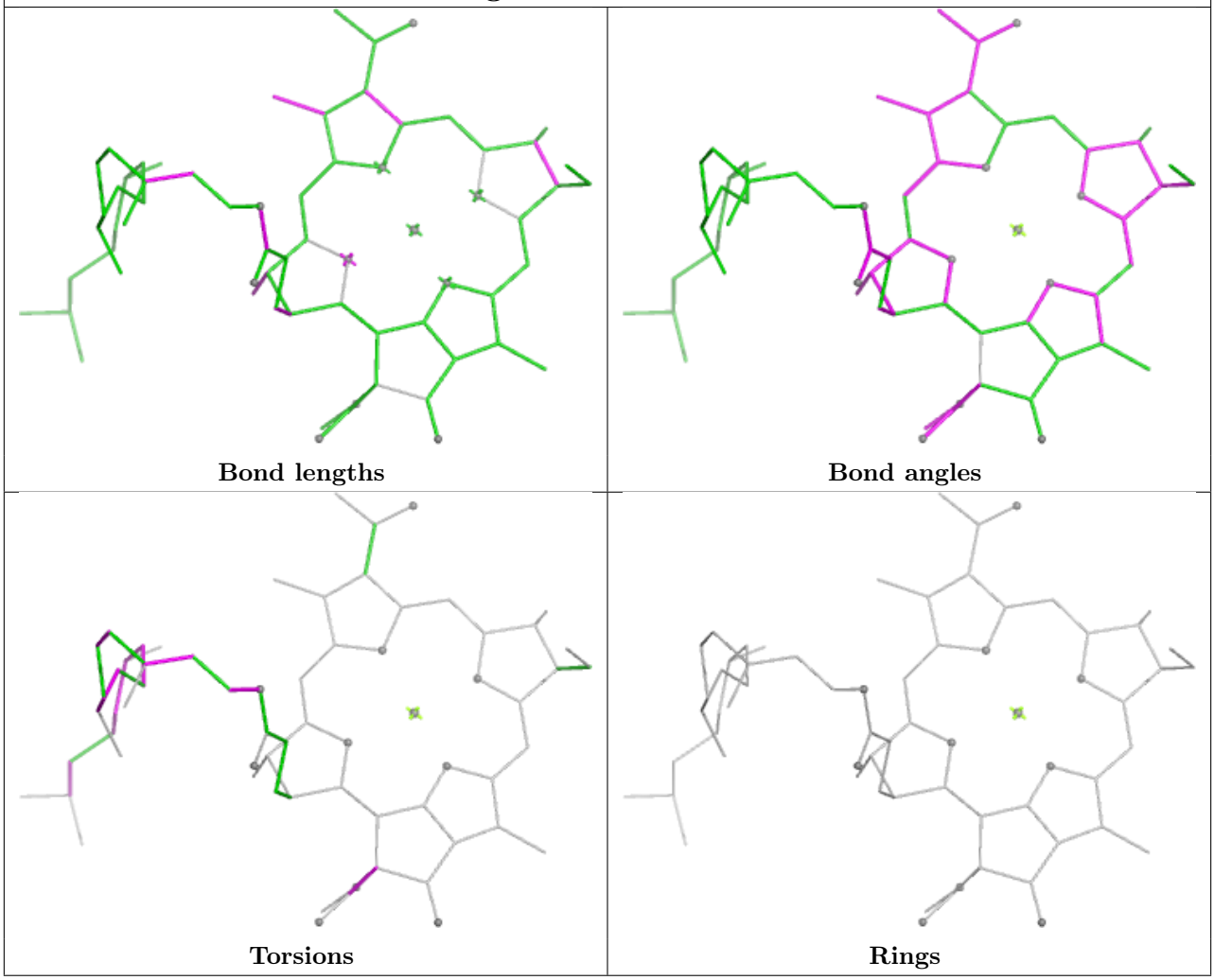
15 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1301	BCL	10	0
5	M	1303	BCL	3	0
7	L	1502	U10	8	0
4	M	1701	LDA	2	0
6	M	1401	BPH	10	0
9	M	1600	SPN	2	0
5	L	1304	BCL	1	0
10	M	1801	PO4	2	0
10	M	1800	PO4	1	0
7	M	1501	U10	3	0
4	M	1703	LDA	5	0
6	L	1402	BPH	6	0
5	L	1302	BCL	4	0
4	M	1706	LDA	4	0
4	M	1702	LDA	2	0

