Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2026 – 05:15 AM EDT

PDB ID	:	8VTM / pdb_00008vtm
Title	:	Crystal structure of R. sphaeroides Photosynthetic Reaction Center variant Y (M210)2-bromophenylalanine
Authors	:	Tran, K.; Mathews, I.; Boxer, S.G.
Deposited on	:	2024-01-26
Resolution	:	3.51 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:

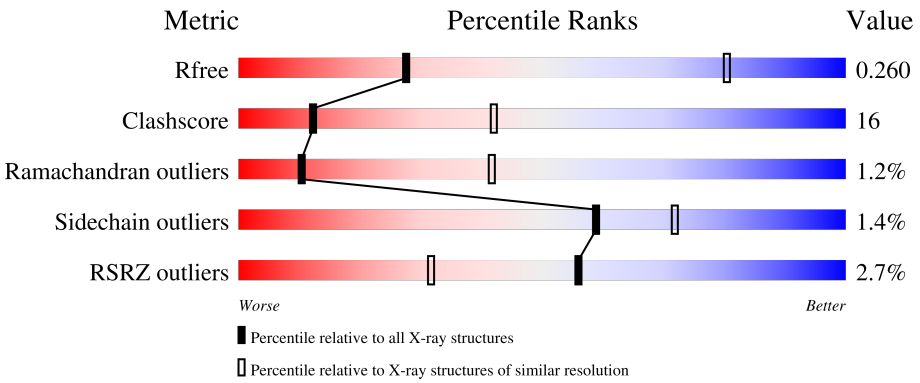
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.51 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	240	2% 66% 30% •
2	L	281	2% 72% 28%
3	M	301	3% 65% 33% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CDL	M	407	X	-	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 6994 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	240	1829	1169	314	337	9	0	0	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	2232	1507	355	362	8	0	0	0

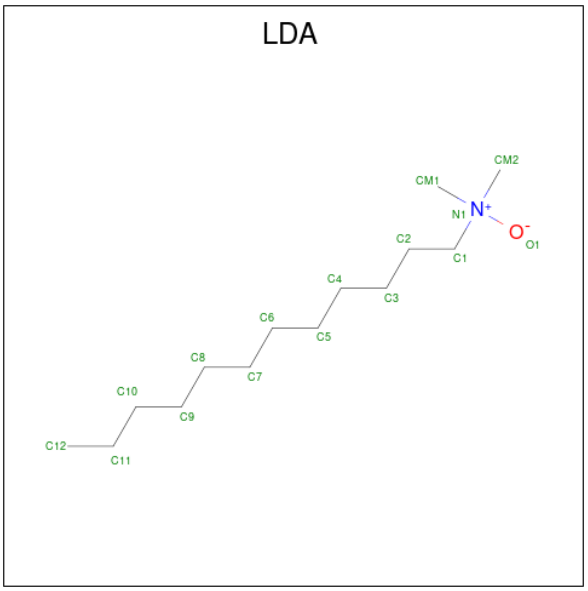
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	Br	C	N	O	S			
3	M	301	2396	1	1598	392	395	10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

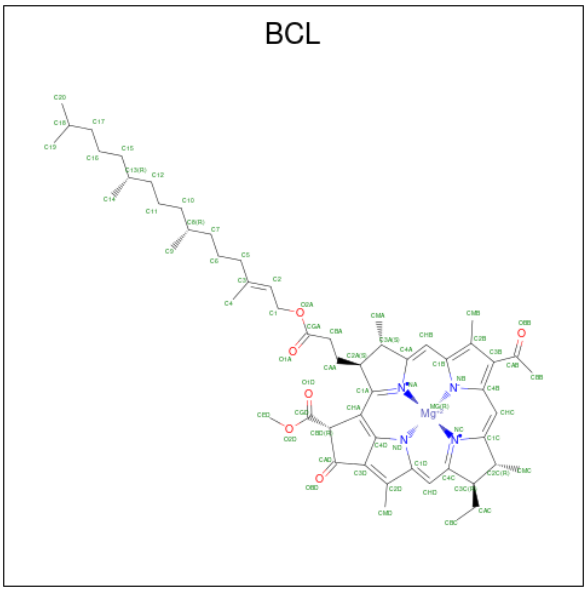
Chain	Residue	Modelled	Actual	Comment	Reference
M	210	6DU	TYR	conflict	UNP P0C0Y9
M	252	VAL	TRP	conflict	UNP P0C0Y9

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



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

- Molecule 5 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
5	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	M	1	51	40	1	4	6	0	0

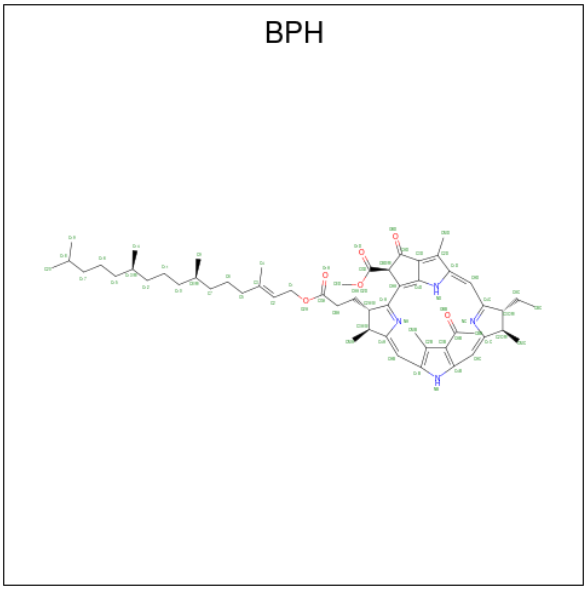
- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
6	L	1	1	1	0	0

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

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

- Molecule 8 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	M	1	55	45	4	6	0	0

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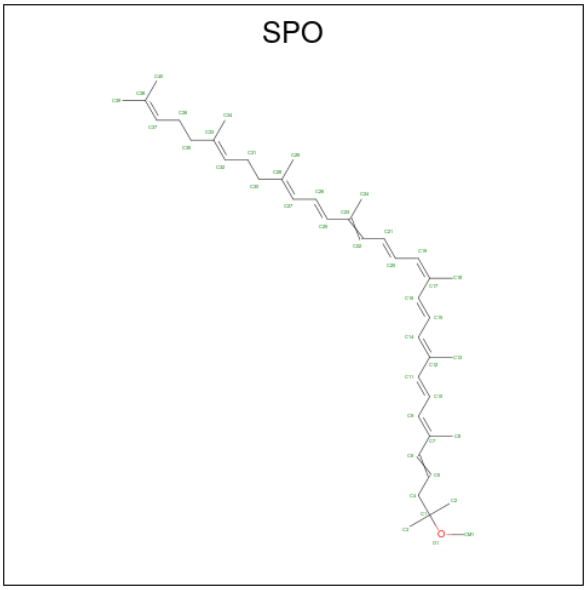
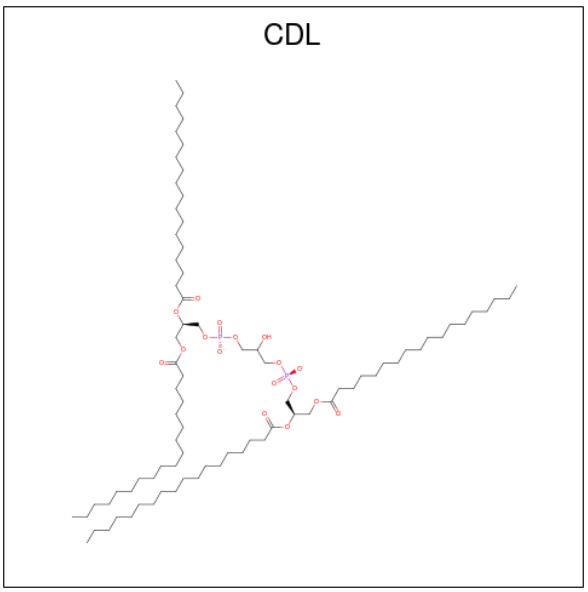
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	M	1	65	55	4	6	0	0

- Molecule 9 is SPHEROIDENE (CCD ID: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 10 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
10	M	1	69	50	17	2	0	0

- Molecule 11 is water.

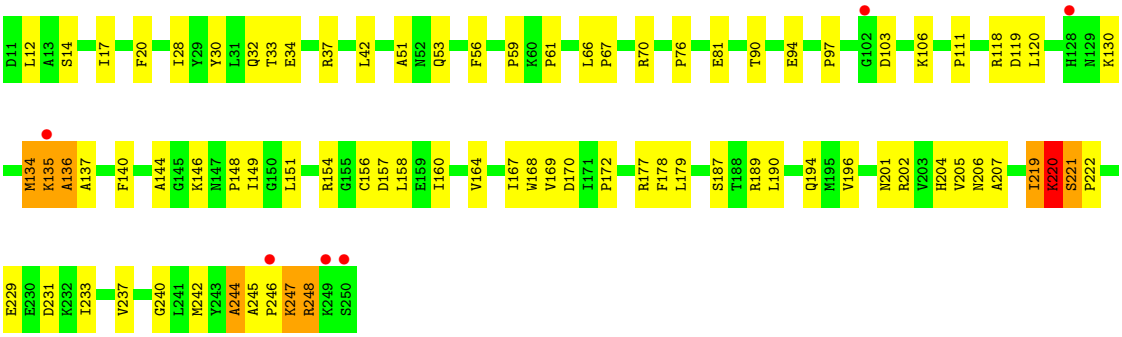
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	H	2	2	2	0	0
			Total	O		
11	L	3	3	3	0	0
			Total	O		
11	M	2	2	2	0	0

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.

