



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:11 pm BST

PDB ID : 4TQQ  
Title : Photosynthetic Reaction Center from *R. sphaeroides* Analyzed at Room Temperature on an X-ray Transparent Microfluidic Chip  
Authors : Schieferstein, J.M.; Khvostichenko, D.S.; Pawate, A.S.; Kenis, P.J.A.  
Deposited on : 2014-06-11  
Resolution : 2.50 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](mailto: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.

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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	:	2.11
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)	:	2.11

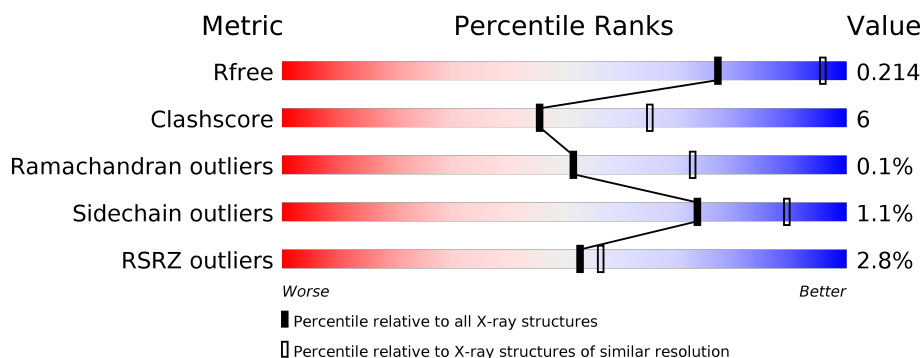
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	240	<div> <div>3%</div> <div>85%</div> <div>14%</div> </div>
2	L	281	<div> <div>3%</div> <div>92%</div> <div>7%</div> </div>
3	M	302	<div> <div>2%</div> <div>91%</div> <div>8%</div> </div>

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
6	UQ1	L	304	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7114 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

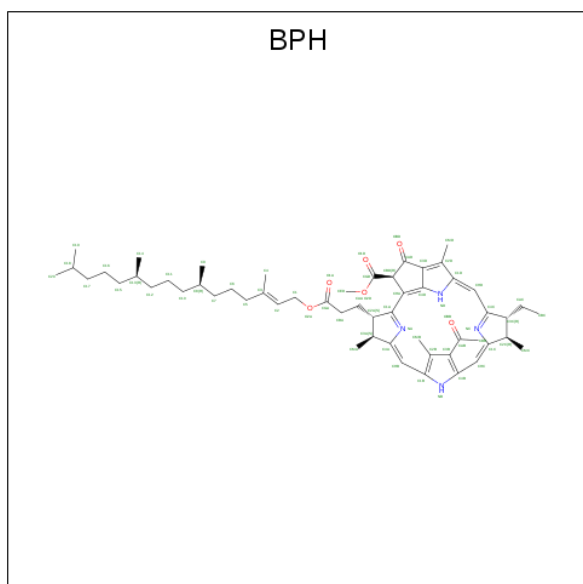
- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2231	1507	355	361	8			

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

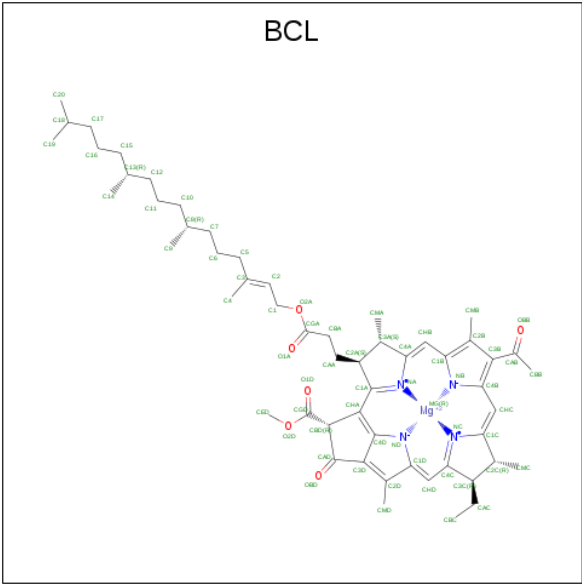
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	0	0
			2408	1607	394	397	10			

- Molecule 4 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



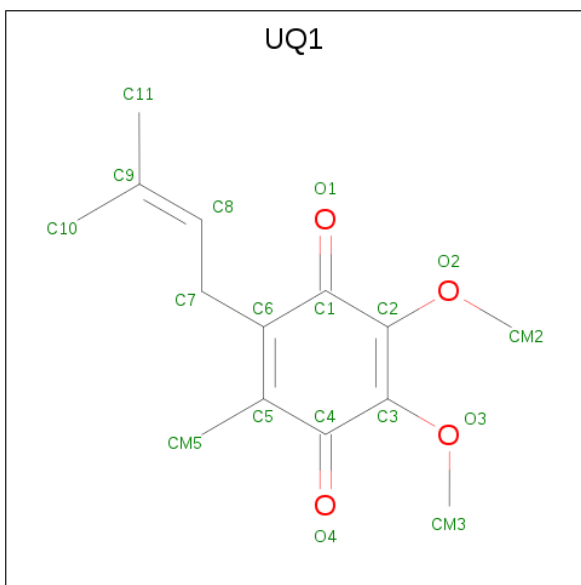
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	L	1	Total	C	N	O	0	0
			65	55	4	6		
4	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



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

- Molecule 6 is UBIQUINONE-1 (three-letter code: UQ1) (formula: C<sub>14</sub>H<sub>18</sub>O<sub>4</sub>).

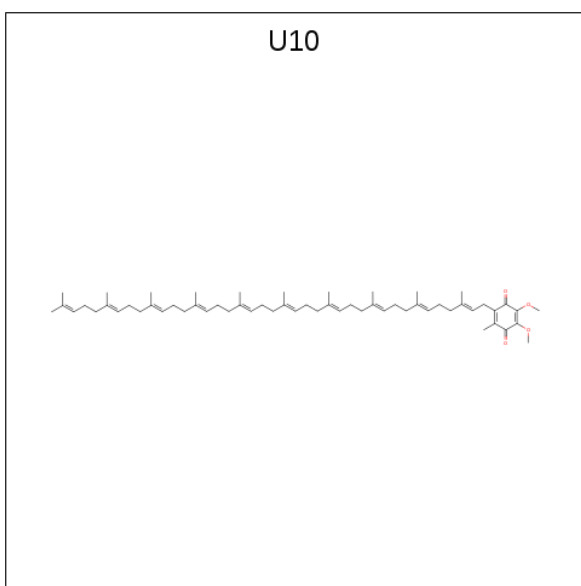


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			18	14	4		

- Molecule 7 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			62	58	4		

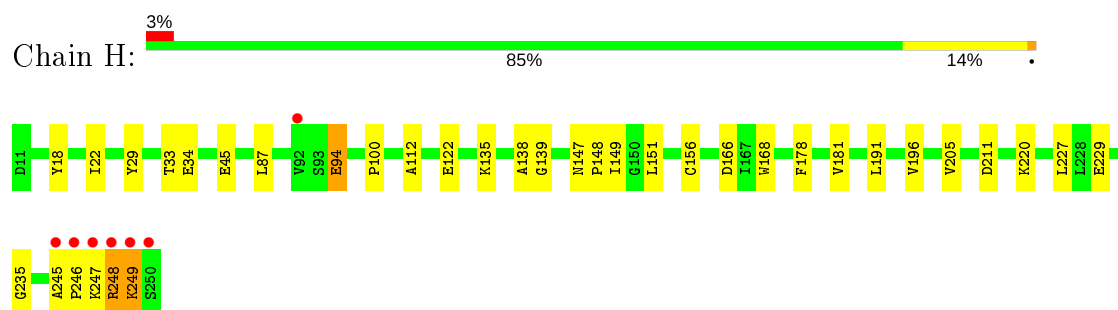
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	64	Total	O	0	0
			64	64		
9	L	53	Total	O	0	0
			53	53		
9	M	69	Total	O	0	0
			69	69		

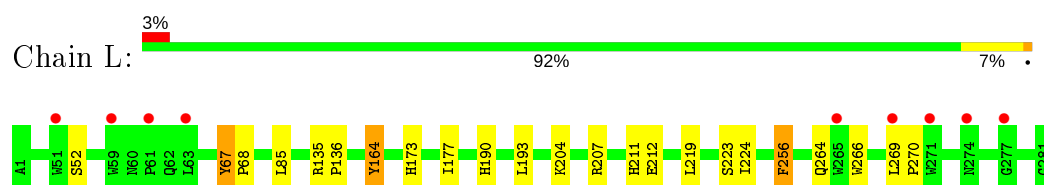
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

