



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:44 AM UTC

PDB ID : 7MH5 / pdb_00007mh5
Title : Crystal structure of R. sphaeroides Photosynthetic Reaction Center variant;
Y(M210)3-iodotyrosine
Authors : Mathews, I.; Weaver, J.; Boxer, S.G.
Deposited on : 2021-04-14
Resolution : 2.85 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

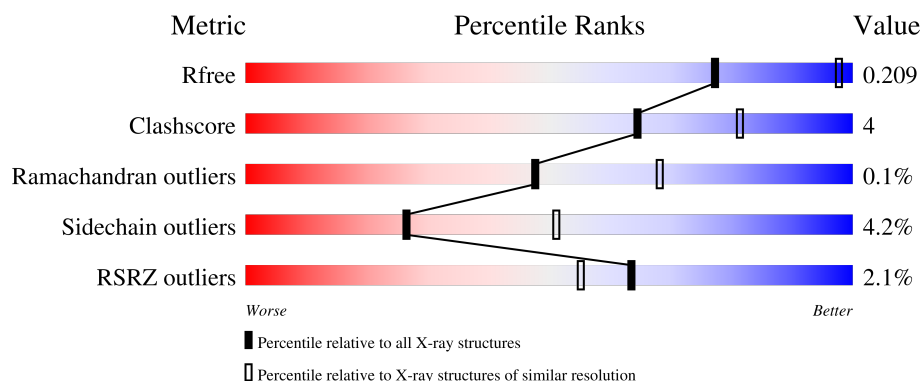
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	266	% 81% 9% 10%
2	L	282	4% 91% 7% .
3	M	308	% 85% 11% ..

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
5	BPH	M	409	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7273 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	239	Total	C	N	O	S	0	2	0
			1844	1180	315	340	9			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	260	VAL	-	expression tag	UNP P0C0Y7
H	261	HIS	-	expression tag	UNP P0C0Y7
H	262	HIS	-	expression tag	UNP P0C0Y7
H	263	HIS	-	expression tag	UNP P0C0Y7
H	264	HIS	-	expression tag	UNP P0C0Y7
H	265	HIS	-	expression tag	UNP P0C0Y7
H	266	HIS	-	expression tag	UNP P0C0Y7

- 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.

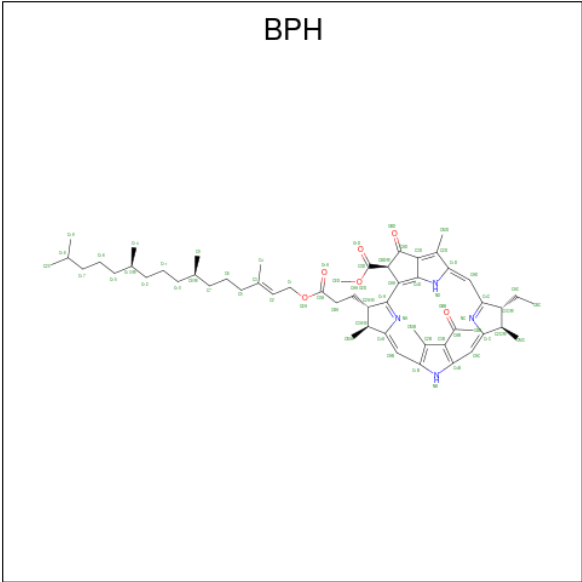
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	M	300	Total	C	I	N	O	S	0	0	0
			2396	1599	2	392	393	10			

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



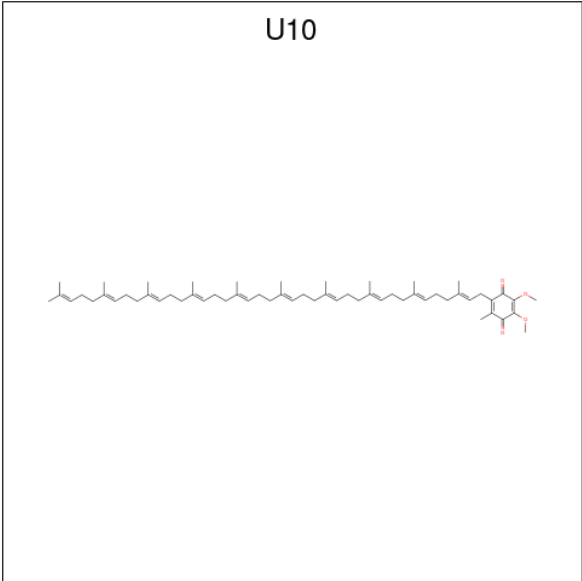
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- 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).



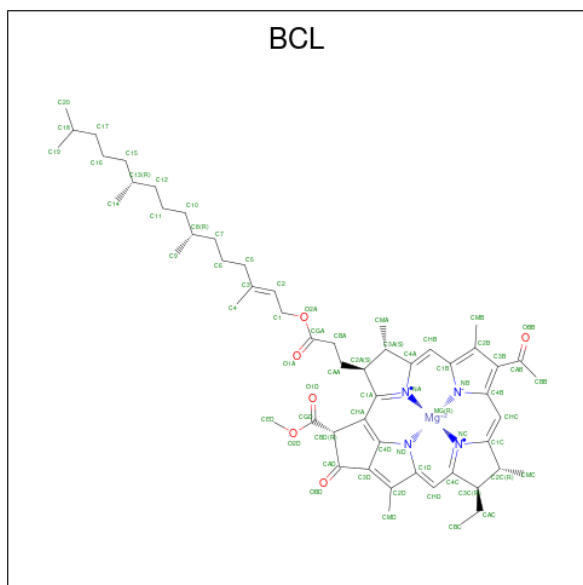
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			18	14	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	C	O	0	0
			38	34	4		

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).

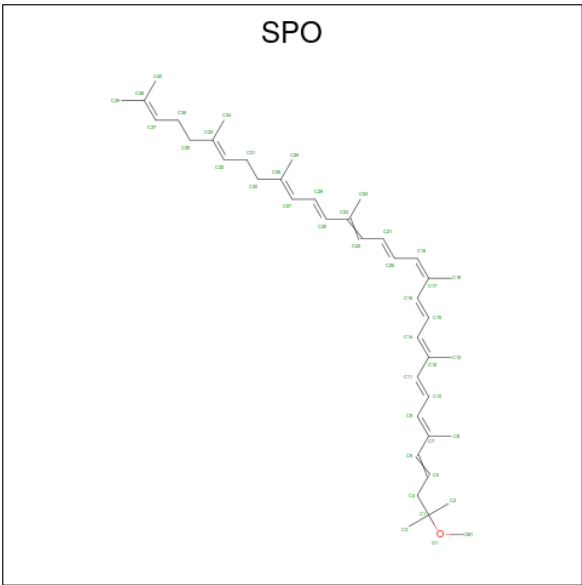


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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

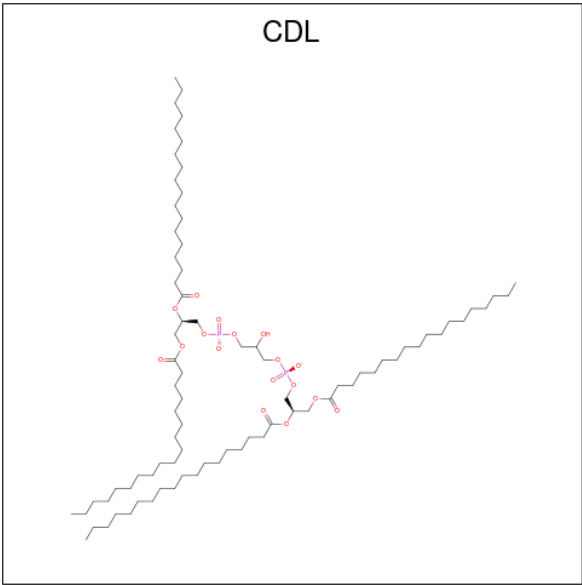
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- 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		

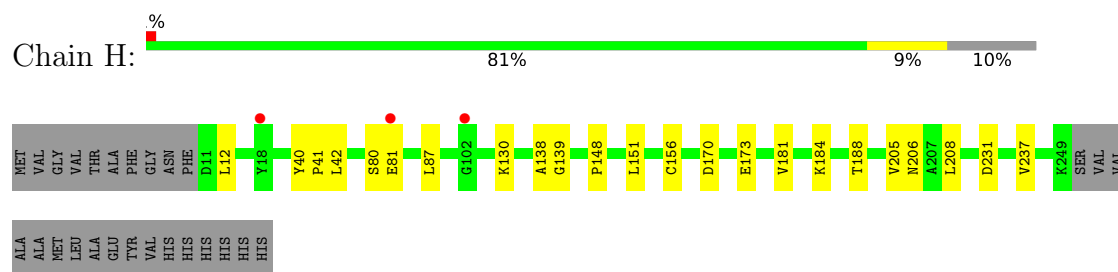
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	82	Total 82	O 82	0	0
11	L	45	Total 45	O 45	0	0
11	M	57	Total 57	O 57	0	0

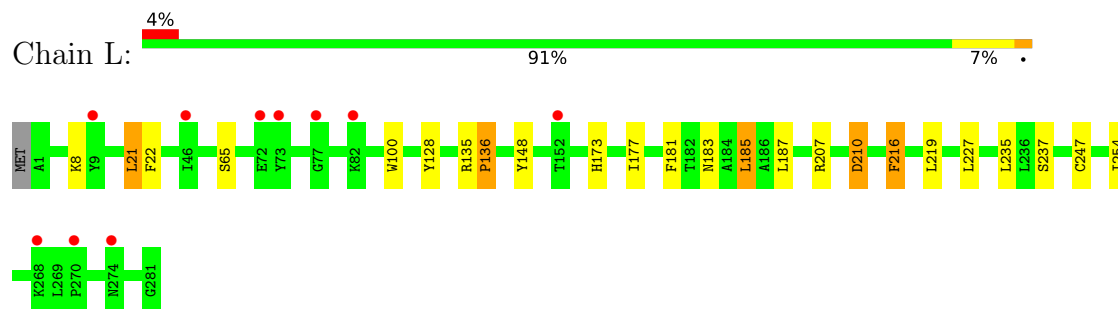
3 Residue-property plots [i](#)

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.

