



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 06:51 AM EDT

PDB ID : 8VTO / pdb_00008vto
Title : Crystal structure of R. sphaeroides Photosynthetic Reaction Center variant Y (M210)2-methylphenylalanine
Authors : Tran, K.; Mathews, I.; Boxer, S.G.
Deposited on : 2024-01-26
Resolution : 3.09 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

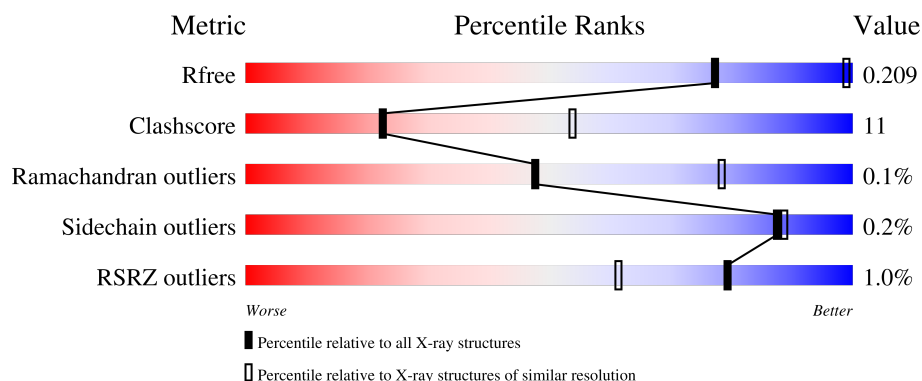
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	 78% 22%
2	L	281	 2% 83% 17%
3	M	301	 75% 25%

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	407	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7026 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	1	0
			2240	1511	356	365	8			

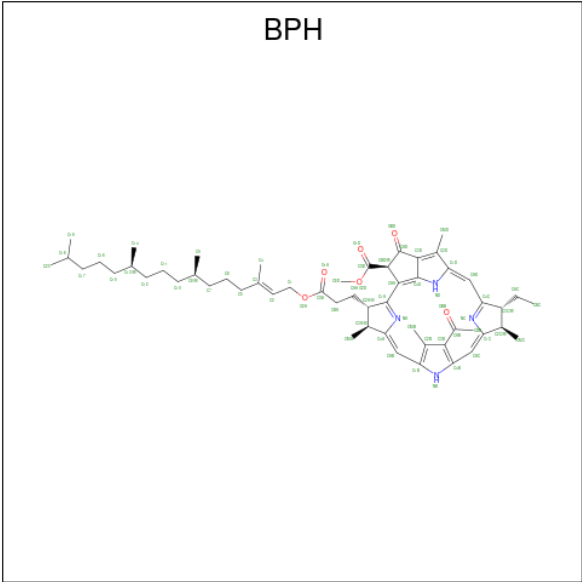
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	301	Total	C	N	O	S	0	0	0
			2396	1599	392	395	10			

There are 2 discrepancies between the modelled and reference sequences:

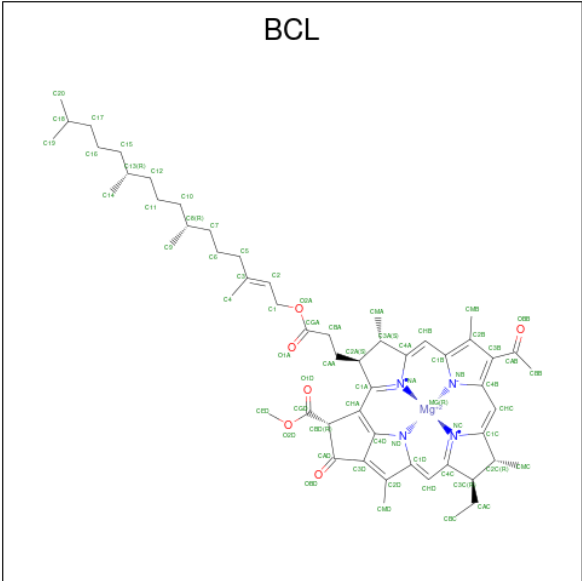
Chain	Residue	Modelled	Actual	Comment	Reference
M	210	A1ADW	TYR	conflict	UNP P0C0Y9
M	252	VAL	TRP	conflict	UNP P0C0Y9

- Molecule 4 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆) (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	L	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).



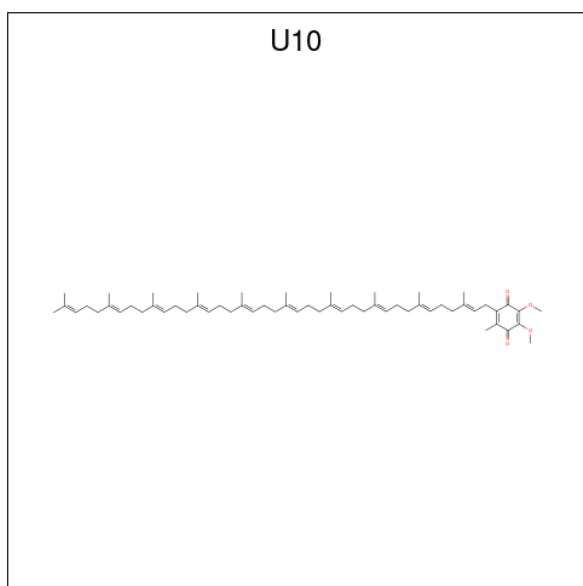
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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

- Molecule 6 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

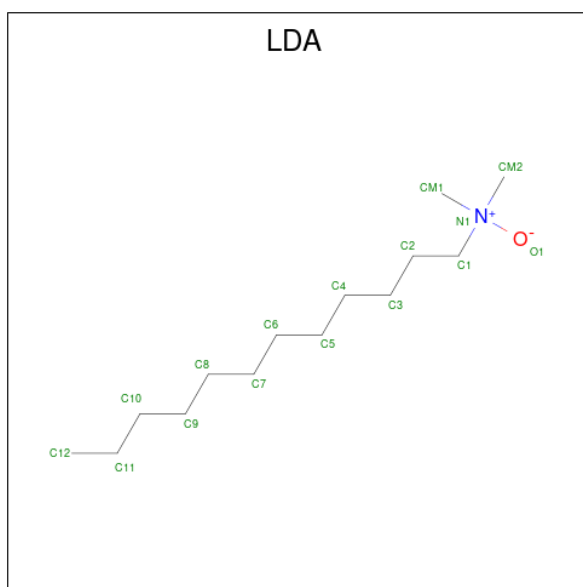


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			18	14	4		

- 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: $C_{14}H_{31}NO$).

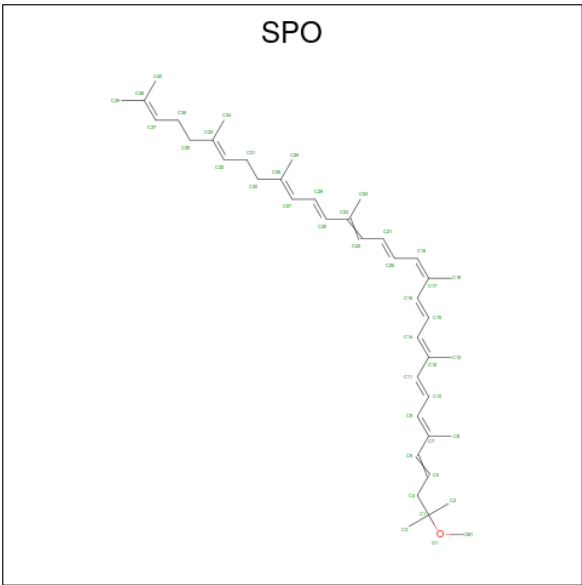


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

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

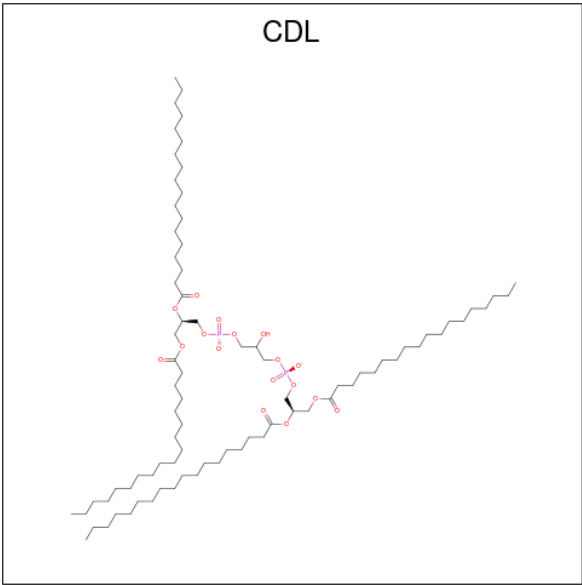
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total	Fe	0	0
			1	1		

- 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		

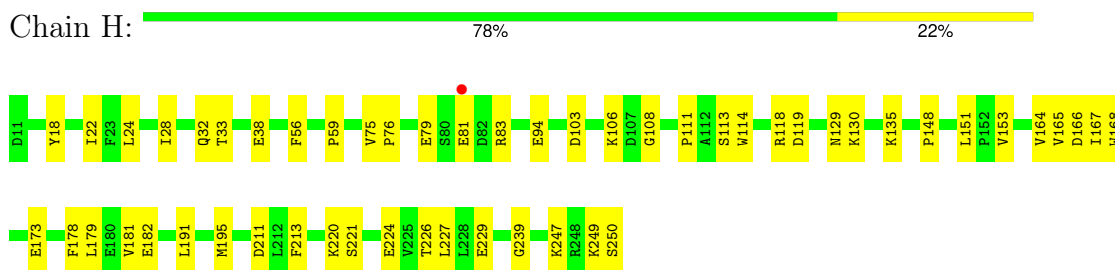
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	H	2	Total 2	O 2	0	0
12	L	8	Total 8	O 8	0	0
12	M	3	Total 3	O 3	0	0

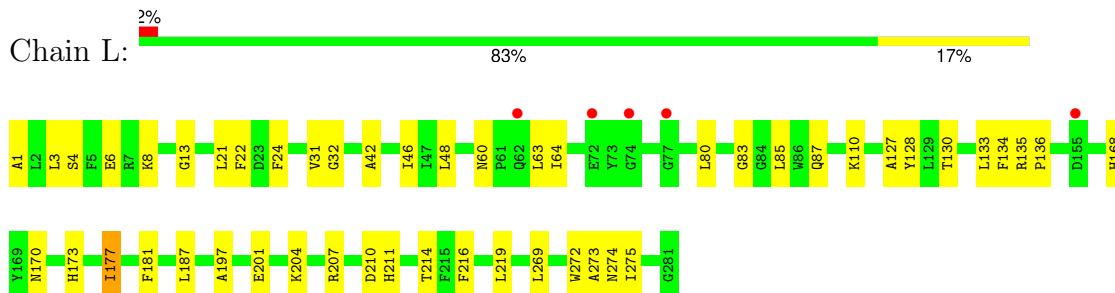
3 Residue-property plots

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.

