



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 11:01 AM UTC

PDB ID : 8VTJ / pdb_00008vtj
Title : Crystal structure of R. sphaeroides Photosynthetic Reaction Center variant Y (M210)2-cyanophenylalanine
Authors : Mathews, I.; Tran, K.; Boxer, S.G.
Deposited on : 2024-01-26
Resolution : 2.81 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

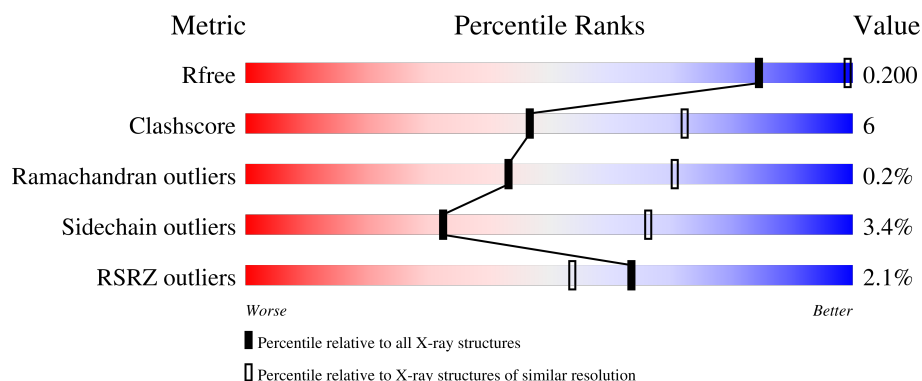
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

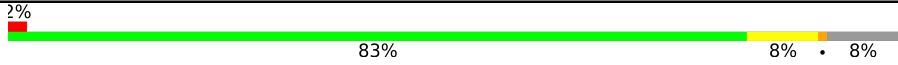
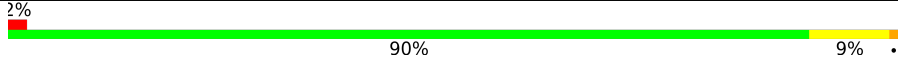
The reported resolution of this entry is 2.81 Å.

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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	260	
2	L	281	
3	M	301	

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
11	CDL	M	408	X	-	-	-
6	U10	L	303	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7117 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	0	0
			2232	1507	355	362	8			

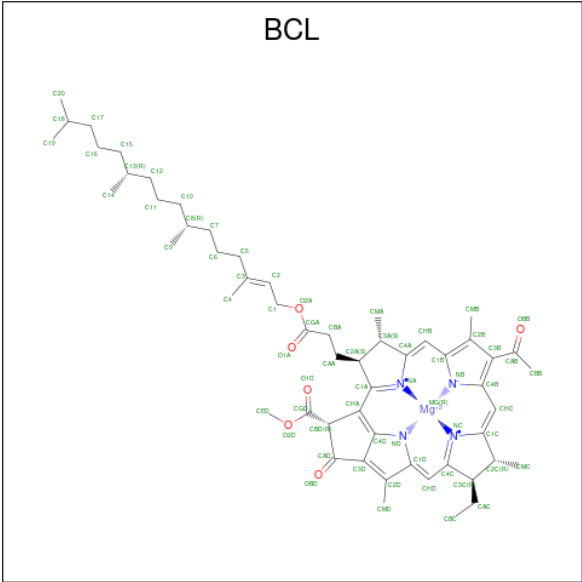
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	301	Total	C	N	O	S	0	0	0
			2397	1599	393	395	10			

There are 2 discrepancies between the modelled and reference sequences:

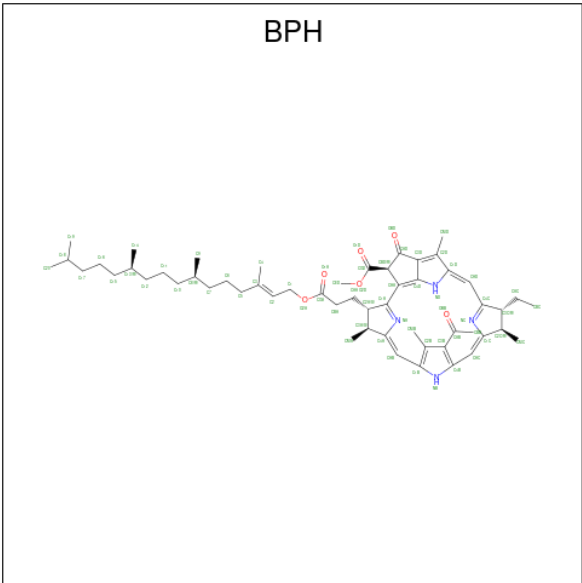
Chain	Residue	Modelled	Actual	Comment	Reference
M	210	9IJ	TYR	conflict	UNP P0C0Y9
M	252	VAL	TRP	conflict	UNP P0C0Y9

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



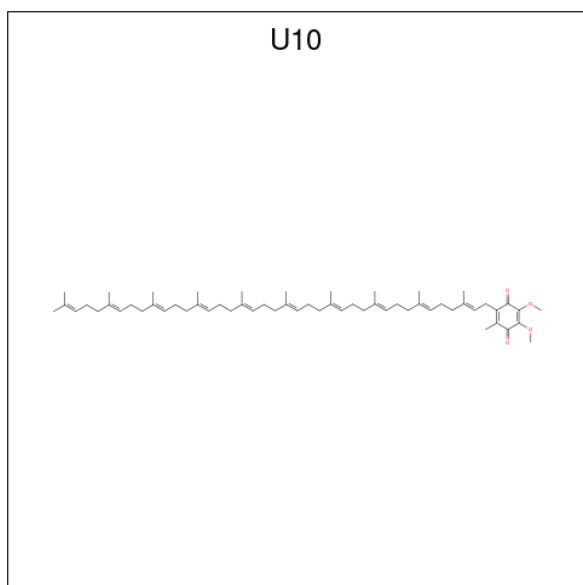
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 51	C 40	Mg 1	N 4	O 6	0	0

- Molecule 5 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
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			55	45	4	6		

- Molecule 6 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).

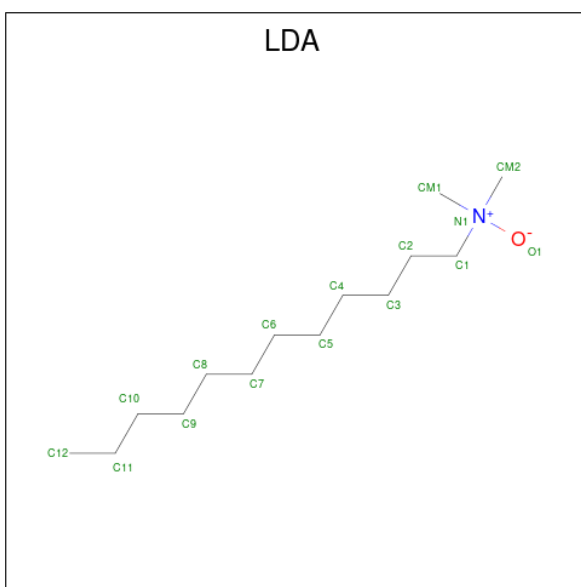


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			18	14	4		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).

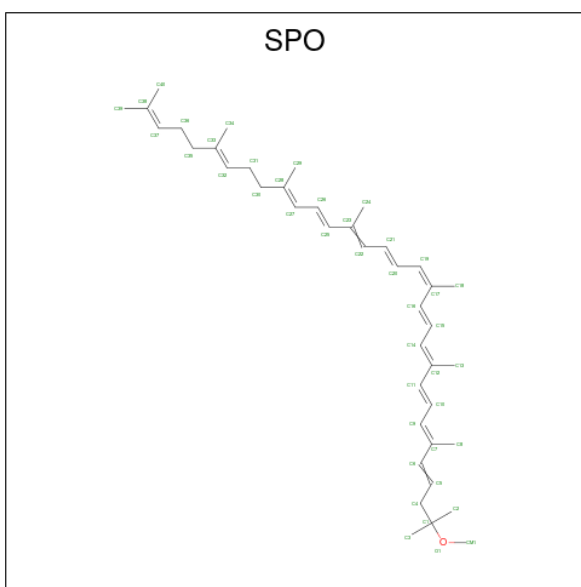


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 is FE (III) ION (CCD ID: FE) (formula: Fe).

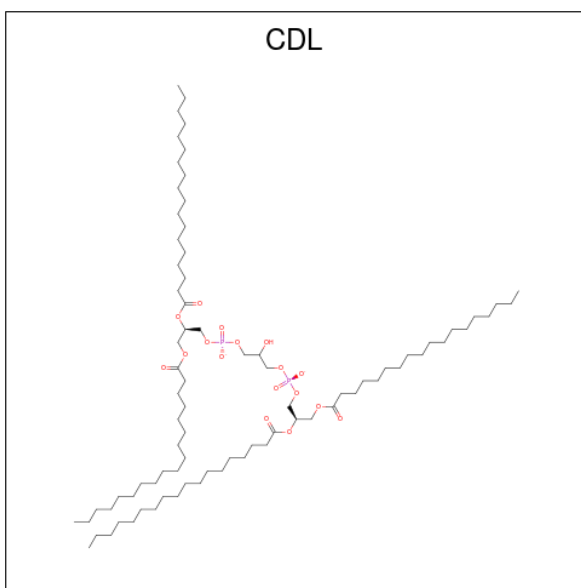
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total	Fe	0	0
			1	1		

- Molecule 10 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).



