Full wwPDB X-ray Structure Validation Report (i)

Apr 21, 2024 – 02:22 am BST

PDB ID	:	2JJ0
Title	:	PHOTOSYNTHETIC REACTION CENTER MUTANT WITH ALA M248 REPLACED WITH TRP (CHAIN M, AM248W)
Authors	:	Fyfe, P.K.; Potter, J.A.; Cheng, J.; Williams, C.M.; Watson, A.J.; Jones, M.R.
Deposited on	:	2007-07-03
Resolution	:	2.80 Å(reported)

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

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

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

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

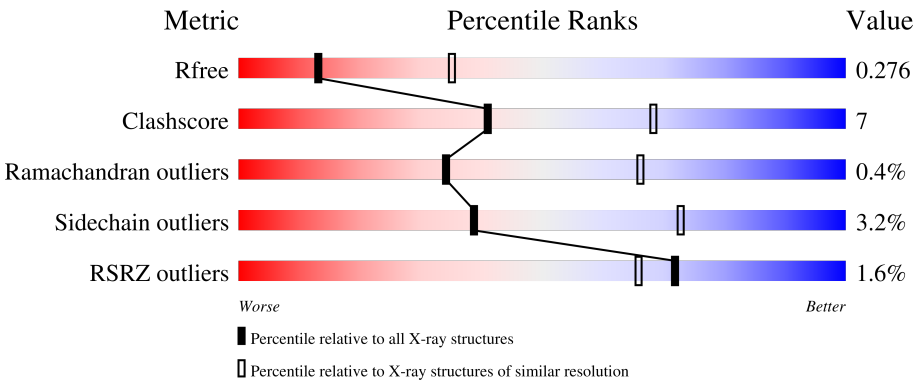
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	H	260	.% 79% 10% • 10%
2	L	281	2% 84% 15% •
3	M	308	.% 87% 11% •

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 7111 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	235	1796	1148	305	334	9	0	1	0

- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	281	2244	1516	356	364	8	0	1	0

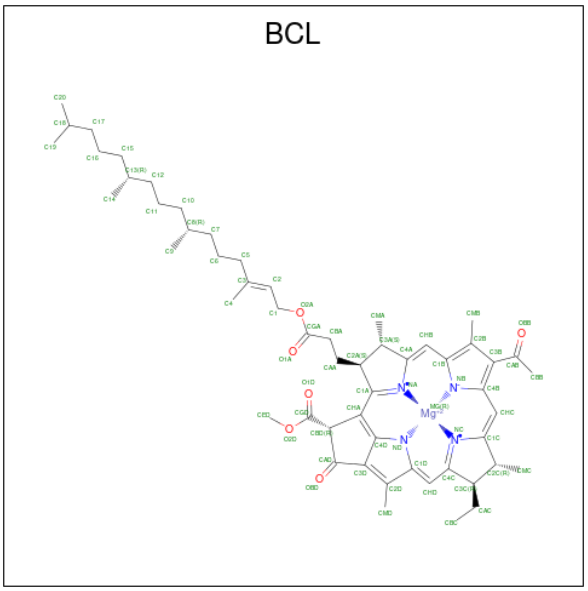
- Molecule 3 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	301	2412	1612	394	396	10	0	0	0

There is a discrepancy between the modelled and reference sequences:

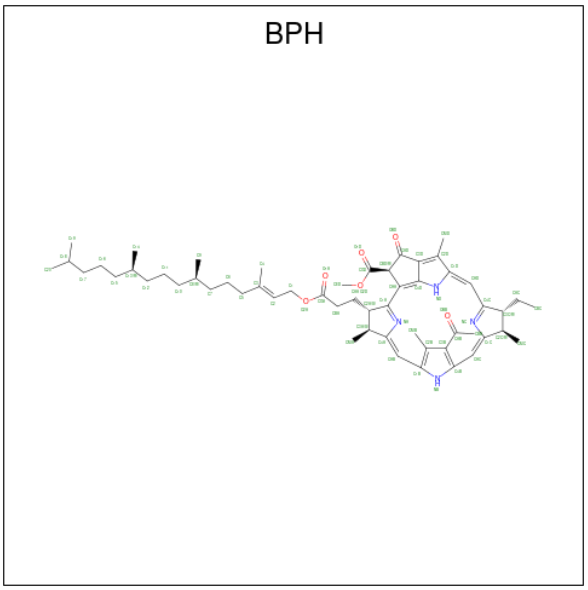
Chain	Residue	Modelled	Actual	Comment	Reference
M	248	TRP	ALA	engineered mutation	UNP P0C0Y9

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



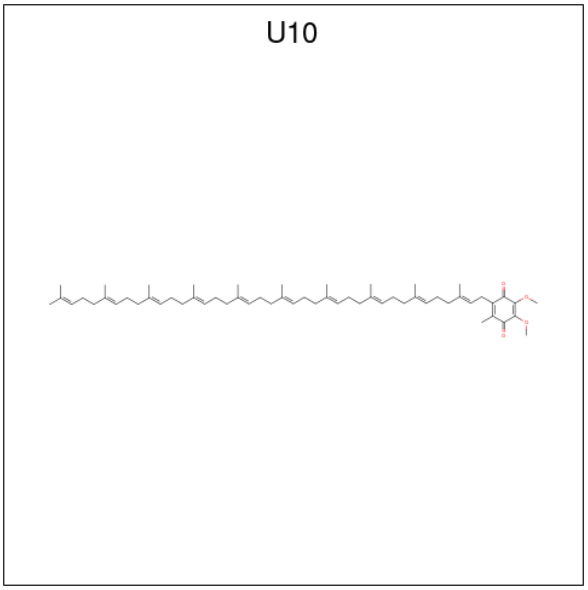
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
4	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
4	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
4	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
4	M	1	66	55	1	4	6	0	0

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



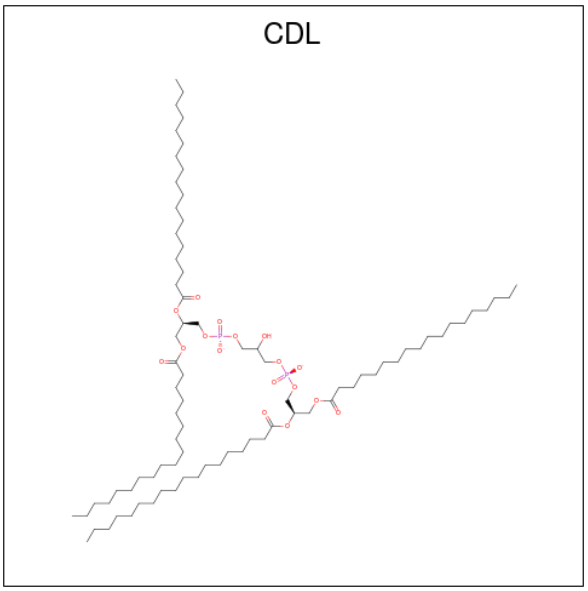
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	L	1	65	55	4	6	0	0
			Total	C	N	O		
5	M	1	65	55	4	6	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	L	1	17	13	4	0	0

- Molecule 7 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

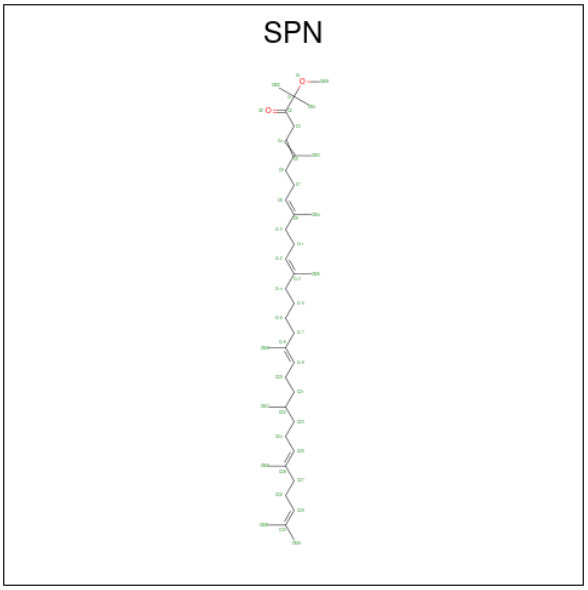


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
7	M	1	81	62	17	2	0	0

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

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

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



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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
10	M	1	1	1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	H	55	55	55	0	0

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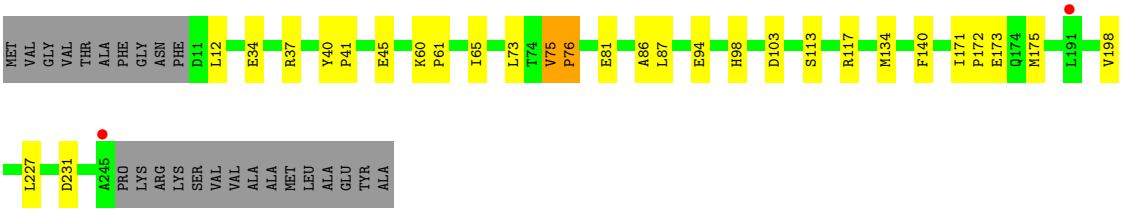
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	L	23	23	23	0	0
			Total	O		
11	M	44	44	44	0	0

3 Residue-property plots (i)

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

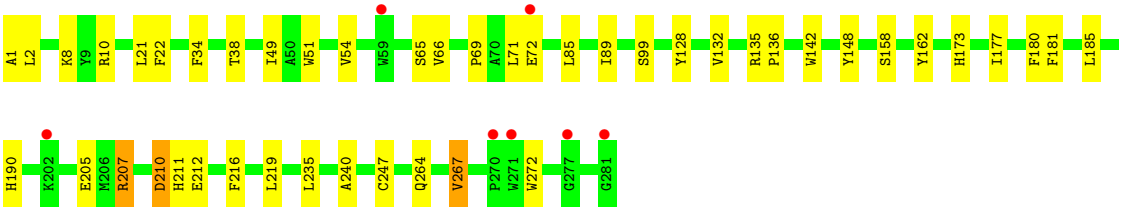
• Molecule 1: REACTION CENTER PROTEIN H CHAIN

Chain H:



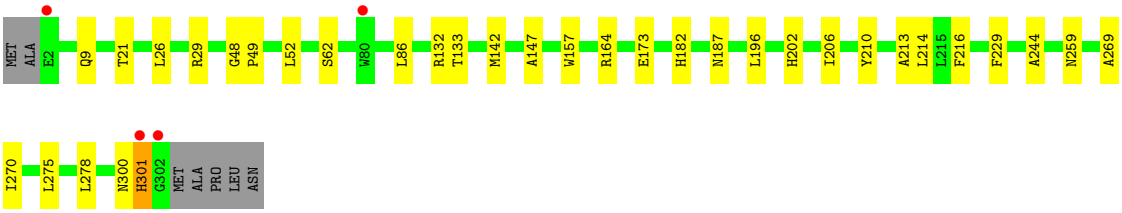
• Molecule 2: REACTION CENTER PROTEIN L CHAIN

Chain L:



• Molecule 3: REACTION CENTER PROTEIN M CHAIN

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.81Å 139.81Å 185.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.90 – 2.80 25.41 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (27.90-2.80) 99.0 (25.41-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.203 , 0.245 0.234 , 0.276	Depositor DCC
R_{free} test set	2573 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	60.5	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7111	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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: BPH, CL, FE, U10, BCL, SPN, CDL

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	0.64	0/1843	0.74	1/2509 (0.0%)
2	L	0.61	0/2333	0.63	0/3194
3	M	0.59	0/2506	0.65	1/3422 (0.0%)
All	All	0.61	0/6682	0.67	2/9125 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	2
3	M	0	2
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	103	ASP	CB-CG-OD1	5.17	122.95	118.30
3	M	29	ARG	NE-CZ-NH2	-5.13	117.74	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	40	TYR	Peptide
1	H	75	VAL	Peptide
3	M	300	ASN	Peptide

