



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 06:08 AM EDT

PDB ID : 4HBH
Title : Bacterial Photosynthetic Reaction Center from Rhodobacter sphaeroides with ILE M265 replaced with ASN
Authors : Mattis, A.J.; Wraight, C.A.
Deposited on : 2012-09-28
Resolution : 2.93 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

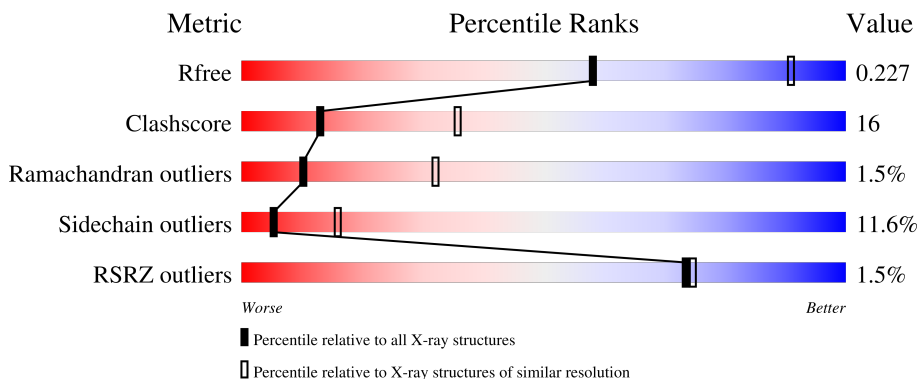
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	L	281	
2	M	313	
3	H	260	

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	L	303	X	-	-	-
6	U10	L	304	-	-	X	-
6	U10	L	305	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6919 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 L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	281	2209	1490	350	361	8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	301	2390	1594	391	395	10	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	265	ASN	ILE	engineered mutation	UNP P0C0Y9
M	303	MET	-	expression tag	UNP P0C0Y9
M	304	ALA	-	expression tag	UNP P0C0Y9
M	305	PRO	-	expression tag	UNP P0C0Y9
M	306	LEU	-	expression tag	UNP P0C0Y9
M	307	ASN	-	expression tag	UNP P0C0Y9
M	308	HIS	-	expression tag	UNP P0C0Y9
M	309	HIS	-	expression tag	UNP P0C0Y9
M	310	HIS	-	expression tag	UNP P0C0Y9
M	311	HIS	-	expression tag	UNP P0C0Y9
M	312	HIS	-	expression tag	UNP P0C0Y9
M	313	HIS	-	expression tag	UNP P0C0Y9

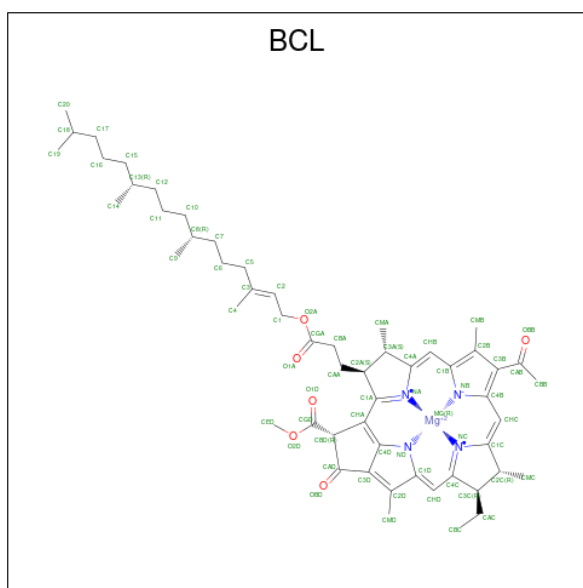
- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	238	1792	1146	305	332	9	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	MET	-	expression tag	UNP P0C0Y7
H	2	VAL	-	expression tag	UNP P0C0Y7
H	3	GLY	-	expression tag	UNP P0C0Y7
H	4	VAL	-	expression tag	UNP P0C0Y7
H	5	THR	-	expression tag	UNP P0C0Y7
H	6	ALA	-	expression tag	UNP P0C0Y7
H	7	PHE	-	expression tag	UNP P0C0Y7
H	8	GLY	-	expression tag	UNP P0C0Y7
H	9	ASN	-	expression tag	UNP P0C0Y7
H	10	PHE	-	expression tag	UNP P0C0Y7
H	251	VAL	-	expression tag	UNP P0C0Y7
H	252	VAL	-	expression tag	UNP P0C0Y7
H	253	ALA	-	expression tag	UNP P0C0Y7
H	254	ALA	-	expression tag	UNP P0C0Y7
H	255	MET	-	expression tag	UNP P0C0Y7
H	256	LEU	-	expression tag	UNP P0C0Y7
H	257	ALA	-	expression tag	UNP P0C0Y7
H	258	GLU	-	expression tag	UNP P0C0Y7
H	259	TYR	-	expression tag	UNP P0C0Y7
H	260	ALA	-	expression tag	UNP P0C0Y7

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



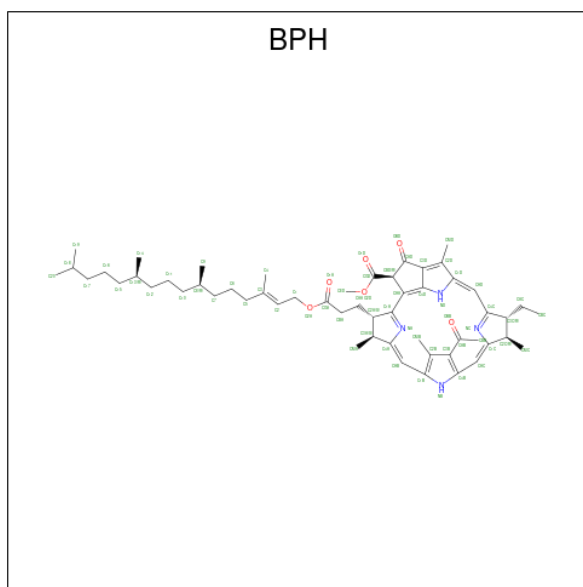
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	Mg	N			O	
4	L	1	Total	66	55	1	4	6	0	0
4	L	1	Total	66	55	1	4	6	0	0

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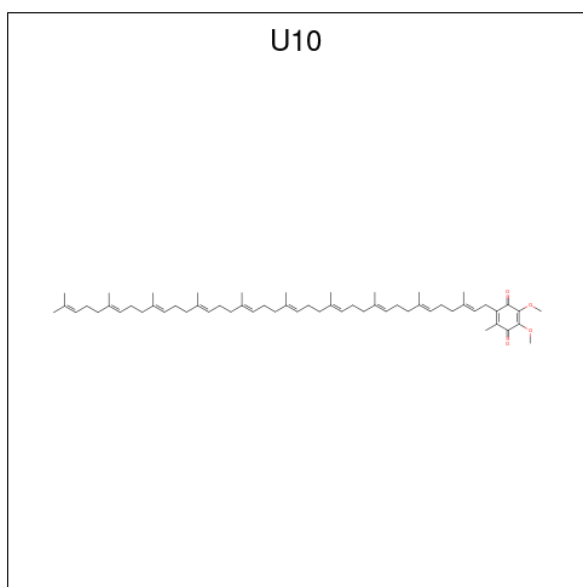
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	M	1	Total	C	Mg	N	O	0	0
			55	44	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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
			53	43	4	6		

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).

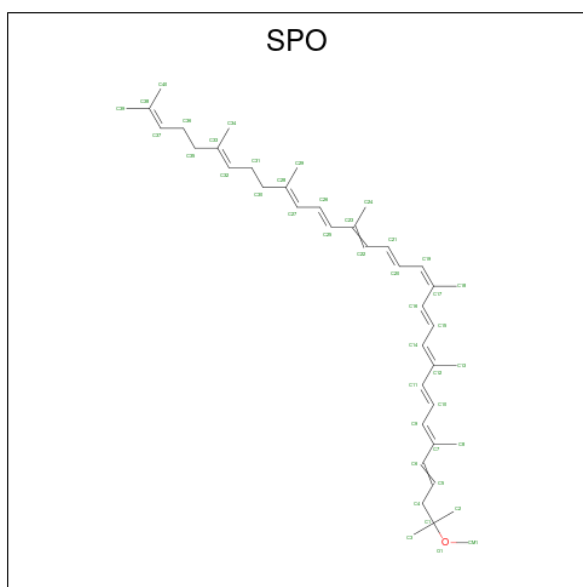


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			26	22	4		
6	L	1	Total	C	O	0	0
			26	22	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 8 is SPHEROIDENE (three-letter code: SPO) (formula: C₄₁H₆₀O).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	C O	0	0
			35	34 1		

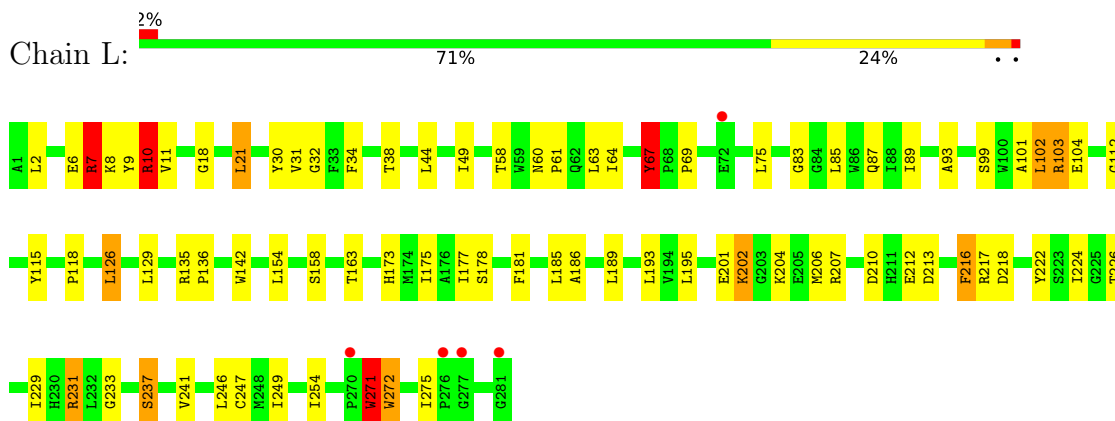
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	8	Total	O	0	0
			8	8		
9	M	11	Total	O	0	0
			11	11		
9	H	2	Total	O	0	0
			2	2		

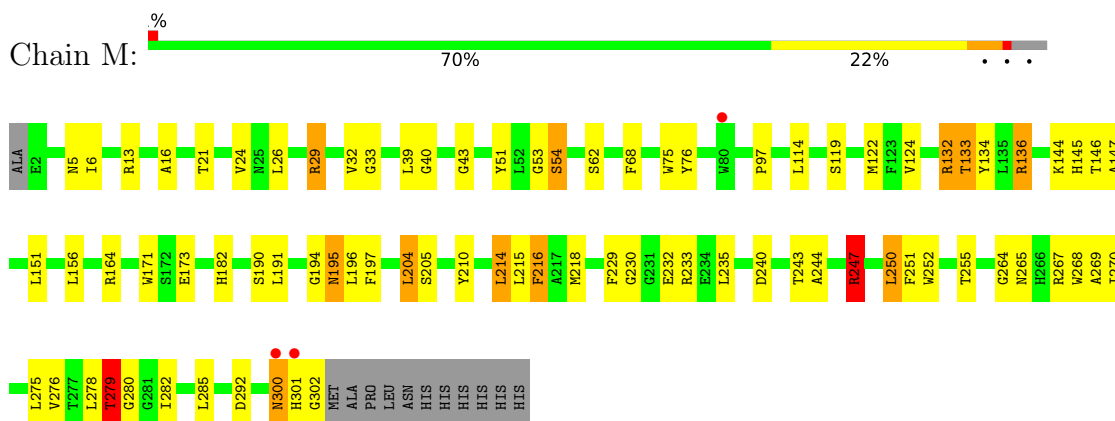
3 Residue-property plots [i](#)

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.