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

- Molecule 11 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

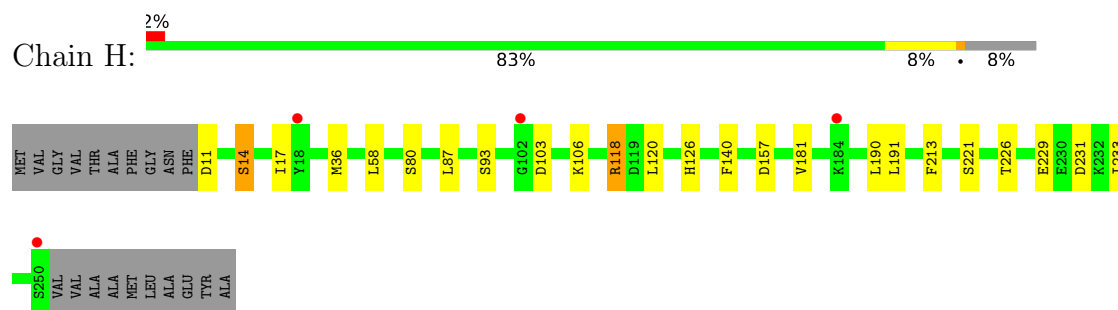
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	H	52	Total 52	O 52	0	0
12	L	29	Total 29	O 29	0	0
12	M	30	Total 30	O 30	0	0

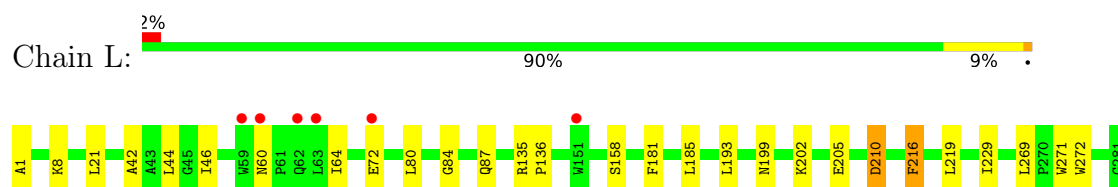
3 Residue-property plots [i](#)

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.

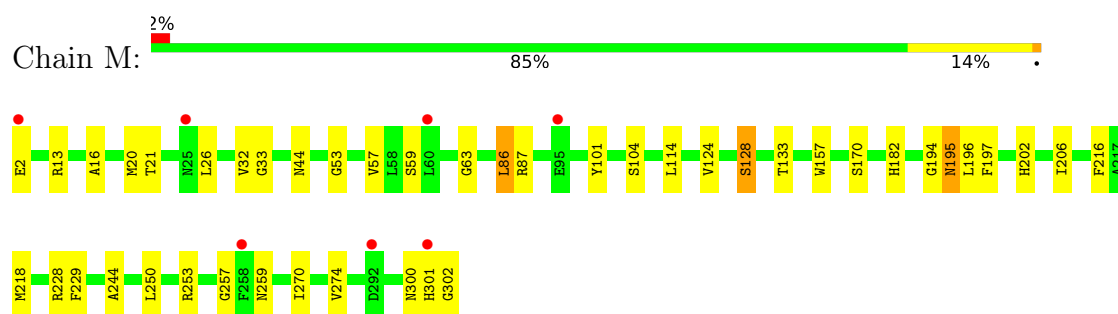
- Molecule 1: Reaction center protein H chain



- 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	141.29Å 141.29Å 187.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.85 – 2.81 39.85 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.85-2.81) 91.7 (39.85-2.81)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.171 , 0.197 0.175 , 0.200	Depositor DCC
R_{free} test set	2637 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7117	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: BCL, FE, CDL, U10, BPH, 9IJ, SPO, CL, LDA

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	0.49	0/1877	0.57	0/2553
2	L	0.42	0/2320	0.54	0/3175
3	M	0.40	0/2472	0.56	2/3372 (0.1%)
All	All	0.44	0/6669	0.55	2/9100 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	257	GLY	CA-C-N	-5.44	113.33	123.01
3	M	257	GLY	C-N-CA	-5.44	113.33	123.01

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1829	0	1836	14	0
2	L	2232	0	2187	22	0
3	M	2397	0	2303	31	0
4	L	132	0	148	5	0
4	M	117	0	115	10	0
5	L	65	0	76	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	55	0	53	6	0
6	L	18	0	15	0	0
7	L	1	0	0	0	0
8	M	48	0	91	4	0
9	M	1	0	0	0	0
10	M	42	0	60	3	0
11	M	69	0	82	3	0
12	H	52	0	0	0	0
12	L	29	0	0	1	0
12	M	30	0	0	1	0
All	All	7117	0	6966	79	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 6.

All (79) 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:197:PHE:HZ	4:M:401:BCL:HBB2	1.53	0.74
2:L:199:ASN:HB3	11:M:408:CDL:HA22	1.72	0.72
5:L:302:BPH:HBB3	5:L:302:BPH:HHC	1.73	0.71
11:M:408:CDL:HB4	11:M:408:CDL:HA62	1.74	0.70
4:M:401:BCL:H41	4:M:409:BCL:HBB3	1.71	0.70
3:M:2:GLU:N	12:M:501:HOH:O	2.27	0.67
3:M:124:VAL:O	3:M:128:SER:OG	2.15	0.65
1:H:181:VAL:HG21	1:H:191:LEU:HD12	1.79	0.65
4:M:409:BCL:HHC	4:M:409:BCL:HBB2	1.78	0.64
4:L:301:BCL:HBB2	4:L:301:BCL:HHC	1.80	0.64
1:H:226:THR:OG1	1:H:229:GLU:HG3	2.00	0.62
3:M:197:PHE:CZ	4:M:401:BCL:HBB2	2.33	0.62
3:M:33:GLY:HA2	8:M:404:LDA:HM13	1.81	0.61
2:L:219:LEU:HD11	3:M:133:THR:HG22	1.82	0.60
1:H:103:ASP:HB3	1:H:106:LYS:HB2	1.83	0.60
3:M:63:GLY:HA3	5:M:406:BPH:H5C1	1.84	0.59
1:H:11:ASP:OD1	1:H:14:SER:OG	2.20	0.58
2:L:181:PHE:HB3	5:M:406:BPH:HBB2	1.88	0.56
1:H:191:LEU:HD11	1:H:213:PHE:HE2	1.71	0.54
4:L:301:BCL:O1D	8:M:402:LDA:H11	2.06	0.54
1:H:36:MET:HE2	1:H:58:LEU:HD23	1.90	0.54
3:M:59:SER:HB2	3:M:128:SER:HB2	1.89	0.54
5:M:406:BPH:HBC3	5:M:406:BPH:HHD	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1:ALA:O	3:M:253:ARG:NH2	2.42	0.53
2:L:210:ASP:OD1	2:L:210:ASP:N	2.40	0.52
4:L:301:BCL:HBB3	4:L:304:BCL:H52	1.92	0.52
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.92	0.52
3:M:53:GLY:O	3:M:57:VAL:HG23	2.10	0.52
11:M:408:CDL:H122	11:M:408:CDL:H311	1.92	0.51
2:L:193:LEU:HD22	2:L:216:PHE:CE2	2.47	0.50
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.92	0.50
2:L:46:ILE:CD1	4:L:301:BCL:H201	2.43	0.49
2:L:181:PHE:CD2	5:M:406:BPH:HBB1	2.49	0.48
5:L:302:BPH:HHC	5:L:302:BPH:CBB	2.43	0.48
4:L:304:BCL:HHC	4:L:304:BCL:OBB	2.14	0.48
4:M:401:BCL:HBB2	4:M:401:BCL:HHC	1.95	0.48
2:L:60:ASN:O	2:L:64:ILE:HG13	2.14	0.47
1:H:87:LEU:HD11	2:L:8:LYS:HA	1.96	0.47
4:M:409:BCL:HHC	4:M:409:BCL:CBB	2.43	0.47
3:M:101:TYR:O	3:M:104:SER:HB3	2.15	0.47
1:H:14:SER:HA	1:H:17:ILE:HG22	1.97	0.46
1:H:190:LEU:HB2	1:H:233:ILE:HD13	1.97	0.46
1:H:140:PHE:HA	3:M:13:ARG:O	2.15	0.46
3:M:300:ASN:C	3:M:302:GLY:H	2.23	0.46
2:L:84:GLY:HA2	2:L:87:GLN:HE21	1.81	0.46
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.50	0.46
2:L:1:ALA:N	12:L:401:HOH:O	2.48	0.45
3:M:300:ASN:C	3:M:302:GLY:N	2.73	0.45
3:M:270:ILE:O	3:M:274:VAL:HG13	2.15	0.45
2:L:272:TRP:NE1	3:M:87:ARG:HG3	2.31	0.45
4:M:401:BCL:HHC	4:M:401:BCL:CBB	2.47	0.45
10:M:407:SPO:H243	4:M:409:BCL:CBB	2.47	0.45
3:M:114:LEU:HD12	3:M:114:LEU:HA	1.79	0.45
8:M:403:LDA:H62	8:M:403:LDA:H91	1.79	0.45
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.52	0.45
1:H:126:HIS:CD2	3:M:20:MET:HE1	2.52	0.45
10:M:407:SPO:H243	4:M:409:BCL:HBB2	1.99	0.45
1:H:118:ARG:HE	1:H:118:ARG:HB2	1.68	0.44
8:M:404:LDA:HM13	8:M:404:LDA:H21	1.74	0.44
2:L:181:PHE:HB3	5:M:406:BPH:CBB	2.46	0.44
4:M:401:BCL:H2	5:M:406:BPH:HHC	1.99	0.44
2:L:72:GLU:OE1	2:L:72:GLU:N	2.50	0.44
1:H:157:ASP:OD1	1:H:157:ASP:N	2.51	0.43
3:M:86:LEU:HD22	3:M:86:LEU:HA	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:218:MET:HE3	3:M:218:MET:HB3	1.84	0.43
1:H:118:ARG:C	1:H:120:LEU:H	2.27	0.43
3:M:194:GLY:O	3:M:195:ASN:CB	2.66	0.42
3:M:300:ASN:O	3:M:302:GLY:N	2.53	0.42
2:L:216:PHE:HD1	2:L:216:PHE:HA	1.76	0.41
2:L:135:ARG:HB3	2:L:136:PRO:HD3	2.02	0.41
3:M:228:ARG:HG3	3:M:229:PHE:CE2	2.56	0.41
2:L:21:LEU:HD12	2:L:21:LEU:HA	1.90	0.41
2:L:42:ALA:O	2:L:46:ILE:HG12	2.20	0.41
3:M:16:ALA:HB1	3:M:32:VAL:HG11	2.03	0.41
2:L:269:LEU:HD13	2:L:271:TRP:CZ2	2.56	0.41
3:M:250:LEU:HD23	3:M:250:LEU:HA	1.92	0.40
2:L:72:GLU:H	2:L:72:GLU:CD	2.28	0.40
3:M:44:ASN:HD22	3:M:44:ASN:HA	1.69	0.40
3:M:157:TRP:CE2	10:M:407:SPO:H293	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	238/260 (92%)	234 (98%)	4 (2%)	0	100	100
2	L	279/281 (99%)	272 (98%)	7 (2%)	0	100	100
3	M	298/301 (99%)	290 (97%)	6 (2%)	2 (1%)	18	45
All	All	815/842 (97%)	796 (98%)	17 (2%)	2 (0%)	43	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	301	HIS
3	M	195	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/208 (94%)	189 (97%)	6 (3%)	35	69
2	L	220/220 (100%)	211 (96%)	9 (4%)	27	60
3	M	235/235 (100%)	228 (97%)	7 (3%)	36	69
All	All	650/663 (98%)	628 (97%)	22 (3%)	32	66