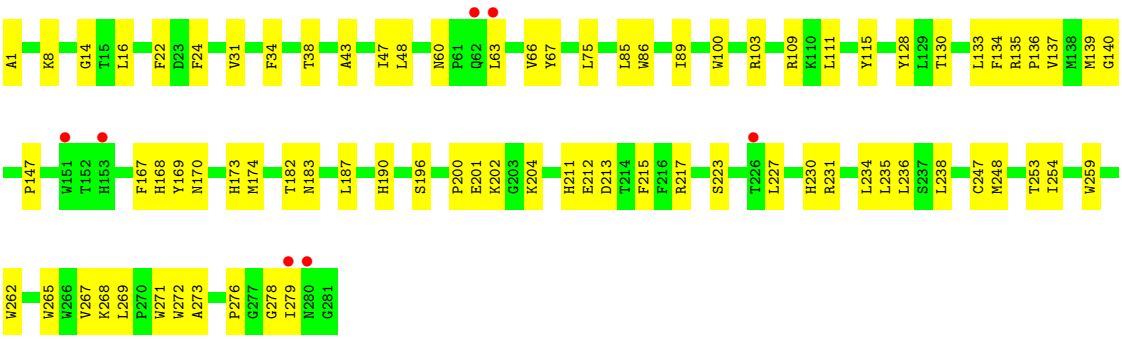
• Molecule 1: Reaction center protein H chain

Chain H:



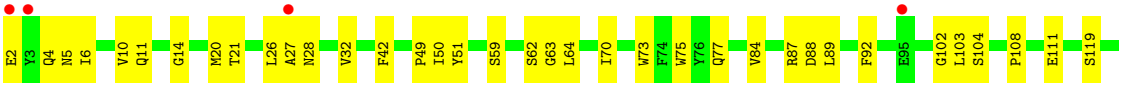
• Molecule 2: Reaction center protein L chain

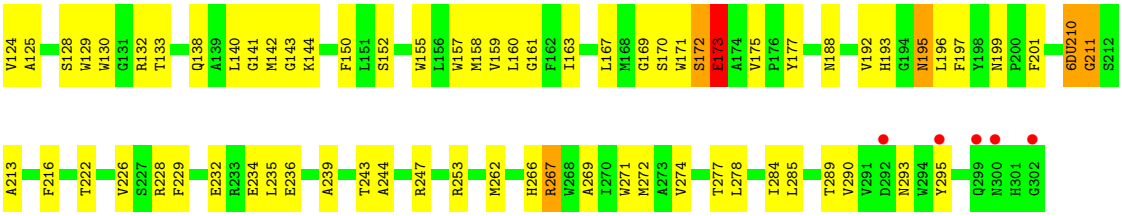
Chain L:



• Molecule 3: Reaction center protein M chain

Chain M:




V124
A125
S128
W129
W130
G131
R132
T133
Q138
A139
L140
G141
M142
G143
K144
F150
L151
S152
W155
L156
W157
M158
V159
L160
G161
F162
I163
L167
M168
G169
S170
W171
S172
E173
A174
V175
P176
Y177
N188
V192
H193
G194
N195
L196
F197
Y198
N199
P200
F201
6DU210
G211
S212
A213
F216
T222
V226
S227
R228
F229
E232
R233
E234
L235
E236
A239
T243
A244
R247
R253
M262
H266
R267
W268
A269
I270
W271
M272
A273
V274
T277
L278
I284
L285
T289
V290
V291
D292
N293
W294
Y295
Q299
N300
H301
G302

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.79Å 141.79Å 187.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.99 – 3.51 39.99 – 3.51	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.99-3.51) 89.3 (39.99-3.51)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.220 , 0.261 0.222 , 0.260	Depositor DCC
R_{free} test set	1387 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	71.1	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 40.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6994	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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, CDL, CL, 6DU, SPO, LDA, FE, 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	H	0.36	0/1877	0.59	4/2553 (0.2%)
2	L	0.15	0/2320	0.32	0/3175
3	M	0.44	0/2472	0.51	2/3372 (0.1%)
All	All	0.34	0/6669	0.48	6/9100 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	M	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	221	SER	CA-C-N	9.76	132.04	119.84
1	H	221	SER	C-N-CA	9.76	132.04	119.84
3	M	267	ARG	N-CA-C	-6.48	104.30	111.36
1	H	244	ALA	N-CA-C	-6.11	97.78	110.80
1	H	136	ALA	N-CA-C	-5.68	98.70	110.80
3	M	172	SER	N-CA-C	-5.04	106.24	112.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	210	6DU	Mainchain,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	1829	0	1836	69	17
2	L	2232	0	2187	67	0
3	M	2396	0	2302	103	17
4	H	16	0	31	1	0
4	M	32	0	62	0	0
5	L	132	0	146	10	0
5	M	117	0	112	5	0
6	L	1	0	0	0	0
7	M	1	0	0	0	0
8	M	120	0	126	6	0
9	M	42	0	54	7	0
10	M	69	0	82	2	0
11	H	2	0	0	0	0
11	L	3	0	0	0	0
11	M	2	0	0	0	0
All	All	6994	0	6938	216	17

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 16.