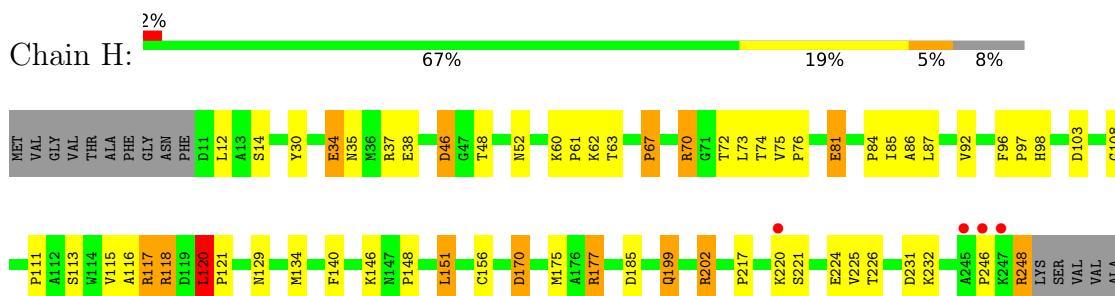
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain



ALA
MET
LEU
ALA
GLU
TYR
ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.72Å 139.72Å 183.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	121.00 – 2.93 19.84 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.6 (121.00-2.93) 100.0 (19.84-2.93)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.93Å)	Xtrriage
Refinement program	REFMAC 5.5.0109, PHENIX	Depositor
R, R_{free}	0.185 , 0.226 0.187 , 0.227	Depositor DCC
R_{free} test set	2250 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtrriage
Anisotropy	0.041	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6919	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: U10, BCL, BPH, SPO, FE

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	L	1.02	1/2295 (0.0%)	0.97	9/3144 (0.3%)
2	M	0.98	0/2480	0.94	4/3386 (0.1%)
3	H	0.99	0/1840	1.02	5/2511 (0.2%)
All	All	1.00	1/6615 (0.0%)	0.97	18/9041 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
2	M	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	67	TYR	CD2-CE2	5.75	1.48	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	247	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	L	231	ARG	NE-CZ-NH1	7.26	123.93	120.30
3	H	120	LEU	CA-CB-CG	6.83	131.01	115.30
2	M	21	THR	C-N-CA	-6.45	105.58	121.70
2	M	132	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	L	126	LEU	CB-CG-CD2	-6.13	100.58	111.00
1	L	231	ARG	NE-CZ-NH2	-5.77	117.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	81	GLU	C-N-CA	-5.77	107.28	121.70
1	L	7	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	L	10	ARG	NE-CZ-NH2	-5.52	117.54	120.30
3	H	170	ASP	CB-CG-OD1	5.50	123.25	118.30
1	L	10	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	L	103	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	L	7	ARG	NE-CZ-NH2	-5.22	117.69	120.30
3	H	46	ASP	CB-CG-OD1	5.13	122.92	118.30
2	M	204	LEU	CB-CG-CD1	5.10	119.67	111.00
1	L	31	VAL	C-N-CA	-5.08	111.63	122.30
3	H	67	PRO	C-N-CA	-5.05	109.06	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	32	GLY	Peptide
2	M	278	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2209	0	2144	76	0
2	M	2390	0	2281	63	0
3	H	1792	0	1760	44	0
4	L	132	0	148	7	0
4	M	121	0	124	19	0
5	L	65	0	76	9	0
5	M	53	0	49	7	0
6	L	52	0	56	47	0
6	M	48	0	63	6	0
7	M	1	0	0	0	0
8	M	35	0	46	6	0
9	H	2	0	0	0	0
9	L	8	0	0	2	0
9	M	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6919	0	6747	224	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 16.

All (224) 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)
6:L:304:U10:C3M	6:L:305:U10:H1M1	1.29	1.60
6:L:304:U10:C3M	6:L:305:U10:C1M	2.23	1.15
3:H:117:ARG:HG2	3:H:117:ARG:HH11	1.07	1.09
6:L:304:U10:H3M1	6:L:305:U10:C1M	1.84	1.06
1:L:7:ARG:HH11	3:H:98:HIS:CD2	1.73	1.06
6:L:304:U10:H3M3	6:L:305:U10:H1M1	1.34	1.06
6:L:304:U10:H3M1	6:L:305:U10:H1M1	1.01	1.01
6:L:304:U10:H1M2	6:L:305:U10:H122	1.43	1.01
1:L:38:THR:HG22	1:L:99:SER:HB3	1.44	1.00
6:L:304:U10:H3M3	6:L:304:U10:H4M2	1.39	1.00
4:M:403:BCL:HHC	4:M:403:BCL:CBB	1.93	0.99
6:L:304:U10:O3	6:L:305:U10:H72	1.64	0.98
2:M:119:SER:HB3	8:M:406:SPO:H32	1.48	0.95
5:L:303:BPH:HBB2	2:M:210:TYR:HB3	1.53	0.90
1:L:216:PHE:CD2	6:L:305:U10:H8	2.05	0.89
3:H:117:ARG:HG2	3:H:117:ARG:NH1	1.88	0.87
3:H:117:ARG:HH11	3:H:117:ARG:CG	1.88	0.86
2:M:275:LEU:O	2:M:279:THR:HB	1.75	0.85
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.59	0.84
1:L:38:THR:HG22	1:L:99:SER:CB	2.06	0.84
1:L:186:ALA:HA	6:L:304:U10:C4M	2.07	0.83
5:M:404:BPH:HHC	5:M:404:BPH:HBB3	1.59	0.83
2:M:197:PHE:CZ	4:M:403:BCL:HBB2	2.15	0.82
1:L:224:ILE:H	6:L:305:U10:H71	1.45	0.81
6:L:304:U10:H3M3	6:L:305:U10:C1M	2.02	0.81
4:M:403:BCL:HHC	4:M:403:BCL:HBB3	1.62	0.81
6:L:304:U10:C3M	6:L:305:U10:C8	2.60	0.79
2:M:197:PHE:HZ	4:M:403:BCL:HBB2	1.43	0.79
3:H:129:ASN:ND2	3:H:224:GLU:HG2	1.98	0.78
4:M:403:BCL:HHC	4:M:403:BCL:HBB2	1.66	0.78
2:M:279:THR:HG22	2:M:280:GLY:N	1.99	0.78
5:L:303:BPH:HBB3	5:L:303:BPH:HHC	1.66	0.78
1:L:60:ASN:HD22	1:L:61:PRO:CD	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:304:U10:H3M3	6:L:304:U10:C4M	2.14	0.78
6:L:304:U10:O2	6:L:305:U10:H103	1.85	0.77
6:L:304:U10:O3	6:L:305:U10:C7	2.32	0.77
1:L:186:ALA:HA	6:L:304:U10:H4M1	1.67	0.76
2:M:240:ASP:O	3:H:117:ARG:NH1	2.19	0.75
1:L:189:LEU:HD12	6:L:304:U10:H4M3	1.68	0.75
1:L:213:ASP:O	1:L:217:ARG:HG3	1.87	0.75
2:M:279:THR:HG22	2:M:280:GLY:H	1.52	0.75
2:M:164:ARG:NH1	2:M:173:GLU:HG3	2.01	0.75
1:L:7:ARG:NH1	3:H:98:HIS:CD2	2.52	0.75
1:L:60:ASN:ND2	1:L:61:PRO:HD2	2.01	0.74
6:L:304:U10:C1M	6:L:305:U10:H122	2.18	0.73
3:H:70:ARG:NH2	3:H:121:PRO:O	2.20	0.73
4:L:302:BCL:HMB1	4:L:302:BCL:HBB2	1.71	0.72
4:L:302:BCL:HMB1	4:L:302:BCL:CBB	2.20	0.72
3:H:46:ASP:OD1	3:H:48:THR:HB	1.89	0.72
6:L:304:U10:O3	6:L:305:U10:C8	2.38	0.71
2:M:164:ARG:HH12	2:M:173:GLU:HG3	1.56	0.71
1:L:60:ASN:HD22	1:L:61:PRO:HD2	1.56	0.70
1:L:38:THR:CG2	1:L:99:SER:HB3	2.20	0.70
4:M:401:BCL:HHC	4:M:401:BCL:CBB	2.22	0.70
1:L:231:ARG:HD3	2:M:5:ASN:O	1.91	0.70
4:M:401:BCL:HHC	4:M:401:BCL:HBB2	1.74	0.70
3:H:37:ARG:O	3:H:38:GLU:HG2	1.90	0.70
2:M:53:GLY:O	2:M:54:SER:HB2	1.91	0.69
3:H:148:PRO:HA	3:H:151:LEU:HD22	1.74	0.69
3:H:156:CYS:SG	3:H:248:ARG:HA	2.32	0.69
1:L:224:ILE:HG22	6:L:305:U10:C7	2.22	0.69
1:L:216:PHE:CG	6:L:305:U10:H8	2.28	0.69
3:H:34:GLU:OE2	3:H:37:ARG:NH1	2.26	0.69
1:L:7:ARG:HH11	3:H:98:HIS:HD2	1.38	0.68
1:L:34:PHE:O	1:L:38:THR:HG23	1.93	0.68
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.75	0.68
2:M:32:VAL:HG12	2:M:33:GLY:O	1.93	0.68
3:H:70:ARG:O	3:H:118:ARG:NH2	2.26	0.67
5:L:303:BPH:CBB	2:M:210:TYR:HB3	2.24	0.67
1:L:201:GLU:O	1:L:202:LYS:HB2	1.94	0.67
6:L:304:U10:O2	6:L:305:U10:C10	2.43	0.67
1:L:181:PHE:HB3	5:M:404:BPH:HBB2	1.76	0.66
6:L:304:U10:O3	6:L:305:U10:H1M1	1.95	0.66
3:H:118:ARG:CD	3:H:120:LEU:HD22	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:181:PHE:HB3	5:M:404:BPH:CBB	2.28	0.64
3:H:118:ARG:HD2	3:H:120:LEU:HD22	1.79	0.64
2:M:194:GLY:O	2:M:195:ASN:HB3	1.98	0.64
3:H:120:LEU:HB3	3:H:121:PRO:CD	2.28	0.64
1:L:69:PRO:HD3	1:L:83:GLY:O	1.98	0.63
4:L:301:BCL:CBB	4:L:301:BCL:HMB1	2.28	0.63
1:L:60:ASN:ND2	1:L:61:PRO:CD	2.59	0.63
1:L:49:ILE:HG13	1:L:89:ILE:HD13	1.80	0.63
2:M:205:SER:HA	2:M:279:THR:HG21	1.80	0.62
2:M:243:THR:O	2:M:247:ARG:HG2	1.98	0.62
1:L:224:ILE:HG22	6:L:305:U10:H71	1.80	0.62
4:M:401:BCL:HBB3	4:M:403:BCL:H41	1.82	0.62
6:L:304:U10:H4M2	6:L:305:U10:C1M	2.30	0.61
3:H:129:ASN:HD21	3:H:224:GLU:HG2	1.65	0.61
2:M:133:THR:HG22	2:M:147:ALA:HB2	1.83	0.61
2:M:164:ARG:HH12	2:M:173:GLU:CG	2.12	0.61
1:L:7:ARG:NH1	3:H:98:HIS:HD2	1.97	0.61
1:L:241:VAL:HG21	5:L:303:BPH:HBC2	1.83	0.61
2:M:279:THR:CG2	2:M:280:GLY:N	2.63	0.61
1:L:216:PHE:CE2	6:L:304:U10:H3M2	2.36	0.60
2:M:119:SER:CB	8:M:406:SPO:H32	2.28	0.60
1:L:201:GLU:O	1:L:202:LYS:CB	2.49	0.60
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.83	0.60
4:L:301:BCL:HMB1	4:L:301:BCL:HBB3	1.83	0.59
6:L:304:U10:H3M1	6:L:305:U10:C8	2.31	0.59
4:M:403:BCL:HAA2	4:M:403:BCL:HBD	1.83	0.59
1:L:186:ALA:HA	6:L:304:U10:H4M3	1.84	0.59
2:M:164:ARG:NH1	2:M:173:GLU:CG	2.66	0.58
1:L:181:PHE:CD2	5:M:404:BPH:HBB1	2.38	0.58
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.33	0.58
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.39	0.57
2:M:76:TYR:C	2:M:76:TYR:CD2	2.78	0.57
1:L:226:THR:HG22	6:L:305:U10:H3M3	1.87	0.57
1:L:231:ARG:HD2	2:M:6:ILE:O	2.05	0.56
3:H:170:ASP:OD2	3:H:177:ARG:NH1	2.31	0.56
2:M:51:TYR:O	2:M:132:ARG:NH2	2.34	0.56
2:M:136:ARG:NE	2:M:136:ARG:HA	2.21	0.56
2:M:247:ARG:NH2	3:H:111:PRO:O	2.36	0.56
1:L:241:VAL:CG2	5:L:303:BPH:HBC2	2.35	0.56
1:L:60:ASN:O	1:L:64:ILE:HG13	2.06	0.55
6:L:304:U10:C3M	6:L:305:U10:C7	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:304:U10:C2	6:L:305:U10:C9	2.84	0.55
3:H:199:GLN:OE1	3:H:202:ARG:HD2	2.07	0.55
2:M:197:PHE:HZ	4:M:403:BCL:CBB	2.18	0.54
3:H:62:LYS:O	3:H:74:THR:HA	2.07	0.54
1:L:222:TYR:CD2	6:L:305:U10:C10	2.91	0.54
4:M:401:BCL:CBB	8:M:406:SPO:H243	2.38	0.53
1:L:186:ALA:CA	6:L:304:U10:H4M1	2.39	0.53
1:L:216:PHE:CD2	6:L:305:U10:C8	2.86	0.53
1:L:272:TRP:HA	1:L:275:ILE:CD1	2.39	0.53
6:L:304:U10:H4M2	6:L:305:U10:H1M2	1.91	0.53
2:M:194:GLY:O	2:M:195:ASN:CB	2.57	0.53
5:L:303:BPH:HBB1	2:M:210:TYR:CD2	2.42	0.53
1:L:101:ALA:O	1:L:104:GLU:HB2	2.09	0.52
1:L:271:TRP:H	1:L:271:TRP:HD1	1.54	0.52
2:M:133:THR:CG2	2:M:147:ALA:HA	2.39	0.52
2:M:232:GLU:OE2	3:H:177:ARG:NH2	2.42	0.52
1:L:103:ARG:NH2	2:M:255:THR:O	2.37	0.52
6:M:405:U10:H272	6:M:405:U10:H322	1.92	0.52
2:M:134:TYR:CE2	2:M:144:LYS:HG2	2.45	0.51
1:L:30:TYR:O	1:L:103:ARG:NH1	2.40	0.51
1:L:9:TYR:O	1:L:11:VAL:N	2.40	0.51
1:L:175:ILE:O	1:L:178:SER:HB3	2.10	0.51
4:M:403:BCL:HBB3	4:M:403:BCL:CHC	2.36	0.51
3:H:63:THR:HA	3:H:73:LEU:O	2.10	0.50
2:M:251:PHE:CD1	2:M:251:PHE:C	2.85	0.50
5:M:404:BPH:HBB3	5:M:404:BPH:CHC	2.37	0.50
2:M:24:VAL:HG11	2:M:29:ARG:NH1	2.27	0.50
1:L:222:TYR:HD2	6:L:305:U10:H101	1.77	0.49
1:L:233:GLY:HA3	2:M:216:PHE:CE1	2.47	0.49
4:L:301:BCL:HBB2	4:M:403:BCL:NA	2.27	0.49
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.12	0.49
1:L:218:ASP:OD1	2:M:29:ARG:HD3	2.13	0.49
3:H:118:ARG:HD3	3:H:120:LEU:HD22	1.95	0.49
6:M:405:U10:H1M1	6:M:405:U10:H8	1.95	0.48
2:M:300:ASN:C	2:M:302:GLY:H	2.15	0.48
1:L:34:PHE:CE1	1:L:102:LEU:HD23	2.49	0.48
4:L:301:BCL:CGA	4:L:302:BCL:HBC1	2.43	0.48
1:L:18:GLY:O	1:L:21:LEU:HB2	2.14	0.48
6:L:304:U10:H3M1	6:L:305:U10:C7	2.44	0.48
2:M:40:GLY:HA2	2:M:43:GLY:O	2.13	0.48
4:M:401:BCL:HBB2	8:M:406:SPO:H243	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:404:BPH:HBC3	5:M:404:BPH:HHD	1.96	0.47
6:L:304:U10:O2	6:L:305:U10:C9	2.63	0.47
2:M:133:THR:HG21	2:M:147:ALA:HA	1.96	0.47
2:M:214:LEU:HD22	2:M:218:MET:SD	2.54	0.47
6:L:304:U10:C2	6:L:305:U10:C11	2.93	0.47
1:L:10:ARG:NH2	9:L:404:HOH:O	2.47	0.47
1:L:8:LYS:NZ	3:H:81:GLU:OE1	2.40	0.47
2:M:16:ALA:HB1	2:M:32:VAL:HG21	1.97	0.47
6:M:405:U10:H272	6:M:405:U10:C32	2.45	0.47
1:L:83:GLY:O	1:L:87:GLN:HG3	2.16	0.46
2:M:250:LEU:HD12	2:M:250:LEU:HA	1.82	0.46
1:L:216:PHE:CE2	6:L:305:U10:H112	2.51	0.46
4:M:401:BCL:HMB1	4:M:401:BCL:OBB	2.15	0.46
6:L:304:U10:H72	6:L:305:U10:C13	2.45	0.46
3:H:37:ARG:C	3:H:38:GLU:HG2	2.35	0.46
3:H:37:ARG:NH2	3:H:60:LYS:O	2.49	0.46
1:L:115:TYR:O	1:L:118:PRO:HG2	2.16	0.46
5:L:303:BPH:HBB1	2:M:210:TYR:CG	2.51	0.45
2:M:230:GLY:O	2:M:233:ARG:HG3	2.16	0.45
3:H:61:PRO:HA	3:H:76:PRO:HD2	1.99	0.45
5:M:404:BPH:H6C1	5:M:404:BPH:H4C1	1.71	0.45
2:M:68:PHE:HE1	8:M:406:SPO:H31	1.81	0.45
2:M:133:THR:HG22	2:M:147:ALA:CB	2.45	0.45
4:M:403:BCL:H2C	4:M:403:BCL:HBC2	1.76	0.45
1:L:38:THR:HG22	1:L:99:SER:HB2	1.96	0.45
4:M:403:BCL:HAA2	4:M:403:BCL:CBD	2.47	0.45
6:M:405:U10:H1M1	6:M:405:U10:C8	2.46	0.45
1:L:75:LEU:HD23	1:L:75:LEU:HA	1.79	0.44
3:H:30:TYR:O	3:H:34:GLU:HB2	2.16	0.44
1:L:193:LEU:HG	1:L:212:GLU:HG2	1.98	0.44
1:L:229:ILE:HD13	6:L:305:U10:H1M2	1.99	0.44
1:L:67:TYR:N	1:L:67:TYR:CD1	2.86	0.44
2:M:197:PHE:CE1	4:M:403:BCL:HBB2	2.53	0.43
6:L:304:U10:C1	6:L:305:U10:H122	2.47	0.43
2:M:13:ARG:O	3:H:140:PHE:HA	2.19	0.43
1:L:135:ARG:HB3	1:L:136:PRO:HD3	2.00	0.43
1:L:93:ALA:HA	5:L:303:BPH:H9C2	2.00	0.43
3:H:96:PHE:HB3	3:H:97:PRO:CD	2.47	0.43
3:H:84:PRO:O	3:H:85:ILE:HD13	2.18	0.42
3:H:118:ARG:CD	3:H:120:LEU:CD2	2.97	0.42
1:L:224:ILE:HG22	6:L:305:U10:H72	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:103:ASP:C	3:H:103:ASP:OD1	2.58	0.42
3:H:120:LEU:HA	3:H:226:THR:HG22	2.00	0.42
1:L:112:GLY:HA2	9:L:401:HOH:O	2.19	0.42
6:L:304:U10:C2	6:L:305:U10:H111	2.50	0.42
2:M:114:LEU:HD23	2:M:114:LEU:HA	1.82	0.41
2:M:145:HIS:O	2:M:146:THR:C	2.58	0.41
1:L:2:LEU:HD13	1:L:6:GLU:HG2	2.03	0.41
1:L:222:TYR:CD2	6:L:305:U10:H101	2.56	0.41
3:H:115:VAL:HG22	3:H:117:ARG:HG3	2.03	0.41
1:L:85:LEU:O	1:L:89:ILE:HG13	2.21	0.41
2:M:268:TRP:CD1	6:M:405:U10:H111	2.55	0.41
2:M:269:ALA:O	2:M:270:ILE:C	2.57	0.41
3:H:75:VAL:HA	3:H:76:PRO:C	2.40	0.41
8:M:406:SPO:H183	8:M:406:SPO:H15	1.88	0.41
1:L:206:MET:O	3:H:67:PRO:HG3	2.20	0.41
1:L:272:TRP:HA	1:L:275:ILE:HD12	2.02	0.41
2:M:282:ILE:H	2:M:282:ILE:HG13	1.74	0.41
1:L:163:THR:HG22	1:L:163:THR:O	2.21	0.41
1:L:271:TRP:CD1	1:L:271:TRP:N	2.82	0.41
2:M:243:THR:OG1	2:M:247:ARG:HD2	2.20	0.41
2:M:252:TRP:CD1	6:M:405:U10:C6	3.03	0.40
2:M:276:VAL:O	2:M:279:THR:HG22	2.21	0.40
2:M:190:SER:HB2	4:M:403:BCL:H3C	2.03	0.40
4:L:302:BCL:C19	5:L:303:BPH:H6C1	2.52	0.40
3:H:108:GLY:O	3:H:113:SER:HA	2.22	0.40
3:H:85:ILE:O	3:H:87:LEU:N	2.48	0.40
1:L:195:LEU:HD11	2:M:267:ARG:HG2	2.03	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	L	279/281 (99%)	253 (91%)	22 (8%)	4 (1%)	11	34
2	M	299/313 (96%)	276 (92%)	19 (6%)	4 (1%)	12	35
3	H	236/260 (91%)	218 (92%)	14 (6%)	4 (2%)	9	29
All	All	814/854 (95%)	747 (92%)	55 (7%)	12 (2%)	10	32

