



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:08 PM EDT

PDB ID : 8VTL / pdb_00008vtl
Title : Crystal structure of R. sphaeroides Photosynthetic Reaction Center variant Y (M210)2-methoxyphenylalanine
Authors : Tran, K.; Mathews, I.; Boxer, S.G.
Deposited on : 2024-01-26
Resolution : 3.05 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 ⓘ 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 ⓘ](#)) 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

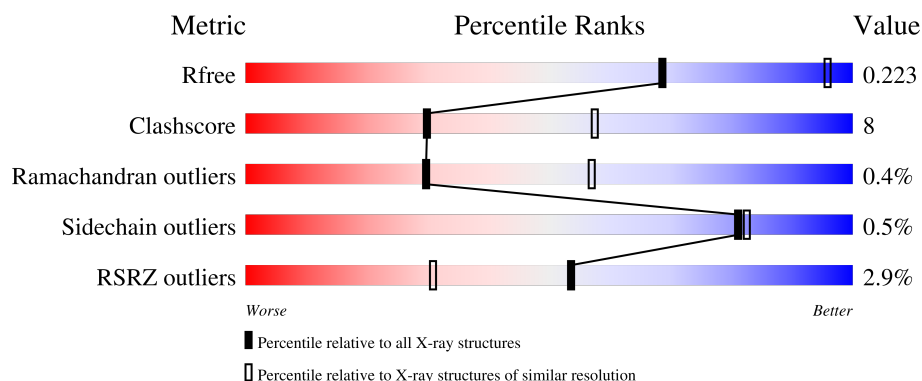
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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 $\leq 5\%$. 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	4% 78% 21%
2	L	281	2% 87% 13%
3	M	301	3% 83% 16%

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

There are 11 unique types of molecules in this entry. The entry contains 7019 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
1	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	2	0
			2248	1517	357	366	8			

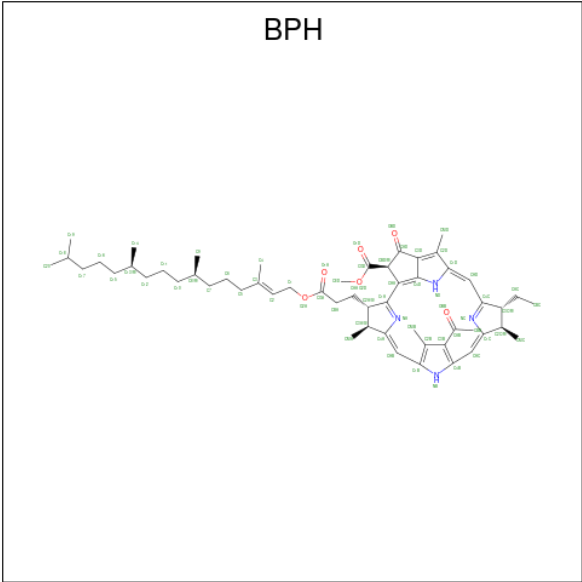
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	301	Total	C	N	O	S	0	0	0
			2397	1599	392	396	10			

There are 2 discrepancies between the modelled and reference sequences:

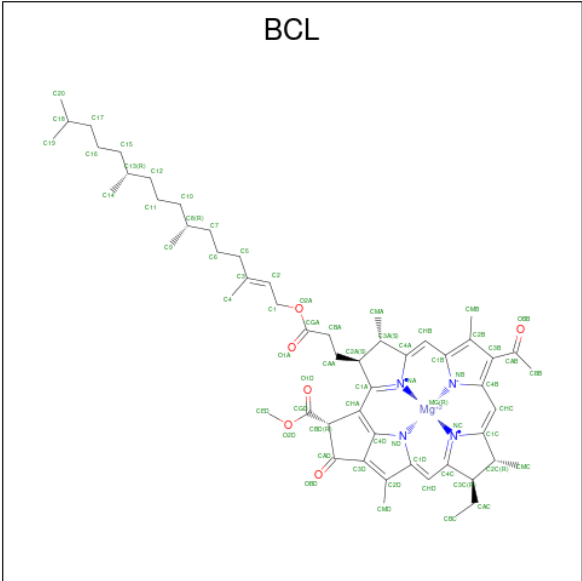
Chain	Residue	Modelled	Actual	Comment	Reference
M	210	A1ADZ	TYR	conflict	UNP P0C0Y9
M	252	VAL	TRP	conflict	UNP P0C0Y9

- Molecule 4 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
4	L	1	Total	C	N	O	0	0
			55	45	4	6		
4	M	1	Total	C	N	O	0	0
			65	55	4	6		

- 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
5	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

Continued on next page...

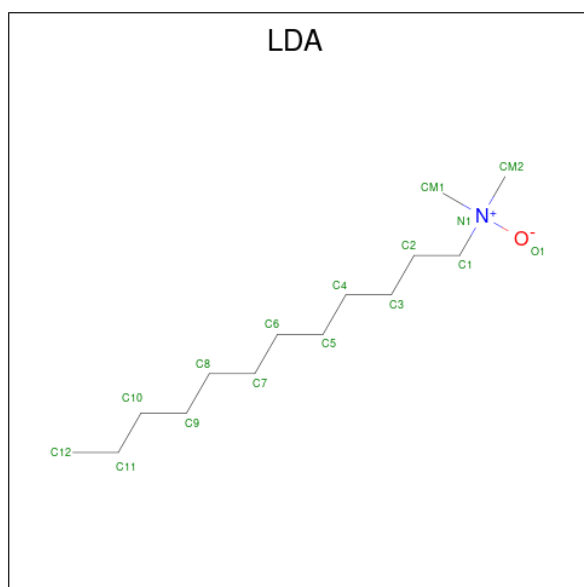
Continued from previous page...

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

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

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

- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).

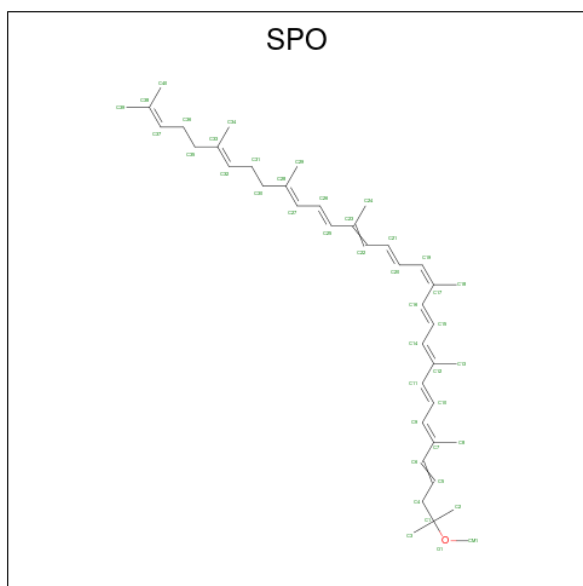


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		

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

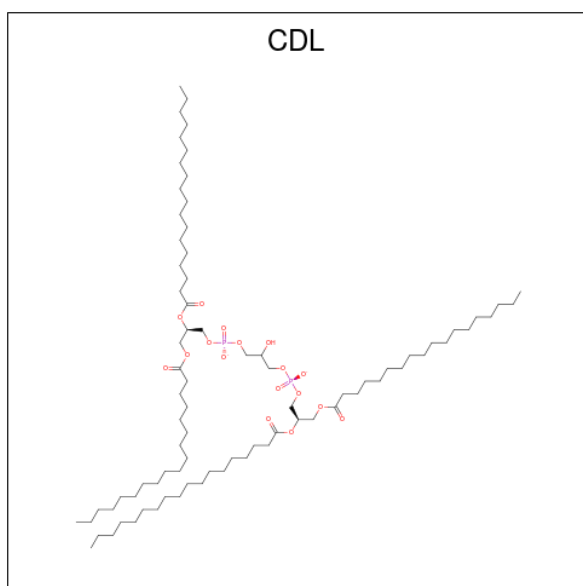
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

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



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

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



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

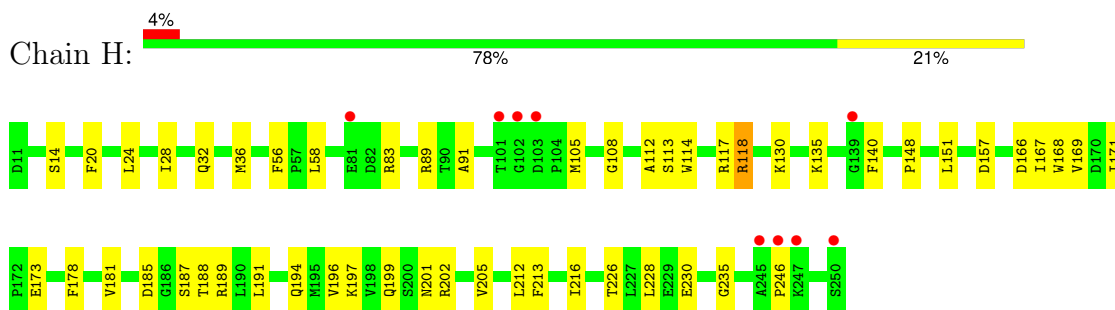
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	5	Total	O	0	0
			5	5		
11	L	5	Total	O	0	0
			5	5		
11	M	5	Total	O	0	0
			5	5		

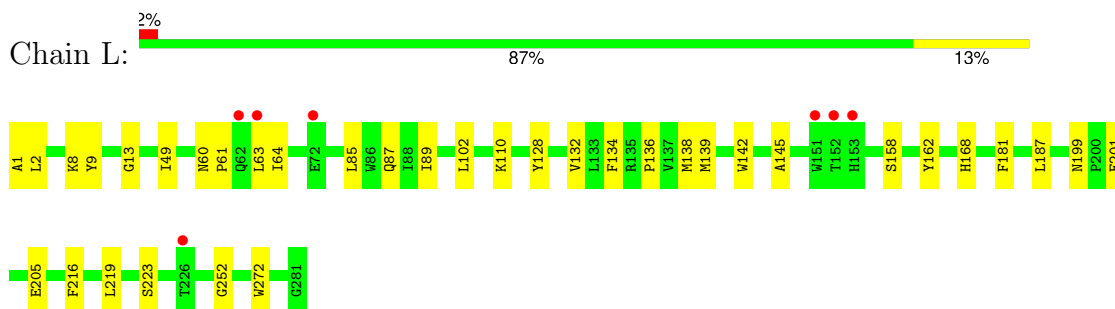
3 Residue-property plots

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.