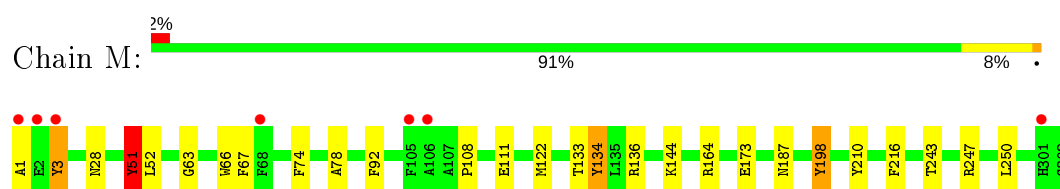
- Molecule 1: Reaction center protein H chain



- 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 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.48Å 102.48Å 239.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.81 – 2.50 42.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (42.81-2.50) 94.7 (42.81-2.50)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.162 , 0.213 0.171 , 0.214	Depositor DCC
$R_{free}$ test set	2000 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 63.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7114	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, BPH, UQ1, FE2, U10

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	H	0.48	0/1877	0.73	2/2553 (0.1%)
2	L	0.46	0/2319	0.61	0/3175
3	M	0.53	2/2500 (0.1%)	0.65	1/3413 (0.0%)
All	All	0.49	2/6696 (0.0%)	0.66	3/9141 (0.0%)

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	H	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	134	TYR	CE1-CZ	-5.54	1.31	1.38
3	M	51	TYR	CE1-CZ	-5.49	1.31	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	94	GLU	CA-CB-CG	8.77	132.69	113.40
1	H	249	LYS	CA-CB-CG	6.32	127.30	113.40
3	M	198	TYR	CB-CG-CD2	-5.14	117.91	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	248	ARG	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	H	1829	0	1836	20	0
2	L	2231	0	2187	27	0
3	M	2408	0	2321	25	0
4	L	65	0	76	4	0
4	M	65	0	76	6	0
5	L	132	0	148	2	0
5	M	117	0	115	4	0
6	L	18	0	18	13	0
7	L	1	0	0	0	0
8	M	62	0	84	6	0
9	H	64	0	0	3	0
9	L	53	0	0	0	0
9	M	69	0	0	4	0
All	All	7114	0	6861	88	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (88) 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:136:ARG:NH1	9:M:548:HOH:O	2.08	0.84
8:M:401:U10:C46	8:M:401:U10:C45	2.58	0.81
8:M:401:U10:C46	8:M:401:U10:C43	2.59	0.81
8:M:401:U10:C45	8:M:401:U10:C43	2.59	0.80
2:L:190:HIS:HD1	6:L:304:UQ1:CM2	2.02	0.72
2:L:190:HIS:HD1	6:L:304:UQ1:HM21	1.56	0.70
2:L:224:ILE:H	6:L:304:UQ1:HM53	1.57	0.70
3:M:134:TYR:HE1	3:M:144:LYS:HE2	1.58	0.68
3:M:108:PRO:HG2	3:M:111:GLU:HB2	1.75	0.67
3:M:52:LEU:O	9:M:510:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:28:ASN:HB2	3:M:51:TYR:CE1	2.33	0.64
4:L:301:BPH:HBB3	4:L:301:BPH:HHC	1.77	0.64
4:L:301:BPH:HBB2	3:M:210:TYR:HB3	1.82	0.62
1:H:211:ASP:OD2	1:H:247:LYS:NZ	2.33	0.60
3:M:63:GLY:HA3	4:M:404:BPH:H5C2	1.84	0.59
2:L:52:SER:HB2	2:L:85:LEU:HD13	1.84	0.58
1:H:45:GLU:HG3	1:H:94:GLU:OE1	2.03	0.58
1:H:34:GLU:OE2	9:H:313:HOH:O	2.17	0.57
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.87	0.57
1:H:34:GLU:HG3	9:H:313:HOH:O	2.04	0.56
3:M:67:PHE:CE1	4:M:404:BPH:H18	2.40	0.56
3:M:67:PHE:HB2	4:M:404:BPH:H101	1.90	0.54
4:L:301:BPH:HHC	4:L:301:BPH:CBB	2.38	0.53
4:M:404:BPH:HBC3	4:M:404:BPH:HHD	1.91	0.53
2:L:269:LEU:HB3	2:L:270:PRO:HD2	1.93	0.51
2:L:164:TYR:N	2:L:164:TYR:CD1	2.80	0.50
5:L:302:BCL:HMB1	5:L:302:BCL:HBB2	1.93	0.49
3:M:136:ARG:NH1	9:M:510:HOH:O	2.40	0.49
1:H:245:ALA:N	1:H:246:PRO:HD2	2.28	0.49
2:L:193:LEU:HD23	6:L:304:UQ1:HM22	1.95	0.49
5:M:403:BCL:HMB1	5:M:403:BCL:HBB3	1.94	0.49
1:H:34:GLU:OE2	9:H:335:HOH:O	2.20	0.48
2:L:269:LEU:HB3	2:L:270:PRO:CD	2.43	0.48
3:M:144:LYS:N	3:M:144:LYS:HD2	2.28	0.48
3:M:164:ARG:HH12	3:M:173:GLU:HG3	1.78	0.48
2:L:190:HIS:HA	6:L:304:UQ1:HM23	1.94	0.48
2:L:223:SER:HA	6:L:304:UQ1:HM52	1.96	0.48
1:H:87:LEU:HD23	1:H:100:PRO:HA	1.94	0.48
2:L:207:ARG:HD2	2:L:211:HIS:CD2	2.49	0.48
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.49	0.48
6:L:304:UQ1:O1	6:L:304:UQ1:HM23	2.14	0.48
6:L:304:UQ1:HM51	6:L:304:UQ1:H72	1.66	0.47
1:H:112:ALA:HA	1:H:235:GLY:O	2.15	0.47
1:H:147:ASN:OD1	1:H:149:ILE:HG12	2.14	0.47
3:M:243:THR:O	3:M:247:ARG:HG3	2.14	0.47
3:M:136:ARG:CZ	9:M:548:HOH:O	2.60	0.46
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.50	0.46
8:M:401:U10:H521	8:M:401:U10:H501	1.65	0.46
2:L:67:TYR:HB3	2:L:68:PRO:HD2	1.98	0.46
2:L:204:LYS:HD2	2:L:207:ARG:HH22	1.81	0.46
5:L:303:BCL:HMB1	5:L:303:BCL:HBB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:190:HIS:ND1	6:L:304:UQ1:HM21	2.27	0.45
3:M:67:PHE:CD1	4:M:404:BPH:H121	2.51	0.45
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.99	0.45
1:H:196:VAL:HG12	1:H:205:VAL:HG22	1.98	0.45
4:L:301:BPH:H161	4:L:301:BPH:H141	1.79	0.45
3:M:187:ASN:HA	5:M:402:BCL:CBC	2.47	0.45
3:M:1:ALA:O	3:M:3:TYR:N	2.49	0.44
3:M:134:TYR:CE1	3:M:144:LYS:HG2	2.52	0.44
2:L:256:PHE:N	2:L:256:PHE:CD1	2.86	0.44
3:M:78:ALA:HB2	3:M:92:PHE:CZ	2.53	0.44
1:H:156:CYS:HB2	1:H:248:ARG:HG3	2.00	0.43
1:H:135:LYS:HG2	1:H:166:ASP:OD2	2.18	0.43
8:M:401:U10:H422	8:M:401:U10:H401	1.53	0.43
1:H:138:ALA:HA	1:H:139:GLY:HA2	1.58	0.43
8:M:401:U10:H272	8:M:401:U10:H251	1.72	0.43
5:M:402:BCL:H2	4:M:404:BPH:HHC	2.00	0.43
1:H:168:TRP:HB2	1:H:178:PHE:HB2	2.00	0.43
2:L:223:SER:OG	6:L:304:UQ1:O4	2.27	0.43
1:H:18:TYR:O	1:H:22:ILE:HG12	2.19	0.42
1:H:29:TYR:O	1:H:33:THR:HG23	2.20	0.42
1:H:220:LYS:HG2	1:H:229:GLU:OE2	2.20	0.42
3:M:164:ARG:NH1	3:M:173:GLU:HG3	2.34	0.42
2:L:219:LEU:HD11	3:M:133:THR:HG22	2.01	0.41
2:L:224:ILE:HG22	6:L:304:UQ1:C4	2.50	0.41
2:L:193:LEU:HD21	2:L:212:GLU:HB3	2.01	0.41
1:H:181:VAL:HG21	1:H:191:LEU:HD12	2.02	0.41
2:L:224:ILE:HG22	6:L:304:UQ1:C5	2.50	0.41
3:M:52:LEU:HA	3:M:52:LEU:HD23	1.89	0.41
2:L:264:GLN:C	2:L:266:TRP:N	2.74	0.41
5:M:402:BCL:HHC	5:M:402:BCL:OBB	2.21	0.41
3:M:74:PHE:CD1	3:M:92:PHE:HB3	2.56	0.41
2:L:193:LEU:HG	2:L:212:GLU:HG2	2.02	0.41
2:L:269:LEU:HD23	2:L:269:LEU:HA	1.89	0.40
1:H:148:PRO:HA	1:H:151:LEU:HD12	2.03	0.40
3:M:250:LEU:HA	3:M:250:LEU:HD23	1.87	0.40
2:L:264:GLN:C	2:L:266:TRP:H	2.23	0.40
2:L:193:LEU:CD2	6:L:304:UQ1:HM22	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	238/240 (99%)	235 (99%)	3 (1%)	0	100	100
2	L	279/281 (99%)	270 (97%)	9 (3%)	0	100	100
3	M	300/302 (99%)	288 (96%)	11 (4%)	1 (0%)	41	61
All	All	817/823 (99%)	793 (97%)	23 (3%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	3	TYR