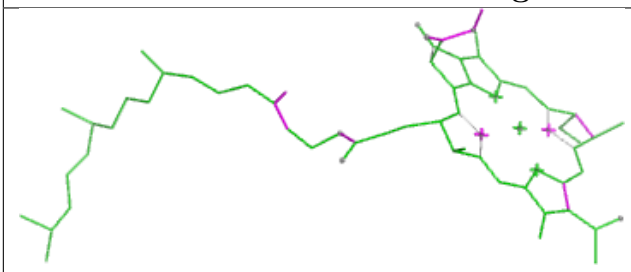
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

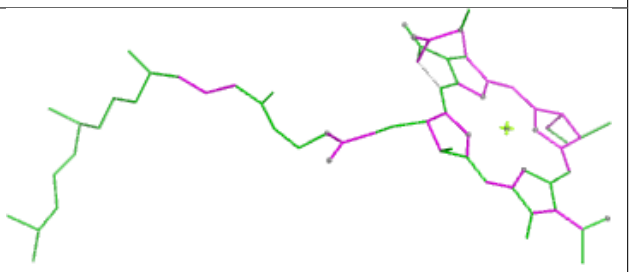
Ligand BCL M 1301



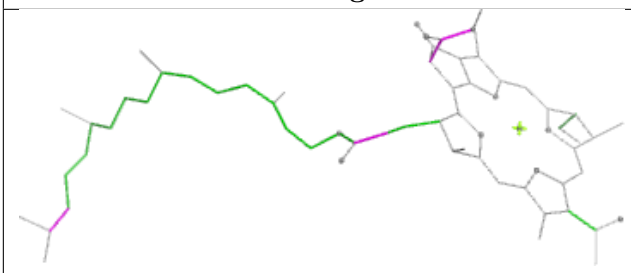
Ligand BCL M 1303



Bond lengths



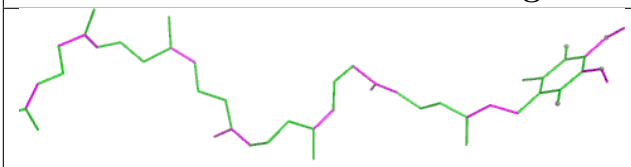
Bond angles



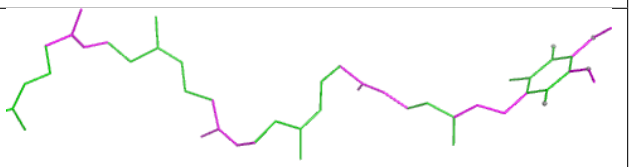
