



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 06:00 pm BST

PDB ID : 2UX5  
Title : X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 9 in the charge-separated state  
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.  
Deposited on : 2007-03-26  
Resolution : 2.21 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

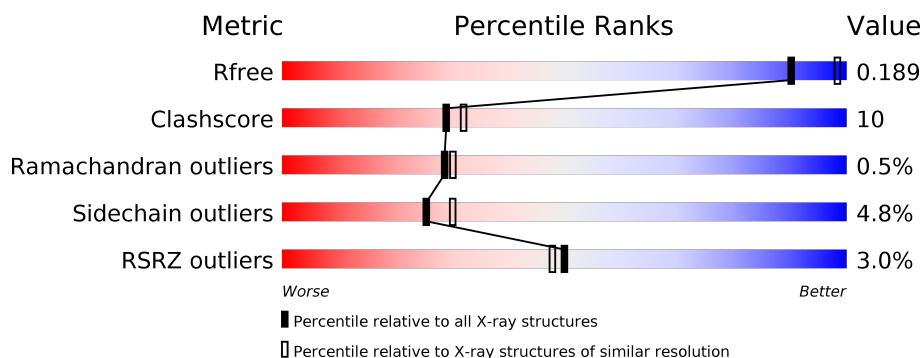
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.21 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	260	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>•</div> <div>7%</div> </div> </div>
2	L	281	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>•</div> </div> </div>
3	M	307	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>••</div> </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
14	CDL	M	1317	-	-	-	X
5	BCL	L	1282	X	-	-	-
5	BCL	L	1287	X	-	-	-
5	BCL	M	1304	X	-	-	-
5	BCL	M	1305	X	-	-	-
6	LDA	L	1283	-	-	-	X
6	LDA	M	1311	-	-	-	X

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 7706 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	241	Total	C	N	O	S	0	3	1
			1846	1181	319	337	9			

- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

- Molecule 3 is a protein called REACTION CENTER PROTEIN M CHAIN.

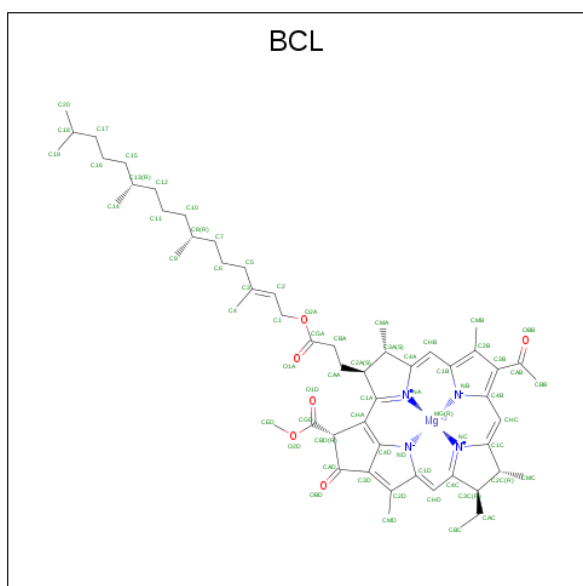
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	M	1	Total	C	O	0	0
			6	3	3		

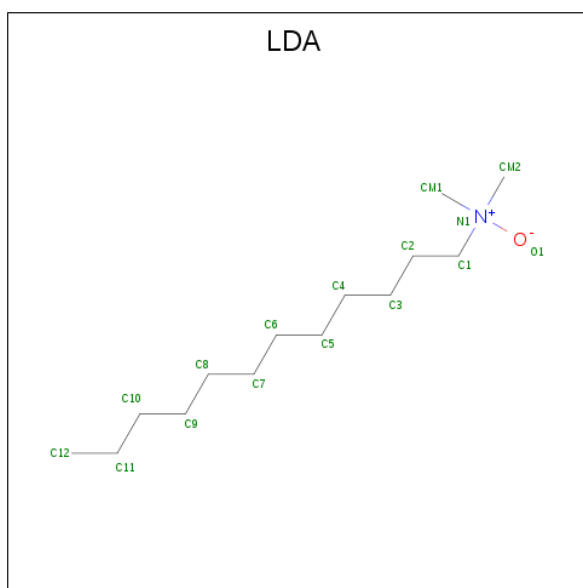
- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula:  $C_{55}H_{74}MgN_4O_6$ ).



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

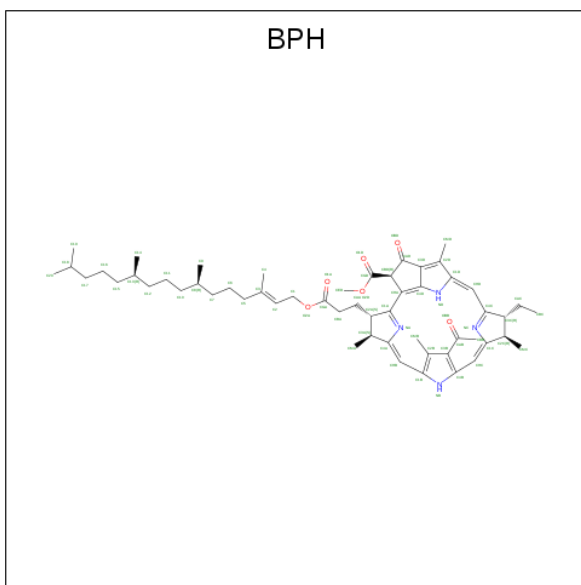
- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

C<sub>14</sub>H<sub>31</sub>NO).