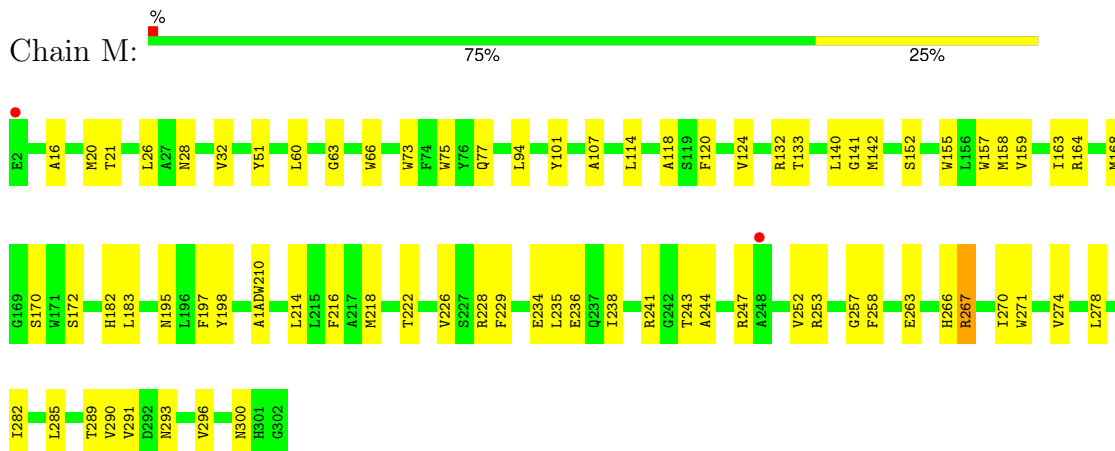
• Molecule 1: Reaction center protein H chain



• 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	140.94Å 140.94Å 186.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.75 – 3.09 39.75 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.75-3.09) 91.3 (39.75-3.09)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 3.06Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.177 , 0.205 0.182 , 0.209	Depositor DCC
R_{free} test set	1992 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	67.8	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7026	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: SPO, CDL, A1ADW, LDA, CL, FE, U10, BPH, 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	0.51	0/1877	0.72	0/2553
2	L	0.51	1/2328 (0.0%)	0.63	0/3186
3	M	0.47	0/2472	0.67	3/3372 (0.1%)
All	All	0.50	1/6677 (0.0%)	0.67	3/9111 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	177	ILE	CG1-CD1	-5.37	1.30	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	267	ARG	N-CA-C	-7.15	102.67	111.40
3	M	257	GLY	CA-C-N	-5.05	113.93	123.27
3	M	257	GLY	C-N-CA	-5.05	113.93	123.27

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	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	2240	0	2190	48	0
3	M	2396	0	2301	56	0
4	L	120	0	129	13	0
5	L	132	0	148	9	0
5	M	117	0	115	9	0
6	L	18	0	15	0	0
7	L	1	0	0	0	0
8	M	48	0	93	2	0
9	M	1	0	0	0	0
10	M	42	0	60	4	0
11	M	69	0	82	3	0
12	H	2	0	0	1	0
12	L	8	0	0	0	0
12	M	3	0	0	2	0
All	All	7026	0	6969	147	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 11.

All (147) 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:75:TRP:HE1	10:M:406:SPO:HM12	1.23	1.04
2:L:187:LEU:HD13	3:M:216:PHE:HB2	1.61	0.83
2:L:272:TRP:HA	2:L:275:ILE:HD12	1.60	0.82
5:L:302:BCL:HBB3	5:L:305:BCL:H52	1.61	0.82
1:H:81:GLU:OE1	2:L:8:LYS:NZ	2.13	0.80
3:M:21:THR:HG23	3:M:26:LEU:HD11	1.66	0.78
1:H:94:GLU:OE1	12:H:301:HOH:O	2.01	0.78
4:L:303:BPH:HBB3	4:L:303:BPH:HHC	1.68	0.75
1:H:135:LYS:HE3	1:H:166:ASP:OD2	1.87	0.73
1:H:249:LYS:HD3	1:H:250:SER:H	1.52	0.71
3:M:300:ASN:ND2	12:M:501:HOH:O	2.21	0.70
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.72	0.70
5:L:302:BCL:HBB2	5:L:302:BCL:HHC	1.76	0.68
3:M:267:ARG:NH1	12:M:502:HOH:O	2.27	0.66
3:M:234:GLU:O	3:M:238:ILE:HG13	1.95	0.65
2:L:133:LEU:HD23	2:L:134:PHE:CE1	2.32	0.65
1:H:148:PRO:HD2	1:H:167:ILE:HD11	1.78	0.65
3:M:197:PHE:HZ	5:M:401:BCL:HBB2	1.61	0.64
2:L:1:ALA:O	3:M:253:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:32:GLN:HG2	1:H:56:PHE:CE1	2.33	0.64
1:H:191:LEU:HD11	1:H:213:PHE:HE2	1.64	0.62
3:M:238:ILE:HD13	3:M:263:GLU:HB2	1.82	0.62
2:L:13:GLY:O	2:L:110:LYS:HE2	2.00	0.62
3:M:157:TRP:CE3	3:M:158:MET:HG2	2.35	0.62
1:H:119:ASP:OD2	1:H:220:LYS:NZ	2.29	0.62
11:M:407:CDL:HB4	11:M:407:CDL:HA62	1.81	0.62
2:L:219:LEU:O	3:M:132:ARG:NH2	2.32	0.61
1:H:181:VAL:HG21	1:H:191:LEU:HD12	1.83	0.60
3:M:197:PHE:CZ	5:M:401:BCL:HBB2	2.37	0.59
2:L:181:PHE:HB3	4:L:301:BPH:HBB2	1.85	0.59
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.85	0.58
1:H:103:ASP:HB3	1:H:106:LYS:HB2	1.84	0.58
3:M:75:TRP:NE1	10:M:406:SPO:HM12	2.07	0.58
4:L:301:BPH:H5C1	3:M:63:GLY:HA3	1.86	0.57
3:M:243:THR:O	3:M:247:ARG:HG3	2.03	0.57
4:L:303:BPH:ND	3:M:214:LEU:HD13	2.20	0.57
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.87	0.56
11:M:407:CDL:HB32	11:M:407:CDL:HA21	1.87	0.56
5:M:401:BCL:H41	5:M:408:BCL:HBB3	1.88	0.56
3:M:285:LEU:O	3:M:289:THR:OG1	2.22	0.56
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.88	0.56
1:H:153:VAL:HG21	1:H:181:VAL:HG22	1.88	0.56
5:M:408:BCL:HHC	5:M:408:BCL:HBB2	1.88	0.55
1:H:165:VAL:HG11	1:H:182:GLU:HB2	1.88	0.55
1:H:221:SER:HB3	1:H:224:GLU:HG2	1.89	0.54
3:M:252:VAL:HG12	3:M:258:PHE:O	2.06	0.54
2:L:42:ALA:O	2:L:46:ILE:HG12	2.08	0.54
4:L:301:BPH:H6C1	5:M:401:BCL:H192	1.90	0.53
2:L:3:LEU:HB2	2:L:6:GLU:HB2	1.90	0.53
3:M:120:PHE:O	3:M:124:VAL:HG23	2.08	0.53
2:L:269:LEU:HB2	2:L:272:TRP:NE1	2.24	0.53
2:L:207:ARG:HG3	3:M:142:MET:HG2	1.91	0.52
1:H:33:THR:O	1:H:59:PRO:HG3	2.09	0.52
1:H:18:TYR:O	1:H:22:ILE:HG13	2.08	0.52
3:M:159:VAL:HA	3:M:163:ILE:HB	1.92	0.52
1:H:113:SER:HB3	2:L:8:LYS:HD2	1.92	0.52
3:M:195:ASN:HB3	3:M:198:TYR:CD2	2.45	0.52
3:M:170:SER:HG	3:M:172:SER:HG	1.56	0.51
2:L:46:ILE:HD11	5:L:302:BCL:H191	1.92	0.51
4:L:301:BPH:HHC	4:L:301:BPH:HBB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:38:GLU:OE1	3:M:241:ARG:NH1	2.38	0.51
1:H:118:ARG:NH2	3:M:236:GLU:OE2	2.44	0.50
2:L:197:ALA:HB1	3:M:235:LEU:HD11	1.93	0.50
2:L:201:GLU:HB2	2:L:204:LYS:HG3	1.93	0.50
3:M:293:ASN:HB3	3:M:296:VAL:HB	1.92	0.50
5:L:305:BCL:OBB	5:L:305:BCL:HHC	2.12	0.49
3:M:290:VAL:HG12	3:M:291:VAL:HG23	1.95	0.49
1:H:165:VAL:CG1	1:H:182:GLU:HB2	2.43	0.49
1:H:111:PRO:HB2	1:H:239:GLY:HA2	1.95	0.49
2:L:272:TRP:HA	2:L:275:ILE:CD1	2.37	0.49
3:M:270:ILE:O	3:M:274:VAL:HG13	2.13	0.48
1:H:249:LYS:HA	1:H:249:LYS:HE2	1.95	0.48
2:L:170:ASN:HB3	2:L:173:HIS:HB2	1.95	0.48
1:H:75:VAL:HA	1:H:76:PRO:C	2.39	0.48
3:M:155:TRP:O	3:M:159:VAL:HG23	2.13	0.47
1:H:211:ASP:OD2	1:H:247:LYS:NZ	2.47	0.47
4:L:301:BPH:HBB3	4:L:301:BPH:CHC	2.45	0.47
5:L:302:BCL:HHC	5:L:302:BCL:CBB	2.43	0.47
2:L:83:GLY:O	2:L:87:GLN:HG3	2.15	0.47
1:H:220:LYS:HE3	1:H:229:GLU:OE2	2.15	0.47
2:L:60:ASN:O	2:L:64:ILE:HG13	2.15	0.47
4:L:301:BPH:HBC3	4:L:301:BPH:HHD	1.97	0.47
2:L:22:PHE:HA	2:L:24:PHE:CE2	2.50	0.47
3:M:66:TRP:HD1	3:M:118:ALA:O	1.99	0.46
3:M:114:LEU:HA	3:M:114:LEU:HD12	1.67	0.46
3:M:228:ARG:HG3	3:M:229:PHE:CE2	2.51	0.46
3:M:94:LEU:HD11	3:M:114:LEU:HB3	1.97	0.46
1:H:195:MET:HB3	1:H:195:MET:HE3	1.74	0.46
2:L:168:HIS:HB3	3:M:183:LEU:HD13	1.97	0.46
4:L:301:BPH:H4C1	3:M:60:LEU:HD12	1.98	0.45
2:L:127:ALA:CB	5:L:305:BCL:H43	2.46	0.45
11:M:407:CDL:H312	11:M:407:CDL:H511	1.99	0.45
3:M:152:SER:O	3:M:155:TRP:HB3	2.17	0.45
1:H:108:GLY:O	1:H:113:SER:HA	2.16	0.45
8:M:403:LDA:H21	8:M:403:LDA:HM11	1.57	0.45
5:M:408:BCL:HHC	5:M:408:BCL:CBB	2.47	0.44
3:M:73:TRP:NE1	3:M:77:GLN:HE21	2.16	0.44
3:M:271:TRP:HA	3:M:274:VAL:HG22	2.00	0.44
1:H:227:LEU:HA	1:H:227:LEU:HD23	1.74	0.44
2:L:133:LEU:HD23	2:L:134:PHE:CD1	2.52	0.44
2:L:127:ALA:HB3	5:L:305:BCL:H43	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:272:TRP:C	2:L:274:ASN:H	2.25	0.44
3:M:164:ARG:NH2	3:M:168:MET:HE2	2.32	0.44
10:M:406:SPO:H243	5:M:408:BCL:CBB	2.48	0.44
2:L:21:LEU:HD23	2:L:22:PHE:CE2	2.53	0.44
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.99	0.44
5:L:305:BCL:H193	5:L:305:BCL:H162	1.70	0.43
2:L:211:HIS:CE1	3:M:20:MET:HE2	2.53	0.43
3:M:234:GLU:OE1	3:M:266:HIS:CE1	2.71	0.43
5:M:401:BCL:HBB2	5:M:401:BCL:HHC	1.99	0.43
1:H:153:VAL:HG21	1:H:181:VAL:CG2	2.48	0.43
2:L:31:VAL:HG12	2:L:32:GLY:N	2.34	0.43
1:H:164:VAL:HG11	1:H:179:LEU:HD22	2.00	0.43
2:L:128:TYR:HD1	5:L:302:BCL:HBB1	1.83	0.43
3:M:51:TYR:C	3:M:51:TYR:CD1	2.96	0.43
2:L:181:PHE:HB3	4:L:301:BPH:CBB	2.48	0.43
10:M:406:SPO:H243	5:M:408:BCL:HBB2	2.01	0.43
2:L:60:ASN:HB3	2:L:63:LEU:HD12	2.00	0.42
1:H:83:ARG:NH1	1:H:114:TRP:O	2.50	0.42
1:H:28:ILE:HD11	8:M:402:LDA:H102	2.02	0.42
2:L:187:LEU:HD13	3:M:216:PHE:CB	2.39	0.42
3:M:218:MET:HE3	3:M:218:MET:HB3	1.72	0.42
2:L:269:LEU:HD23	2:L:269:LEU:HA	1.79	0.42
2:L:201:GLU:HG3	3:M:141:GLY:HA2	2.01	0.42
1:H:79:GLU:OE1	2:L:4:SER:OG	2.27	0.41
2:L:210:ASP:OD1	2:L:210:ASP:N	2.53	0.41
3:M:222:THR:O	3:M:226:VAL:HG22	2.19	0.41
1:H:130:LYS:HZ1	1:H:173:GLU:HG3	1.86	0.41
3:M:28:ASN:O	3:M:51:TYR:HA	2.20	0.41
2:L:173:HIS:O	2:L:177:ILE:HG12	2.21	0.41
1:H:129:ASN:ND2	1:H:224:GLU:HB2	2.35	0.41
2:L:181:PHE:CD2	4:L:301:BPH:HBB1	2.54	0.41
2:L:219:LEU:HD21	3:M:133:THR:HG22	2.01	0.41
3:M:236:GLU:O	3:M:236:GLU:HG3	2.21	0.41
1:H:24:LEU:O	1:H:28:ILE:HG12	2.20	0.41
2:L:48:LEU:N	2:L:48:LEU:HD23	2.36	0.41
2:L:197:ALA:CB	3:M:235:LEU:HD11	2.51	0.41
4:L:303:BPH:H121	4:L:303:BPH:H8	1.89	0.41
2:L:80:LEU:HD13	2:L:85:LEU:HD21	2.03	0.40
2:L:127:ALA:O	2:L:130:THR:HB	2.21	0.40
2:L:214:THR:HG21	3:M:140:LEU:HD21	2.04	0.40
2:L:272:TRP:O	2:L:274:ASN:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:303:BPH:HHC	4:L:303:BPH:CBB	2.46	0.40
1:H:226:THR:OG1	1:H:229:GLU:HG3	2.21	0.40
2:L:216:PHE:HD1	2:L:216:PHE:HA	1.74	0.40
3:M:101:TYR:CE2	3:M:107:ALA:HA	2.57	0.40
3:M:278:LEU:O	3:M:282:ILE:HG13	2.22	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%)	229 (96%)	9 (4%)	0	100	100
2	L	280/281 (100%)	268 (96%)	11 (4%)	1 (0%)	30	61
3	M	296/301 (98%)	284 (96%)	12 (4%)	0	100	100
All	All	814/822 (99%)	781 (96%)	32 (4%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	273	ALA