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	202	LYS
2	M	279	THR
2	M	301	HIS
3	H	86	ALA
3	H	185	ASP
2	M	54	SER
1	L	237	SER
2	M	195	ASN
1	L	10	ARG
1	L	271	TRP
3	H	116	ALA
3	H	246	PRO

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	L	215/220 (98%)	192 (89%)	23 (11%)	6	19
2	M	231/246 (94%)	205 (89%)	26 (11%)	6	17
3	H	186/208 (89%)	162 (87%)	24 (13%)	4	12
All	All	632/674 (94%)	559 (88%)	73 (12%)	5	16

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	ARG

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Mol	Chain	Res	Type
1	L	21	LEU
1	L	44	LEU
1	L	58	THR
1	L	63	LEU
1	L	67	TYR
1	L	102	LEU
1	L	126	LEU
1	L	129	LEU
1	L	154	LEU
1	L	158	SER
1	L	185	LEU
1	L	204	LYS
1	L	207	ARG
1	L	210	ASP
1	L	216	PHE
1	L	237	SER
1	L	246	LEU
1	L	247	CYS
1	L	249	ILE
1	L	254	ILE
1	L	271	TRP
1	L	272	TRP
2	M	26	LEU
2	M	29	ARG
2	M	39	LEU
2	M	62	SER
2	M	75	TRP
2	M	122	MET
2	M	124	VAL
2	M	133	THR
2	M	136	ARG
2	M	151	LEU
2	M	156	LEU
2	M	182	HIS
2	M	191	LEU
2	M	196	LEU
2	M	204	LEU
2	M	214	LEU
2	M	215	LEU
2	M	216	PHE
2	M	235	LEU
2	M	247	ARG

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Mol	Chain	Res	Type
2	M	250	LEU
2	M	265	ASN
2	M	279	THR
2	M	285	LEU
2	M	292	ASP
2	M	300	ASN
3	H	12	LEU
3	H	14	SER
3	H	34	GLU
3	H	52	ASN
3	H	70	ARG
3	H	72	THR
3	H	92	VAL
3	H	117	ARG
3	H	118	ARG
3	H	120	LEU
3	H	134	MET
3	H	146	LYS
3	H	151	LEU
3	H	175	MET
3	H	177	ARG
3	H	199	GLN
3	H	202	ARG
3	H	217	PRO
3	H	220	LYS
3	H	221	SER
3	H	225	VAL
3	H	231	ASP
3	H	232	LYS
3	H	248	ARG

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

Mol	Chain	Res	Type
1	L	60	ASN
3	H	52	ASN
3	H	98	HIS

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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$
6	U10	L	304	-	26,26,63	2.79	9 (34%)	31,34,79	2.25	8 (25%)
4	BCL	M	401	-	47,63,74	1.99	4 (8%)	55,101,115	2.47	17 (30%)
5	BPH	L	303	-	51,70,70	0.87	0	52,101,101	1.86	12 (23%)
4	BCL	L	302	-	58,74,74	1.49	5 (8%)	69,115,115	2.10	20 (28%)
6	U10	L	305	-	26,26,63	3.09	12 (46%)	31,34,79	2.56	13 (41%)
6	U10	M	405	-	48,48,63	2.84	14 (29%)	58,61,79	1.72	16 (27%)
8	SPO	M	406	-	33,34,41	1.30	3 (9%)	38,41,50	2.19	10 (26%)
4	BCL	L	301	-	58,74,74	1.56	4 (6%)	69,115,115	1.41	10 (14%)
4	BCL	M	403	-	58,74,74	1.32	4 (6%)	69,115,115	1.75	19 (27%)
5	BPH	M	404	-	39,58,70	1.17	3 (7%)	37,86,101	2.41	14 (37%)

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
6	U10	L	304	-	-	11/19/43/87	0/1/1/1
4	BCL	M	401	-	-	2/24/124/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	L	302	-	-	7/37/137/137	-
5	BPH	L	303	-	2/2/18/22	14/37/105/105	0/5/6/6
6	U10	L	305	-	-	10/19/43/87	0/1/1/1
6	U10	M	405	-	-	20/45/69/87	0/1/1/1
8	SPO	M	406	-	-	14/39/39/47	-
4	BCL	L	301	-	-	5/37/137/137	-
4	BCL	M	403	-	-	10/37/137/137	-
5	BPH	M	404	-	-	8/23/91/105	0/5/6/6