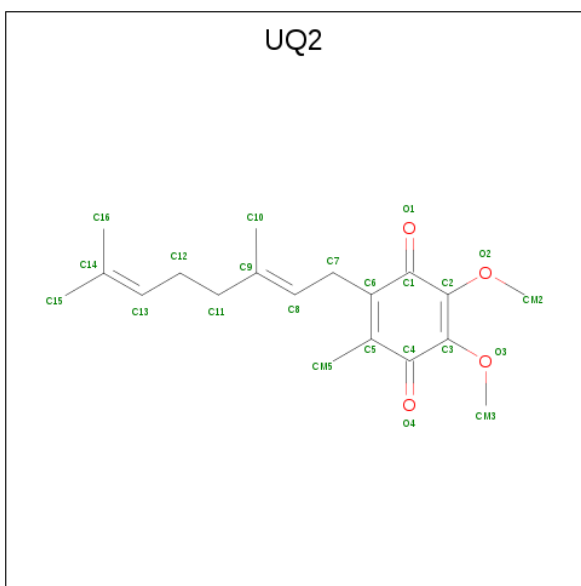
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1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

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>).



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

- Molecule 8 is UBIQUINONE-2 (three-letter code: UQ2) (formula:  $C_{19}H_{26}O_4$ ).



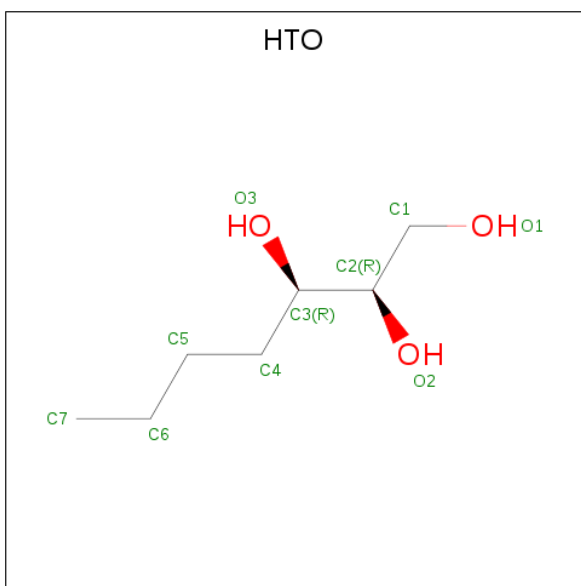
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula:  $C_7H_{16}O_3$ ).



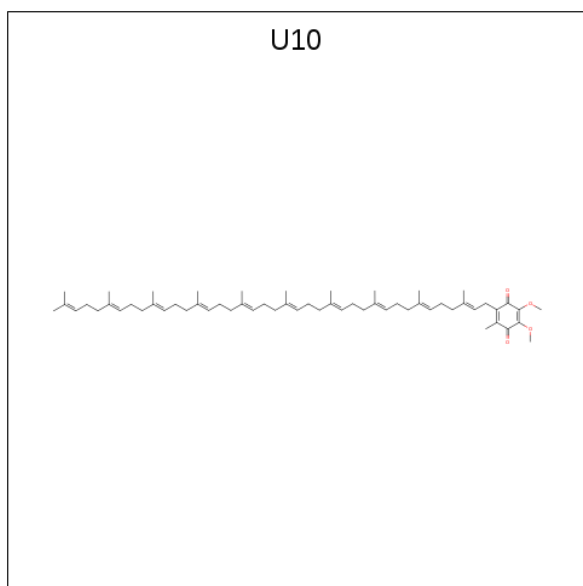
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).



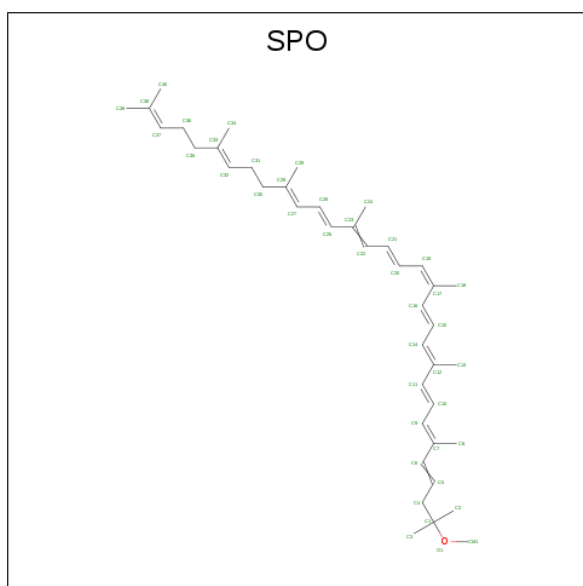
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