Torsions

Rings

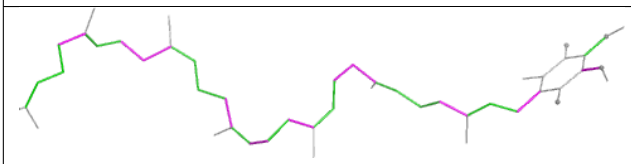
Ligand U10 L 1502



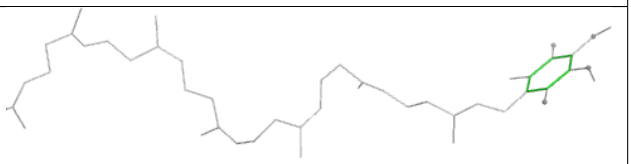
Bond lengths



Bond angles

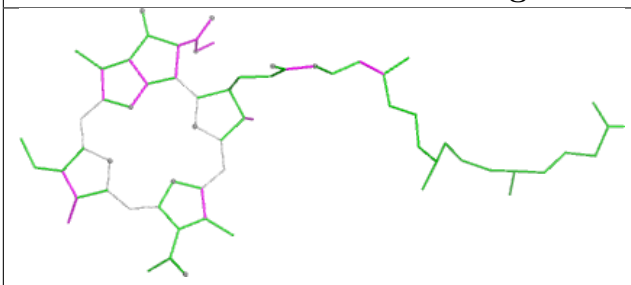


Torsions

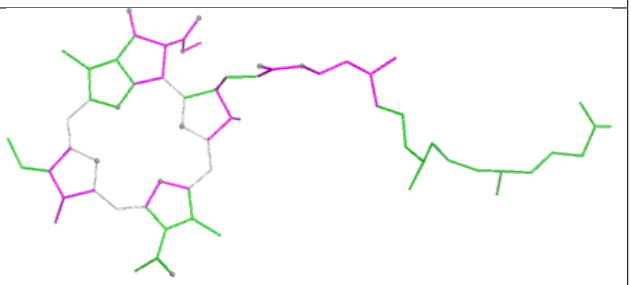


Rings

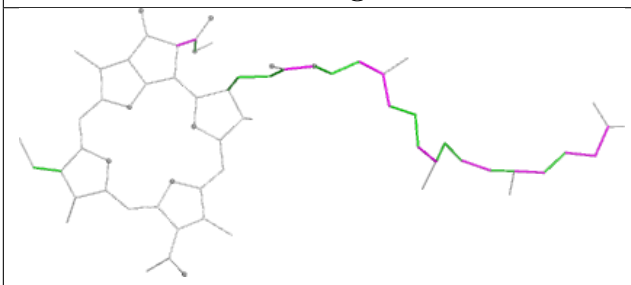