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Mol	Chain	Res	Type	Group
3	M	48	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1796	0	1790	20	0
2	L	2244	0	2196	33	0
3	M	2412	0	2318	28	0
4	L	198	0	222	17	0
4	M	66	0	74	7	0
5	L	65	0	76	7	0
5	M	65	0	76	8	0
6	L	17	0	15	2	0
7	M	81	0	106	2	0
8	M	1	0	0	0	0
9	M	43	0	69	9	0
10	M	1	0	0	0	0
11	H	55	0	0	1	0
11	L	23	0	0	0	0
11	M	44	0	0	1	0
All	All	7111	0	6942	99	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (99) 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)
3:M:275:LEU:HD23	3:M:278:LEU:HD23	1.53	0.88
4:L:1283:BCL:HBB3	4:L:1283:BCL:HMB1	1.61	0.80
5:L:1285:BPH:HHC	5:L:1285:BPH:HBB3	1.62	0.80
5:M:1307:BPH:HHC	5:M:1307:BPH:HBB3	1.64	0.79
2:L:181:PHE:CD2	5:M:1307:BPH:HBB1	2.20	0.77
1:H:41:PRO:HD2	11:H:2008:HOH:O	1.85	0.77
2:L:181:PHE:HB3	5:M:1307:BPH:HBB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1285:BPH:HBB2	3:M:210:TYR:HB3	1.71	0.73
4:L:1283:BCL:HMB1	4:L:1283:BCL:CBB	2.18	0.73
3:M:157:TRP:CD1	9:M:1308:SPN:H202	2.24	0.73
1:H:173[B]:GLU:OE2	1:H:175:MET:HE3	1.91	0.70
1:H:198:VAL:H	3:M:9:GLN:HE22	1.39	0.69
1:H:198:VAL:H	3:M:9:GLN:NE2	1.91	0.67
3:M:133:THR:HG21	3:M:147:ALA:HA	1.78	0.66
4:L:1284:BCL:HMD1	3:M:206:ILE:HD13	1.78	0.66
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.77	0.65
1:H:61:PRO:HA	1:H:76:PRO:HD3	1.77	0.65
2:L:264:GLN:HA	2:L:267:VAL:HG13	1.77	0.65
2:L:21:LEU:HD23	2:L:22:PHE:CE1	2.33	0.63
4:L:1284:BCL:CBB	4:L:1284:BCL:HMB1	2.28	0.63
2:L:38:THR:HG22	2:L:99:SER:HB2	1.80	0.62
3:M:133:THR:CG2	3:M:147:ALA:HA	2.30	0.61
4:L:1284:BCL:HMB1	4:L:1284:BCL:HBB2	1.82	0.61
1:H:37:ARG:NH2	1:H:60:LYS:O	2.33	0.61
2:L:71:LEU:H	2:L:71:LEU:HD12	1.66	0.60
2:L:190:HIS:HA	6:L:1286:U10:O2	2.03	0.59
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.86	0.58
1:H:173[B]:GLU:OE2	1:H:175:MET:CE	2.51	0.58
4:L:1282:BCL:H62	4:M:1304:BCL:H203	1.84	0.58
2:L:51:TRP:O	2:L:54:VAL:HG22	2.04	0.57
4:L:1282:BCL:C6	4:M:1304:BCL:H203	2.34	0.57
3:M:157:TRP:NE1	9:M:1308:SPN:H202	2.19	0.56
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.87	0.56
4:L:1282:BCL:HMB1	4:L:1282:BCL:HBB2	1.88	0.55
3:M:133:THR:HG22	3:M:147:ALA:HB2	1.87	0.55
1:H:34:GLU:O	1:H:37:ARG:HG3	2.08	0.54
4:M:1304:BCL:CBB	4:M:1304:BCL:HMB1	2.38	0.54
4:L:1282:BCL:HMB1	4:L:1282:BCL:CBB	2.38	0.53
2:L:38:THR:HG22	2:L:99:SER:CB	2.37	0.53
1:H:117:ARG:NH2	1:H:227:LEU:HD22	2.25	0.52
2:L:128:TYR:CE2	2:L:132:VAL:HG21	2.44	0.52
9:M:1308:SPN:HMA3	9:M:1308:SPN:H32	1.91	0.52
1:H:86:ALA:O	1:H:87:LEU:HD23	2.10	0.52
4:L:1282:BCL:CAB	9:M:1308:SPN:H162	2.40	0.52
2:L:207:ARG:HG3	3:M:142:MET:HG2	1.92	0.51
1:H:45:GLU:HG3	1:H:94:GLU:OE2	2.11	0.51
3:M:164:ARG:HH12	3:M:173:GLU:HG3	1.75	0.51
4:L:1282:BCL:C3B	9:M:1308:SPN:H152	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1285:BPH:HBB1	3:M:210:TYR:CD2	2.46	0.51
4:L:1282:BCL:H141	9:M:1308:SPN:H101	1.92	0.50
2:L:219:LEU:HD12	3:M:132:ARG:NH1	2.27	0.50
4:M:1304:BCL:H202	5:M:1307:BPH:HMA3	1.92	0.50
3:M:270:ILE:HD13	7:M:1305:CDL:H311	1.94	0.50
3:M:157:TRP:CE2	9:M:1308:SPN:HM73	2.47	0.49
2:L:181:PHE:HB3	5:M:1307:BPH:CBB	2.40	0.48
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.46	0.48
2:L:177:ILE:HG12	4:L:1283:BCL:HMB3	1.95	0.47
5:L:1285:BPH:CMC	3:M:213:ALA:HB3	2.44	0.47
3:M:278:LEU:HD13	7:M:1305:CDL:H391	1.97	0.47
1:H:87:LEU:HD13	1:H:98:HIS:HB2	1.95	0.47
2:L:34:PHE:O	2:L:38:THR:HG23	2.14	0.47
3:M:206:ILE:HG12	4:M:1304:BCL:HMB3	1.97	0.47
1:H:140:PHE:CE2	1:H:171:ILE:HG23	2.50	0.47
2:L:85:LEU:O	2:L:89:ILE:HG13	2.15	0.47
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.49	0.47
1:H:65:ILE:HB	2:L:205:GLU:HA	1.98	0.46
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.97	0.46
2:L:210:ASP:OD1	2:L:210:ASP:N	2.49	0.46
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.51	0.46
1:H:61:PRO:HA	1:H:76:PRO:CD	2.46	0.46
2:L:207:ARG:HB3	2:L:211:HIS:CG	2.51	0.46
4:L:1282:BCL:OBB	9:M:1308:SPN:HM63	2.16	0.45
2:L:66:VAL:HG11	2:L:89:ILE:HD12	1.97	0.45
5:L:1285:BPH:HHC	5:L:1285:BPH:CBB	2.40	0.45
1:H:117:ARG:CZ	1:H:227:LEU:HD22	2.47	0.45
2:L:1:ALA:O	2:L:2:LEU:HD23	2.17	0.44
1:H:73:LEU:HG	1:H:75:VAL:HG13	2.00	0.44
1:H:171:ILE:HB	1:H:172:PRO:CD	2.48	0.43
4:L:1282:BCL:C14	9:M:1308:SPN:H101	2.49	0.42
3:M:133:THR:HG22	3:M:147:ALA:CB	2.49	0.42
5:M:1307:BPH:HHC	5:M:1307:BPH:CBB	2.44	0.42
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.55	0.42
4:L:1284:BCL:CMD	3:M:206:ILE:HD13	2.47	0.42
5:L:1285:BPH:HBB3	5:L:1285:BPH:CHC	2.43	0.42
3:M:259:ASN:ND2	11:M:2036:HOH:O	2.52	0.42
2:L:128:TYR:O	2:L:132:VAL:HG22	2.20	0.41
4:M:1304:BCL:HMB1	4:M:1304:BCL:HBB3	2.02	0.41
5:M:1307:BPH:HBB3	5:M:1307:BPH:CHC	2.43	0.41
4:L:1282:BCL:H61	4:M:1304:BCL:H203	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.55	0.41
2:L:2:LEU:CD2	2:L:10:ARG:CZ	2.98	0.41
1:H:75:VAL:HG23	1:H:75:VAL:O	2.20	0.41
1:H:81:GLU:OE2	2:L:8:LYS:NZ	2.31	0.41
2:L:212:GLU:OE2	6:L:1286:U10:H3M2	2.21	0.41
2:L:65:SER:HA	2:L:148:TYR:O	2.20	0.41
5:M:1307:BPH:H6C1	5:M:1307:BPH:H4C1	1.58	0.41
5:L:1285:BPH:ND	3:M:214:LEU:HD13	2.36	0.40
2:L:49:ILE:HG13	2:L:89:ILE:HD13	2.03	0.40
3:M:269:ALA:O	3:M:270:ILE:C	2.59	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	234/260 (90%)	224 (96%)	9 (4%)	1 (0%)	34	66
2	L	280/281 (100%)	265 (95%)	15 (5%)	0	100	100
3	M	299/308 (97%)	284 (95%)	13 (4%)	2 (1%)	22	53
All	All	813/849 (96%)	773 (95%)	37 (5%)	3 (0%)	34	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	49	PRO
3	M	301	HIS
1	H	76	PRO

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	191/208 (92%)	187 (98%)	4 (2%)	53	84
2	L	221/220 (100%)	211 (96%)	10 (4%)	27	60
3	M	237/242 (98%)	230 (97%)	7 (3%)	41	75
All	All	649/670 (97%)	628 (97%)	21 (3%)	39	73

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

Mol	Chain	Res	Type
1	H	12	LEU
1	H	113	SER
1	H	134	MET
1	H	231	ASP
2	L	72	GLU
2	L	158	SER
2	L	185	LEU
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	235	LEU
2	L	247	CYS
2	L	267	VAL
2	L	272	TRP
3	M	52	LEU
3	M	62	SER
3	M	86	LEU
3	M	182	HIS
3	M	196	LEU
3	M	216	PHE
3	M	301	HIS

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

Mol	Chain	Res	Type
1	H	68	HIS
2	L	183	ASN
2	L	280	ASN
3	M	4	GLN
3	M	9	GLN
3	M	28	ASN
3	M	187	ASN
3	M	193	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	L	1282	3	64,74,74	1.34	3 (4%)	78,115,115	1.64	18 (23%)
5	BPH	M	1307	-	51,70,70	0.72	1 (1%)	52,101,101	1.80	12 (23%)
6	U10	L	1286	-	17,17,63	2.20	2 (11%)	19,23,79	1.29	3 (15%)
7	CDL	M	1305	-	80,80,99	1.11	4 (5%)	86,92,111	1.11	7 (8%)
4	BCL	L	1284	2	64,74,74	1.17	5 (7%)	78,115,115	1.72	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	SPN	M	1308	-	40,42,42	3.70	16 (40%)	50,52,52	2.14	20 (40%)
4	BCL	M	1304	3	64,74,74	1.25	4 (6%)	78,115,115	1.40	12 (15%)
5	BPH	L	1285	-	51,70,70	0.81	1 (1%)	52,101,101	1.46	8 (15%)
4	BCL	L	1283	2	64,74,74	1.19	3 (4%)	78,115,115	1.27	10 (12%)