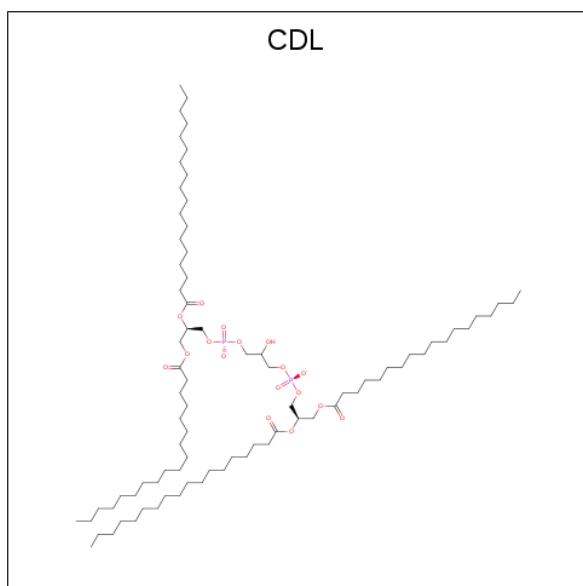
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 13 is SPHEROIDENE (three-letter code: SPO) (formula:  $C_{41}H_{60}O$ ).



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

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	M	1	Total	C	O	P	0	0
			81	62	17	2		

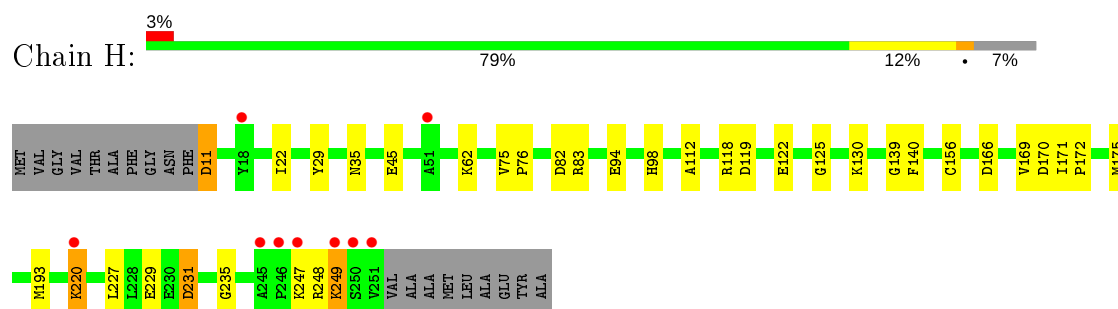
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	167	Total	O	0	0
			167	167		
15	L	115	Total	O	0	0
			115	115		
15	M	124	Total	O	0	0
			124	124		

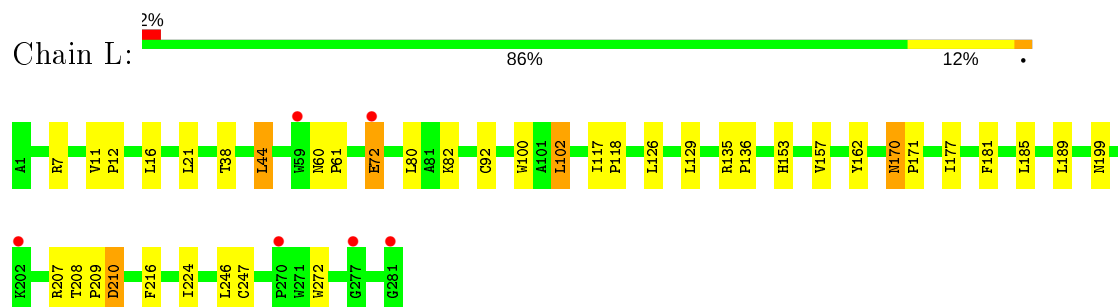
### 3 Residue-property plots [i](#)

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.

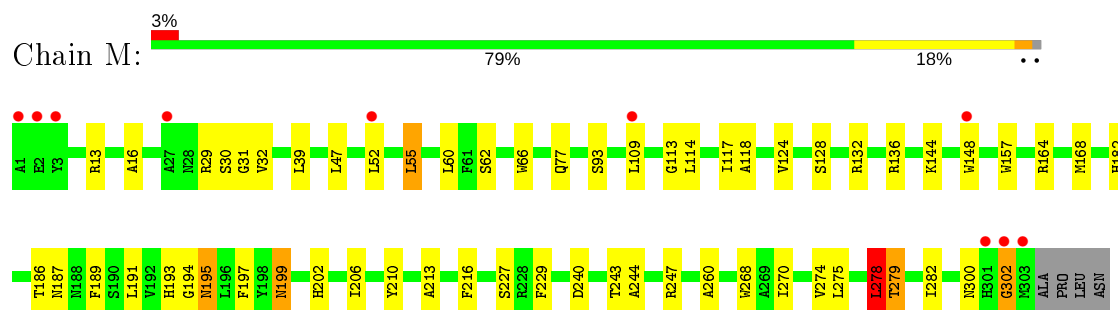
#### • Molecule 1: REACTION CENTER PROTEIN H CHAIN



#### • 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 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.46Å 139.46Å 184.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.21 19.86 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.21) 96.3 (19.86-2.21)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.37 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.202 , 0.236 0.196 , 0.189	Depositor DCC
$R_{free}$ test set	3118 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7706	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, GOL, LDA, CDL, BPH, PO4, HTO, FE, SPO, U10, UQ2

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	0.88	0/1906	0.92	6/2591 (0.2%)
2	L	0.91	0/2320	0.78	1/3175 (0.0%)
3	M	0.88	3/2501 (0.1%)	0.80	2/3415 (0.1%)
All	All	0.89	3/6727 (0.0%)	0.83	9/9181 (0.1%)