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%)	195 (100%)	0	100	100
2	L	221/220 (100%)	221 (100%)	0	100	100
3	M	235/235 (100%)	234 (100%)	1 (0%)	84	86
All	All	651/650 (100%)	650 (100%)	1 (0%)	87	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	182	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	52	ASN
2	L	280	ASN
3	M	188	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	A1ADW	M	210	3	11,12,13	0.96	1 (9%)	9,15,17	0.34	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	A1ADW	M	210	3	-	1/5/6/8	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	A1ADW	O1-C3	2.98	1.31	1.20

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	210	A1ADW	C2-C5-C6-C7

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 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	$\# Z > 2$
5	BCL	L	305	2	69,74,74	1.26	6 (8%)	79,115,115	1.40	11 (13%)
4	BPH	L	301	-	49,60,70	1.34	6 (12%)	47,89,101	2.45	10 (21%)
8	LDA	M	402	-	13,15,15	2.09	2 (15%)	14,17,17	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BCL	M	408	3	54,59,74	1.67	11 (20%)	61,97,115	1.87	14 (22%)
8	LDA	M	403	-	13,15,15	2.14	2 (15%)	14,17,17	0.31	0
8	LDA	M	404	-	13,15,15	2.14	2 (15%)	14,17,17	0.53	0
5	BCL	L	302	2	69,74,74	1.42	10 (14%)	79,115,115	1.41	12 (15%)
11	CDL	M	407	-	68,68,99	1.10	6 (8%)	74,80,111	1.05	4 (5%)
5	BCL	M	401	3	69,74,74	1.27	5 (7%)	79,115,115	1.43	9 (11%)
6	U10	L	304	-	18,18,63	2.68	8 (44%)	24,25,79	2.19	8 (33%)
10	SPO	M	406	-	41,41,41	0.39	0	47,50,50	0.61	0
4	BPH	L	303	-	59,70,70	1.42	7 (11%)	59,101,101	2.35	12 (20%)

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	305	2	-	6/41/137/137	-
4	BPH	L	301	-	-	2/25/93/105	0/5/6/6
8	LDA	M	402	-	-	6/13/13/13	-
5	BCL	M	408	3	-	2/23/119/137	-
8	LDA	M	403	-	-	5/13/13/13	-
8	LDA	M	404	-	-	4/13/13/13	-
5	BCL	L	302	2	-	3/41/137/137	-
11	CDL	M	407	-	1/1/9/9	42/79/79/110	-
5	BCL	M	401	3	-	4/41/137/137	-
6	U10	L	304	-	-	4/9/33/87	0/1/1/1
10	SPO	M	406	-	-	7/47/47/47	-
4	BPH	L	303	-	-	4/37/105/105	0/5/6/6

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	402	LDA	O1-N1	-6.48	1.26	1.42
8	M	404	LDA	O1-N1	-6.44	1.26	1.42
6	L	304	U10	C8-C9	6.16	1.50	1.32
8	M	403	LDA	O1-N1	-6.11	1.27	1.42
4	L	303	BPH	CBD-CGD	-6.00	1.44	1.52
5	L	305	BCL	MG-NA	5.72	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	401	BCL	MG-NA	5.61	2.19	2.06
5	L	302	BCL	MG-NA	5.11	2.18	2.06
6	L	304	U10	O4-C4	-4.73	1.25	1.36
4	L	303	BPH	C3D-CAD	-4.66	1.38	1.47
8	M	403	LDA	C1-N1	-4.43	1.46	1.51
5	M	408	BCL	MG-NA	4.43	2.16	2.06
5	L	302	BCL	MG-NC	4.32	2.16	2.06
5	L	305	BCL	MG-NC	4.26	2.16	2.06
8	M	404	LDA	C1-N1	-4.13	1.47	1.51
5	M	408	BCL	OBD-CAD	4.13	1.29	1.22
6	L	304	U10	C6-C1	4.09	1.42	1.35
5	M	408	BCL	MG-NC	3.99	2.15	2.06
6	L	304	U10	O3-C3	-3.85	1.27	1.36
4	L	301	BPH	C4D-CHA	3.85	1.45	1.39
5	M	401	BCL	MG-NC	3.82	2.15	2.06
5	M	408	BCL	C1-C2	3.69	1.59	1.49
8	M	402	LDA	C1-N1	-3.61	1.47	1.51
4	L	301	BPH	CBD-CGD	-3.60	1.48	1.52
5	M	408	BCL	O1A-CGA	-3.46	1.12	1.22
4	L	301	BPH	C3D-CAD	-3.24	1.41	1.47
5	L	302	BCL	CHD-C1D	3.05	1.44	1.38
5	M	408	BCL	C3B-C4B	3.02	1.47	1.41
11	M	407	CDL	PA1-OA4	-3.01	1.41	1.55
11	M	407	CDL	PB2-OB5	2.97	1.71	1.59
11	M	407	CDL	PA1-OA5	2.81	1.70	1.59
5	M	408	BCL	O2A-CGA	2.78	1.41	1.33
5	M	408	BCL	CHD-C1D	2.77	1.43	1.38
11	M	407	CDL	PB2-OB4	-2.76	1.42	1.55
6	L	304	U10	C3-C2	-2.73	1.41	1.48
5	L	305	BCL	C3B-C4B	2.73	1.46	1.41
5	L	302	BCL	O1A-CGA	-2.72	1.14	1.22
5	L	302	BCL	C3B-C4B	2.71	1.46	1.41
4	L	303	BPH	C1B-C2B	2.70	1.42	1.39
5	L	302	BCL	OBD-CAD	2.67	1.27	1.22
11	M	407	CDL	PB2-OB3	-2.63	1.41	1.50
5	L	302	BCL	C1D-ND	2.60	1.41	1.37
5	M	401	BCL	C3B-C4B	2.57	1.46	1.41
6	L	304	U10	C7-C8	2.57	1.54	1.50
5	L	302	BCL	MG-NB	2.52	2.10	2.05
4	L	301	BPH	CHA-CBD	2.48	1.54	1.51
4	L	301	BPH	C1D-C2D	2.45	1.42	1.39
5	L	305	BCL	C5-C3	2.44	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	301	BPH	C3B-CAB	-2.42	1.42	1.49
6	L	304	U10	C4-C3	2.41	1.45	1.36
5	M	408	BCL	C1D-ND	2.40	1.41	1.37
6	L	304	U10	C7-C6	2.36	1.55	1.51
4	L	303	BPH	C3B-C4B	2.33	1.45	1.41
4	L	303	BPH	C4D-CHA	2.32	1.43	1.39
5	M	408	BCL	C1B-NB	2.24	1.40	1.37
5	M	408	BCL	O2A-C1	2.17	1.52	1.46
5	L	302	BCL	C1-C2	2.15	1.55	1.49
5	M	401	BCL	C1D-ND	2.13	1.40	1.37
4	L	303	BPH	C1A-C2A	2.09	1.54	1.51
4	L	303	BPH	C1C-C2C	-2.08	1.47	1.51
5	L	305	BCL	C1D-C2D	-2.07	1.41	1.45
5	L	302	BCL	C1B-NB	2.05	1.40	1.37
5	M	401	BCL	CHD-C1D	2.04	1.42	1.38
5	L	305	BCL	C1B-NB	2.02	1.40	1.37
11	M	407	CDL	CA3-CA4	2.01	1.57	1.50