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	14	SER
1	H	80	SER
1	H	93	SER
1	H	118	ARG
1	H	221	SER
1	H	231	ASP
2	L	44	LEU
2	L	80	LEU
2	L	158	SER
2	L	185	LEU
2	L	202	LYS
2	L	205	GLU
2	L	210	ASP
2	L	216	PHE
2	L	229	ILE
3	M	86	LEU
3	M	128	SER
3	M	170	SER
3	M	182	HIS
3	M	196	LEU
3	M	216	PHE
3	M	259	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	206	ASN
2	L	20	ASN
2	L	87	GLN
2	L	258	GLN
3	M	44	ASN
3	M	138	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	BCL	M	401	-	69,74,74	1.17	5 (7%)	79,115,115	1.40	8 (10%)
6	U10	L	303	-	18,18,63	2.48	8 (44%)	24,25,79	1.82	5 (20%)
8	LDA	M	402	-	13,15,15	2.26	2 (15%)	14,17,17	0.54	0
4	BCL	L	304	-	69,74,74	1.11	4 (5%)	79,115,115	1.36	11 (13%)
8	LDA	M	404	-	13,15,15	2.27	2 (15%)	14,17,17	0.64	0
4	BCL	M	409	-	54,59,74	1.37	9 (16%)	61,97,115	1.63	11 (18%)
10	SPO	M	407	-	41,41,41	0.34	0	47,50,50	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CDL	M	408	-	68,68,99	1.16	7 (10%)	74,80,111	0.98	5 (6%)
5	BPH	L	302	-	59,70,70	1.19	5 (8%)	59,101,101	2.18	12 (20%)
4	BCL	L	301	-	69,74,74	1.25	6 (8%)	79,115,115	1.43	10 (12%)
8	LDA	M	403	-	13,15,15	2.13	2 (15%)	14,17,17	0.45	0
5	BPH	M	406	-	49,60,70	1.28	4 (8%)	47,89,101	2.17	10 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	M	401	-	-	3/41/137/137	-
6	U10	L	303	-	-	4/9/33/87	0/1/1/1
8	LDA	M	402	-	-	9/13/13/13	-
4	BCL	L	304	-	-	4/41/137/137	-
8	LDA	M	404	-	-	7/13/13/13	-
4	BCL	M	409	-	-	1/23/119/137	-
11	CDL	M	408	-	1/1/9/9	32/79/79/110	-
10	SPO	M	407	-	-	4/47/47/47	-
5	BPH	L	302	-	-	4/37/105/105	0/5/6/6
4	BCL	L	301	-	-	8/41/137/137	-
8	LDA	M	403	-	-	8/13/13/13	-
5	BPH	M	406	-	-	5/25/93/105	0/5/6/6

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	402	LDA	O1-N1	-6.53	1.26	1.42
8	M	404	LDA	O1-N1	-6.48	1.26	1.42
8	M	403	LDA	O1-N1	-6.13	1.27	1.42
4	M	401	BCL	MG-NA	5.43	2.19	2.06
6	L	303	U10	O3-C3	-5.16	1.24	1.36
6	L	303	U10	C8-C9	5.03	1.47	1.32
8	M	404	LDA	C1-N1	-4.92	1.46	1.51
8	M	402	LDA	C1-N1	-4.76	1.46	1.51
6	L	303	U10	O4-C4	-4.51	1.25	1.36
8	M	403	LDA	C1-N1	-4.44	1.46	1.51
4	M	409	BCL	MG-NA	4.38	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	301	BCL	OBD-CAD	4.35	1.30	1.22
4	L	301	BCL	MG-NA	4.35	2.16	2.06
5	L	302	BPH	C3D-CAD	-4.16	1.39	1.47
5	L	302	BPH	CBD-CGD	-3.99	1.47	1.52
4	L	304	BCL	MG-NA	3.93	2.15	2.06
5	M	406	BPH	C1D-C2D	3.81	1.43	1.39
4	L	304	BCL	MG-NC	3.75	2.15	2.06
4	M	409	BCL	MG-NC	3.67	2.15	2.06
5	M	406	BPH	CBD-CGD	-3.64	1.47	1.52
4	L	301	BCL	MG-NC	3.44	2.14	2.06
11	M	408	CDL	PA1-OA5	3.30	1.72	1.59
11	M	408	CDL	PA1-OA4	-3.21	1.40	1.55
11	M	408	CDL	PA1-OA3	-3.16	1.39	1.50
5	L	302	BPH	C3B-C4B	3.09	1.46	1.41
4	L	304	BCL	C3B-C4B	2.97	1.47	1.41
5	M	406	BPH	C3D-CAD	-2.95	1.42	1.47
11	M	408	CDL	PB2-OB4	-2.89	1.42	1.55
11	M	408	CDL	PB2-OB5	2.87	1.70	1.59
4	M	401	BCL	OBD-CAD	2.86	1.27	1.22
11	M	408	CDL	PB2-OB3	-2.74	1.41	1.50
4	M	409	BCL	O2A-CGA	2.69	1.41	1.33
6	L	303	U10	C6-C1	2.66	1.39	1.35
6	L	303	U10	C3-C2	-2.61	1.41	1.48
4	M	401	BCL	C3B-C4B	2.59	1.46	1.41
4	M	409	BCL	C4-C3	2.59	1.57	1.50
6	L	303	U10	C4-C5	-2.58	1.41	1.48
5	M	406	BPH	C4D-CHA	2.37	1.43	1.39
4	M	401	BCL	MG-NC	2.34	2.11	2.06
6	L	303	U10	C1-C2	-2.33	1.39	1.47
4	M	409	BCL	C3B-C4B	2.31	1.45	1.41
4	M	409	BCL	C1B-NB	2.28	1.40	1.37
11	M	408	CDL	CA3-CA4	2.25	1.57	1.50
4	M	409	BCL	OBD-CAD	2.24	1.26	1.22
5	L	302	BPH	C1-C2	2.19	1.55	1.49
4	L	301	BCL	C1D-C2D	-2.18	1.41	1.45
4	M	409	BCL	C1-C2	2.16	1.55	1.49
5	L	302	BPH	C1B-C2B	2.13	1.41	1.39
4	L	301	BCL	C1D-ND	2.12	1.40	1.37
4	M	401	BCL	C3D-C4D	-2.06	1.39	1.44
4	L	304	BCL	C3D-C4D	-2.05	1.39	1.44
4	L	301	BCL	C4-C3	2.05	1.55	1.50
6	L	303	U10	C6-C5	-2.04	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	409	BCL	CHD-C1D	2.01	1.42	1.38

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	302	BPH	C4D-CHA-CBD	-12.23	102.59	108.45
5	M	406	BPH	C4D-CHA-CBD	-10.48	103.43	108.45
4	M	401	BCL	C4D-CHA-C1A	5.19	127.43	121.24
6	L	303	U10	C7-C6-C1	-4.97	116.37	124.89
4	M	409	BCL	C4D-CHA-C1A	4.62	126.75	121.24
4	L	301	BCL	C1D-ND-C4D	-4.60	103.08	106.31
4	M	409	BCL	C1-O2A-CGA	4.26	126.96	116.65
4	M	409	BCL	C1D-ND-C4D	-4.17	103.39	106.31
4	L	304	BCL	C4D-CHA-C1A	3.95	125.96	121.24
5	M	406	BPH	O2D-CGD-CBD	3.91	115.25	110.95
4	L	301	BCL	C4D-CHA-C1A	3.90	125.89	121.24
5	L	302	BPH	C4D-ND-C1D	-3.81	104.31	108.87
4	L	304	BCL	C1D-ND-C4D	-3.79	103.66	106.31
4	M	409	BCL	CHD-C1D-ND	-3.74	119.54	124.80
5	M	406	BPH	C4D-ND-C1D	-3.71	104.43	108.87
4	L	301	BCL	C16-C15-C13	-3.66	103.80	115.97
4	M	401	BCL	CHD-C1D-ND	-3.64	119.68	124.80
6	L	303	U10	C7-C8-C9	-3.58	117.12	127.25
4	L	301	BCL	CHD-C1D-ND	-3.58	119.77	124.80
5	L	302	BPH	C1-C2-C3	-3.54	120.39	126.20
4	M	401	BCL	C4A-NA-C1A	3.54	108.29	106.68
4	M	401	BCL	C1D-ND-C4D	-3.51	103.85	106.31
4	L	301	BCL	C2A-C1A-CHA	3.44	129.84	123.87
5	M	406	BPH	C3D-C4D-ND	3.44	112.12	107.71
4	L	304	BCL	CHD-C1D-ND	-3.41	120.00	124.80
4	M	401	BCL	C1-C2-C3	-3.29	120.81	126.20
5	M	406	BPH	OBD-CAD-CBD	-3.26	121.04	125.82
4	M	401	BCL	CHA-C1A-NA	-3.18	119.18	126.39
5	L	302	BPH	C2D-C1D-ND	3.12	111.69	109.43
4	L	301	BCL	CHA-C1A-NA	-3.11	119.34	126.39
5	L	302	BPH	C3D-C4D-ND	3.07	111.64	107.71
4	L	304	BCL	C16-C15-C13	-3.01	105.95	115.97
4	L	301	BCL	O2D-CGD-CBD	2.93	116.35	111.23
11	M	408	CDL	OA4-PA1-OA3	2.93	126.06	112.44
5	L	302	BPH	O2D-CGD-CBD	2.91	114.14	110.95
11	M	408	CDL	OB4-PB2-OB3	2.90	125.96	112.44
4	M	409	BCL	C1-C2-C3	-2.89	122.08	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	304	BCL	CHA-C1A-NA	-2.84	119.95	126.39
4	M	409	BCL	CHA-C1A-NA	-2.82	120.01	126.39
5	L	302	BPH	OBD-CAD-CBD	-2.78	121.74	125.82
5	L	302	BPH	OBB-CAB-C3B	2.76	124.60	119.99
4	M	409	BCL	C2A-C1A-CHA	2.64	128.45	123.87
6	L	303	U10	C11-C9-C10	2.63	120.64	114.59
5	M	406	BPH	OBB-CAB-C3B	2.63	124.38	119.99
5	L	302	BPH	CMD-C2D-C3D	2.60	129.88	124.68
4	L	304	BCL	C2A-C1A-CHA	2.59	128.36	123.87
4	M	401	BCL	C2A-C1A-CHA	2.59	128.35	123.87
4	M	409	BCL	O2D-CGD-O1D	-2.59	118.82	123.85
4	L	304	BCL	CAB-C3B-C2B	2.58	133.10	127.74
5	L	302	BPH	OBB-CAB-CBB	-2.51	114.85	120.19
11	M	408	CDL	CA4-OA6-CA5	2.50	123.79	117.80
4	L	301	BCL	OBB-CAB-CBB	-2.42	114.36	119.77
5	M	406	BPH	CMD-C2D-C3D	2.41	129.50	124.68
11	M	408	CDL	OB8-CB7-OB9	-2.39	117.65	123.63
5	M	406	BPH	C1-C2-C3	-2.38	122.29	126.20
5	M	406	BPH	C2D-C1D-ND	2.37	111.14	109.43
6	L	303	U10	C4M-O4-C4	2.32	124.62	116.47
4	L	304	BCL	O2A-CGA-O1A	-2.31	117.84	123.63
5	L	302	BPH	C4C-C3C-C2C	-2.27	100.68	102.84
4	M	409	BCL	OBB-CAB-CBB	-2.19	114.87	119.77
4	L	301	BCL	O2D-CGD-O1D	-2.18	119.60	123.85
4	L	304	BCL	C11-C10-C8	-2.17	108.75	115.97
4	M	401	BCL	OBB-CAB-CBB	-2.17	114.91	119.77
5	L	302	BPH	C1C-C2C-C3C	-2.16	100.78	102.84
6	L	303	U10	C1M-C1-C6	-2.12	120.96	124.45
4	M	409	BCL	CHC-C1C-NC	-2.08	121.39	124.40
4	L	304	BCL	OBB-CAB-CBB	-2.08	115.11	119.77
11	M	408	CDL	OA6-CA5-OA7	-2.07	118.88	123.70
4	M	409	BCL	O2D-CGD-CBD	2.06	114.83	111.23
4	L	301	BCL	C2D-C1D-ND	2.06	112.16	110.13
4	L	304	BCL	C15-C13-C12	-2.04	101.71	112.07
5	M	406	BPH	CMB-C2B-C3B	2.00	128.68	124.68

