Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2026 – 06:36 am BST

PDB ID	:	2BNP / pdb_00002bnp
Title	:	Lipidic cubic phase grown reaction centre from Rhodobacter sphaeroides, ground state
Authors	:	Katona, G.; Snijder, A.; Gourdon, P.; Andreasson, U.; Hansson, O.; Andreasson, L.E.; Neutze, R.
Deposited on	:	2005-03-31
Resolution	:	2.70 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:

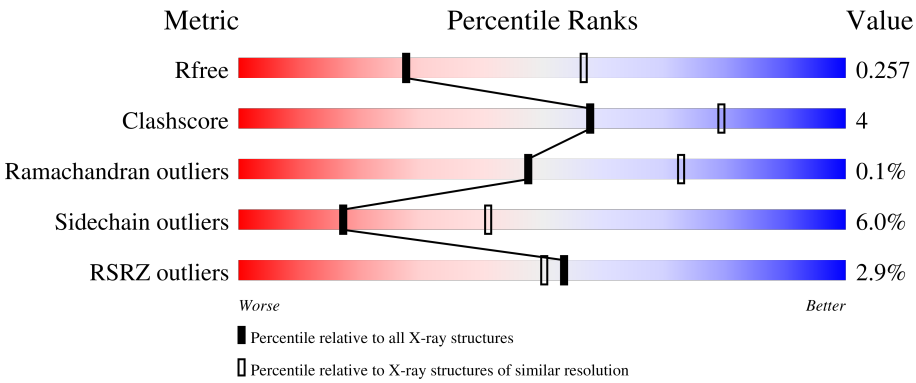
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	A	281	4% 86% 13% •
2	B	307	2% 86% 11% • •
3	C	260	3% 82% 8% 9%

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
6	MST	A	1285	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 6935 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	A	281	2232	1507	355	362	8	4	0	0

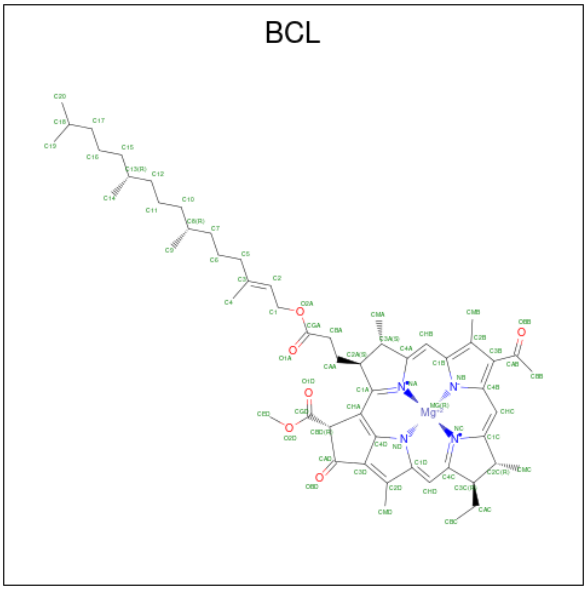
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	302	2405	1605	394	396	10	19	0	1

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

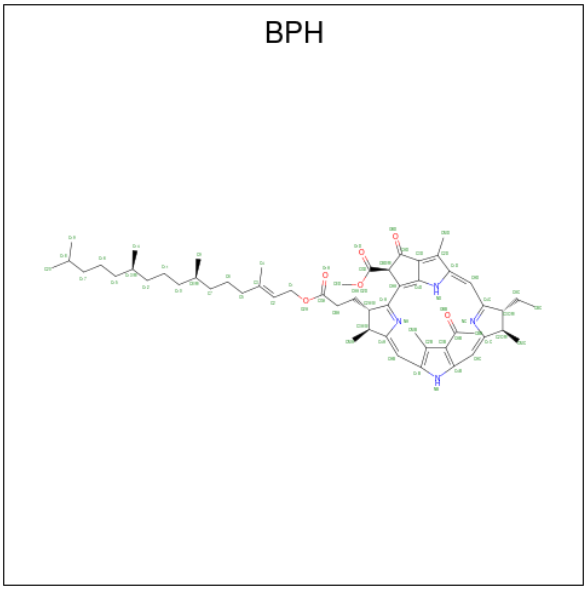
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	237	1803	1154	307	333	9	31	0	0

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



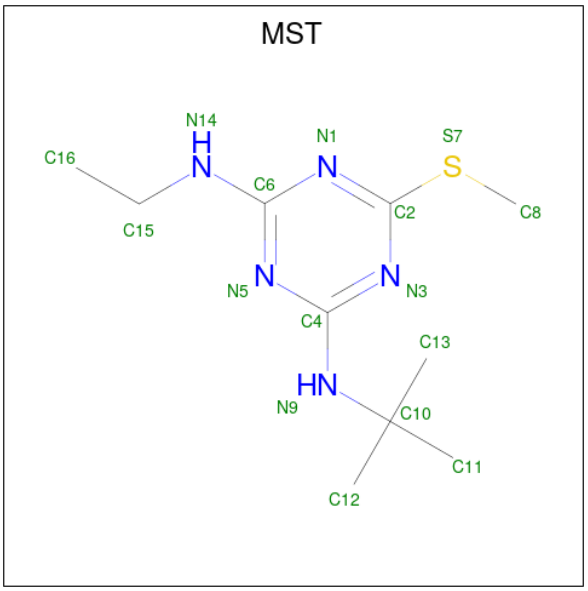
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
4	A	1	66	55	1	4	6	0	0
4	A	1	66	55	1	4	6	0	0
4	B	1	51	40	1	4	6	0	0
4	B	1	66	55	1	4	6	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	65	55	4	6	0	0
5	B	1	51	41	4	6	0	0

- Molecule 6 is 2-T-BUTYLAMINO-4-ETHYLAMINO-6-METHYLTHIO-S-TRIAZINE (CCD ID: MST) (formula: $C_{10}H_{19}N_5S$).

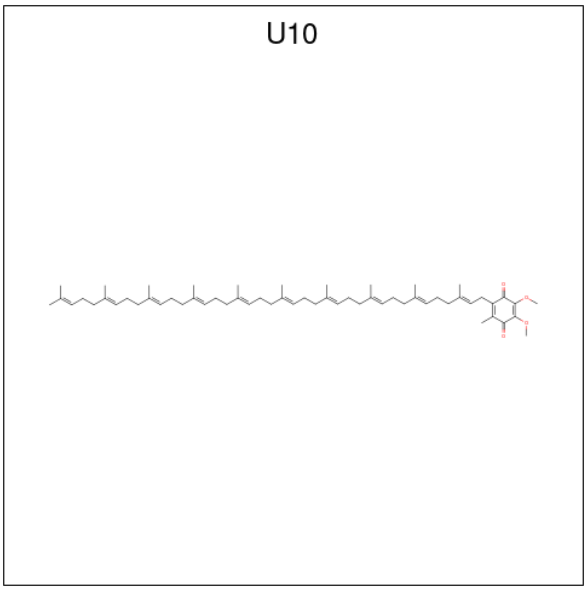


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
6	A	1	16	10	5	1	0	0

- Molecule 7 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
7	B	1	1	1	0	0

- Molecule 8 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).

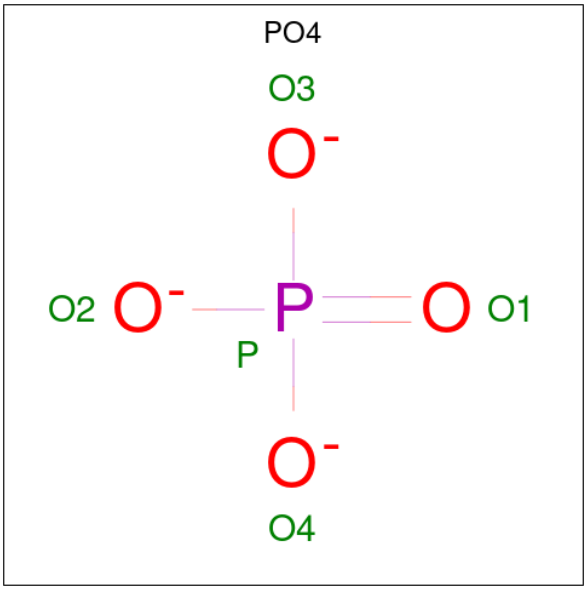


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	B	1	38	34	4	0	0

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
9	B	1	1	1	0	0

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 11 is water.

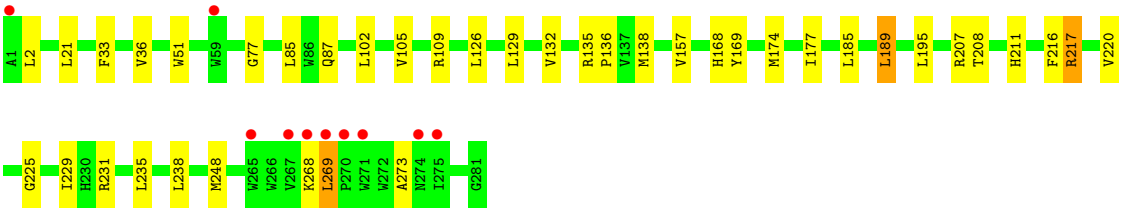
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	22	22	22	0	0
			Total	O		
11	B	22	22	22	0	0
			Total	O		
11	C	20	20	20	0	0

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.