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
3	M	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	278	LEU	CG-CD2	7.91	1.81	1.51
3	M	213	ALA	CA-CB	6.24	1.65	1.52
3	M	227	SER	CA-CB	5.32	1.60	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	278	LEU	CA-CB-CG	-13.19	84.97	115.30
1	H	11	ASP	CB-CG-OD2	8.98	126.38	118.30
1	H	166	ASP	CB-CG-OD2	8.16	125.64	118.30
1	H	83	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	H	231	ASP	CB-CG-OD2	7.12	124.71	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	300	ASN	Peptide

## 5.2 Too-close contacts

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	1846	0	1861	24	0
2	L	2232	0	2187	28	0
3	M	2409	0	2321	53	0
4	H	24	0	32	4	0
4	L	12	0	16	1	0
4	M	6	0	8	1	0
5	L	132	0	148	6	0
5	M	132	0	148	20	0
6	L	32	0	62	2	0
6	M	112	0	217	8	0
7	L	65	0	76	6	0
7	M	65	0	76	14	0
8	L	46	0	52	6	0
9	L	5	0	0	0	0
10	L	10	0	16	0	0
11	M	1	0	0	0	0
12	M	48	0	63	3	0
13	M	42	0	60	2	0
14	M	81	0	86	4	0
15	H	167	0	0	3	0
15	L	115	0	0	2	0
15	M	124	0	0	2	0
All	All	7706	0	7429	141	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 10.

The worst 5 of 141 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:278:LEU:CG	3:M:278:LEU:CD2	1.81	1.56
3:M:278:LEU:CD2	3:M:279:THR:H	1.18	1.55
3:M:278:LEU:CD2	3:M:279:THR:N	1.74	1.38
3:M:278:LEU:HA	3:M:278:LEU:CD2	1.61	1.28
3:M:278:LEU:CA	3:M:278:LEU:CD2	2.11	1.27

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	242/260 (93%)	235 (97%)	6 (2%)	1 (0%)	34	37
2	L	279/281 (99%)	272 (98%)	7 (2%)	0	100	100
3	M	301/307 (98%)	289 (96%)	9 (3%)	3 (1%)	15	13
All	All	822/848 (97%)	796 (97%)	22 (3%)	4 (0%)	29	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249	LYS
3	M	195	ASN
3	M	279	THR
3	M	302	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	198/208 (95%)	193 (98%)	5 (2%)	47	58
2	L	220/220 (100%)	204 (93%)	16 (7%)	14	14
3	M	236/240 (98%)	225 (95%)	11 (5%)	26	31
All	All	654/668 (98%)	622 (95%)	32 (5%)	25	29