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/195 (100%)	194 (100%)	1 (0%)	88	96
2	L	220/220 (100%)	217 (99%)	3 (1%)	67	86
3	M	236/236 (100%)	233 (99%)	3 (1%)	69	87
All	All	651/651 (100%)	644 (99%)	7 (1%)	73	89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	249	LYS
2	L	67	TYR

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Mol	Chain	Res	Type
2	L	164	TYR
2	L	256	PHE
3	M	51	TYR
3	M	198	TYR
3	M	216	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	UQ1	L	304	-	18,18,18	1.95	7 (38%)	22,25,25	1.79	4 (18%)
4	BPH	M	404	-	64,70,70	1.07	5 (7%)	76,101,101	1.53	10 (13%)
5	BCL	L	303	-	58,74,74	1.25	4 (6%)	69,115,115	1.50	12 (17%)
4	BPH	L	301	-	64,70,70	1.00	3 (4%)	76,101,101	1.15	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BCL	M	403	-	43,59,74	1.38	5 (11%)	51,97,115	1.53	10 (19%)
5	BCL	L	302	-	58,74,74	1.22	4 (6%)	69,115,115	1.29	11 (15%)
5	BCL	M	402	-	58,74,74	1.39	5 (8%)	69,115,115	1.54	13 (18%)
8	U10	M	401	-	60,60,63	2.64	16 (26%)	70,74,79	1.73	16 (22%)

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	UQ1	L	304	-	-	3/9/33/33	0/1/1/1
4	BPH	M	404	-	-	23/54/105/105	0/5/6/6
5	BCL	L	303	-	-	2/37/137/137	-
4	BPH	L	301	-	-	5/54/105/105	0/5/6/6
5	BCL	M	403	-	-	2/19/119/137	-
5	BCL	L	302	-	-	4/37/137/137	-
5	BCL	M	402	-	-	6/37/137/137	-
8	U10	M	401	-	-	21/57/81/87	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	401	U10	C33-C34	6.15	1.47	1.33
8	M	401	U10	C13-C14	6.11	1.47	1.33
5	M	402	BCL	MG-NA	6.10	2.20	2.06
8	M	401	U10	C48-C49	6.08	1.47	1.33
8	M	401	U10	C38-C39	6.07	1.47	1.33
8	M	401	U10	C18-C19	6.01	1.47	1.33
8	M	401	U10	C28-C29	5.89	1.47	1.33
8	M	401	U10	C23-C24	5.82	1.46	1.33
8	M	401	U10	C8-C9	5.80	1.46	1.33
8	M	401	U10	C53-C54	5.43	1.48	1.32
8	M	401	U10	O4-C4	-5.12	1.24	1.36
8	M	401	U10	O3-C3	-5.09	1.24	1.36
5	L	302	BCL	C1B-NB	5.03	1.39	1.35
5	M	403	BCL	C1B-NB	5.03	1.39	1.35
5	M	402	BCL	C1B-NB	4.93	1.39	1.35
5	L	302	BCL	MG-NA	4.75	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	303	BCL	C1B-NB	4.65	1.39	1.35
5	L	303	BCL	MG-NC	4.24	2.16	2.06
5	L	303	BCL	MG-NA	4.04	2.15	2.06
5	M	403	BCL	MG-NA	3.93	2.15	2.06
6	L	304	UQ1	C3-C4	-3.64	1.38	1.48
6	L	304	UQ1	O2-CM2	-3.49	1.37	1.45
8	M	401	U10	C3-C2	-3.42	1.39	1.48
4	L	301	BPH	C3D-CAD	-3.28	1.40	1.47
5	M	403	BCL	MG-NC	3.17	2.13	2.06
8	M	401	U10	C4-C5	-3.07	1.40	1.48
6	L	304	UQ1	C6-C1	-3.00	1.38	1.46
6	L	304	UQ1	C2-C1	-2.97	1.40	1.48
4	M	404	BPH	OBD-CAD	2.93	1.26	1.22
5	M	402	BCL	MG-NC	2.85	2.13	2.06
8	M	401	U10	C6-C1	2.84	1.40	1.35
5	L	302	BCL	OBD-CAD	2.69	1.26	1.22
6	L	304	UQ1	O3-CM3	-2.67	1.39	1.45
5	M	402	BCL	O1A-CGA	-2.67	1.14	1.22
5	L	303	BCL	C4B-NB	2.66	1.37	1.35
4	M	404	BPH	CHC-C1C	2.54	1.41	1.36
4	M	404	BPH	C1B-C2B	-2.51	1.40	1.45
4	M	404	BPH	C3D-CAD	-2.50	1.42	1.47
5	L	302	BCL	MG-NC	2.49	2.12	2.06
5	M	402	BCL	C4B-NB	2.47	1.37	1.35
6	L	304	UQ1	C6-C5	2.46	1.39	1.35
4	L	301	BPH	O1A-CGA	-2.25	1.15	1.22
5	M	403	BCL	O1A-CGA	-2.22	1.16	1.22
8	M	401	U10	C6-C5	-2.22	1.40	1.46
4	M	404	BPH	C16-C15	2.20	1.61	1.52
8	M	401	U10	C1-C2	-2.11	1.39	1.47
5	M	403	BCL	OBD-CAD	2.08	1.25	1.22
4	L	301	BPH	C1B-C2B	-2.05	1.41	1.45
6	L	304	UQ1	C5-C4	-2.01	1.40	1.47