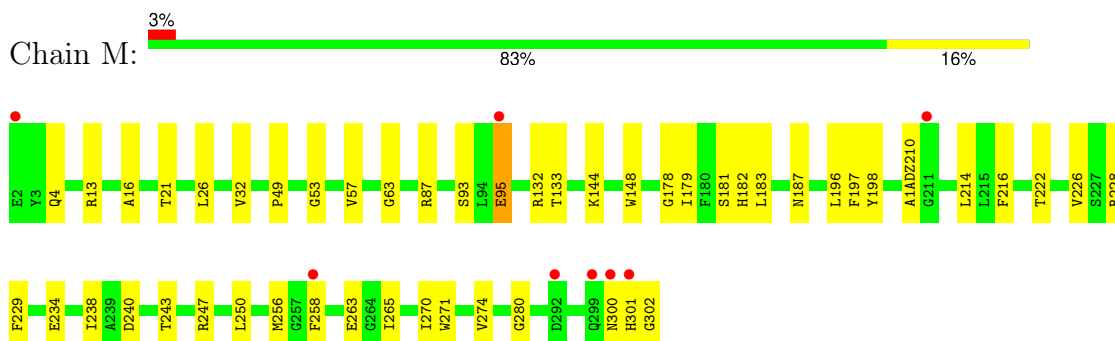
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.43Å 141.43Å 187.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.89 – 3.05 39.89 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.89-3.05) 91.3 (39.89-3.05)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.06Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.181 , 0.216 0.186 , 0.223	Depositor DCC
R_{free} test set	2104 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	66.0	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7019	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, BCL, BPH, CL, CDL, A1ADZ, LDA, SPO

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	0.53	0/1877	0.67	1/2553 (0.0%)
2	L	0.43	0/2336	0.58	0/3197
3	M	0.49	0/2472	0.62	0/3372
All	All	0.48	0/6685	0.62	1/9122 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	228	LEU	N-CA-C	-5.09	105.64	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1829	0	1834	41	0
2	L	2248	0	2200	27	0
3	M	2397	0	2300	45	0
4	L	55	0	53	8	0
4	M	65	0	76	3	0
5	L	132	0	148	5	0
5	M	117	0	115	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	1	0	0	0	0
7	M	48	0	93	3	0
8	M	1	0	0	0	0
9	M	42	0	60	1	0
10	M	69	0	82	2	0
11	H	5	0	0	0	0
11	L	5	0	0	0	0
11	M	5	0	0	2	0
All	All	7019	0	6961	118	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 8.

All (118) 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:93:SER:OG	3:M:95:GLU:OE2	1.69	1.09
1:H:118:ARG:HG3	1:H:118:ARG:HH11	1.19	1.05
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.60	0.81
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.68	0.76
3:M:197:PHE:HZ	5:M:401:BCL:HBB2	1.51	0.75
2:L:199:ASN:HB3	10:M:407:CDL:HA22	1.69	0.73
1:H:118:ARG:HG3	1:H:118:ARG:NH1	1.93	0.71
1:H:118:ARG:HH12	3:M:240:ASP:HB2	1.53	0.70
3:M:234:GLU:O	3:M:238:ILE:HG13	1.91	0.70
2:L:219:LEU:O	3:M:132:ARG:NH2	2.24	0.70
4:L:301:BPH:H6C1	5:M:401:BCL:H192	1.74	0.70
1:H:189:ARG:HD2	1:H:216:ILE:HB	1.74	0.69
2:L:49:ILE:HD12	2:L:89:ILE:HD13	1.73	0.69
3:M:214:LEU:HD13	4:M:408:BPH:ND	2.11	0.66
4:M:408:BPH:HBB3	4:M:408:BPH:HHC	1.77	0.65
3:M:197:PHE:CZ	5:M:401:BCL:HBB2	2.31	0.65
1:H:105:MET:HE3	1:H:212:LEU:HD22	1.79	0.64
3:M:4:GLN:NE2	11:M:501:HOH:O	2.30	0.63
5:L:302:BCL:HBB2	5:L:302:BCL:HHC	1.82	0.61
1:H:135:LYS:HE3	1:H:166:ASP:OD2	2.01	0.61
3:M:238:ILE:HD13	3:M:263:GLU:HB2	1.83	0.60
4:L:301:BPH:H5C1	3:M:63:GLY:HA3	1.85	0.59
1:H:118:ARG:NH1	3:M:240:ASP:HB2	2.18	0.58
3:M:243:THR:O	3:M:247:ARG:HG3	2.02	0.58
2:L:134:PHE:O	2:L:138:MET:HG3	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:32:VAL:HG12	3:M:49:PRO:HD3	1.85	0.57
1:H:197:LYS:HD3	1:H:199:GLN:HE21	1.69	0.57
3:M:256:MET:HE2	3:M:258:PHE:CD1	2.39	0.57
5:M:401:BCL:H41	5:M:409:BCL:HBB3	1.86	0.57
1:H:148:PRO:HD2	1:H:167:ILE:HD11	1.87	0.57
2:L:85:LEU:O	2:L:89:ILE:HG13	2.05	0.56
1:H:191:LEU:HD11	1:H:213:PHE:HE2	1.70	0.56
1:H:118:ARG:NH1	3:M:240:ASP:OD2	2.39	0.55
2:L:61:PRO:HA	2:L:64:ILE:HD12	1.87	0.55
5:M:409:BCL:HHC	5:M:409:BCL:HBB2	1.88	0.55
2:L:181:PHE:HB3	4:L:301:BPH:HBB2	1.89	0.55
5:M:401:BCL:CBB	5:M:401:BCL:HHC	2.36	0.55
1:H:83:ARG:HD2	1:H:114:TRP:CH2	2.41	0.55
5:L:302:BCL:HBB3	5:L:303:BCL:H52	1.91	0.53
1:H:83:ARG:NH1	1:H:114:TRP:O	2.41	0.53
5:L:303:BCL:HHC	5:L:303:BCL:OBB	2.08	0.52
1:H:89:ARG:HD3	1:H:91:ALA:O	2.09	0.52
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.45	0.52
3:M:300:ASN:C	3:M:302:GLY:H	2.18	0.52
1:H:169:VAL:HG23	1:H:171:ILE:HD12	1.92	0.52
1:H:28:ILE:HD11	7:M:402:LDA:H112	1.93	0.51
1:H:181:VAL:HG21	1:H:191:LEU:HD12	1.93	0.50
4:L:301:BPH:HBC3	4:L:301:BPH:HHD	1.92	0.50
1:H:130:LYS:HZ1	1:H:173:GLU:HG3	1.76	0.49
3:M:178:GLY:HA3	3:M:181:SER:HB3	1.94	0.49
3:M:228:ARG:HG3	3:M:229:PHE:CE2	2.47	0.49
1:H:194:GLN:OE1	1:H:194:GLN:N	2.36	0.49
1:H:157:ASP:OD1	1:H:157:ASP:N	2.46	0.48
1:H:118:ARG:HH12	3:M:240:ASP:CB	2.22	0.48
2:L:136:PRO:HG3	2:L:145:ALA:HB2	1.95	0.48
3:M:93:SER:CB	3:M:95:GLU:OE2	2.61	0.48
3:M:197:PHE:CE1	5:M:401:BCL:HMC2	2.48	0.48
2:L:168:HIS:HB3	3:M:183:LEU:HD13	1.95	0.47
2:L:181:PHE:HB3	4:L:301:BPH:CBB	2.44	0.47
3:M:270:ILE:O	3:M:274:VAL:HG13	2.14	0.47
5:M:409:BCL:HHC	5:M:409:BCL:CBB	2.45	0.47
3:M:300:ASN:C	3:M:302:GLY:N	2.71	0.47
1:H:185:ASP:OD1	1:H:187:SER:OG	2.24	0.47
1:H:196:VAL:HG12	1:H:205:VAL:HG22	1.96	0.47
1:H:201:ASN:HD21	1:H:202:ARG:NH2	2.12	0.47
2:L:219:LEU:HD11	3:M:133:THR:HG22	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:36:MET:HE2	1:H:58:LEU:HD23	1.98	0.46
1:H:20:PHE:CE2	1:H:24:LEU:HD22	2.51	0.45
2:L:139:MET:HE3	2:L:252:GLY:HA3	1.97	0.45
1:H:14:SER:OG	3:M:302:GLY:HA3	2.17	0.45
2:L:8:LYS:HE2	2:L:9:TYR:CE2	2.52	0.45
2:L:216:PHE:HB2	2:L:223:SER:HB2	1.98	0.45
4:M:408:BPH:HHC	4:M:408:BPH:CBB	2.44	0.45
3:M:144:LYS:NZ	11:M:502:HOH:O	2.39	0.45
1:H:118:ARG:HG3	3:M:240:ASP:OD2	2.17	0.44
5:M:401:BCL:HBB2	5:M:401:BCL:HHC	1.98	0.44
1:H:140:PHE:HA	3:M:13:ARG:O	2.18	0.44
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.99	0.44
5:M:401:BCL:HAA2	5:M:409:BCL:HBC1	1.98	0.44
3:M:148:TRP:CD1	10:M:407:CDL:H522	2.52	0.44
3:M:300:ASN:O	3:M:302:GLY:N	2.51	0.44
2:L:60:ASN:HB3	2:L:63:LEU:HD12	1.98	0.44
3:M:196:LEU:C	3:M:198:TYR:N	2.74	0.44
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.99	0.44
2:L:158:SER:HA	5:L:303:BCL:HBC1	1.99	0.44
5:L:302:BCL:HHC	5:L:302:BCL:CBB	2.47	0.44
7:M:404:LDA:HM13	7:M:404:LDA:H21	1.77	0.44
3:M:222:THR:O	3:M:226:VAL:HG22	2.18	0.43
2:L:162:TYR:OH	3:M:187:ASN:OD1	2.26	0.43
2:L:187:LEU:HD13	3:M:216:PHE:CG	2.54	0.43
3:M:271:TRP:HA	3:M:274:VAL:HG22	2.01	0.43
1:H:130:LYS:NZ	1:H:173:GLU:HG3	2.33	0.42
2:L:1:ALA:C	2:L:2:LEU:HD12	2.43	0.42
2:L:102:LEU:HD23	2:L:102:LEU:HA	1.89	0.42
3:M:53:GLY:O	3:M:57:VAL:HG23	2.19	0.42
9:M:406:SPO:H243	5:M:409:BCL:HBB2	2.01	0.42
2:L:128:TYR:O	2:L:132:VAL:HG22	2.19	0.42
1:H:188:THR:C	1:H:189:ARG:HG2	2.45	0.42
2:L:13:GLY:O	2:L:110:LYS:NZ	2.44	0.42
2:L:181:PHE:CD2	4:L:301:BPH:HBB1	2.55	0.42
1:H:112:ALA:HA	1:H:235:GLY:O	2.20	0.41
4:L:301:BPH:HHC	5:M:401:BCL:H2	2.01	0.41
1:H:118:ARG:NH1	1:H:118:ARG:CG	2.72	0.41
2:L:201:GLU:OE2	3:M:144:LYS:NZ	2.49	0.41
3:M:250:LEU:HD23	3:M:250:LEU:HA	1.94	0.41
3:M:265:ILE:O	3:M:265:ILE:HG13	2.21	0.41
1:H:117:ARG:O	1:H:118:ARG:C	2.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:191:LEU:HA	1:H:191:LEU:HD23	1.86	0.41
2:L:205:GLU:H	2:L:205:GLU:HG3	1.73	0.41
2:L:87:GLN:HE21	2:L:142:TRP:CD1	2.39	0.41
1:H:32:GLN:HG2	1:H:56:PHE:CE2	2.55	0.41
4:L:301:BPH:HHC	4:L:301:BPH:HBB3	2.03	0.40
7:M:403:LDA:H21	7:M:403:LDA:HM11	1.73	0.40
1:H:213:PHE:O	1:H:216:ILE:HG13	2.21	0.40
1:H:226:THR:O	1:H:230:GLU:HG3	2.21	0.40
3:M:196:LEU:O	3:M:198:TYR:N	2.54	0.40
3:M:280:GLY:O	5:M:401:BCL:HED3	2.21	0.40
1:H:108:GLY:O	1:H:113:SER:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	238/240 (99%)	232 (98%)	5 (2%)	1 (0%)	30	57
2	L	281/281 (100%)	271 (96%)	10 (4%)	0	100	100
3	M	296/301 (98%)	283 (96%)	11 (4%)	2 (1%)	18	45
All	All	815/822 (99%)	786 (96%)	26 (3%)	3 (0%)	30	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	301	HIS
1	H	246	PRO
3	M	179	ILE