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	401	BCL	C1B-NB	9.13	1.43	1.35
6	L	305	U10	C8-C9	8.12	1.52	1.33
6	L	305	U10	C13-C14	8.03	1.52	1.33
4	M	401	BCL	C4B-NB	7.88	1.42	1.35
4	L	301	BCL	C4B-NB	7.87	1.42	1.35
6	M	405	U10	C33-C34	7.65	1.51	1.33
4	L	302	BCL	C4B-NB	7.09	1.41	1.35
4	L	301	BCL	C1B-NB	6.79	1.41	1.35
6	M	405	U10	C13-C14	6.78	1.49	1.33
6	L	304	U10	C13-C14	6.75	1.49	1.33
6	M	405	U10	C28-C29	6.56	1.48	1.33
6	L	304	U10	C8-C9	6.47	1.48	1.33
6	M	405	U10	C38-C39	6.45	1.50	1.32
6	M	405	U10	C23-C24	6.36	1.48	1.33
6	M	405	U10	C18-C19	6.26	1.48	1.33
4	M	403	BCL	C1B-NB	6.05	1.40	1.35
4	L	302	BCL	C1B-NB	5.70	1.40	1.35
4	M	403	BCL	C4B-NB	5.62	1.40	1.35
6	M	405	U10	C8-C9	5.36	1.45	1.33
6	L	304	U10	O4-C4	-5.25	1.24	1.36
6	L	304	U10	O3-C3	-4.80	1.25	1.36
6	L	305	U10	O4-C4	-4.56	1.25	1.36
6	M	405	U10	O4-C4	-4.49	1.25	1.36
8	M	406	SPO	C27-C28	3.94	1.38	1.34
6	L	305	U10	C6-C1	3.92	1.42	1.35
6	L	304	U10	C6-C1	3.83	1.42	1.35
6	M	405	U10	O3-C3	-3.81	1.27	1.36
6	L	305	U10	C7-C6	3.68	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	405	U10	C6-C1	3.63	1.41	1.35
6	L	304	U10	C3-C2	-3.24	1.39	1.48
6	L	304	U10	C4-C5	-3.07	1.40	1.48
4	M	401	BCL	C5-C3	3.01	1.57	1.51
6	L	305	U10	C19-C18	2.98	1.48	1.28
6	L	304	U10	C19-C18	2.91	1.48	1.28
8	M	406	SPO	C25-C23	2.78	1.51	1.45
6	L	305	U10	C11-C9	2.77	1.57	1.51
6	L	305	U10	O3-C3	-2.77	1.30	1.36
6	L	304	U10	C6-C5	-2.74	1.39	1.46
5	M	404	BPH	O2A-CGA	2.69	1.41	1.33
6	L	305	U10	C3-C2	-2.69	1.41	1.48
6	L	305	U10	C16-C14	2.58	1.56	1.51
4	L	302	BCL	C2D-C1D	-2.47	1.37	1.42
6	L	305	U10	C7-C8	2.46	1.54	1.50
5	M	404	BPH	C1A-C2A	2.40	1.54	1.51
4	M	401	BCL	C6-C5	2.36	1.60	1.52
6	M	405	U10	C4-C5	-2.34	1.42	1.48
4	L	301	BCL	C2D-C1D	-2.26	1.37	1.42
8	M	406	SPO	C26-C27	2.23	1.50	1.43
6	L	305	U10	C4-C5	-2.23	1.42	1.48
6	M	405	U10	C36-C34	2.13	1.55	1.51
6	M	405	U10	C31-C29	2.08	1.55	1.51
6	M	405	U10	C3-C2	-2.08	1.42	1.48
4	L	302	BCL	O2D-CGD	2.06	1.38	1.33
4	M	403	BCL	O2D-CGD	2.05	1.38	1.33
4	M	403	BCL	C4B-CHC	-2.05	1.35	1.41
4	L	302	BCL	C1A-CHA	-2.05	1.34	1.43
5	M	404	BPH	C5-C3	2.02	1.55	1.51
4	L	301	BCL	CHD-C4C	-2.01	1.35	1.41

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	401	BCL	C1-C2-C3	8.10	140.04	126.04
6	L	304	U10	C7-C6-C5	-7.46	109.51	118.48
4	L	302	BCL	O2D-CGD-CBD	7.24	124.14	111.27
4	L	302	BCL	O1D-CGD-CBD	-6.87	110.44	124.48
6	L	305	U10	C1-C6-C5	-6.84	113.14	119.58
4	M	401	BCL	O2A-C1-C2	6.13	124.76	108.64
5	L	303	BPH	C6-C5-C3	5.76	128.56	113.45
5	M	404	BPH	C1-O2A-CGA	5.67	131.31	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	401	BCL	C1C-NC-C4C	5.63	109.24	106.71
5	M	404	BPH	C5-C3-C2	5.54	132.32	121.12
8	M	406	SPO	C20-C21-C22	-5.50	112.21	123.47
8	M	406	SPO	C16-C17-C19	5.47	127.34	118.94
6	L	304	U10	C7-C8-C9	-5.40	117.80	126.79
5	L	303	BPH	CBC-CAC-C3C	-5.25	103.19	113.77
4	M	401	BCL	C4-C3-C2	-5.15	110.45	123.68
4	M	401	BCL	C5-C3-C2	5.10	131.44	121.12
6	L	305	U10	C6-C1-C2	4.92	123.07	119.18
4	M	403	BCL	O2D-CGD-CBD	4.83	119.85	111.27
5	M	404	BPH	C1A-C2A-C3A	-4.82	98.25	102.84
4	L	302	BCL	C1C-NC-C4C	4.53	108.74	106.71
4	M	403	BCL	CHD-C4C-NC	4.52	130.10	125.08
4	M	401	BCL	O2D-CGD-CBD	4.48	119.23	111.27
6	M	405	U10	C35-C34-C36	4.39	122.66	115.27
5	L	303	BPH	CAC-C3C-C4C	-4.27	104.20	113.73
4	M	401	BCL	C6-C5-C3	4.20	124.46	113.45
6	L	305	U10	C8-C7-C6	4.18	123.30	112.05
4	M	403	BCL	CAD-C3D-C4D	-4.15	106.15	108.47
8	M	406	SPO	C24-C23-C25	4.12	124.56	118.08
6	M	405	U10	C30-C29-C31	4.10	122.17	115.27
6	L	305	U10	C3M-O3-C3	4.04	130.78	116.47
5	M	404	BPH	CAC-C3C-C2C	-4.01	104.23	114.26
4	L	302	BCL	OBD-CAD-CBD	3.99	131.60	125.89
5	M	404	BPH	CMA-C3A-C4A	-3.96	105.70	114.38
8	M	406	SPO	C15-C16-C17	-3.83	115.65	126.42
5	L	303	BPH	C11-C10-C8	3.78	128.13	115.92
6	M	405	U10	C15-C14-C16	3.78	121.62	115.27
8	M	406	SPO	C18-C17-C19	-3.77	117.64	122.92
4	L	302	BCL	C4C-CHD-C1D	-3.71	120.41	125.88
6	L	305	U10	O2-C2-C3	-3.67	113.14	120.93
5	M	404	BPH	O2D-CGD-CBD	3.63	115.59	111.00
4	L	302	BCL	OBD-CAD-C3D	-3.60	122.00	127.98
6	L	305	U10	C11-C9-C8	3.57	128.35	121.12
6	L	304	U10	C10-C9-C11	3.57	121.28	115.27
5	M	404	BPH	C4-C3-C5	-3.55	109.31	115.27
5	M	404	BPH	CMD-C2D-C3D	3.55	131.31	124.68
6	L	305	U10	C15-C14-C16	3.43	121.04	115.27
4	L	302	BCL	O2A-CGA-CBA	3.39	122.56	111.91
6	M	405	U10	C17-C18-C19	-3.30	119.72	127.66
8	M	406	SPO	C2-C1-C4	-3.28	105.82	110.86
4	M	401	BCL	CAD-C3D-C4D	-3.28	106.64	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	302	BCL	CHD-C4C-NC	3.27	128.71	125.08
6	M	405	U10	C1M-C1-C6	-3.27	119.07	124.40
4	M	401	BCL	O2A-CGA-CBA	3.24	122.09	111.91
6	L	305	U10	C4-C3-C2	-3.16	114.47	120.68
5	L	303	BPH	CMD-C2D-C3D	3.15	130.58	124.68
4	M	403	BCL	OBB-CAB-C3B	3.13	125.55	119.99
6	M	405	U10	C12-C13-C14	-3.13	120.13	127.66
4	M	401	BCL	OBD-CAD-C3D	-3.09	122.85	127.98
4	L	301	BCL	C1-O2A-CGA	3.04	124.41	116.44
8	M	406	SPO	C29-C28-C30	3.01	120.34	115.27
4	M	403	BCL	CED-O2D-CGD	2.99	122.71	115.94
4	L	302	BCL	C4-C3-C5	2.98	120.29	115.27
4	L	301	BCL	C4C-CHD-C1D	-2.98	121.49	125.88
6	L	304	U10	C15-C14-C16	2.96	120.26	115.27
6	L	304	U10	O4-C4-C3	-2.95	112.51	123.64
4	L	301	BCL	O2A-C1-C2	-2.94	100.90	108.64
4	M	403	BCL	O2A-C1-C2	2.92	116.30	108.64
4	M	403	BCL	O2A-CGA-CBA	2.91	121.05	111.91
4	L	302	BCL	C5-C3-C2	-2.90	115.26	121.12
4	M	403	BCL	C1C-NC-C4C	2.85	107.99	106.71
6	L	305	U10	C10-C9-C8	-2.84	116.38	123.68
6	M	405	U10	C7-C8-C9	-2.84	122.06	126.79
6	L	304	U10	C12-C13-C14	-2.81	120.89	127.66
4	L	301	BCL	O2D-CGD-CBD	2.77	116.19	111.27
4	M	401	BCL	CHB-C4A-NA	2.77	128.34	124.51
4	L	301	BCL	C1C-NC-C4C	2.73	107.94	106.71
5	M	404	BPH	C6-C5-C3	2.72	120.59	113.45
4	M	403	BCL	O2D-CGD-O1D	-2.70	118.55	123.84
8	M	406	SPO	C24-C23-C22	-2.67	119.19	122.92
4	M	403	BCL	C4C-CHD-C1D	-2.67	121.95	125.88
5	L	303	BPH	C1A-C2A-C3A	-2.67	100.30	102.84
4	L	301	BCL	O2A-CGA-CBA	2.67	120.27	111.91
6	L	304	U10	O5-C5-C6	-2.66	116.89	121.55
5	M	404	BPH	OBD-CAD-CBD	-2.63	121.96	125.82
5	L	303	BPH	CAA-CBA-CGA	-2.59	105.68	113.25
6	M	405	U10	C30-C29-C28	-2.58	117.06	123.68
4	M	401	BCL	CHD-C4C-NC	2.58	127.94	125.08
4	L	302	BCL	CED-O2D-CGD	2.57	121.75	115.94
6	L	305	U10	C1M-C1-C6	-2.55	120.24	124.40
4	L	302	BCL	CHB-C4A-NA	2.55	128.04	124.51
6	M	405	U10	C10-C9-C11	2.53	119.53	115.27
4	M	401	BCL	C1B-CHB-C4A	-2.52	125.13	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	305	U10	C16-C17-C18	2.50	119.07	112.63
6	M	405	U10	C4M-O4-C4	2.50	125.32	116.47
8	M	406	SPO	C15-C14-C12	-2.49	123.76	127.31
4	M	401	BCL	C4C-CHD-C1D	-2.48	122.22	125.88
4	M	403	BCL	O2A-CGA-O1A	-2.47	117.36	123.59
6	M	405	U10	C22-C23-C24	-2.47	121.72	127.66
5	L	303	BPH	C6-C7-C8	2.47	123.89	115.92
4	M	403	BCL	C11-C10-C8	-2.41	108.12	115.92
6	L	304	U10	C10-C9-C8	-2.40	117.51	123.68
4	L	302	BCL	CMB-C2B-C1B	-2.40	124.78	128.46
4	M	401	BCL	C1-O2A-CGA	2.38	122.68	116.44
4	L	302	BCL	O2A-CGA-O1A	-2.37	117.61	123.59
4	L	302	BCL	C11-C12-C13	-2.35	108.32	115.92
4	L	301	BCL	C2A-C1A-CHA	-2.35	119.75	123.86
4	L	301	BCL	C4A-NA-C1A	-2.34	105.65	106.71
4	L	302	BCL	OBB-CAB-C3B	2.34	124.14	119.99
4	M	403	BCL	C4B-C3B-CAB	-2.33	122.63	127.13
5	L	303	BPH	CMC-C2C-C1C	-2.32	109.30	114.38
4	M	401	BCL	O1A-CGA-CBA	-2.31	114.74	123.73
6	L	305	U10	C4M-O4-C4	2.30	124.62	116.47
6	M	405	U10	C3M-O3-C3	2.29	124.58	116.47
4	M	403	BCL	CBC-CAC-C3C	-2.26	108.44	113.47
5	M	404	BPH	C3D-CAD-CBD	2.24	110.55	107.61
4	L	301	BCL	C4-C3-C5	2.23	119.03	115.27
4	L	301	BCL	CHD-C4C-NC	2.23	127.55	125.08
6	M	405	U10	C15-C14-C13	-2.22	117.99	123.68
5	M	404	BPH	C7-C6-C5	2.21	123.51	113.44
4	L	302	BCL	C1-O2A-CGA	2.21	122.24	116.44
4	M	401	BCL	O2D-CGD-O1D	-2.20	119.54	123.84
4	M	403	BCL	C16-C15-C13	-2.16	108.93	115.92
4	L	302	BCL	C2A-C1A-CHA	-2.16	120.09	123.86
4	M	403	BCL	OBD-CAD-C3D	-2.15	124.42	127.98
4	L	302	BCL	C16-C17-C18	-2.13	105.96	115.98
4	M	403	BCL	C3C-C4C-CHD	-2.12	118.85	123.39
5	M	404	BPH	C4C-C3C-C2C	-2.12	100.82	102.84
4	M	403	BCL	C16-C17-C18	-2.09	106.12	115.98
6	M	405	U10	C27-C28-C29	-2.09	122.64	127.66
5	L	303	BPH	CMA-C3A-C4A	-2.08	109.82	114.38
5	M	404	BPH	C4-C3-C2	-2.07	118.36	123.68
6	M	405	U10	C35-C34-C33	-2.07	118.38	123.68
8	M	406	SPO	C26-C25-C23	2.06	132.21	126.42
5	L	303	BPH	C10-C8-C7	2.06	122.95	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	305	U10	O5-C5-C4	-2.03	116.62	120.93
4	L	302	BCL	C4B-CHC-C1C	-2.03	126.10	130.12
5	L	303	BPH	C4-C3-C5	-2.01	111.90	115.27
4	M	403	BCL	C11-C12-C13	-2.01	109.44	115.92
6	M	405	U10	C20-C19-C21	2.00	118.64	115.27