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	404	BPH	C16-C15-C13	5.31	133.07	115.92
4	M	404	BPH	C11-C10-C8	5.07	132.31	115.92
5	L	303	BCL	C17-C16-C15	-4.59	92.15	113.24
6	L	304	UQ1	C8-C7-C6	4.55	124.32	112.05
5	M	402	BCL	CMB-C2B-C1B	-4.41	121.69	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	403	BCL	CMB-C2B-C1B	-4.05	122.25	128.46
5	M	402	BCL	C4A-NA-C1A	4.03	108.52	106.71
8	M	401	U10	C27-C28-C29	-3.95	118.15	127.66
8	M	401	U10	C42-C41-C39	-3.91	108.23	114.62
4	L	301	BPH	C1C-NC-C4C	-3.78	107.21	110.54
8	M	401	U10	C22-C23-C24	-3.75	118.63	127.66
8	M	401	U10	C17-C18-C19	-3.58	119.03	127.66
5	M	402	BCL	OBD-CAD-CBD	-3.55	120.82	125.89
5	L	302	BCL	CMB-C2B-C1B	-3.50	123.08	128.46
4	M	404	BPH	OBD-CAD-CBD	-3.48	120.92	125.89
5	L	303	BCL	CMB-C2B-C1B	-3.39	123.25	128.46
8	M	401	U10	C10-C9-C11	3.35	120.91	115.27
5	M	403	BCL	OBD-CAD-CBD	-3.33	121.13	125.89
6	L	304	UQ1	O1-C1-C6	-3.33	115.71	121.55
5	L	303	BCL	C4A-NA-C1A	3.28	108.18	106.71
5	M	402	BCL	CHA-C1A-NA	-3.28	118.88	126.40
5	L	303	BCL	C4D-C3D-CAD	-3.26	106.65	108.47
8	M	401	U10	C12-C13-C14	-3.24	119.85	127.66
5	M	402	BCL	CMB-C2B-C3B	3.23	130.72	124.68
5	M	402	BCL	C4D-C3D-CAD	-3.19	106.69	108.47
8	M	401	U10	C30-C29-C31	3.11	120.50	115.27
5	M	403	BCL	CMB-C2B-C3B	3.10	130.47	124.68
8	M	401	U10	C50-C49-C51	3.10	120.48	115.27
4	M	404	BPH	C17-C16-C15	3.07	127.34	113.24
5	L	302	BCL	OBD-CAD-CBD	-3.06	121.52	125.89
8	M	401	U10	C20-C19-C21	3.01	120.33	115.27
5	L	302	BCL	CHA-C1A-NA	-2.99	119.56	126.40
4	M	404	BPH	CHC-C1C-NC	-2.96	121.69	125.20
6	L	304	UQ1	CM5-C5-C6	-2.95	119.59	124.40
5	L	303	BCL	C2A-C1A-CHA	2.93	128.98	123.86
5	M	403	BCL	C1-O2A-CGA	2.90	124.06	116.44
6	L	304	UQ1	C7-C8-C9	-2.87	118.27	127.26
5	M	403	BCL	C4D-C3D-CAD	-2.85	106.88	108.47
4	M	404	BPH	CAC-C3C-C2C	-2.85	107.15	114.26
5	L	303	BCL	CHA-C1A-NA	-2.84	119.90	126.40
5	M	402	BCL	C2A-C1A-CHA	2.82	128.79	123.86
4	M	404	BPH	CAC-C3C-C4C	2.81	119.89	112.67
5	L	303	BCL	CMD-C2D-C3D	2.81	129.93	124.68
4	L	301	BPH	OBD-CAD-CBD	-2.79	121.90	125.89
5	L	303	BCL	OBD-CAD-CBD	-2.78	121.92	125.89
8	M	401	U10	C7-C8-C9	-2.77	122.18	126.79
5	M	403	BCL	CHA-C1A-NA	-2.76	120.07	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	302	BCL	C2A-C1A-CHA	2.76	128.69	123.86
4	L	301	BPH	C1-C2-C3	-2.73	121.31	126.04
8	M	401	U10	C25-C24-C26	2.73	119.86	115.27
5	L	302	BCL	C1-C2-C3	-2.72	121.34	126.04
8	M	401	U10	C35-C34-C36	2.71	119.84	115.27
5	M	403	BCL	C2A-C1A-CHA	2.71	128.60	123.86
8	M	401	U10	C32-C33-C34	-2.70	121.16	127.66
5	M	402	BCL	C16-C15-C13	-2.61	107.49	115.92
5	L	302	BCL	O2D-CGD-O1D	-2.60	118.76	123.84
5	L	302	BCL	CMB-C2B-C3B	2.56	129.46	124.68
5	M	402	BCL	CMD-C2D-C3D	2.52	129.38	124.68
5	M	403	BCL	CMD-C2D-C3D	2.48	129.32	124.68
5	M	403	BCL	C4A-NA-C1A	2.48	107.82	106.71
5	L	303	BCL	CMB-C2B-C3B	2.47	129.31	124.68
4	L	301	BPH	C17-C16-C15	2.43	124.40	113.24
4	M	404	BPH	C6-C5-C3	2.39	119.72	113.45
5	L	302	BCL	CMD-C2D-C3D	2.37	129.12	124.68
5	L	303	BCL	C1D-CHD-C4C	2.36	129.38	125.88
4	L	301	BPH	CHC-C1C-NC	-2.35	122.41	125.20
5	M	402	BCL	C4B-C3B-CAB	-2.30	122.68	127.13
5	L	303	BCL	O2A-CGA-O1A	-2.28	117.84	123.59
5	M	402	BCL	OBB-CAB-CBB	-2.27	115.06	120.17
5	M	402	BCL	CED-O2D-CGD	2.25	121.03	115.94
5	L	303	BCL	OBB-CAB-CBB	-2.24	115.12	120.17
4	M	404	BPH	C1C-NC-C4C	-2.22	108.59	110.54
5	L	302	BCL	C4D-C3D-CAD	-2.21	107.24	108.47
4	L	301	BPH	CHD-C4C-NC	-2.16	122.64	125.20
4	L	301	BPH	C3A-C4A-CHB	2.13	125.51	121.83
8	M	401	U10	C30-C29-C28	-2.09	118.31	123.68
5	M	403	BCL	C1C-NC-C4C	2.09	107.65	106.71
8	M	401	U10	C56-C54-C55	2.08	119.20	114.60
4	L	301	BPH	OBB-CAB-CBB	-2.08	115.13	119.73
5	L	302	BCL	C4A-NA-C1A	2.06	107.63	106.71
5	M	402	BCL	CBC-CAC-C3C	-2.05	108.91	113.47
4	M	404	BPH	CHD-C4C-NC	-2.03	122.79	125.20
8	M	401	U10	C15-C14-C16	2.01	118.64	115.27
5	L	302	BCL	O1D-CGD-CBD	2.00	128.58	124.48

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	304	UQ1	C3-C2-O2-CM2
6	L	304	UQ1	C7-C8-C9-C11
4	M	404	BPH	C4B-C3B-CAB-CBB
4	M	404	BPH	C4B-C3B-CAB-OB
4	M	404	BPH	C2B-C3B-CAB-CBB
4	M	404	BPH	C2B-C3B-CAB-OB
4	M	404	BPH	C2-C3-C5-C6
4	M	404	BPH	C4-C3-C5-C6
5	M	402	BCL	C4C-C3C-CAC-CBC
8	M	401	U10	C23-C24-C26-C27
8	M	401	U10	C25-C24-C26-C27
8	M	401	U10	C29-C31-C32-C33
8	M	401	U10	C38-C39-C41-C42
8	M	401	U10	C40-C39-C41-C42
8	M	401	U10	C48-C49-C51-C52
8	M	401	U10	C50-C49-C51-C52
8	M	401	U10	C19-C21-C22-C23
8	M	401	U10	C49-C51-C52-C53
6	L	304	UQ1	C7-C8-C9-C10
4	M	404	BPH	C6-C7-C8-C9
4	M	404	BPH	C11-C10-C8-C9
4	M	404	BPH	C11-C12-C13-C14
4	M	404	BPH	C14-C13-C15-C16
4	M	404	BPH	C8-C10-C11-C12
4	M	404	BPH	C5-C6-C7-C8
4	L	301	BPH	C13-C15-C16-C17
8	M	401	U10	C24-C26-C27-C28
5	M	402	BCL	C16-C17-C18-C20
4	L	301	BPH	C4-C3-C5-C6
5	L	302	BCL	C14-C13-C15-C16
4	M	404	BPH	C11-C10-C8-C7
4	L	301	BPH	C2-C3-C5-C6
5	M	402	BCL	C16-C17-C18-C19
5	M	402	BCL	C2C-C3C-CAC-CBC
4	M	404	BPH	C16-C17-C18-C19
5	L	302	BCL	C12-C13-C15-C16
5	L	302	BCL	C15-C16-C17-C18
4	M	404	BPH	C2-C1-O2A-CGA
4	M	404	BPH	C12-C13-C15-C16
5	L	303	BCL	CAD-CBD-CGD-O2D
5	M	403	BCL	CAD-CBD-CGD-O2D
8	M	401	U10	C35-C34-C36-C37
4	M	404	BPH	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
4	M	404	BPH	C11-C12-C13-C15
8	M	401	U10	C33-C34-C36-C37
8	M	401	U10	C3-C4-O4-C4M
4	M	404	BPH	C15-C16-C17-C18
4	M	404	BPH	NC-C1C-CHC-C4B
8	M	401	U10	C14-C16-C17-C18
8	M	401	U10	C39-C41-C42-C43
5	M	402	BCL	C14-C13-C15-C16
4	L	301	BPH	C4C-C3C-CAC-CBC
5	M	403	BCL	C4C-C3C-CAC-CBC
8	M	401	U10	C37-C38-C39-C40
5	L	303	BCL	C2A-CAA-CBA-CGA
5	M	402	BCL	C12-C13-C15-C16
5	L	302	BCL	C13-C15-C16-C17
4	M	404	BPH	CAD-CBD-CGD-O2D
8	M	401	U10	C5-C4-O4-C4M
4	L	301	BPH	O2A-C1-C2-C3
8	M	401	U10	C51-C52-C53-C54
8	M	401	U10	C37-C38-C39-C41
8	M	401	U10	C34-C36-C37-C38
8	M	401	U10	C16-C17-C18-C19
4	M	404	BPH	C6-C7-C8-C10
4	M	404	BPH	C10-C11-C12-C13