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%)	194 (100%)	1 (0%)	81	82
2	L	222/220 (101%)	222 (100%)	0	100	100
3	M	235/235 (100%)	233 (99%)	2 (1%)	70	78
All	All	652/650 (100%)	649 (100%)	3 (0%)	81	82

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	118	ARG
3	M	95	GLU
3	M	182	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	M	145	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](#)

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	A1ADZ	M	210	3	12,13,14	1.49	1 (8%)	11,16,18	0.48	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	A1ADZ	M	210	3	-	3/7/8/10	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	A1ADZ	O1-C3	5.07	1.39	1.20

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	210	A1ADZ	C2-C5-C6-C7
3	M	210	A1ADZ	C2-C5-C6-C8
3	M	210	A1ADZ	C3-C2-C5-C6

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	L	303	2	69,74,74	1.22	8 (11%)	79,115,115	1.40	11 (13%)
5	BCL	L	302	2	69,74,74	1.32	7 (10%)	79,115,115	1.44	12 (15%)
9	SPO	M	406	-	41,41,41	0.33	0	47,50,50	0.44	0
7	LDA	M	403	-	13,15,15	2.02	2 (15%)	14,17,17	0.63	0
7	LDA	M	404	-	13,15,15	2.30	2 (15%)	14,17,17	0.36	0
4	BPH	L	301	-	49,60,70	1.36	8 (16%)	47,89,101	2.29	11 (23%)
4	BPH	M	408	-	59,70,70	1.24	6 (10%)	59,101,101	2.14	13 (22%)
10	CDL	M	407	3	68,68,99	1.18	7 (10%)	74,80,111	1.03	5 (6%)
5	BCL	M	401	3	69,74,74	1.26	8 (11%)	79,115,115	1.41	9 (11%)
7	LDA	M	402	-	13,15,15	2.08	2 (15%)	14,17,17	0.56	0
5	BCL	M	409	3	54,59,74	1.52	9 (16%)	61,97,115	1.57	9 (14%)

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	L	303	2	-	4/41/137/137	-
5	BCL	L	302	2	-	4/41/137/137	-
9	SPO	M	406	-	-	4/47/47/47	-
7	LDA	M	403	-	-	7/13/13/13	-
7	LDA	M	404	-	-	7/13/13/13	-
4	BPH	L	301	-	-	4/25/93/105	0/5/6/6
10	CDL	M	407	3	1/1/9/9	33/79/79/110	-
4	BPH	M	408	-	-	3/37/105/105	0/5/6/6
5	BCL	M	401	3	-	5/41/137/137	-
7	LDA	M	402	-	-	8/13/13/13	-
5	BCL	M	409	3	-	1/23/119/137	-

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	404	LDA	O1-N1	-6.55	1.26	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	402	LDA	O1-N1	-6.37	1.26	1.42
7	M	403	LDA	O1-N1	-6.35	1.26	1.42
5	M	401	BCL	MG-NA	5.34	2.19	2.06
7	M	404	LDA	C1-N1	-4.93	1.46	1.51
5	L	302	BCL	MG-NA	4.83	2.17	2.06
5	M	409	BCL	MG-NA	4.77	2.17	2.06
5	L	303	BCL	MG-NA	4.73	2.17	2.06
4	M	408	BPH	CBD-CGD	-4.28	1.47	1.52
5	M	409	BCL	MG-NC	4.15	2.16	2.06
4	M	408	BPH	C3D-CAD	-3.91	1.40	1.47
7	M	402	LDA	C1-N1	-3.79	1.47	1.51
4	L	301	BPH	C1D-C2D	3.62	1.43	1.39
5	M	409	BCL	OBD-CAD	3.57	1.28	1.22
5	L	303	BCL	MG-NC	3.55	2.14	2.06
5	M	409	BCL	O2A-CGA	3.46	1.43	1.33
7	M	403	LDA	C1-N1	-3.29	1.48	1.51
5	L	302	BCL	OBD-CAD	3.23	1.28	1.22
10	M	407	CDL	PA1-OA4	-3.23	1.40	1.55
5	L	302	BCL	MG-NC	3.19	2.13	2.06
10	M	407	CDL	PA1-OA5	3.16	1.71	1.59
4	L	301	BPH	C3D-CAD	-3.09	1.41	1.47
10	M	407	CDL	PB2-OB5	3.07	1.71	1.59
5	L	303	BCL	C3B-C4B	3.07	1.47	1.41
4	M	408	BPH	C3B-C4B	3.07	1.46	1.41
4	L	301	BPH	C4D-CHA	2.95	1.44	1.39
5	M	409	BCL	CHD-C1D	2.94	1.44	1.38
5	L	302	BCL	CAC-C3C	2.93	1.59	1.54
10	M	407	CDL	PB2-OB4	-2.88	1.42	1.55
4	L	301	BPH	CHA-CBD	2.85	1.55	1.51
10	M	407	CDL	PB2-OB3	-2.81	1.41	1.50
5	M	401	BCL	C1D-C2D	-2.77	1.39	1.45
5	M	409	BCL	C1D-ND	2.77	1.41	1.37
5	M	401	BCL	MG-NC	2.74	2.12	2.06
4	M	408	BPH	C1D-C2D	2.72	1.42	1.39
5	M	401	BCL	C1D-ND	2.63	1.41	1.37
5	L	303	BCL	C1B-NB	2.59	1.41	1.37
5	M	409	BCL	C3B-C4B	2.58	1.46	1.41
5	L	302	BCL	CHD-C1D	2.55	1.43	1.38
4	L	301	BPH	C3B-C4B	2.49	1.45	1.41
5	L	303	BCL	C5-C3	2.36	1.56	1.51
5	M	401	BCL	OBD-CAD	2.21	1.26	1.22
5	M	401	BCL	C1B-NB	2.19	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	303	BCL	CHD-C1D	2.19	1.42	1.38
10	M	407	CDL	CA3-CA4	2.18	1.57	1.50
4	L	301	BPH	CMD-C2D	2.16	1.55	1.51
5	L	302	BCL	MG-NB	2.15	2.10	2.05
5	M	409	BCL	C1-C2	2.15	1.55	1.49
5	L	303	BCL	C1D-C2D	-2.13	1.41	1.45
10	M	407	CDL	OB6-CB5	2.13	1.40	1.34
4	M	408	BPH	C1C-C2C	-2.12	1.47	1.51
4	M	408	BPH	CHA-CBD	2.12	1.54	1.51
5	M	409	BCL	C5-C3	2.11	1.56	1.50
5	L	303	BCL	C3D-C4D	-2.10	1.39	1.44
4	L	301	BPH	C1D-ND	2.08	1.42	1.38
5	L	302	BCL	C3B-C4B	2.07	1.45	1.41
5	M	401	BCL	OBB-CAB	2.06	1.27	1.23
5	M	401	BCL	C1-C2	2.05	1.55	1.49
4	L	301	BPH	C4-C3	2.00	1.55	1.50