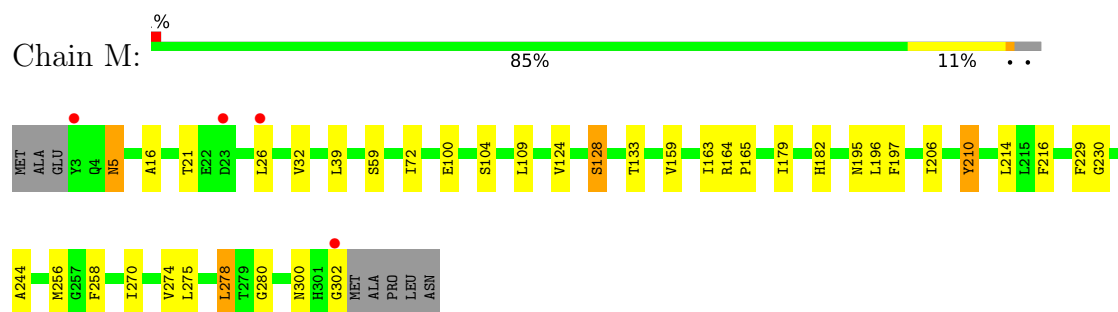
- Molecule 1: Reaction center protein H chain



- 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	141.41Å 141.41Å 186.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.95 – 2.85 38.95 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.95-2.85) 99.9 (38.95-2.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.180 , 0.205 0.187 , 0.209	Depositor DCC
R_{free} test set	2495 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	69.1	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.0	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	7273	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: BPH, BCL, U10, FE, CDL, TYI, 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	1.01	0/1893	1.38	1/2575 (0.0%)
2	L	1.00	0/2320	1.48	0/3175
3	M	0.99	0/2472	1.48	2/3373 (0.1%)
All	All	1.00	0/6685	1.45	3/9123 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	230	GLY	CA-C-N	5.18	125.83	120.03
3	M	230	GLY	C-N-CA	5.18	125.83	120.03
1	H	170	ASP	CA-CB-CG	5.17	117.77	112.60

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	1844	0	1844	10	0
2	L	2232	0	2187	20	0
3	M	2396	0	2304	22	0
4	H	16	0	31	2	0
4	M	64	0	124	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	65	0	76	1	0
5	M	55	0	53	2	0
6	L	18	0	15	2	0
6	M	38	0	47	2	0
7	L	66	0	74	1	0
7	M	183	0	189	14	0
8	M	1	0	0	0	0
9	M	42	0	60	0	0
10	M	69	0	82	0	0
11	H	82	0	0	1	0
11	L	45	0	0	0	0
11	M	57	0	0	0	0
All	All	7273	0	7086	55	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 4.

All (55) 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:210:TYI:I2	7:M:401:BCL:C4D	2.77	1.03
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.43	0.96
3:M:210:TYI:I2	7:M:401:BCL:C1D	2.95	0.79
3:M:197:PHE:HZ	7:M:403:BCL:HBB2	1.59	0.67
3:M:256:MET:HE3	3:M:258:PHE:CZ	2.30	0.65
7:M:402:BCL:HHC	7:M:402:BCL:HBB2	1.76	0.65
5:L:301:BPH:HHC	5:L:301:BPH:HBB3	1.78	0.64
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.77	0.64
3:M:197:PHE:CZ	7:M:403:BCL:HBB2	2.32	0.64
3:M:256:MET:HE3	3:M:258:PHE:CE1	2.34	0.63
7:M:401:BCL:HBB2	7:M:401:BCL:HHC	1.81	0.61
1:H:156:CYS:HB3	1:H:206:ASN:O	2.01	0.61
3:M:124:VAL:O	3:M:128:SER:OG	2.15	0.59
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.86	0.58
1:H:181:VAL:O	1:H:188:THR:HA	2.05	0.57
2:L:227:LEU:HD21	3:M:5:ASN:HD21	1.71	0.56
3:M:179:ILE:HG23	7:M:402:BCL:HED1	1.92	0.51
2:L:187:LEU:HD13	3:M:216:PHE:CG	2.45	0.51
2:L:181:PHE:CD2	5:M:409:BPH:HBB1	2.46	0.50
7:M:403:BCL:HAA2	7:M:403:BCL:HBD	1.94	0.49
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:81:GLU:OE1	2:L:8:LYS:NZ	2.41	0.48
1:H:208:LEU:HD11	1:H:237:VAL:HG22	1.96	0.47
2:L:128:TYR:HD1	7:M:401:BCL:HBB1	1.79	0.47
3:M:270:ILE:O	3:M:274:VAL:HG13	2.15	0.47
3:M:300:ASN:C	3:M:302:GLY:H	2.22	0.47
2:L:135:ARG:HB3	2:L:136:PRO:CD	2.45	0.47
2:L:183:ASN:ND2	2:L:237:SER:HB3	2.30	0.46
1:H:130:LYS:NZ	11:H:405:HOH:O	2.41	0.46
2:L:216:PHE:CZ	6:L:302:U10:H72	2.51	0.46
4:H:301:LDA:H123	6:M:410:U10:H202	1.98	0.46
2:L:21:LEU:HD13	2:L:22:PHE:CE2	2.51	0.45
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.52	0.45
3:M:159:VAL:HA	3:M:163:ILE:HB	1.98	0.45
2:L:100:TRP:CH2	6:M:410:U10:H251	2.51	0.45
1:H:42:LEU:HD11	4:H:301:LDA:HM23	1.99	0.44
2:L:65:SER:HA	2:L:148:TYR:O	2.18	0.44
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.99	0.43
3:M:197:PHE:CE1	7:M:403:BCL:HMC2	2.53	0.43
7:L:303:BCL:HMB3	7:L:303:BCL:CBB	2.49	0.43
2:L:210:ASP:N	2:L:210:ASP:OD1	2.52	0.43
2:L:185:LEU:HD12	2:L:185:LEU:O	2.19	0.43
1:H:40:TYR:HA	1:H:41:PRO:C	2.45	0.42
3:M:275:LEU:HD23	3:M:278:LEU:HD12	2.01	0.41
1:H:138:ALA:HA	1:H:139:GLY:HA2	1.81	0.41
6:L:302:U10:O5	6:L:302:U10:H8	2.19	0.41
2:L:219:LEU:HD11	3:M:133:THR:HG22	2.01	0.41
3:M:280:GLY:HA2	7:M:403:BCL:HED3	2.02	0.41
1:H:87:LEU:HD11	2:L:8:LYS:HA	2.03	0.41
1:H:148:PRO:HA	1:H:151:LEU:HD12	2.03	0.41
2:L:177:ILE:HD13	7:M:402:BCL:HMD2	2.03	0.41
2:L:185:LEU:HD13	5:M:409:BPH:C1D	2.50	0.41
3:M:206:ILE:HD13	7:M:401:BCL:HMD2	2.02	0.41
2:L:185:LEU:HD12	2:L:185:LEU:C	2.46	0.41
7:M:402:BCL:HHC	7:M:402:BCL:CBB	2.46	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	239/266 (90%)	237 (99%)	2 (1%)	0	100	100
2	L	279/282 (99%)	269 (96%)	10 (4%)	0	100	100
3	M	297/308 (96%)	281 (95%)	15 (5%)	1 (0%)	36	54
All	All	815/856 (95%)	787 (97%)	27 (3%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	196/215 (91%)	190 (97%)	6 (3%)	35	60
2	L	220/221 (100%)	211 (96%)	9 (4%)	27	52
3	M	234/240 (98%)	222 (95%)	12 (5%)	21	43
All	All	650/676 (96%)	623 (96%)	27 (4%)	26	51

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	LEU
1	H	80	SER

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Mol	Chain	Res	Type
1	H	173	GLU
1	H	184	LYS
1	H	205	VAL
1	H	231	ASP
2	L	21	LEU
2	L	136	PRO
2	L	185	LEU
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	235	LEU
2	L	247	CYS
2	L	254	ILE
3	M	5	ASN
3	M	39	LEU
3	M	59	SER
3	M	72	ILE
3	M	100	GLU
3	M	104	SER
3	M	109	LEU
3	M	128	SER
3	M	182	HIS
3	M	196	LEU
3	M	214	LEU
3	M	278	LEU

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

Mol	Chain	Res	Type
2	L	183	ASN
2	L	258	GLN
2	L	264	GLN
3	M	4	GLN
3	M	5	ASN
3	M	202	HIS

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	TYI	M	210	3	13,14,15	0.93	1 (7%)	14,19,21	2.16	5 (35%)

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	TYI	M	210	3	-	2/5/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	210	TYI	CE2-I2	-2.52	2.04	2.10

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	210	TYI	CB-CG-CD1	3.84	127.02	120.43
3	M	210	TYI	CZ-CE1-I1	3.58	124.55	119.35
3	M	210	TYI	CD2-CE2-I2	-3.21	112.44	118.46
3	M	210	TYI	CB-CG-CD2	-2.82	115.59	120.43
3	M	210	TYI	CZ-CE2-I2	2.66	123.22	119.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	210	TYI	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	LDA	M	406	-	13,15,15	0.14	0	14,17,17	0.17	0
4	LDA	M	404	-	13,15,15	0.20	0	14,17,17	0.23	0
7	BCL	M	401	-	69,74,74	1.72	14 (20%)	79,115,115	2.23	25 (31%)
4	LDA	M	405	-	13,15,15	0.14	0	14,17,17	0.29	0
6	U10	M	410	-	38,38,63	0.75	2 (5%)	48,49,79	0.57	0
7	BCL	M	402	-	54,59,74	2.02	16 (29%)	61,97,115	2.39	23 (37%)
9	SPO	M	411	-	41,41,41	1.23	7 (17%)	47,50,50	1.13	5 (10%)
5	BPH	L	301	-	59,70,70	0.79	2 (3%)	59,101,101	0.99	4 (6%)
10	CDL	M	412	-	68,68,99	0.34	0	74,80,111	0.46	0
7	BCL	M	403	-	69,74,74	1.75	13 (18%)	79,115,115	2.14	23 (29%)
4	LDA	M	407	-	13,15,15	0.21	0	14,17,17	0.16	0
5	BPH	M	409	-	49,60,70	0.88	3 (6%)	47,89,101	1.14	3 (6%)
7	BCL	L	303	-	69,74,74	1.72	14 (20%)	79,115,115	2.10	21 (26%)
4	LDA	H	301	-	13,15,15	0.11	0	14,17,17	0.27	0
6	U10	L	302	-	18,18,63	0.97	2 (11%)	24,25,79	1.31	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	M	406	-	-	3/13/13/13	-
4	LDA	M	404	-	-	3/13/13/13	-
7	BCL	M	401	-	-	10/41/137/137	-
4	LDA	M	405	-	-	3/13/13/13	-
6	U10	M	410	-	-	3/33/57/87	0/1/1/1
7	BCL	M	402	-	-	7/23/119/137	-
9	SPO	M	411	-	-	8/47/47/47	-
5	BPH	L	301	-	-	6/37/105/105	0/5/6/6
10	CDL	M	412	-	-	21/79/79/110	-
7	BCL	M	403	-	-	8/41/137/137	-
5	BPH	M	409	-	1/1/16/22	8/25/93/105	0/5/6/6
4	LDA	M	407	-	-	4/13/13/13	-
7	BCL	L	303	-	-	2/41/137/137	-
4	LDA	H	301	-	-	4/13/13/13	-
6	U10	L	302	-	-	6/9/33/87	0/1/1/1