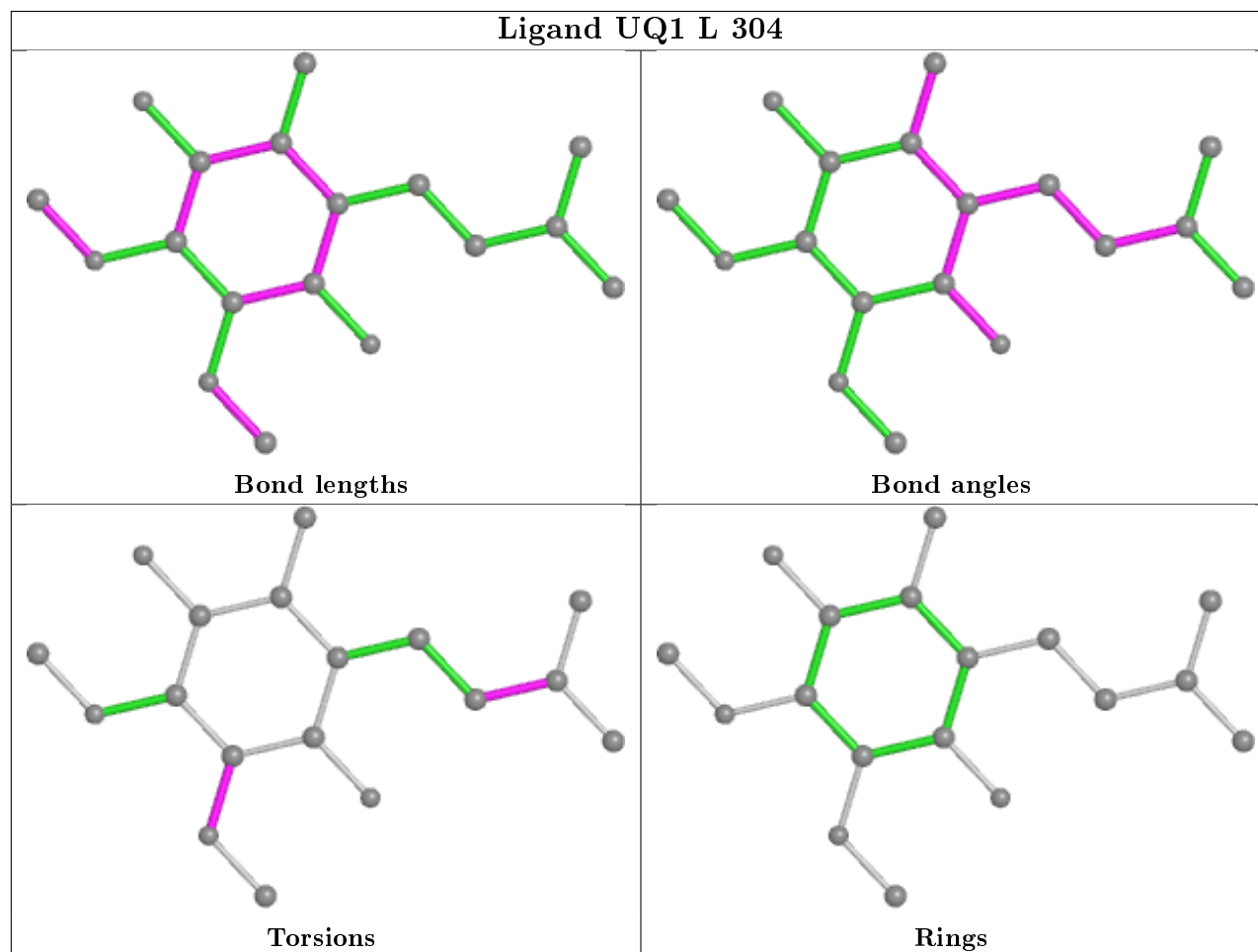
There are no ring outliers.

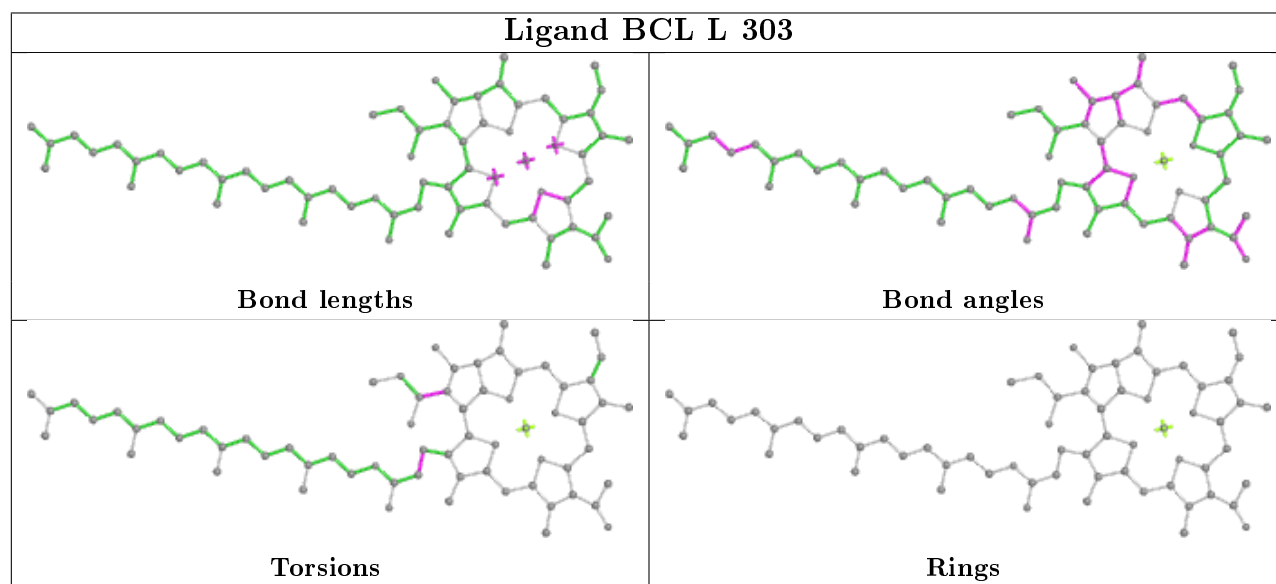
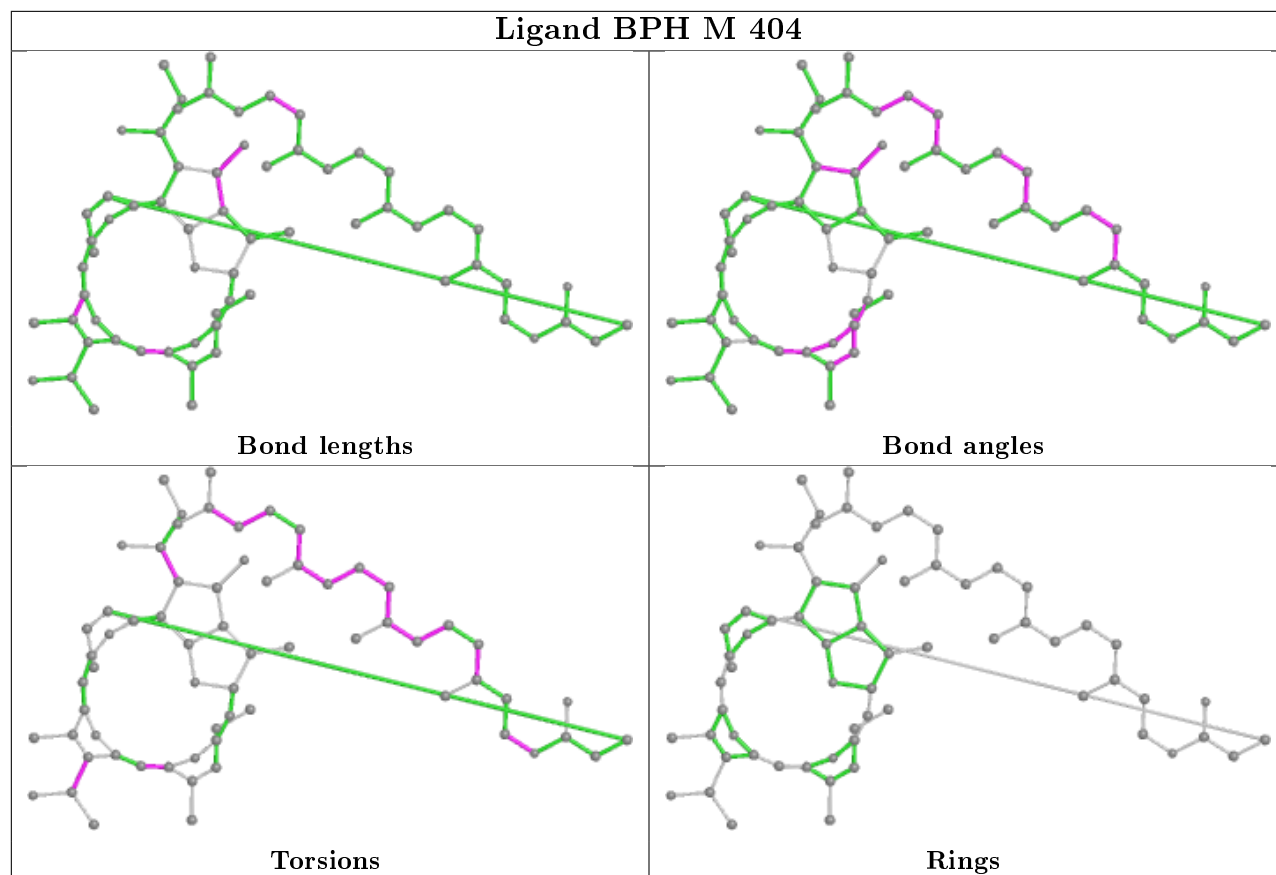
8 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	304	UQ1	13	0
4	M	404	BPH	6	0
5	L	303	BCL	1	0
4	L	301	BPH	4	0
5	M	403	BCL	1	0
5	L	302	BCL	1	0
5	M	402	BCL	3	0
8	M	401	U10	6	0