Ligand BPH M 1401



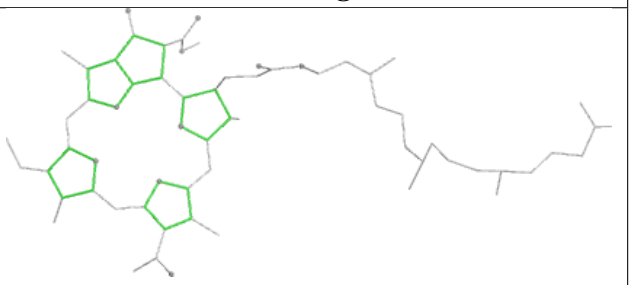
Bond lengths



Bond angles

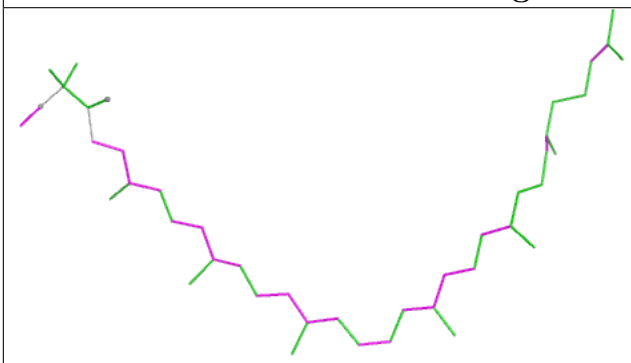


Torsions

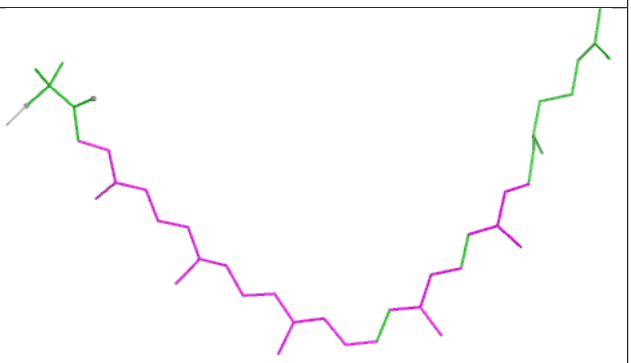


Rings

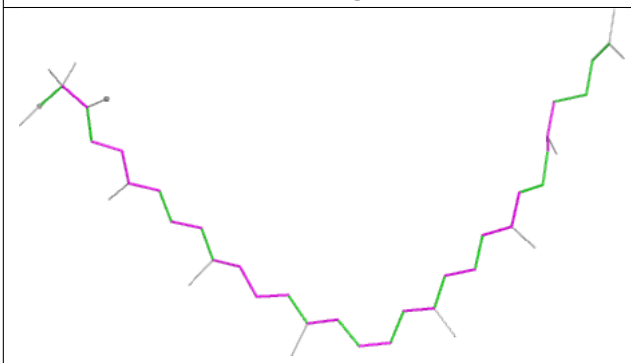
Ligand SPN M 1600



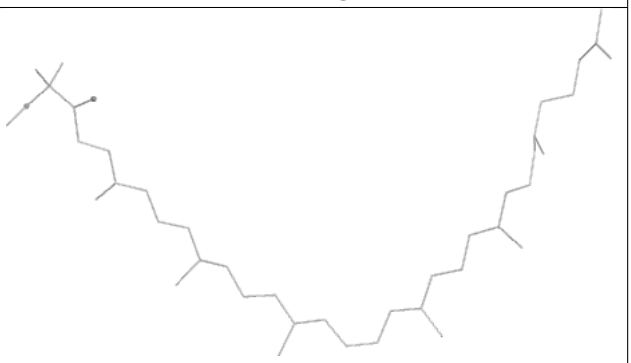
Bond lengths



Bond angles