All (216) 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)
1:H:240:GLY:O	1:H:244:ALA:HB2	1.66	0.96
2:L:231:ARG:NE	3:M:6:ILE:O	2.03	0.91
1:H:248:ARG:HB2	1:H:248:ARG:CZ	1.98	0.91
1:H:156:CYS:SG	1:H:206:ASN:HA	2.11	0.90
1:H:30:TYR:OH	3:M:267:ARG:NH1	2.08	0.86
2:L:170:ASN:HB3	2:L:173:HIS:HB2	1.58	0.86
3:M:234:GLU:HG2	3:M:262:MET:HE3	1.59	0.85
1:H:240:GLY:O	1:H:244:ALA:CB	2.26	0.84
1:H:81:GLU:OE1	2:L:8:LYS:NZ	2.10	0.84
3:M:26:LEU:O	3:M:28:ASN:N	2.16	0.76
2:L:202:LYS:H	2:L:202:LYS:HD2	1.50	0.75
3:M:170:SER:OG	3:M:172:SER:OG	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.71	0.73
3:M:63:GLY:HA3	8:M:405:BPH:H5C1	1.72	0.72
2:L:231:ARG:CD	3:M:6:ILE:O	2.39	0.70
1:H:220:LYS:HG2	1:H:229:GLU:OE2	1.91	0.70
1:H:248:ARG:HB2	1:H:248:ARG:NH1	2.06	0.70
1:H:246:PRO:O	1:H:247:LYS:HG3	1.91	0.69
3:M:103:LEU:HD12	3:M:170:SER:HA	1.72	0.69
3:M:103:LEU:HA	3:M:171:TRP:NE1	2.07	0.69
1:H:111:PRO:HG3	1:H:242:MET:HE3	1.75	0.69
3:M:234:GLU:OE1	3:M:266:HIS:NE2	2.17	0.69
2:L:278:GLY:HA3	3:M:84:VAL:HG21	1.75	0.68
3:M:138:GLN:HB2	3:M:144:LYS:HE3	1.76	0.68
2:L:75:LEU:HD21	2:L:137:VAL:HA	1.76	0.67
1:H:201:ASN:HD21	1:H:202:ARG:HH21	1.42	0.67
1:H:42:LEU:O	1:H:53:GLN:NE2	2.28	0.66
2:L:231:ARG:HD3	3:M:6:ILE:O	1.95	0.66
2:L:66:VAL:HG12	2:L:86:TRP:HB2	1.79	0.65
1:H:34:GLU:OE2	1:H:37:ARG:NH2	2.27	0.65
3:M:26:LEU:O	3:M:27:ALA:HB3	1.97	0.64
2:L:109:ARG:NH1	2:L:115:TYR:OH	2.29	0.64
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.79	0.63
3:M:130:TRP:HD1	3:M:150:PHE:HD2	1.44	0.63
2:L:272:TRP:O	3:M:87:ARG:NH1	2.32	0.62
2:L:170:ASN:HD22	2:L:247:CYS:HB2	1.66	0.61
2:L:170:ASN:ND2	2:L:247:CYS:HB2	2.16	0.61
2:L:212:GLU:OE2	3:M:235:LEU:HD11	2.01	0.61
2:L:128:TYR:HD1	5:L:301:BCL:HBB1	1.64	0.61
2:L:231:ARG:NH1	3:M:42:PHE:O	2.33	0.61
1:H:66:LEU:HD21	3:M:239:ALA:HB1	1.83	0.61
2:L:38:THR:HG21	2:L:100:TRP:HE3	1.66	0.60
3:M:124:VAL:O	3:M:128:SER:OG	2.15	0.59
2:L:201:GLU:HB2	2:L:204:LYS:HG3	1.85	0.59
1:H:231:ASP:OD1	3:M:243:THR:HG22	2.02	0.59
1:H:130:LYS:NZ	1:H:170:ASP:OD2	2.36	0.58
1:H:90:THR:OG1	1:H:97:PRO:O	2.14	0.58
1:H:28:ILE:HD11	4:H:301:LDA:H112	1.85	0.58
2:L:213:ASP:OD1	2:L:223:SER:OG	2.15	0.57
8:M:408:BPH:HHC	8:M:408:BPH:HBB3	1.86	0.56
2:L:234:LEU:O	2:L:238:LEU:HG	2.05	0.56
3:M:75:TRP:HE1	9:M:406:SPO:HM12	1.68	0.56
2:L:211:HIS:CE1	3:M:20:MET:HE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:215:PHE:HB2	3:M:142:MET:HE1	1.86	0.56
3:M:160:LEU:HD23	3:M:284:ILE:HG21	1.86	0.56
1:H:144:ALA:H	3:M:11:GLN:HB2	1.71	0.56
5:L:301:BCL:HBB2	5:L:301:BCL:HHC	1.89	0.55
2:L:187:LEU:HD11	3:M:269:ALA:HB1	1.88	0.55
3:M:199:ASN:OD1	3:M:201:PHE:N	2.40	0.55
2:L:231:ARG:CZ	3:M:6:ILE:O	2.54	0.55
1:H:67:PRO:O	1:H:70:ARG:HG3	2.06	0.55
1:H:12:LEU:HD13	3:M:290:VAL:HG21	1.87	0.55
2:L:1:ALA:O	3:M:253:ARG:NH2	2.38	0.54
3:M:108:PRO:HG2	3:M:111:GLU:HB2	1.88	0.54
3:M:159:VAL:HA	3:M:163:ILE:HB	1.88	0.54
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.90	0.54
1:H:118:ARG:NH2	3:M:236:GLU:OE2	2.41	0.54
1:H:219:ILE:HB	1:H:229:GLU:OE1	2.08	0.54
3:M:161:GLY:HA3	9:M:406:SPO:H26	1.90	0.54
1:H:134:MET:O	1:H:137:ALA:HB3	2.09	0.53
1:H:148:PRO:HD3	3:M:10:VAL:HG11	1.90	0.53
1:H:156:CYS:SG	1:H:204:HIS:CD2	3.01	0.53
2:L:85:LEU:O	2:L:89:ILE:HG13	2.09	0.53
3:M:119:SER:HB3	9:M:406:SPO:H32	1.89	0.53
5:L:301:BCL:HBB3	5:L:302:BCL:H61	1.91	0.53
3:M:103:LEU:CD1	3:M:170:SER:HA	2.39	0.53
1:H:248:ARG:NH1	1:H:248:ARG:CB	2.72	0.52
3:M:293:ASN:OD1	3:M:295:TYR:HB3	2.09	0.52
1:H:148:PRO:HA	1:H:151:LEU:HD13	1.91	0.52
1:H:94:GLU:OE1	1:H:94:GLU:N	2.43	0.52
2:L:248:MET:HE1	5:L:302:BCL:HMD2	1.92	0.52
1:H:156:CYS:C	1:H:158:LEU:H	2.18	0.51
1:H:156:CYS:SG	1:H:205:VAL:O	2.69	0.51
3:M:4:GLN:O	3:M:6:ILE:N	2.43	0.51
1:H:119:ASP:O	1:H:120:LEU:HD23	2.10	0.51
1:H:229:GLU:O	1:H:233:ILE:HG13	2.11	0.51
2:L:130:THR:HA	2:L:134:PHE:HB2	1.93	0.51
1:H:248:ARG:CZ	1:H:248:ARG:CB	2.83	0.50
3:M:32:VAL:HG12	3:M:49:PRO:HD3	1.92	0.50
1:H:156:CYS:CB	1:H:248:ARG:HH11	2.25	0.50
2:L:168:HIS:NE2	5:L:302:BCL:HHC	2.27	0.50
3:M:285:LEU:O	3:M:289:THR:OG1	2.27	0.50
3:M:103:LEU:HD12	3:M:170:SER:CA	2.41	0.49
3:M:175:VAL:HG21	9:M:406:SPO:H242	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:267:VAL:HA	3:M:87:ARG:HG3	1.93	0.49
1:H:156:CYS:HB3	1:H:248:ARG:HH11	1.76	0.48
3:M:51:TYR:O	3:M:132:ARG:NH1	2.30	0.48
1:H:246:PRO:HB2	1:H:247:LYS:HD2	1.94	0.48
1:H:196:VAL:HG12	1:H:205:VAL:HG22	1.95	0.48
1:H:246:PRO:C	1:H:247:LYS:HG3	2.39	0.48
1:H:33:THR:O	1:H:59:PRO:HG3	2.13	0.48
1:H:187:SER:HB2	1:H:189:ARG:HH12	1.78	0.48
2:L:196:SER:HB2	3:M:143:GLY:O	2.14	0.48
8:M:405:BPH:HMA3	5:M:409:BCL:H43	1.96	0.48
2:L:111:LEU:O	3:M:247:ARG:NH1	2.38	0.48
2:L:182:THR:HG22	2:L:236:LEU:HD13	1.96	0.47
3:M:228:ARG:HG3	3:M:229:PHE:CD1	2.48	0.47
2:L:75:LEU:HD11	2:L:140:GLY:HA2	1.95	0.47
2:L:135:ARG:O	2:L:139:MET:HG3	2.14	0.47
3:M:103:LEU:HA	3:M:171:TRP:CE2	2.49	0.47
3:M:89:LEU:HA	3:M:92:PHE:HE1	1.80	0.47
3:M:152:SER:OG	3:M:277:THR:OG1	2.32	0.47
3:M:195:ASN:C	3:M:197:PHE:N	2.72	0.47
3:M:64:LEU:HD23	8:M:405:BPH:H7C2	1.96	0.46
3:M:103:LEU:HD13	3:M:169:GLY:C	2.40	0.46
1:H:134:MET:HG3	1:H:169:VAL:CG1	2.45	0.46
2:L:269:LEU:HB2	2:L:272:TRP:NE1	2.30	0.46
2:L:60:ASN:HB3	2:L:63:LEU:HD12	1.96	0.46
2:L:253:THR:OG1	2:L:254:ILE:N	2.49	0.46
1:H:37:ARG:HD3	1:H:76:PRO:HD3	1.97	0.46
2:L:269:LEU:HD13	2:L:271:TRP:CZ2	2.51	0.46
1:H:134:MET:HE2	1:H:149:ILE:HD11	1.97	0.46
2:L:133:LEU:C	2:L:136:PRO:HD2	2.40	0.46
2:L:230:HIS:NE2	3:M:234:GLU:OE2	2.48	0.46
2:L:279:ILE:HD12	2:L:279:ILE:H	1.81	0.46
1:H:240:GLY:O	1:H:244:ALA:HB3	2.13	0.46
3:M:89:LEU:HA	3:M:92:PHE:CE1	2.51	0.46
3:M:193:HIS:O	3:M:293:ASN:HA	2.15	0.46
8:M:405:BPH:CMB	5:M:409:BCL:H2	2.46	0.46
1:H:118:ARG:HE	1:H:118:ARG:HB2	1.58	0.45
3:M:26:LEU:C	3:M:28:ASN:N	2.75	0.45
1:H:194:GLN:H	1:H:194:GLN:CD	2.24	0.45
3:M:228:ARG:HG3	3:M:229:PHE:CE1	2.52	0.45
3:M:140:LEU:HB2	3:M:142:MET:HE2	1.98	0.45
1:H:32:GLN:HG2	1:H:56:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:167:PHE:HB3	5:L:302:BCL:HMC3	1.99	0.45
2:L:170:ASN:O	2:L:174:MET:HG3	2.17	0.45
1:H:61:PRO:HA	1:H:76:PRO:HD2	1.99	0.44
2:L:43:ALA:O	2:L:47:ILE:HD13	2.16	0.44
2:L:34:PHE:HB2	2:L:103:ARG:HB2	1.97	0.44
3:M:73:TRP:HE1	3:M:77:GLN:NE2	2.15	0.44
2:L:67:TYR:HA	2:L:147:PRO:HB3	2.00	0.44
2:L:183:ASN:ND2	3:M:213:ALA:HA	2.33	0.44
3:M:102:GLY:O	3:M:104:SER:N	2.39	0.44
1:H:178:PHE:CD2	1:H:190:LEU:HB3	2.53	0.44
3:M:272:MET:HE2	3:M:272:MET:HB2	1.85	0.44
1:H:103:ASP:OD2	1:H:106:LYS:HG3	2.18	0.44
2:L:16:LEU:HD23	2:L:16:LEU:HA	1.79	0.44
2:L:227:LEU:O	2:L:231:ARG:HG3	2.18	0.44
3:M:130:TRP:CD1	3:M:150:PHE:HD2	2.30	0.44
1:H:170:ASP:OD1	1:H:172:PRO:HD2	2.18	0.43
2:L:268:LYS:HA	2:L:273:ALA:HB2	2.00	0.43
3:M:171:TRP:C	3:M:173:GLU:N	2.73	0.43
1:H:164:VAL:HG11	1:H:179:LEU:HD22	1.99	0.43
5:L:302:BCL:CHB	5:M:401:BCL:HMB2	2.48	0.43
3:M:87:ARG:HG2	3:M:88:ASP:OD1	2.18	0.43
1:H:20:PHE:HD1	10:M:407:CDL:H401	1.83	0.43
3:M:26:LEU:HB3	3:M:27:ALA:H	1.55	0.43
3:M:103:LEU:CD1	3:M:170:SER:CA	2.97	0.43
3:M:157:TRP:CE3	3:M:158:MET:HG2	2.54	0.43
3:M:75:TRP:HE1	9:M:406:SPO:H32A	1.83	0.43
3:M:129:TRP:O	3:M:133:THR:HG23	2.18	0.43
2:L:202:LYS:HD2	2:L:202:LYS:N	2.27	0.43
2:L:235:LEU:HD22	3:M:42:PHE:CZ	2.54	0.43
3:M:130:TRP:HD1	3:M:150:PHE:CD2	2.32	0.43
5:L:302:BCL:H61	5:L:302:BCL:H41	1.91	0.42
3:M:271:TRP:HA	3:M:274:VAL:HG22	2.00	0.42
2:L:22:PHE:HA	2:L:24:PHE:CE1	2.55	0.42
1:H:154:ARG:HA	1:H:160:ILE:HA	2.02	0.42
3:M:155:TRP:O	3:M:159:VAL:HG23	2.19	0.42
3:M:278:LEU:HD21	10:M:407:CDL:H371	2.00	0.42
2:L:272:TRP:CD2	3:M:87:ARG:HB2	2.55	0.42
1:H:134:MET:HG3	1:H:169:VAL:HG11	2.02	0.42
1:H:221:SER:HA	1:H:222:PRO:HD2	1.70	0.42
2:L:169:TYR:HA	2:L:174:MET:HE3	2.01	0.42
2:L:202:LYS:H	2:L:202:LYS:CD	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:59:SER:HB2	3:M:128:SER:HB2	2.02	0.42
3:M:195:ASN:C	3:M:197:PHE:H	2.26	0.42
1:H:157:ASP:HA	1:H:248:ARG:HG3	0.94	0.42
1:H:177:ARG:NH1	3:M:232:GLU:OE2	2.38	0.42
2:L:190:HIS:NE2	3:M:266:HIS:HE1	2.18	0.42
3:M:163:ILE:O	3:M:167:LEU:HG	2.20	0.42
2:L:34:PHE:O	2:L:38:THR:OG1	2.26	0.41
2:L:262:TRP:O	2:L:265:TRP:HD1	2.03	0.41
3:M:267:ARG:HH11	3:M:267:ARG:HD3	1.68	0.41
9:M:406:SPO:H26	9:M:406:SPO:H241	1.86	0.41
1:H:14:SER:HA	1:H:17:ILE:HG22	2.02	0.41
5:L:302:BCL:H2C	5:M:401:BCL:HBC2	2.02	0.41
3:M:70:ILE:HD13	3:M:177:TYR:HB3	2.02	0.41
1:H:140:PHE:CE1	3:M:14:GLY:HA3	2.56	0.41
1:H:148:PRO:HG2	1:H:167:ILE:HD11	2.03	0.41
2:L:217:ARG:O	3:M:50:ILE:HA	2.21	0.41
2:L:170:ASN:OD1	2:L:259:TRP:CE2	2.73	0.41
3:M:102:GLY:C	3:M:104:SER:H	2.25	0.41
3:M:103:LEU:CD1	3:M:170:SER:N	2.83	0.41
3:M:196:LEU:HA	3:M:196:LEU:HD23	1.66	0.41
3:M:188:ASN:O	3:M:192:VAL:HG23	2.19	0.41
1:H:146:LYS:HD2	1:H:146:LYS:HA	1.81	0.41
2:L:269:LEU:HD23	2:L:269:LEU:HA	1.81	0.41
3:M:175:VAL:CG2	9:M:406:SPO:H242	2.51	0.41
5:L:302:BCL:C1C	5:M:401:BCL:HBB3	2.51	0.41
3:M:195:ASN:HD22	3:M:195:ASN:HA	1.72	0.41
3:M:211:GLY:HA3	3:M:272:MET:SD	2.61	0.41
1:H:156:CYS:SG	1:H:204:HIS:NE2	2.94	0.40
2:L:14:GLY:O	2:L:109:ARG:HD3	2.21	0.40
2:L:201:GLU:HG3	3:M:141:GLY:HA2	2.02	0.40
1:H:17:ILE:HD12	1:H:17:ILE:HA	1.95	0.40
2:L:47:ILE:HG22	2:L:48:LEU:HD23	2.02	0.40
3:M:62:SER:HB2	3:M:125:ALA:HB2	2.04	0.40
1:H:30:TYR:HH	3:M:267:ARG:NH1	2.12	0.40
1:H:207:ALA:HB1	1:H:237:VAL:O	2.22	0.40
1:H:246:PRO:C	1:H:247:LYS:CG	2.94	0.40
3:M:102:GLY:HA2	3:M:170:SER:HB2	2.03	0.40
2:L:183:ASN:OD1	3:M:216:PHE:HD2	2.05	0.40
3:M:222:THR:O	3:M:226:VAL:HG22	2.22	0.40
8:M:405:BPH:HBA2	8:M:405:BPH:H3A	1.89	0.40