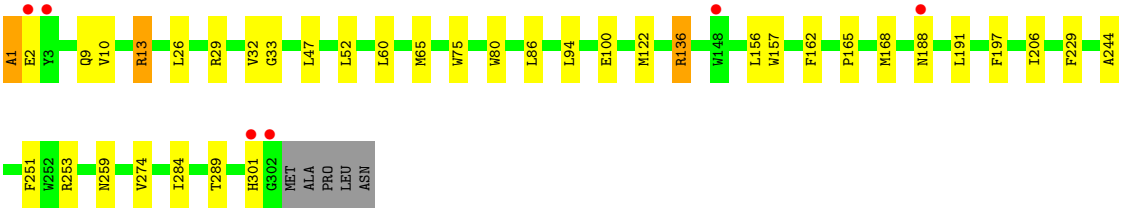
• Molecule 1: Reaction center protein L chain

Chain A:



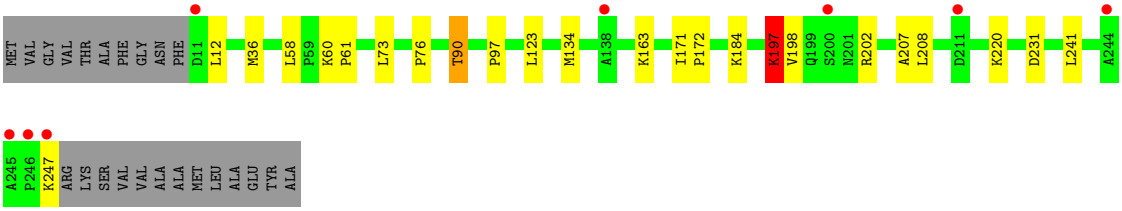
• Molecule 2: Reaction center protein M chain

Chain B:



• Molecule 3: Reaction center protein H chain

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	100.14Å 100.14Å 238.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.53 – 2.70 39.53 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.53-2.70) 99.3 (39.53-2.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.210 , 0.249 0.226 , 0.257	Depositor DCC
R_{free} test set	1696 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.8	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 25.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6935	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: CL, PO4, FE2, BPH, U10, MST, BCL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.78	1/2320 (0.0%)	0.91	1/3175 (0.0%)
2	B	1.10	6/2497 (0.2%)	1.13	6/3410 (0.2%)
3	C	1.13	5/1851 (0.3%)	1.01	3/2520 (0.1%)
All	All	1.01	12/6668 (0.2%)	1.03	10/9105 (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
2	B	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	52	LEU	CB-CG	-24.66	1.04	1.53
3	C	247	LYS	CB-CG	23.27	2.22	1.52
2	B	1	ALA	C-N	-21.51	1.03	1.33
3	C	60	LYS	CG-CD	-20.21	0.91	1.52
2	B	13	ARG	CD-NE	-17.25	1.22	1.46
3	C	197	LYS	CG-CD	-11.33	1.18	1.52
2	B	188	ASN	CB-CG	-9.84	1.27	1.52
2	B	65	MET	SD-CE	7.29	1.97	1.79
1	A	138	MET	SD-CE	6.78	1.96	1.79
2	B	301	HIS	C-N	-6.11	1.24	1.33
3	C	36	MET	SD-CE	5.83	1.94	1.79
3	C	134	MET	SD-CE	5.50	1.93	1.79

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	ALA	O-C-N	-25.03	82.96	123.00
2	B	1	ALA	CA-C-N	21.87	163.31	121.54
2	B	1	ALA	C-N-CA	21.87	163.31	121.54
3	C	184	LYS	CA-CB-CG	-18.18	77.74	114.10
1	A	268	LYS	CA-CB-CG	12.62	139.35	114.10
3	C	60	LYS	CB-CG-CD	11.54	137.84	111.30
2	B	13	ARG	CD-NE-CZ	-9.92	110.52	124.40
2	B	188	ASN	CA-CB-CG	8.19	120.79	112.60
3	C	220	LYS	CB-CG-CD	-8.16	92.53	111.30
2	B	13	ARG	CG-CD-NE	-6.78	97.09	112.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1	ALA	Mainchain,Peptide
2	B	13	ARG	Sidechain

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	A	2232	0	2187	19	0
2	B	2405	0	2317	18	0
3	C	1803	0	1805	7	0
4	A	132	0	148	5	0
4	B	117	0	115	9	0
5	A	65	0	76	4	0
5	B	51	0	45	6	0
6	A	16	0	19	9	0
7	B	1	0	0	0	0
8	B	38	0	47	2	0
9	B	1	0	0	0	0
10	B	10	0	0	0	0
11	A	22	0	0	0	0
11	B	22	0	0	1	0
11	C	20	0	0	0	0
All	All	6935	0	6759	60	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (60) 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:A:1285:MST:H121	6:A:1285:MST:C8	2.14	0.77
6:A:1285:MST:H121	6:A:1285:MST:H82	1.72	0.72
2:B:9:GLN:HE22	3:C:197:LYS:HA	1.53	0.71
4:B:1302:BCL:HHC	4:B:1302:BCL:HBB3	1.74	0.70
1:A:216:PHE:CE2	6:A:1285:MST:H132	2.32	0.64
2:B:197:PHE:CZ	4:B:1303:BCL:HBB2	2.34	0.62
2:B:136:ARG:NE	2:B:136:ARG:HA	2.16	0.61
5:A:1284:BPH:HMB1	5:A:1284:BPH:HBB3	1.82	0.61
6:A:1285:MST:H121	6:A:1285:MST:H81	1.82	0.61
1:A:135:ARG:HB3	1:A:136:PRO:HD3	1.87	0.56
3:C:90:THR:HB	3:C:97:PRO:O	2.05	0.56
1:A:229:ILE:HD13	6:A:1285:MST:H81	1.87	0.56
1:A:177:ILE:HG12	4:A:1282:BCL:HMB3	1.88	0.55
2:B:32:VAL:HG12	2:B:33:GLY:O	2.06	0.55
1:A:208:THR:H	1:A:211:HIS:HD2	1.54	0.55
2:B:9:GLN:NE2	3:C:198:VAL:H	2.04	0.55
4:A:1283:BCL:HBB3	5:A:1284:BPH:H141	1.88	0.55
3:C:171:ILE:HB	3:C:172:PRO:HD3	1.89	0.55
5:A:1284:BPH:NC	5:A:1284:BPH:ND	2.55	0.54
6:A:1285:MST:H121	6:A:1285:MST:N3	2.23	0.54
5:B:1304:BPH:HHD	5:B:1304:BPH:HBC3	1.92	0.52
2:B:75:TRP:HB3	2:B:80:TRP:CZ3	2.45	0.52
1:A:229:ILE:CD1	6:A:1285:MST:H81	2.40	0.52
2:B:168:MET:HA	2:B:168:MET:HE2	1.90	0.51
1:A:217:ARG:HD2	11:B:2007:HOH:O	2.10	0.51
1:A:269:LEU:O	1:A:273:ALA:HB2	2.11	0.50
2:B:197:PHE:HZ	4:B:1303:BCL:HBB2	1.76	0.50
1:A:157:VAL:HG11	4:B:1303:BCL:HBB1	1.93	0.50
1:A:33:PHE:O	1:A:36:VAL:HG22	2.11	0.49
1:A:168:HIS:NE2	4:A:1282:BCL:OBB	2.42	0.49
4:B:1303:BCL:CBB	4:B:1303:BCL:HHC	2.43	0.48
1:A:225:GLY:C	6:A:1285:MST:H151	2.38	0.48
2:B:168:MET:HE3	2:B:289:THR:HG22	1.95	0.48
5:B:1304:BPH:HMB1	5:B:1304:BPH:HBB3	1.96	0.47
2:B:197:PHE:CE1	4:B:1303:BCL:HBB2	2.49	0.47
4:B:1303:BCL:H2	5:B:1304:BPH:HHC	1.95	0.47
4:A:1283:BCL:HMD2	2:B:206:ILE:HD13	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:O	1:A:109:ARG:HG3	2.14	0.47
4:A:1282:BCL:NC	4:B:1303:BCL:HBB3	2.30	0.47
1:A:189:LEU:HG	1:A:216:PHE:HZ	1.80	0.46
2:B:9:GLN:HE22	3:C:198:VAL:H	1.61	0.46
5:B:1304:BPH:NC	5:B:1304:BPH:ND	2.64	0.46
2:B:122:MET:HE3	2:B:157:TRP:HE1	1.80	0.46
2:B:284:ILE:HG12	4:B:1303:BCL:HED3	1.98	0.46
1:A:208:THR:H	1:A:211:HIS:CD2	2.33	0.45
2:B:253:ARG:HD2	2:B:259:ASN:OD1	2.17	0.45
1:A:185:LEU:HD13	5:B:1304:BPH:ND	2.33	0.44
1:A:169:TYR:HA	1:A:174:MET:HE3	2.00	0.44
5:A:1284:BPH:HBB3	5:A:1284:BPH:CMB	2.46	0.44
1:A:135:ARG:HD2	1:A:248:MET:O	2.18	0.43
5:B:1304:BPH:HBB3	5:B:1304:BPH:CMB	2.48	0.43
2:B:251:PHE:CD2	2:B:251:PHE:C	2.97	0.43
1:A:77:GLY:HA2	1:A:87:GLN:HE22	1.84	0.43
2:B:162:PHE:C	2:B:165:PRO:HD2	2.44	0.43
8:B:1306:U10:C3M	8:B:1306:U10:H4M2	2.50	0.42
6:A:1285:MST:N3	6:A:1285:MST:C12	2.81	0.42
2:B:229:PHE:HB2	2:B:244:ALA:HB2	2.02	0.42
3:C:61:PRO:HA	3:C:76:PRO:HD2	2.02	0.41
8:B:1306:U10:H4M2	8:B:1306:U10:O3	2.20	0.41
3:C:207:ALA:HA	3:C:241:LEU:HD23	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	279/281 (99%)	268 (96%)	11 (4%)	0	100 100
2	B	300/307 (98%)	291 (97%)	8 (3%)	1 (0%)	36 60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	235/260 (90%)	226 (96%)	9 (4%)	0	100	100
All	All	814/848 (96%)	785 (96%)	28 (3%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	2	GLU

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	A	220/220 (100%)	203 (92%)	17 (8%)	12	30
2	B	236/240 (98%)	224 (95%)	12 (5%)	21	48
3	C	192/208 (92%)	182 (95%)	10 (5%)	21	47
All	All	648/668 (97%)	609 (94%)	39 (6%)	17	41