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	303	BCL	O2D-CGD	5.40	1.46	1.33
7	M	401	BCL	O2D-CGD	5.05	1.45	1.33
7	M	403	BCL	O2D-CGD	4.87	1.45	1.33
7	M	402	BCL	O2D-CGD	4.82	1.45	1.33
7	M	402	BCL	O2A-CGA	4.82	1.47	1.33
7	M	401	BCL	C3D-C4D	-4.67	1.33	1.44
7	M	402	BCL	C3D-C4D	-4.53	1.34	1.44
7	L	303	BCL	C3D-C4D	-4.52	1.34	1.44
7	M	403	BCL	C3B-C4B	4.48	1.50	1.41
7	M	401	BCL	O2A-CGA	4.45	1.46	1.33
7	M	403	BCL	C3D-C4D	-4.44	1.34	1.44
7	M	402	BCL	C3B-C4B	4.23	1.49	1.41
7	L	303	BCL	OBD-CAD	4.19	1.29	1.22
7	L	303	BCL	O2A-CGA	4.07	1.45	1.33
7	M	401	BCL	C3B-C4B	4.00	1.49	1.41
7	M	403	BCL	O2A-CGA	3.98	1.45	1.33
5	M	409	BPH	C4D-CHA	3.86	1.45	1.39
7	M	403	BCL	OBD-CAD	3.80	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	401	BCL	CHB-C1B	3.79	1.47	1.39
7	L	303	BCL	C3B-C4B	3.71	1.48	1.41
7	M	403	BCL	CHD-C1D	3.68	1.45	1.38
7	M	402	BCL	CHB-C1B	3.62	1.47	1.39
7	M	402	BCL	CHD-C1D	3.56	1.45	1.38
7	L	303	BCL	CHC-C4B	3.45	1.47	1.39
5	L	301	BPH	C1B-C2B	3.40	1.43	1.39
7	M	402	BCL	OBD-CAD	3.38	1.28	1.22
7	M	401	BCL	CHC-C4B	3.36	1.46	1.39
7	M	401	BCL	CHD-C1D	3.29	1.44	1.38
7	M	402	BCL	CHC-C4B	3.27	1.46	1.39
7	M	403	BCL	C3D-C2D	3.23	1.47	1.39
7	M	403	BCL	CHC-C4B	3.22	1.46	1.39
7	L	303	BCL	CHB-C1B	3.18	1.46	1.39
7	M	402	BCL	C3D-C2D	3.16	1.47	1.39
7	M	401	BCL	OBD-CAD	3.14	1.27	1.22
7	M	403	BCL	CHB-C1B	3.10	1.46	1.39
7	L	303	BCL	CHD-C1D	3.05	1.44	1.38
7	M	401	BCL	C3D-C2D	3.03	1.47	1.39
5	L	301	BPH	C4D-CHA	3.00	1.44	1.39
7	M	402	BCL	CHD-C4C	2.92	1.47	1.39
7	L	303	BCL	C3D-C2D	2.89	1.46	1.39
7	M	402	BCL	C1D-ND	-2.77	1.34	1.37
7	L	303	BCL	CHD-C4C	2.73	1.46	1.39
5	M	409	BPH	C1B-C2B	2.71	1.42	1.39
9	M	411	SPO	C16-C17	-2.70	1.40	1.46
7	M	402	BCL	C1B-C2B	2.65	1.49	1.43
7	M	402	BCL	C1D-C2D	2.64	1.50	1.45
9	M	411	SPO	C25-C23	-2.63	1.40	1.46
7	M	403	BCL	CHD-C4C	2.63	1.46	1.39
7	M	401	BCL	CHD-C4C	2.61	1.46	1.39
7	M	403	BCL	C1D-C2D	2.52	1.50	1.45
7	M	401	BCL	C1B-C2B	2.51	1.49	1.43
9	M	411	SPO	C11-C12	-2.48	1.40	1.46
7	L	303	BCL	C4B-NB	-2.41	1.34	1.37
7	M	401	BCL	MG-NA	-2.39	2.00	2.06
7	L	303	BCL	C1B-C2B	2.36	1.48	1.43
7	M	403	BCL	C1B-NB	-2.33	1.34	1.37
7	L	303	BCL	C1D-ND	-2.32	1.34	1.37
6	L	302	U10	C3-C2	-2.30	1.42	1.48
9	M	411	SPO	C9-C7	2.29	1.41	1.35
6	M	410	U10	C6-C1	2.26	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	303	BCL	C1D-C2D	2.22	1.49	1.45
6	M	410	U10	C4-C5	-2.22	1.42	1.48
7	M	402	BCL	MG-NA	-2.21	2.01	2.06
7	M	402	BCL	MG-NC	-2.21	2.01	2.06
7	M	401	BCL	MG-NC	-2.19	2.01	2.06
6	L	302	U10	C6-C1	2.17	1.39	1.35
7	M	402	BCL	C4B-NB	-2.16	1.35	1.37
9	M	411	SPO	C14-C12	2.12	1.40	1.35
7	M	401	BCL	C1D-C2D	2.11	1.49	1.45
7	M	403	BCL	C1D-ND	-2.10	1.35	1.37
9	M	411	SPO	C6-C7	-2.08	1.41	1.46
9	M	411	SPO	C19-C17	2.07	1.40	1.35
5	M	409	BPH	C3D-C2D	2.01	1.43	1.39

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	303	BCL	CMD-C2D-C1D	7.83	138.51	124.73
7	M	403	BCL	CMD-C2D-C1D	7.39	137.74	124.73
7	M	402	BCL	CMD-C2D-C1D	7.35	137.66	124.73
7	M	401	BCL	CMD-C2D-C1D	7.09	137.21	124.73
7	M	403	BCL	C2B-C1B-NB	6.16	116.72	110.33
7	L	303	BCL	C2B-C1B-NB	5.76	116.30	110.33
7	M	401	BCL	O2D-CGD-CBD	5.60	121.02	111.23
7	M	402	BCL	O2D-CGD-CBD	5.59	120.99	111.23
7	M	402	BCL	CHD-C1D-ND	-5.57	116.97	124.80
7	M	402	BCL	C2B-C1B-NB	5.48	116.00	110.33
7	M	401	BCL	C2B-C1B-NB	5.15	115.67	110.33
7	M	401	BCL	CHD-C1D-ND	-5.14	117.57	124.80
7	M	401	BCL	C3D-C2D-C1D	-5.11	98.86	105.83
7	M	403	BCL	CHD-C1D-ND	-4.83	118.01	124.80
7	M	403	BCL	O2D-CGD-CBD	4.77	119.58	111.23
7	M	402	BCL	C3D-C2D-C1D	-4.65	99.49	105.83
7	L	303	BCL	CHD-C1D-ND	-4.61	118.32	124.80
7	L	303	BCL	C3D-C2D-C1D	-4.55	99.62	105.83
7	M	403	BCL	C3D-C2D-C1D	-4.53	99.65	105.83
7	M	401	BCL	C3C-C4C-CHD	-4.41	114.10	123.39
5	M	409	BPH	C4D-CHA-CBD	-4.23	106.42	108.45
7	L	303	BCL	C3C-C4C-CHD	-4.17	114.60	123.39
7	M	401	BCL	C1D-ND-C4D	-4.11	103.43	106.31
7	M	402	BCL	C1D-ND-C4D	-4.11	103.43	106.31
7	M	403	BCL	C3C-C4C-CHD	-4.05	114.86	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	401	BCL	C3B-C4B-NB	3.99	115.03	109.76
7	M	401	BCL	C2D-C1D-ND	3.93	114.02	110.13
7	L	303	BCL	C1D-ND-C4D	-3.87	103.60	106.31
5	L	301	BPH	C2B-C1B-NB	-3.81	106.68	109.43
7	M	402	BCL	C3D-C4D-ND	3.79	116.14	109.99
7	M	402	BCL	C3C-C4C-CHD	-3.73	115.53	123.39
7	L	303	BCL	CED-O2D-CGD	3.68	124.25	115.92
7	M	401	BCL	C4A-NA-C1A	3.66	108.35	106.68
7	M	403	BCL	CHC-C1C-NC	3.63	129.64	124.40
7	M	401	BCL	CHC-C1C-NC	3.61	129.61	124.40
7	M	402	BCL	C2D-C1D-ND	3.61	113.70	110.13
5	M	409	BPH	C2B-C1B-NB	-3.61	106.82	109.43
5	L	301	BPH	C4D-CHA-CBD	-3.59	106.73	108.45
6	L	302	U10	C7-C6-C5	3.58	122.67	118.52
7	L	303	BCL	C3B-C4B-NB	3.56	114.46	109.76
7	M	403	BCL	O2D-CGD-O1D	-3.55	116.94	123.85
7	L	303	BCL	C2D-C1D-ND	3.51	113.60	110.13
6	L	302	U10	C7-C6-C1	-3.48	118.92	124.89
7	M	401	BCL	CHB-C4A-NA	3.46	129.40	124.40
7	M	403	BCL	C3D-C4D-ND	3.36	115.45	109.99
7	M	403	BCL	C1D-ND-C4D	-3.29	104.01	106.31
7	L	303	BCL	C3D-C4D-ND	3.24	115.26	109.99
7	M	403	BCL	C3B-C4B-NB	3.21	114.00	109.76
7	M	402	BCL	C1-O2A-CGA	3.18	124.36	116.65
7	M	402	BCL	C3B-C4B-NB	3.17	113.94	109.76
7	M	403	BCL	C2D-C1D-ND	3.13	113.22	110.13
7	L	303	BCL	CHB-C4A-NA	3.11	128.89	124.40
7	M	401	BCL	C1-O2A-CGA	3.09	124.13	116.65
7	M	403	BCL	CHB-C4A-NA	3.09	128.85	124.40
7	M	401	BCL	C1C-NC-C4C	-3.03	105.30	106.68
7	M	402	BCL	CHC-C1C-NC	3.01	128.75	124.40
7	M	401	BCL	C3D-C4D-ND	3.01	114.88	109.99
7	L	303	BCL	CHC-C1C-NC	2.99	128.71	124.40
7	L	303	BCL	O2A-CGA-CBA	2.97	120.90	111.83
7	M	401	BCL	C1D-CHD-C4C	-2.94	119.53	126.62
7	M	403	BCL	CHC-C4B-NB	-2.90	119.70	124.05
7	L	303	BCL	C1D-CHD-C4C	-2.87	119.69	126.62
7	M	402	BCL	CHB-C4A-NA	2.85	128.51	124.40
7	L	303	BCL	C4-C3-C5	2.78	120.05	115.23
7	M	403	BCL	C1D-CHD-C4C	-2.77	119.94	126.62
7	M	401	BCL	O1D-CGD-CBD	-2.64	119.32	124.52
7	M	403	BCL	O2A-CGA-CBA	2.63	119.86	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	409	BPH	C1A-C2A-C3A	-2.62	100.34	102.84
7	M	402	BCL	O1D-CGD-CBD	-2.62	119.35	124.52
7	L	303	BCL	C2A-C1A-CHA	-2.62	119.32	123.87
7	M	403	BCL	C4-C3-C5	2.60	119.74	115.23
7	L	303	BCL	CMD-C2D-C3D	-2.54	121.87	127.69
7	L	303	BCL	O2A-CGA-O1A	-2.54	117.28	123.63
7	M	403	BCL	CHB-C1B-C2B	-2.54	120.06	127.43
7	M	401	BCL	C4-C3-C5	2.53	119.62	115.23
7	M	402	BCL	CMB-C2B-C1B	2.50	129.22	125.42
5	L	301	BPH	C1A-C2A-C3A	-2.48	100.48	102.84
7	M	401	BCL	CMB-C2B-C1B	2.45	129.15	125.42
7	M	401	BCL	OBD-CAD-C3D	-2.35	122.92	128.42
9	M	411	SPO	C10-C9-C7	2.34	130.56	127.28
7	M	402	BCL	O2A-CGA-CBA	2.28	118.77	111.83
7	M	403	BCL	CED-O2D-CGD	2.27	121.07	115.92
6	L	302	U10	C8-C7-C6	2.25	117.62	112.08
7	M	402	BCL	CHC-C4B-NB	-2.25	120.68	124.05
7	L	303	BCL	CMB-C2B-C1B	2.25	128.84	125.42
7	M	401	BCL	O2A-CGA-CBA	2.23	118.65	111.83
7	M	403	BCL	C4A-NA-C1A	2.22	107.69	106.68
7	M	403	BCL	CMD-C2D-C3D	-2.21	122.61	127.69
7	M	401	BCL	CHC-C4B-NB	-2.21	120.74	124.05
7	L	303	BCL	O2D-CGD-CBD	2.20	115.07	111.23
7	M	402	BCL	C2A-C1A-CHA	-2.19	120.06	123.87
5	L	301	BPH	C2D-C1D-ND	-2.16	107.87	109.43
7	M	401	BCL	O2D-CGD-O1D	-2.16	119.65	123.85
7	M	402	BCL	O2D-CGD-O1D	-2.16	119.65	123.85
7	L	303	BCL	C5-C3-C2	-2.15	116.35	121.17
7	M	402	BCL	C1D-CHD-C4C	-2.14	121.45	126.62
7	M	401	BCL	C5-C3-C2	-2.13	116.38	121.17
7	M	401	BCL	C6-C5-C3	-2.13	108.29	113.47
7	M	402	BCL	CMD-C2D-C3D	-2.12	122.84	127.69
7	M	402	BCL	C1-C2-C3	-2.11	123.34	126.76
7	M	403	BCL	C1-C2-C3	-2.09	122.78	126.20
9	M	411	SPO	C21-C20-C19	2.07	127.76	123.52
9	M	411	SPO	C21-C22-C23	2.06	130.16	127.28
7	M	402	BCL	CHB-C1B-C2B	-2.03	121.53	127.43
9	M	411	SPO	C24-C23-C22	-2.02	119.54	122.82
9	M	411	SPO	C20-C19-C17	2.01	130.10	127.28
7	M	403	BCL	C1C-NC-C4C	-2.01	105.76	106.68