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	408	BPH	C4D-CHA-CBD	-11.34	103.02	108.45
4	L	301	BPH	C4D-CHA-CBD	-10.73	103.31	108.45
5	M	401	BCL	C4D-CHA-C1A	5.26	127.52	121.24
5	M	409	BCL	C4D-CHA-C1A	4.96	127.16	121.24
5	L	302	BCL	C1D-ND-C4D	-4.53	103.13	106.31
5	L	303	BCL	C4D-CHA-C1A	4.32	126.40	121.24
4	L	301	BPH	O2D-CGD-CBD	4.24	115.60	110.95
5	M	401	BCL	C1D-ND-C4D	-4.23	103.34	106.31
5	M	409	BCL	C1D-ND-C4D	-4.23	103.34	106.31
4	M	408	BPH	C11-C10-C8	-4.11	102.30	115.97
4	L	301	BPH	C1-C2-C3	-4.07	119.54	126.20
4	M	408	BPH	C4D-ND-C1D	-4.05	104.02	108.87
5	L	302	BCL	CHD-C1D-ND	-3.94	119.25	124.80
5	L	302	BCL	C4D-CHA-C1A	3.88	125.87	121.24
5	L	303	BCL	C1D-ND-C4D	-3.86	103.60	106.31
5	M	409	BCL	CHD-C1D-ND	-3.79	119.47	124.80
4	L	301	BPH	C4D-ND-C1D	-3.64	104.51	108.87
5	M	401	BCL	CHD-C1D-ND	-3.55	119.80	124.80
4	M	408	BPH	C4C-C3C-C2C	-3.55	99.46	102.84
5	M	409	BCL	C1-O2A-CGA	3.51	125.16	116.65
5	L	303	BCL	C11-C12-C13	-3.38	104.73	115.97
5	L	302	BCL	C2A-C1A-CHA	3.36	129.71	123.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	408	BPH	C3D-C4D-ND	3.36	112.01	107.71
4	L	301	BPH	OBD-CAD-CBD	-3.33	120.94	125.82
5	M	401	BCL	C4A-NA-C1A	3.31	108.19	106.68
5	L	303	BCL	CHD-C1D-ND	-3.20	120.30	124.80
5	M	409	BCL	C2A-C1A-CHA	3.13	129.31	123.87
4	L	301	BPH	C3D-C4D-ND	3.12	111.70	107.71
10	M	407	CDL	OA4-PA1-OA3	3.10	126.85	112.44
5	M	401	BCL	CHA-C1A-NA	-3.08	119.42	126.39
4	M	408	BPH	OBD-CAD-CBD	-3.07	121.32	125.82
5	L	303	BCL	C17-C16-C15	-3.01	99.77	113.28
5	M	409	BCL	CHA-C1A-NA	-3.00	119.59	126.39
5	L	302	BCL	CHA-C1A-NA	-3.00	119.60	126.39
5	L	302	BCL	C16-C15-C13	2.91	125.62	115.97
5	L	303	BCL	CHA-C1A-NA	-2.88	119.87	126.39
5	M	401	BCL	C1-C2-C3	-2.87	121.49	126.20
5	M	409	BCL	C1-C2-C3	-2.85	122.15	126.76
5	L	303	BCL	C2A-C1A-CHA	2.84	128.79	123.87
4	M	408	BPH	OBB-CAB-CBB	-2.77	114.28	120.19
5	L	303	BCL	C16-C15-C13	2.71	124.97	115.97
5	L	302	BCL	C4A-NA-C1A	2.63	107.88	106.68
5	L	303	BCL	CAB-C3B-C2B	2.63	133.22	127.74
10	M	407	CDL	OB4-PB2-OB3	2.55	124.33	112.44
5	L	302	BCL	OBB-CAB-CBB	-2.55	114.07	119.77
10	M	407	CDL	OB8-CB7-OB9	-2.53	117.29	123.63
5	M	401	BCL	C2A-C1A-CHA	2.52	128.25	123.87
5	L	302	BCL	O2D-CGD-CBD	2.51	115.62	111.23
4	L	301	BPH	O2D-CGD-O1D	-2.37	119.23	123.85
5	L	303	BCL	C11-C10-C8	-2.35	108.16	115.97
4	L	301	BPH	CMA-C3A-C4A	-2.35	109.55	114.61
4	L	301	BPH	C2D-C1D-ND	2.32	111.11	109.43
4	M	408	BPH	OBB-CAB-C3B	2.31	123.85	119.99
10	M	407	CDL	OB6-CB5-OB7	-2.30	118.33	123.70
5	M	401	BCL	OBB-CAB-CBB	-2.26	114.72	119.77
10	M	407	CDL	CA4-OA6-CA5	2.25	123.19	117.80
4	L	301	BPH	CMD-C2D-C3D	2.25	129.19	124.68
5	L	302	BCL	CAC-C3C-C4C	2.24	117.56	112.58
5	M	409	BCL	OBB-CAB-CBB	-2.23	114.78	119.77
4	M	408	BPH	CMB-C2B-C3B	2.18	129.04	124.68
5	L	302	BCL	O2D-CGD-O1D	-2.18	119.61	123.85
4	M	408	BPH	C1C-C2C-C3C	-2.16	100.78	102.84
4	M	408	BPH	C2D-C1D-ND	2.15	110.98	109.43
4	L	301	BPH	OBB-CAB-C3B	2.10	123.51	119.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	303	BCL	O2D-CGD-CBD	2.10	114.90	111.23
5	M	409	BCL	C4A-NA-C1A	2.08	107.63	106.68
4	M	408	BPH	C16-C15-C13	-2.08	109.04	115.97
4	M	408	BPH	CMC-C2C-C1C	-2.06	110.18	114.61
5	L	302	BCL	C2D-C1D-ND	2.06	112.16	110.13
5	M	401	BCL	C2D-C1D-ND	2.04	112.14	110.13

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	M	407	CDL	CA4

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	402	LDA	C2-C1-N1-O1
7	M	402	LDA	C2-C1-N1-CM1
7	M	402	LDA	C2-C1-N1-CM2
7	M	403	LDA	C2-C1-N1-O1
7	M	403	LDA	C2-C1-N1-CM1
10	M	407	CDL	CA2-OA2-PA1-OA3
10	M	407	CDL	CA2-OA2-PA1-OA4
10	M	407	CDL	CA2-OA2-PA1-OA5
10	M	407	CDL	CA3-OA5-PA1-OA4
10	M	407	CDL	CA6-CA4-OA6-CA5
10	M	407	CDL	C11-CA5-OA6-CA4
10	M	407	CDL	OA7-CA5-OA6-CA4
10	M	407	CDL	C31-CA7-OA8-CA6
10	M	407	CDL	OA9-CA7-OA8-CA6
7	M	403	LDA	C1-C2-C3-C4
5	M	401	BCL	C14-C13-C15-C16
10	M	407	CDL	CB5-C51-C52-C53
10	M	407	CDL	CB7-C71-C72-C73
10	M	407	CDL	CA5-C11-C12-C13
5	M	401	BCL	C13-C15-C16-C17
10	M	407	CDL	OB6-CB4-CB6-OB8
7	M	403	LDA	C6-C7-C8-C9
7	M	404	LDA	C6-C7-C8-C9
7	M	402	LDA	C3-C4-C5-C6
7	M	404	LDA	C2-C3-C4-C5
10	M	407	CDL	C33-C34-C35-C36
7	M	404	LDA	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	M	404	LDA	C5-C6-C7-C8
7	M	402	LDA	C7-C8-C9-C10
10	M	407	CDL	C34-C35-C36-C37
7	M	403	LDA	C7-C8-C9-C10
7	M	402	LDA	C4-C5-C6-C7
4	L	301	BPH	C2-C3-C5-C6
10	M	407	CDL	CB3-CB4-CB6-OB8
4	L	301	BPH	C4-C3-C5-C6
4	M	408	BPH	O2A-C1-C2-C3
7	M	404	LDA	C4-C5-C6-C7
4	M	408	BPH	C15-C16-C17-C18
9	M	406	SPO	C34-C33-C35-C36
9	M	406	SPO	C32-C33-C35-C36
10	M	407	CDL	CA7-C31-C32-C33
7	M	402	LDA	C6-C7-C8-C9
10	M	407	CDL	C17-C18-C19-C20
7	M	404	LDA	C1-C2-C3-C4
10	M	407	CDL	C39-C40-C41-C42
5	M	401	BCL	C15-C16-C17-C18
7	M	403	LDA	C5-C6-C7-C8
7	M	402	LDA	C1-C2-C3-C4
7	M	403	LDA	C2-C1-N1-CM2
10	M	407	CDL	C72-C73-C74-C75
10	M	407	CDL	OB5-CB3-CB4-OB6
4	M	408	BPH	C8-C10-C11-C12
10	M	407	CDL	CA3-OA5-PA1-OA2
10	M	407	CDL	CA3-OA5-PA1-OA3
10	M	407	CDL	CB2-OB2-PB2-OB3
9	M	406	SPO	C5-C6-C7-C8
10	M	407	CDL	C12-C13-C14-C15
5	L	303	BCL	C16-C17-C18-C19
5	M	401	BCL	C12-C13-C15-C16
7	M	404	LDA	C7-C8-C9-C10
10	M	407	CDL	C14-C15-C16-C17
10	M	407	CDL	C71-C72-C73-C74
5	L	303	BCL	C2A-CAA-CBA-CGA
5	L	302	BCL	C15-C16-C17-C18
5	L	303	BCL	C16-C17-C18-C20
4	L	301	BPH	C5-C6-C7-C8
10	M	407	CDL	C1-CB2-OB2-PB2
4	L	301	BPH	CHA-CBD-CGD-O1D
10	M	407	CDL	OB5-CB3-CB4-CB6

Continued on next page...

Continued from previous page...