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	L	1282	3	-	9/37/137/137	-
5	BPH	M	1307	-	-	15/37/105/105	0/5/6/6
6	U10	L	1286	-	-	3/8/32/87	0/1/1/1
7	CDL	M	1305	-	-	44/91/91/110	-
4	BCL	L	1284	2	-	5/37/137/137	-
9	SPN	M	1308	-	-	15/50/51/51	-
4	BCL	M	1304	3	-	1/37/137/137	-
5	BPH	L	1285	-	-	15/37/105/105	0/5/6/6
4	BCL	L	1283	2	-	6/37/137/137	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1308	SPN	C3-C4	-9.51	1.36	1.50
6	L	1286	U10	C6-C1	8.07	1.50	1.35
9	M	1308	SPN	C10-C9	-7.71	1.35	1.51
9	M	1308	SPN	C14-C13	-7.35	1.36	1.51
9	M	1308	SPN	C6-C5	-7.24	1.36	1.51
9	M	1308	SPN	C17-C18	-6.92	1.36	1.51
4	L	1282	BCL	MG-NA	6.13	2.20	2.06
9	M	1308	SPN	C4-C5	6.06	1.47	1.33
9	M	1308	SPN	C19-C18	5.93	1.47	1.33
9	M	1308	SPN	C8-C9	5.83	1.47	1.33
4	M	1304	BCL	MG-NA	5.64	2.19	2.06
4	L	1283	BCL	MG-NA	5.62	2.19	2.06
9	M	1308	SPN	C12-C13	5.50	1.46	1.33
4	L	1282	BCL	C1B-NB	5.24	1.39	1.35
4	M	1304	BCL	C4B-NB	4.97	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1305	CDL	OB8-CB7	4.80	1.47	1.33
7	M	1305	CDL	OA6-CA5	4.63	1.47	1.34
9	M	1308	SPN	C7-C8	-4.55	1.35	1.50
9	M	1308	SPN	C11-C12	-4.51	1.35	1.50
9	M	1308	SPN	C20-C19	-4.20	1.36	1.50
7	M	1305	CDL	OA8-CA7	4.05	1.45	1.33
7	M	1305	CDL	OB6-CB5	4.04	1.45	1.34
4	L	1283	BCL	C1B-NB	3.63	1.38	1.35
4	L	1283	BCL	C4B-NB	3.35	1.38	1.35
9	M	1308	SPN	C21-C22	-3.31	1.35	1.52
4	L	1284	BCL	MG-NA	3.29	2.14	2.06
6	L	1286	U10	C4-C3	3.19	1.49	1.36
4	L	1282	BCL	C4B-NB	3.06	1.37	1.35
4	L	1284	BCL	C4D-ND	-3.05	1.33	1.37
4	L	1284	BCL	C4B-NB	2.75	1.37	1.35
9	M	1308	SPN	C16-C15	-2.69	1.36	1.51
4	L	1284	BCL	C3C-C4C	-2.55	1.48	1.51
5	L	1285	BPH	C2C-C3C	2.53	1.57	1.54
9	M	1308	SPN	C1-C2	-2.45	1.51	1.53
4	M	1304	BCL	C1B-CHB	-2.42	1.34	1.41
4	M	1304	BCL	C4D-ND	-2.36	1.34	1.37
5	M	1307	BPH	C3A-C2A	-2.25	1.52	1.54
4	L	1284	BCL	C1B-NB	2.18	1.37	1.35
9	M	1308	SPN	C6-C7	-2.05	1.46	1.53

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1307	BPH	O2D-CGD-CBD	6.38	119.08	111.00
9	M	1308	SPN	CM5-C13-C14	4.98	123.64	115.27
4	L	1284	BCL	O2D-CGD-CBD	4.94	120.04	111.27
4	L	1282	BCL	CMB-C2B-C1B	-4.85	121.01	128.46
5	M	1307	BPH	C1-O2A-CGA	4.76	128.94	116.44
5	L	1285	BPH	CMA-C3A-C4A	-4.39	104.76	114.38
7	M	1305	CDL	OA6-CA5-C11	4.31	120.80	111.50
4	M	1304	BCL	CHD-C1D-ND	-4.30	120.50	124.45
4	L	1284	BCL	O1D-CGD-CBD	-4.28	115.73	124.48
4	L	1282	BCL	CHD-C1D-ND	-4.23	120.57	124.45
4	L	1283	BCL	CHD-C1D-ND	-4.22	120.58	124.45
7	M	1305	CDL	OB6-CB5-C51	4.14	120.43	111.50
9	M	1308	SPN	CM6-C18-C17	4.07	122.11	115.27
4	M	1304	BCL	C4D-CHA-C1A	4.07	126.20	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	1284	BCL	CHD-C1D-ND	-4.00	120.78	124.45
5	L	1285	BPH	O2D-CGD-CBD	3.87	115.89	111.00
4	L	1282	BCL	CMB-C2B-C3B	3.80	131.78	124.68
5	M	1307	BPH	C1-C2-C3	-3.67	119.70	126.04
9	M	1308	SPN	C15-C14-C13	3.59	122.86	113.45
9	M	1308	SPN	CM3-C5-C6	3.57	121.27	115.27
4	L	1284	BCL	CAC-C3C-C2C	-3.55	105.39	114.26
9	M	1308	SPN	CM4-C9-C10	3.52	121.19	115.27
4	L	1284	BCL	CMB-C2B-C1B	-3.51	123.08	128.46
9	M	1308	SPN	C15-C16-C17	3.45	125.61	113.19
9	M	1308	SPN	C16-C17-C18	3.44	122.48	113.45
4	L	1282	BCL	C1-O2A-CGA	3.42	125.41	116.44
4	L	1284	BCL	CAC-C3C-C4C	-3.41	105.01	112.58
9	M	1308	SPN	C11-C10-C9	3.33	123.94	112.98
5	M	1307	BPH	OBD-CAD-CBD	-3.29	121.00	125.82
4	M	1304	BCL	CHA-C1A-NA	-3.29	118.87	126.40
4	M	1304	BCL	CMB-C2B-C1B	-3.26	123.46	128.46
9	M	1308	SPN	C7-C6-C5	3.24	123.63	112.98
9	M	1308	SPN	C16-C15-C14	3.16	124.54	113.19
4	L	1282	BCL	C4D-CHA-C1A	3.15	125.08	121.25
4	L	1284	BCL	CAA-C2A-C3A	-3.12	104.23	112.78
4	L	1284	BCL	C2C-C3C-C4C	3.07	105.94	101.34
4	L	1282	BCL	O2A-C1-C2	3.01	116.55	108.64
4	L	1284	BCL	C4D-CHA-C1A	2.98	124.87	121.25
4	L	1283	BCL	C4A-NA-C1A	-2.92	105.39	106.71
7	M	1305	CDL	OB6-CB5-OB7	-2.90	116.69	123.70
5	L	1285	BPH	C1-C2-C3	-2.87	121.09	126.04
4	L	1284	BCL	C5-C3-C2	-2.86	115.33	121.12
9	M	1308	SPN	C3-C4-C5	-2.84	122.06	126.79
4	L	1282	BCL	O2D-CGD-CBD	2.83	116.30	111.27
5	M	1307	BPH	CAA-C2A-C3A	-2.81	105.08	112.78
4	L	1283	BCL	CAA-C2A-C3A	-2.80	105.12	112.78
5	M	1307	BPH	C4B-NB-C1B	2.76	112.76	107.09
4	L	1284	BCL	CAA-CBA-CGA	2.76	121.32	113.25
9	M	1308	SPN	CM7-C22-C21	2.73	121.18	111.29
4	M	1304	BCL	CAC-C3C-C4C	-2.70	106.59	112.58
4	L	1282	BCL	CHA-C1A-NA	-2.70	120.22	126.40
4	L	1282	BCL	CHD-C1D-C2D	2.64	131.01	125.48
5	M	1307	BPH	O1D-CGD-CBD	-2.63	120.36	124.74
4	L	1283	BCL	CHD-C1D-C2D	2.62	130.98	125.48
4	L	1283	BCL	CHA-C1A-NA	-2.62	120.39	126.40
5	M	1307	BPH	CMB-C2B-C3B	2.58	129.50	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1307	BPH	C5-C3-C2	2.57	126.33	121.12
4	M	1304	BCL	C1D-ND-C4D	2.54	108.14	106.33
5	L	1285	BPH	C1A-C2A-C3A	-2.53	100.43	102.84
7	M	1305	CDL	OA8-CA7-C31	2.53	119.86	111.91
4	L	1284	BCL	C1D-ND-C4D	2.53	108.13	106.33
4	L	1282	BCL	CAA-C2A-C3A	-2.51	105.90	112.78
9	M	1308	SPN	C10-C9-C8	-2.50	116.06	121.12
7	M	1305	CDL	OB8-CB7-C71	2.50	119.74	111.91
5	L	1285	BPH	CMB-C2B-C3B	2.48	129.32	124.68
4	M	1304	BCL	CAC-C3C-C2C	-2.47	108.10	114.26
4	L	1284	BCL	CHA-C1A-NA	-2.45	120.78	126.40
9	M	1308	SPN	C21-C20-C19	2.42	118.62	112.23
6	L	1286	U10	O5-C5-C6	-2.40	117.34	121.55
7	M	1305	CDL	OA8-CA7-OA9	-2.40	117.54	123.59
4	L	1282	BCL	CMA-C3A-C2A	-2.40	104.16	113.83
4	L	1284	BCL	C6-C5-C3	-2.39	107.20	113.45
9	M	1308	SPN	C14-C13-C12	-2.38	116.30	121.12
9	M	1308	SPN	CMB-C30-CM9	2.37	119.83	114.60
9	M	1308	SPN	CM7-C22-C23	2.33	119.73	111.29
6	L	1286	U10	C1M-C1-C6	-2.31	120.63	124.40
5	M	1307	BPH	CMA-C3A-C4A	-2.30	109.35	114.38
4	L	1282	BCL	O1D-CGD-CBD	-2.29	119.80	124.48
4	L	1282	BCL	C2D-C1D-ND	-2.28	108.42	110.10
4	L	1284	BCL	C1C-NC-C4C	2.28	107.73	106.71
4	L	1283	BCL	C2D-C1D-ND	-2.28	108.43	110.10
4	L	1284	BCL	CHD-C1D-C2D	2.27	130.25	125.48
4	L	1282	BCL	C5-C3-C2	2.25	125.66	121.12
5	M	1307	BPH	CAA-CBA-CGA	2.24	119.79	113.25
4	L	1282	BCL	C1D-ND-C4D	2.23	107.92	106.33
4	L	1283	BCL	C4D-CHA-C1A	2.22	123.95	121.25
4	L	1283	BCL	C1D-ND-C4D	2.22	107.91	106.33
4	M	1304	BCL	C4B-C3B-CAB	-2.22	122.84	127.13
4	L	1282	BCL	CAA-CBA-CGA	2.21	119.71	113.25
4	M	1304	BCL	CHD-C1D-C2D	2.20	130.09	125.48
4	L	1283	BCL	CMD-C2D-C1D	2.20	128.58	124.71
9	M	1308	SPN	C20-C21-C22	2.19	123.33	115.76
4	L	1284	BCL	CMB-C2B-C3B	2.18	128.76	124.68
9	M	1308	SPN	C6-C7-C8	2.17	119.00	111.88
4	L	1282	BCL	C4B-C3B-CAB	-2.16	122.96	127.13
4	L	1282	BCL	CAC-C3C-C2C	-2.14	108.90	114.26
5	L	1285	BPH	CAC-C3C-C2C	2.14	119.61	114.26
7	M	1305	CDL	CB4-OB6-CB5	-2.14	112.53	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	1304	BCL	CMB-C2B-C3B	2.12	128.64	124.68
5	L	1285	BPH	C4B-NB-C1B	2.10	111.41	107.09
4	L	1284	BCL	OBB-CAB-C3B	2.10	123.71	119.99
9	M	1308	SPN	C7-C8-C9	-2.09	122.62	127.66
4	L	1283	BCL	CMA-C3A-C2A	-2.08	105.43	113.83
5	M	1307	BPH	C4-C3-C2	-2.07	118.36	123.68
4	M	1304	BCL	C2A-C1A-CHA	2.04	127.43	123.86
6	L	1286	U10	C3M-O3-C3	2.04	123.69	116.47
5	L	1285	BPH	CMC-C2C-C3C	2.02	122.14	113.99
4	M	1304	BCL	C1-C2-C3	-2.01	122.56	126.04