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	303	BPH	C4D-CHA-CBD	-13.81	101.83	108.45
4	L	301	BPH	C4D-CHA-CBD	-12.54	102.44	108.45
6	L	304	U10	C6-C1-C2	6.69	124.45	119.17
5	M	401	BCL	C4D-CHA-C1A	5.23	127.48	121.24
5	M	408	BCL	C1-C2-C3	4.92	134.73	126.76
4	L	301	BPH	C1-C2-C3	-4.87	118.22	126.20
4	L	303	BPH	C11-C10-C8	-4.75	100.19	115.97
5	M	408	BCL	C4D-CHA-C1A	4.64	126.78	121.24
5	L	302	BCL	C1D-ND-C4D	-4.57	103.11	106.31
5	L	302	BCL	C4D-CHA-C1A	4.32	126.40	121.24
4	L	303	BPH	C4D-ND-C1D	-4.05	104.02	108.87
5	L	305	BCL	C16-C15-C13	-4.04	102.54	115.97
5	M	408	BCL	C1D-ND-C4D	-4.00	103.51	106.31
5	L	302	BCL	CHD-C1D-ND	-3.90	119.31	124.80
5	L	305	BCL	C4D-CHA-C1A	3.80	125.78	121.24
5	M	408	BCL	CBA-CAA-C2A	3.79	125.07	113.79
5	M	401	BCL	C1D-ND-C4D	-3.71	103.71	106.31
6	L	304	U10	C1-C6-C5	-3.69	116.03	119.62
5	L	305	BCL	C1D-ND-C4D	-3.69	103.72	106.31
4	L	301	BPH	C4D-ND-C1D	-3.64	104.51	108.87
5	M	401	BCL	CHD-C1D-ND	-3.64	119.67	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	408	BCL	CHD-C1D-ND	-3.60	119.74	124.80
5	M	401	BCL	C1-C2-C3	-3.50	120.45	126.20
5	M	408	BCL	O2A-CGA-O1A	-3.48	114.93	123.63
5	M	401	BCL	CHA-C1A-NA	-3.40	118.69	126.39
5	M	408	BCL	O2A-CGA-CBA	3.32	121.94	111.83
5	M	408	BCL	C1-O2A-CGA	3.29	124.61	116.65
4	L	301	BPH	OBD-CAD-CBD	-3.27	121.02	125.82
6	L	304	U10	C1M-C1-C6	-3.24	119.13	124.45
5	L	302	BCL	O2D-CGD-CBD	3.23	116.89	111.23
5	L	305	BCL	CHA-C1A-NA	-3.21	119.13	126.39
5	L	305	BCL	C2A-C1A-CHA	3.18	129.38	123.87
4	L	301	BPH	C3D-C4D-ND	3.11	111.69	107.71
5	L	305	BCL	CHD-C1D-ND	-3.07	120.48	124.80
5	M	408	BCL	CAA-C2A-C1A	-3.01	102.10	111.97
6	L	304	U10	C7-C6-C5	3.01	122.01	118.52
5	L	302	BCL	C2A-C1A-CHA	2.98	129.04	123.87
4	L	303	BPH	CMC-C2C-C1C	-2.97	108.22	114.61
5	L	302	BCL	CHA-C1A-NA	-2.96	119.69	126.39
5	L	305	BCL	CAB-C3B-C2B	2.93	133.84	127.74
5	M	408	BCL	CHA-C1A-NA	-2.90	119.83	126.39
4	L	301	BPH	O2D-CGD-CBD	2.86	114.08	110.95
5	M	408	BCL	C5-C3-C4	-2.81	108.11	114.59
11	M	407	CDL	OB4-PB2-OB3	2.80	125.48	112.44
6	L	304	U10	C8-C7-C6	2.73	118.81	112.08
5	M	401	BCL	C2A-C1A-CHA	2.72	128.58	123.87
5	L	305	BCL	C15-C13-C12	-2.71	98.31	112.07
4	L	303	BPH	OBD-CAD-CBD	-2.71	121.85	125.82
5	M	408	BCL	O2D-CGD-O1D	-2.71	118.58	123.85
4	L	303	BPH	OBB-CAB-C3B	2.67	124.45	119.99
6	L	304	U10	C3M-O3-C3	2.65	125.80	116.47
5	M	408	BCL	O2D-CGD-CBD	2.63	115.83	111.23
4	L	303	BPH	C3D-C4D-ND	2.60	111.04	107.71
4	L	301	BPH	C2D-C1D-ND	2.53	111.26	109.43
4	L	303	BPH	C2D-C1D-ND	2.51	111.24	109.43
5	L	305	BCL	C11-C10-C8	-2.50	107.64	115.97
11	M	407	CDL	OA4-PA1-OA3	2.48	123.99	112.44
5	L	305	BCL	CHC-C1C-NC	-2.46	120.84	124.40
4	L	303	BPH	CMA-C3A-C4A	-2.44	109.35	114.61
6	L	304	U10	C4-C3-C2	-2.43	116.24	120.69
5	M	408	BCL	OBB-CAB-CBB	-2.40	114.39	119.77
4	L	301	BPH	CMD-C2D-C3D	2.38	129.44	124.68
4	L	303	BPH	C16-C15-C13	-2.37	108.10	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	401	BCL	C4A-NA-C1A	2.37	107.76	106.68
5	L	305	BCL	O2D-CGD-CBD	2.36	115.36	111.23
11	M	407	CDL	CA4-OA6-CA5	2.30	123.31	117.80
6	L	304	U10	O5-C5-C6	-2.29	117.37	121.79
4	L	301	BPH	OBB-CAB-CBB	-2.28	115.34	120.19
5	L	302	BCL	CED-O2D-CGD	2.26	121.04	115.92
4	L	303	BPH	OBB-CAB-CBB	-2.25	115.39	120.19
5	L	302	BCL	C16-C17-C18	-2.24	105.92	115.94
5	M	401	BCL	C11-C10-C8	-2.22	108.60	115.97
4	L	303	BPH	CMD-C2D-C3D	2.19	129.06	124.68
4	L	301	BPH	CMB-C2B-C3B	2.11	128.91	124.68
5	L	302	BCL	OBB-CAB-CBB	-2.07	115.14	119.77
5	L	302	BCL	C15-C13-C12	-2.06	101.63	112.07
5	M	401	BCL	C11-C12-C13	-2.05	109.15	115.97
5	L	302	BCL	C4A-NA-C1A	2.04	107.61	106.68
5	L	302	BCL	O2D-CGD-O1D	-2.03	119.89	123.85
11	M	407	CDL	OB6-CB5-OB7	-2.03	118.96	123.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	M	407	CDL	CA4

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	305	BCL	C4C-C3C-CAC-CBC
8	M	402	LDA	C2-C1-N1-O1
8	M	402	LDA	C2-C1-N1-CM1
8	M	402	LDA	C2-C1-N1-CM2
8	M	403	LDA	C2-C1-N1-O1
8	M	403	LDA	C2-C1-N1-CM1
8	M	403	LDA	N1-C1-C2-C3
10	M	406	SPO	C5-C6-C7-C8
10	M	406	SPO	C5-C6-C7-C9
11	M	407	CDL	CA2-C1-CB2-OB2
11	M	407	CDL	CA3-OA5-PA1-OA2
11	M	407	CDL	CA3-OA5-PA1-OA3
11	M	407	CDL	CA3-OA5-PA1-OA4
11	M	407	CDL	C11-CA5-OA6-CA4
11	M	407	CDL	CB2-OB2-PB2-OB3
11	M	407	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
11	M	407	CDL	CB2-OB2-PB2-OB5
11	M	407	CDL	CB3-OB5-PB2-OB2
11	M	407	CDL	OA9-CA7-OA8-CA6
11	M	407	CDL	OB9-CB7-OB8-CB6
11	M	407	CDL	OA7-CA5-OA6-CA4
11	M	407	CDL	C31-CA7-OA8-CA6
11	M	407	CDL	C71-CB7-OB8-CB6
6	L	304	U10	C7-C8-C9-C11
5	M	401	BCL	C14-C13-C15-C16
6	L	304	U10	C7-C8-C9-C10
11	M	407	CDL	CA7-C31-C32-C33
11	M	407	CDL	CB2-C1-CA2-OA2
5	L	305	BCL	C13-C15-C16-C17
11	M	407	CDL	O1-C1-CA2-OA2
11	M	407	CDL	CA6-CA4-OA6-CA5
11	M	407	CDL	OB7-CB5-OB6-CB4
11	M	407	CDL	C51-CB5-OB6-CB4
5	M	401	BCL	C16-C17-C18-C20
5	L	305	BCL	C15-C16-C17-C18
8	M	403	LDA	C6-C7-C8-C9
8	M	404	LDA	C2-C3-C4-C5
11	M	407	CDL	C31-C32-C33-C34
4	L	303	BPH	C4-C3-C5-C6
8	M	402	LDA	C1-C2-C3-C4
11	M	407	CDL	C71-C72-C73-C74
8	M	403	LDA	C1-C2-C3-C4
5	M	401	BCL	C16-C17-C18-C19
4	L	303	BPH	C2-C3-C5-C6
5	L	305	BCL	C2C-C3C-CAC-CBC
11	M	407	CDL	CA3-CA4-CA6-OA8
11	M	407	CDL	CB3-CB4-CB6-OB8
11	M	407	CDL	C13-C14-C15-C16
4	L	301	BPH	C2-C3-C5-C6
5	M	408	BCL	O2A-C1-C2-C3
8	M	404	LDA	N1-C1-C2-C3
11	M	407	CDL	C17-C18-C19-C20
4	L	301	BPH	C4-C3-C5-C6
10	M	406	SPO	C34-C33-C35-C36
8	M	402	LDA	C3-C4-C5-C6
11	M	407	CDL	C33-C34-C35-C36
11	M	407	CDL	C51-C52-C53-C54
8	M	404	LDA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
8	M	402	LDA	C7-C8-C9-C10
10	M	406	SPO	C32-C33-C35-C36
11	M	407	CDL	OA6-CA4-CA6-OA8
11	M	407	CDL	C40-C41-C42-C43
11	M	407	CDL	O1-C1-CB2-OB2
8	M	404	LDA	C4-C5-C6-C7
11	M	407	CDL	C75-C76-C77-C78
11	M	407	CDL	OB6-CB4-CB6-OB8
11	M	407	CDL	CA5-C11-C12-C13
11	M	407	CDL	C52-C53-C54-C55
11	M	407	CDL	C74-C75-C76-C77
11	M	407	CDL	C36-C37-C38-C39
6	L	304	U10	C1-C6-C7-C8
10	M	406	SPO	C33-C35-C36-C37
4	L	303	BPH	C16-C17-C18-C20
5	L	302	BCL	C11-C10-C8-C9
11	M	407	CDL	CB5-C51-C52-C53
5	L	302	BCL	C12-C13-C15-C16
11	M	407	CDL	C73-C74-C75-C76
11	M	407	CDL	C14-C15-C16-C17
5	L	302	BCL	C14-C13-C15-C16
4	L	303	BPH	O2A-C1-C2-C3
11	M	407	CDL	C32-C33-C34-C35
5	M	408	BCL	C2A-CAA-CBA-CGA
5	L	305	BCL	C2-C1-O2A-CGA
5	L	305	BCL	C5-C6-C7-C8
10	M	406	SPO	C2-C1-C4-C5
6	L	304	U10	C6-C7-C8-C9
10	M	406	SPO	C28-C30-C31-C32
11	M	407	CDL	C35-C36-C37-C38
5	M	401	BCL	CAA-CBA-CGA-O2A