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	303	BPH	C13
5	L	303	BPH	C8

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	401	BCL	O2A-C1-C2-C3
5	L	303	BPH	O2A-C1-C2-C3
5	L	303	BPH	C6-C7-C8-C10
5	M	404	BPH	C4-C3-C5-C6
6	L	304	U10	C7-C8-C9-C10
6	L	304	U10	C7-C8-C9-C11
6	L	304	U10	C9-C11-C12-C13
6	L	304	U10	C12-C13-C14-C15
6	L	304	U10	C14-C16-C17-C18
6	L	305	U10	C7-C8-C9-C11
6	M	405	U10	C14-C16-C17-C18
6	M	405	U10	C24-C26-C27-C28
6	M	405	U10	C27-C28-C29-C30
6	M	405	U10	C27-C28-C29-C31
8	M	406	SPO	C2-C1-O1-CM1
8	M	406	SPO	C1-C4-C5-C6
6	M	405	U10	C37-C38-C39-C40
6	M	405	U10	C37-C38-C39-C41
6	L	305	U10	C15-C14-C16-C17
5	M	404	BPH	C2-C3-C5-C6
6	L	305	U10	C7-C8-C9-C10
6	M	405	U10	C12-C13-C14-C15
6	M	405	U10	C32-C33-C34-C35
6	L	304	U10	C12-C13-C14-C16
6	M	405	U10	C12-C13-C14-C16
6	M	405	U10	C32-C33-C34-C36
6	L	305	U10	C12-C11-C9-C10

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Mol	Chain	Res	Type	Atoms
6	L	305	U10	C12-C11-C9-C8
6	L	305	U10	C14-C16-C17-C18
8	M	406	SPO	C28-C30-C31-C32
5	L	303	BPH	C14-C13-C15-C16
4	L	301	BCL	C15-C16-C17-C18
5	M	404	BPH	C3-C5-C6-C7
4	L	302	BCL	C13-C15-C16-C17
5	L	303	BPH	C5-C6-C7-C8
6	L	305	U10	C13-C14-C16-C17
5	L	303	BPH	C4-C3-C5-C6
6	M	405	U10	C28-C29-C31-C32
5	L	303	BPH	C15-C16-C17-C18
4	M	403	BCL	C6-C7-C8-C10
5	L	303	BPH	C2-C3-C5-C6
5	M	404	BPH	CBA-CGA-O2A-C1
6	M	405	U10	C30-C29-C31-C32
4	M	403	BCL	C6-C7-C8-C9
5	M	404	BPH	O1A-CGA-O2A-C1
4	L	302	BCL	C15-C16-C17-C18
5	M	404	BPH	C5-C6-C7-C8
8	M	406	SPO	C3-C1-O1-CM1
8	M	406	SPO	C2-C1-C4-C5
6	M	405	U10	C20-C19-C21-C22
5	L	303	BPH	C3-C5-C6-C7
6	M	405	U10	C18-C19-C21-C22
4	M	403	BCL	C11-C10-C8-C9
4	M	403	BCL	C11-C10-C8-C7
8	M	406	SPO	C12-C14-C15-C16
5	L	303	BPH	CAD-CBD-CGD-O2D
6	M	405	U10	C15-C14-C16-C17
6	L	304	U10	C5-C4-O4-C4M
4	M	403	BCL	CHA-CBD-CGD-O1D
5	L	303	BPH	C13-C15-C16-C17
8	M	406	SPO	C10-C11-C12-C13
8	M	406	SPO	C24-C23-C25-C26
4	M	403	BCL	C3-C5-C6-C7
4	L	301	BCL	C12-C13-C15-C16
5	L	303	BPH	C11-C12-C13-C15
4	L	301	BCL	C14-C13-C15-C16
4	L	302	BCL	C14-C13-C15-C16
4	L	302	BCL	C12-C13-C15-C16
4	L	302	BCL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
6	L	305	U10	C2-C3-O3-C3M
5	L	303	BPH	C6-C7-C8-C9
8	M	406	SPO	C18-C17-C19-C20
4	M	403	BCL	C11-C12-C13-C15
4	L	301	BCL	C16-C17-C18-C19
6	L	305	U10	C16-C17-C18-C19
4	M	403	BCL	C10-C11-C12-C13
5	L	303	BPH	C8-C10-C11-C12
6	L	304	U10	C2-C3-O3-C3M
8	M	406	SPO	C16-C17-C19-C20
6	M	405	U10	C9-C11-C12-C13
4	L	302	BCL	C16-C17-C18-C20
8	M	406	SPO	C30-C31-C32-C33
6	L	304	U10	C12-C11-C9-C10
5	L	303	BPH	C10-C11-C12-C13
4	L	301	BCL	C16-C17-C18-C20
4	M	403	BCL	CAA-CBA-CGA-O2A
6	M	405	U10	C5-C4-O4-C4M
6	L	304	U10	C4-C3-O3-C3M
4	L	302	BCL	CAD-CBD-CGD-O2D
4	M	401	BCL	CAD-CBD-CGD-O2D
5	M	404	BPH	CAD-CBD-CGD-O2D
8	M	406	SPO	C22-C23-C25-C26
5	M	404	BPH	O2A-C1-C2-C3
6	M	405	U10	C13-C14-C16-C17
8	M	406	SPO	C3-C1-C4-C5
6	L	304	U10	C12-C11-C9-C8
6	L	305	U10	C4-C3-O3-C3M
6	M	405	U10	C34-C36-C37-C38
4	M	403	BCL	C11-C12-C13-C14
8	M	406	SPO	C5-C6-C7-C9
6	M	405	U10	C29-C31-C32-C33

There are no ring outliers.

10 monomers are involved in 97 short contacts:

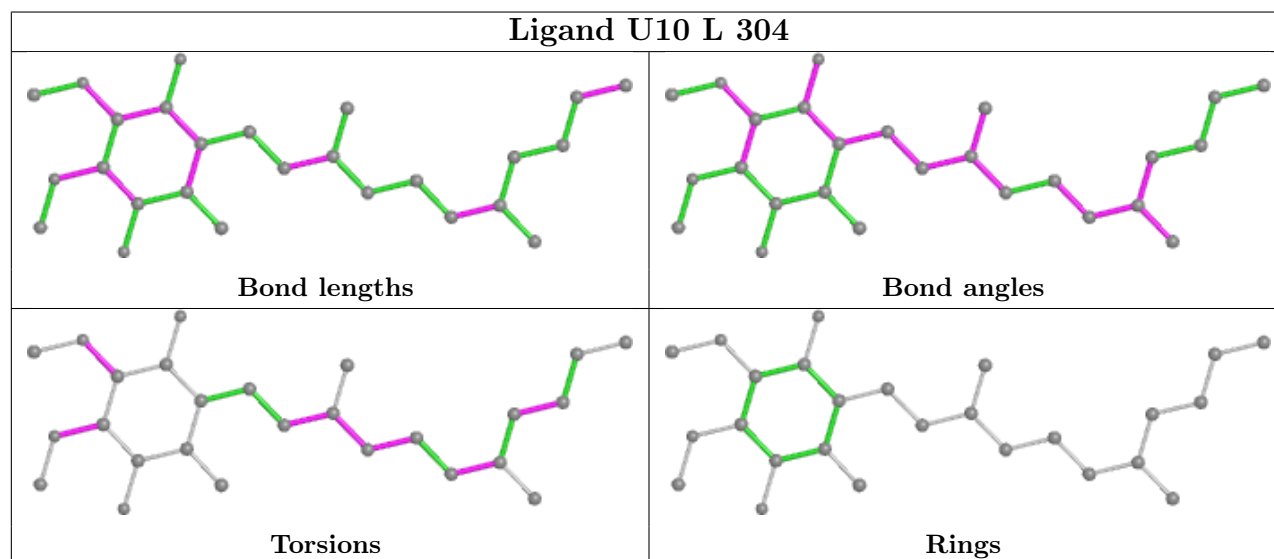
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	304	U10	34	0
4	M	401	BCL	6	0
5	L	303	BPH	9	0
4	L	302	BCL	4	0
6	L	305	U10	39	0

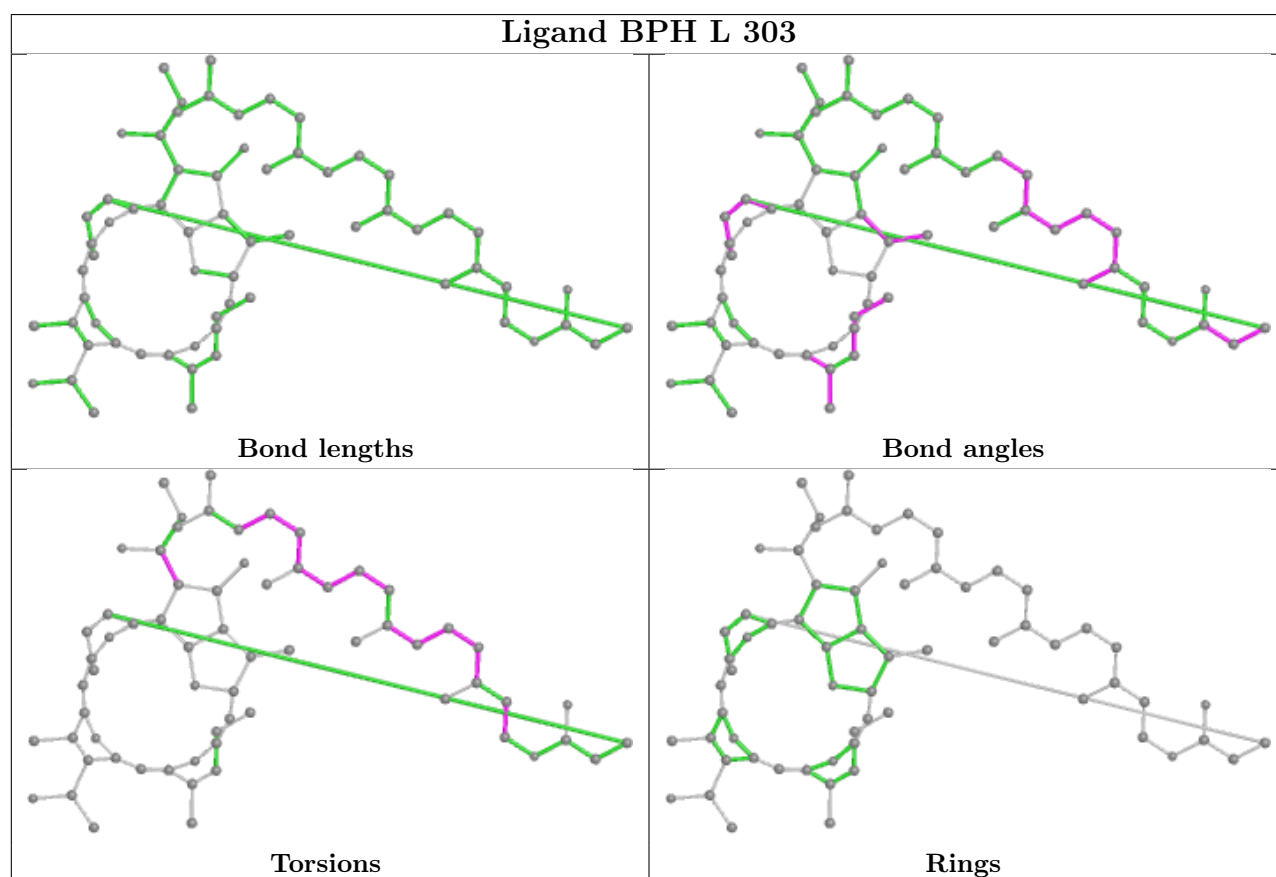
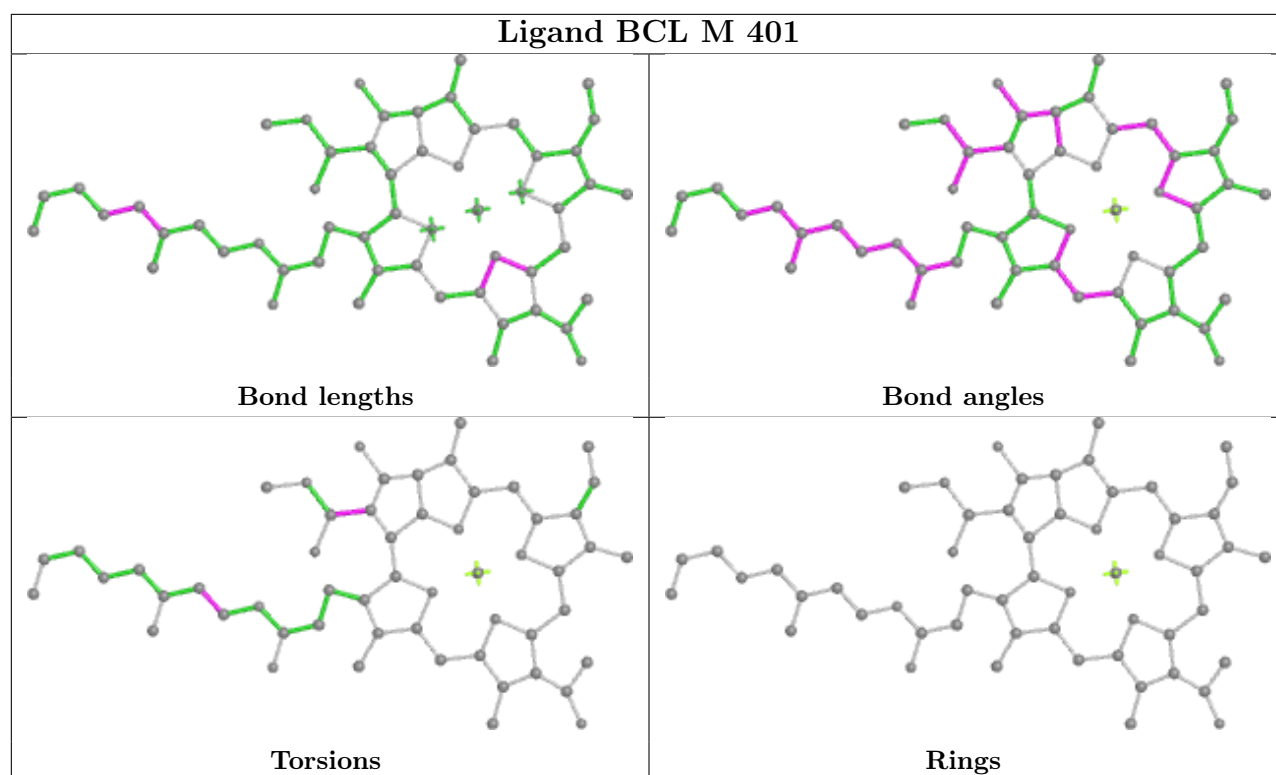
Continued on next page...