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	1307	BPH	C4C-C3C-CAC-CBC
6	L	1286	U10	C6-C7-C8-C9
7	M	1305	CDL	CA2-OA2-PA1-OA3
7	M	1305	CDL	CB2-OB2-PB2-OB3
7	M	1305	CDL	CB2-OB2-PB2-OB4
7	M	1305	CDL	CB2-OB2-PB2-OB5
9	M	1308	SPN	C20-C21-C22-CM7
9	M	1308	SPN	C14-C15-C16-C17
5	M	1307	BPH	C4-C3-C5-C6
9	M	1308	SPN	CM3-C5-C6-C7
9	M	1308	SPN	C11-C10-C9-CM4
9	M	1308	SPN	CM5-C13-C14-C15
9	M	1308	SPN	C16-C17-C18-CM6
5	M	1307	BPH	C2-C3-C5-C6
9	M	1308	SPN	C4-C5-C6-C7
9	M	1308	SPN	C11-C10-C9-C8
9	M	1308	SPN	C12-C13-C14-C15
9	M	1308	SPN	C16-C17-C18-C19
5	M	1307	BPH	C15-C16-C17-C18
4	L	1282	BCL	C15-C16-C17-C18
4	L	1283	BCL	C13-C15-C16-C17
7	M	1305	CDL	CA7-C31-C32-C33
4	L	1283	BCL	C5-C6-C7-C8
4	L	1282	BCL	C8-C10-C11-C12
5	M	1307	BPH	C10-C11-C12-C13
4	L	1282	BCL	C13-C15-C16-C17
7	M	1305	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
7	M	1305	CDL	C14-C15-C16-C17
7	M	1305	CDL	C58-C59-C60-C61
7	M	1305	CDL	C76-C77-C78-C79
7	M	1305	CDL	OB7-CB5-OB6-CB4
7	M	1305	CDL	C51-CB5-OB6-CB4
7	M	1305	CDL	C12-C13-C14-C15
4	L	1283	BCL	C15-C16-C17-C18
7	M	1305	CDL	C38-C39-C40-C41
5	L	1285	BPH	C16-C17-C18-C20
7	M	1305	CDL	C11-C12-C13-C14
5	L	1285	BPH	O2A-C1-C2-C3
7	M	1305	CDL	CB2-C1-CA2-OA2
7	M	1305	CDL	C53-C54-C55-C56
4	L	1284	BCL	C15-C16-C17-C18
7	M	1305	CDL	C35-C36-C37-C38
7	M	1305	CDL	C55-C56-C57-C58
5	M	1307	BPH	C2C-C3C-CAC-CBC
5	L	1285	BPH	C16-C17-C18-C19
7	M	1305	CDL	CA2-OA2-PA1-OA5
7	M	1305	CDL	OB5-CB3-CB4-CB6
7	M	1305	CDL	C54-C55-C56-C57
5	L	1285	BPH	C6-C7-C8-C10
7	M	1305	CDL	C80-C81-C82-C83
5	M	1307	BPH	C6-C7-C8-C9
7	M	1305	CDL	C33-C34-C35-C36
9	M	1308	SPN	C5-C6-C7-C8
7	M	1305	CDL	O1-C1-CA2-OA2
5	M	1307	BPH	C11-C12-C13-C15
4	L	1282	BCL	CAD-CBD-CGD-O2D
7	M	1305	CDL	C51-C52-C53-C54
7	M	1305	CDL	OB5-CB3-CB4-OB6
5	L	1285	BPH	C11-C10-C8-C9
5	M	1307	BPH	C11-C12-C13-C14
4	L	1282	BCL	C3-C5-C6-C7
7	M	1305	CDL	CA2-OA2-PA1-OA4
4	L	1284	BCL	C16-C17-C18-C19
7	M	1305	CDL	C31-CA7-OA8-CA6
7	M	1305	CDL	C13-C14-C15-C16
5	M	1307	BPH	C16-C17-C18-C19
4	L	1282	BCL	C12-C13-C15-C16
5	M	1307	BPH	C12-C13-C15-C16
7	M	1305	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
5	L	1285	BPH	C4C-C3C-CAC-CBC
7	M	1305	CDL	C1-CB2-OB2-PB2
4	L	1282	BCL	C11-C10-C8-C9
5	M	1307	BPH	C11-C10-C8-C9
7	M	1305	CDL	OA9-CA7-OA8-CA6
7	M	1305	CDL	CB5-C51-C52-C53
7	M	1305	CDL	C40-C41-C42-C43
7	M	1305	CDL	C60-C61-C62-C63
7	M	1305	CDL	C71-C72-C73-C74
4	L	1282	BCL	C14-C13-C15-C16
5	L	1285	BPH	C6-C7-C8-C9
5	M	1307	BPH	C16-C17-C18-C20
4	L	1284	BCL	C16-C17-C18-C20
4	L	1283	BCL	C2A-CAA-CBA-CGA
9	M	1308	SPN	CM7-C22-C23-C24
5	L	1285	BPH	C3-C5-C6-C7
5	L	1285	BPH	C12-C13-C15-C16
5	L	1285	BPH	C8-C10-C11-C12
4	L	1282	BCL	C4C-C3C-CAC-CBC
6	L	1286	U10	C7-C8-C9-C10
5	L	1285	BPH	C11-C10-C8-C7
7	M	1305	CDL	OA6-CA4-CA6-OA8
7	M	1305	CDL	CA3-OA5-PA1-OA2
5	L	1285	BPH	C14-C13-C15-C16
4	L	1283	BCL	CAD-CBD-CGD-O2D
5	L	1285	BPH	CAD-CBD-CGD-O2D
7	M	1305	CDL	C32-C31-CA7-OA8
7	M	1305	CDL	C79-C80-C81-C82
4	M	1304	BCL	CAA-CBA-CGA-O2A
4	L	1284	BCL	CHA-CBD-CGD-O1D
4	L	1284	BCL	CHA-CBD-CGD-O2D
5	L	1285	BPH	CHA-CBD-CGD-O2D
5	L	1285	BPH	C2-C3-C5-C6
7	M	1305	CDL	C32-C33-C34-C35
5	M	1307	BPH	C14-C13-C15-C16
6	L	1286	U10	C5-C4-O4-C4M
9	M	1308	SPN	C10-C11-C12-C13
7	M	1305	CDL	C32-C31-CA7-OA9
9	M	1308	SPN	C6-C7-C8-C9
4	L	1283	BCL	C2-C1-O2A-CGA
5	M	1307	BPH	C11-C10-C8-C7
7	M	1305	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
9	M	1308	SPN	C7-C8-C9-CM4
7	M	1305	CDL	C72-C71-CB7-OB8

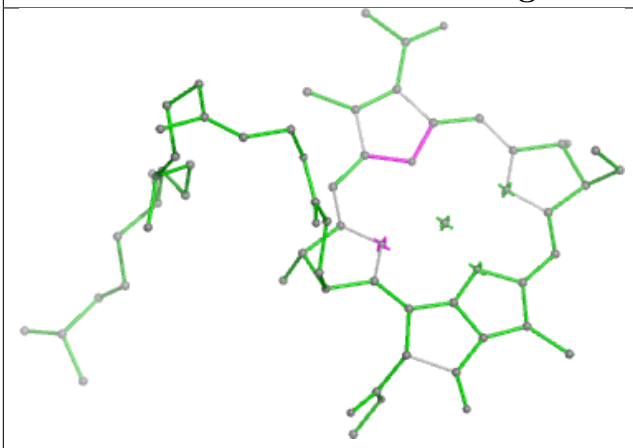
There are no ring outliers.

9 monomers are involved in 43 short contacts:

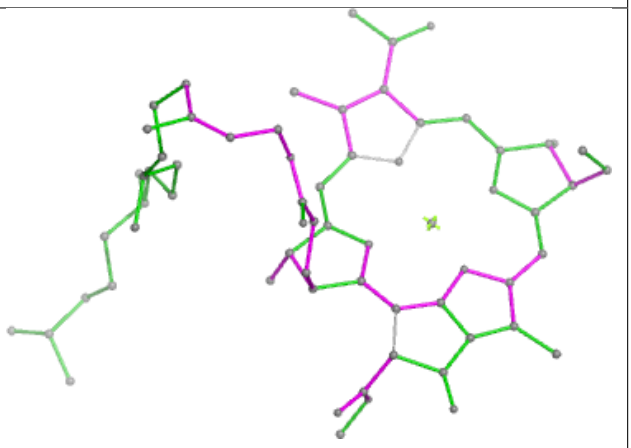
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1282	BCL	10	0
5	M	1307	BPH	8	0
6	L	1286	U10	2	0
7	M	1305	CDL	2	0
4	L	1284	BCL	4	0
9	M	1308	SPN	9	0
4	M	1304	BCL	7	0
5	L	1285	BPH	7	0
4	L	1283	BCL	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