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	409	BPH	C8

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	301	LDA	C2-C1-N1-CM1
4	M	405	LDA	N1-C1-C2-C3
5	M	409	BPH	C2C-C3C-CAC-CBC
6	L	302	U10	C1-C6-C7-C8
6	L	302	U10	C5-C6-C7-C8
7	M	401	BCL	CHA-CBD-CGD-O1D
7	M	401	BCL	CHA-CBD-CGD-O2D
7	M	402	BCL	CHA-CBD-CGD-O1D
7	M	402	BCL	CHA-CBD-CGD-O2D
7	M	403	BCL	CBD-CGD-O2D-CED
9	M	411	SPO	C4-C1-O1-CM1
10	M	412	CDL	CA3-OA5-PA1-OA2
10	M	412	CDL	CA3-OA5-PA1-OA3
10	M	412	CDL	CA3-OA5-PA1-OA4
10	M	412	CDL	CB2-OB2-PB2-OB3
7	M	401	BCL	CBD-CGD-O2D-CED
7	M	403	BCL	O1D-CGD-O2D-CED
7	M	402	BCL	CBD-CGD-O2D-CED
7	M	401	BCL	O1D-CGD-O2D-CED
7	M	402	BCL	O1D-CGD-O2D-CED
5	L	301	BPH	C11-C12-C13-C15
6	M	410	U10	C24-C26-C27-C28
10	M	412	CDL	CA7-C31-C32-C33
5	M	409	BPH	C5-C6-C7-C8
6	L	302	U10	C7-C8-C9-C10
10	M	412	CDL	C33-C34-C35-C36
4	M	404	LDA	C4-C5-C6-C7
4	H	301	LDA	C6-C7-C8-C9
4	M	405	LDA	C1-C2-C3-C4
4	M	406	LDA	C1-C2-C3-C4
10	M	412	CDL	C11-CA5-OA6-CA4
4	M	407	LDA	C1-C2-C3-C4
10	M	412	CDL	C13-C14-C15-C16
7	L	303	BCL	C2A-CAA-CBA-CGA
6	L	302	U10	C7-C8-C9-C11
7	M	401	BCL	C15-C16-C17-C18
7	M	401	BCL	C2B-C3B-CAB-CBB
10	M	412	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
4	M	406	LDA	C9-C10-C11-C12
4	M	404	LDA	C1-C2-C3-C4
9	M	411	SPO	C3-C1-O1-CM1
4	H	301	LDA	C9-C10-C11-C12
5	L	301	BPH	C13-C15-C16-C17
7	M	403	BCL	C13-C15-C16-C17
10	M	412	CDL	OA7-CA5-OA6-CA4
4	M	407	LDA	C3-C4-C5-C6
4	M	407	LDA	C9-C10-C11-C12
10	M	412	CDL	C17-C18-C19-C20
10	M	412	CDL	C39-C40-C41-C42
7	M	401	BCL	C4B-C3B-CAB-OB
7	M	401	BCL	C4B-C3B-CAB-CBB
7	M	402	BCL	C4C-C3C-CAC-CBC
4	M	405	LDA	C6-C7-C8-C9
9	M	411	SPO	C18-C17-C19-C20
7	M	401	BCL	C2B-C3B-CAB-OB
7	L	303	BCL	C15-C16-C17-C18
7	M	403	BCL	C16-C17-C18-C19
5	L	301	BPH	C5-C6-C7-C8
5	L	301	BPH	C4-C3-C5-C6
5	M	409	BPH	C4-C3-C5-C6
7	M	403	BCL	CAD-CBD-CGD-O2D
7	M	403	BCL	CAD-CBD-CGD-O1D
10	M	412	CDL	CB2-OB2-PB2-OB4
10	M	412	CDL	CB2-OB2-PB2-OB5
5	L	301	BPH	O2A-C1-C2-C3
10	M	412	CDL	OA5-CA3-CA4-CA6
5	M	409	BPH	C6-C7-C8-C9
9	M	411	SPO	C34-C33-C35-C36
6	M	410	U10	C14-C16-C17-C18
9	M	411	SPO	C2-C1-O1-CM1
10	M	412	CDL	C72-C71-CB7-OB8
6	L	302	U10	C5-C4-O4-C4M
5	M	409	BPH	C6-C7-C8-C10
4	H	301	LDA	C11-C10-C9-C8
5	L	301	BPH	C2-C3-C5-C6
9	M	411	SPO	C32-C33-C35-C36
4	M	406	LDA	C2-C3-C4-C5
5	M	409	BPH	C2-C3-C5-C6
10	M	412	CDL	C72-C73-C74-C75
5	M	409	BPH	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	L	302	U10	C3-C4-O4-C4M
6	M	410	U10	C3-C4-O4-C4M
7	M	401	BCL	C12-C13-C15-C16
4	M	404	LDA	C11-C10-C9-C8
10	M	412	CDL	C36-C37-C38-C39
9	M	411	SPO	C1-C4-C5-C6
7	M	402	BCL	C2B-C3B-CAB-OB5
7	M	403	BCL	C16-C17-C18-C20
10	M	412	CDL	C71-C72-C73-C74
10	M	412	CDL	C52-C51-CB5-OB6
4	M	407	LDA	C6-C7-C8-C9
7	M	403	BCL	C11-C12-C13-C15
7	M	402	BCL	C2B-C3B-CAB-CBB
9	M	411	SPO	C16-C17-C19-C20
10	M	412	CDL	C52-C51-CB5-OB7
5	M	409	BPH	C4C-C3C-CAC-CBC