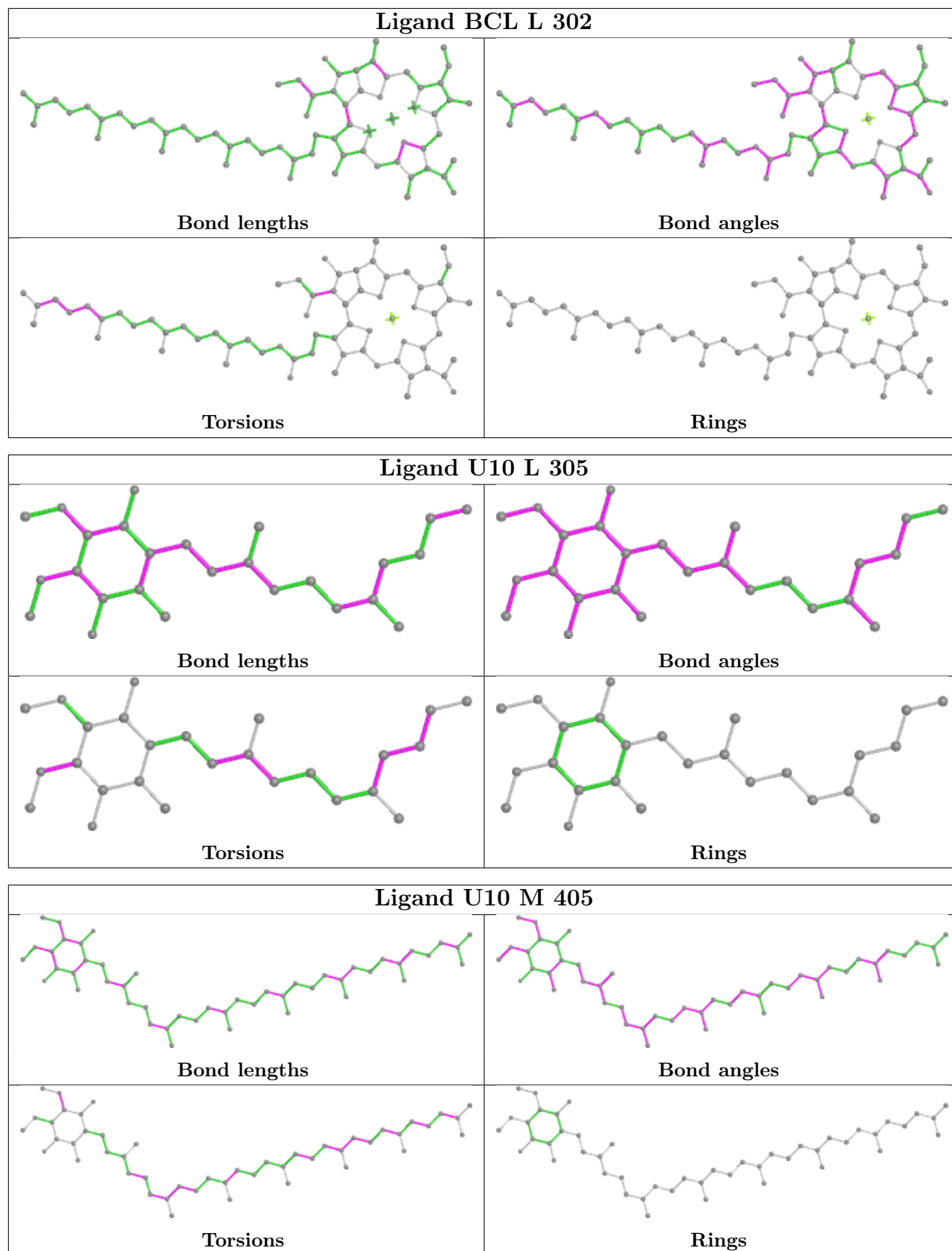
Continued from previous page...

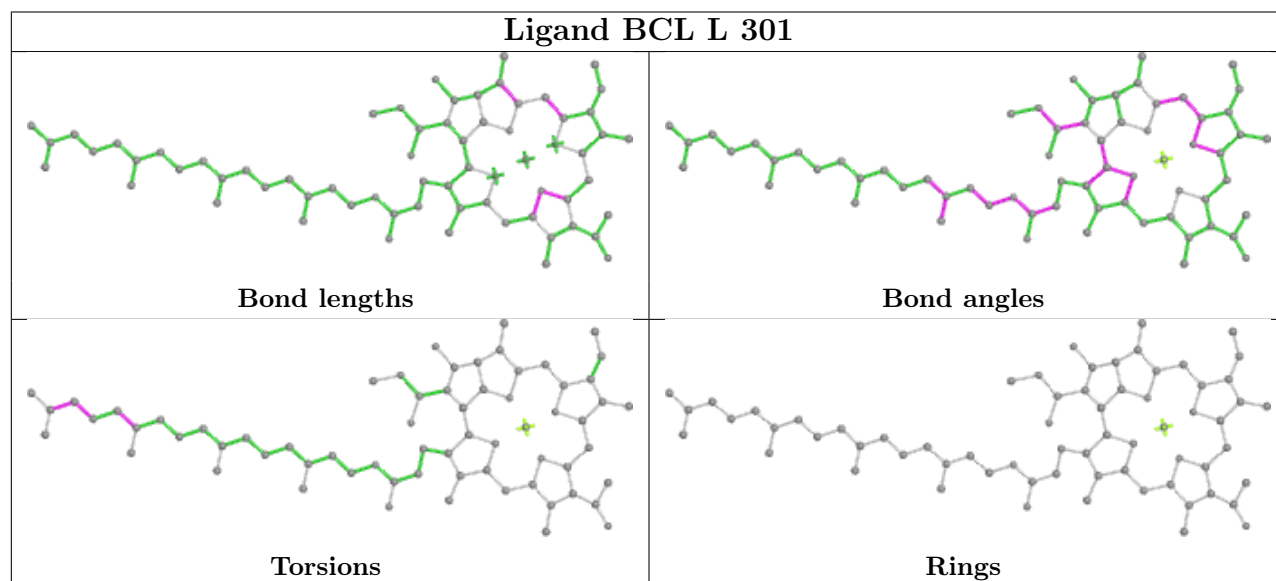
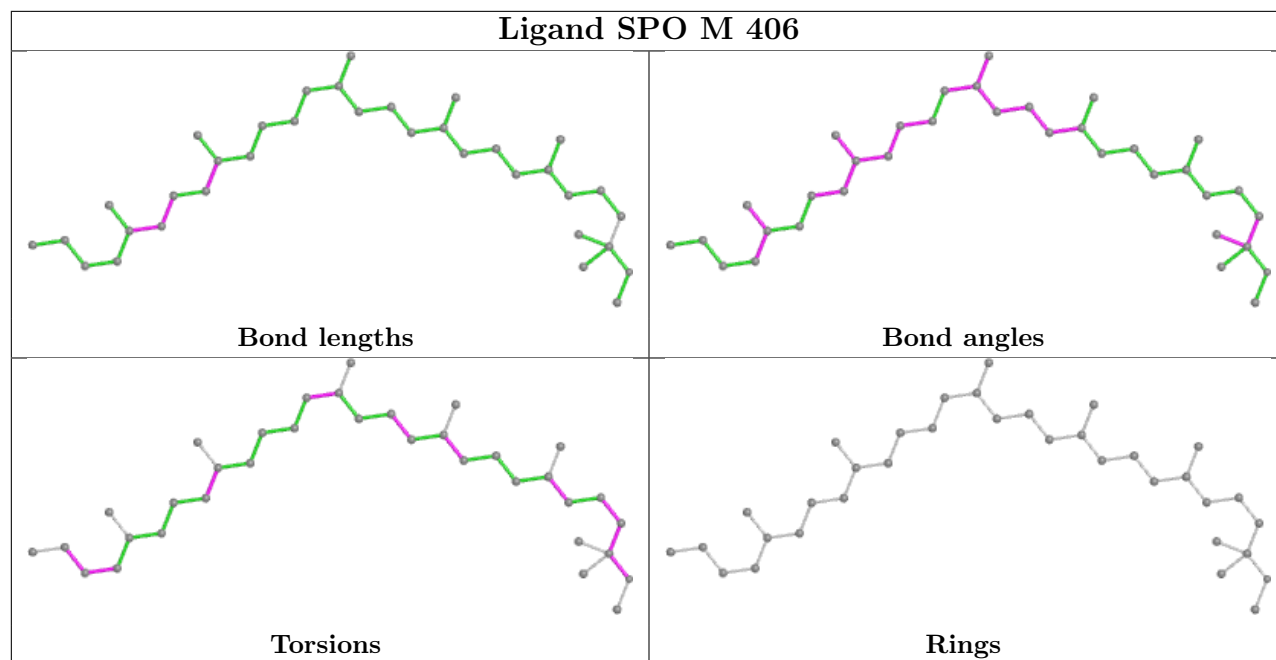
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	405	U10	6	0
8	M	406	SPO	6	0
4	L	301	BCL	4	0
4	M	403	BCL	14	0
5	M	404	BPH	7	0