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	M	408	CDL	CA4

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	303	U10	C1-C6-C7-C8
8	M	402	LDA	C2-C1-N1-CM1
8	M	402	LDA	C2-C1-N1-CM2
8	M	402	LDA	N1-C1-C2-C3
8	M	404	LDA	N1-C1-C2-C3
10	M	407	SPO	C1-C4-C5-C6
11	M	408	CDL	CA2-OA2-PA1-OA5
11	M	408	CDL	C11-CA5-OA6-CA4
11	M	408	CDL	CB2-OB2-PB2-OB3
11	M	408	CDL	CB2-OB2-PB2-OB5
11	M	408	CDL	OA7-CA5-OA6-CA4
6	L	303	U10	C7-C8-C9-C11
11	M	408	CDL	C31-CA7-OA8-CA6
11	M	408	CDL	O1-C1-CB2-OB2
11	M	408	CDL	CB7-C71-C72-C73
11	M	408	CDL	OA9-CA7-OA8-CA6
11	M	408	CDL	CA2-C1-CB2-OB2
6	L	303	U10	C7-C8-C9-C10
4	L	301	BCL	C13-C15-C16-C17
11	M	408	CDL	CA6-CA4-OA6-CA5
11	M	408	CDL	C51-CB5-OB6-CB4
8	M	404	LDA	C7-C8-C9-C10
11	M	408	CDL	OB7-CB5-OB6-CB4
4	M	401	BCL	C16-C17-C18-C20
8	M	403	LDA	C11-C10-C9-C8
8	M	403	LDA	C1-C2-C3-C4
11	M	408	CDL	C13-C14-C15-C16
11	M	408	CDL	CB5-C51-C52-C53
8	M	404	LDA	C3-C4-C5-C6
8	M	404	LDA	C11-C10-C9-C8
5	M	406	BPH	C4-C3-C5-C6
5	M	406	BPH	C2-C3-C5-C6
5	M	406	BPH	C5-C6-C7-C8
4	M	401	BCL	C16-C17-C18-C19
11	M	408	CDL	C31-C32-C33-C34
8	M	404	LDA	C1-C2-C3-C4
10	M	407	SPO	C2-C1-C4-C5
5	L	302	BPH	C13-C15-C16-C17
8	M	403	LDA	C6-C7-C8-C9
11	M	408	CDL	CA5-C11-C12-C13
8	M	403	LDA	C4-C5-C6-C7
4	L	301	BCL	C2B-C3B-CAB-CBB
11	M	408	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
11	M	408	CDL	C39-C40-C41-C42
8	M	403	LDA	C7-C8-C9-C10
11	M	408	CDL	C52-C53-C54-C55
8	M	403	LDA	C9-C10-C11-C12
5	L	302	BPH	C4-C3-C5-C6
5	L	302	BPH	C2-C3-C5-C6
11	M	408	CDL	C32-C33-C34-C35
11	M	408	CDL	C71-C72-C73-C74
4	L	301	BCL	C4B-C3B-CAB-OBB
4	L	301	BCL	C4B-C3B-CAB-CBB
8	M	404	LDA	C9-C10-C11-C12
8	M	402	LDA	C4-C5-C6-C7
8	M	402	LDA	C2-C3-C4-C5
4	L	301	BCL	C2B-C3B-CAB-OBB
4	L	301	BCL	C16-C17-C18-C19
11	M	408	CDL	C35-C36-C37-C38
4	L	304	BCL	C15-C16-C17-C18
8	M	402	LDA	C2-C1-N1-O1
11	M	408	CDL	CA2-OA2-PA1-OA3
8	M	402	LDA	C9-C10-C11-C12
8	M	403	LDA	N1-C1-C2-C3
4	L	304	BCL	C11-C12-C13-C14
6	L	303	U10	C5-C4-O4-C4M
10	M	407	SPO	C34-C33-C35-C36
5	L	302	BPH	C15-C16-C17-C18
11	M	408	CDL	C17-C18-C19-C20
8	M	402	LDA	C7-C8-C9-C10
4	L	304	BCL	C2A-CAA-CBA-CGA
11	M	408	CDL	C51-C52-C53-C54
11	M	408	CDL	CA7-C31-C32-C33
4	L	301	BCL	C16-C17-C18-C20
10	M	407	SPO	C32-C33-C35-C36
11	M	408	CDL	OB6-CB4-CB6-OB8
8	M	402	LDA	C11-C10-C9-C8
11	M	408	CDL	CB3-CB4-CB6-OB8
8	M	404	LDA	C4-C5-C6-C7
11	M	408	CDL	C14-C15-C16-C17
5	M	406	BPH	C6-C7-C8-C9
4	M	409	BCL	C2-C1-O2A-CGA
5	M	406	BPH	C2-C1-O2A-CGA
4	L	304	BCL	C11-C12-C13-C15
8	M	403	LDA	C2-C1-N1-O1