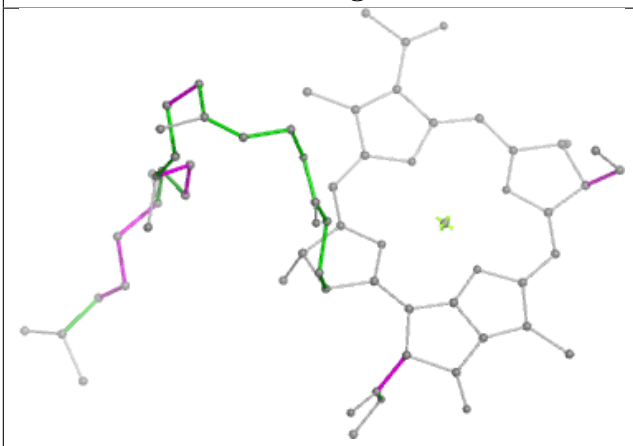
Ligand BCL L 1282



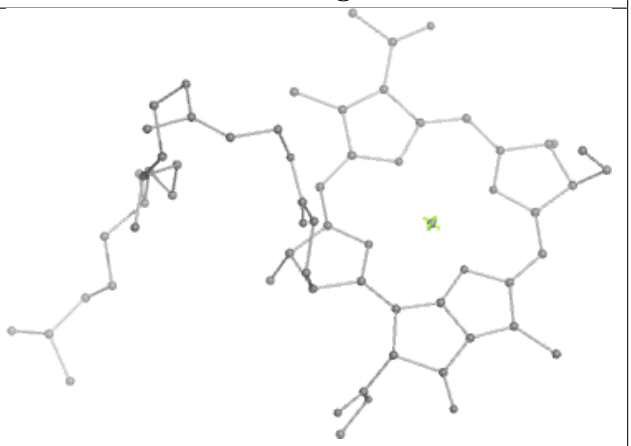
Bond lengths



Bond angles

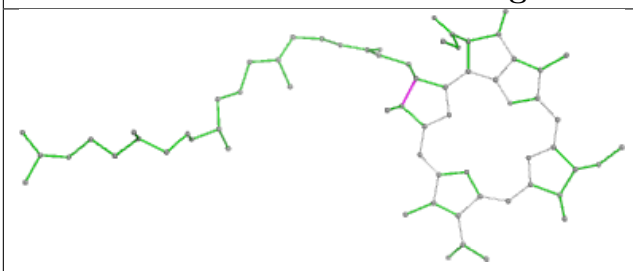


Torsions

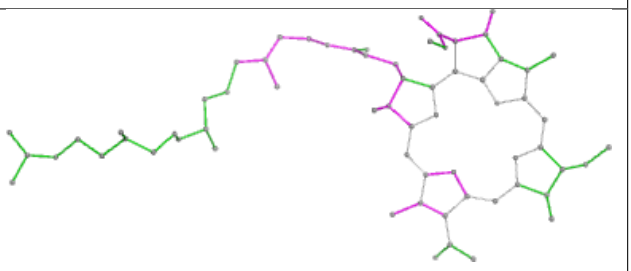


Rings

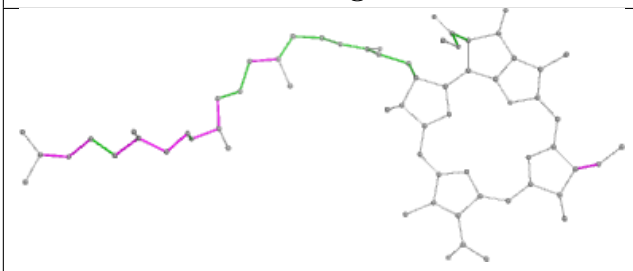
Ligand BPH M 1307



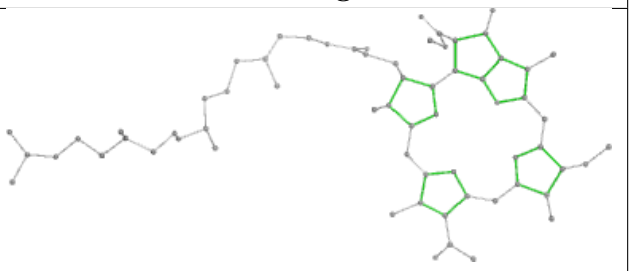
Bond lengths



Bond angles

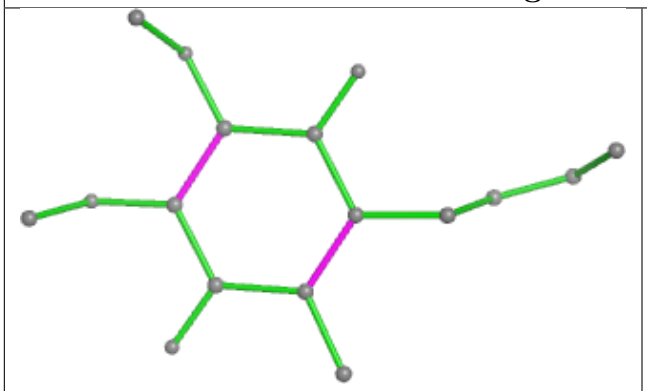


Torsions

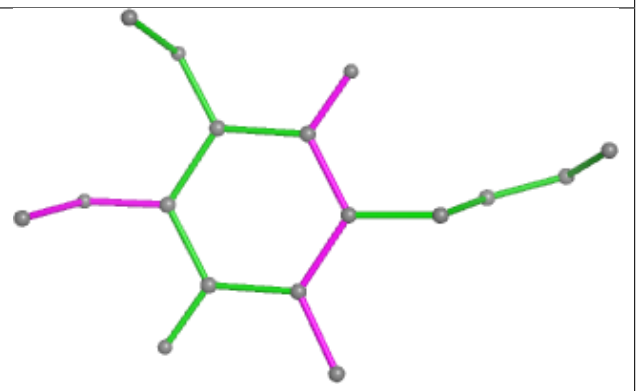


Rings

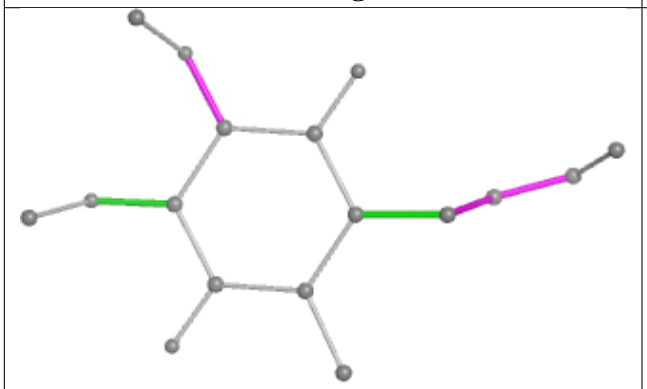
Ligand U10 L 1286



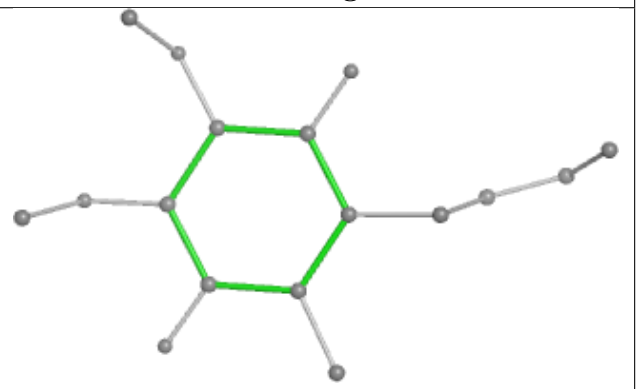
Bond lengths



Bond angles

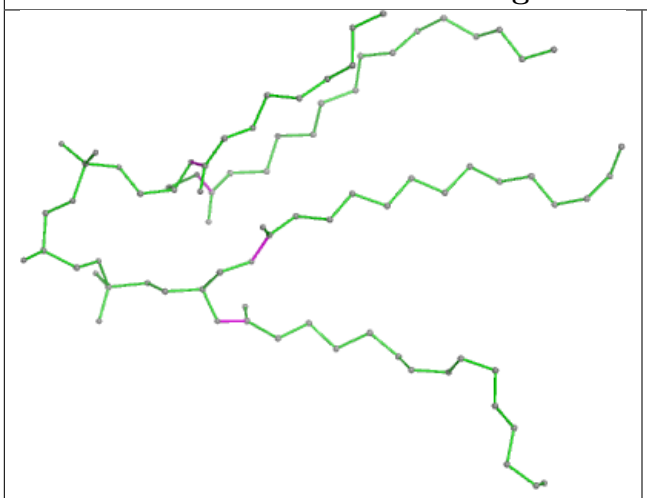


Torsions

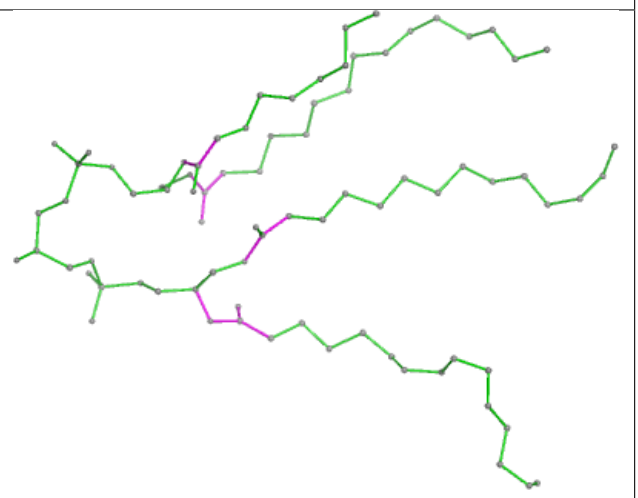


Rings

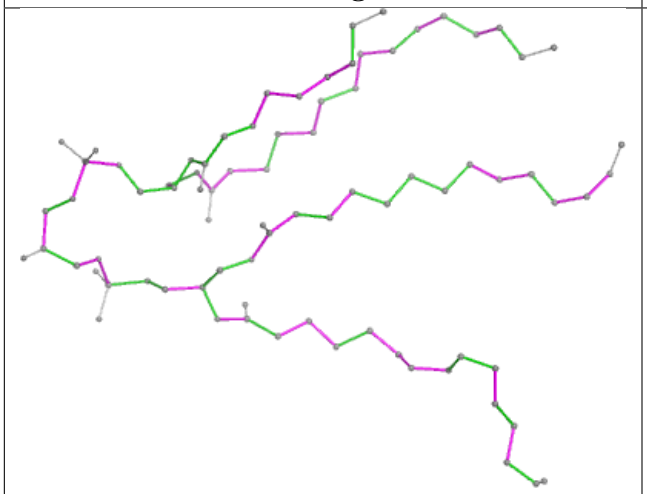
Ligand CDL M 1305



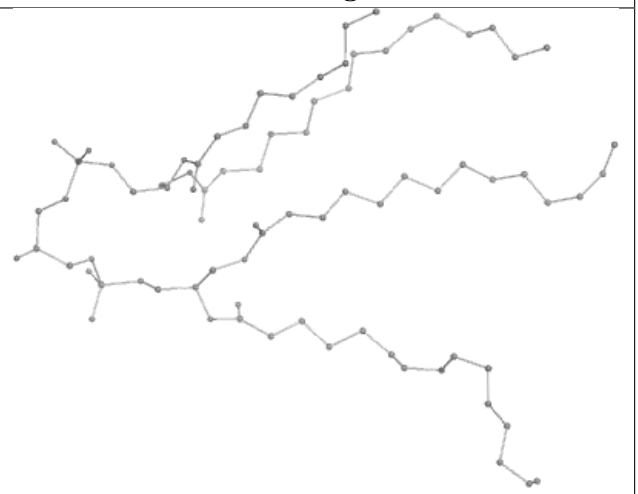
Bond lengths



Bond angles

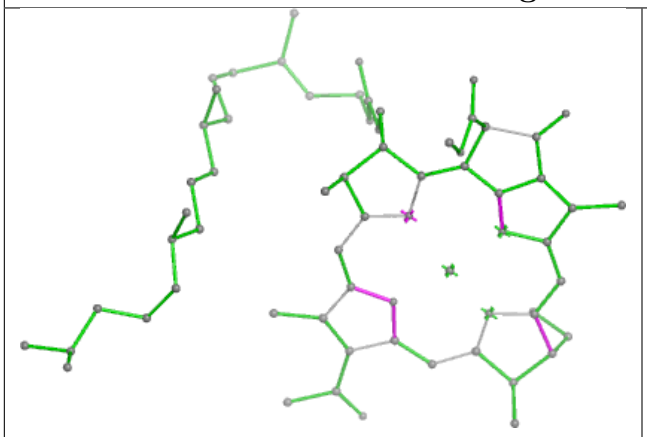


Torsions

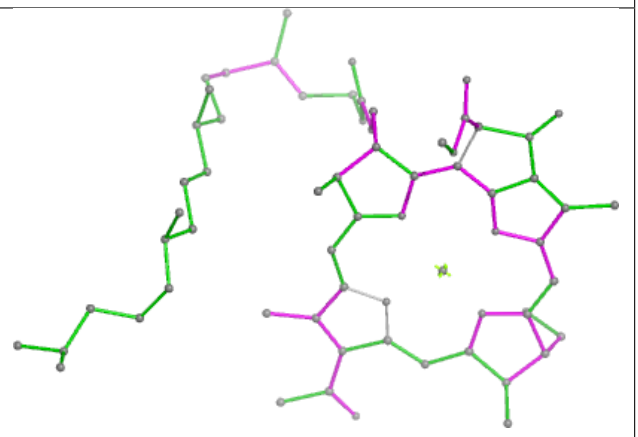


Rings

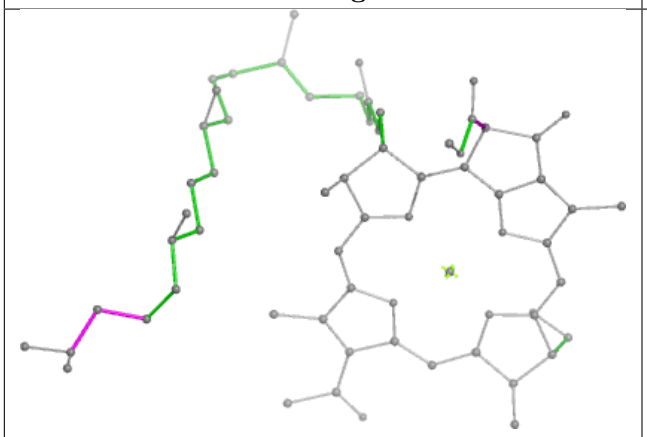