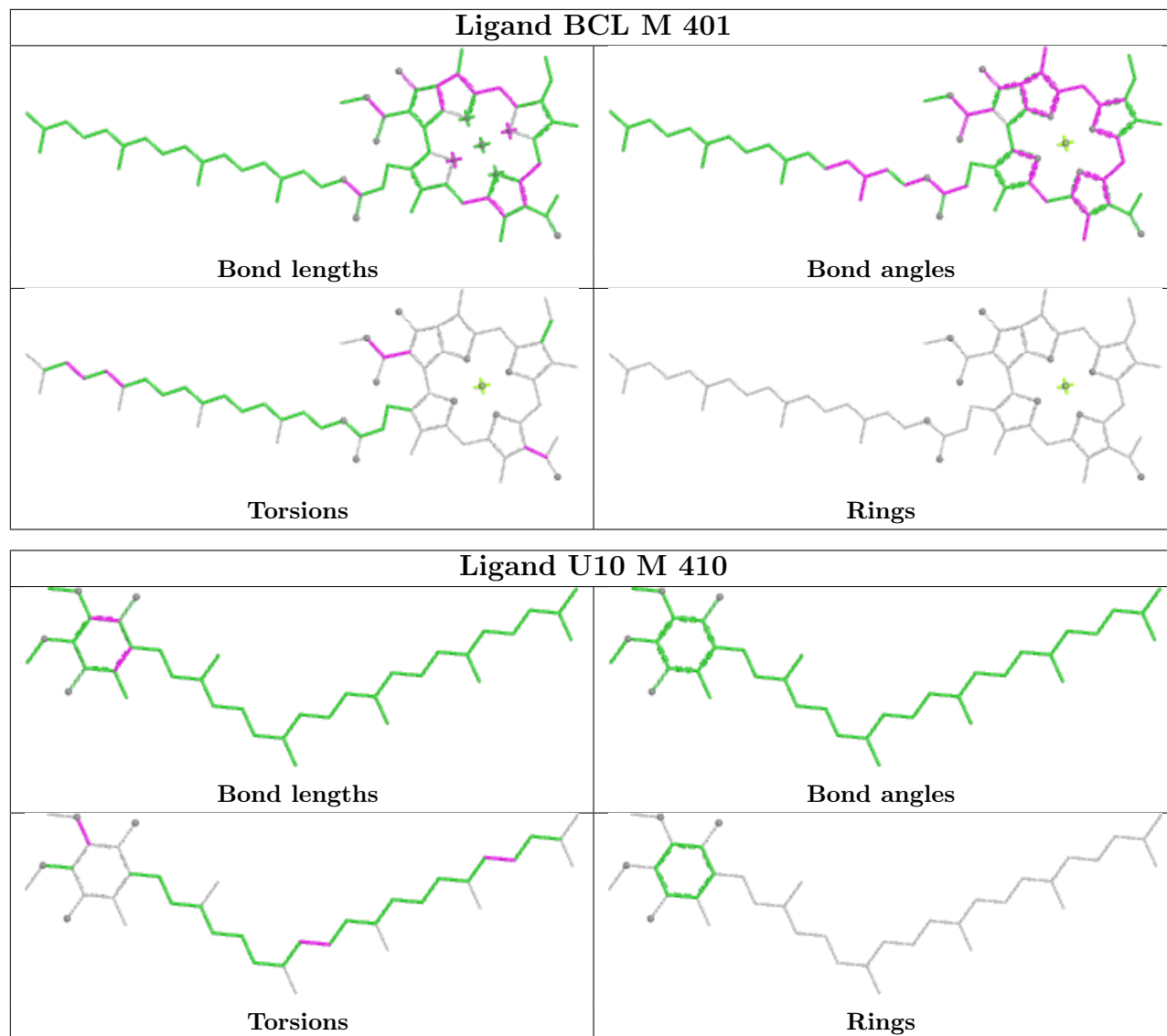
There are no ring outliers.

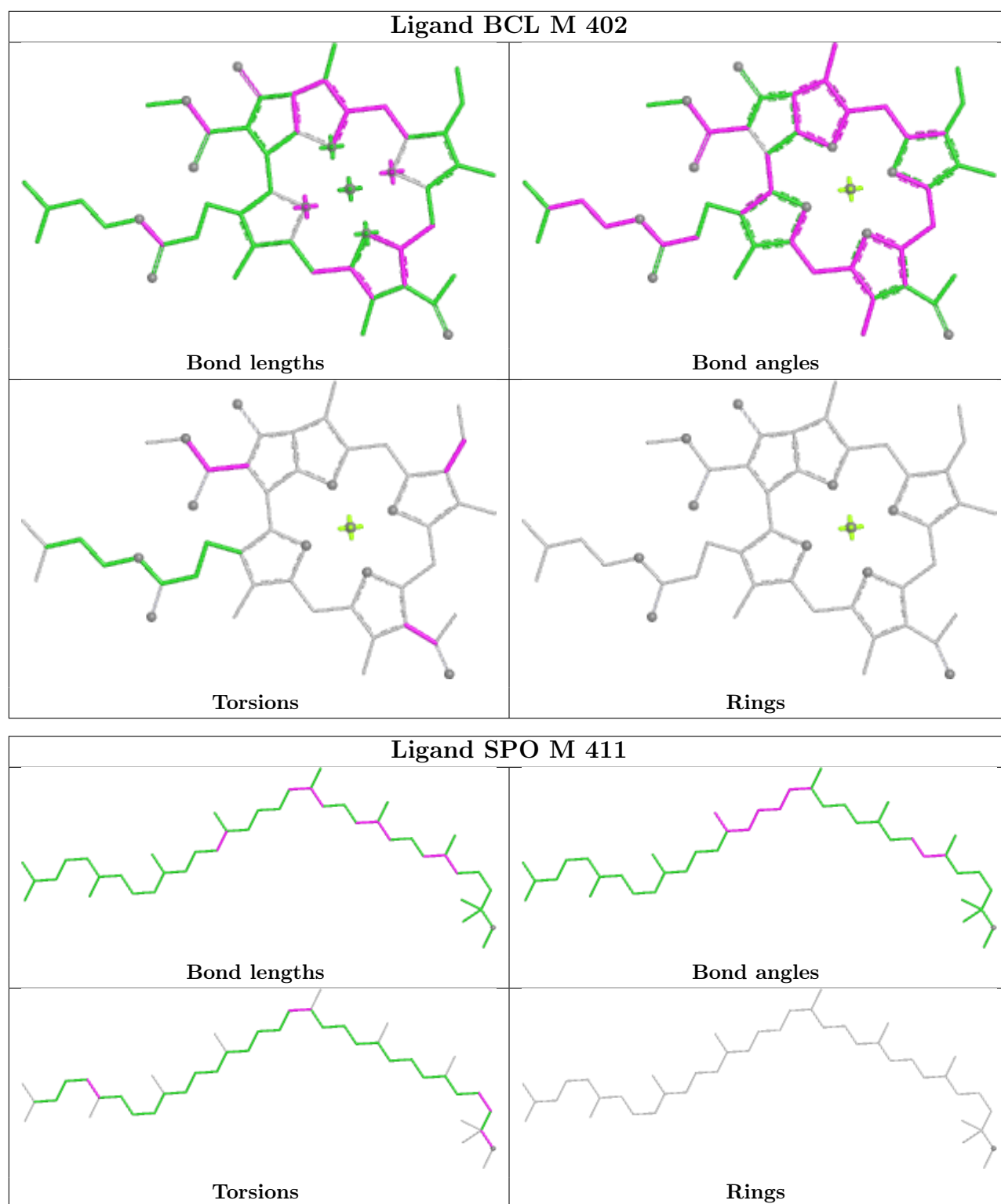
9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	401	BCL	5	0
6	M	410	U10	2	0
7	M	402	BCL	4	0
5	L	301	BPH	1	0
7	M	403	BCL	5	0
5	M	409	BPH	2	0
7	L	303	BCL	1	0
4	H	301	LDA	2	0
6	L	302	U10	2	0

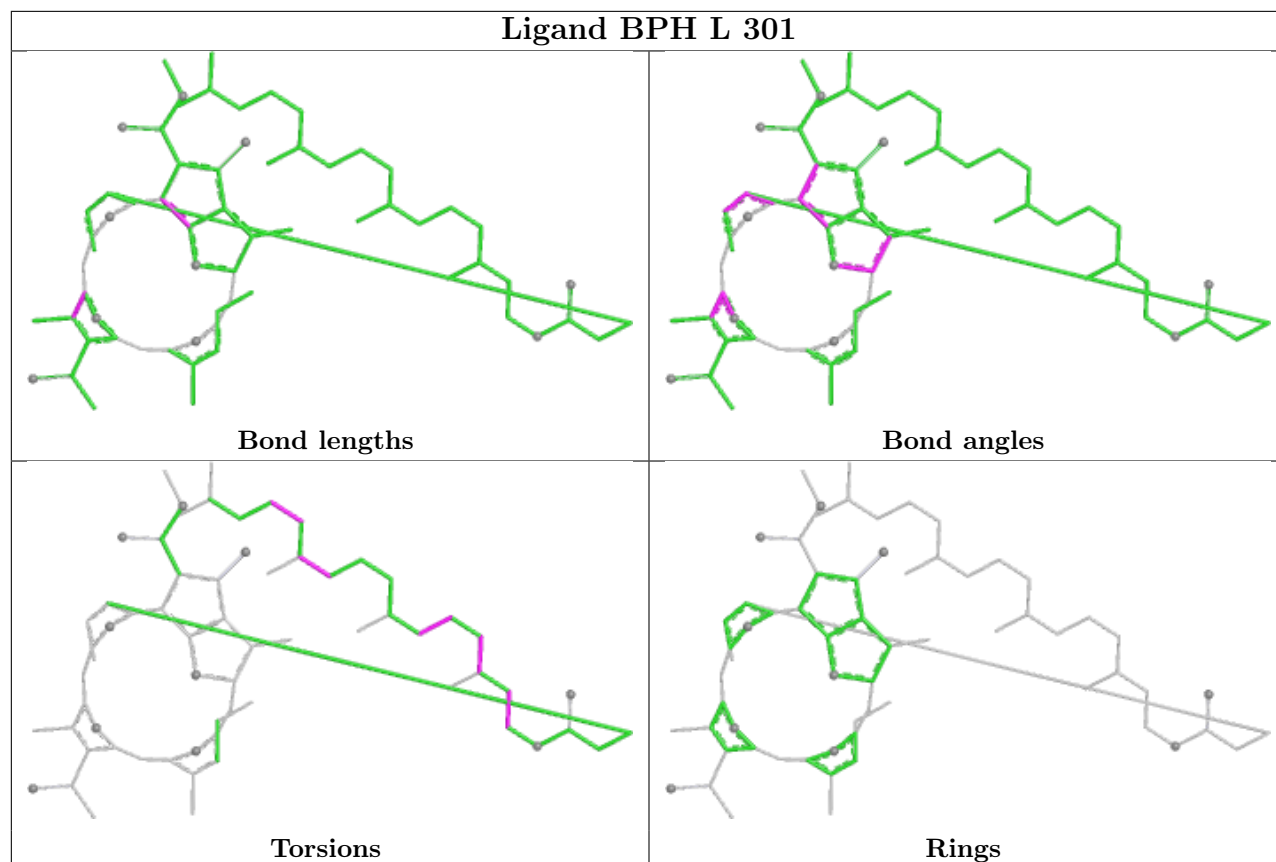
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