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	21	LEU
1	A	51	TRP
1	A	85	LEU
1	A	102	LEU
1	A	126	LEU
1	A	129	LEU
1	A	132	VAL
1	A	189	LEU
1	A	195	LEU
1	A	207	ARG
1	A	217	ARG
1	A	220	VAL
1	A	231	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	235	LEU
1	A	238	LEU
1	A	269	LEU
2	B	10	VAL
2	B	26	LEU
2	B	29	ARG
2	B	47	LEU
2	B	60	LEU
2	B	86	LEU
2	B	94	LEU
2	B	100	GLU
2	B	136	ARG
2	B	156	LEU
2	B	191	LEU
2	B	274	VAL
3	C	12	LEU
3	C	58	LEU
3	C	73	LEU
3	C	90	THR
3	C	123	LEU
3	C	163	LYS
3	C	197	LYS
3	C	202	ARG
3	C	208	LEU
3	C	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	183	ASN
1	A	211	HIS
1	A	274	ASN
2	B	9	GLN
2	B	25	ASN
2	B	138	GLN
2	B	195	ASN
2	B	202	HIS
3	C	204	HIS
3	C	206	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BCL	B	1302	2	54,59,74	1.80	12 (22%)	65,97,115	2.35	20 (30%)
4	BCL	A	1283	1	69,74,74	2.04	15 (21%)	83,115,115	1.91	19 (22%)
8	U10	B	1306	-	38,38,63	2.78	12 (31%)	46,49,79	1.44	7 (15%)
4	BCL	B	1303	2	69,74,74	2.34	11 (15%)	83,115,115	2.24	22 (26%)
10	PO4	B	1308	-	4,4,4	1.35	1 (25%)	6,6,6	0.87	0
6	MST	A	1285	-	16,16,16	3.20	3 (18%)	22,22,22	3.76	7 (31%)
10	PO4	B	1309	-	4,4,4	0.59	0	6,6,6	0.72	0
5	BPH	A	1284	-	59,70,70	1.62	9 (15%)	61,101,101	2.62	15 (24%)
4	BCL	A	1282	1	69,74,74	1.64	9 (13%)	83,115,115	1.97	16 (19%)
5	BPH	B	1304	-	45,56,70	1.96	7 (15%)	44,84,101	3.05	15 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	B	1302	2	-	9/23/119/137	-
4	BCL	A	1283	1	-	4/41/137/137	-
8	U10	B	1306	-	-	9/33/57/87	0/1/1/1
4	BCL	B	1303	2	-	12/41/137/137	-
6	MST	A	1285	-	-	6/10/10/10	0/1/1/1
5	BPH	A	1284	-	-	10/37/105/105	0/5/6/6
4	BCL	A	1282	1	-	8/41/137/137	-
5	BPH	B	1304	-	-	1/21/89/105	0/5/6/6

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1303	BCL	MG-NC	-14.55	1.71	2.06
6	A	1285	MST	C2-S7	-11.05	1.66	1.75
4	A	1283	BCL	MG-NA	-9.15	1.84	2.06
4	A	1282	BCL	MG-NC	-6.68	1.90	2.06
8	B	1306	U10	C8-C9	6.55	1.48	1.33
8	B	1306	U10	C18-C19	6.24	1.47	1.33
4	A	1283	BCL	MG-NB	6.09	2.17	2.05
8	B	1306	U10	C13-C14	6.03	1.47	1.33
8	B	1306	U10	C23-C24	5.85	1.47	1.33
5	B	1304	BPH	O2D-CGD	5.76	1.47	1.33
8	B	1306	U10	C28-C29	5.57	1.48	1.32
8	B	1306	U10	O3-C3	-5.35	1.23	1.36
5	B	1304	BPH	C4D-CHA	5.09	1.47	1.39
8	B	1306	U10	O4-C4	-5.07	1.24	1.36
4	A	1283	BCL	C3D-C4D	-5.00	1.32	1.44
4	B	1303	BCL	C3D-C4D	-4.96	1.33	1.44
4	B	1303	BCL	O2D-CGD	4.94	1.45	1.33
5	B	1304	BPH	C3D-C4D	-4.88	1.34	1.41
4	A	1282	BCL	C3D-C4D	-4.86	1.33	1.44
4	A	1282	BCL	O2D-CGD	4.81	1.44	1.33
5	A	1284	BPH	C4D-CHA	4.72	1.47	1.39
4	B	1302	BCL	O2A-CGA	4.71	1.47	1.33
4	B	1302	BCL	C3D-C4D	-4.71	1.33	1.44
5	A	1284	BPH	C3D-C4D	-4.62	1.34	1.41
4	A	1283	BCL	O2A-CGA	4.54	1.46	1.33
5	B	1304	BPH	O2A-CGA	4.52	1.46	1.33
4	B	1303	BCL	O2A-CGA	4.44	1.46	1.33
5	A	1284	BPH	OBD-CAD	4.27	1.28	1.22
6	A	1285	MST	C10-N9	4.26	1.55	1.48
5	A	1284	BPH	O2D-CGD	4.22	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1302	BCL	O2D-CGD	4.17	1.43	1.33
4	B	1302	BCL	MG-NB	-4.14	1.97	2.05
5	B	1304	BPH	C3A-C2A	-4.07	1.51	1.54
4	A	1283	BCL	O2D-CGD	4.03	1.43	1.33
5	B	1304	BPH	OBD-CAD	3.98	1.27	1.22
4	B	1303	BCL	C3C-C4C	-3.94	1.46	1.51
4	B	1302	BCL	MG-NC	-3.92	1.96	2.06
4	A	1282	BCL	O2A-CGA	3.81	1.44	1.33
4	B	1302	BCL	MG-NA	-3.70	1.97	2.06
4	B	1303	BCL	C4D-ND	-3.62	1.32	1.37
4	A	1283	BCL	MG-NC	-3.61	1.97	2.06
5	B	1304	BPH	C2C-C3C	-3.60	1.51	1.54
5	A	1284	BPH	O2A-CGA	3.58	1.43	1.33
4	A	1283	BCL	C4D-ND	-3.50	1.32	1.37
4	A	1282	BCL	OBD-CAD	3.47	1.28	1.22
5	A	1284	BPH	C3A-C2A	-3.44	1.51	1.54
6	A	1285	MST	C4-N9	3.22	1.39	1.34
8	B	1306	U10	C3-C2	-3.17	1.39	1.48
4	A	1282	BCL	C3C-C4C	-3.14	1.47	1.51
8	B	1306	U10	C6-C1	3.13	1.40	1.35
4	A	1283	BCL	OBD-CAD	3.12	1.27	1.22
8	B	1306	U10	C4-C5	-3.05	1.40	1.48
5	A	1284	BPH	C2C-C3C	-3.03	1.51	1.54
4	B	1302	BCL	OBD-CAD	2.89	1.27	1.22
4	A	1283	BCL	C3C-C4C	-2.86	1.48	1.51
4	A	1283	BCL	MG-ND	-2.80	2.00	2.05
4	B	1302	BCL	C2A-C1A	-2.79	1.45	1.52
4	B	1303	BCL	MG-NB	2.73	2.11	2.05
4	B	1302	BCL	C3C-C4C	-2.71	1.48	1.51
4	B	1303	BCL	C1D-C2D	-2.54	1.40	1.45
4	A	1282	BCL	C4D-CHA	2.50	1.47	1.38
4	B	1303	BCL	C4D-CHA	2.44	1.47	1.38
4	B	1302	BCL	C4D-ND	-2.43	1.34	1.37
4	A	1283	BCL	C2A-C1A	-2.41	1.46	1.52
4	A	1282	BCL	C4D-ND	-2.38	1.34	1.37
5	A	1284	BPH	CBD-CGD	-2.38	1.49	1.52
4	A	1282	BCL	C2A-C1A	-2.37	1.46	1.52
4	A	1283	BCL	C1B-NB	-2.36	1.34	1.37
8	B	1306	U10	C6-C5	-2.35	1.40	1.46
4	B	1303	BCL	OBD-CAD	2.32	1.26	1.22
4	A	1283	BCL	C1D-C2D	-2.26	1.40	1.45
4	B	1302	BCL	C4D-CHA	2.21	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1283	BCL	C4D-CHA	2.19	1.46	1.38
5	A	1284	BPH	CHA-CBD	-2.18	1.49	1.51
4	B	1303	BCL	MG-ND	-2.14	2.01	2.05
4	B	1302	BCL	C1D-C2D	-2.13	1.41	1.45
4	A	1283	BCL	C3B-C2B	-2.10	1.35	1.42
8	B	1306	U10	C1-C2	-2.09	1.39	1.47
10	B	1308	PO4	P-O3	-2.08	1.48	1.54