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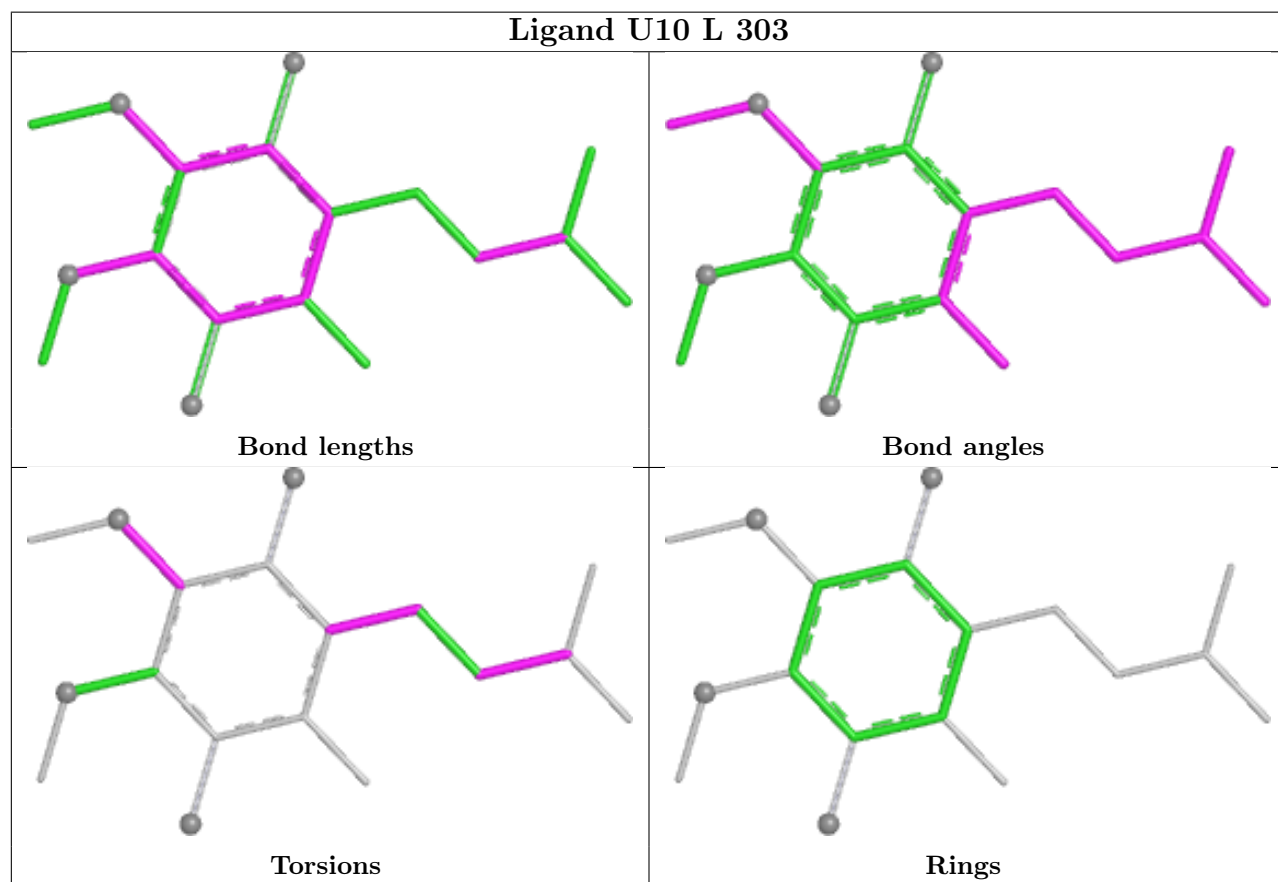
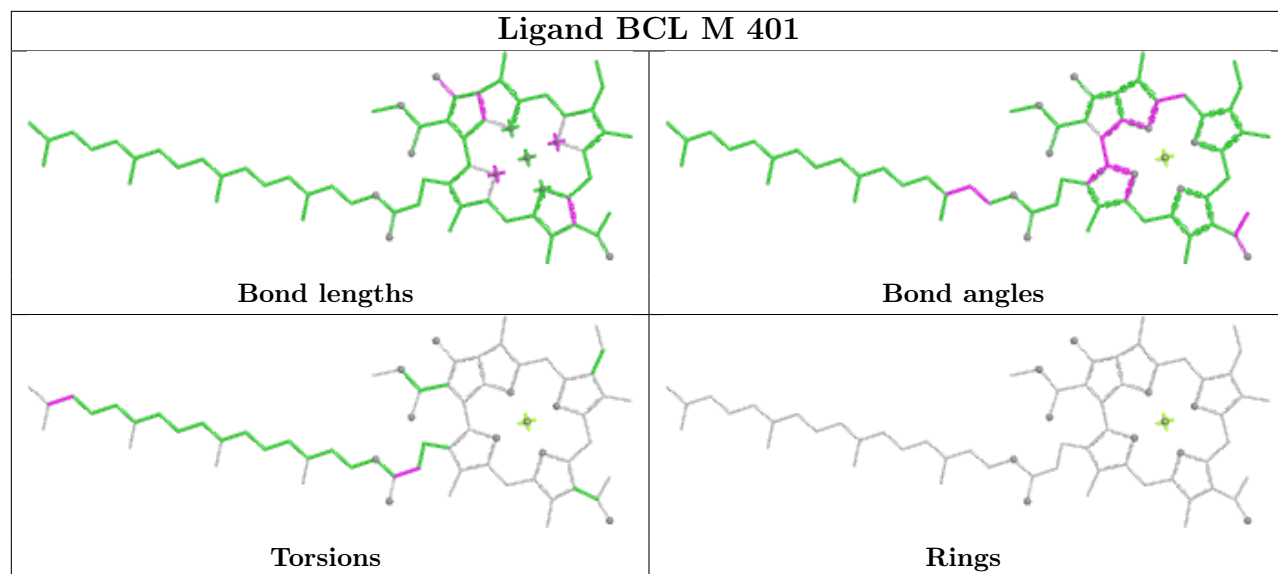
Mol	Chain	Res	Type	Atoms
4	L	301	BCL	CAD-CBD-CGD-O2D
4	M	401	BCL	CAA-CBA-CGA-O2A
11	M	408	CDL	C72-C71-CB7-OB8
11	M	408	CDL	C74-C75-C76-C77

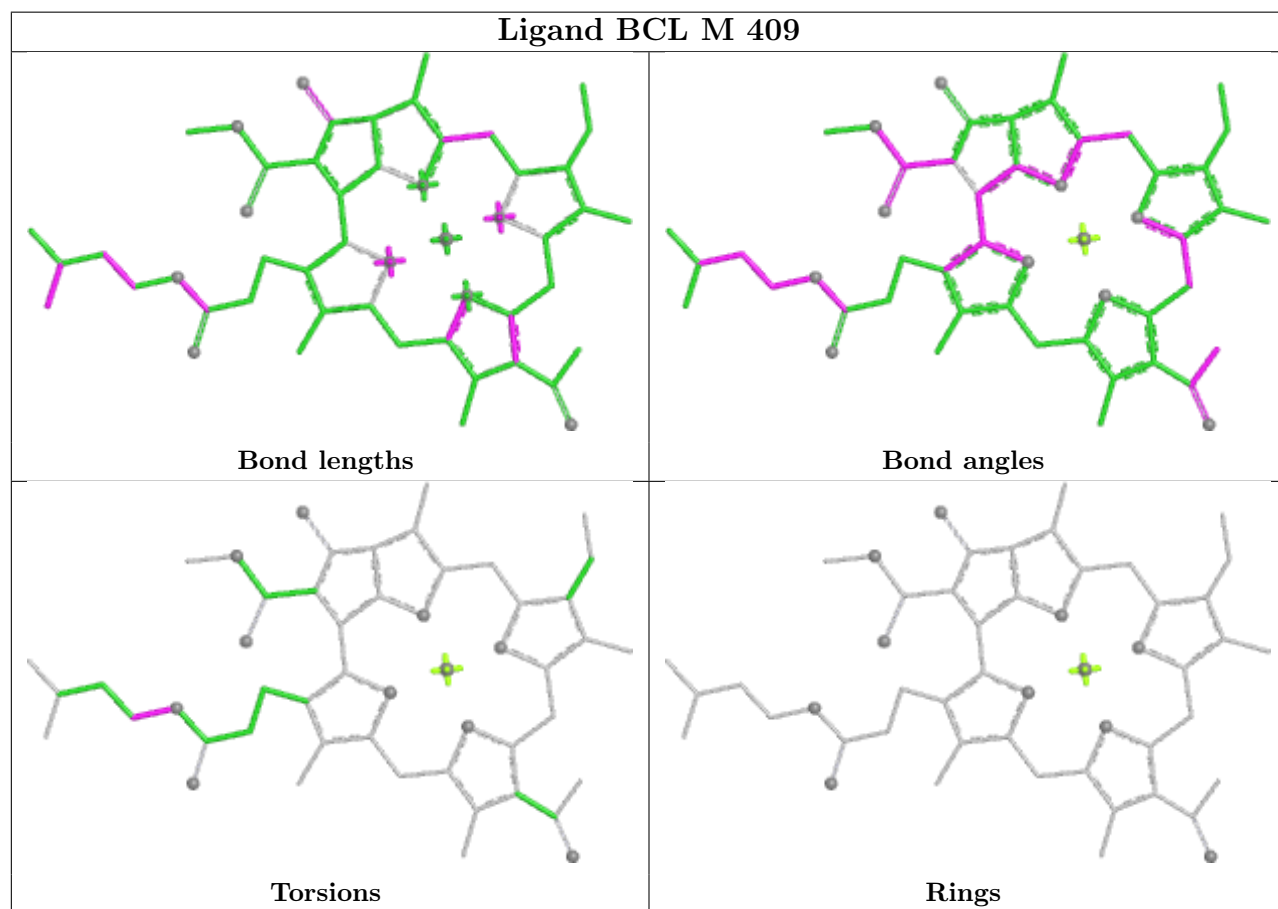
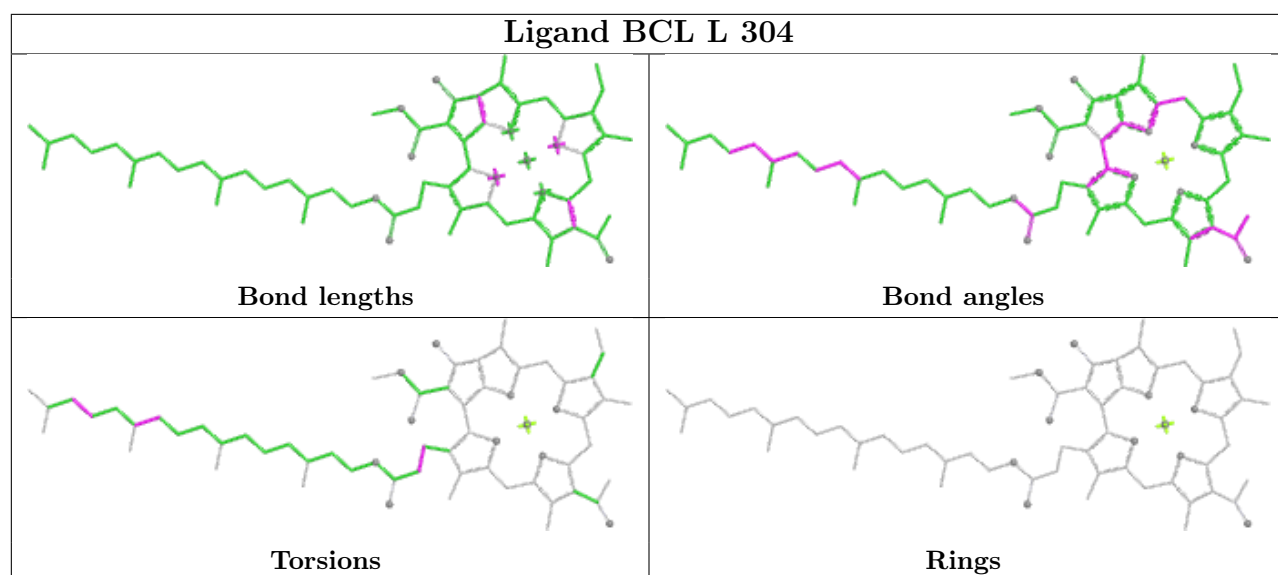
There are no ring outliers.