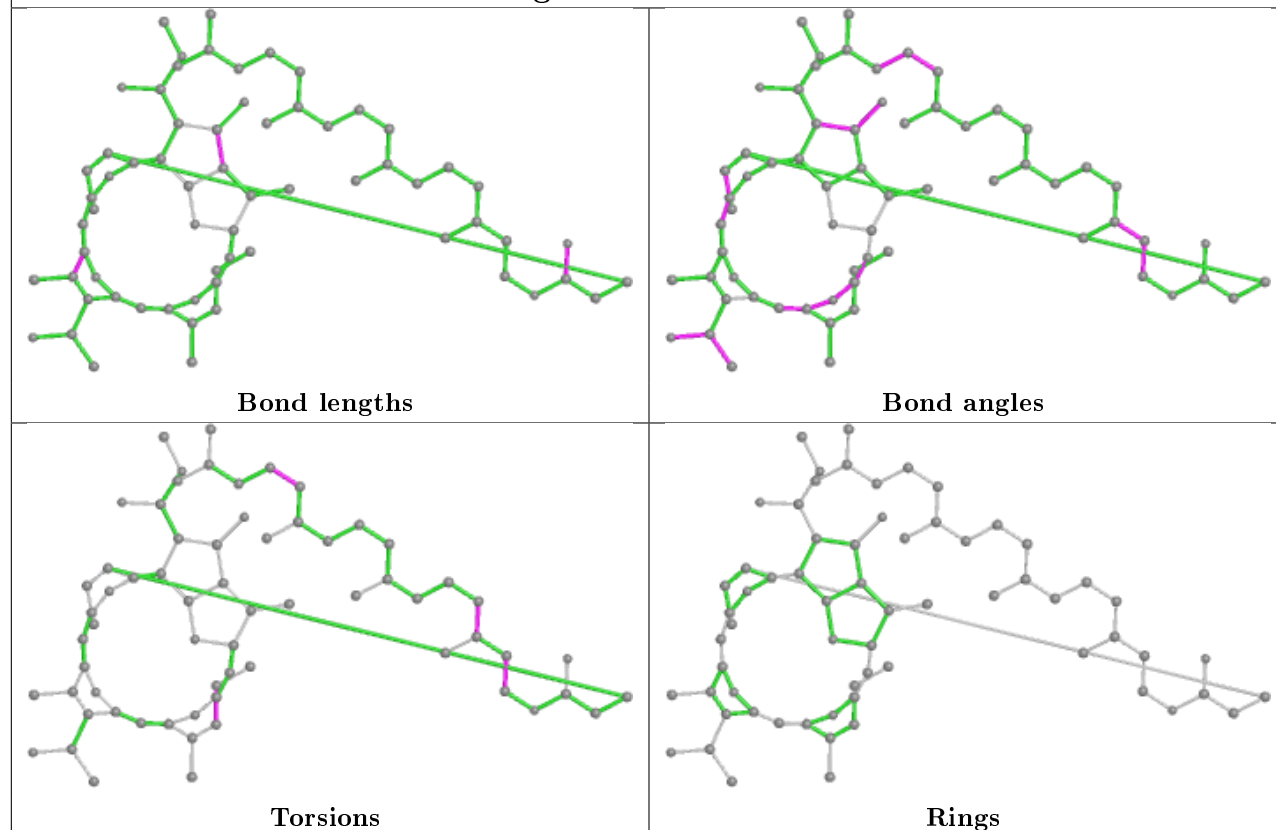
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