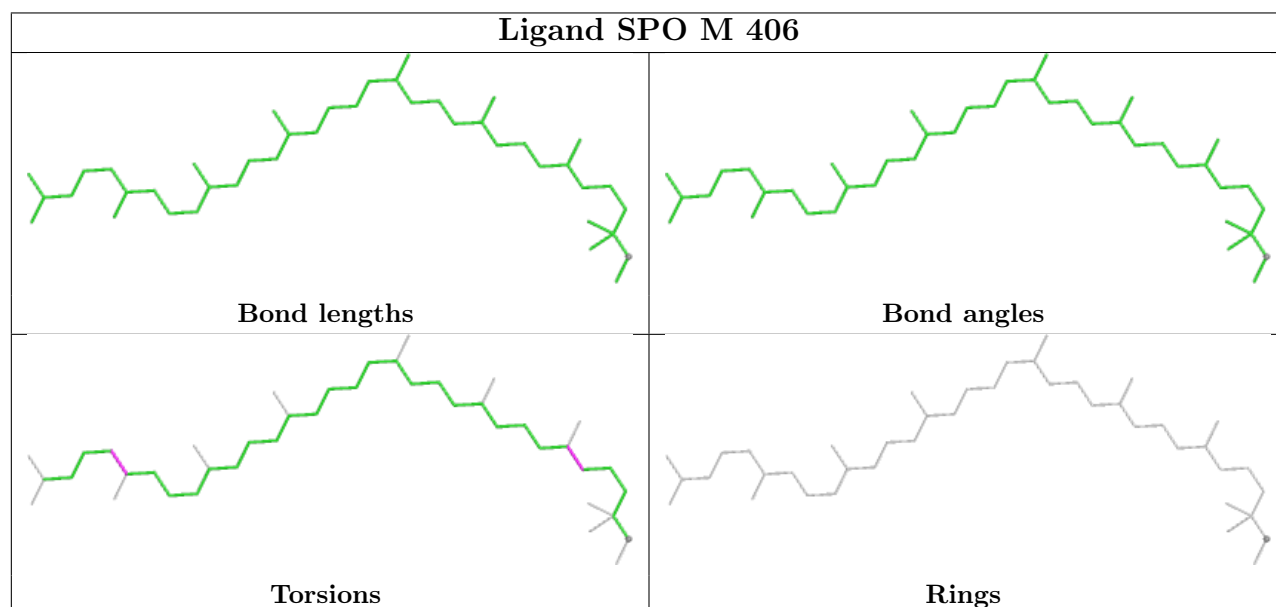
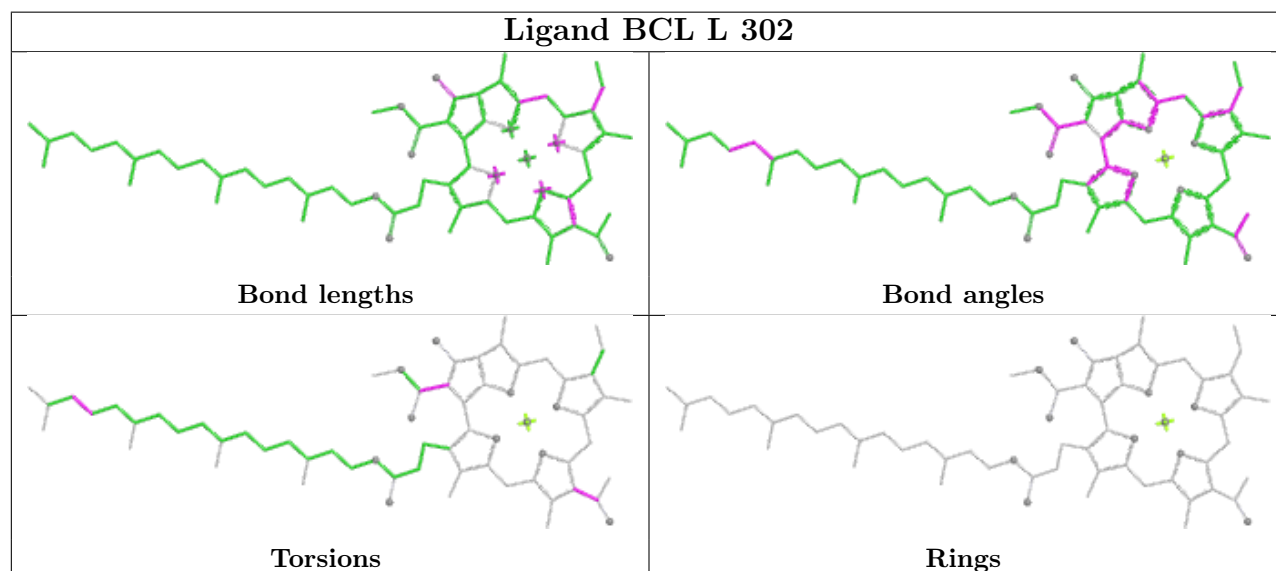
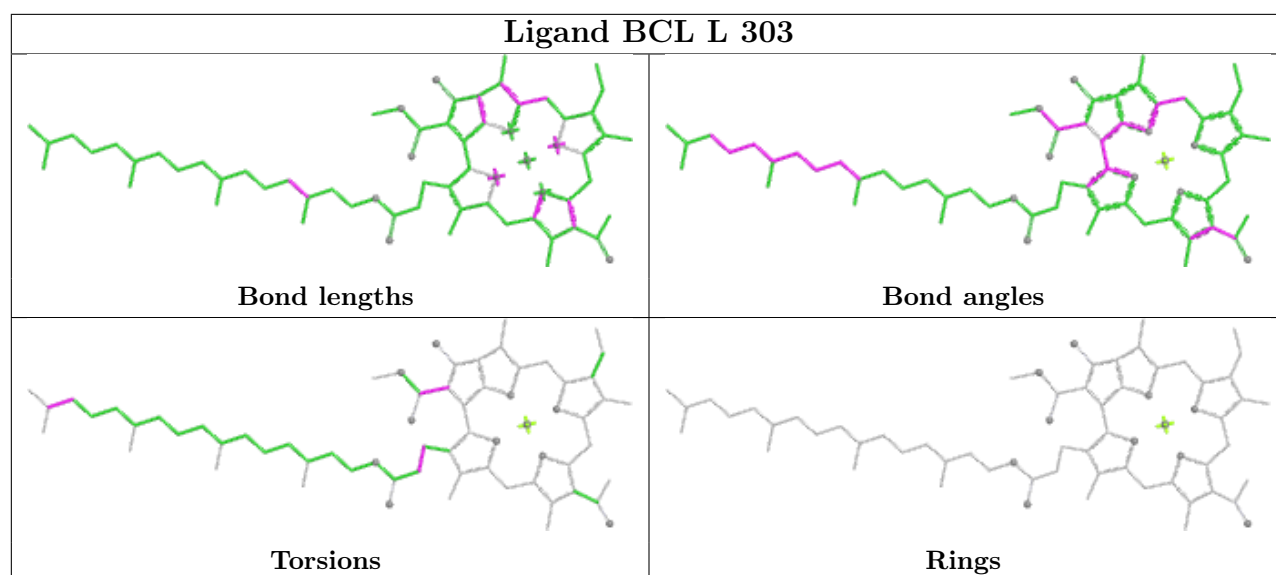
Mol	Chain	Res	Type	Atoms
10	M	407	CDL	C15-C16-C17-C18
5	L	302	BCL	C2B-C3B-CAB-OBB
10	M	407	CDL	C72-C71-CB7-OB8
10	M	407	CDL	C51-C52-C53-C54
9	M	406	SPO	C5-C6-C7-C9
10	M	407	CDL	C76-C77-C78-C79
5	L	302	BCL	C2B-C3B-CAB-CBB
5	M	401	BCL	CAA-CBA-CGA-O2A
5	L	302	BCL	CAD-CBD-CGD-O2D
5	L	303	BCL	CAD-CBD-CGD-O2D
5	M	409	BCL	C2-C1-O2A-CGA

There are no ring outliers.

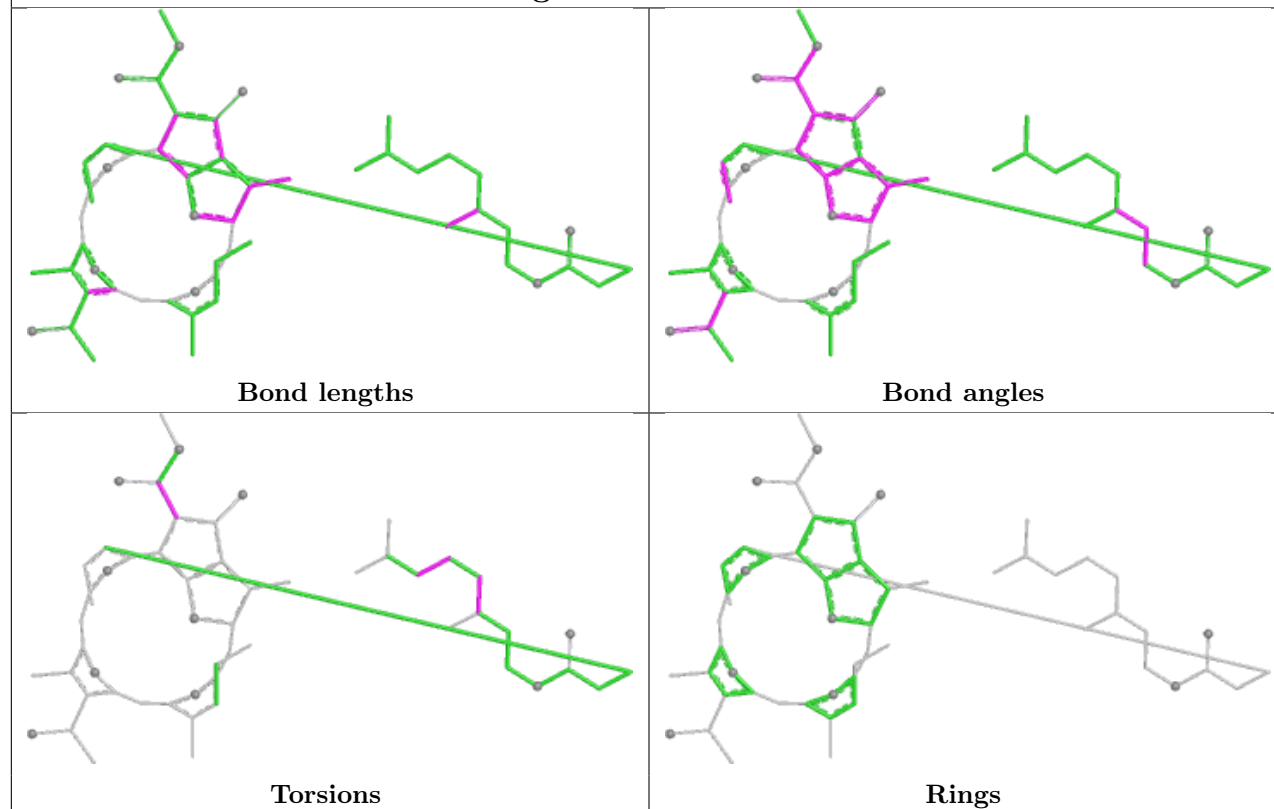
11 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	303	BCL	3	0
5	L	302	BCL	3	0
9	M	406	SPO	1	0
7	M	403	LDA	1	0
7	M	404	LDA	1	0
4	L	301	BPH	8	0
4	M	408	BPH	3	0
10	M	407	CDL	2	0
5	M	401	BCL	10	0
7	M	402	LDA	1	0
5	M	409	BCL	5	0