All (17) symmetry-related close contacts are listed below. The label for Atom-2 includes the

symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:135:LYS:CE	3:M:295:TYR:CZ[4_565]	0.51	1.69
1:H:135:LYS:NZ	3:M:295:TYR:CG[4_565]	0.83	1.37
1:H:135:LYS:CD	3:M:295:TYR:CE1[4_565]	0.85	1.35
1:H:135:LYS:CE	3:M:295:TYR:CE2[4_565]	1.00	1.20
1:H:135:LYS:NZ	3:M:295:TYR:CD2[4_565]	1.06	1.14
1:H:135:LYS:CD	3:M:295:TYR:CZ[4_565]	1.22	0.98
1:H:135:LYS:NZ	3:M:295:TYR:CD1[4_565]	1.31	0.89
1:H:135:LYS:CE	3:M:295:TYR:CE1[4_565]	1.36	0.84
1:H:135:LYS:NZ	3:M:295:TYR:CE2[4_565]	1.65	0.55
1:H:135:LYS:CD	3:M:295:TYR:OH[4_565]	1.74	0.46
1:H:135:LYS:CE	3:M:295:TYR:OH[4_565]	1.83	0.37
1:H:135:LYS:NZ	3:M:295:TYR:CE1[4_565]	1.83	0.37
1:H:135:LYS:CE	3:M:295:TYR:CD2[4_565]	1.85	0.35
1:H:135:LYS:NZ	3:M:295:TYR:CZ[4_565]	1.95	0.25
1:H:135:LYS:CG	3:M:295:TYR:OH[4_565]	2.05	0.15
1:H:135:LYS:CE	3:M:295:TYR:CD1[4_565]	2.06	0.14
1:H:135:LYS:CD	3:M:295:TYR:CD1[4_565]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	238/240 (99%)	220 (92%)	14 (6%)	4 (2%)	7 35
2	L	279/281 (99%)	263 (94%)	13 (5%)	3 (1%)	11 44
3	M	298/301 (99%)	276 (93%)	19 (6%)	3 (1%)	12 45
All	All	815/822 (99%)	759 (93%)	46 (6%)	10 (1%)	10 42

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	245	ALA

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Mol	Chain	Res	Type
3	M	5	ASN
1	H	136	ALA
3	M	211	GLY
2	L	276	PRO
3	M	173	GLU
1	H	51	ALA
1	H	220	LYS
2	L	200	PRO
2	L	31	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/195 (100%)	189 (97%)	6 (3%)	35	60
2	L	220/220 (100%)	220 (100%)	0	100	100
3	M	235/235 (100%)	232 (99%)	3 (1%)	61	72
All	All	650/650 (100%)	641 (99%)	9 (1%)	59	72

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	134	MET
1	H	135	LYS
1	H	219	ILE
1	H	220	LYS
1	H	247	LYS
1	H	248	ARG
3	M	2	GLU
3	M	173	GLU
3	M	195	ASN

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

Mol	Chain	Res	Type
1	H	174	GLN
1	H	201	ASN
2	L	170	ASN
3	M	195	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\| > 2$
3	6DU	M	210	3	11,12,13	0.90	1 (9%)	10,15,17	0.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6DU	M	210	3	-	2/5/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	210	6DU	O-C	2.89	1.31	1.20

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	210	6DU	CA-CB-CG-CD1
3	M	210	6DU	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	BCL	M	409	9,3	54,59,74	1.26	3 (5%)	61,97,115	1.42	6 (9%)
4	LDA	M	403	-	13,15,15	2.35	2 (15%)	14,17,17	0.57	0
4	LDA	M	402	-	13,15,15	2.33	2 (15%)	14,17,17	0.66	0
10	CDL	M	407	3	68,68,99	1.08	6 (8%)	74,80,111	0.87	4 (5%)
8	BPH	M	405	-	49,60,70	1.18	5 (10%)	47,89,101	2.01	7 (14%)
5	BCL	L	301	2	69,74,74	1.11	5 (7%)	79,115,115	1.38	7 (8%)
5	BCL	M	401	3	69,74,74	1.17	4 (5%)	79,115,115	1.43	10 (12%)
9	SPO	M	406	3,5	41,41,41	0.19	0	47,50,50	0.44	0
8	BPH	M	408	3	59,70,70	1.15	5 (8%)	59,101,101	1.87	8 (13%)
4	LDA	H	301	-	13,15,15	2.45	2 (15%)	14,17,17	0.57	0
5	BCL	L	302	2	69,74,74	1.12	3 (4%)	79,115,115	1.26	7 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	M	409	9,3	-	6/23/119/137	-
4	LDA	M	403	-	-	7/13/13/13	-
4	LDA	M	402	-	-	8/13/13/13	-
10	CDL	M	407	3	1/1/9/9	34/79/79/110	-
8	BPH	M	405	-	-	1/25/93/105	0/5/6/6
5	BCL	L	301	2	-	7/41/137/137	-
5	BCL	M	401	3	-	5/41/137/137	-
9	SPO	M	406	3,5	-	8/47/47/47	-
8	BPH	M	408	3	-	9/37/105/105	0/5/6/6
4	LDA	H	301	-	-	5/13/13/13	-
5	BCL	L	302	2	-	5/41/137/137	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	403	LDA	O1-N1	-6.79	1.25	1.42
4	H	301	LDA	O1-N1	-6.78	1.25	1.42
4	M	402	LDA	O1-N1	-6.75	1.25	1.42
4	H	301	LDA	C1-N1	-5.60	1.45	1.51
5	M	401	BCL	MG-NA	5.11	2.18	2.06
4	M	403	LDA	C1-N1	-5.02	1.46	1.51
4	M	402	LDA	C1-N1	-4.92	1.46	1.51
5	M	409	BCL	MG-NA	4.90	2.17	2.06
5	L	302	BCL	MG-NA	4.88	2.17	2.06
5	L	301	BCL	MG-NA	4.65	2.17	2.06
8	M	405	BPH	CBD-CGD	-4.12	1.47	1.52
8	M	408	BPH	CBD-CGD	-4.12	1.47	1.52
5	L	302	BCL	MG-NC	3.82	2.15	2.06
5	M	409	BCL	MG-NC	3.66	2.15	2.06
5	M	401	BCL	MG-NC	3.45	2.14	2.06
5	L	301	BCL	MG-NC	3.43	2.14	2.06
8	M	408	BPH	C3D-CAD	-3.27	1.41	1.47
10	M	407	CDL	PA1-OA4	-3.17	1.40	1.55
8	M	408	BPH	C3B-C4B	3.10	1.46	1.41
5	M	401	BCL	C3B-C4B	3.06	1.47	1.41
5	L	301	BCL	C3B-C4B	2.94	1.46	1.41
10	M	407	CDL	PB2-OB4	-2.92	1.41	1.55
10	M	407	CDL	PB2-OB3	-2.86	1.40	1.50
8	M	405	BPH	C3D-CAD	-2.83	1.42	1.47
10	M	407	CDL	PA1-OA5	2.77	1.70	1.59
10	M	407	CDL	PA1-OA3	-2.68	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	407	CDL	PB2-OB5	2.57	1.69	1.59
8	M	405	BPH	C3B-C4B	2.54	1.45	1.41
5	M	409	BCL	CHD-C1D	2.46	1.43	1.38
8	M	405	BPH	OBD-CAD	2.28	1.25	1.22
5	M	401	BCL	CHD-C1D	2.27	1.42	1.38
5	L	301	BCL	CHD-C1D	2.18	1.42	1.38
8	M	405	BPH	C1D-C2D	2.18	1.42	1.39
8	M	408	BPH	C1D-C2D	2.17	1.42	1.39
5	L	302	BCL	C1D-C2D	-2.14	1.41	1.45
8	M	408	BPH	CHA-CBD	2.08	1.54	1.51
5	L	301	BCL	C1D-C2D	-2.07	1.41	1.45

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	408	BPH	C4D-CHA-CBD	-10.14	103.59	108.45
8	M	405	BPH	C4D-CHA-CBD	-9.76	103.78	108.45
5	M	401	BCL	C4D-CHA-C1A	5.27	127.53	121.24
5	L	301	BCL	C4D-CHA-C1A	5.12	127.35	121.24
5	M	409	BCL	C4D-CHA-C1A	5.04	127.26	121.24
5	L	302	BCL	C4D-CHA-C1A	4.24	126.30	121.24
5	M	401	BCL	C1-C2-C3	-4.23	119.26	126.20
8	M	408	BPH	C4D-ND-C1D	-4.02	104.06	108.87
5	L	301	BCL	CHD-C1D-ND	-4.02	119.15	124.80
8	M	405	BPH	C4D-ND-C1D	-3.99	104.09	108.87
5	L	301	BCL	C1D-ND-C4D	-3.91	103.57	106.31
8	M	405	BPH	C3D-C4D-ND	3.68	112.43	107.71
5	M	409	BCL	CHD-C1D-ND	-3.67	119.63	124.80
5	M	409	BCL	C1D-ND-C4D	-3.63	103.76	106.31
5	M	401	BCL	CHD-C1D-ND	-3.59	119.75	124.80
5	L	302	BCL	C1D-ND-C4D	-3.59	103.80	106.31
5	M	401	BCL	C1D-ND-C4D	-3.54	103.83	106.31
5	L	302	BCL	CHD-C1D-ND	-3.47	119.92	124.80
8	M	408	BPH	C3D-C4D-ND	3.40	112.07	107.71
5	M	401	BCL	C4A-NA-C1A	3.29	108.18	106.68
8	M	405	BPH	OBD-CAD-CBD	-3.23	121.09	125.82
5	M	401	BCL	CHA-C1A-NA	-3.21	119.11	126.39
5	L	302	BCL	CHA-C1A-NA	-3.14	119.28	126.39
5	M	409	BCL	CHA-C1A-NA	-3.03	119.54	126.39
10	M	407	CDL	OA4-PA1-OA3	3.01	126.47	112.44
8	M	408	BPH	OBD-CAD-CBD	-3.00	121.42	125.82
5	M	409	BCL	C2A-C1A-CHA	2.99	129.06	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	302	BCL	C2A-C1A-CHA	2.98	129.05	123.87
5	L	301	BCL	CHA-C1A-NA	-2.93	119.75	126.39
5	L	301	BCL	C2A-C1A-CHA	2.93	128.96	123.87
10	M	407	CDL	OB4-PB2-OB3	2.89	125.88	112.44
5	L	301	BCL	C4A-NA-C1A	2.86	107.98	106.68
5	L	302	BCL	CAB-C3B-C2B	2.84	133.65	127.74
8	M	405	BPH	C2D-C1D-ND	2.80	111.45	109.43
5	M	409	BCL	C4A-NA-C1A	2.64	107.88	106.68
8	M	408	BPH	C2D-C1D-ND	2.59	111.30	109.43
5	M	401	BCL	CAA-CBA-CGA	-2.52	106.04	113.21
5	L	301	BCL	C16-C15-C13	-2.52	107.58	115.97
5	M	401	BCL	C2A-C1A-CHA	2.45	128.13	123.87
10	M	407	CDL	OA6-CA5-OA7	-2.45	117.97	123.70
5	L	302	BCL	O2D-CGD-CBD	2.37	115.37	111.23
8	M	405	BPH	O2D-CGD-CBD	2.36	113.54	110.95
8	M	405	BPH	CMD-C2D-C3D	2.36	129.39	124.68
8	M	408	BPH	CMD-C2D-C3D	2.24	129.15	124.68
10	M	407	CDL	OB6-CB5-OB7	-2.23	118.50	123.70
8	M	408	BPH	OBB-CAB-CBB	-2.12	115.68	120.19
8	M	408	BPH	CMB-C2B-C3B	2.11	128.90	124.68
5	M	401	BCL	OBB-CAB-CBB	-2.10	115.06	119.77
5	M	401	BCL	CHC-C4B-NB	-2.05	120.97	124.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	M	407	CDL	CA4