There are no ring outliers.

10 monomers are involved in 37 short contacts:

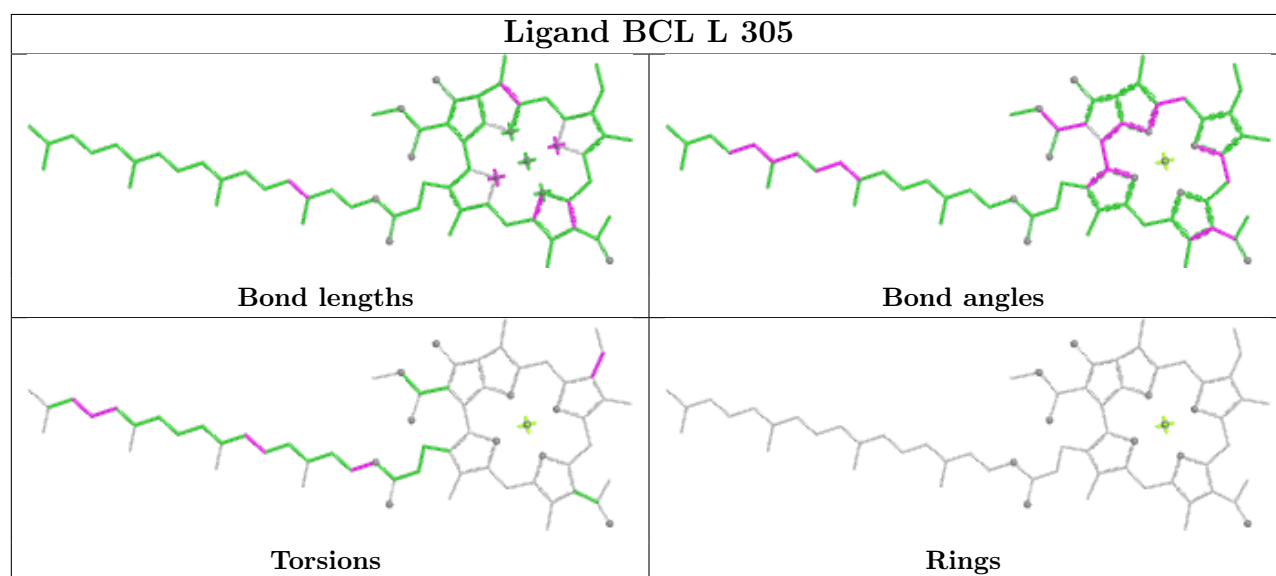
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	305	BCL	5	0
4	L	301	BPH	9	0
8	M	402	LDA	1	0
5	M	408	BCL	5	0
8	M	403	LDA	1	0
5	L	302	BCL	5	0

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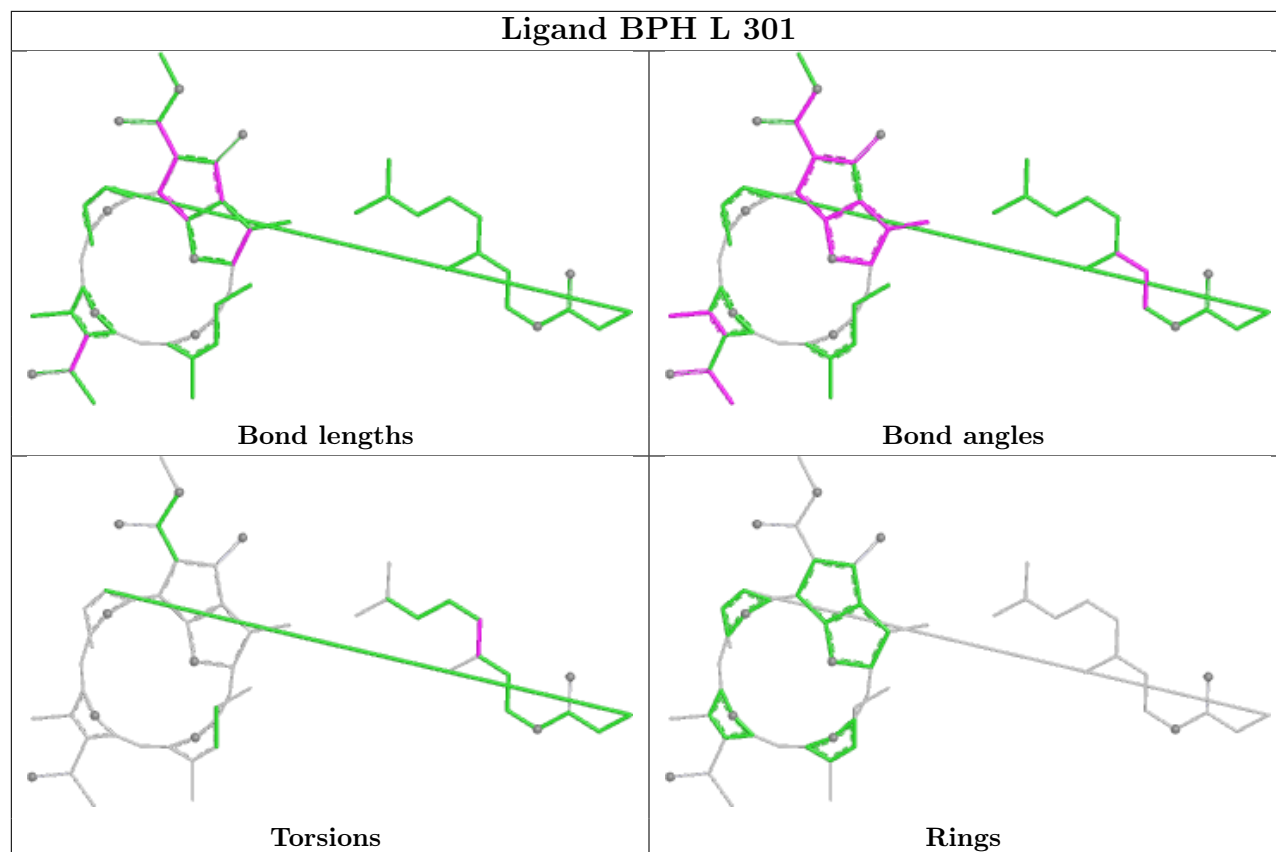
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	407	CDL	3	0
5	M	401	BCL	5	0
10	M	406	SPO	4	0
4	L	303	BPH	4	0

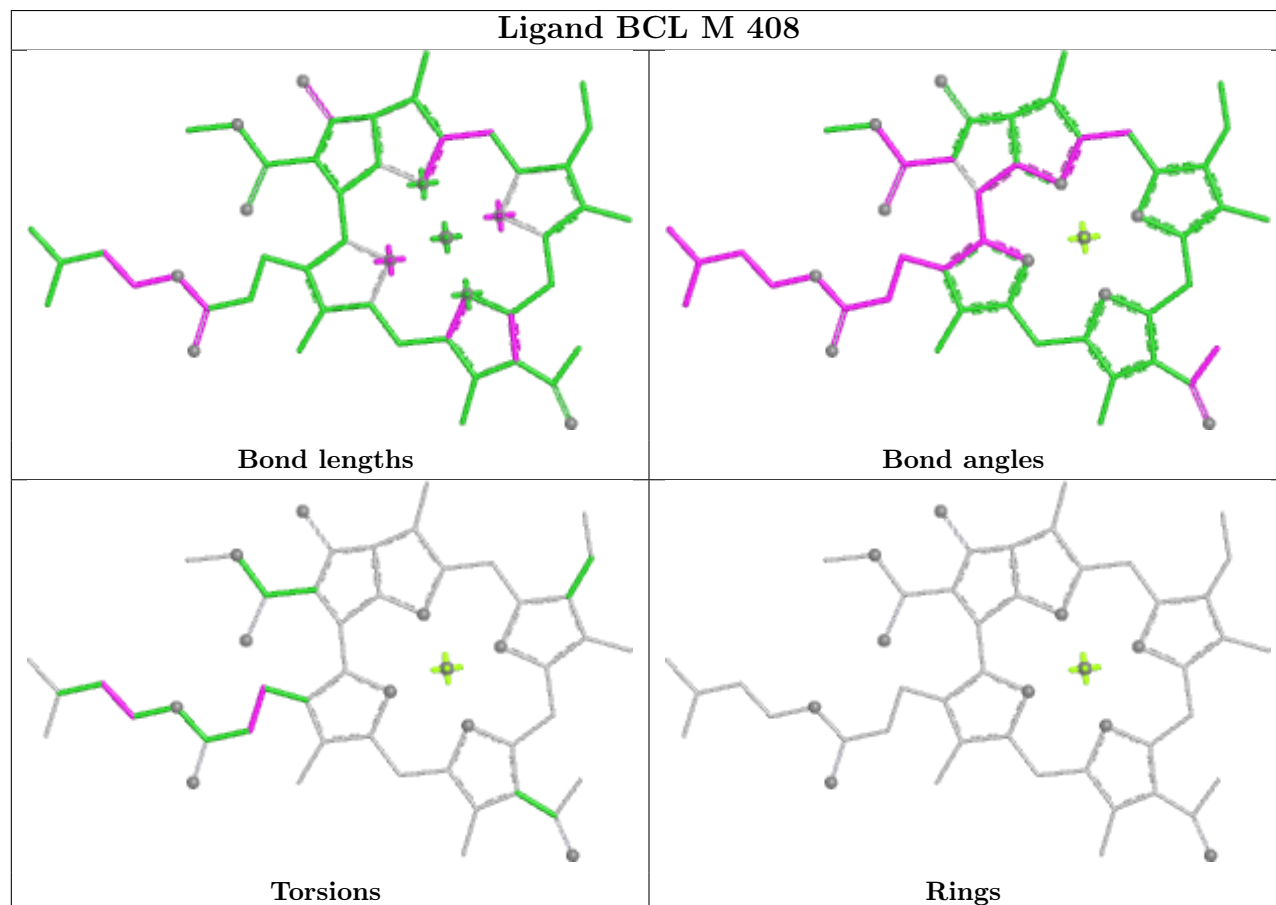
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