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	170	ASN
2	L	216	PHE
3	M	199	ASN
2	L	210	ASP
2	L	246	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	264	GLN
3	M	199	ASN
3	M	187	ASN
2	L	170	ASN
3	M	77	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 1 is monoatomic - leaving 29 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	LDA	M	1311	-	12,15,15	2.03	1 (8%)	14,17,17	0.55	0
6	LDA	M	1306	-	12,15,15	2.13	1 (8%)	14,17,17	0.67	1 (7%)
4	GOL	M	1318	-	5,5,5	0.35	0	5,5,5	0.36	0
4	GOL	H	1253	-	5,5,5	0.52	0	5,5,5	0.56	0
6	LDA	M	1307	-	12,15,15	2.04	1 (8%)	14,17,17	0.49	0
8	UQ2	L	1286[A]	-	23,23,23	2.71	8 (34%)	28,31,31	1.29	3 (10%)
6	LDA	M	1309	-	12,15,15	2.02	1 (8%)	14,17,17	0.41	0
7	BPH	L	1285	-	64,70,70	3.03	18 (28%)	76,101,101	2.03	18 (23%)
8	UQ2	L	1286[B]	-	23,23,23	2.62	8 (34%)	28,31,31	1.80	7 (25%)
9	PO4	L	1288	-	4,4,4	0.73	0	6,6,6	0.49	0
5	BCL	L	1287	2	58,74,74	2.45	7 (12%)	69,115,115	2.03	19 (27%)
6	LDA	M	1310	-	12,15,15	2.03	1 (8%)	14,17,17	0.57	0
6	LDA	M	1308	-	12,15,15	1.93	1 (8%)	14,17,17	0.52	0
6	LDA	M	1312	-	12,15,15	2.00	1 (8%)	14,17,17	0.54	0
4	GOL	L	1291	-	5,5,5	0.34	0	5,5,5	0.27	0
13	SPO	M	1316	-	40,41,41	3.95	12 (30%)	47,50,50	2.20	17 (36%)
12	U10	M	1315	-	48,48,63	2.66	12 (25%)	58,61,79	1.82	13 (22%)
4	GOL	H	1254	-	5,5,5	0.36	0	5,5,5	0.39	0
6	LDA	L	1283	-	12,15,15	2.00	1 (8%)	14,17,17	0.46	0
4	GOL	L	1290	-	5,5,5	0.44	0	5,5,5	0.85	0
10	HTO	L	1289	-	9,9,9	0.47	0	10,10,10	0.61	0
5	BCL	L	1282	2	58,74,74	2.32	8 (13%)	69,115,115	2.01	18 (26%)
4	GOL	H	1252	-	5,5,5	0.61	0	5,5,5	1.10	0
6	LDA	L	1284	-	12,15,15	2.07	1 (8%)	14,17,17	0.68	0
5	BCL	M	1304	3	58,74,74	2.27	9 (15%)	69,115,115	1.98	18 (26%)
7	BPH	M	1314	-	64,70,70	2.92	16 (25%)	76,101,101	1.90	14 (18%)
5	BCL	M	1305	3	58,74,74	2.40	11 (18%)	69,115,115	2.15	17 (24%)
14	CDL	M	1317	-	80,80,99	2.13	17 (21%)	86,92,111	3.42	17 (19%)
4	GOL	H	1255	-	5,5,5	0.38	0	5,5,5	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LDA	M	1311	-	-	6/13/13/13	-
6	LDA	M	1306	-	-	4/13/13/13	-
4	GOL	H	1254	-	-	2/4/4/4	-
4	GOL	H	1253	-	-	2/4/4/4	-
6	LDA	M	1307	-	-	6/13/13/13	-
8	UQ2	L	1286[A]	-	-	6/15/39/39	0/1/1/1
6	LDA	M	1309	-	-	5/13/13/13	-
7	BPH	L	1285	-	-	7/54/105/105	0/5/6/6
8	UQ2	L	1286[B]	-	-	5/15/39/39	0/1/1/1
5	BCL	L	1287	2	2/2/21/25	9/37/137/137	-
6	LDA	M	1310	-	-	5/13/13/13	-
6	LDA	M	1308	-	-	6/13/13/13	-
6	LDA	M	1312	-	-	8/13/13/13	-
4	GOL	L	1291	-	-	4/4/4/4	-
13	SPO	M	1316	-	-	13/47/47/47	-
12	U10	M	1315	-	-	13/45/69/87	0/1/1/1
4	GOL	M	1318	-	-	1/4/4/4	-
6	LDA	L	1283	-	-	5/13/13/13	-
4	GOL	L	1290	-	-	2/4/4/4	-
10	HTO	L	1289	-	-	5/10/10/10	-
5	BCL	L	1282	2	2/2/21/25	8/37/137/137	-
4	GOL	H	1252	-	-	0/4/4/4	-
6	LDA	L	1284	-	-	9/13/13/13	-
5	BCL	M	1304	3	2/2/21/25	14/37/137/137	-
7	BPH	M	1314	-	-	22/54/105/105	0/5/6/6
5	BCL	M	1305	3	2/2/21/25	6/37/137/137	-
14	CDL	M	1317	-	-	46/91/91/110	-
4	GOL	H	1255	-	-	1/4/4/4	-

The worst 5 of 135 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1305	BCL	OBD-CAD	14.12	1.42	1.22
5	L	1287	BCL	OBD-CAD	13.32	1.40	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1282	BCL	OBD-CAD	12.98	1.40	1.22
5	M	1304	BCL	OBD-CAD	12.96	1.40	1.22
7	L	1285	BPH	OBD-CAD	12.74	1.40	1.22

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	1317	CDL	C33-C32-C31	18.11	178.30	113.19
14	M	1317	CDL	C17-C16-C15	11.38	172.22	114.42
14	M	1317	CDL	C12-C11-CA5	10.77	152.78	113.62
14	M	1317	CDL	C20-C19-C18	10.10	165.72	114.42
14	M	1317	CDL	C35-C34-C33	8.41	157.13	114.42

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1287	BCL	C8
5	L	1287	BCL	C13
5	L	1282	BCL	C8
5	L	1282	BCL	C13
5	M	1304	BCL	C8

5 of 220 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1253	GOL	O1-C1-C2-C3
6	M	1307	LDA	C2-C1-N1-CM1
6	M	1307	LDA	C2-C1-N1-CM2
8	L	1286[A]	UQ2	C12-C13-C14-C15
8	L	1286[B]	UQ2	C7-C8-C9-C10

There are no ring outliers.

20 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	1306	LDA	3	0
4	M	1318	GOL	1	0
4	H	1253	GOL	1	0
8	L	1286[A]	UQ2	2	0
6	M	1309	LDA	2	0
7	L	1285	BPH	6	0