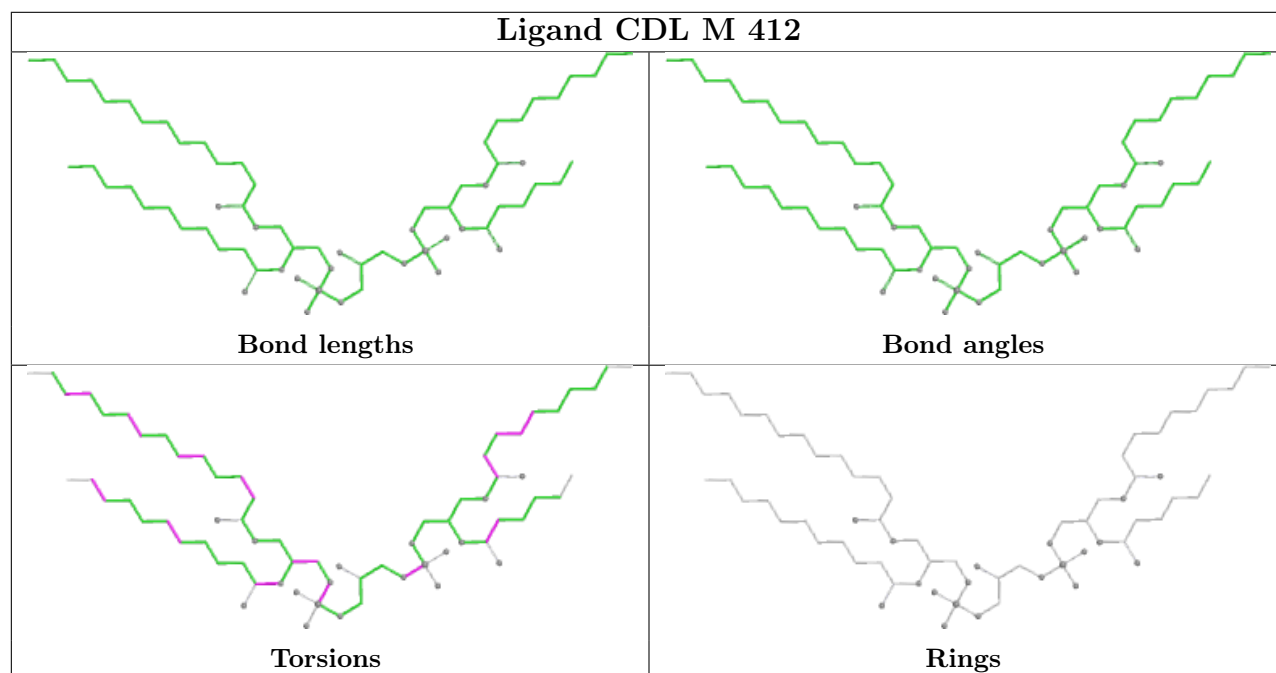


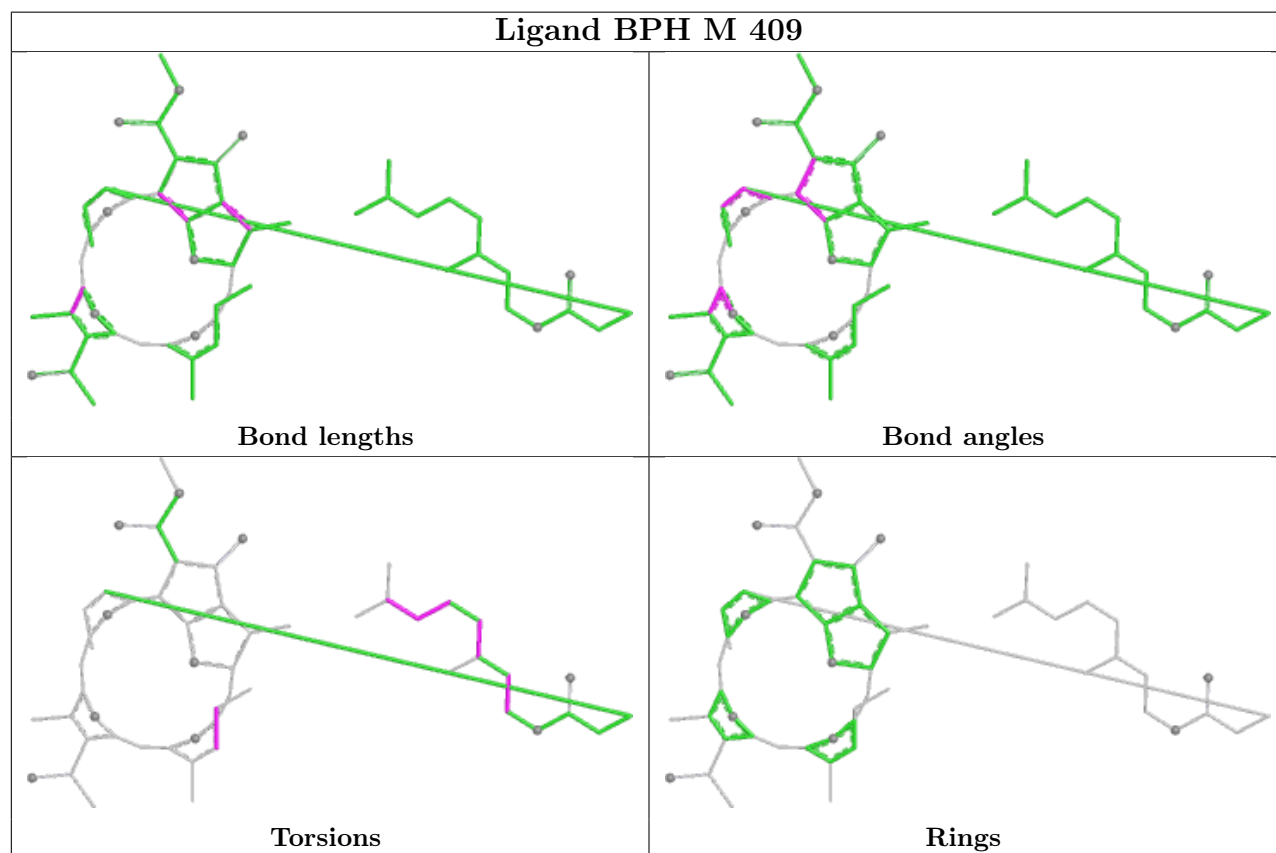
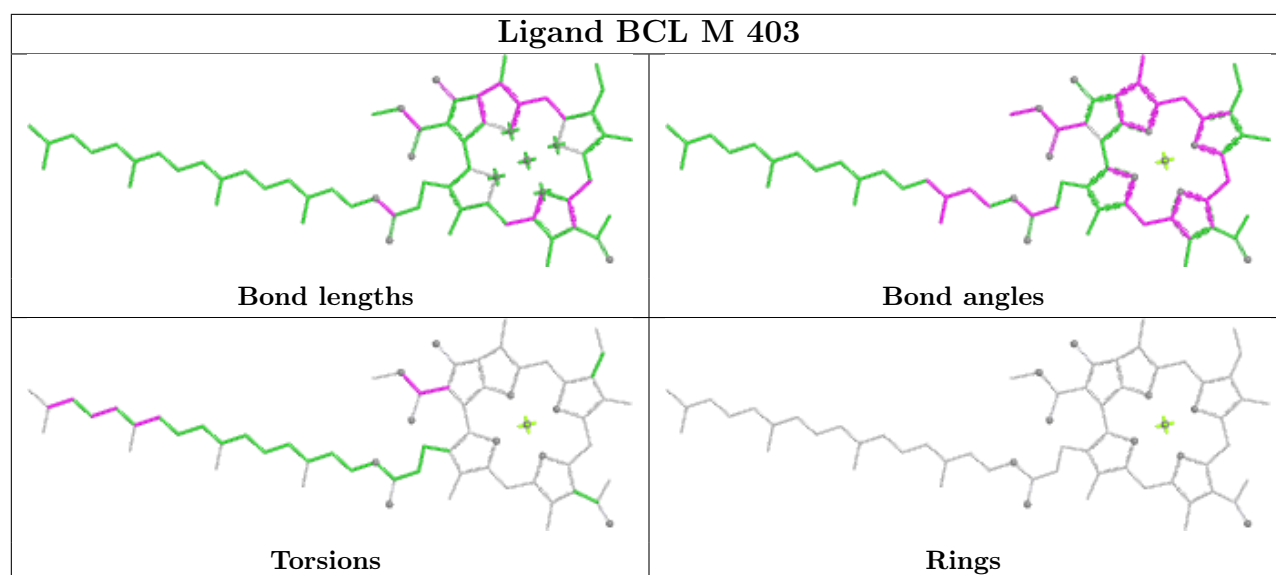