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1285	MST	C2-N3-C4	13.83	121.64	113.85
5	A	1284	BPH	C4D-ND-C1D	-9.75	98.91	108.83
4	B	1303	BCL	C1C-NC-C4C	-9.42	102.47	106.71
5	B	1304	BPH	C4D-ND-C1D	-9.31	99.36	108.83
5	A	1284	BPH	C2D-C1D-ND	8.96	115.71	109.53
5	B	1304	BPH	C2D-C1D-ND	8.68	115.52	109.53
4	B	1302	BCL	C1C-NC-C4C	-8.09	103.07	106.71
5	B	1304	BPH	O2D-CGD-CBD	7.95	121.07	111.00
4	A	1283	BCL	C4A-NA-C1A	-7.62	103.28	106.71
4	A	1282	BCL	C1C-NC-C4C	-7.34	103.41	106.71
4	B	1302	BCL	C4A-NA-C1A	-7.30	103.42	106.71
6	A	1285	MST	N5-C4-N3	-7.17	114.89	126.23
4	B	1302	BCL	C1D-ND-C4D	-7.15	101.25	106.33
4	B	1303	BCL	C4A-NA-C1A	-7.08	103.52	106.71
4	A	1282	BCL	C4A-NA-C1A	-7.08	103.53	106.71
4	B	1303	BCL	C1D-ND-C4D	-6.06	102.03	106.33
4	A	1282	BCL	C1D-ND-C4D	-5.85	102.18	106.33
5	A	1284	BPH	C2B-C1B-NB	5.83	113.55	109.53
4	A	1283	BCL	C1D-ND-C4D	-5.77	102.24	106.33
5	B	1304	BPH	C2B-C1B-NB	5.33	113.21	109.53
5	A	1284	BPH	O2D-CGD-CBD	5.17	117.55	111.00
5	A	1284	BPH	C3D-C4D-ND	5.05	114.60	107.72
6	A	1285	MST	C6-N5-C4	4.95	122.29	113.89
4	B	1302	BCL	O2D-CGD-CBD	4.78	119.76	111.27
5	B	1304	BPH	C3D-C4D-ND	4.73	114.17	107.72
4	B	1303	BCL	CHC-C1C-NC	4.65	130.94	124.51
8	B	1306	U10	C25-C24-C26	4.47	122.79	115.27
5	A	1284	BPH	C4D-CHA-CBD	4.11	110.38	108.52
4	B	1302	BCL	C1-O2A-CGA	4.09	127.17	116.44
4	B	1303	BCL	CHD-C1D-ND	-4.07	120.71	124.45
5	A	1284	BPH	C1B-NB-C4B	-3.93	102.75	108.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1303	BCL	O2A-CGA-CBA	3.91	124.19	111.91
4	A	1283	BCL	CHC-C1C-NC	3.88	129.88	124.51
5	B	1304	BPH	C1B-NB-C4B	-3.84	102.89	108.83
4	B	1303	BCL	O2D-CGD-CBD	3.82	118.05	111.27
4	A	1282	BCL	C2A-C3A-C4A	3.82	108.03	101.87
4	B	1302	BCL	C3D-C4D-ND	3.75	116.30	110.24
5	B	1304	BPH	C4D-CHA-CBD	3.74	110.21	108.52
4	A	1283	BCL	CHD-C1D-ND	-3.73	121.02	124.45
4	B	1303	BCL	C1D-CHD-C4C	-3.69	117.72	126.62
4	A	1283	BCL	C1C-NC-C4C	-3.68	105.05	106.71
5	A	1284	BPH	C4C-C3C-C2C	-3.61	99.41	102.84
5	B	1304	BPH	CED-O2D-CGD	3.56	123.98	115.94
5	A	1284	BPH	C7-C6-C5	-3.45	104.00	113.36
4	A	1282	BCL	CHA-C1A-NA	-3.40	118.62	126.40
4	A	1283	BCL	C3D-C4D-ND	3.39	115.72	110.24
4	B	1302	BCL	CMB-C2B-C1B	-3.39	120.21	125.37
8	B	1306	U10	C17-C18-C19	-3.37	119.54	127.66
4	A	1283	BCL	CAC-C3C-C2C	-3.35	105.88	114.26
4	A	1282	BCL	C3D-C4D-ND	3.35	115.66	110.24
4	A	1282	BCL	CHD-C1D-ND	-3.34	121.38	124.45
4	B	1303	BCL	CMB-C2B-C1B	-3.28	120.37	125.37
5	B	1304	BPH	C1A-C2A-C3A	-3.24	99.76	102.84
5	A	1284	BPH	C1-C2-C3	-3.21	120.50	126.04
4	B	1303	BCL	C3D-C4D-ND	3.17	115.36	110.24
5	B	1304	BPH	C1-O2A-CGA	3.16	124.74	116.44
4	B	1302	BCL	C4D-C3D-CAD	3.16	111.81	108.10
5	A	1284	BPH	C3B-C4B-NB	3.09	112.66	108.04
4	A	1283	BCL	C2A-C3A-C4A	3.08	106.85	101.87
4	A	1283	BCL	C2C-C3C-C4C	3.06	105.92	101.34
4	B	1303	BCL	CED-O2D-CGD	3.05	122.84	115.94
6	A	1285	MST	N9-C4-N5	3.05	126.43	117.52
4	A	1282	BCL	O2A-CGA-CBA	3.04	121.46	111.91
4	B	1303	BCL	C3C-C2C-C1C	3.02	106.75	101.87
4	A	1282	BCL	CMB-C2B-C1B	-3.01	120.79	125.37
5	A	1284	BPH	O2A-CGA-O1A	-2.98	116.08	123.59
4	B	1302	BCL	C1D-CHD-C4C	-2.97	119.47	126.62
4	A	1282	BCL	CED-O2D-CGD	2.96	122.63	115.94
6	A	1285	MST	N5-C6-N1	-2.96	121.56	126.23
4	A	1283	BCL	CMB-C2B-C1B	-2.93	120.90	125.37
4	A	1283	BCL	C1D-CHD-C4C	-2.91	119.61	126.62
4	B	1303	BCL	CHA-C1A-NA	-2.85	119.87	126.40
4	A	1283	BCL	CHB-C4A-NA	2.84	128.43	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1304	BPH	O2D-CGD-O1D	-2.76	118.45	123.84
4	B	1302	BCL	CHD-C1D-ND	-2.74	121.94	124.45
5	B	1304	BPH	C3B-C4B-NB	2.72	112.11	108.04
4	A	1283	BCL	CAA-C2A-C3A	-2.69	105.41	112.78
5	A	1284	BPH	C1A-C2A-C3A	-2.68	100.29	102.84
4	B	1302	BCL	CHC-C4B-NB	2.66	127.08	124.26
4	B	1303	BCL	CAC-C3C-C2C	-2.64	107.66	114.26
4	A	1282	BCL	CMB-C2B-C3B	2.64	133.05	125.93
4	B	1302	BCL	C2B-C1B-NB	-2.63	108.47	110.23
5	B	1304	BPH	C4-C3-C5	2.61	118.97	115.98
6	A	1285	MST	C15-N14-C6	-2.61	120.63	123.85
5	B	1304	BPH	O1D-CGD-CBD	-2.56	120.47	124.74
4	B	1303	BCL	CMB-C2B-C3B	2.54	132.80	125.93
4	B	1303	BCL	CBB-CAB-C3B	2.48	125.72	120.43
6	A	1285	MST	S7-C2-N1	2.46	124.50	116.01
4	B	1302	BCL	C3D-C4D-CHA	-2.44	107.14	112.72
8	B	1306	U10	C31-C29-C30	2.41	119.92	114.60
4	B	1302	BCL	CMB-C2B-C3B	2.39	132.37	125.93
4	B	1302	BCL	C2A-C3A-C4A	2.37	105.70	101.87
4	B	1302	BCL	O2A-CGA-CBA	2.35	119.29	111.91
4	B	1303	BCL	C4D-C3D-CAD	2.35	110.87	108.10
8	B	1306	U10	C22-C23-C24	-2.34	122.02	127.66
4	A	1283	BCL	C3C-C2C-C1C	2.32	105.61	101.87
4	B	1302	BCL	O2D-CGD-O1D	-2.31	119.32	123.84
4	A	1282	BCL	C2C-C3C-C4C	2.31	104.80	101.34
4	A	1282	BCL	C4-C3-C5	2.29	119.13	115.27
4	A	1282	BCL	CHB-C4A-NA	2.29	127.68	124.51
5	A	1284	BPH	CMA-C3A-C4A	-2.28	109.38	114.38
4	B	1302	BCL	C4D-CHA-C1A	-2.28	118.48	121.25
4	A	1283	BCL	O2D-CGD-CBD	2.26	115.29	111.27
5	A	1284	BPH	O2D-CGD-O1D	-2.24	119.46	123.84
4	B	1303	BCL	C2A-C3A-C4A	2.22	105.45	101.87
4	B	1303	BCL	OBB-CAB-CBB	-2.22	114.82	119.73
8	B	1306	U10	C6-C1-C2	2.21	120.93	119.18
4	A	1283	BCL	C2B-C1B-NB	-2.21	108.75	110.23
8	B	1306	U10	C27-C28-C29	-2.21	120.20	127.75
4	B	1303	BCL	O2D-CGD-O1D	-2.20	119.54	123.84
4	A	1283	BCL	CMB-C2B-C3B	2.17	131.79	125.93
8	B	1306	U10	C12-C13-C14	-2.16	122.47	127.66
4	A	1282	BCL	CAA-C2A-C3A	-2.15	106.89	112.78
4	B	1302	BCL	O2A-CGA-O1A	-2.14	118.19	123.59
4	A	1283	BCL	CHA-C1A-NA	-2.14	121.50	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1302	BCL	CHC-C4B-C3B	-2.13	124.78	132.35
4	B	1303	BCL	CMD-C2D-C1D	2.09	128.40	124.71
5	B	1304	BPH	C4C-C3C-C2C	-2.07	100.87	102.84
4	A	1283	BCL	C5-C3-C2	-2.05	116.96	121.12
4	B	1303	BCL	CGD-CBD-CAD	-2.04	104.14	110.73
4	A	1282	BCL	OBB-CAB-C3B	2.03	124.17	120.41