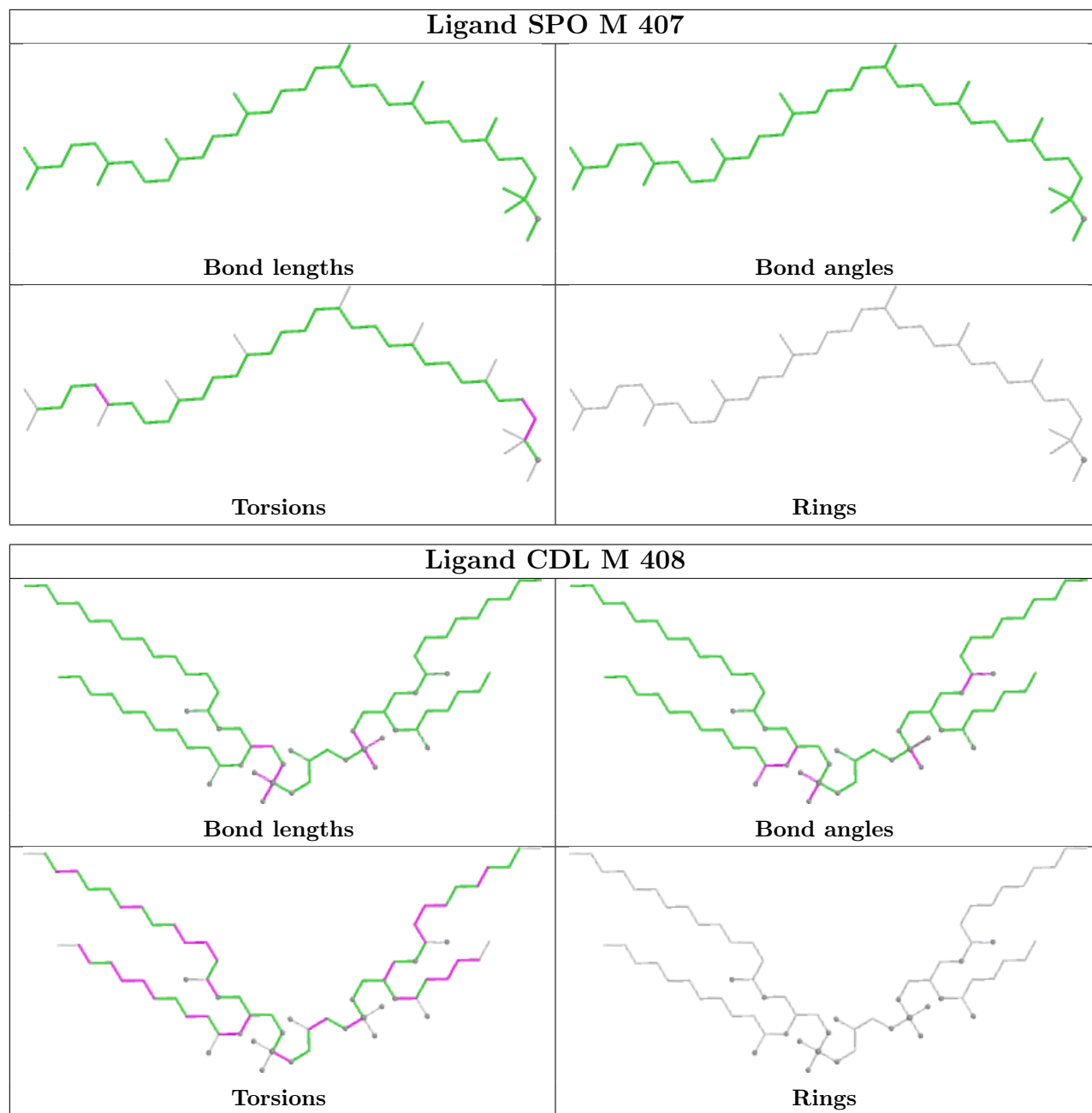
11 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	401	BCL	6	0
8	M	402	LDA	1	0
4	L	304	BCL	2	0
8	M	404	LDA	2	0
4	M	409	BCL	5	0
10	M	407	SPO	3	0
11	M	408	CDL	3	0
5	L	302	BPH	2	0
4	L	301	BCL	4	0
8	M	403	LDA	1	0
5	M	406	BPH	6	0

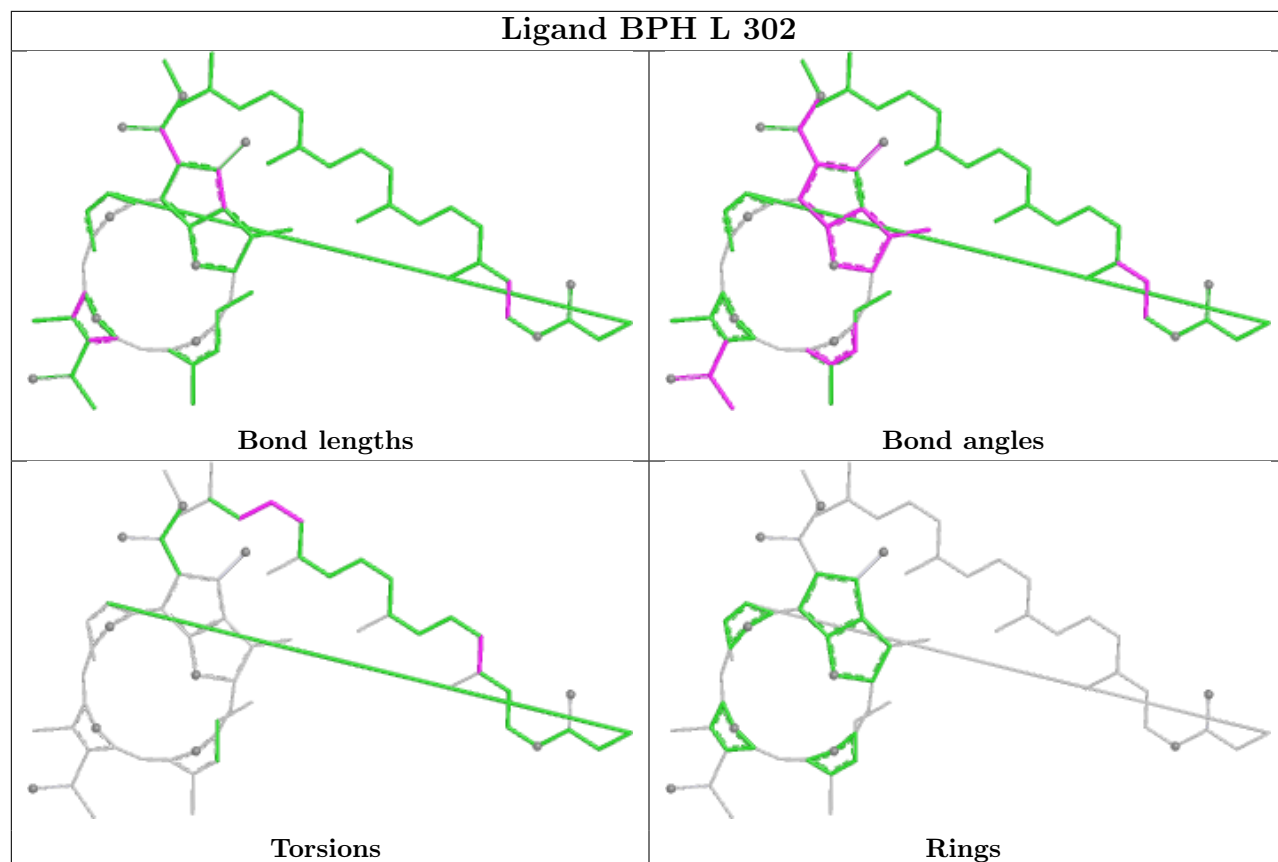
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