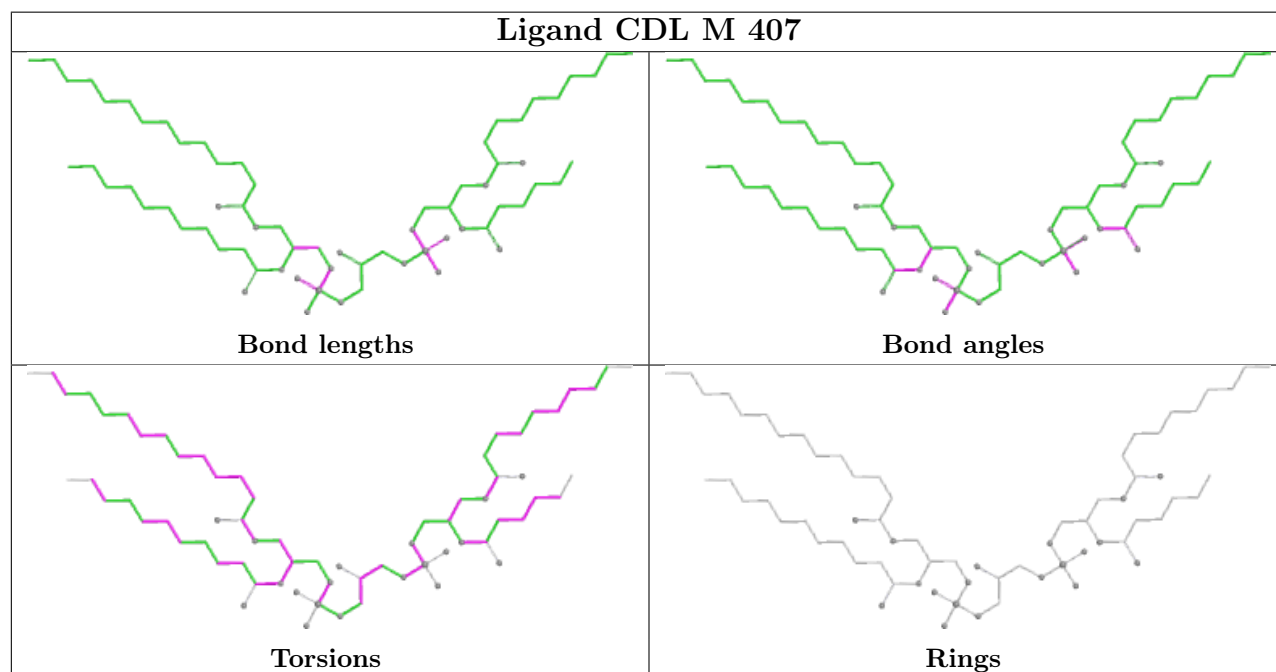
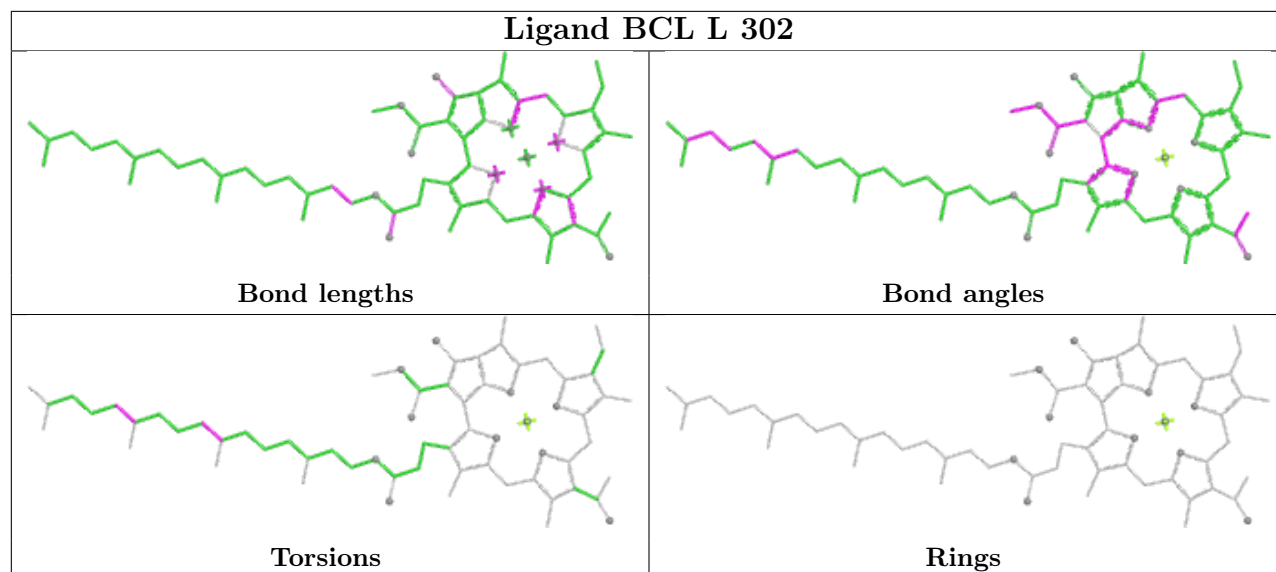


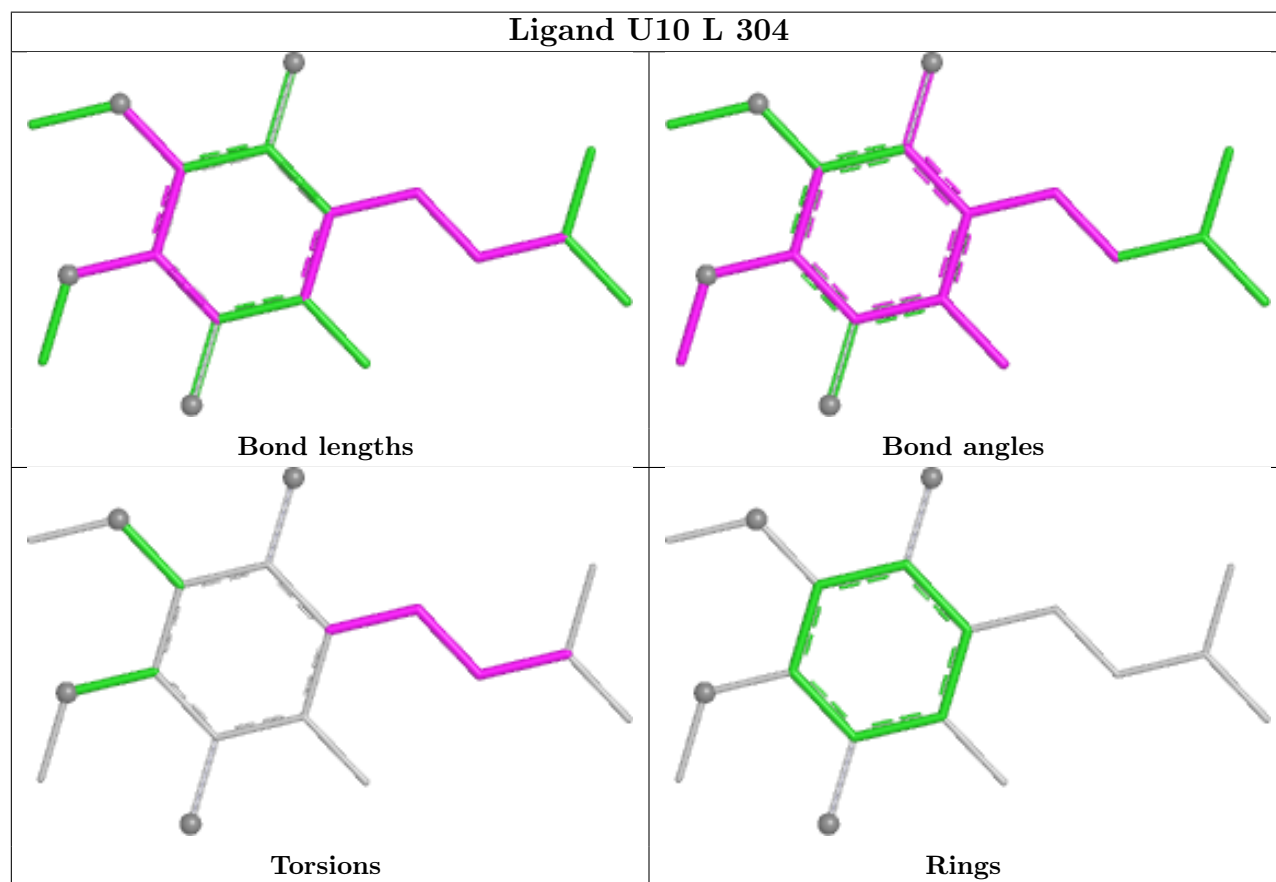
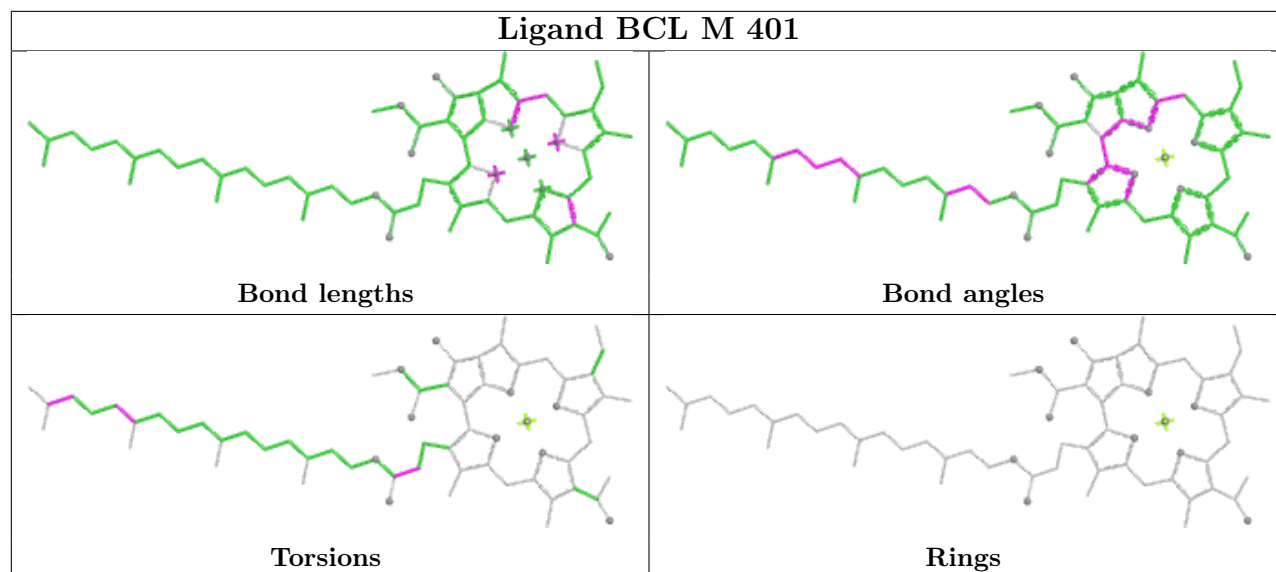
Ligand BPH L 301