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	402	LDA	C2-C1-N1-O1
4	M	402	LDA	C2-C1-N1-CM1
4	M	402	LDA	C2-C1-N1-CM2
4	M	403	LDA	C2-C1-N1-O1
4	M	403	LDA	C2-C1-N1-CM1
4	M	403	LDA	C2-C1-N1-CM2
5	L	301	BCL	C2C-C3C-CAC-CBC
5	M	401	BCL	CAD-CBD-CGD-O1D
5	M	401	BCL	CAD-CBD-CGD-O2D
5	M	409	BCL	C2B-C3B-CAB-OBB
5	M	409	BCL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
9	M	406	SPO	C5-C6-C7-C8
9	M	406	SPO	C5-C6-C7-C9
9	M	406	SPO	C25-C26-C27-C28
10	M	407	CDL	CA2-OA2-PA1-OA5
10	M	407	CDL	CA3-OA5-PA1-OA4
10	M	407	CDL	C11-CA5-OA6-CA4
10	M	407	CDL	CB3-OB5-PB2-OB2
10	M	407	CDL	CB3-OB5-PB2-OB4
10	M	407	CDL	OA7-CA5-OA6-CA4
9	M	406	SPO	C28-C30-C31-C32
8	M	408	BPH	C11-C12-C13-C14
4	M	403	LDA	C4-C5-C6-C7
10	M	407	CDL	C31-CA7-OA8-CA6
10	M	407	CDL	CA7-C31-C32-C33
10	M	407	CDL	OA9-CA7-OA8-CA6
5	M	409	BCL	C4B-C3B-CAB-OBB
10	M	407	CDL	O1-C1-CA2-OA2
8	M	408	BPH	C8-C10-C11-C12
8	M	408	BPH	C15-C16-C17-C18
4	M	402	LDA	C11-C10-C9-C8
10	M	407	CDL	CB2-C1-CA2-OA2
10	M	407	CDL	CB5-C51-C52-C53
4	M	402	LDA	C7-C8-C9-C10
4	H	301	LDA	C6-C7-C8-C9
10	M	407	CDL	C71-C72-C73-C74
10	M	407	CDL	OB6-CB4-CB6-OB8
4	H	301	LDA	C5-C6-C7-C8
4	M	402	LDA	C4-C5-C6-C7
4	H	301	LDA	C7-C8-C9-C10
10	M	407	CDL	C13-C14-C15-C16
10	M	407	CDL	CA2-C1-CB2-OB2
4	M	403	LDA	C1-C2-C3-C4
8	M	408	BPH	C11-C10-C8-C7
8	M	408	BPH	C11-C12-C13-C15
5	M	401	BCL	C16-C17-C18-C20
5	M	409	BCL	C4B-C3B-CAB-CBB
4	M	403	LDA	C2-C3-C4-C5
8	M	408	BPH	C2-C3-C5-C6
10	M	407	CDL	C35-C36-C37-C38
8	M	405	BPH	O2A-C1-C2-C3
10	M	407	CDL	CA6-CA4-OA6-CA5
10	M	407	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
8	M	408	BPH	C10-C11-C12-C13
4	H	301	LDA	C9-C10-C11-C12
8	M	408	BPH	C4-C3-C5-C6
8	M	408	BPH	C11-C10-C8-C9
4	M	403	LDA	C11-C10-C9-C8
10	M	407	CDL	CB3-CB4-CB6-OB8
5	L	302	BCL	C4-C3-C5-C6
5	M	401	BCL	C16-C17-C18-C19
10	M	407	CDL	OB5-CB3-CB4-CB6
9	M	406	SPO	C29-C28-C30-C31
10	M	407	CDL	C14-C15-C16-C17
4	M	402	LDA	C9-C10-C11-C12
9	M	406	SPO	C27-C28-C30-C31
10	M	407	CDL	O1-C1-CB2-OB2
5	L	301	BCL	C12-C13-C15-C16
10	M	407	CDL	OB5-CB3-CB4-OB6
10	M	407	CDL	C36-C37-C38-C39
5	M	409	BCL	CHA-CBD-CGD-O2D
10	M	407	CDL	CA2-OA2-PA1-OA3
10	M	407	CDL	C17-C18-C19-C20
4	M	402	LDA	C6-C7-C8-C9
5	L	302	BCL	C2-C3-C5-C6
5	L	302	BCL	C2A-CAA-CBA-CGA
5	M	401	BCL	C14-C13-C15-C16
10	M	407	CDL	C39-C40-C41-C42
5	L	301	BCL	C11-C12-C13-C15
5	L	302	BCL	C11-C12-C13-C15
10	M	407	CDL	C12-C13-C14-C15
5	L	301	BCL	C14-C13-C15-C16
5	L	301	BCL	C2B-C3B-CAB-OBB
10	M	407	CDL	OB7-CB5-OB6-CB4
5	L	301	BCL	C11-C12-C13-C14
5	L	302	BCL	C11-C12-C13-C14
10	M	407	CDL	C72-C71-CB7-OB8
10	M	407	CDL	C51-CB5-OB6-CB4
4	H	301	LDA	C2-C3-C4-C5
9	M	406	SPO	C3-C1-O1-CM1
9	M	406	SPO	C34-C33-C35-C36
5	M	409	BCL	C2-C1-O2A-CGA
5	L	301	BCL	C2B-C3B-CAB-CBB
10	M	407	CDL	C38-C39-C40-C41
10	M	407	CDL	C72-C71-CB7-OB9

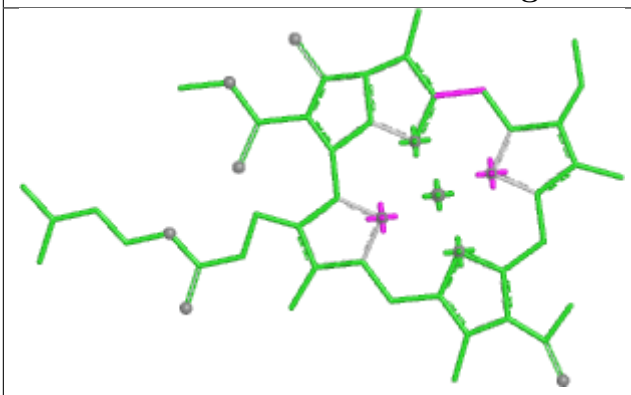
There are no ring outliers.

9 monomers are involved in 26 short contacts:

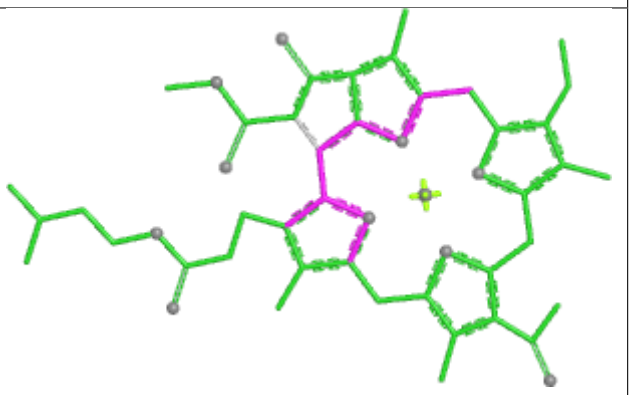
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	409	BCL	2	0
10	M	407	CDL	2	0
8	M	405	BPH	5	0
5	L	301	BCL	3	0
5	M	401	BCL	3	0
9	M	406	SPO	7	0
8	M	408	BPH	1	0
4	H	301	LDA	1	0
5	L	302	BCL	8	0