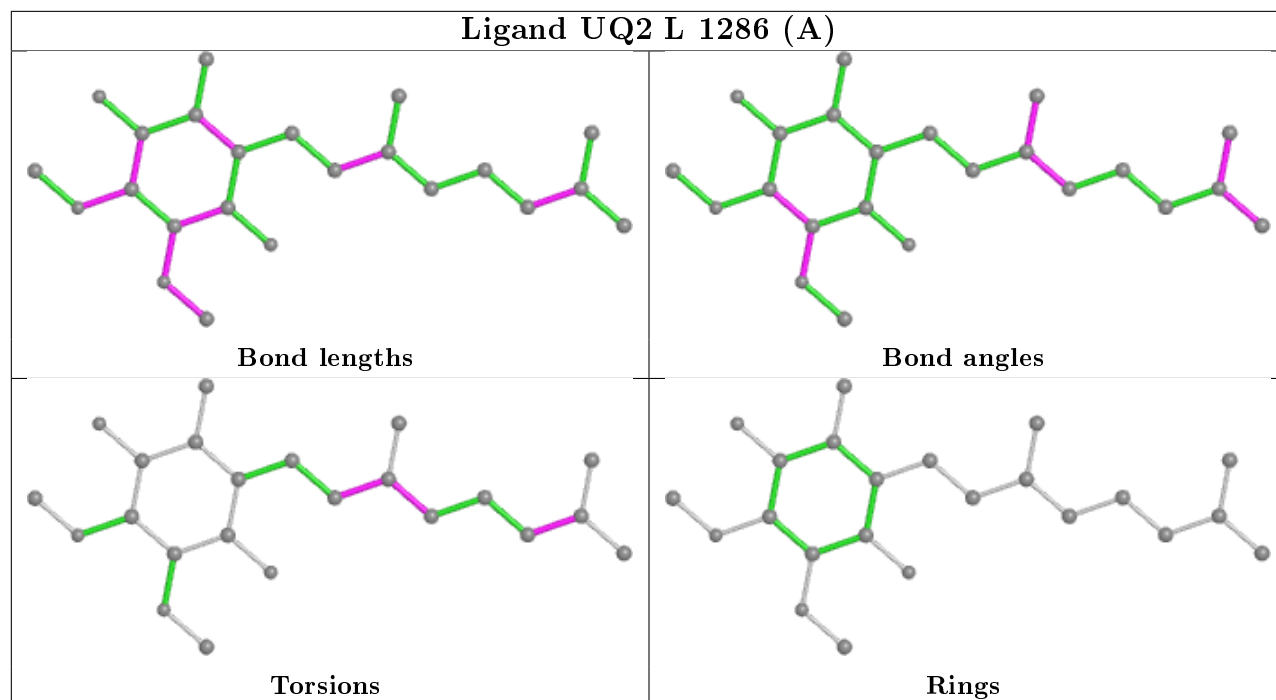
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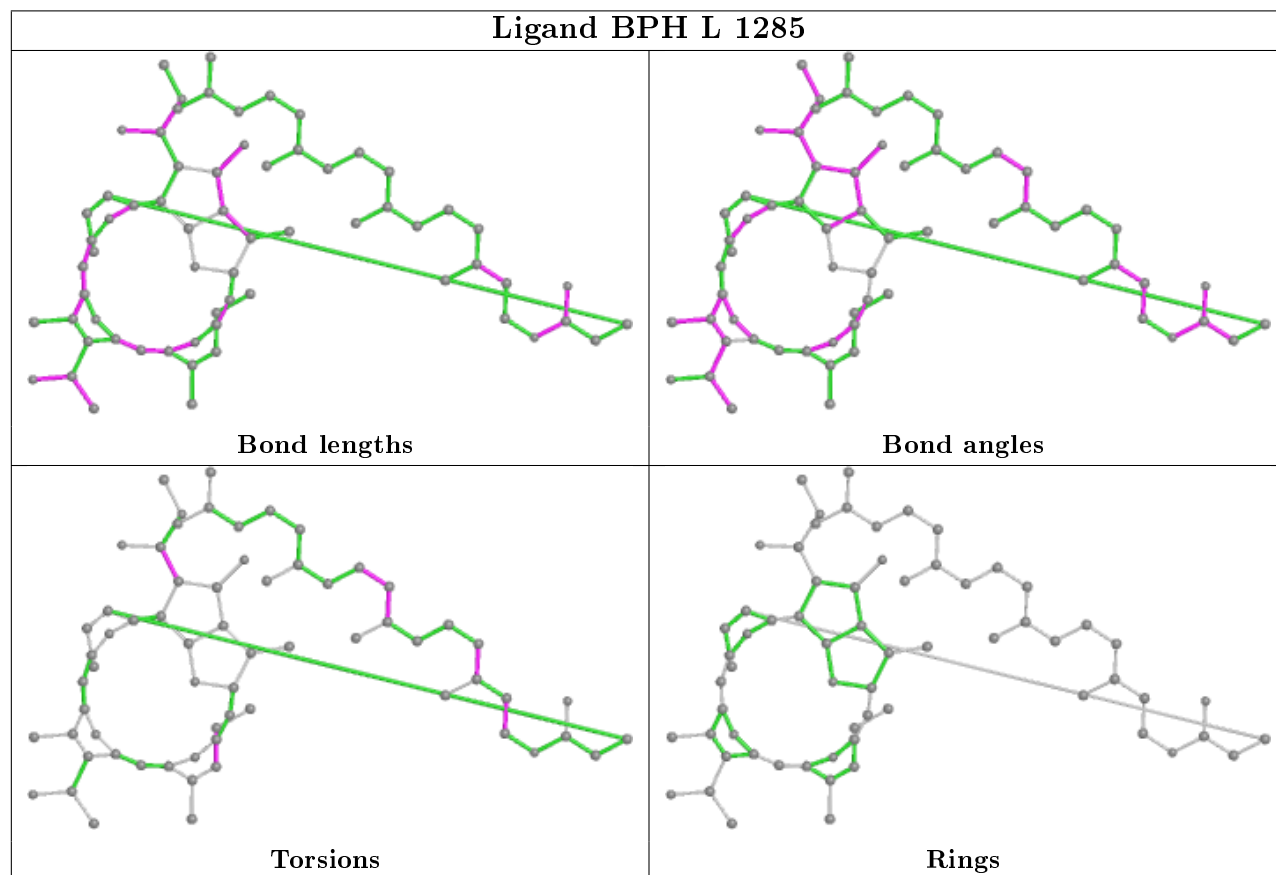
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	1286[B]	UQ2	4	0
5	L	1287	BCL	4	0
6	M	1310	LDA	2	0
6	M	1308	LDA	4	0
13	M	1316	SPO	2	0
12	M	1315	U10	3	0
4	L	1290	GOL	1	0
5	L	1282	BCL	3	0
4	H	1252	GOL	3	0
6	L	1284	LDA	2	0
5	M	1304	BCL	8	0
7	M	1314	BPH	14	0
5	M	1305	BCL	14	0
14	M	1317	CDL	4	0