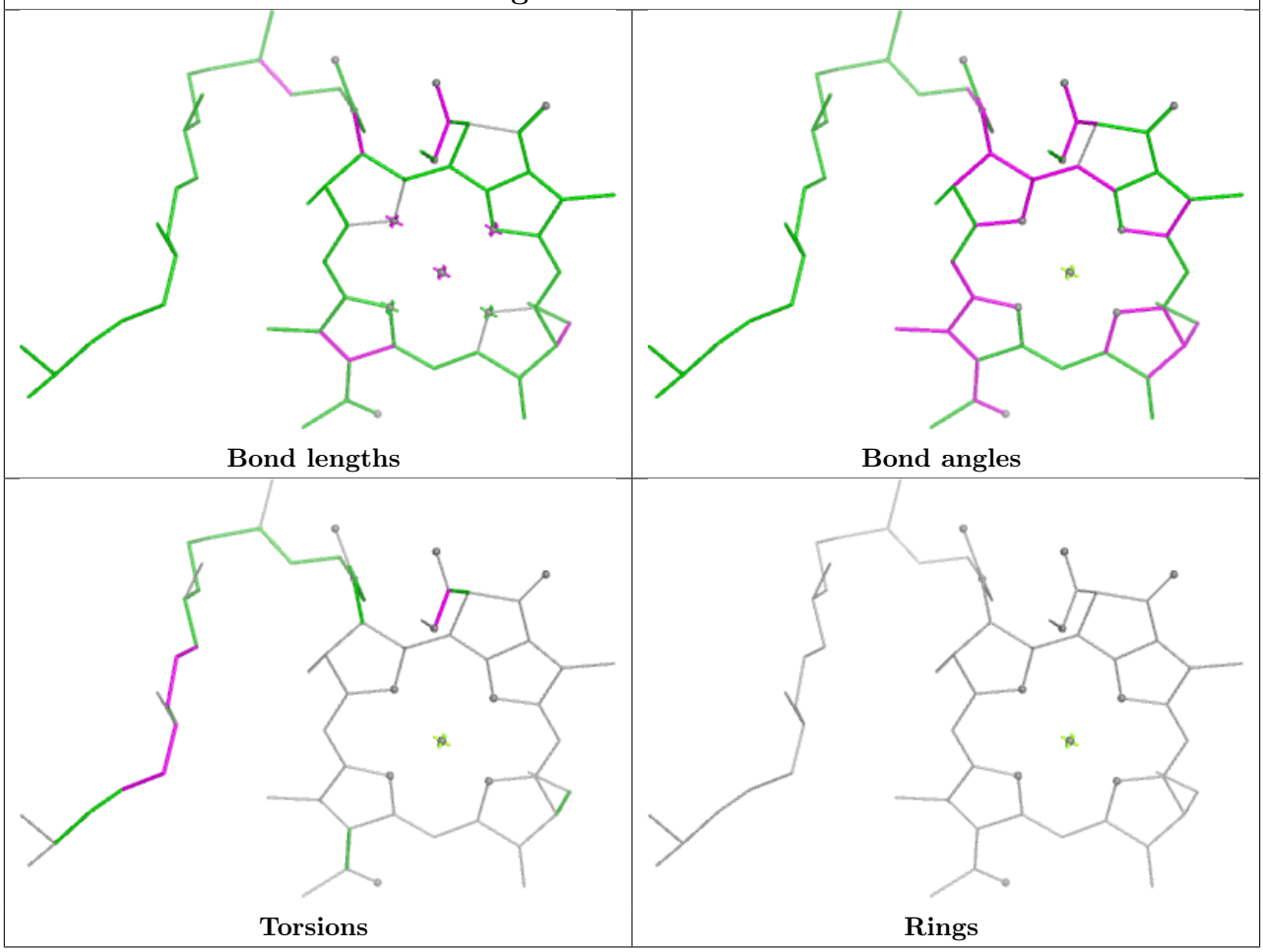


Torsions

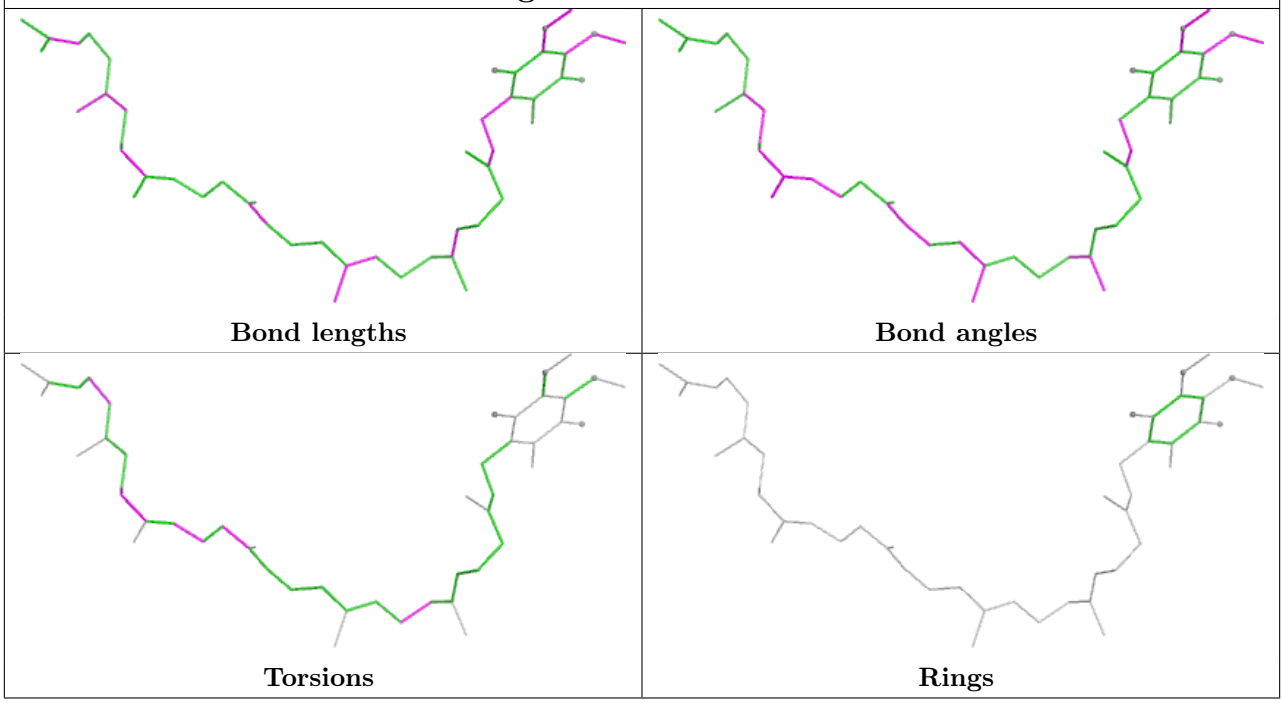


Rings

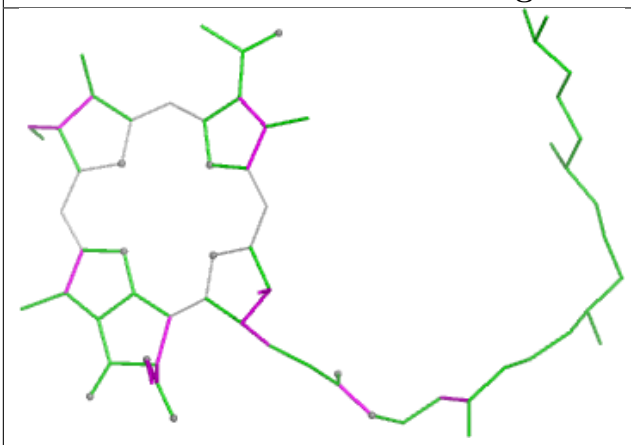
Ligand BCL L 1304



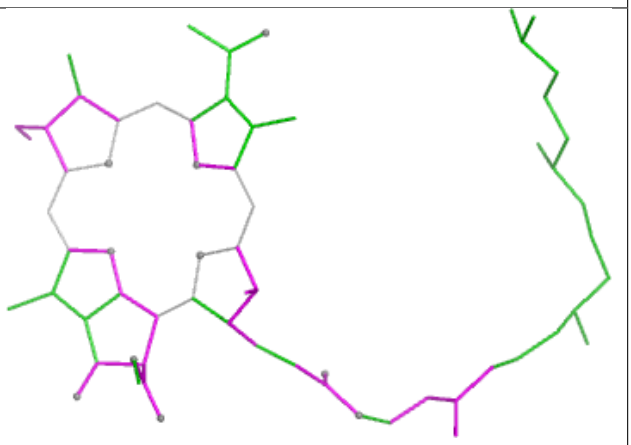
Ligand U10 M 1501



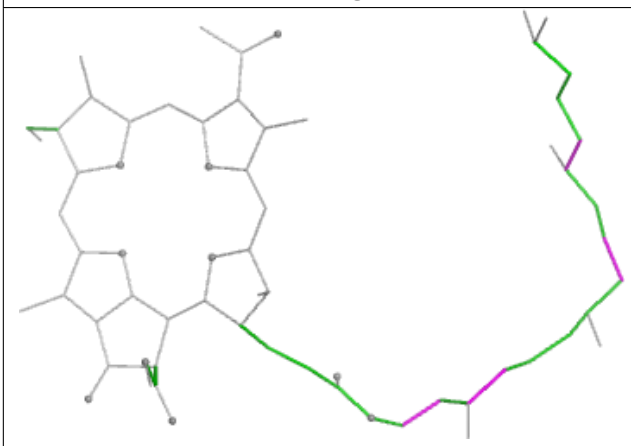
Ligand BPH L 1402



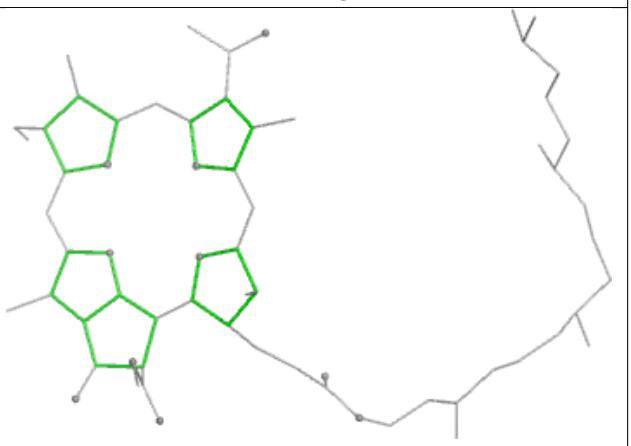