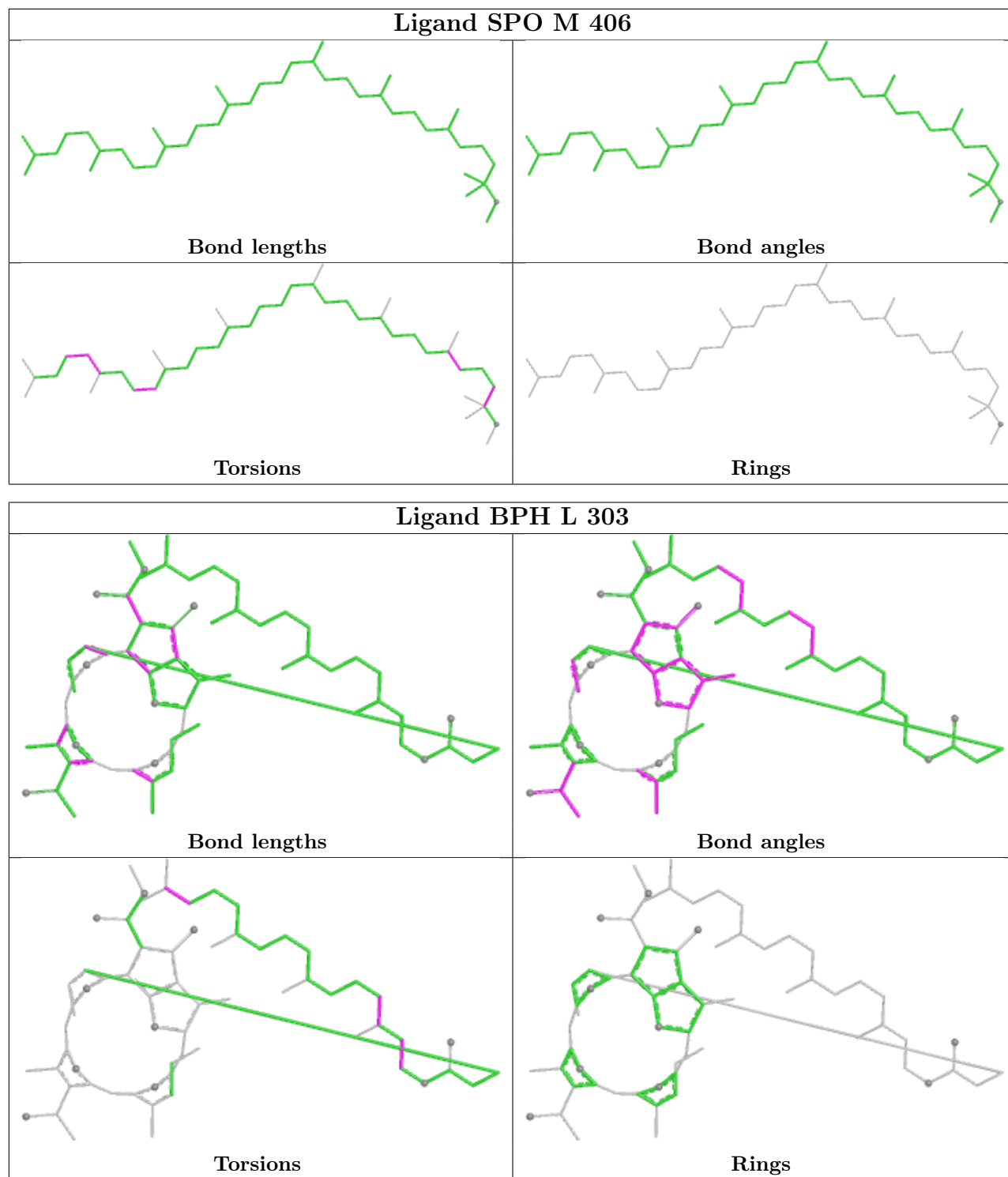


Ligand BCL M 408









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.40	1 (0%) 88 76	50, 64, 93, 138	0
2	L	281/281 (100%)	-0.31	5 (1%) 67 47	40, 59, 94, 128	1 (0%)
3	M	300/301 (99%)	-0.43	2 (0%) 84 68	47, 62, 95, 130	0
All	All	821/822 (99%)	-0.38	8 (0%) 79 61	40, 62, 94, 138	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	72	GLU	5.4
2	L	155[A]	ASP	4.6
2	L	62	GLN	2.8
2	L	77	GLY	2.5
2	L	74	GLY	2.5
1	H	81	GLU	2.5
3	M	2	GLU	2.4
3	M	248	ALA	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	A1ADW	M	210	12/13	0.98	0.07	44,48,50,52	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

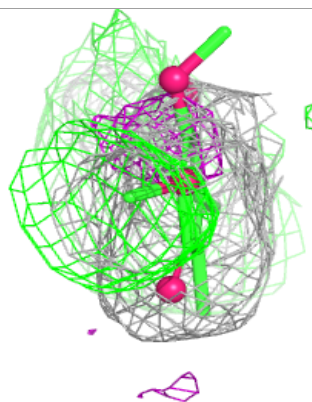
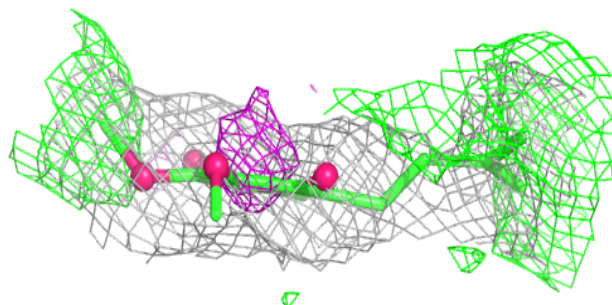
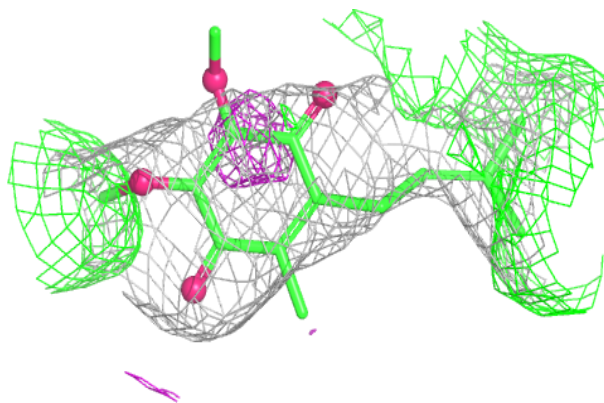
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	U10	L	304	18/63	0.59	0.39	88,116,131,133	0
8	LDA	M	404	16/16	0.81	0.22	60,82,136,136	0
8	LDA	M	403	16/16	0.87	0.20	80,85,98,100	0
11	CDL	M	407	69/100	0.90	0.15	65,84,101,114	0
10	SPO	M	406	42/42	0.92	0.17	51,67,82,87	0
8	LDA	M	402	16/16	0.93	0.19	71,79,98,98	0
7	CL	L	306	1/1	0.95	0.12	97,97,97,97	0
5	BCL	M	408	51/66	0.96	0.09	40,52,65,80	0
4	BPH	L	301	55/65	0.96	0.09	42,55,74,84	0
4	BPH	L	303	65/65	0.97	0.08	38,50,59,65	0
5	BCL	M	401	66/66	0.98	0.09	43,52,69,94	0
5	BCL	L	302	66/66	0.98	0.07	43,51,69,74	0
5	BCL	L	305	66/66	0.98	0.07	43,52,58,64	0
9	FE	M	405	1/1	1.00	0.02	42,42,42,42	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.

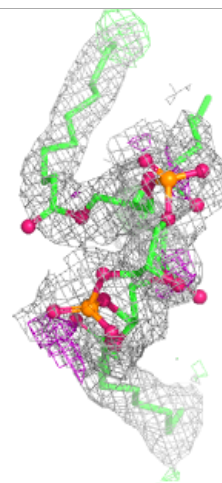
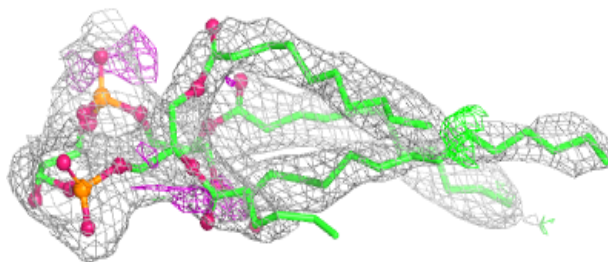
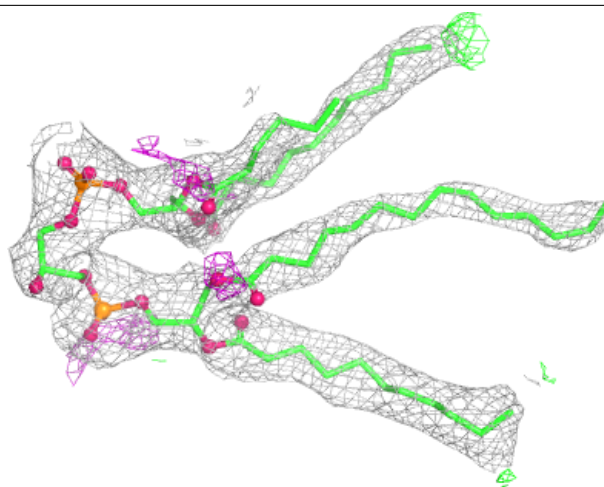
Electron density around U10 L 304:

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



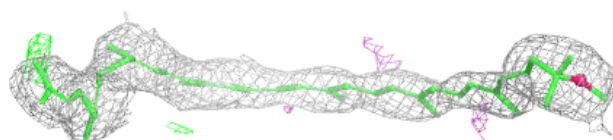
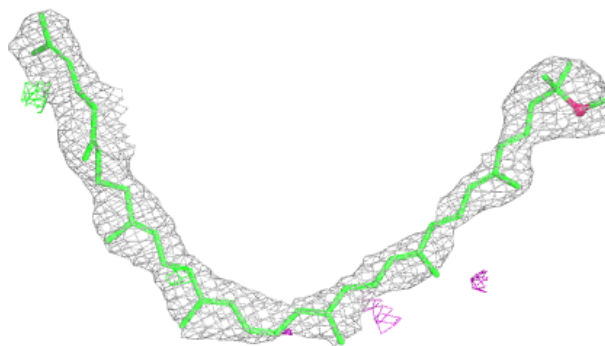
Electron density around CDL M 407:

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



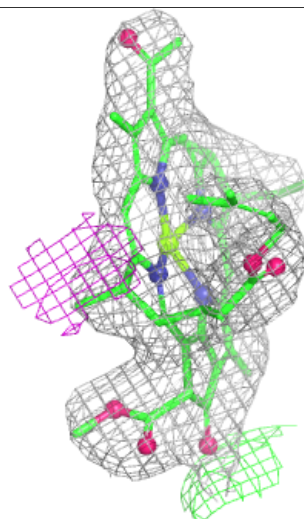
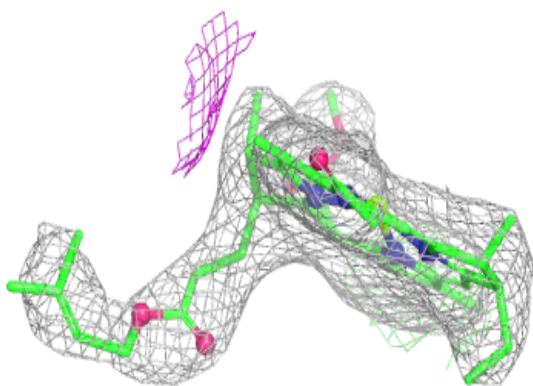
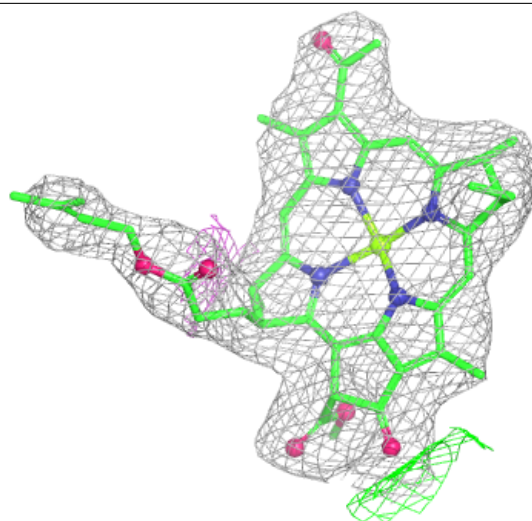
Electron density around SPO M 406:

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



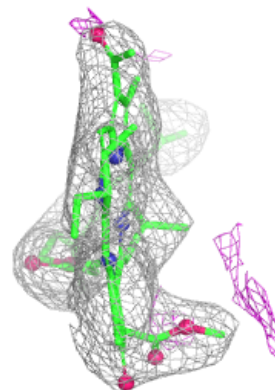
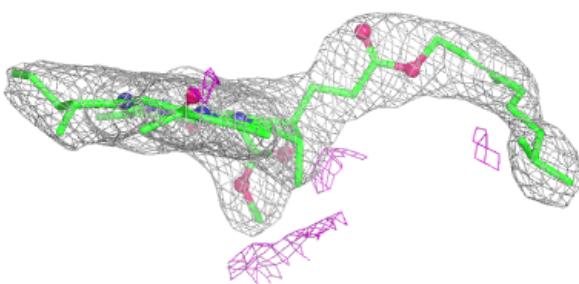
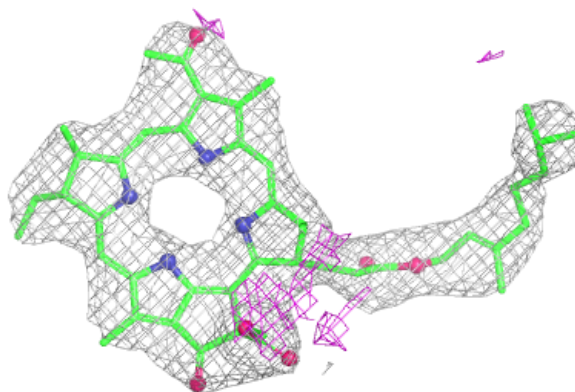
Electron density around BCL M 408:

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



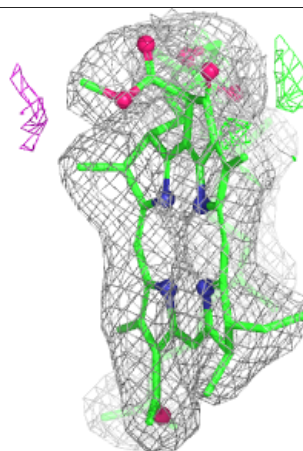
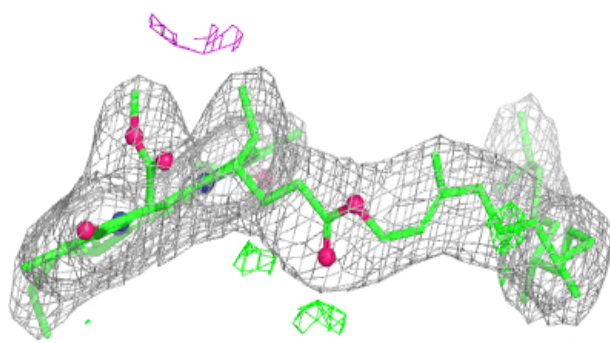
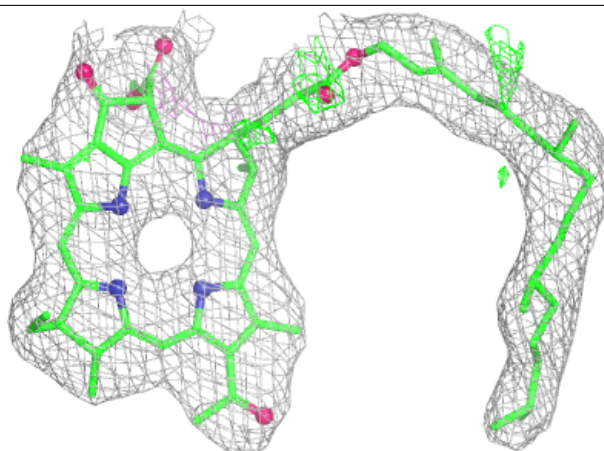
Electron density around BPH L 301:

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



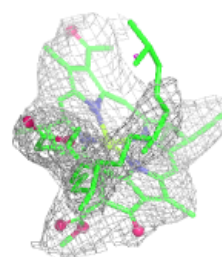
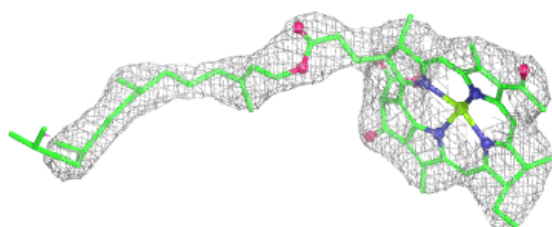
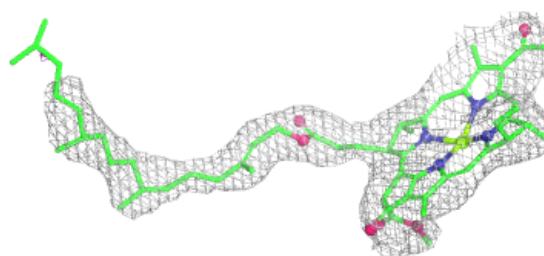
Electron density around BPH L 303:

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

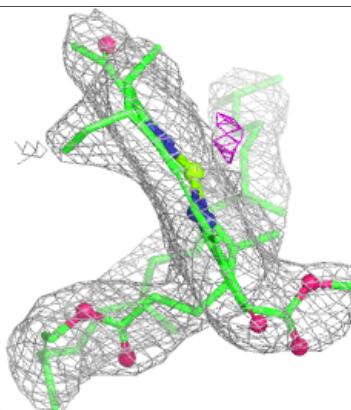
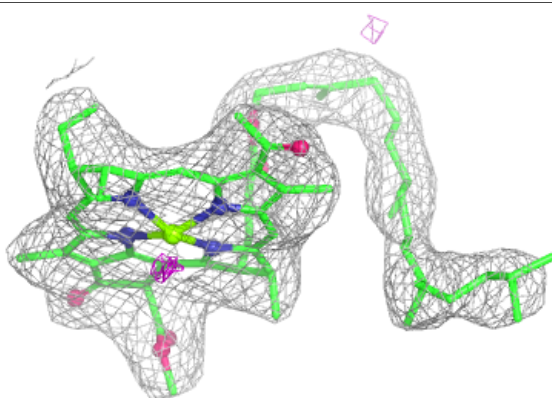
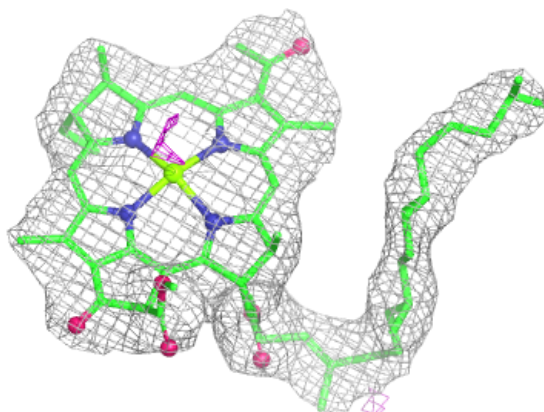


Electron density around BCL M 401:

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

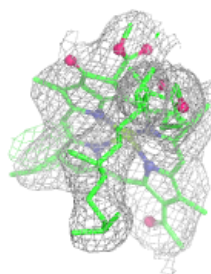
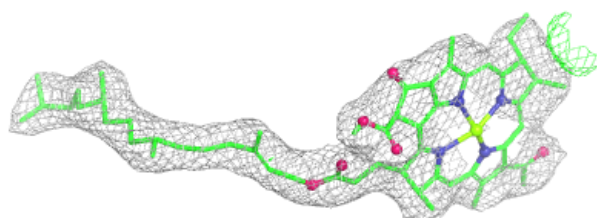
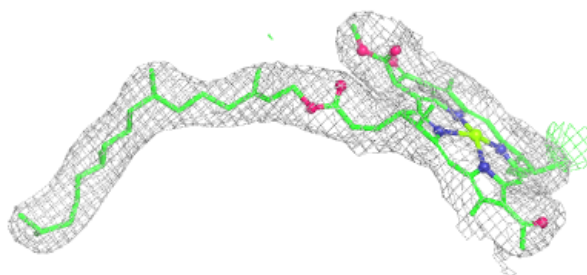
**Electron density around BCL L 302:**

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



Electron density around BCL L 305:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.