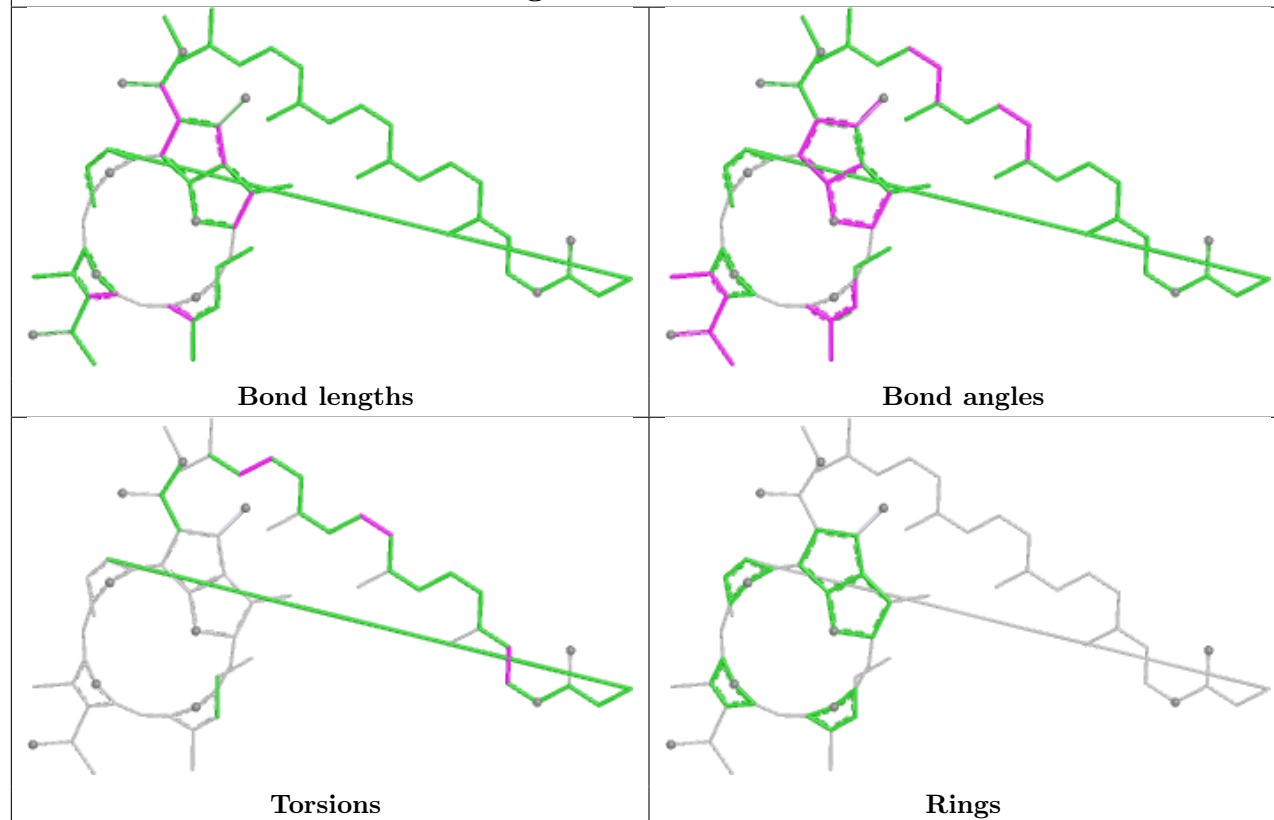
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

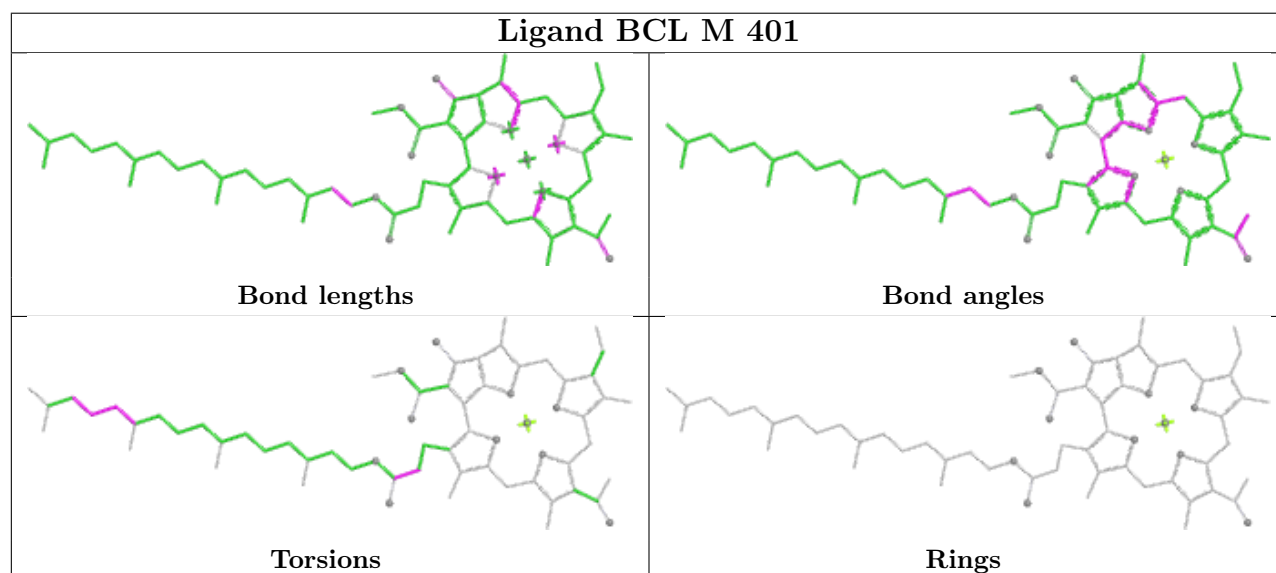
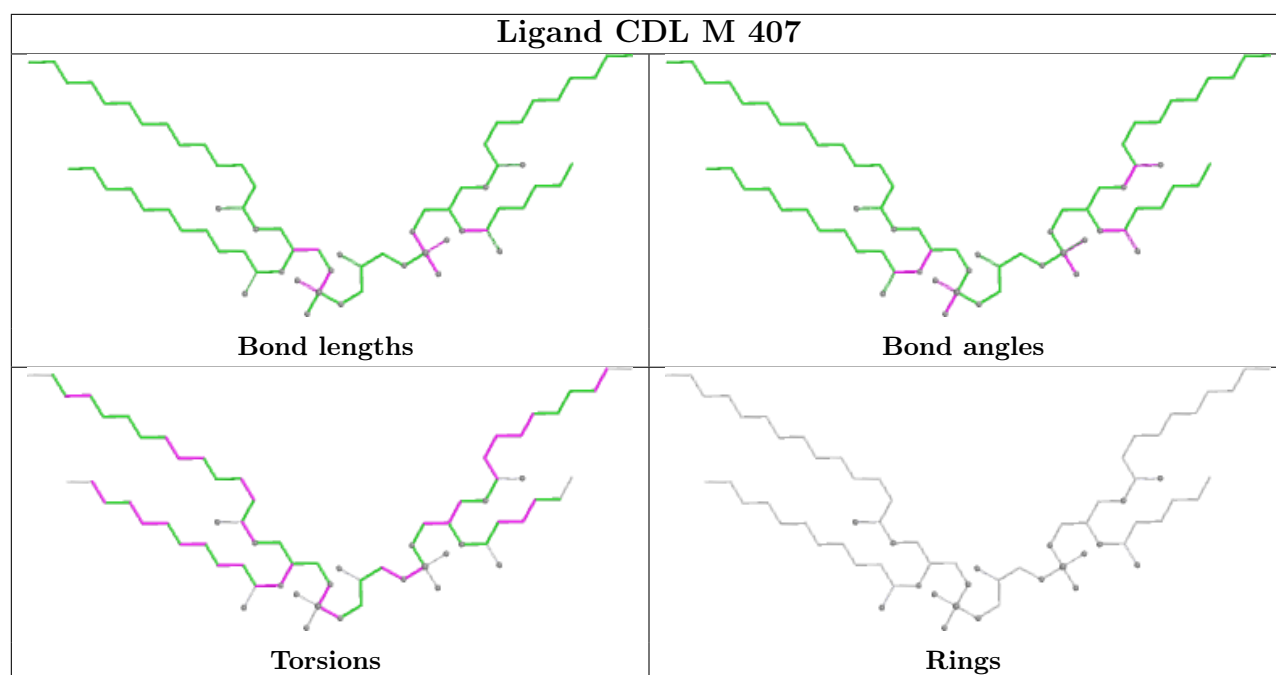