Bond lengths



Bond angles

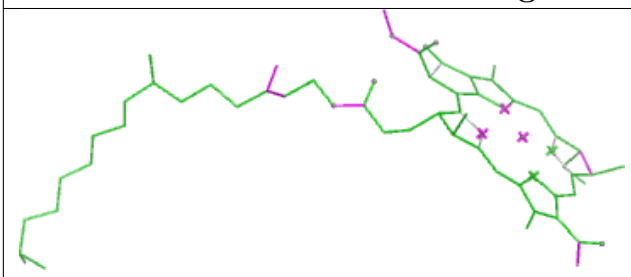


Torsions

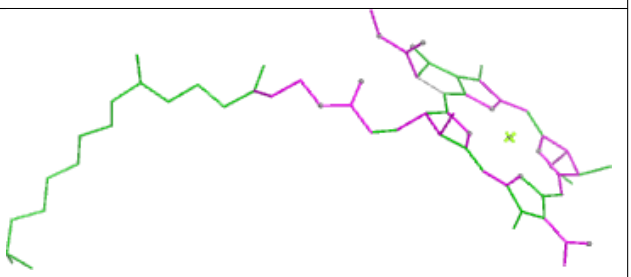


Rings

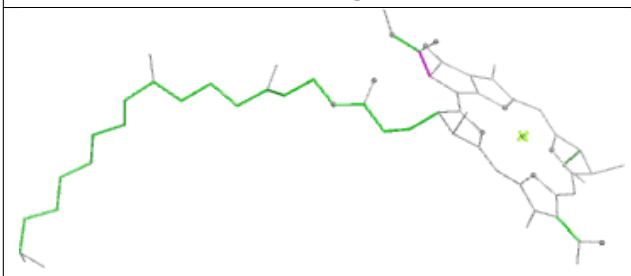
Ligand BCL L 1302



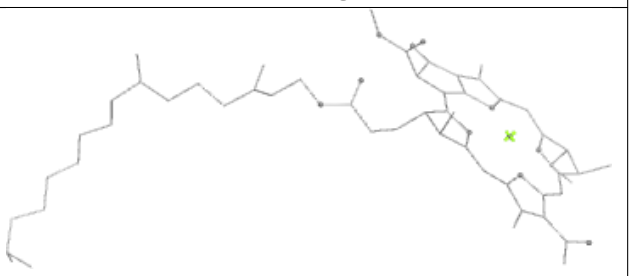
Bond lengths



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.