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

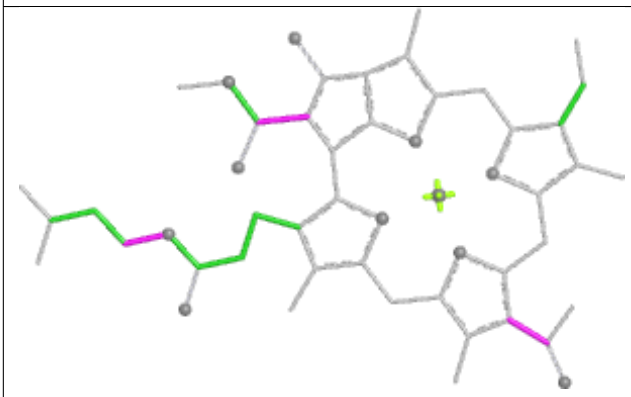
Ligand BCL M 409



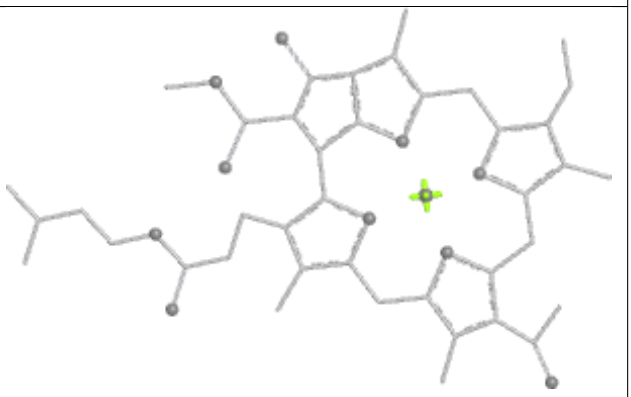
Bond lengths



Bond angles

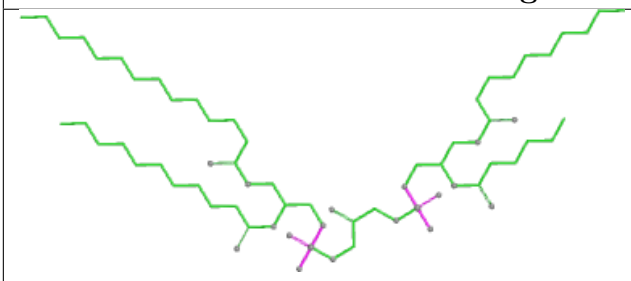


Torsions

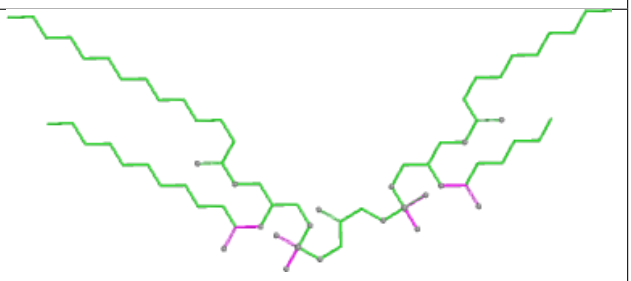


Rings

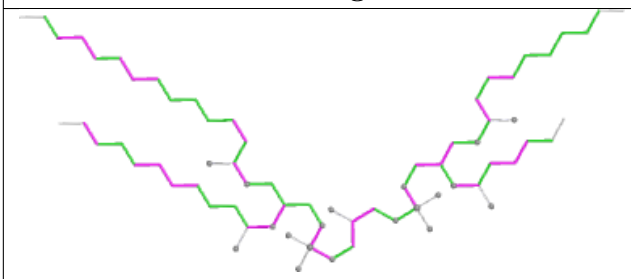
Ligand CDL M 407



Bond lengths



Bond angles



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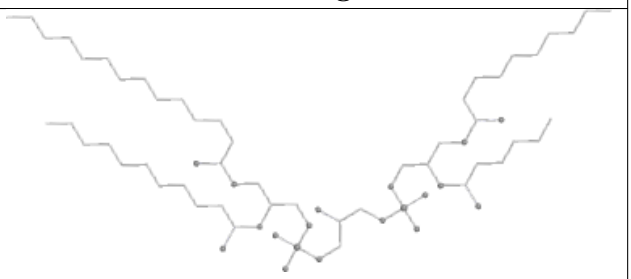
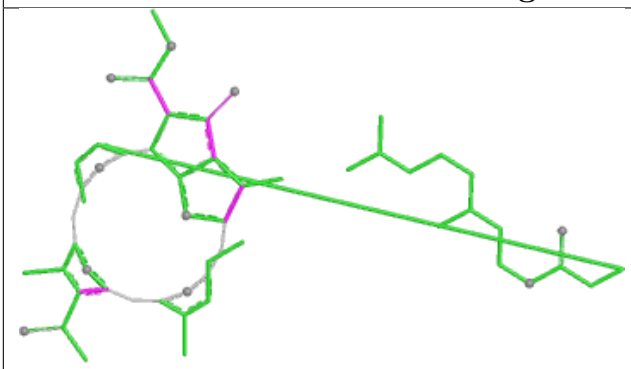
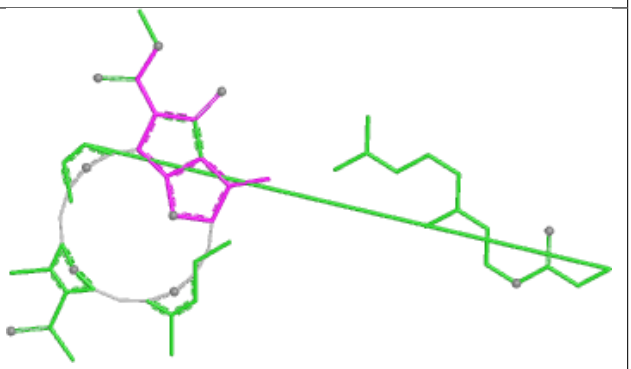