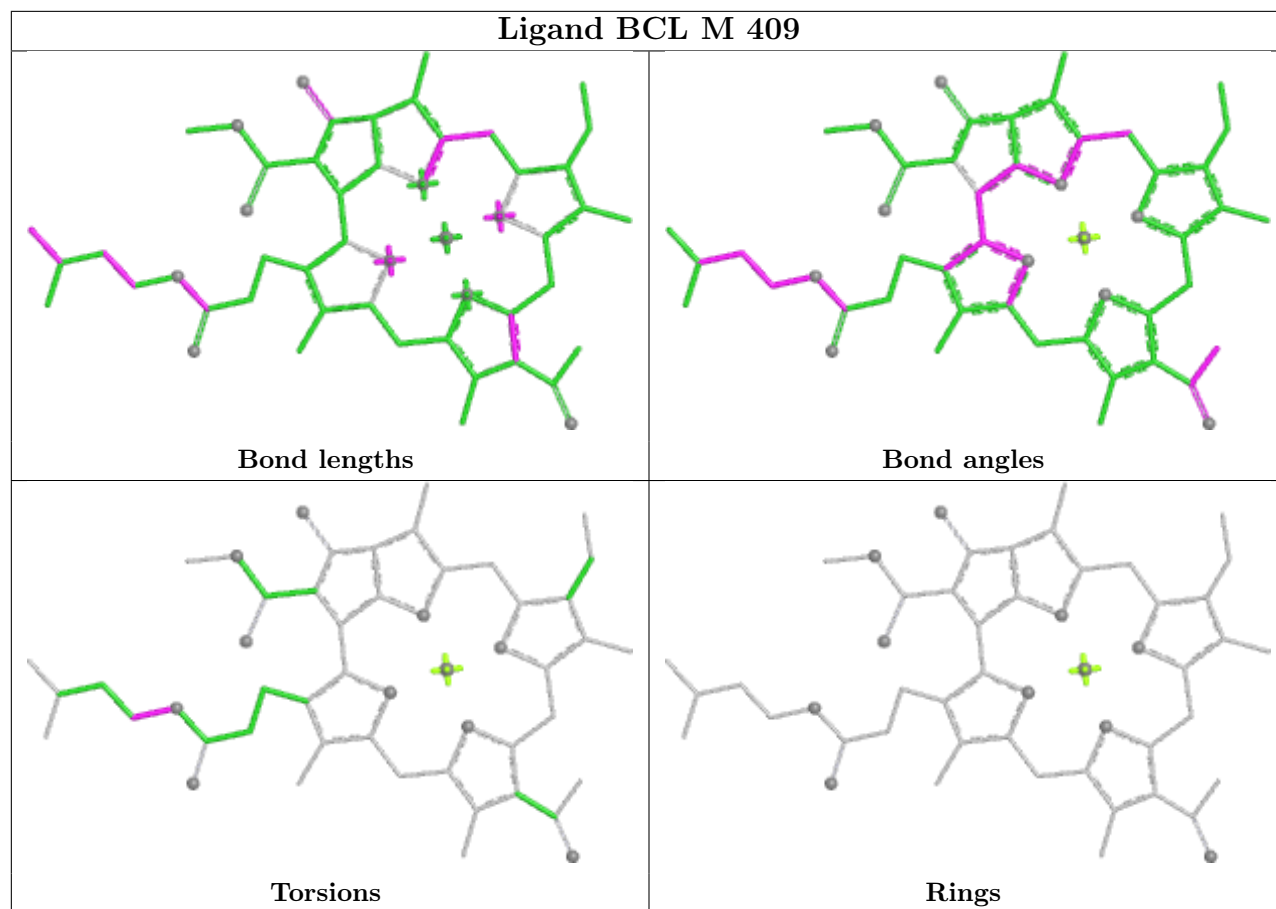
Ligand BPH L 301



Ligand BPH M 408







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

6.1 Protein, DNA and RNA chains

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%)	-0.10	9 (3%)	44	24	49, 62, 87, 146	0
2	L	281/281 (100%)	-0.18	7 (2%)	58	35	27, 57, 91, 123	2 (0%)
3	M	300/301 (99%)	-0.15	8 (2%)	56	33	44, 62, 90, 128	0
All	All	821/822 (99%)	-0.15	24 (2%)	53	31	27, 60, 90, 146	2 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	2	GLU	4.8
2	L	62	GLN	4.5
1	H	102	GLY	4.1
2	L	72	GLU	3.8
3	M	301	HIS	3.4
2	L	153	HIS	3.1
3	M	258	PHE	2.9
1	H	250	SER	2.8
1	H	247	LYS	2.8
3	M	299	GLN	2.8
3	M	300	ASN	2.8
1	H	246	PRO	2.7
3	M	95	GLU	2.6
2	L	151	TRP	2.5
2	L	226	THR	2.3
1	H	139	GLY	2.2
1	H	81	GLU	2.2
2	L	63	LEU	2.1
3	M	211	GLY	2.1
1	H	245	ALA	2.1
3	M	292	ASP	2.1
1	H	103	ASP	2.1
2	L	152	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	101	THR	2.0

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	A1ADZ	M	210	13/14	0.90	0.17	46,49,67,71	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.

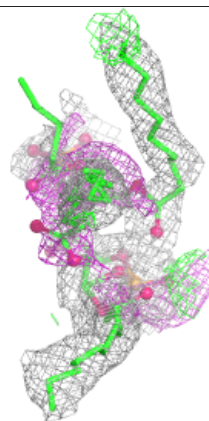
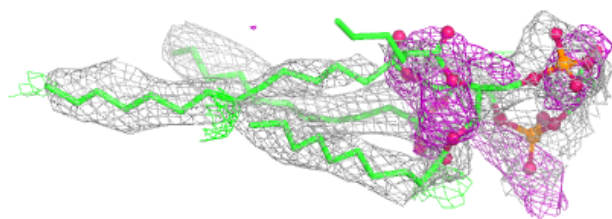
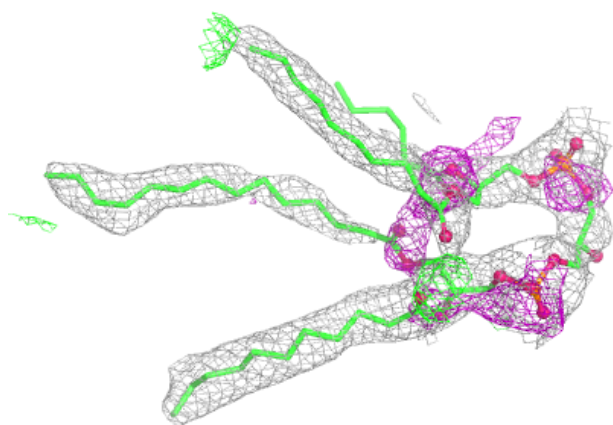
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	LDA	M	404	16/16	0.75	0.30	78,90,105,110	0
10	CDL	M	407	69/100	0.77	0.24	69,93,115,123	0
7	LDA	M	403	16/16	0.87	0.21	82,93,106,108	0
9	SPO	M	406	42/42	0.92	0.18	55,70,86,93	0
7	LDA	M	402	16/16	0.93	0.18	71,78,90,97	0
4	BPH	L	301	55/65	0.94	0.12	45,54,78,88	0
5	BCL	M	409	51/66	0.95	0.10	46,52,63,70	0
4	BPH	M	408	65/65	0.96	0.10	45,49,64,66	0
5	BCL	M	401	66/66	0.97	0.10	44,50,70,85	0
5	BCL	L	302	66/66	0.97	0.09	44,52,67,75	0
6	CL	L	304	1/1	0.97	0.10	89,89,89,89	0
5	BCL	L	303	66/66	0.97	0.09	43,50,58,69	0
8	FE	M	405	1/1	1.00	0.03	44,44,44,44	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.

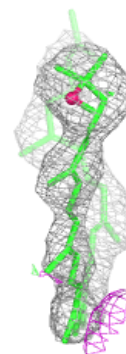
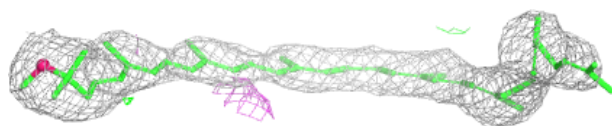
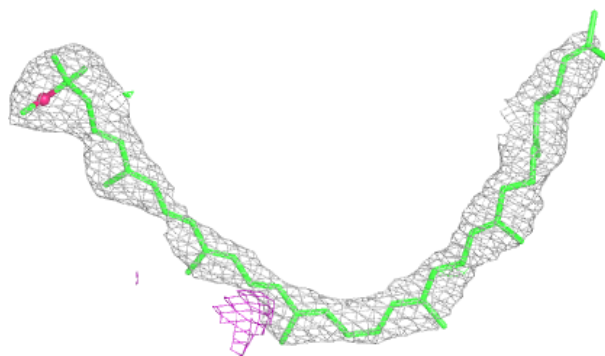
Electron density around CDL M 407:

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



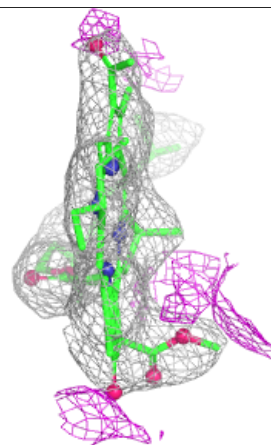
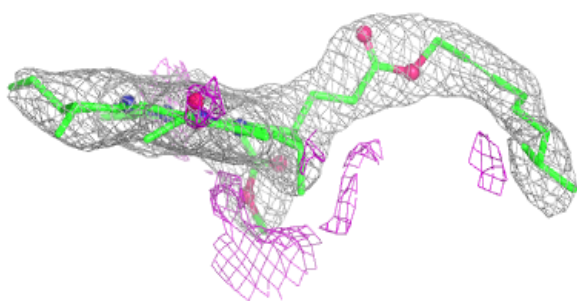
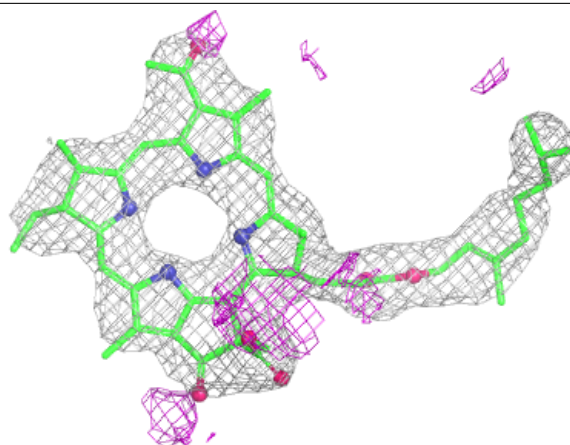
Electron density around SPO M 406:

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



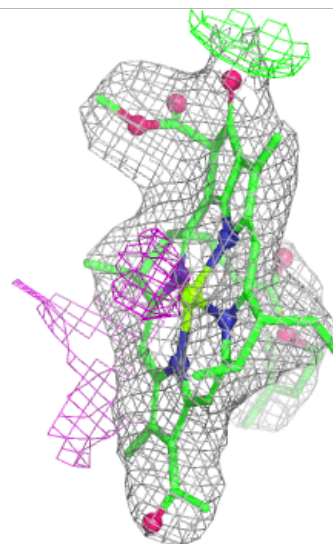
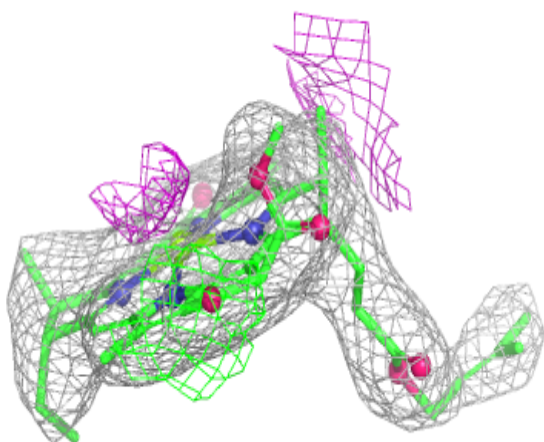
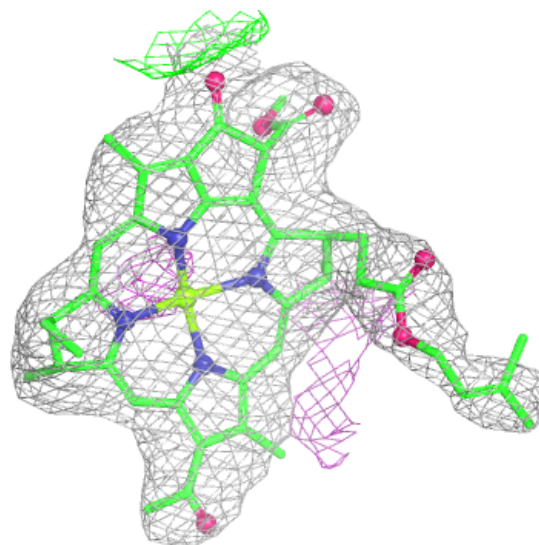
Electron density around BPH L 301:

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



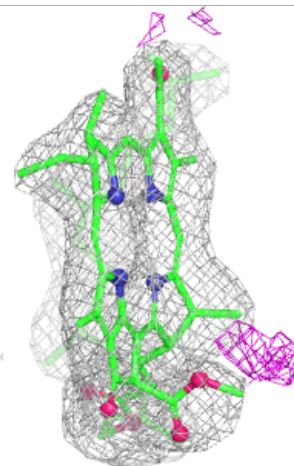
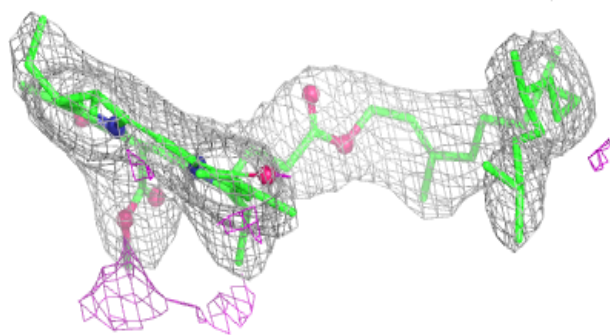
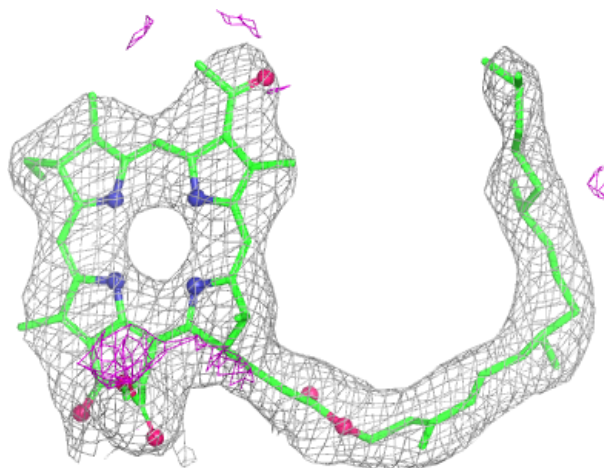
Electron density around BCL M 409:

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



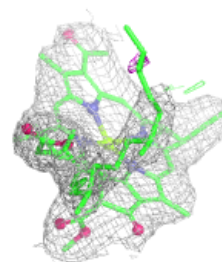
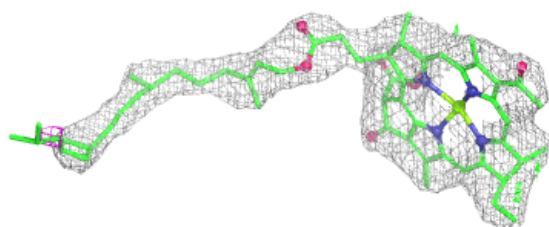
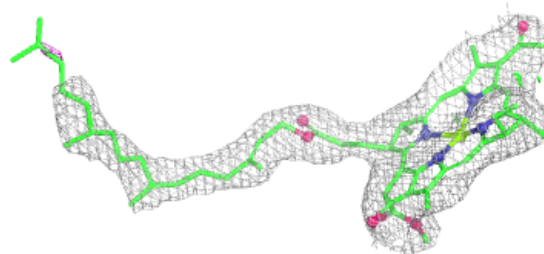
Electron density around BPH M 408:

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



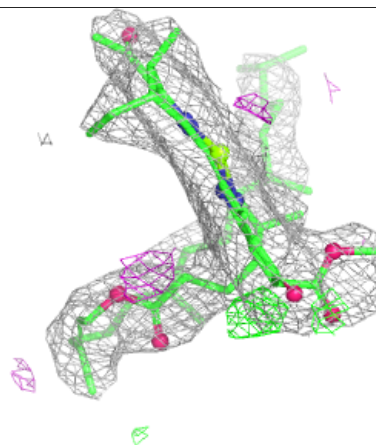
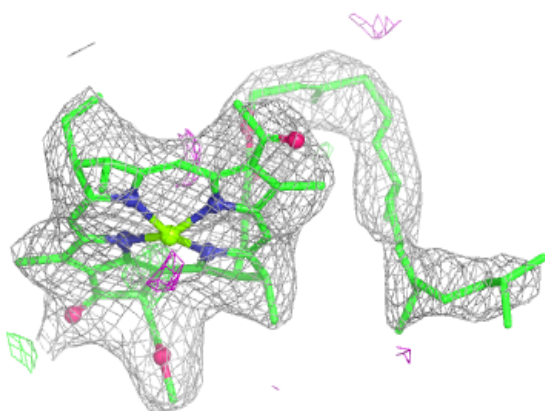
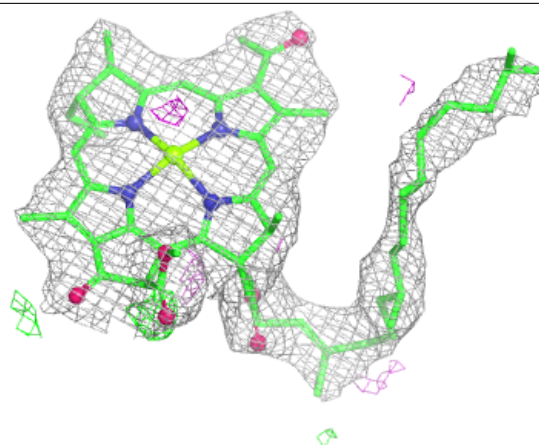
Electron density around BCL M 401:

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



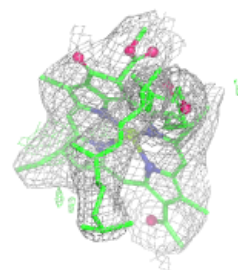
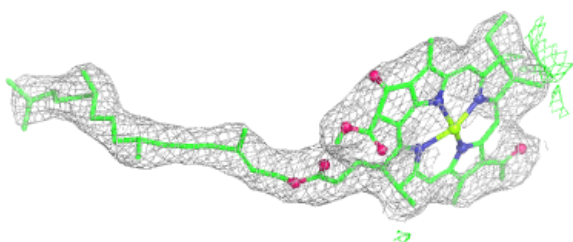
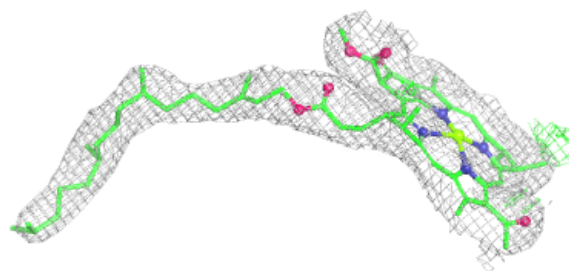
Electron density around BCL L 302:

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



Electron density around BCL L 303:

$2mF_o-DF_c$ (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.