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1302	BCL	C2B-C3B-CAB-OBB
4	B	1302	BCL	C2B-C3B-CAB-CBB
4	B	1302	BCL	C4B-C3B-CAB-OBB
4	B	1302	BCL	C4B-C3B-CAB-CBB
4	B	1303	BCL	C12-C13-C15-C16
6	A	1285	MST	C11-C10-N9-C4
6	A	1285	MST	C12-C10-N9-C4
6	A	1285	MST	C13-C10-N9-C4
6	A	1285	MST	N1-C6-N14-C15
6	A	1285	MST	N5-C6-N14-C15
8	B	1306	U10	C14-C16-C17-C18
8	B	1306	U10	C22-C23-C24-C25
8	B	1306	U10	C22-C23-C24-C26
8	B	1306	U10	C23-C24-C26-C27
8	B	1306	U10	C25-C24-C26-C27
4	B	1303	BCL	C3-C5-C6-C7
8	B	1306	U10	C27-C28-C29-C30
4	B	1302	BCL	CBD-CGD-O2D-CED
8	B	1306	U10	C27-C28-C29-C31
4	A	1282	BCL	C2A-CAA-CBA-CGA
4	B	1303	BCL	C15-C16-C17-C18
4	B	1302	BCL	O1D-CGD-O2D-CED
4	A	1282	BCL	C15-C16-C17-C18
5	A	1284	BPH	C4-C3-C5-C6
4	B	1303	BCL	C16-C17-C18-C19
4	A	1282	BCL	C16-C17-C18-C20
5	A	1284	BPH	C8-C10-C11-C12
4	B	1302	BCL	C2A-CAA-CBA-CGA
5	A	1284	BPH	C2-C3-C5-C6
4	B	1303	BCL	C16-C17-C18-C20
4	A	1283	BCL	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	1303	BCL	C14-C13-C15-C16
4	A	1282	BCL	C16-C17-C18-C19
4	B	1303	BCL	C6-C7-C8-C10
4	B	1302	BCL	C2-C1-O2A-CGA
4	B	1303	BCL	C6-C7-C8-C9
8	B	1306	U10	C5-C4-O4-C4M
5	A	1284	BPH	O2A-C1-C2-C3
4	A	1283	BCL	C11-C12-C13-C15
4	A	1283	BCL	C2A-CAA-CBA-CGA
4	B	1303	BCL	CAA-CBA-CGA-O2A
4	B	1303	BCL	C11-C10-C8-C7
4	A	1282	BCL	CAD-CBD-CGD-O2D
4	B	1302	BCL	CAD-CBD-CGD-O2D
5	A	1284	BPH	C16-C17-C18-C19
5	B	1304	BPH	O2A-C1-C2-C3
4	A	1282	BCL	C12-C13-C15-C16
4	A	1282	BCL	C14-C13-C15-C16
4	A	1283	BCL	C11-C12-C13-C14
4	B	1303	BCL	C11-C10-C8-C9
5	A	1284	BPH	C11-C12-C13-C14
5	A	1284	BPH	C14-C13-C15-C16
6	A	1285	MST	N1-C2-S7-C8
8	B	1306	U10	C21-C22-C23-C24
5	A	1284	BPH	C11-C10-C8-C9
5	A	1284	BPH	C11-C10-C8-C7
5	A	1284	BPH	C12-C13-C15-C16
4	A	1282	BCL	O1D-CGD-O2D-CED
4	B	1303	BCL	C13-C15-C16-C17

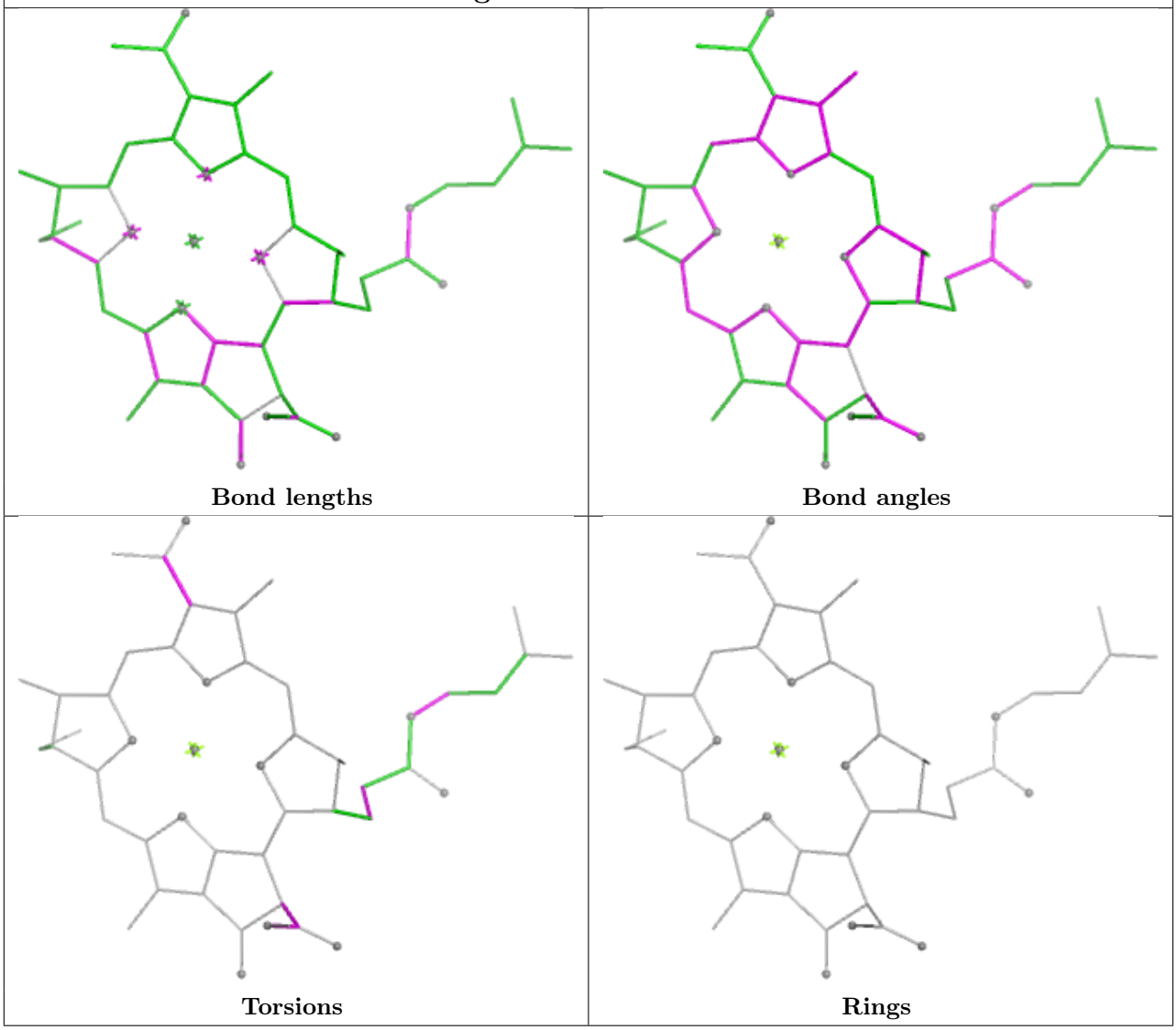
There are no ring outliers.

8 monomers are involved in 32 short contacts:

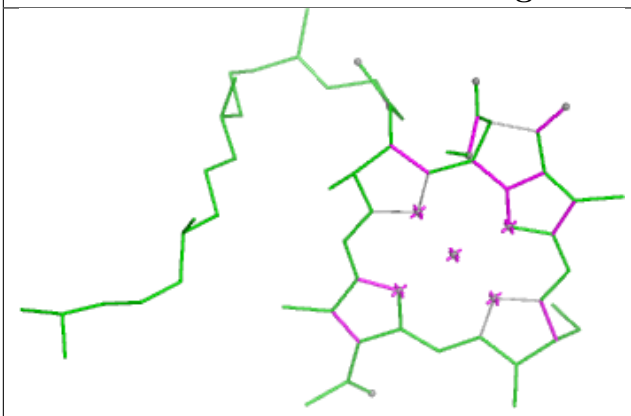
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1302	BCL	1	0
4	A	1283	BCL	2	0
8	B	1306	U10	2	0
4	B	1303	BCL	8	0
6	A	1285	MST	9	0
5	A	1284	BPH	4	0
4	A	1282	BCL	3	0
5	B	1304	BPH	6	0

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.