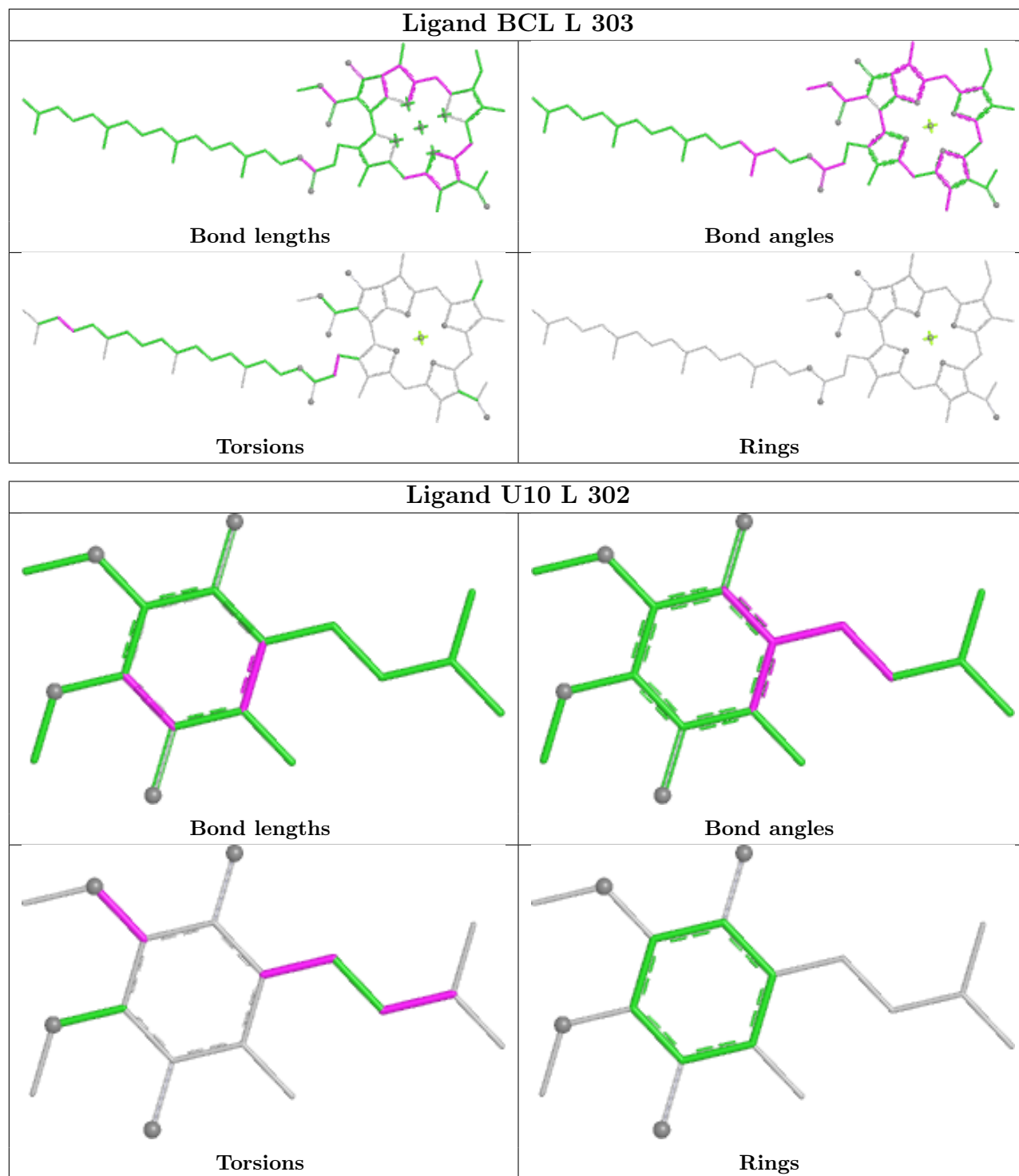
Ligand BPH L 301



Ligand CDL M 412







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	239/266 (89%)	-0.03	3 (1%) 75 68	36, 69, 93, 114	2 (0%)
2	L	281/282 (99%)	0.16	10 (3%) 46 36	51, 69, 107, 120	0
3	M	299/308 (97%)	0.00	4 (1%) 75 68	47, 72, 106, 125	0
All	All	819/856 (95%)	0.05	17 (2%) 63 55	36, 69, 104, 125	2 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	72	GLU	4.4
2	L	270	PRO	3.8
2	L	73	TYR	3.8
3	M	3	TYR	3.4
1	H	81	GLU	3.3
1	H	102	GLY	2.9
2	L	274	ASN	2.9
1	H	18[A]	TYR	2.6
3	M	23	ASP	2.6
2	L	9	TYR	2.5
3	M	26	LEU	2.4
2	L	77	GLY	2.3
2	L	46	ILE	2.3
3	M	302	GLY	2.3
2	L	82	LYS	2.1
2	L	268	LYS	2.1
2	L	152	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	TYI	M	210	14/15	0.99	0.07	56,59,62,62	2

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

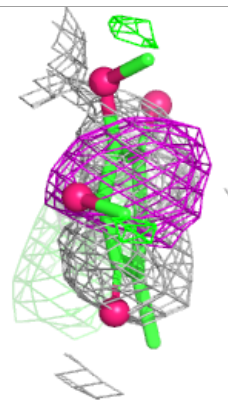
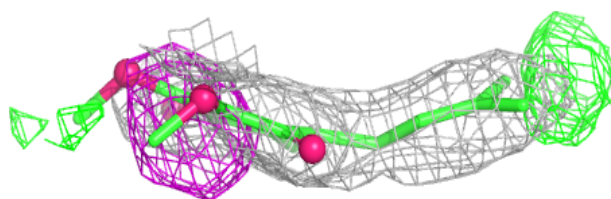
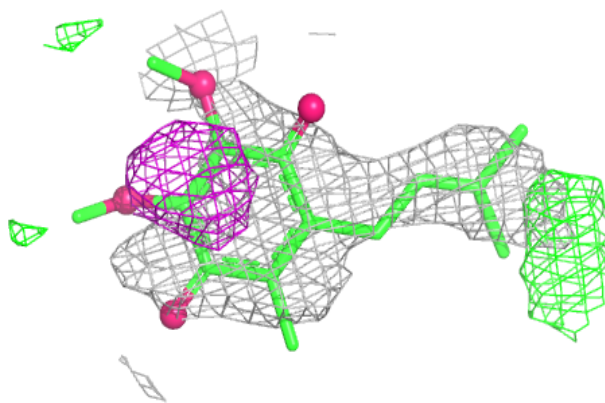
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	LDA	M	407	16/16	0.82	0.37	104,110,135,135	0
4	LDA	M	406	16/16	0.85	0.32	98,114,125,126	0
6	U10	L	302	18/63	0.89	0.27	105,124,135,138	0
10	CDL	M	412	69/100	0.90	0.18	77,99,114,127	0
4	LDA	M	405	16/16	0.91	0.23	86,93,125,128	0
6	U10	M	410	38/63	0.93	0.17	51,66,94,100	0
4	LDA	M	404	16/16	0.93	0.20	83,94,98,101	0
5	BPH	M	409	55/65	0.94	0.14	65,77,110,114	0
7	BCL	M	401	66/66	0.94	0.12	49,58,87,91	0
9	SPO	M	411	42/42	0.94	0.18	75,90,111,116	0
5	BPH	L	301	65/65	0.94	0.13	46,57,84,87	0
4	LDA	H	301	16/16	0.95	0.16	73,81,105,106	0
7	BCL	M	403	66/66	0.96	0.11	52,59,95,105	0
7	BCL	L	303	66/66	0.96	0.11	48,58,85,90	0
7	BCL	M	402	51/66	0.96	0.10	55,60,78,80	0
8	FE	M	408	1/1	0.99	0.02	57,57,57,57	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.

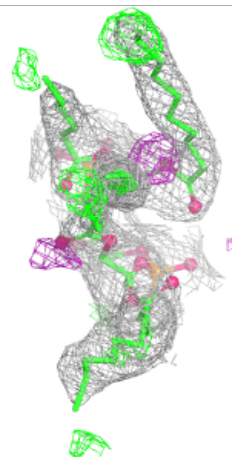
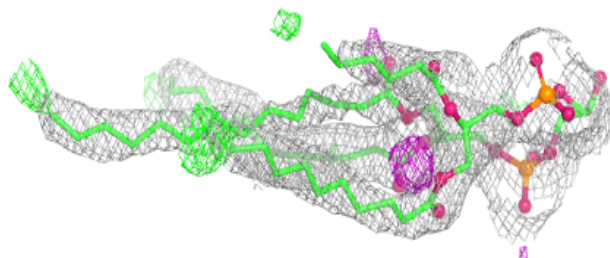
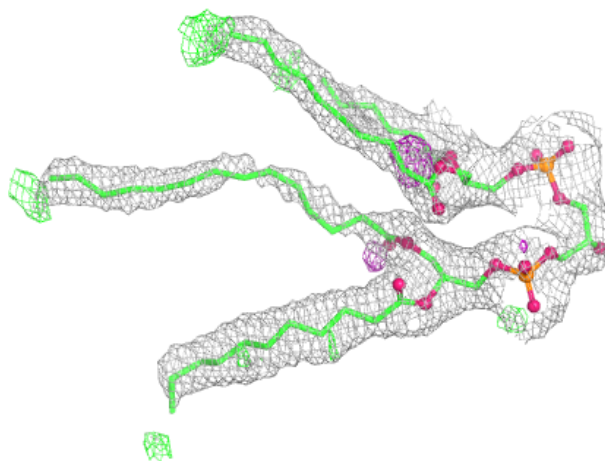
Electron density around U10 L 302:

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



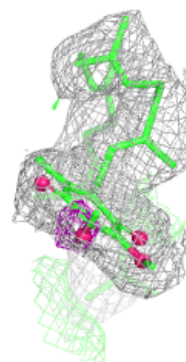
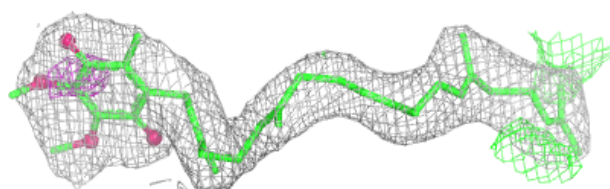
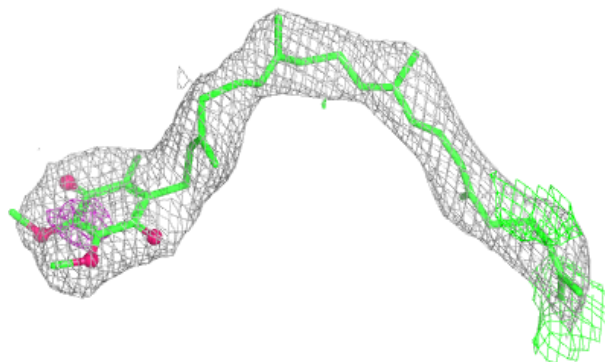
Electron density around CDL M 412:

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

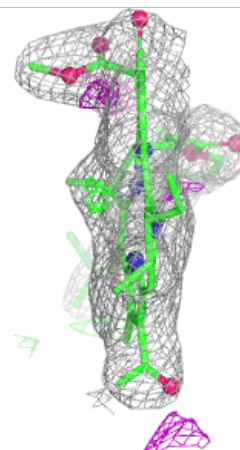
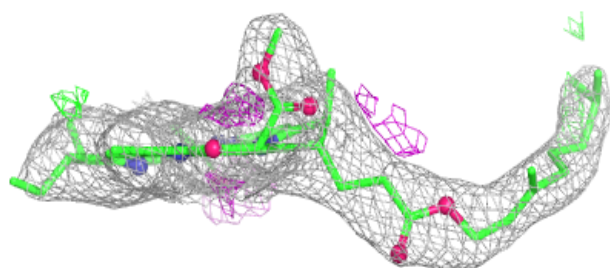
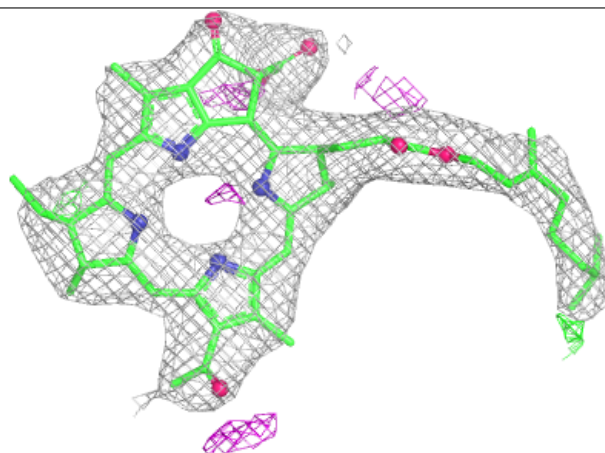