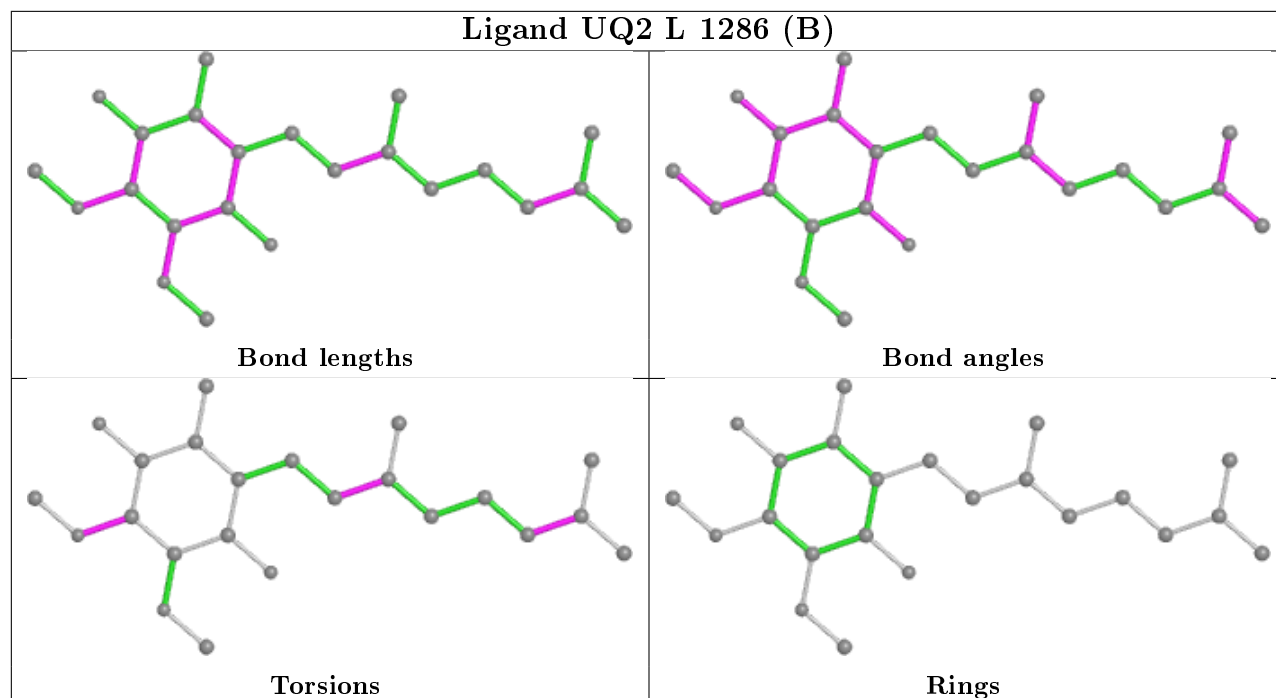
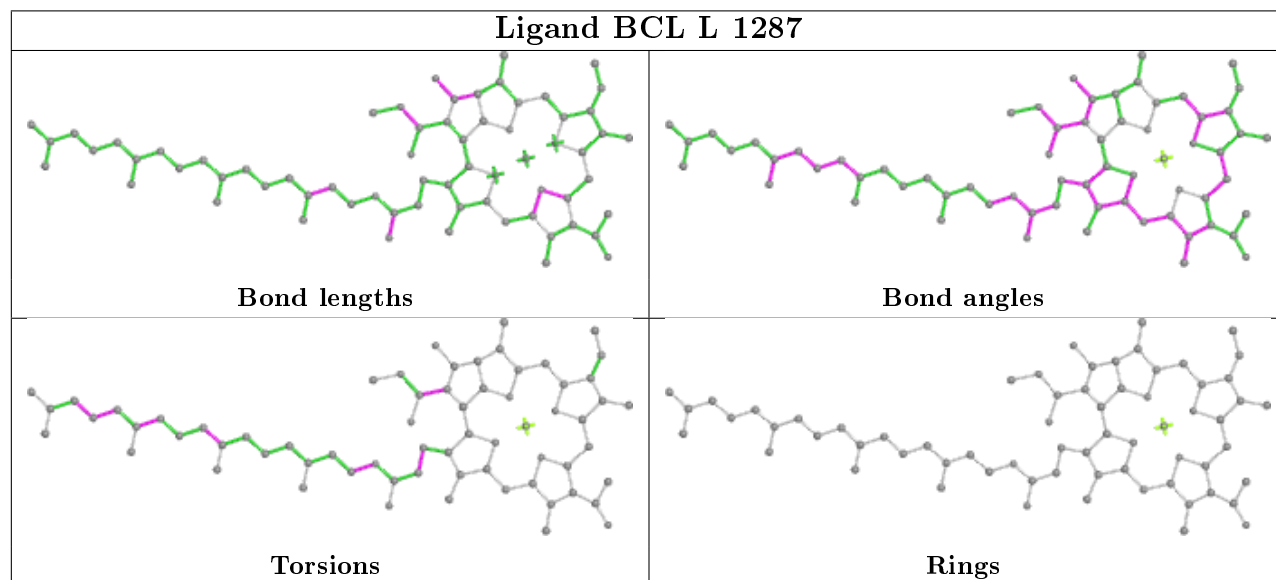
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