Ligand BCL L 1284



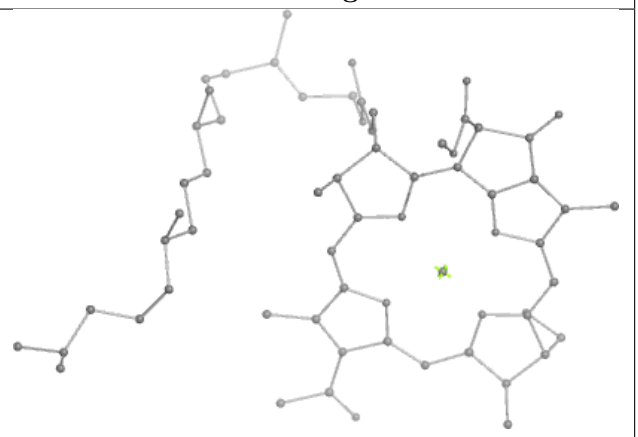
Bond lengths



Bond angles

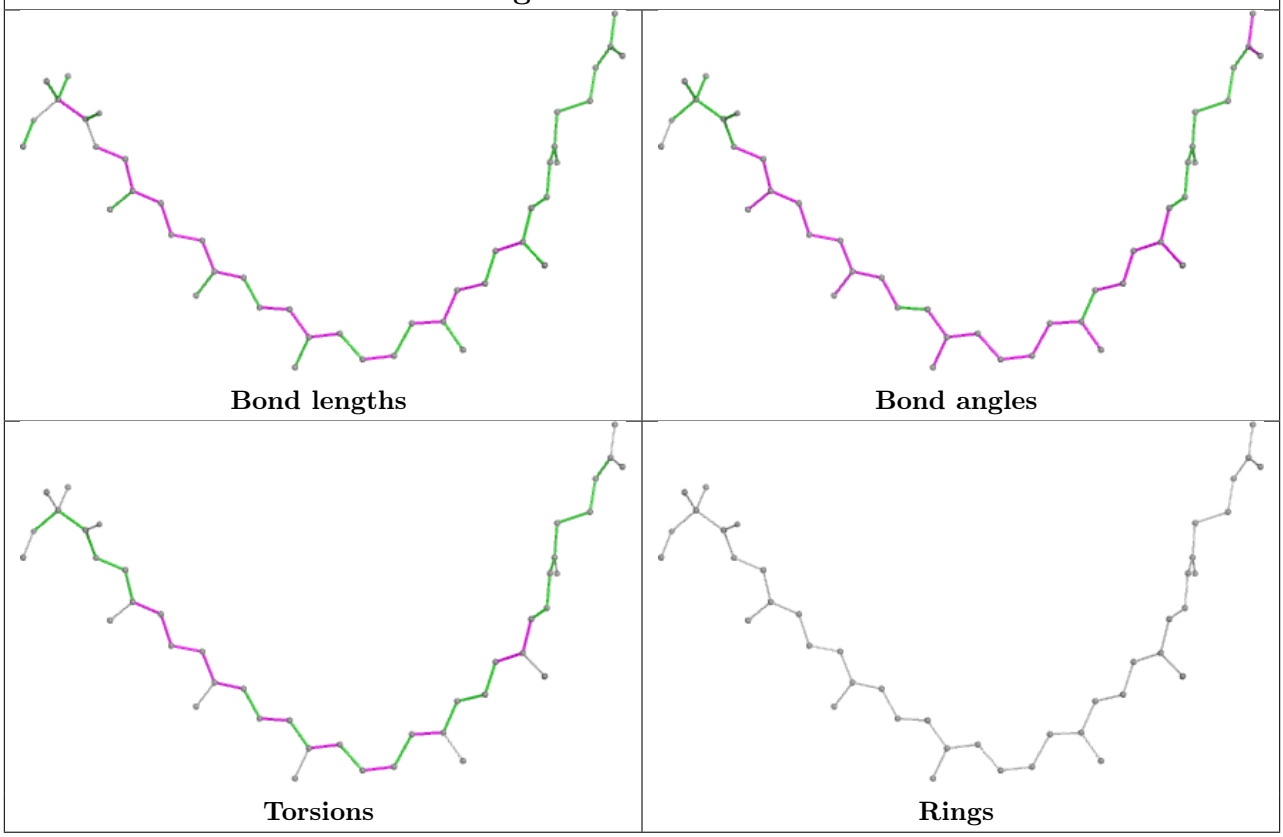


Torsions

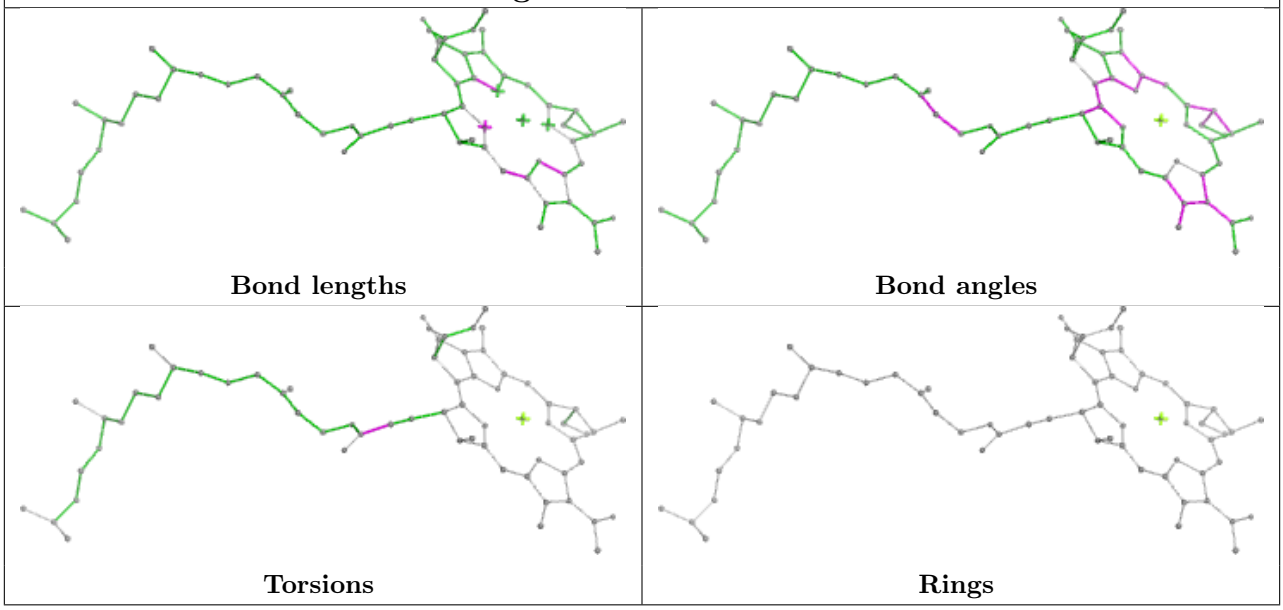


Rings

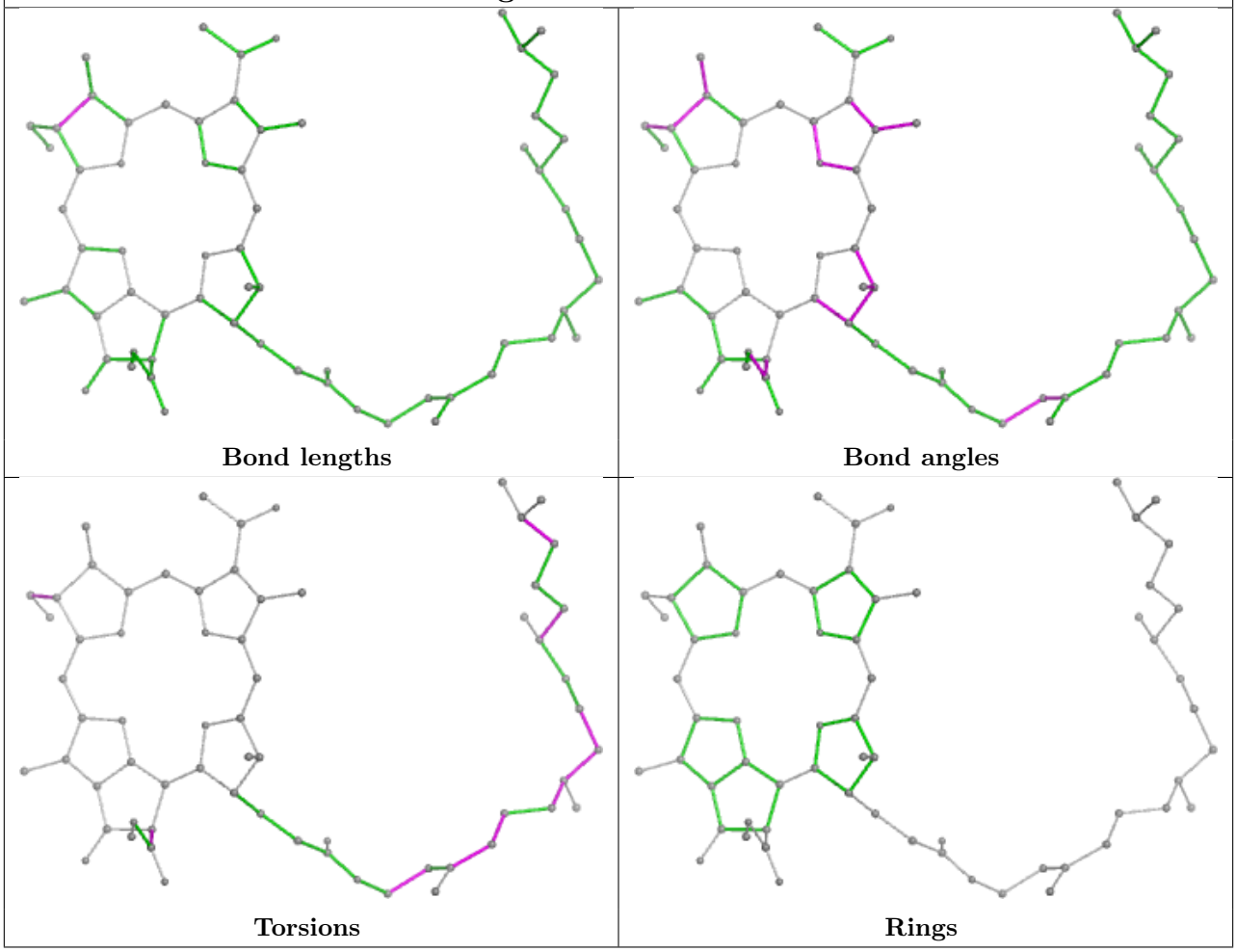
Ligand SPN M 1308



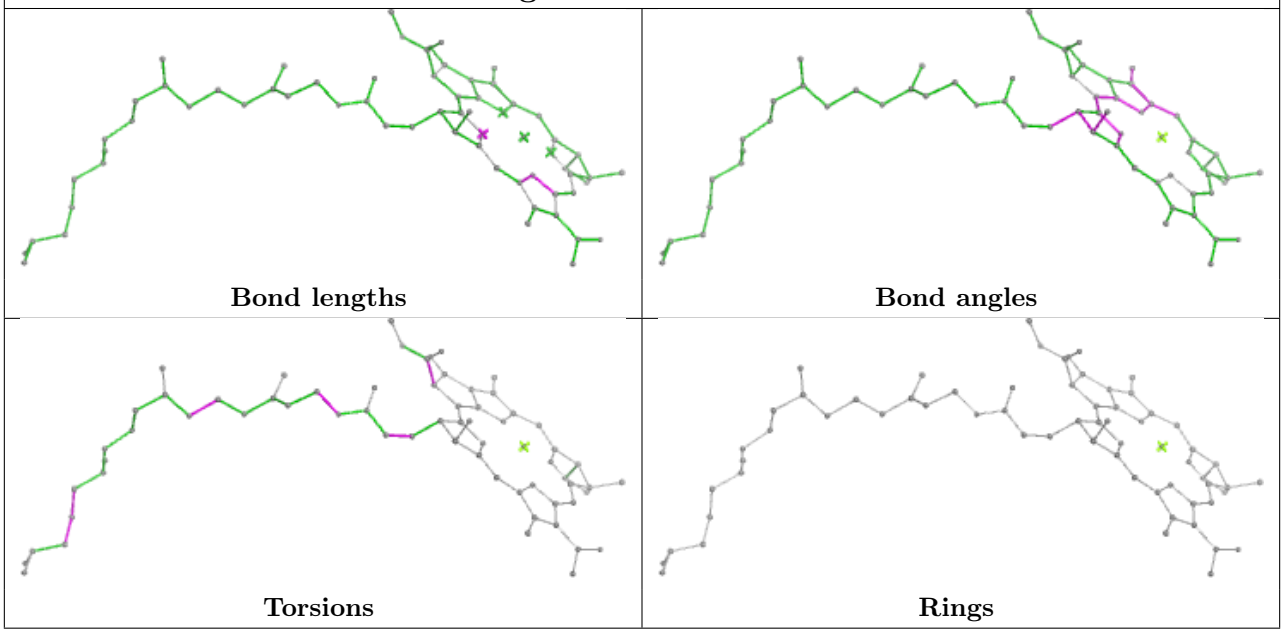
Ligand BCL M 1304



Ligand BPH L 1285



Ligand BCL L 1283



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	H	235/260 (90%)	-0.29	2 (0%)	84	80	36, 43, 53, 58	4 (1%)
2	L	281/281 (100%)	-0.16	7 (2%)	57	47	32, 44, 56, 63	1 (0%)
3	M	301/308 (97%)	-0.28	4 (1%)	77	72	36, 44, 54, 79	1 (0%)
All	All	817/849 (96%)	-0.24	13 (1%)	72	66	32, 44, 54, 79	6 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	245	ALA	3.9
2	L	59	TRP	3.7
3	M	302	GLY	3.6
2	L	281	GLY	3.0
2	L	270	PRO	2.7
2	L	277	GLY	2.7
3	M	301	HIS	2.6
2	L	202	LYS	2.3
3	M	80	TRP	2.3
2	L	72	GLU	2.1
3	M	2	GLU	2.1
2	L	271	TRP	2.0
1	H	191	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