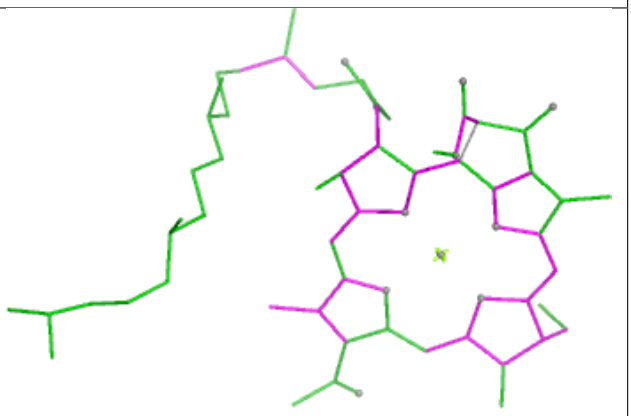
Ligand BCL B 1302



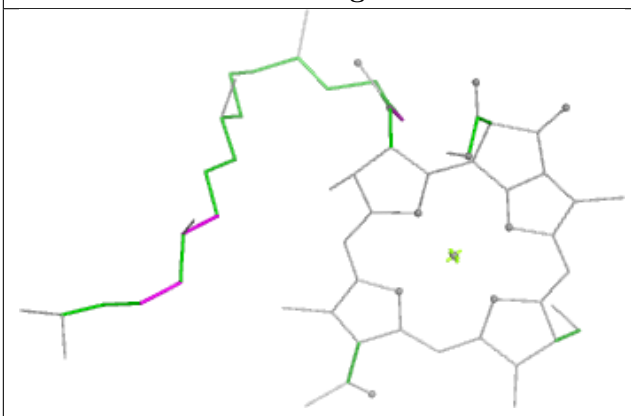
Ligand BCL A 1283



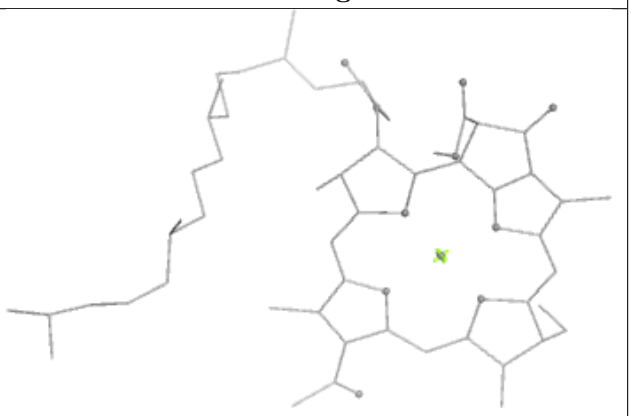
Bond lengths



Bond angles

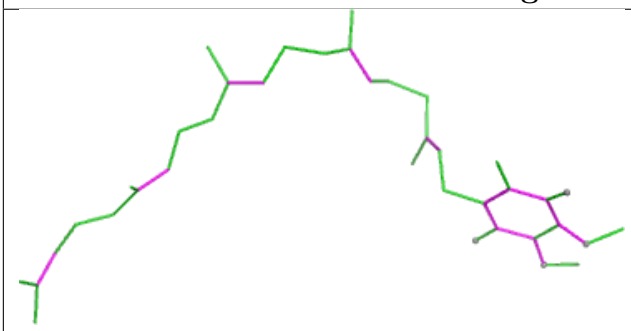


Torsions

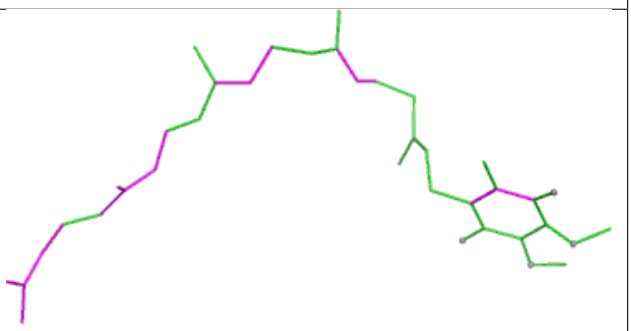


Rings

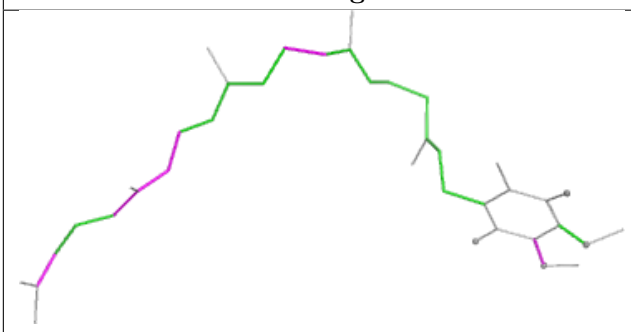
Ligand U10 B 1306



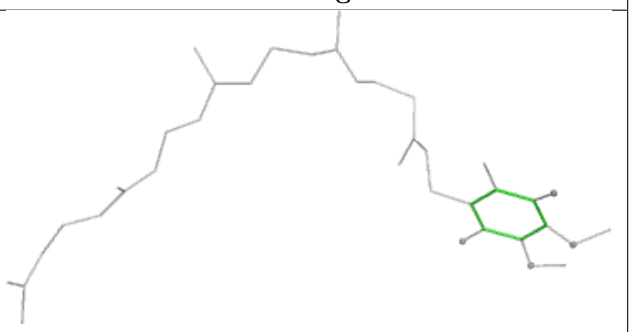
Bond lengths



Bond angles

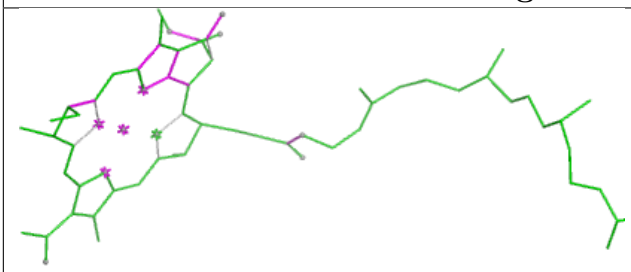


Torsions

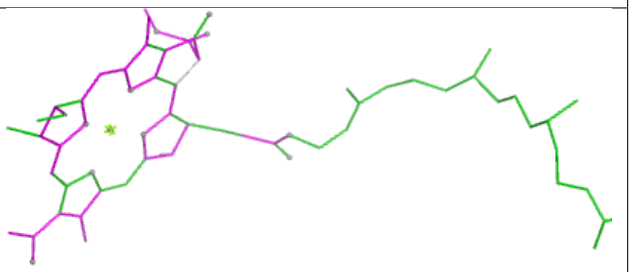


Rings

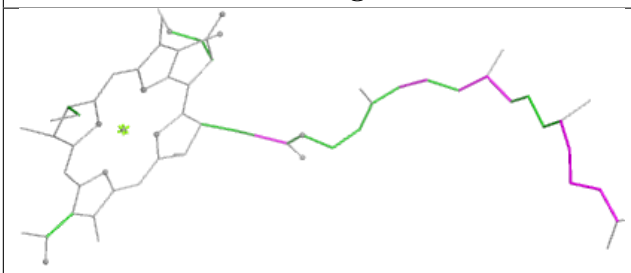
Ligand BCL B 1303



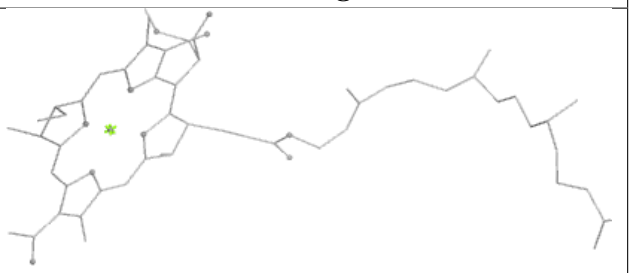
Bond lengths



Bond angles

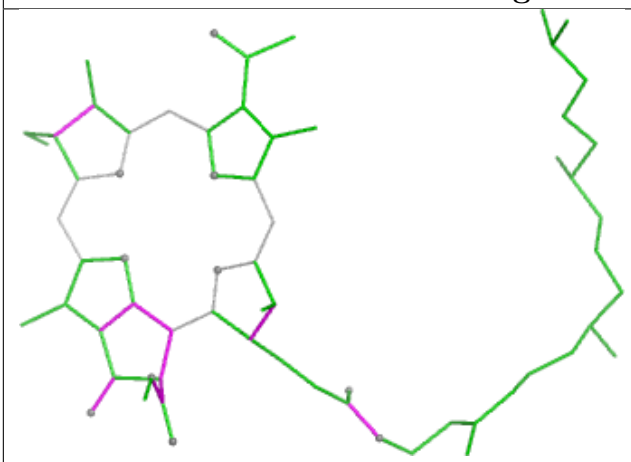


Torsions

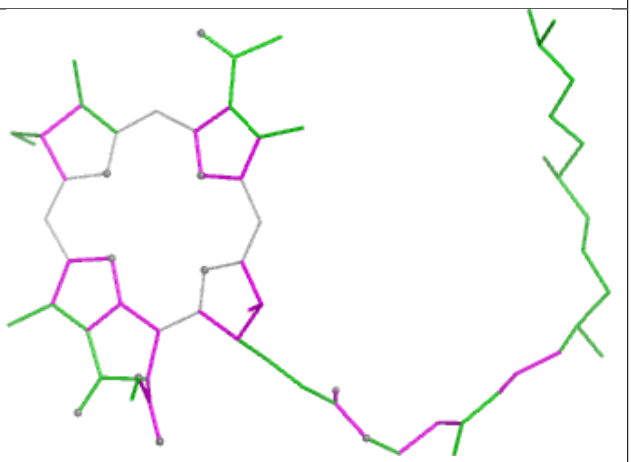


Rings

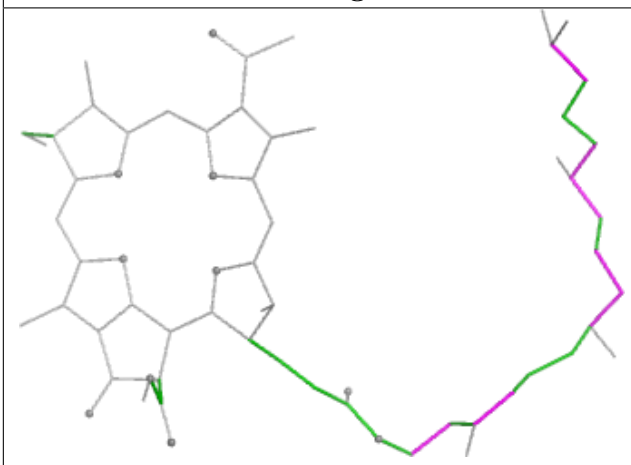
Ligand BPH A 1284



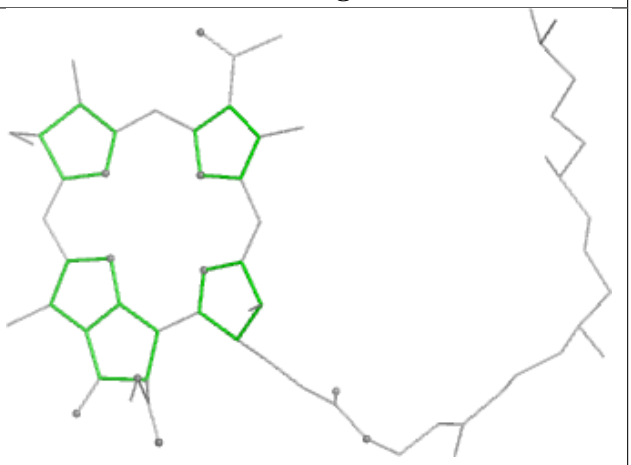
Bond lengths



Bond angles

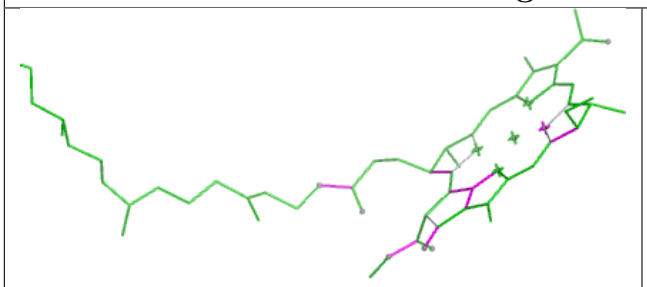


Torsions

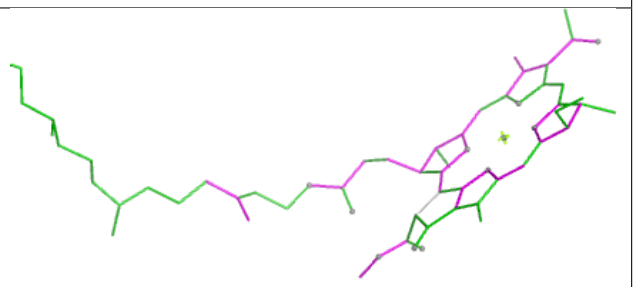


Rings

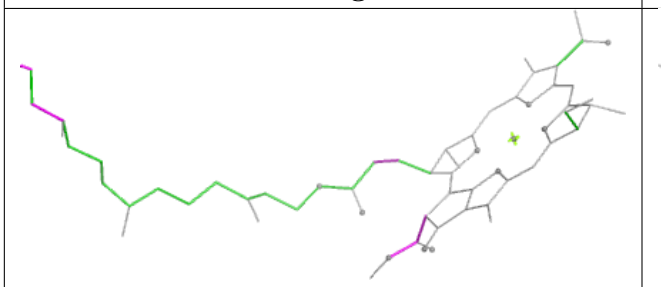
Ligand BCL A 1282



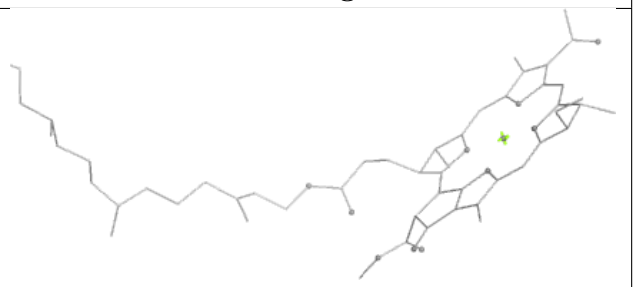
Bond lengths



Bond angles

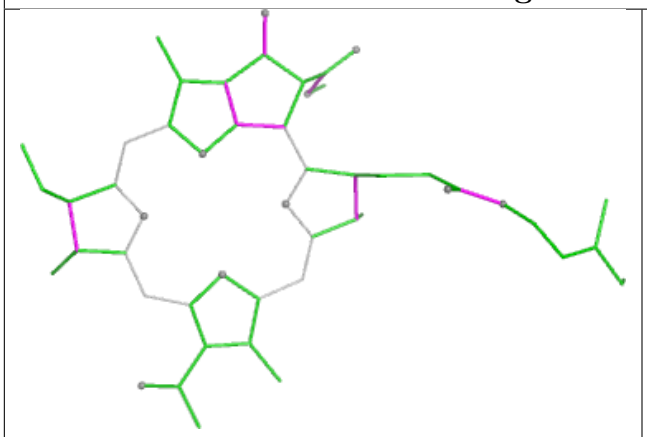


Torsions

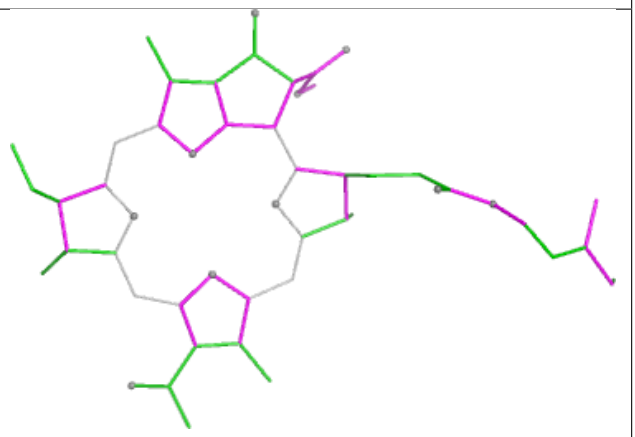


Rings

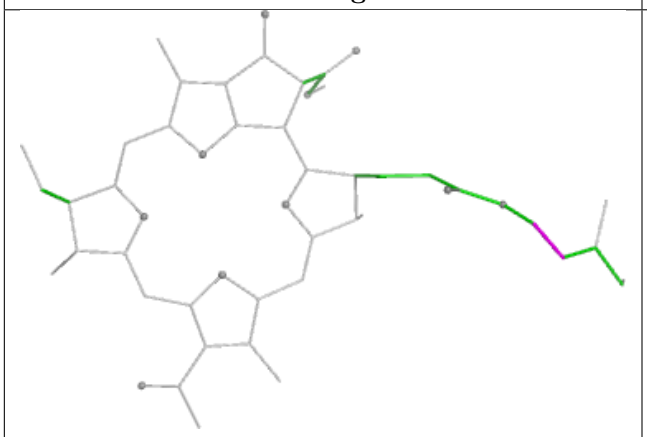
Ligand BPH B 1304



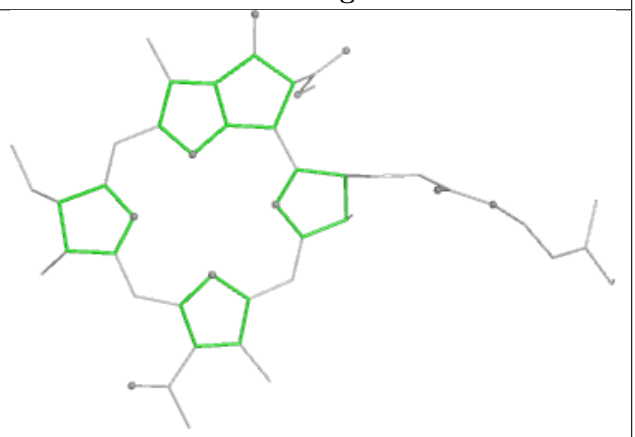
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1:ALA	C	2:GLU	N	1.03

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	A	281/281 (100%)	0.17	10 (3%)	46	42	20, 29, 53, 58	1 (0%)