Rings

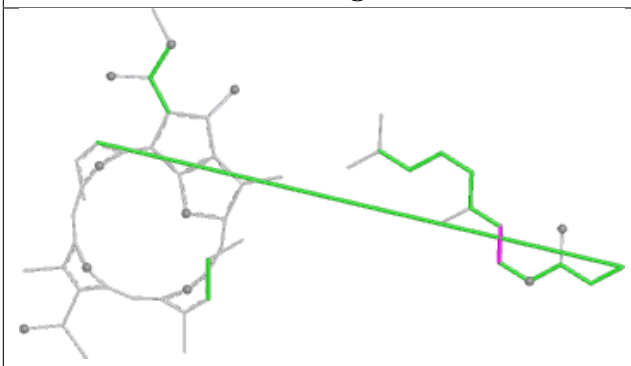
Ligand BPH M 405



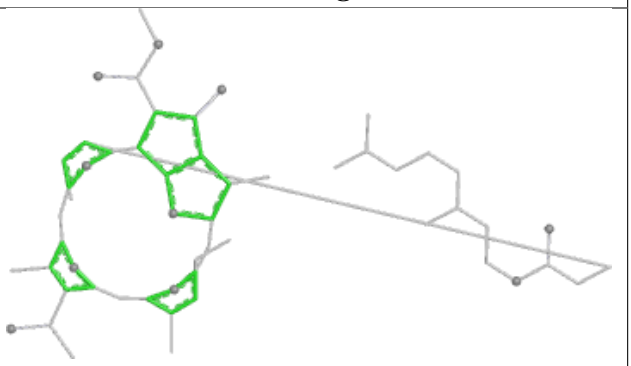
Bond lengths



Bond angles

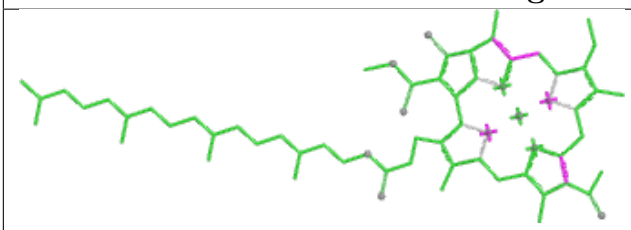


Torsions

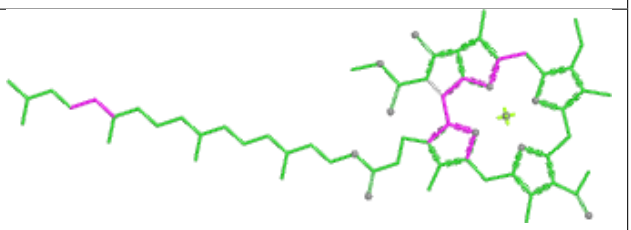


Rings

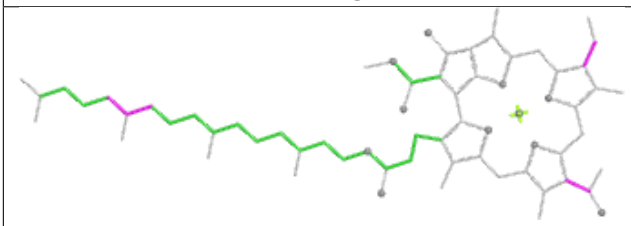
Ligand BCL L 301



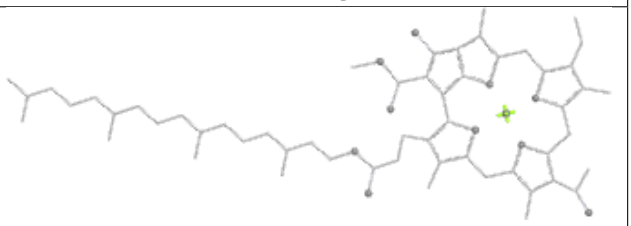
Bond lengths



Bond angles

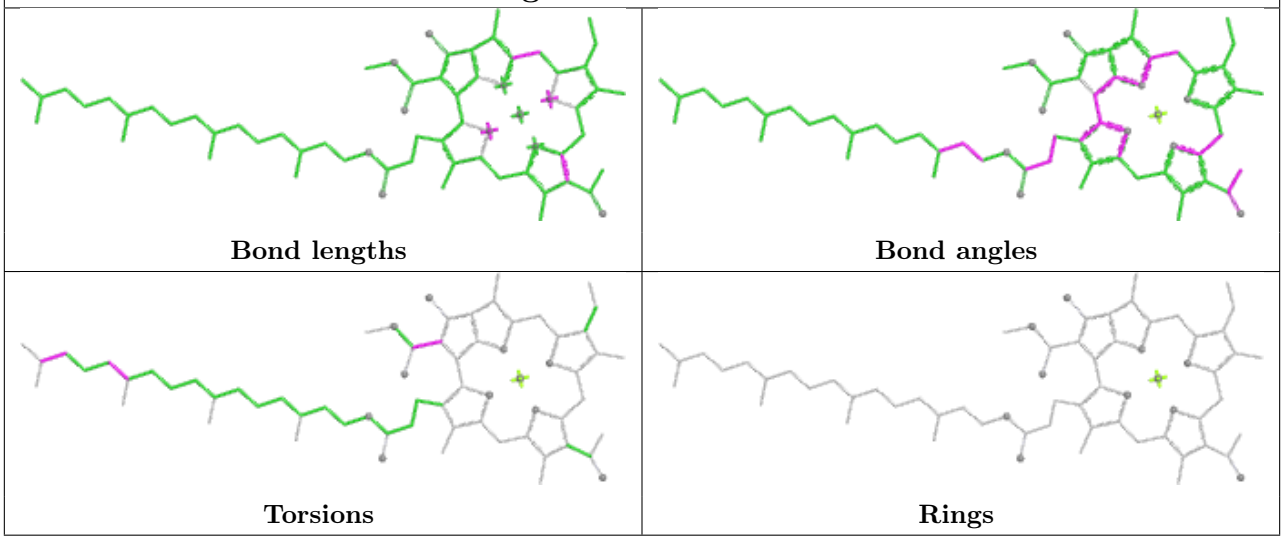


Torsions

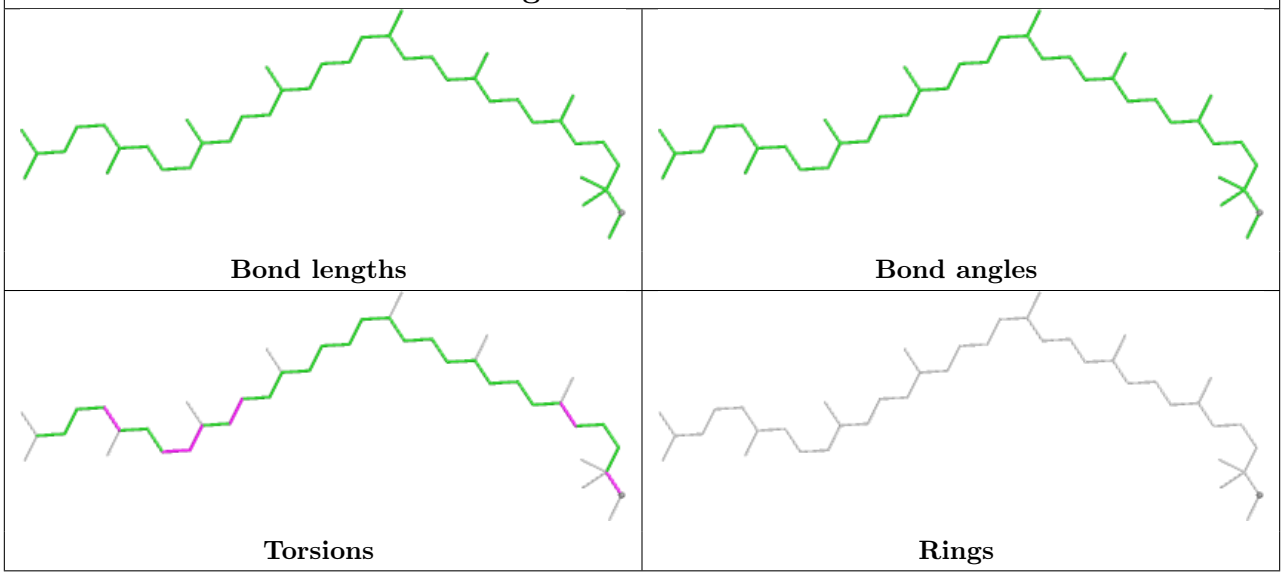


Rings

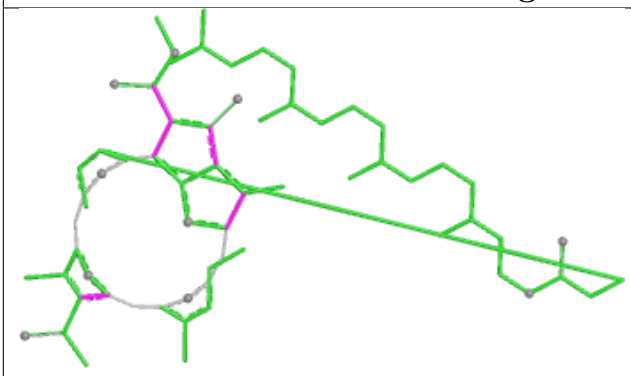
Ligand BCL M 401



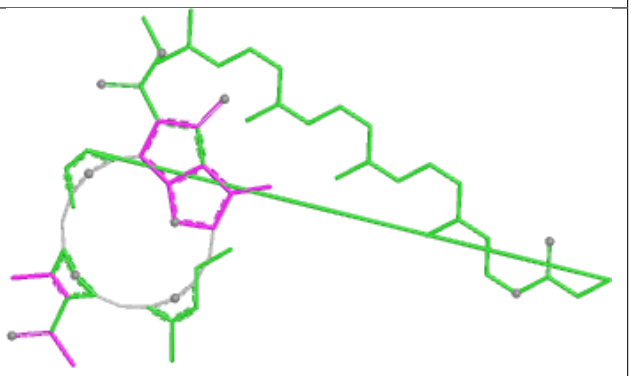
Ligand SPO M 406



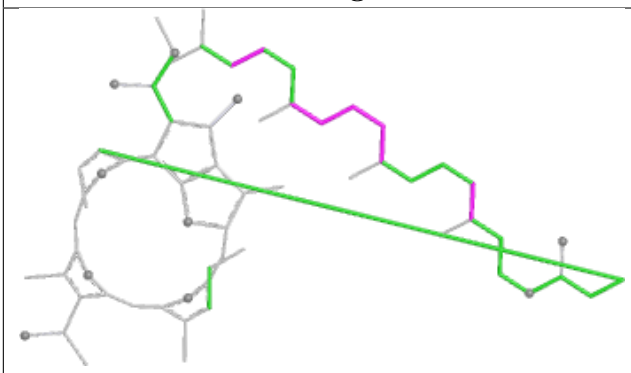
Ligand BPH M 408



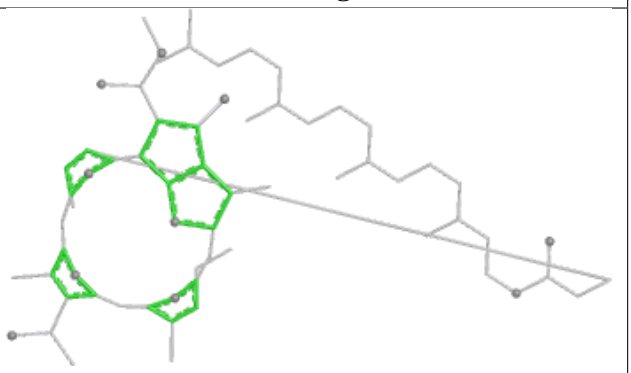
Bond lengths



Bond angles

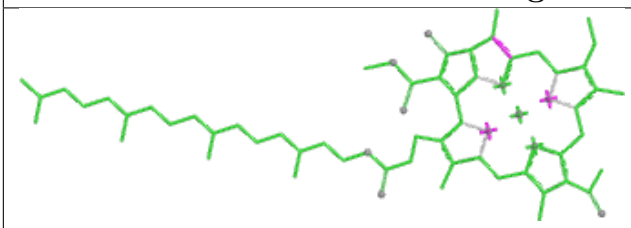


Torsions

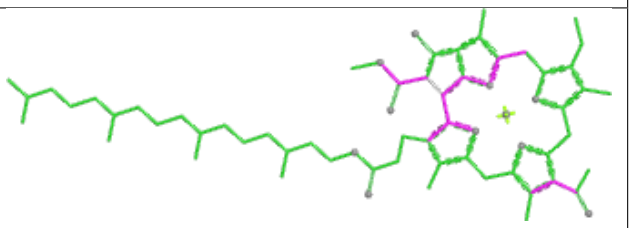


Rings

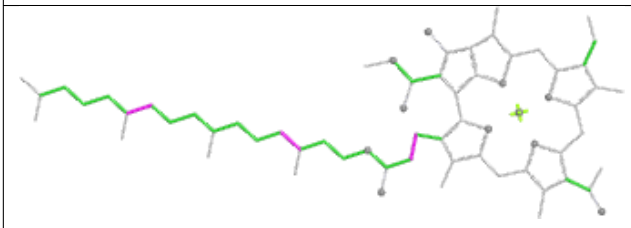
Ligand BCL L 302



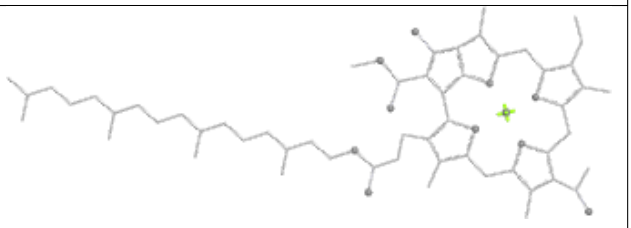
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	H	240/240 (100%)	0.28	6 (2%)	58	33	54, 68, 103, 206	0
2	L	281/281 (100%)	0.04	7 (2%)	58	33	46, 62, 96, 161	0
3	M	300/301 (99%)	0.18	9 (3%)	52	29	50, 68, 100, 142	0
All	All	821/822 (99%)	0.16	22 (2%)	56	32	46, 66, 101, 206	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	102	GLY	5.7
3	M	292	ASP	4.4
3	M	299	GLN	3.8
3	M	300	ASN	3.8
2	L	279	ILE	3.6
3	M	302	GLY	3.5
3	M	2	GLU	3.4
1	H	249	LYS	3.4
1	H	246	PRO	3.3
2	L	62	GLN	3.1
2	L	151	TRP	2.9
1	H	135	LYS	2.7
3	M	27	ALA	2.6
1	H	250	SER	2.5
3	M	95	GLU	2.5
3	M	295	TYR	2.5
2	L	63	LEU	2.4
1	H	128	HIS	2.3
2	L	226	THR	2.2
2	L	280	ASN	2.2
2	L	153	HIS	2.2
3	M	3	TYR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
3	6DU	M	210	12/13	0.89	0.21	58,66,80,90	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

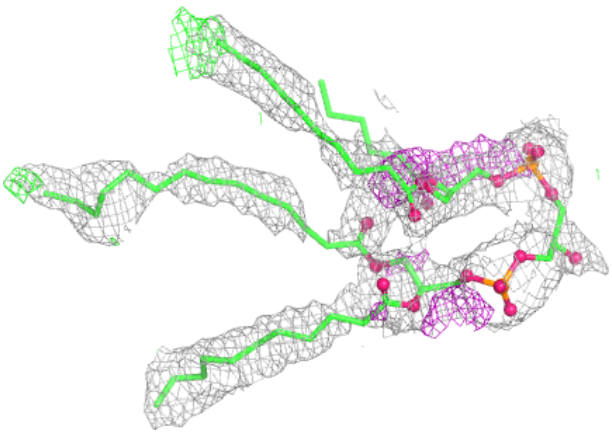
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

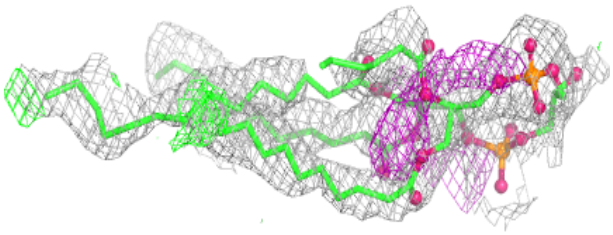
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	LDA	M	403	16/16	0.75	0.28	68,87,118,118	0
10	CDL	M	407	69/100	0.76	0.24	72,93,116,118	0
4	LDA	H	301	16/16	0.84	0.27	75,81,97,99	0
4	LDA	M	402	16/16	0.84	0.21	69,78,92,93	0
9	SPO	M	406	42/42	0.91	0.19	54,69,77,79	0
8	BPH	M	405	55/65	0.93	0.15	50,59,75,82	0
8	BPH	M	408	65/65	0.94	0.13	49,55,59,68	0
5	BCL	M	409	51/66	0.94	0.12	50,56,62,69	0
5	BCL	L	302	66/66	0.94	0.13	43,54,63,67	0
5	BCL	L	301	66/66	0.95	0.12	48,56,64,70	0
5	BCL	M	401	66/66	0.96	0.11	45,55,63,71	0
6	CL	L	303	1/1	0.97	0.10	85,85,85,85	0
7	FE	M	404	1/1	1.00	0.04	46,46,46,46	0

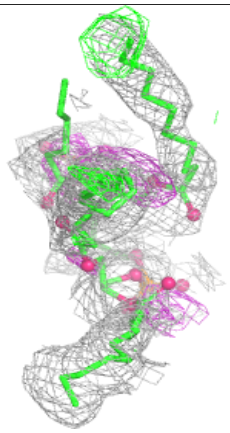
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CDL M 407:

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

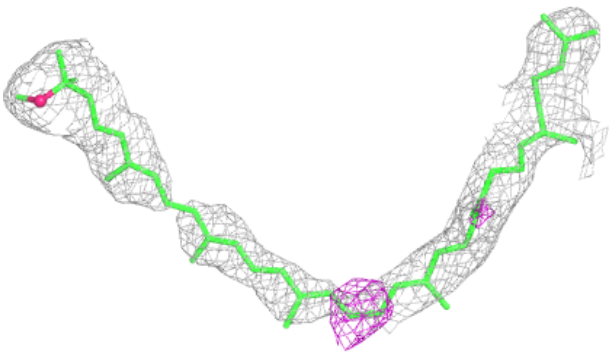


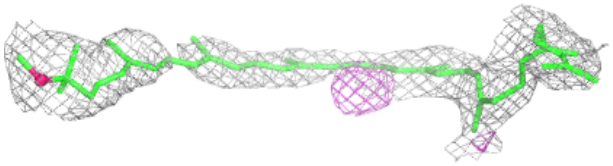




Electron density around SPO M 406:

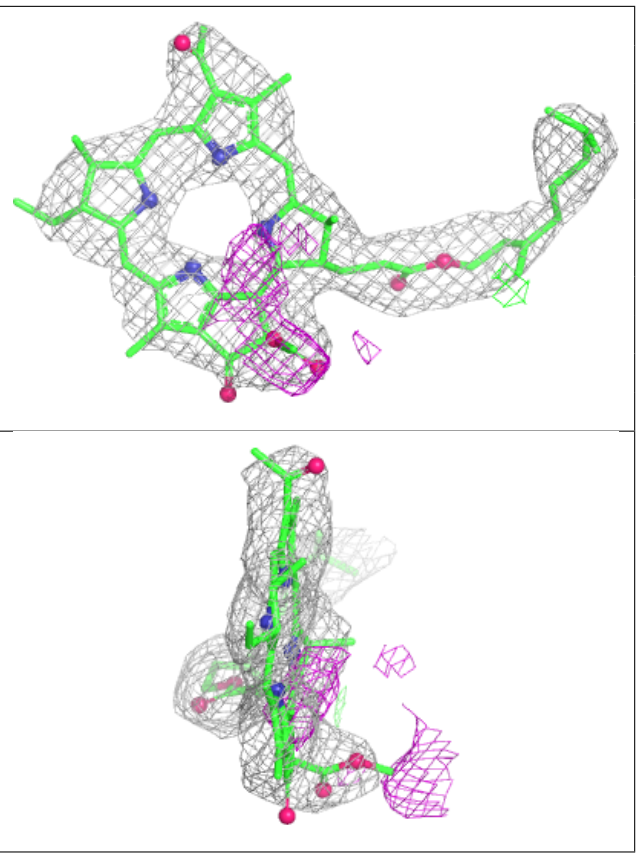
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





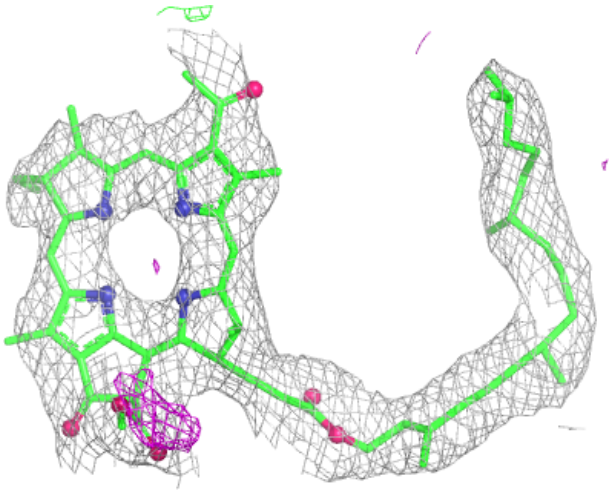
Electron density around BPH M 405:

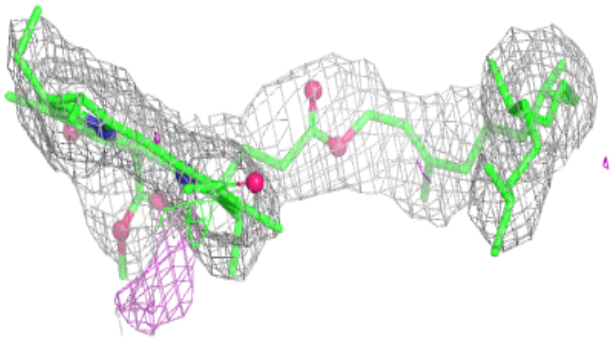
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BPH M 408:

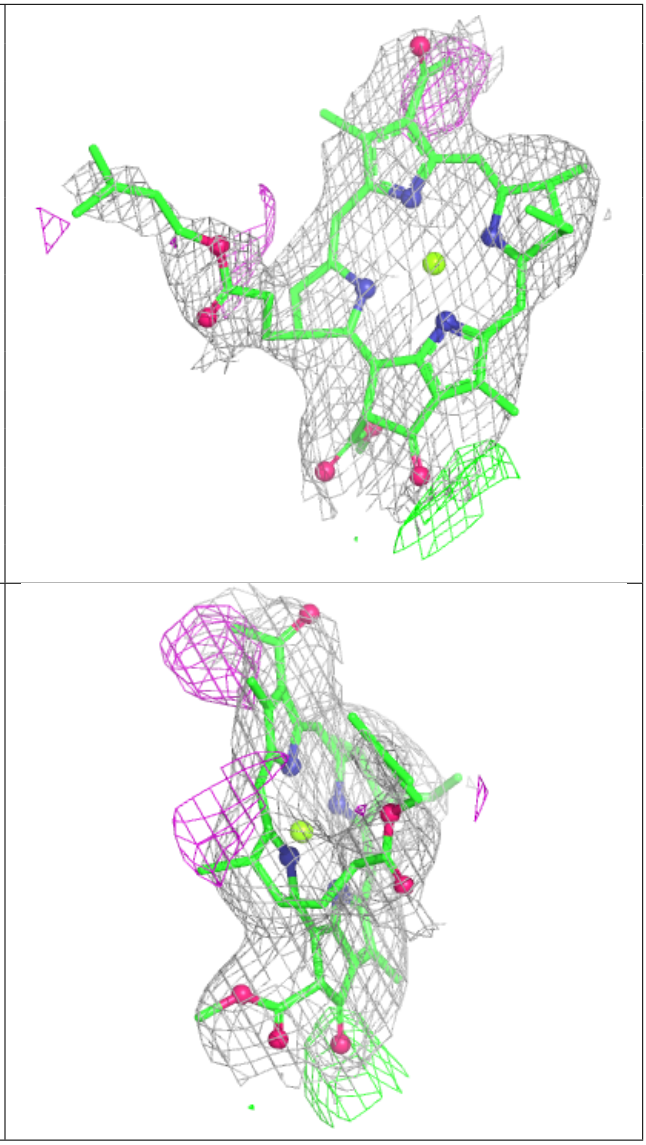
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





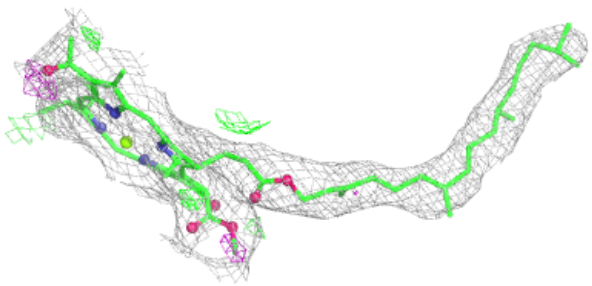
Electron density around BCL M 409:

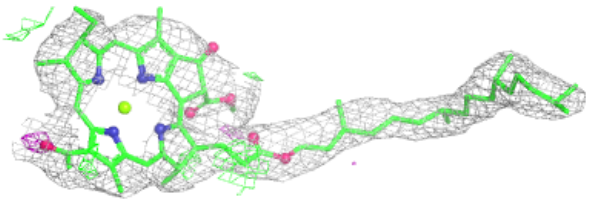
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

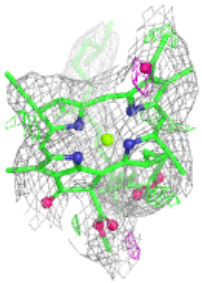


Electron density around BCL L 302:

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







Electron density around BCL L 301:

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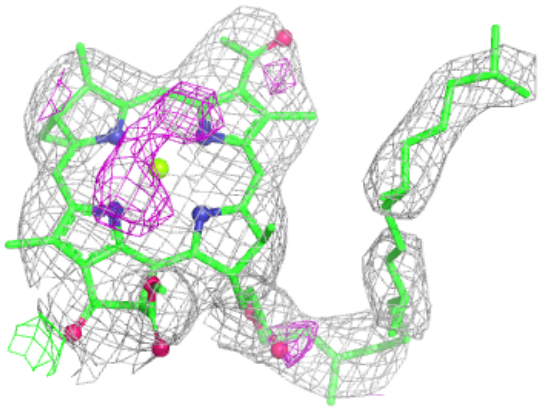
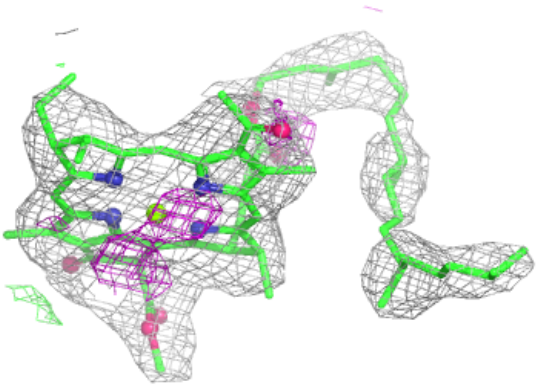
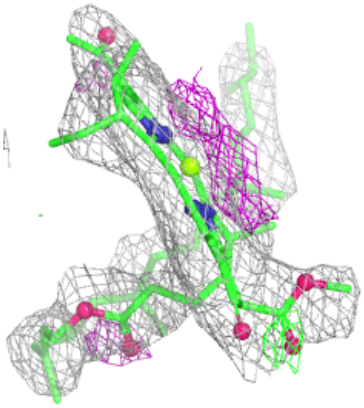
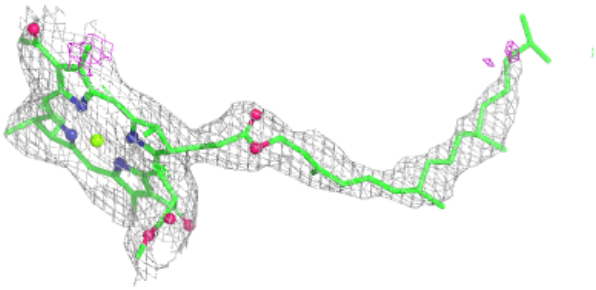
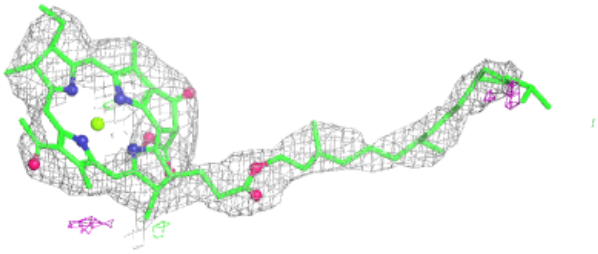
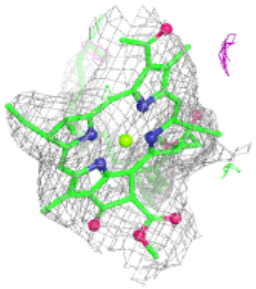
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around BCL M 401: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.