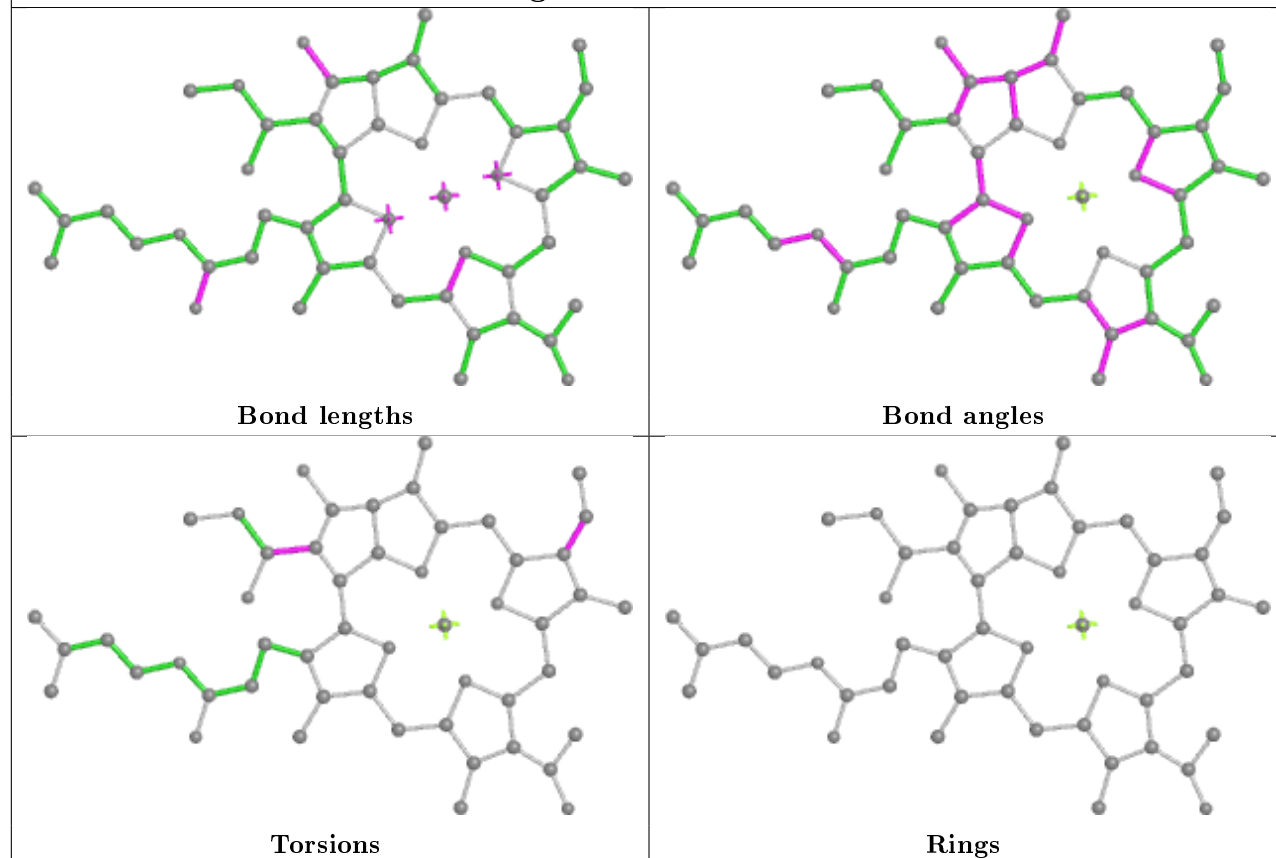




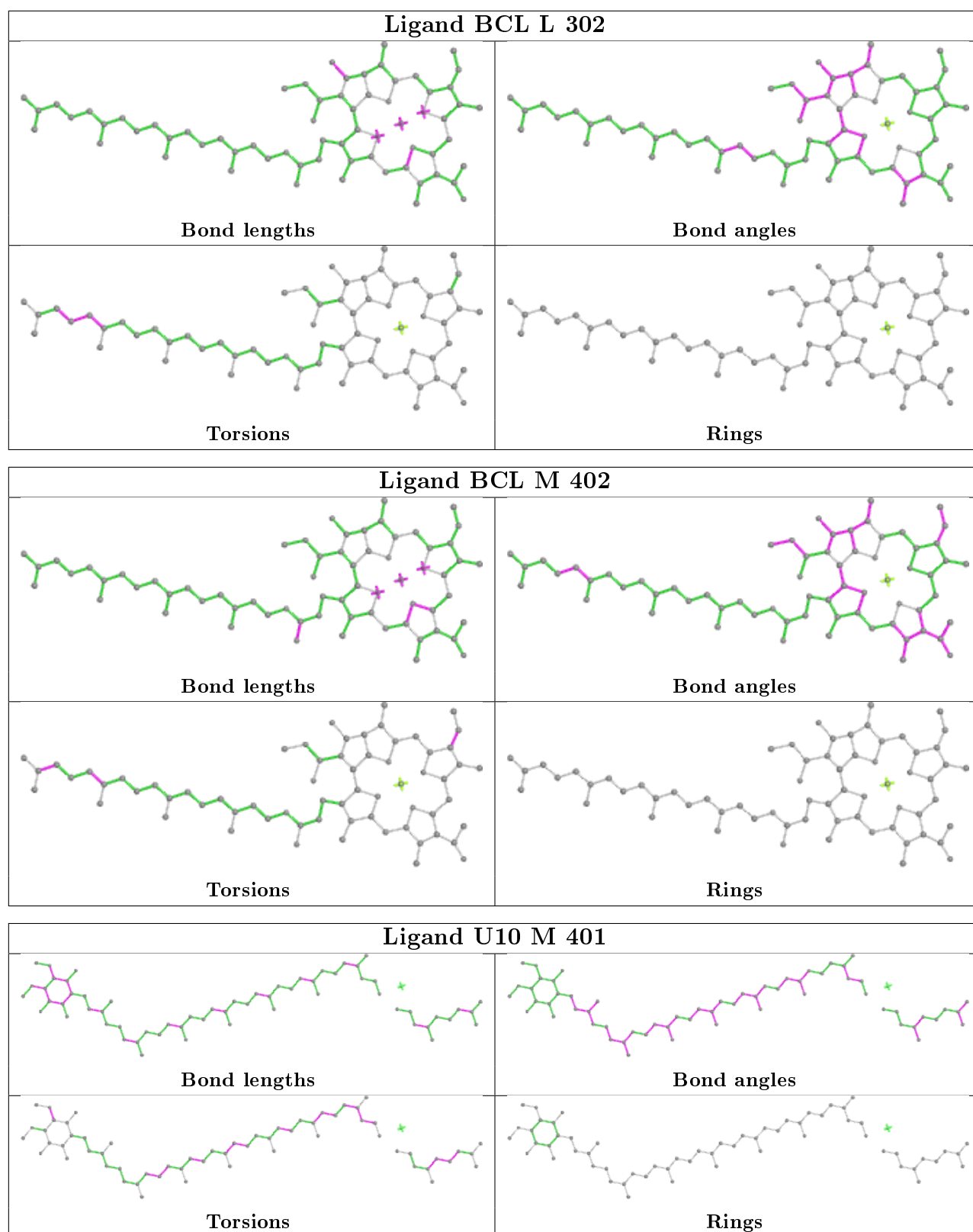
## Ligand BPH L 301



## Ligand BCL M 403







## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	H	240/240 (100%)	-0.38	7 (2%)	51	55	22, 35, 57, 134	0
2	L	281/281 (100%)	-0.42	9 (3%)	47	51	19, 30, 66, 99	0
3	M	302/302 (100%)	-0.40	7 (2%)	60	63	18, 32, 58, 123	0
All	All	823/823 (100%)	-0.40	23 (2%)	53	56	18, 32, 61, 134	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	9.5
1	H	249	LYS	7.7
3	M	1	ALA	7.4
1	H	245	ALA	5.4
2	L	59	TRP	5.3
2	L	265	TRP	4.8
2	L	271	TRP	4.3
1	H	248	ARG	4.2
2	L	51	TRP	3.7
3	M	105	PHE	3.2
2	L	63	LEU	2.8
1	H	247	LYS	2.8
3	M	301	HIS	2.7
2	L	61	PRO	2.6
3	M	3	TYR	2.6
2	L	274	ASN	2.6
3	M	2	GLU	2.4
2	L	269	LEU	2.3
3	M	106	ALA	2.2
1	H	246	PRO	2.1
3	M	68	PHE	2.1
2	L	277	GLY	2.1
1	H	92	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

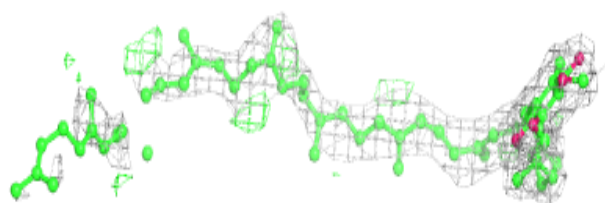
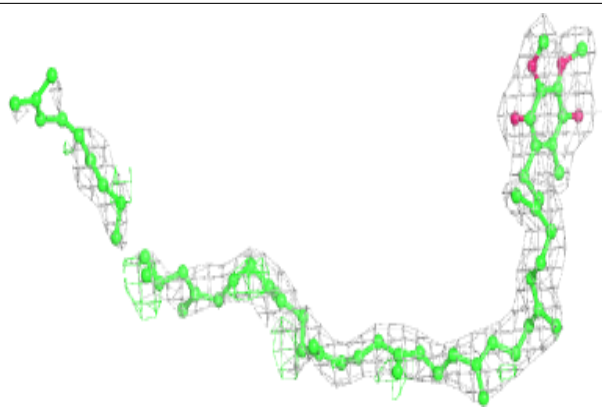
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	U10	M	401	62/63	0.89	0.23	17,44,85,94	14
6	UQ1	L	304	18/18	0.94	0.21	27,29,32,34	11
4	BPH	M	404	65/65	0.95	0.17	19,27,97,129	0
4	BPH	L	301	65/65	0.97	0.15	15,22,35,40	7
5	BCL	M	403	51/66	0.97	0.13	18,26,38,45	0
5	BCL	M	402	66/66	0.97	0.12	19,25,44,63	0
5	BCL	L	303	66/66	0.97	0.12	20,25,37,54	0
5	BCL	L	302	66/66	0.98	0.13	18,24,45,55	13
7	FE2	L	305	1/1	1.00	0.13	19,19,19,19	0

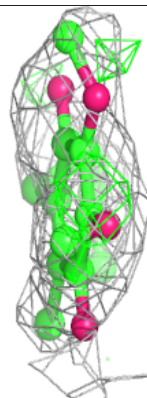
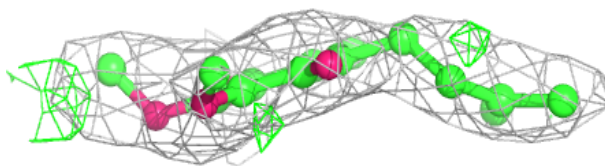
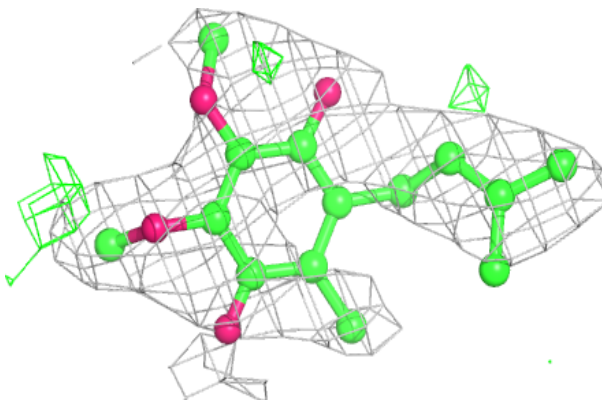
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around U10 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)

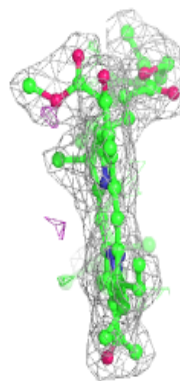
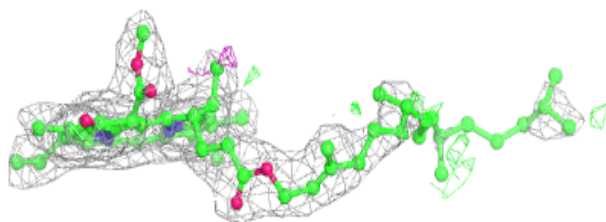
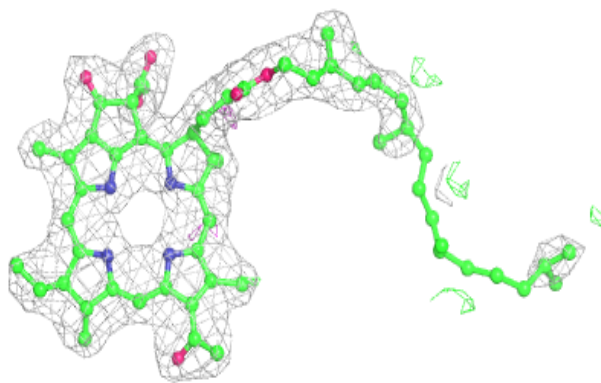
**Electron density around UQ1 L 304:**

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



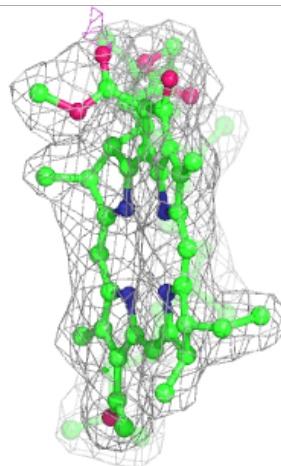
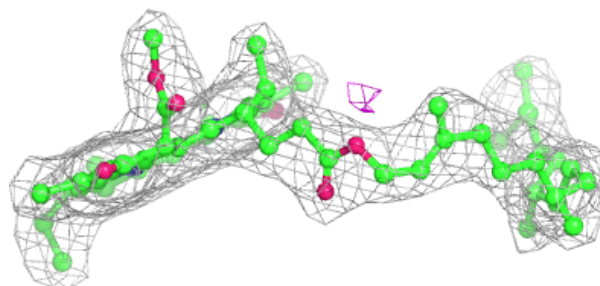
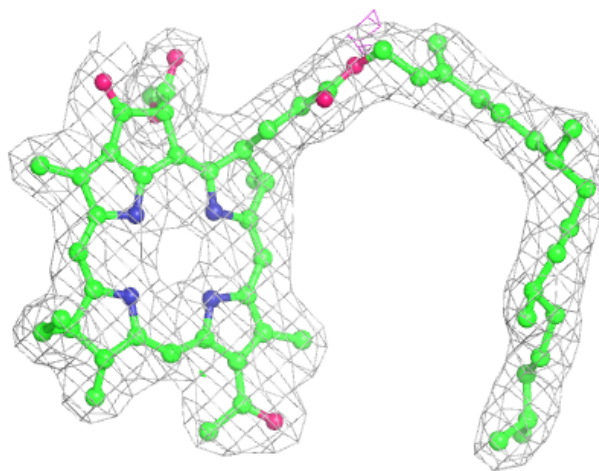
**Electron density around BPH M 404:**