2	B	301/307 (98%)	0.13	6 (1%)	65	62	16, 27, 44, 53	4 (1%)
3	C	237/260 (91%)	0.41	8 (3%)	48	44	13, 36, 42, 52	8 (3%)
All	All	819/848 (96%)	0.23	24 (2%)	53	50	13, 30, 44, 58	13 (1%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	302	GLY	6.1
1	A	268	LYS	4.7
2	B	3	TYR	4.1
2	B	301	HIS	3.8
1	A	265	TRP	3.7
3	C	247	LYS	3.5
1	A	270	PRO	3.5
1	A	271	TRP	3.1
3	C	245	ALA	2.9
3	C	246	PRO	2.9
1	A	267	VAL	2.9
1	A	269	LEU	2.9
3	C	138	ALA	2.9
3	C	244	ALA	2.9
3	C	200	SER	2.8
2	B	148	TRP	2.8
3	C	11	ASP	2.5
2	B	2	GLU	2.5
1	A	274	ASN	2.3
1	A	1	ALA	2.3
2	B	188	ASN	2.3
1	A	59	TRP	2.3
3	C	211	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	275	ILE	2.1

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

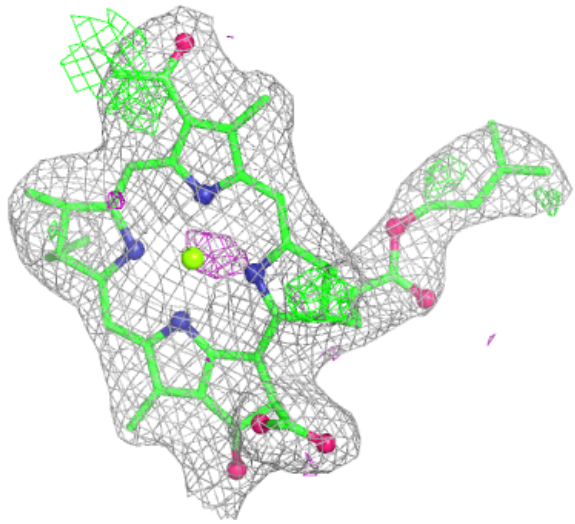
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

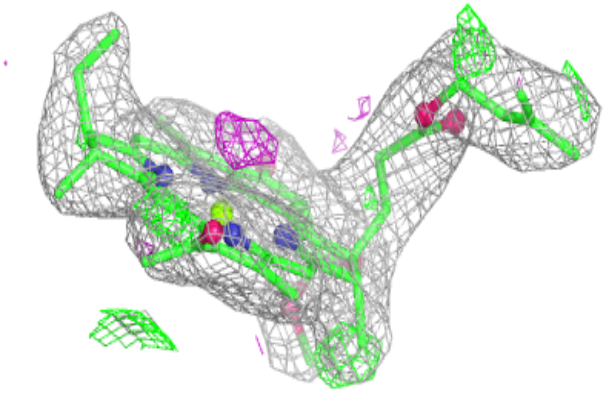
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MST	A	1285	16/16	0.74	0.28	52,56,58,60	0
4	BCL	B	1302	51/66	0.90	0.15	38,42,48,50	0
4	BCL	A	1282	66/66	0.91	0.14	39,41,47,49	0
4	BCL	B	1303	66/66	0.92	0.15	37,40,49,51	0
4	BCL	A	1283	66/66	0.92	0.14	37,40,50,50	0
5	BPH	B	1304	51/65	0.93	0.14	43,46,52,54	0
5	BPH	A	1284	65/65	0.93	0.14	35,37,46,48	0
8	U10	B	1306	38/63	0.93	0.17	43,47,60,60	0
10	PO4	B	1309	5/5	0.94	0.11	55,56,56,56	0
10	PO4	B	1308	5/5	0.96	0.12	35,36,38,39	0
9	CL	B	1307	1/1	0.96	0.26	52,52,52,52	0
7	FE2	B	1305	1/1	1.00	0.02	30,30,30,30	0

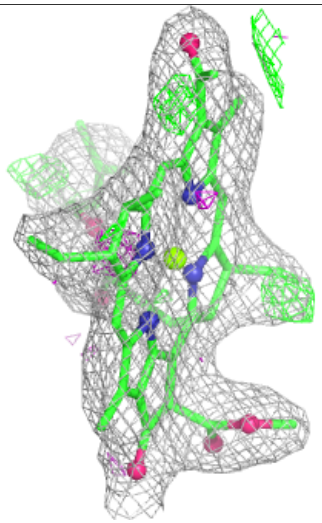
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BCL B 1302:

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

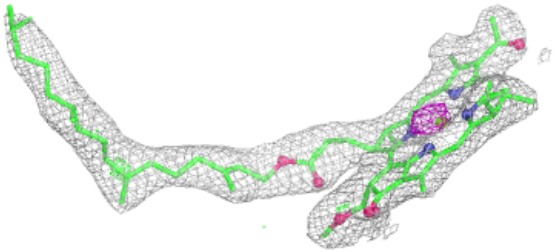


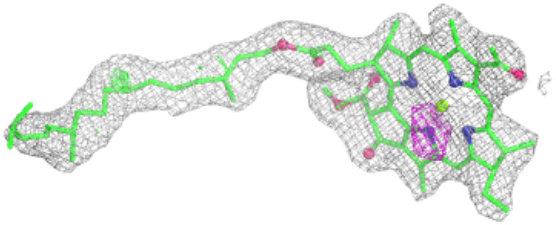


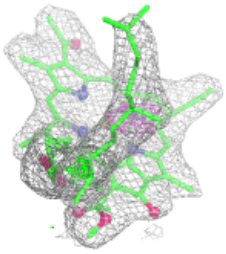


Electron density around BCL A 1282:

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

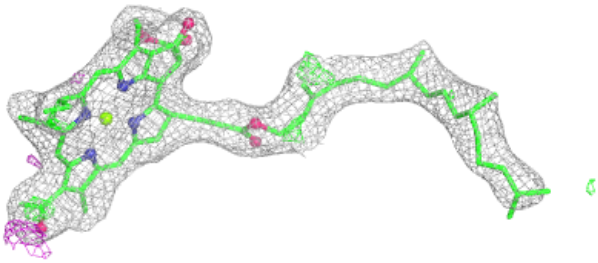


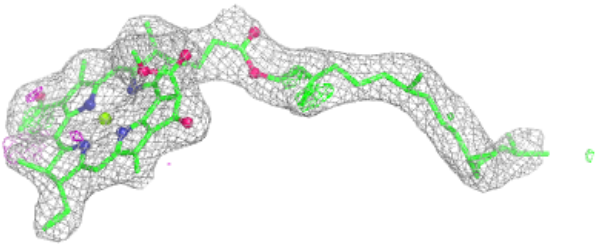


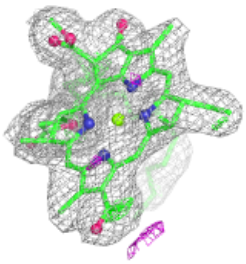


Electron density around BCL B 1303:

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

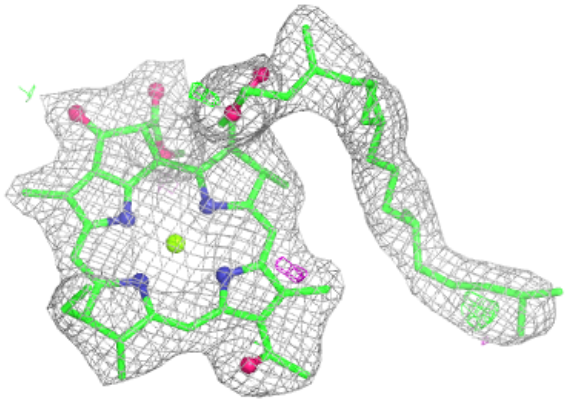


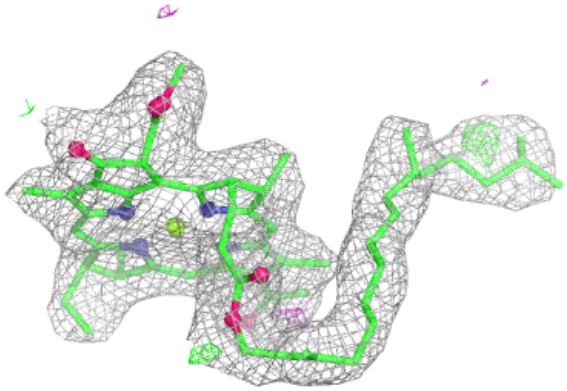


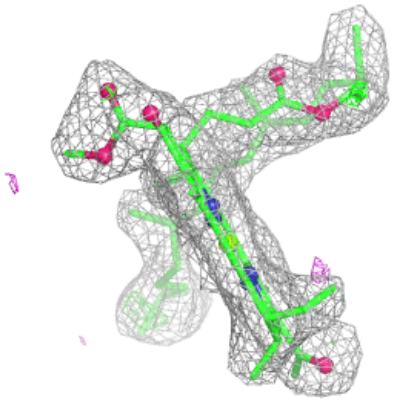


Electron density around BCL A 1283:

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

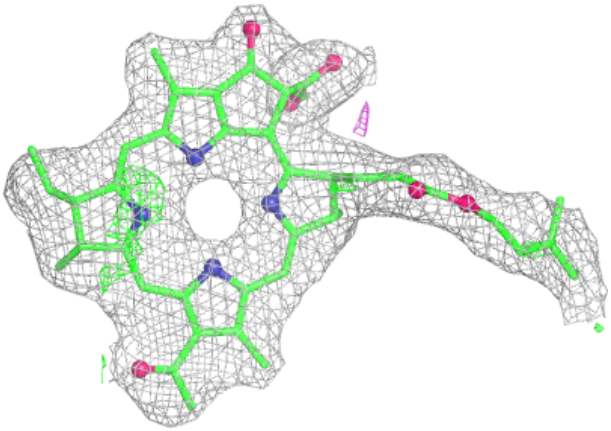


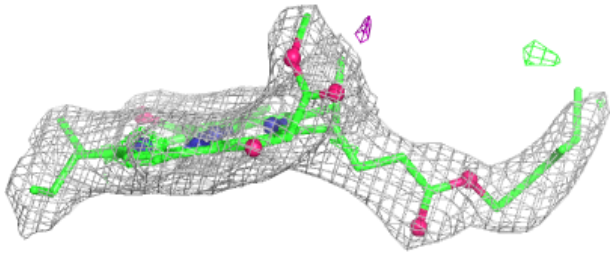


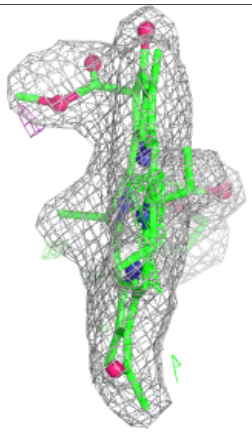


Electron density around BPH B 1304:

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

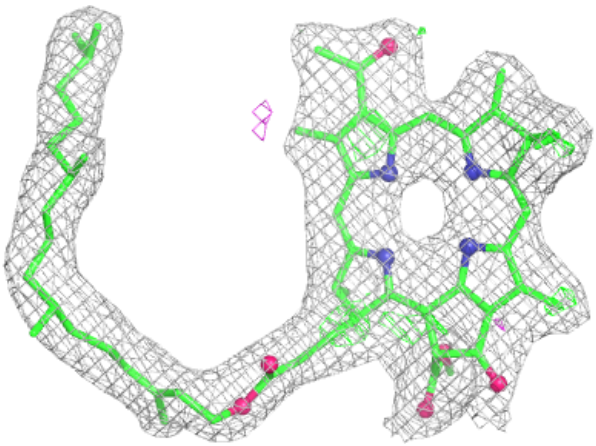


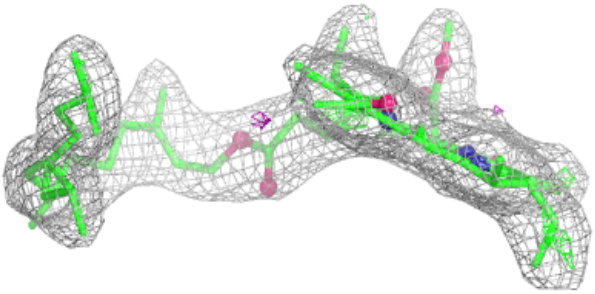


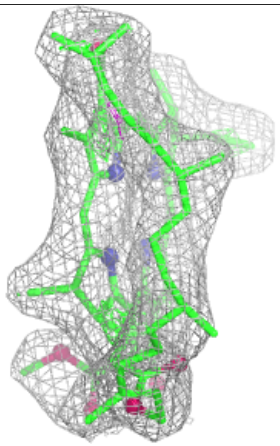


Electron density around BPH A 1284:

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

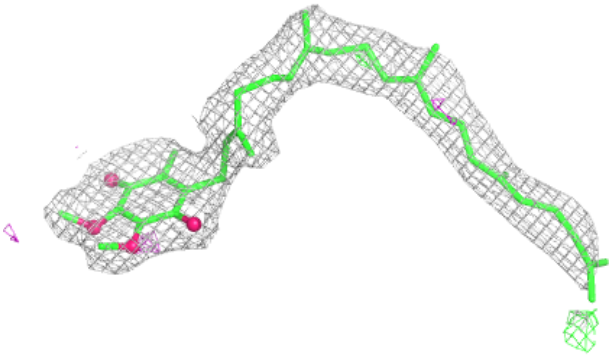


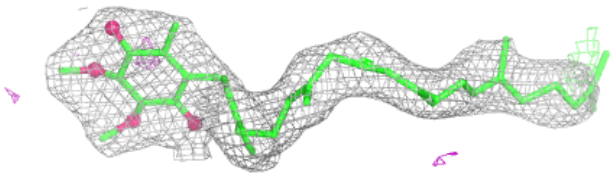


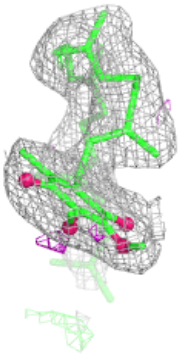


Electron density around U10 B 1306:

$2mF_o$-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.