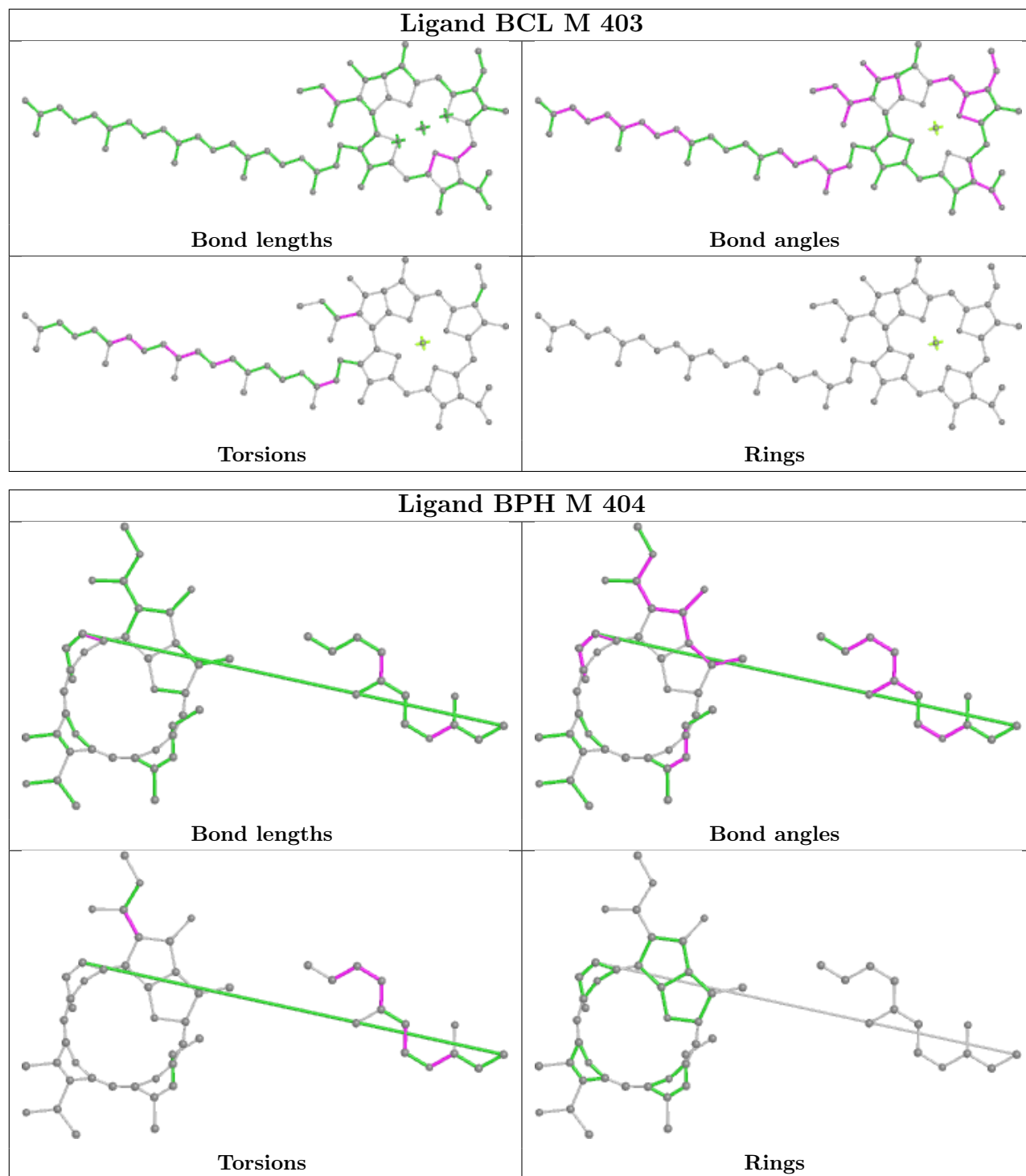
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [\(i\)](#)

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	L	281/281 (100%)	-0.65	5 (1%) 68 69	30, 44, 77, 91	0
2	M	301/313 (96%)	-0.73	3 (0%) 82 83	29, 47, 75, 82	0
3	H	238/260 (91%)	-0.54	4 (1%) 70 71	34, 46, 61, 94	0
All	All	820/854 (96%)	-0.65	12 (1%) 73 75	29, 46, 74, 94	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	246	PRO	4.2
1	L	281	GLY	3.9
1	L	270	PRO	3.3
2	M	301	HIS	2.9
1	L	72	GLU	2.5
1	L	276	PRO	2.5
3	H	245	ALA	2.4
2	M	300	ASN	2.3
1	L	277	GLY	2.3
3	H	247	LYS	2.2
2	M	80	TRP	2.2
3	H	220	LYS	2.1

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 [i](#)

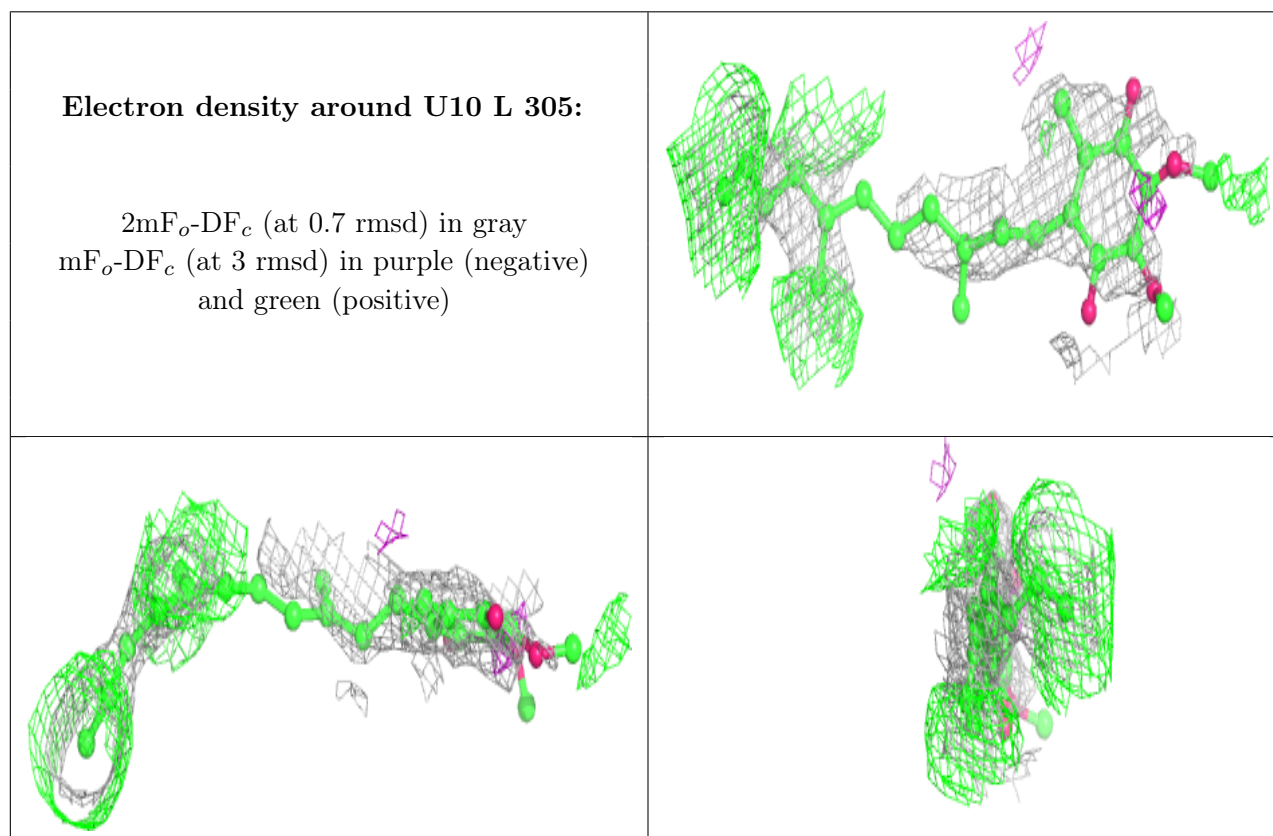
There are no monosaccharides in this entry.

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.

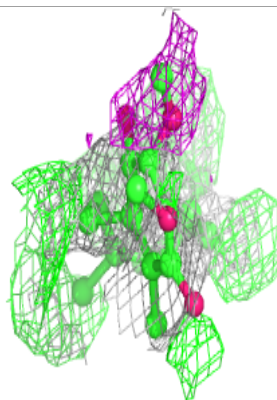
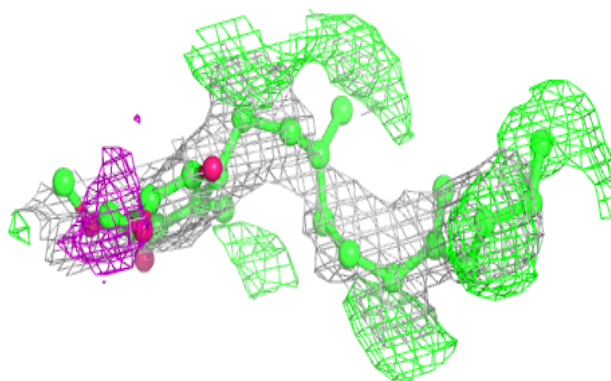
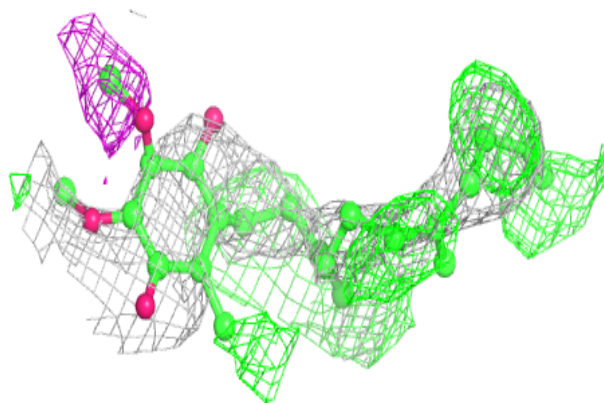
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	U10	L	305	26/63	0.70	0.40	46,55,66,67	26
6	U10	L	304	26/63	0.81	0.37	67,90,94,99	26
8	SPO	M	406	35/42	0.90	0.21	54,68,86,87	0
6	U10	M	405	48/63	0.91	0.17	41,52,83,85	0
4	BCL	M	401	55/66	0.94	0.15	33,39,69,71	0
4	BCL	M	403	66/66	0.97	0.15	32,41,55,70	0
5	BPH	M	404	53/65	0.97	0.12	33,46,59,64	0
4	BCL	L	301	66/66	0.97	0.15	29,39,43,55	0
5	BPH	L	303	65/65	0.98	0.12	26,35,40,46	0
4	BCL	L	302	66/66	0.98	0.09	27,33,48,55	0
7	FE	M	402	1/1	1.00	0.07	35,35,35,35	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.

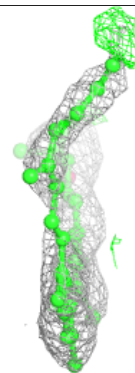
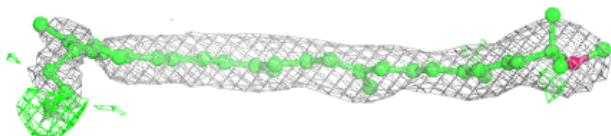
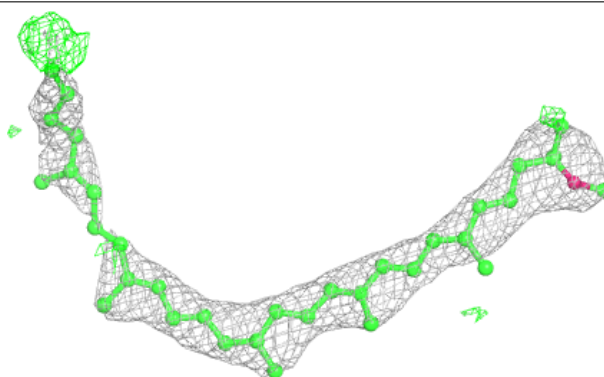


Electron density around U10 L 304:

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

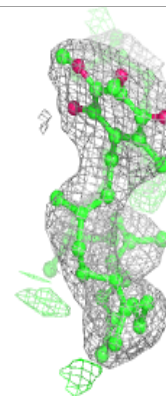
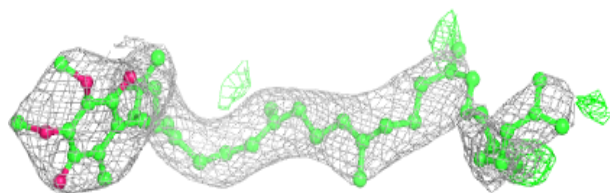
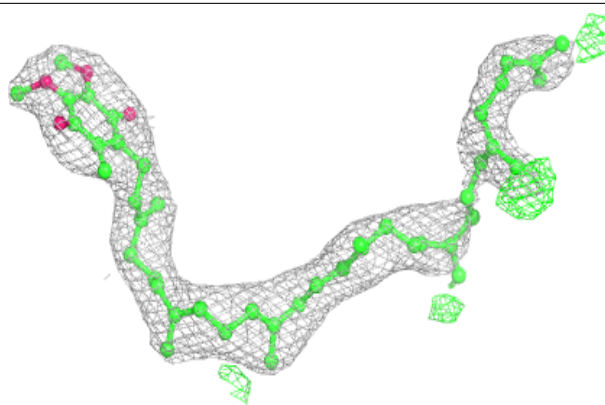
**Electron density around SPO M 406:**