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



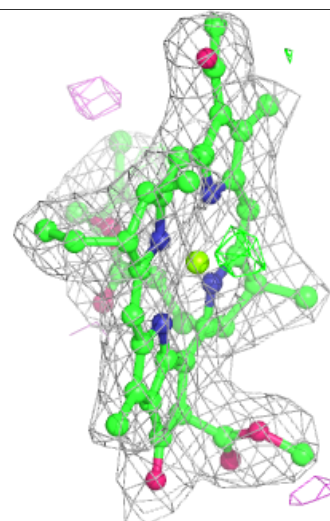
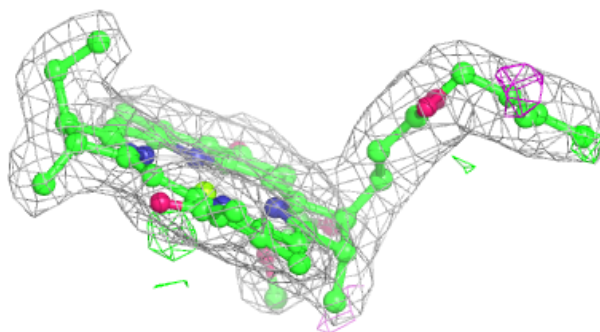
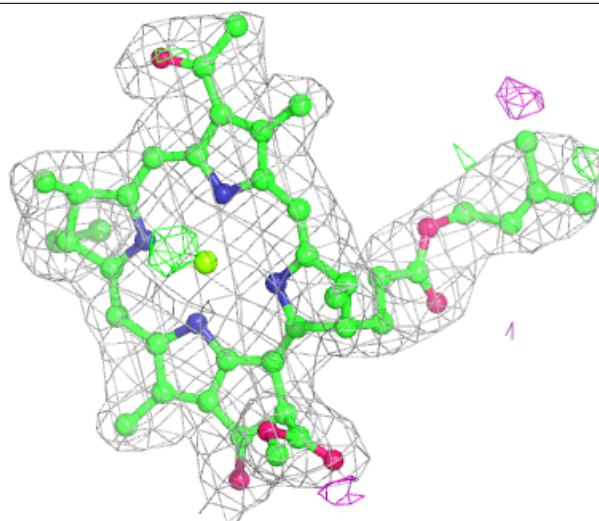
**Electron density around BPH L 301:**

$2mF_o-DF_c$  (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:**

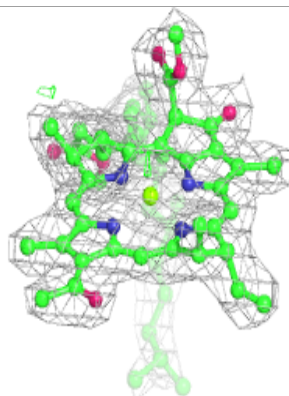
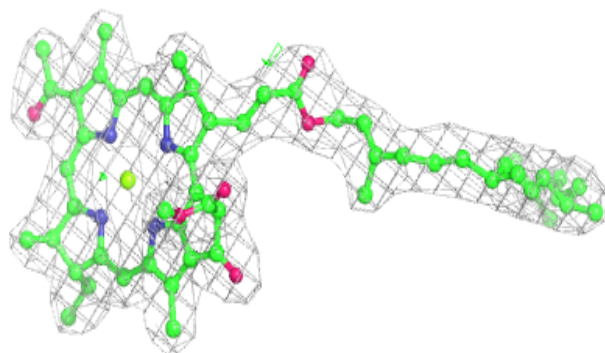
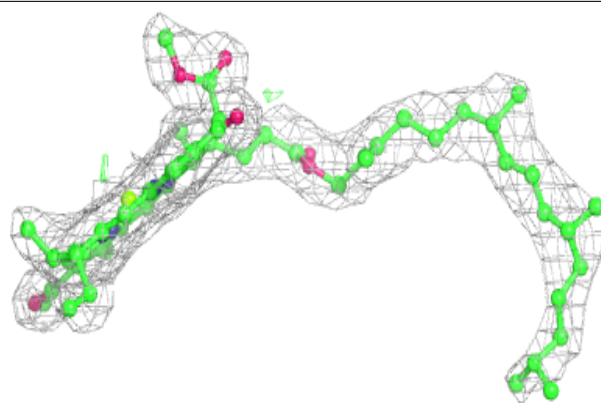
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



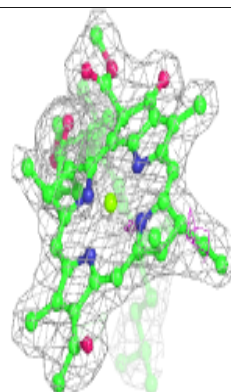
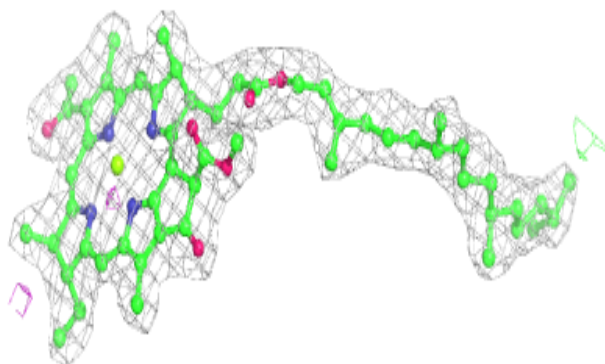
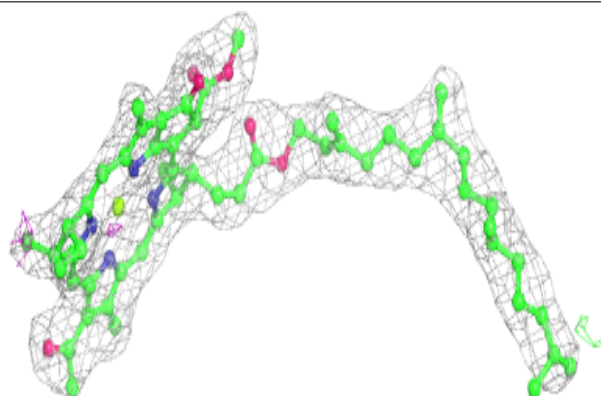


**Electron density around BCL M 402:**

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

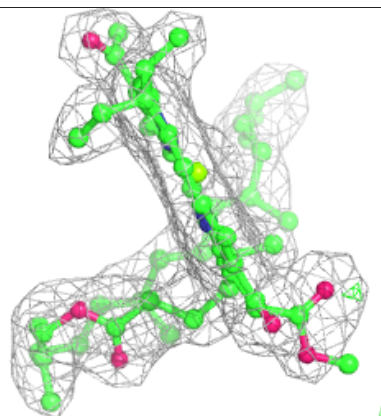
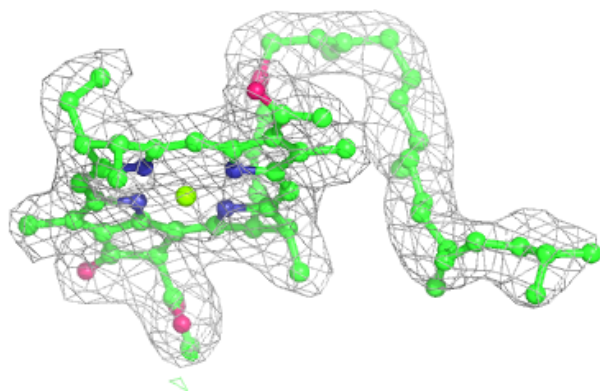
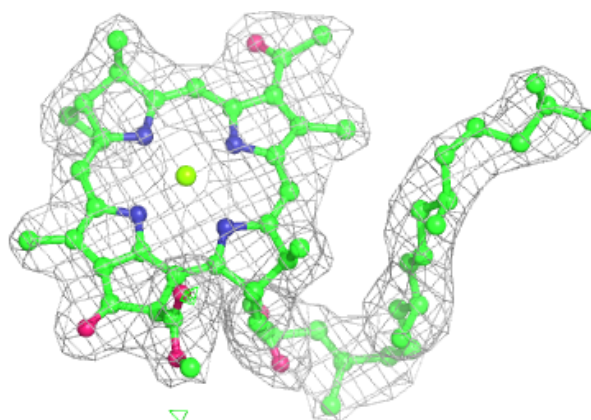
**Electron density around BCL L 303:**

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



**Electron density around BCL 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)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.