Electron density around U10 M 410:

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

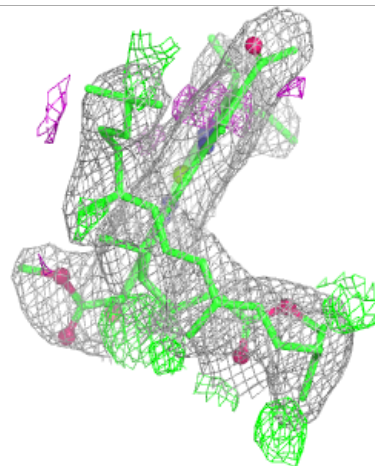
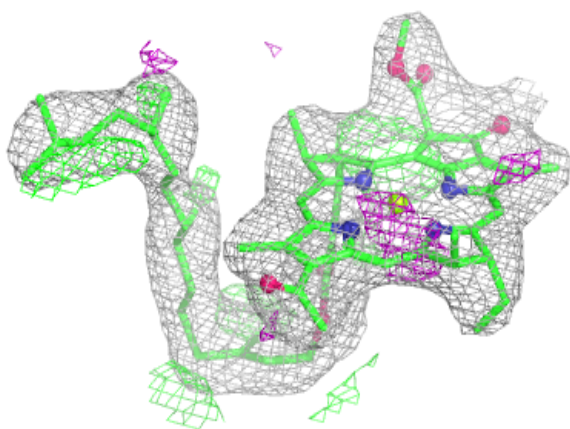
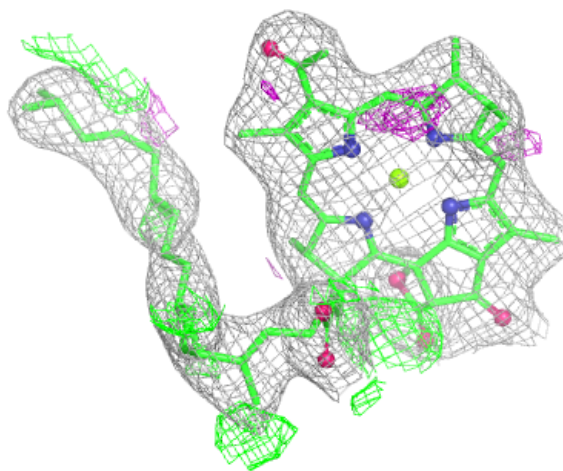
**Electron density around BPH M 409:**

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



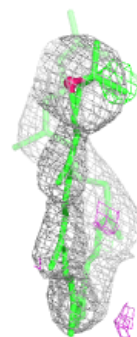
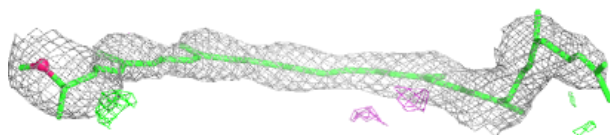
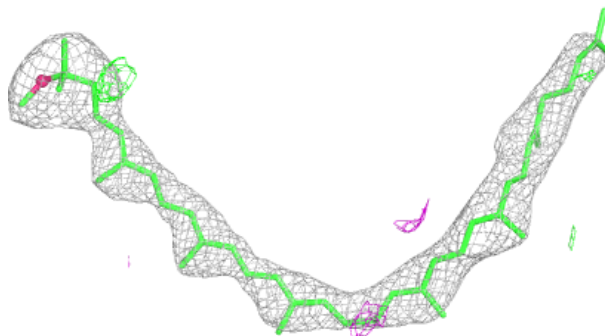
Electron density around BCL M 401:

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



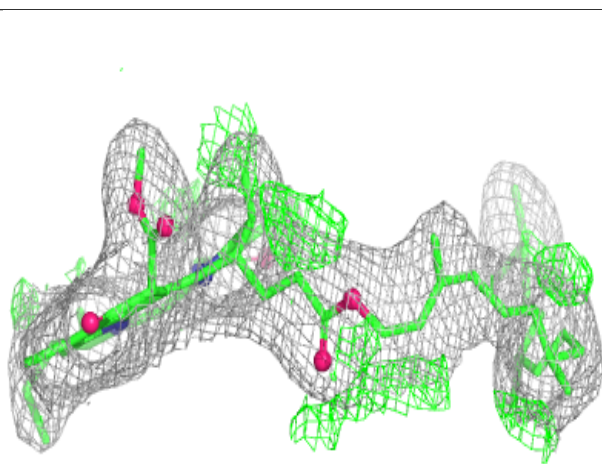
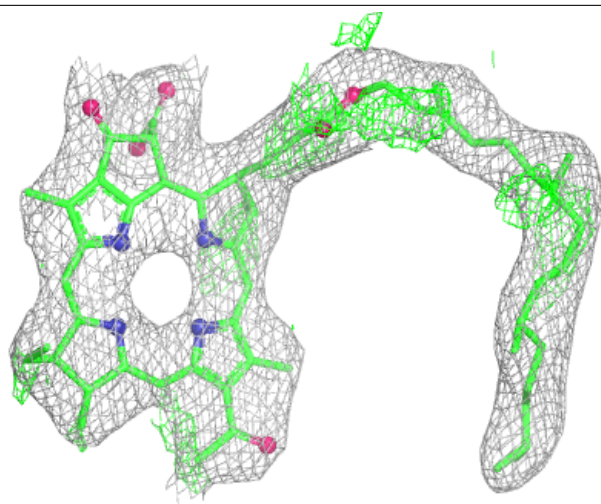
Electron density around SPO M 411:

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



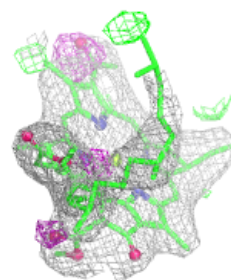
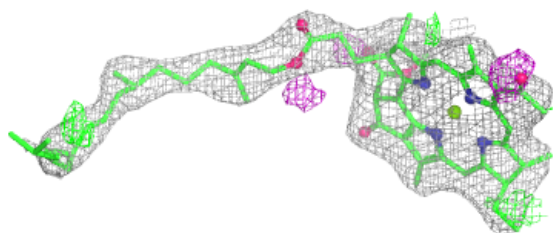
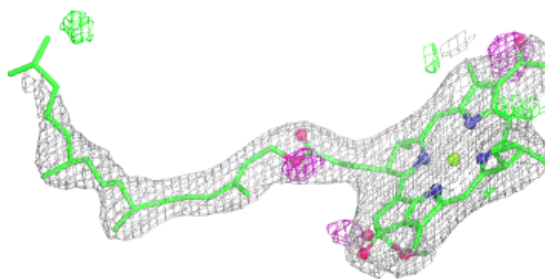
Electron density around BPH L 301:

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

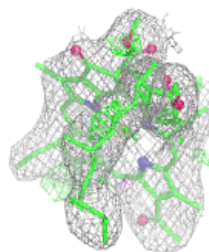
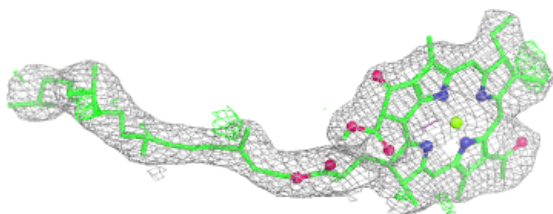
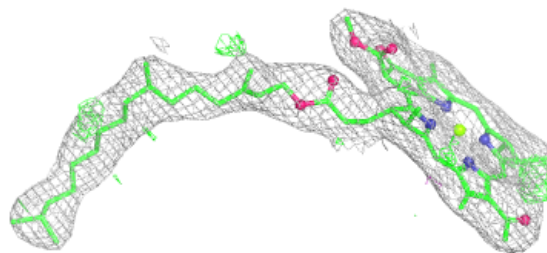


Electron density around BCL M 403:

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

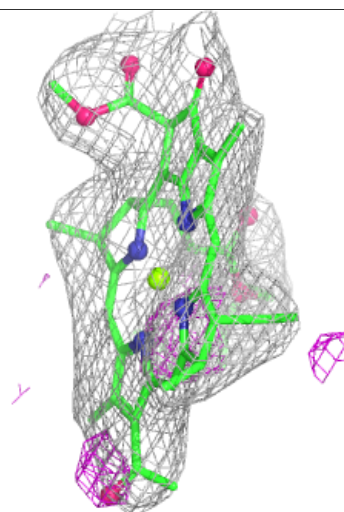
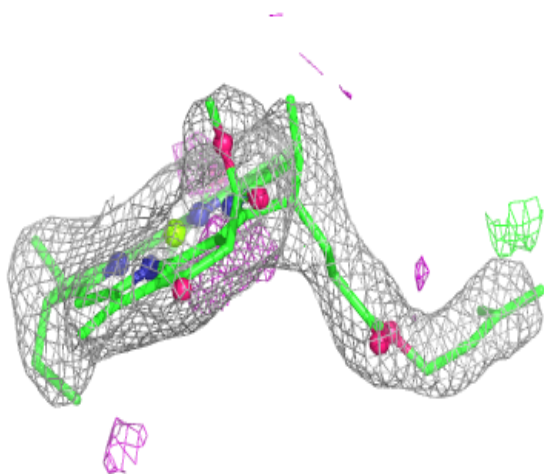
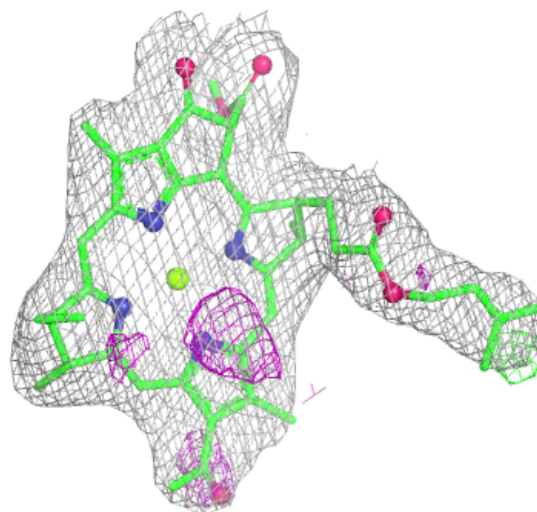
**Electron density around BCL L 303:**

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



Electron density around BCL M 402:

$2mF_o-DF_c$ (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.