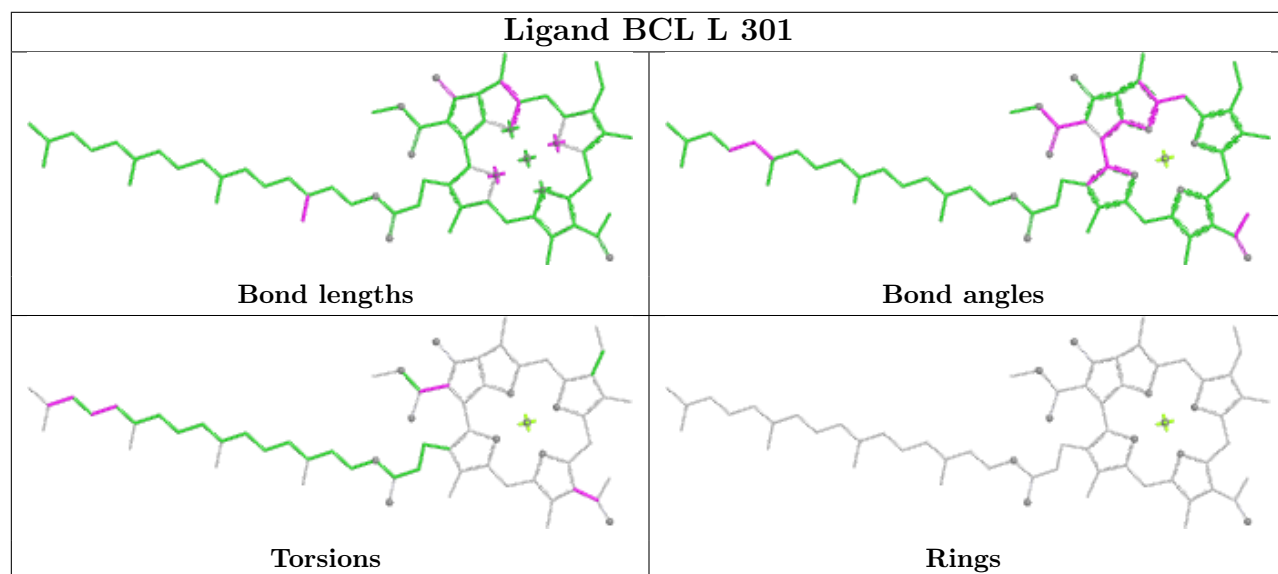


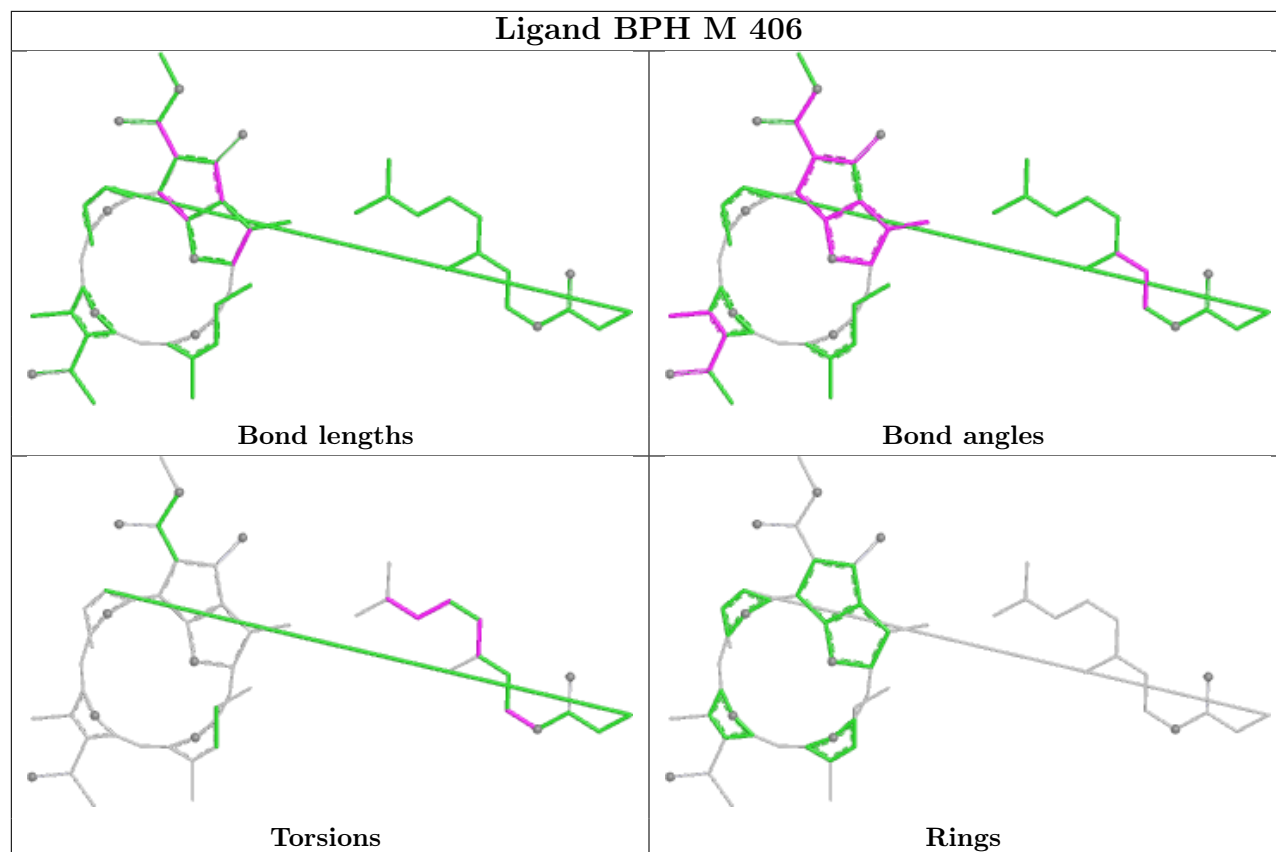


Ligand BPH L 302



Ligand BCL L 301





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	240/260 (92%)	-0.28	4 (1%) 69 60	40, 52, 74, 122	0
2	L	281/281 (100%)	-0.22	6 (2%) 63 54	37, 48, 81, 106	0
3	M	300/301 (99%)	-0.18	7 (2%) 61 51	35, 52, 81, 129	0
All	All	821/842 (97%)	-0.22	17 (2%) 63 54	35, 51, 81, 129	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	6.0
3	M	2	GLU	5.3
3	M	301	HIS	4.9
2	L	62	GLN	4.7
2	L	72	GLU	4.0
1	H	102	GLY	3.5
3	M	292	ASP	3.0
3	M	95	GLU	2.6
3	M	258	PHE	2.6
2	L	151	TRP	2.5
2	L	59	TRP	2.2
3	M	60	LEU	2.2
1	H	184	LYS	2.2
2	L	63	LEU	2.1
2	L	60	ASN	2.1
3	M	25	ASN	2.1
1	H	18	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

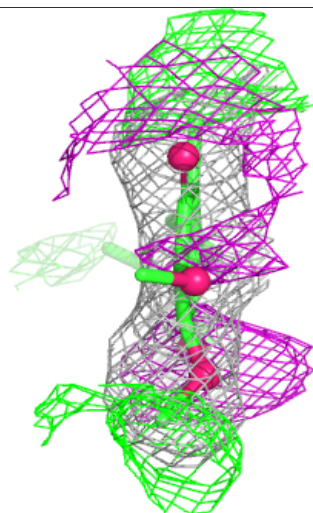
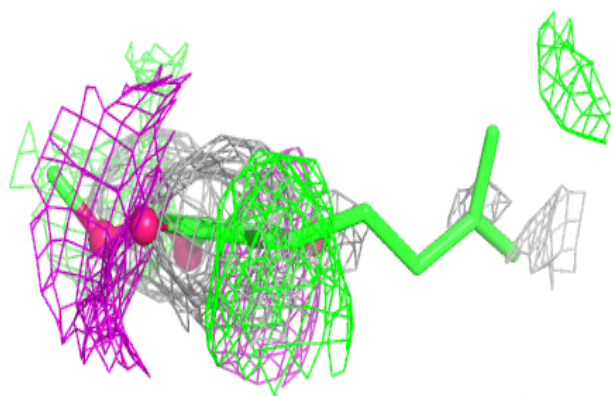
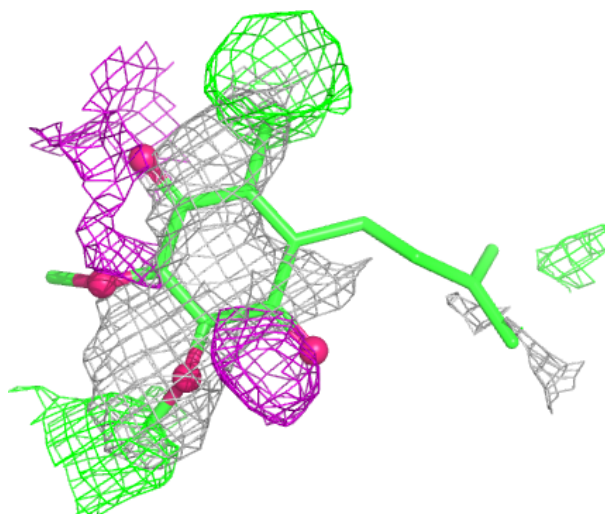
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	U10	L	303	18/63	0.69	0.42	93,117,123,123	0
8	LDA	M	403	16/16	0.81	0.25	75,81,91,97	0
8	LDA	M	404	16/16	0.84	0.28	84,94,111,116	0
11	CDL	M	408	69/100	0.85	0.19	55,78,93,105	0
8	LDA	M	402	16/16	0.91	0.19	71,77,89,94	0
7	CL	L	305	1/1	0.92	0.12	92,92,92,92	0
10	SPO	M	407	42/42	0.93	0.15	43,60,77,83	0
5	BPH	M	406	55/65	0.95	0.10	38,45,73,83	0
5	BPH	L	302	65/65	0.96	0.09	32,39,52,54	0
4	BCL	L	301	66/66	0.96	0.09	34,43,67,72	0
4	BCL	M	409	51/66	0.96	0.09	36,43,55,61	0
4	BCL	M	401	66/66	0.97	0.08	35,40,63,79	0
4	BCL	L	304	66/66	0.98	0.07	35,41,60,66	0
9	FE	M	405	1/1	1.00	0.04	32,32,32,32	0

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

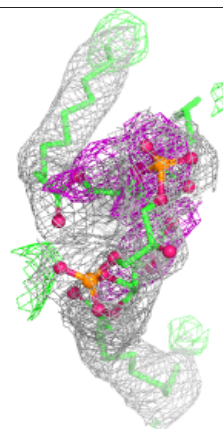
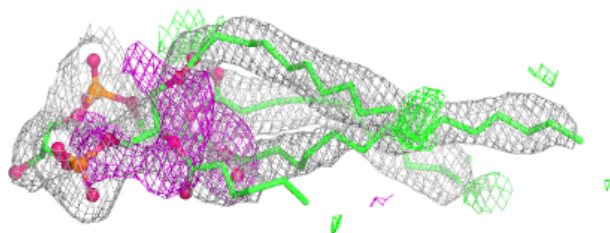
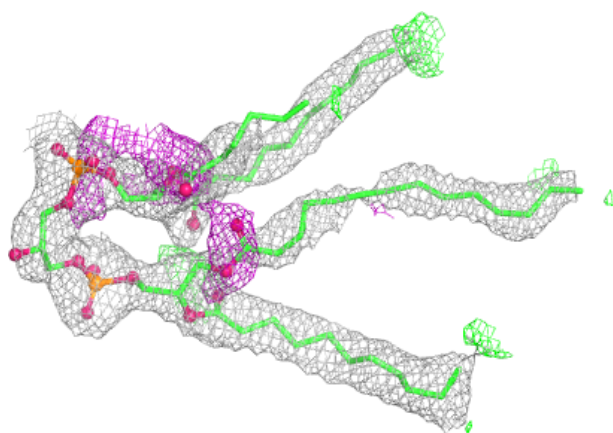
Electron density around U10 L 303:

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

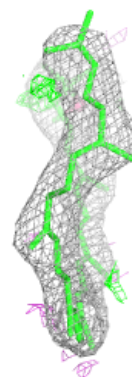
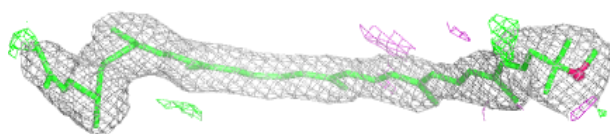
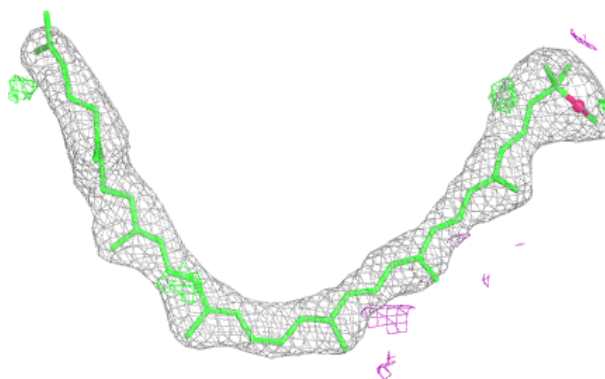


Electron density around CDL M 408:

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

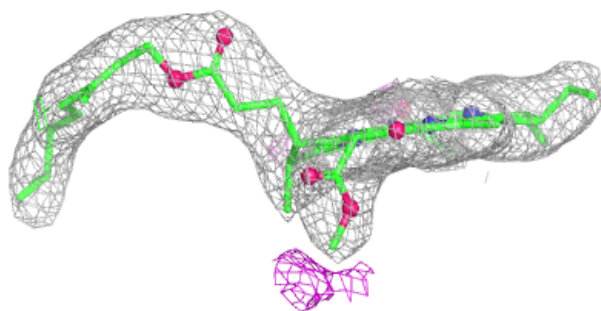
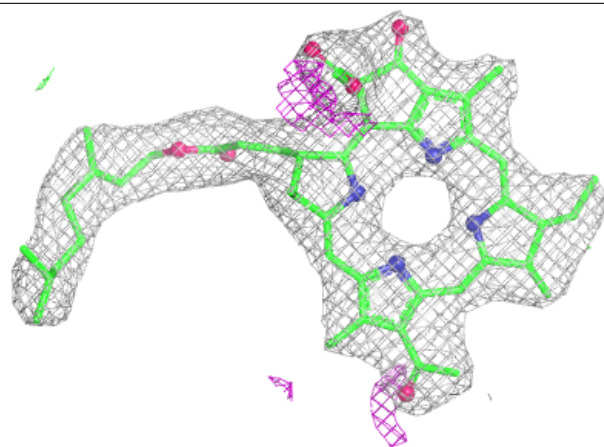
**Electron density around SPO M 407:**

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



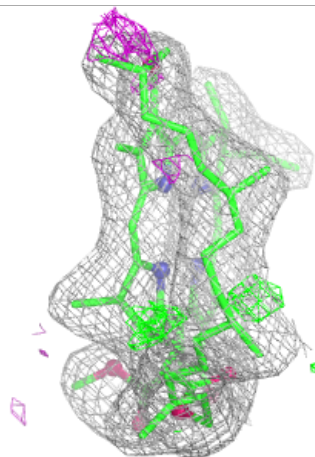
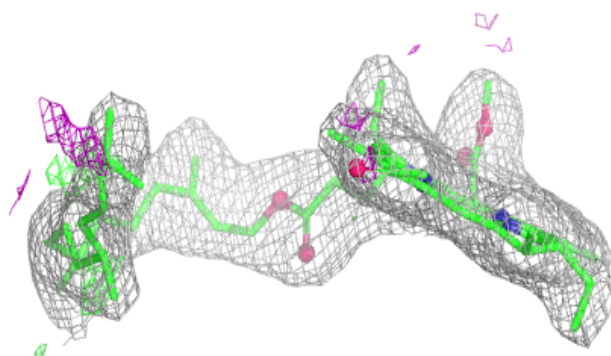
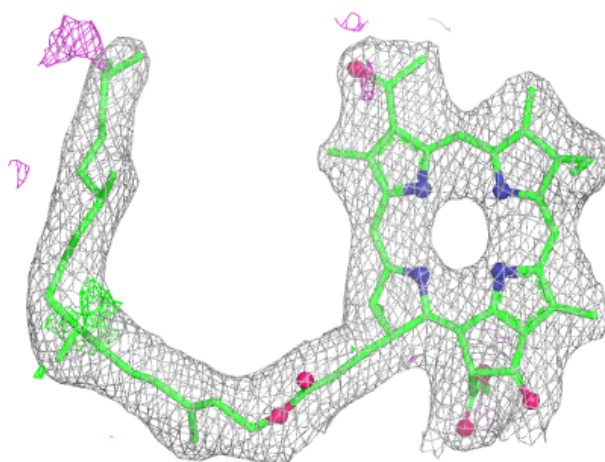
Electron density around BPH M 406:

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



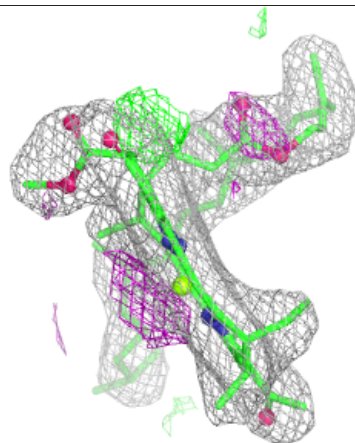
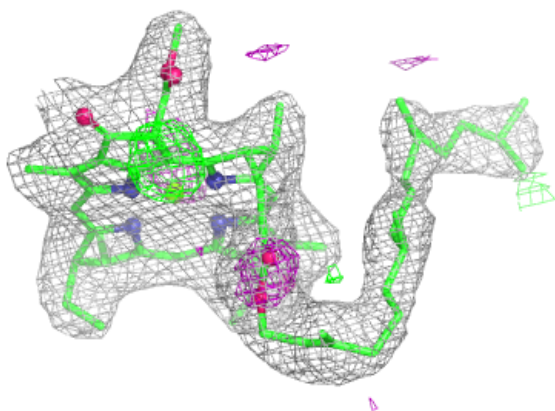
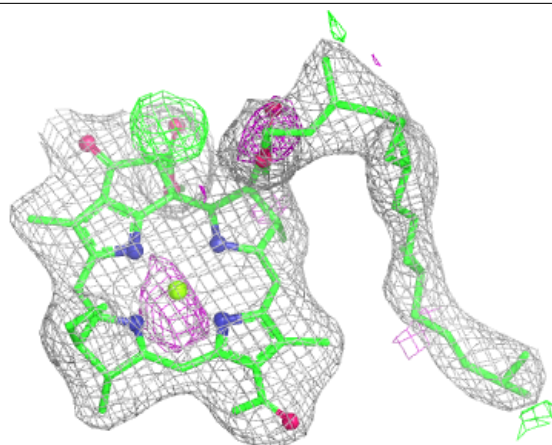
Electron density around BPH L 302:

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



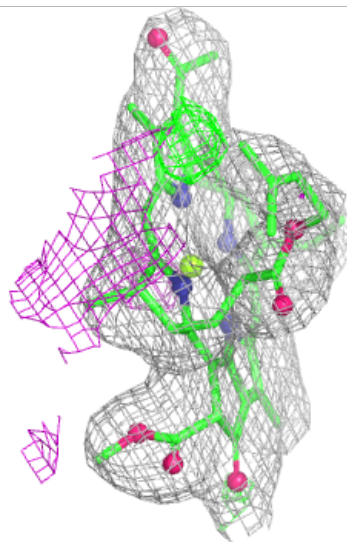
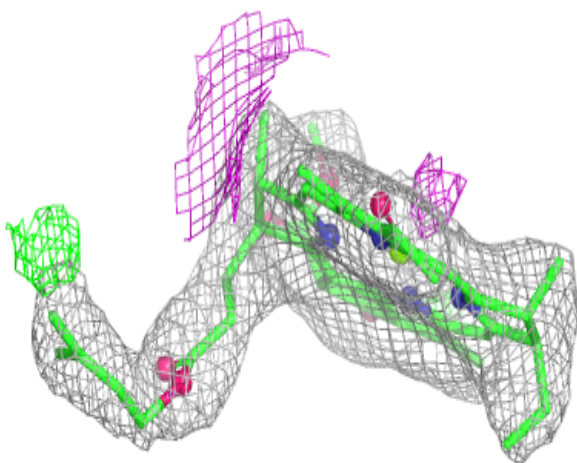
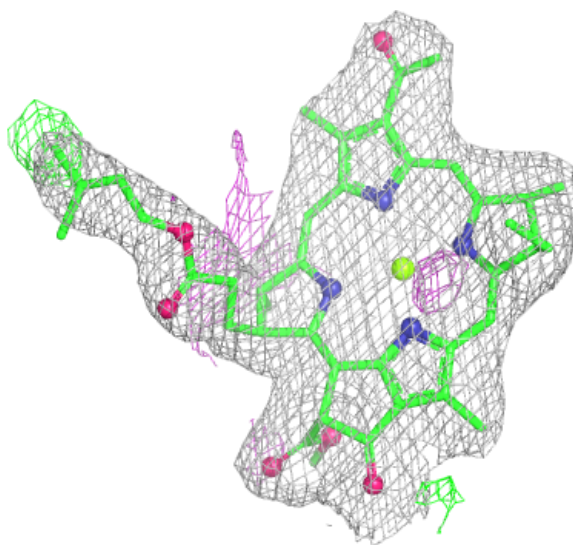
Electron density around BCL L 301:

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



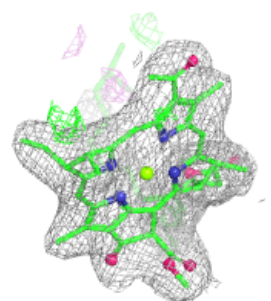
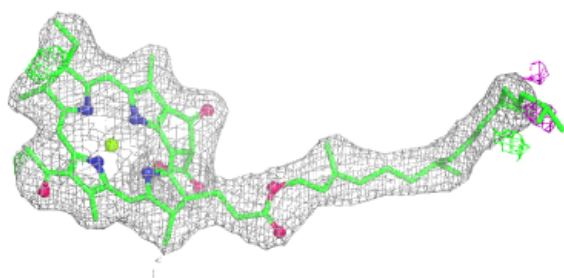
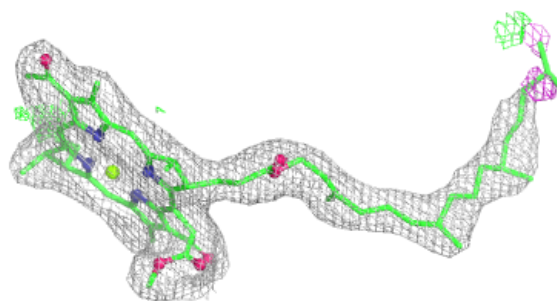
Electron density around BCL M 409:

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

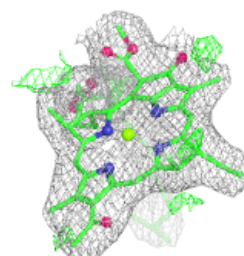
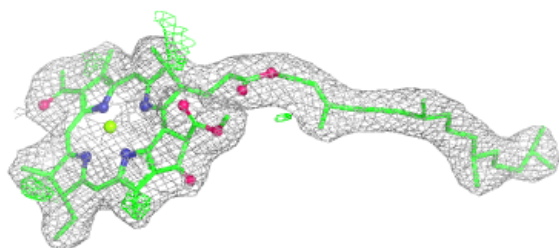
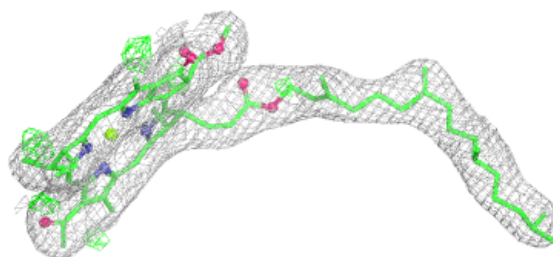


Electron density around BCL M 401:

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

**Electron density around BCL L 304:**

$2mF_o-DF_c$ (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.