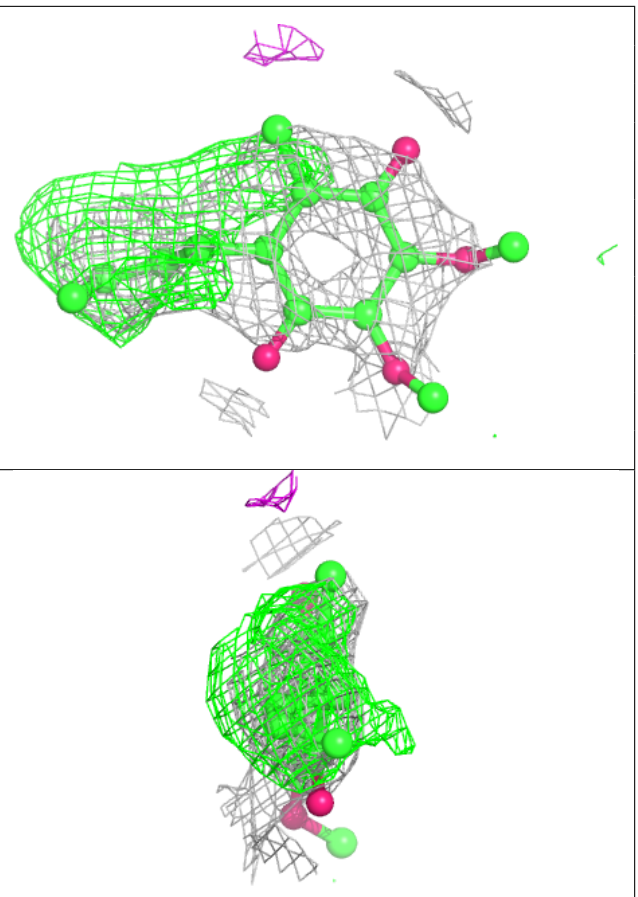
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

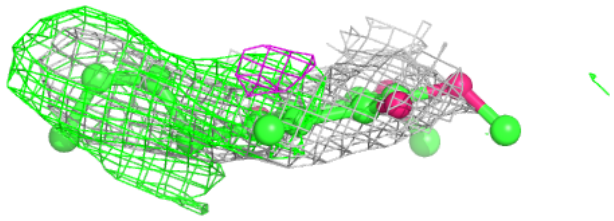
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	U10	L	1286	17/63	0.83	0.56	29,32,33,33	17
7	CDL	M	1305	81/100	0.83	0.33	24,39,52,54	81
5	BPH	M	1307	65/65	0.87	0.23	38,44,85,86	0
9	SPN	M	1308	43/43	0.89	0.22	37,43,51,52	0
4	BCL	L	1282	66/66	0.93	0.20	37,44,69,69	0
4	BCL	L	1284	66/66	0.95	0.17	29,36,50,54	0
4	BCL	M	1304	66/66	0.95	0.22	36,40,51,54	0
4	BCL	L	1283	66/66	0.95	0.21	29,39,53,56	0
5	BPH	L	1285	65/65	0.97	0.15	33,40,43,46	0
8	FE	M	1306	1/1	0.98	0.15	44,44,44,44	0
10	CL	M	1309	1/1	0.99	0.13	39,39,39,39	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 U10 L 1286:

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





Electron density around CDL M 1305:

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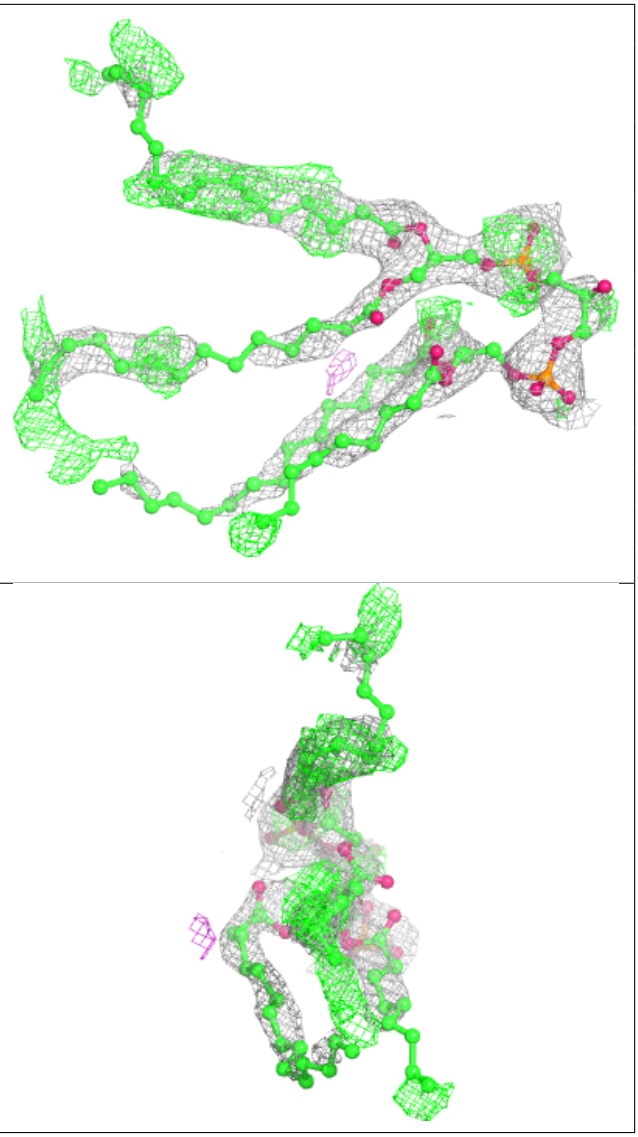
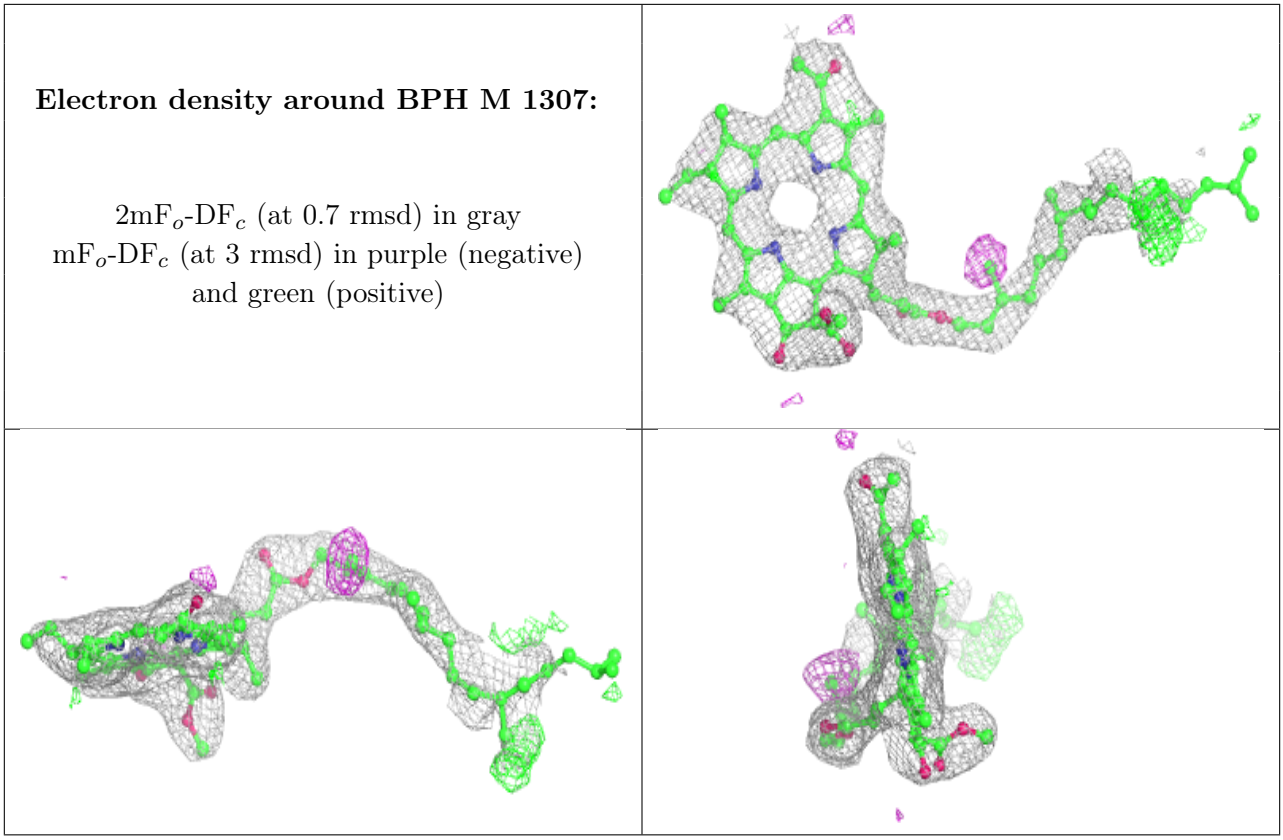
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



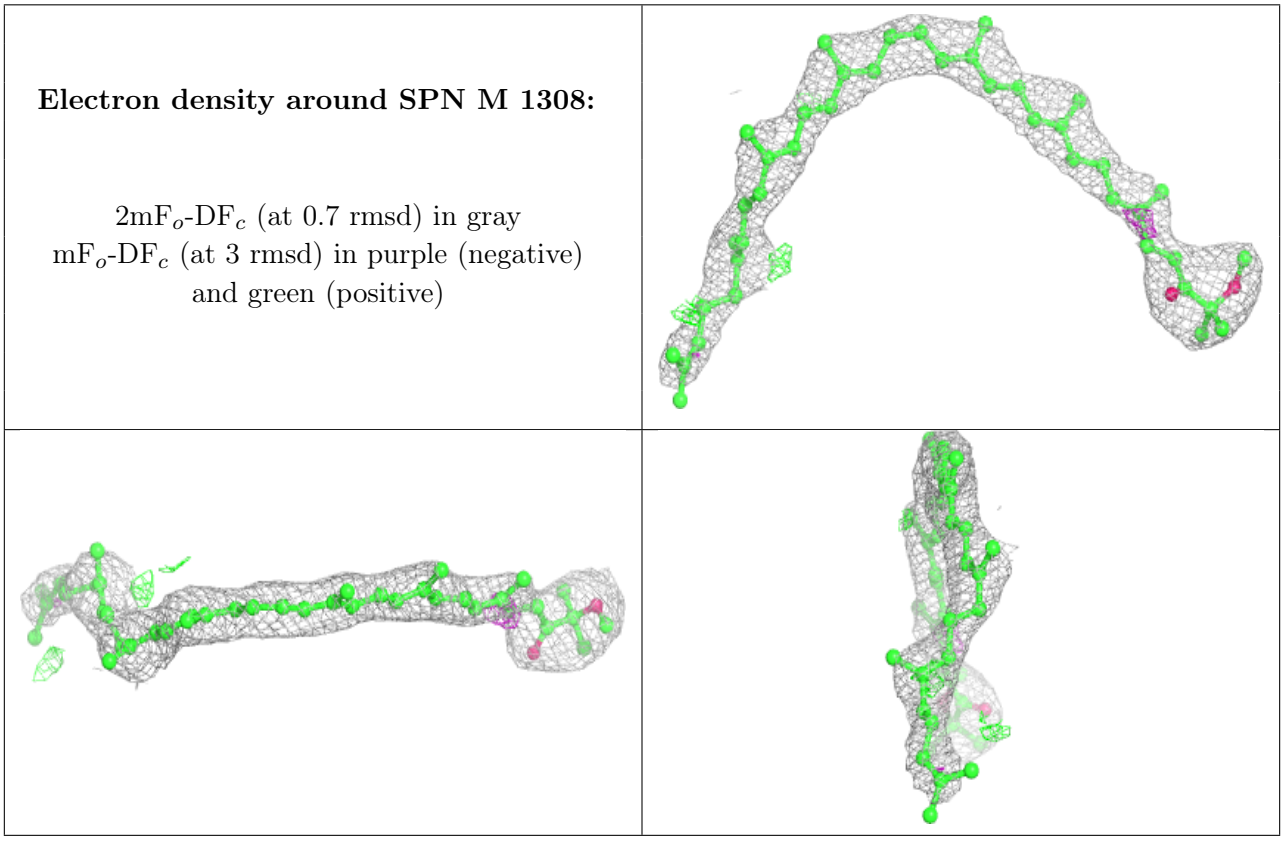
Electron density around BPH M 1307:

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



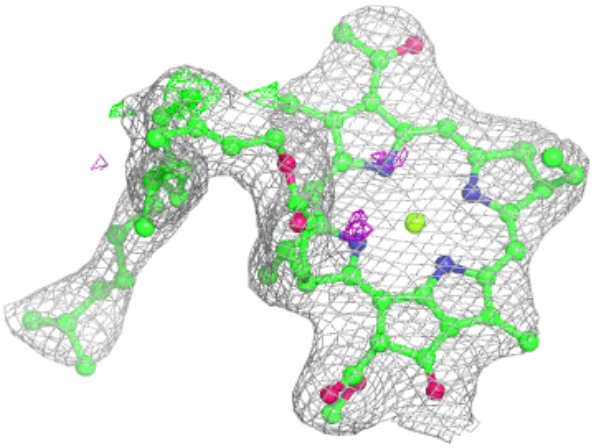
Electron density around SPN M 1308:

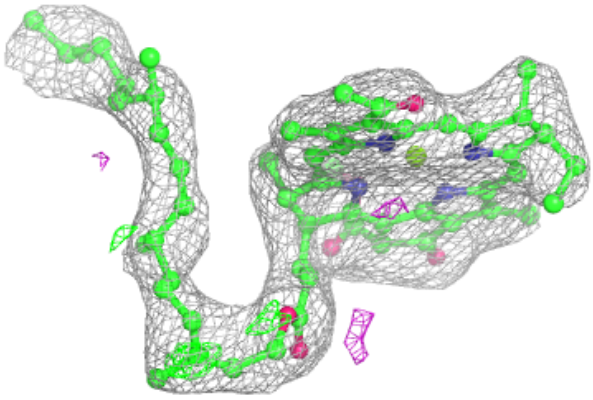
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

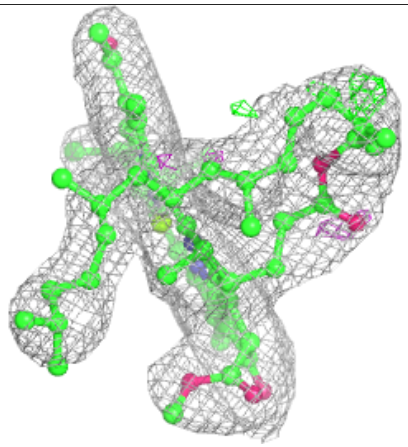


Electron density around BCL L 1282:

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

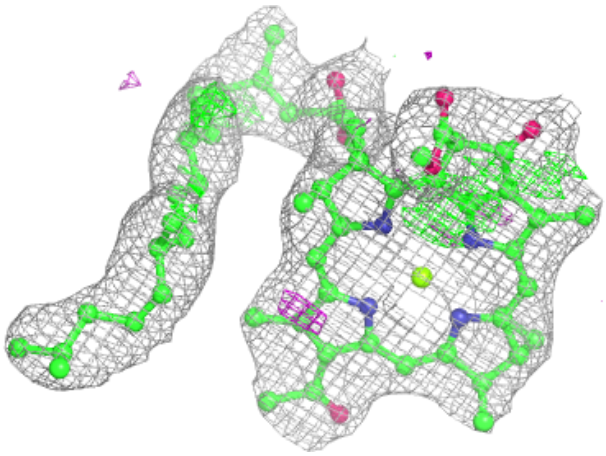


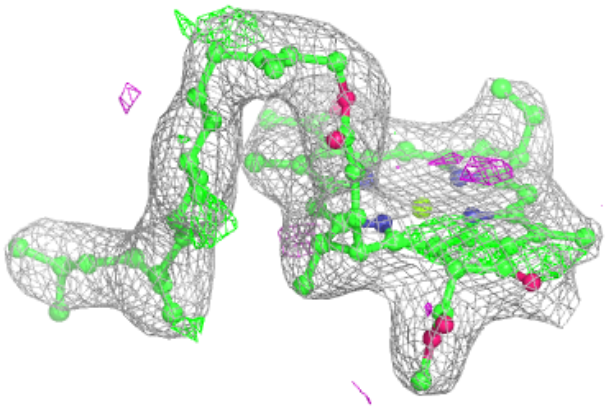




Electron density around BCL L 1284:

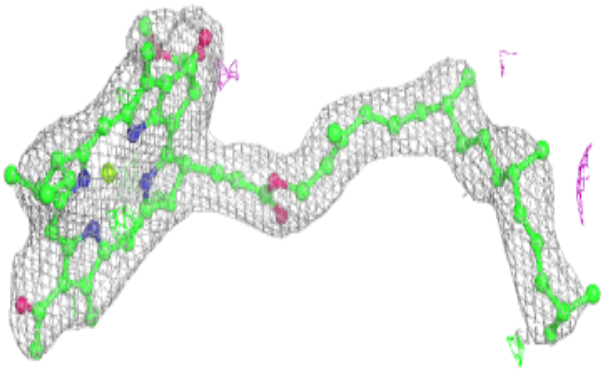
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

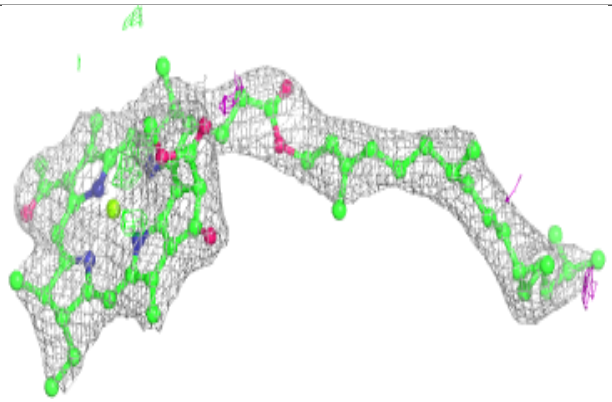


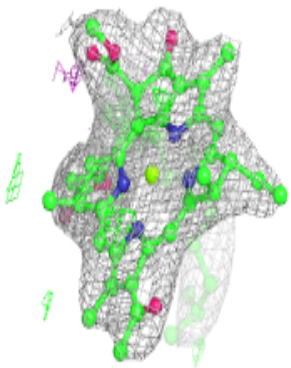


Electron density around BCL M 1304:

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

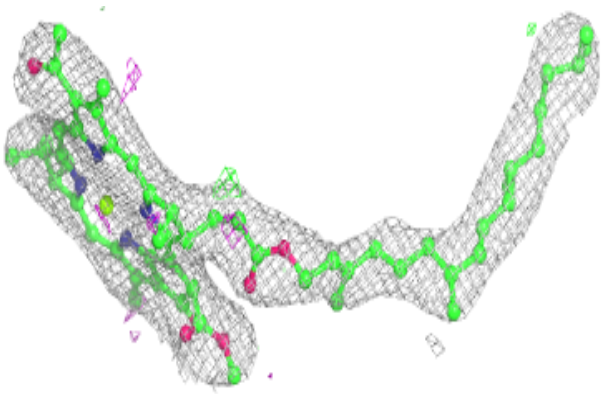


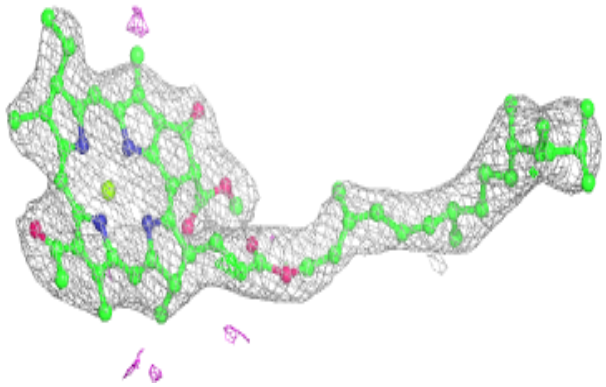


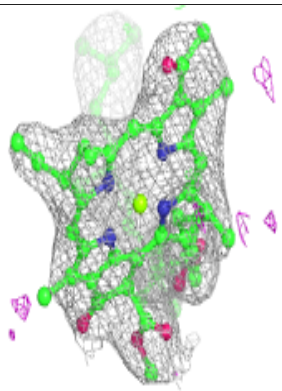


Electron density around BCL L 1283:

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

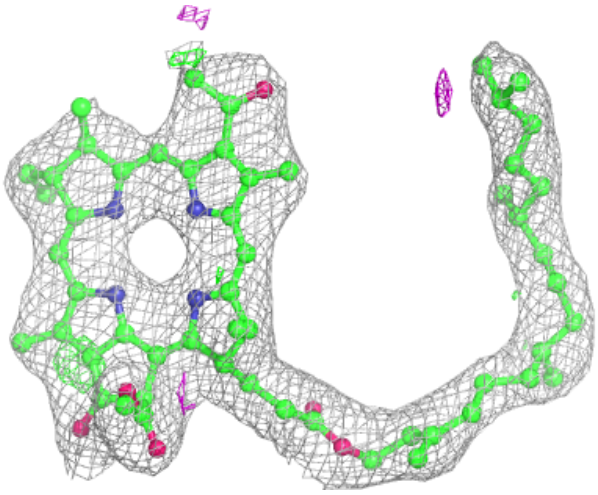


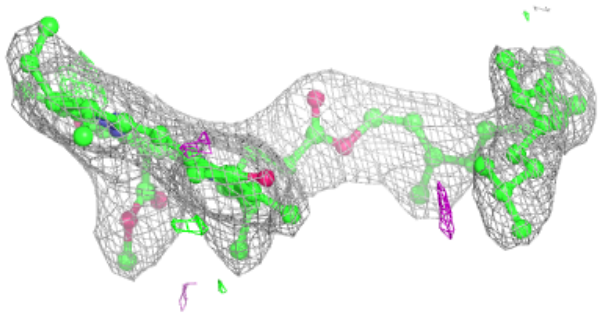


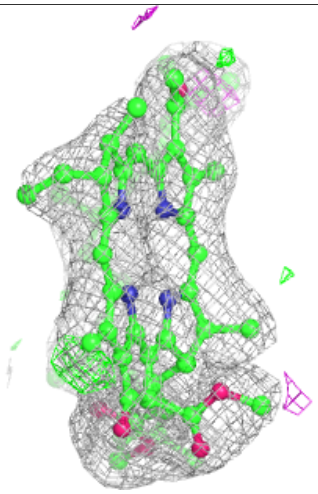


Electron density around BPH L 1285:

$2mF_o$-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.