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



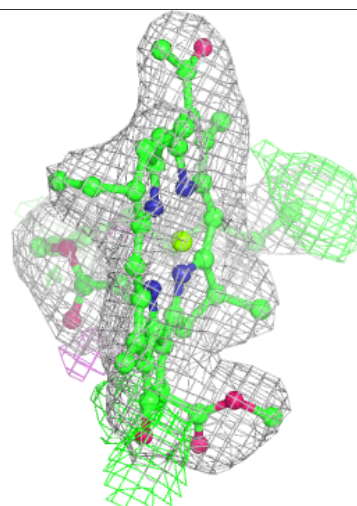
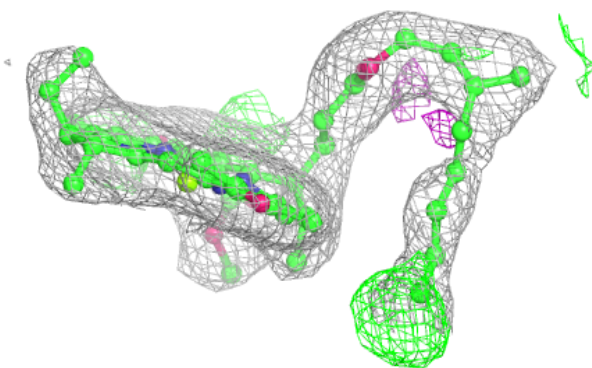
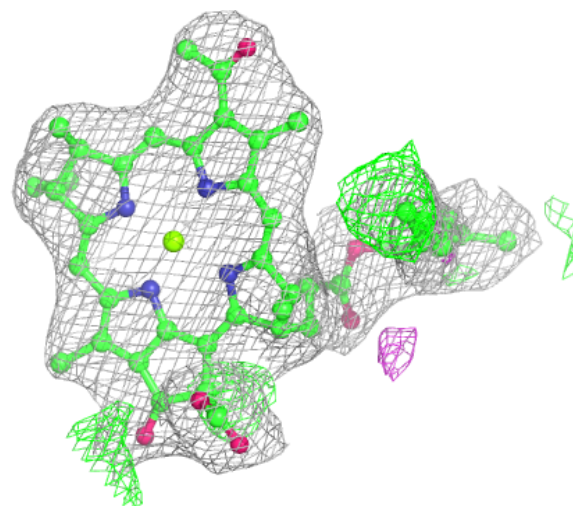
Electron density around U10 M 405:

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



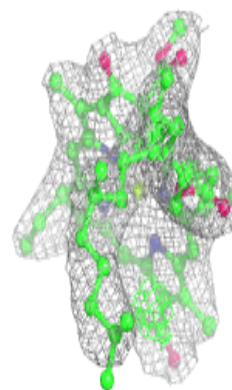
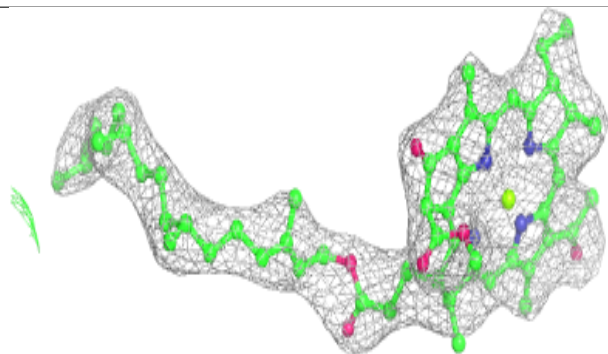
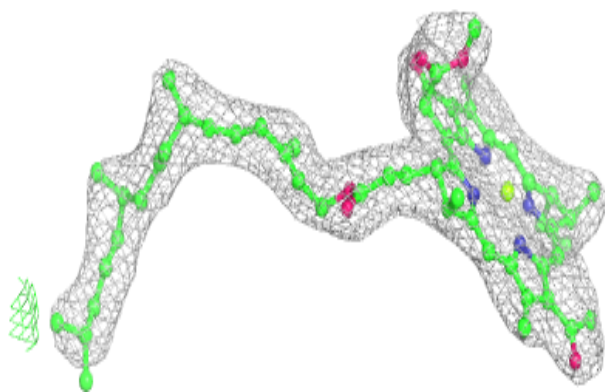
Electron density around BCL M 401:

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

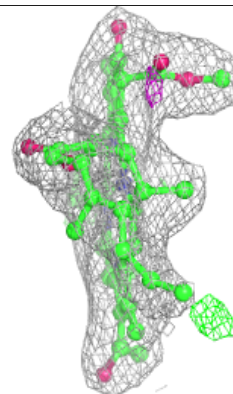
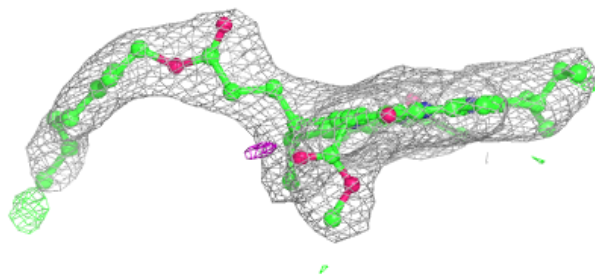
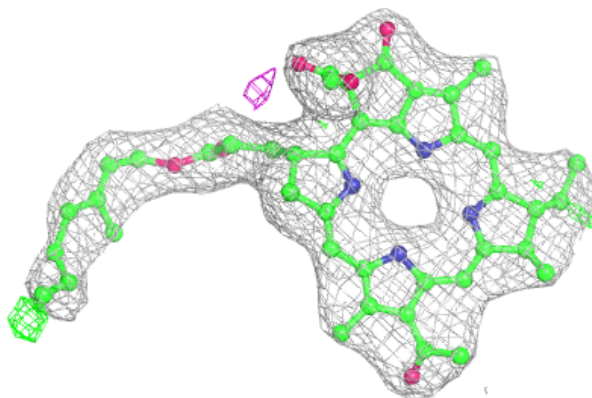


Electron density around BCL M 403:

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

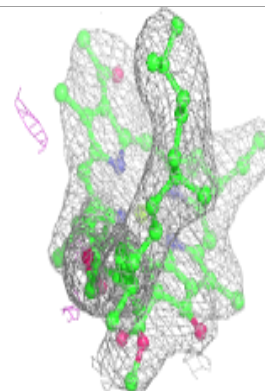
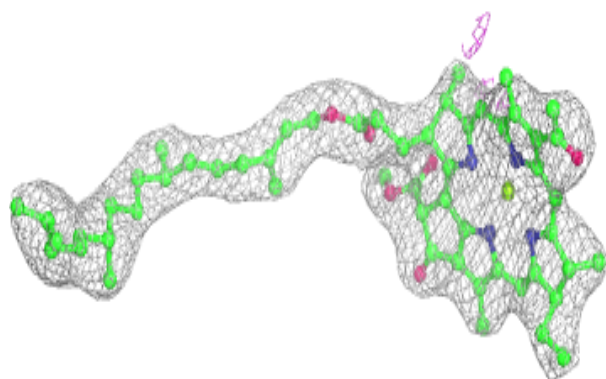
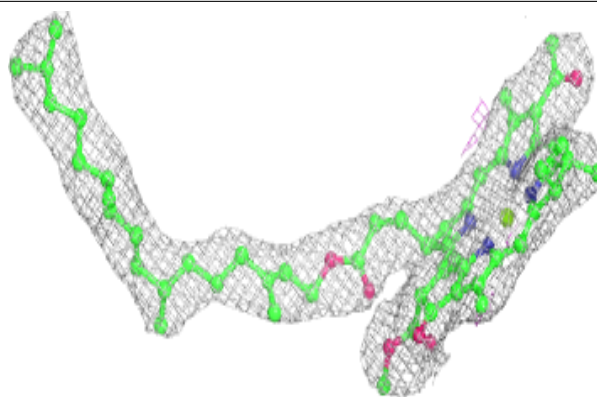
**Electron density around BPH M 404:**

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

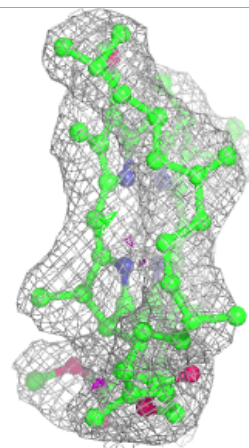
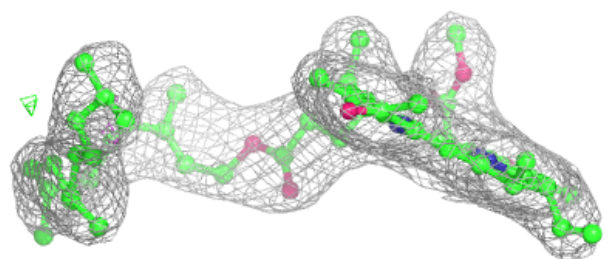
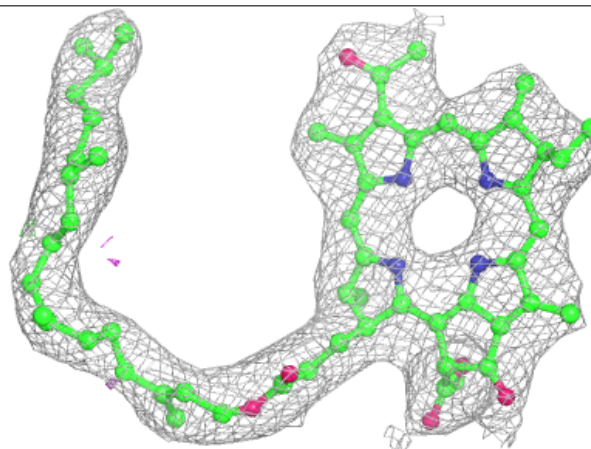


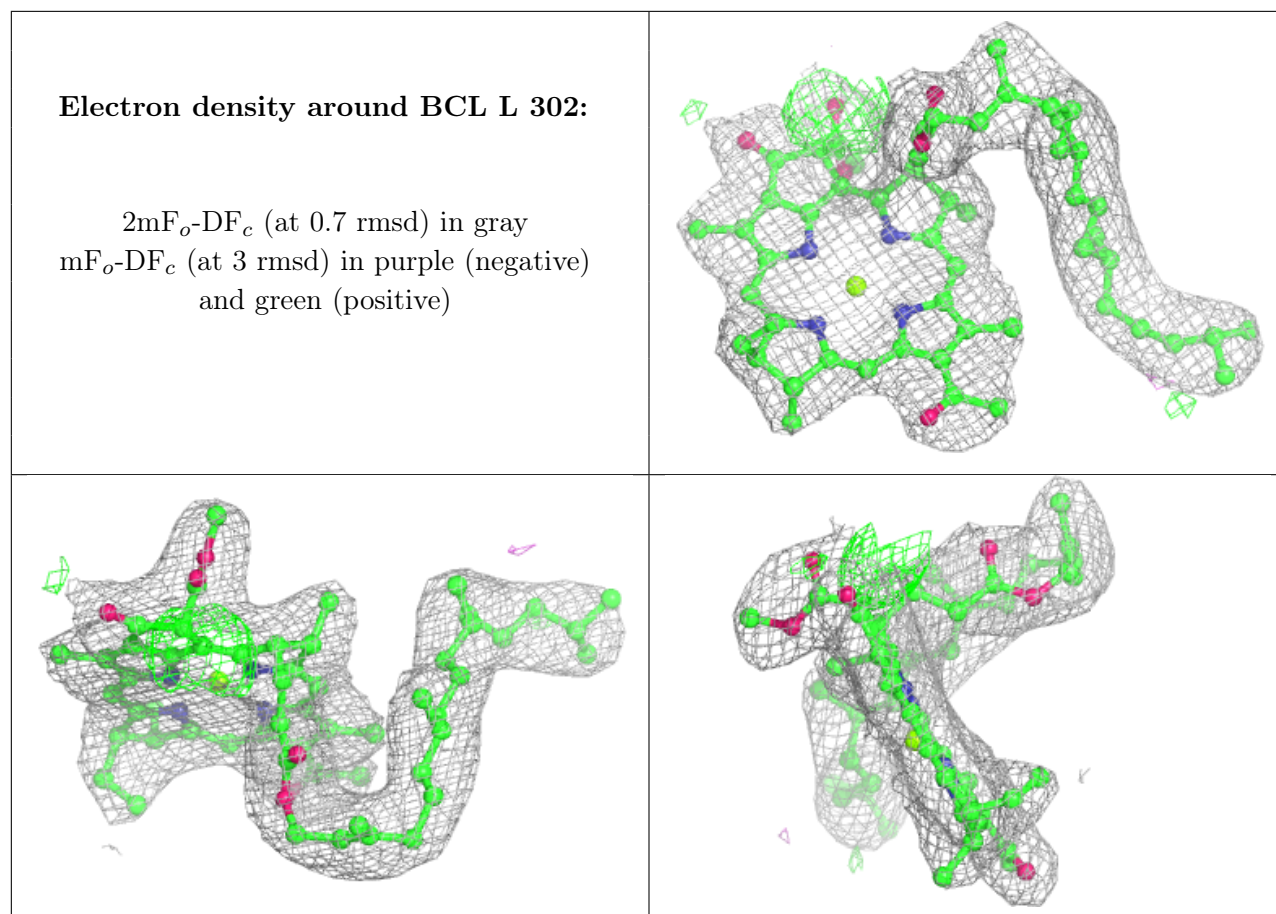
Electron density around BCL L 301:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.