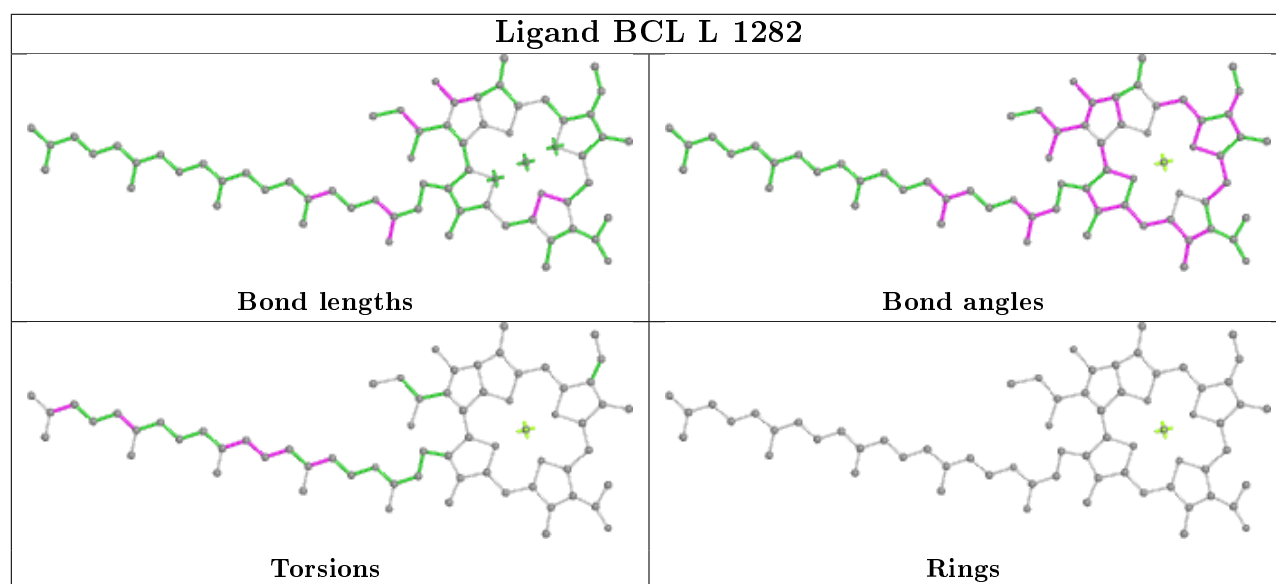
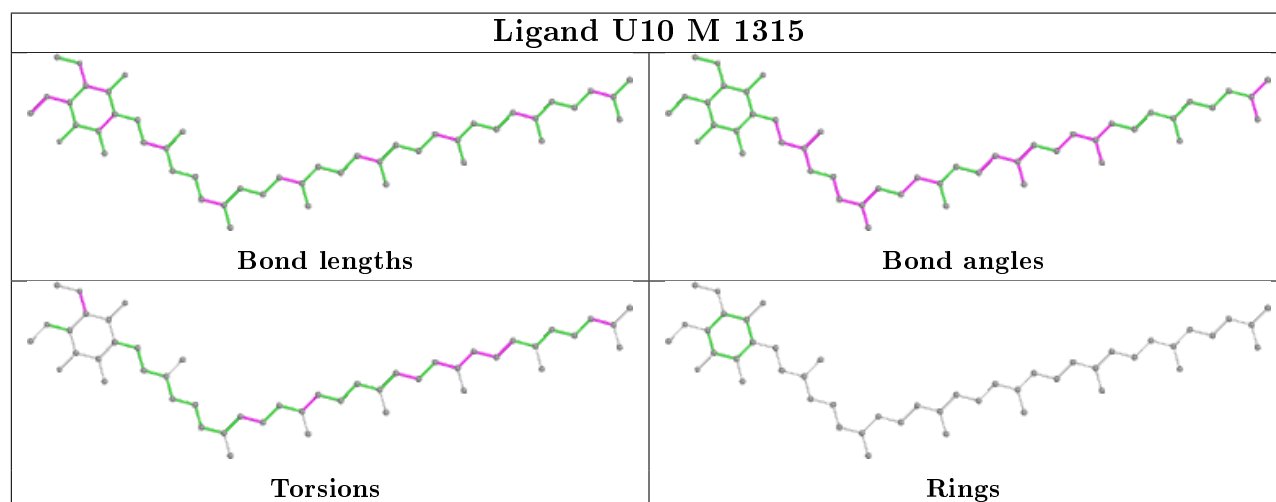
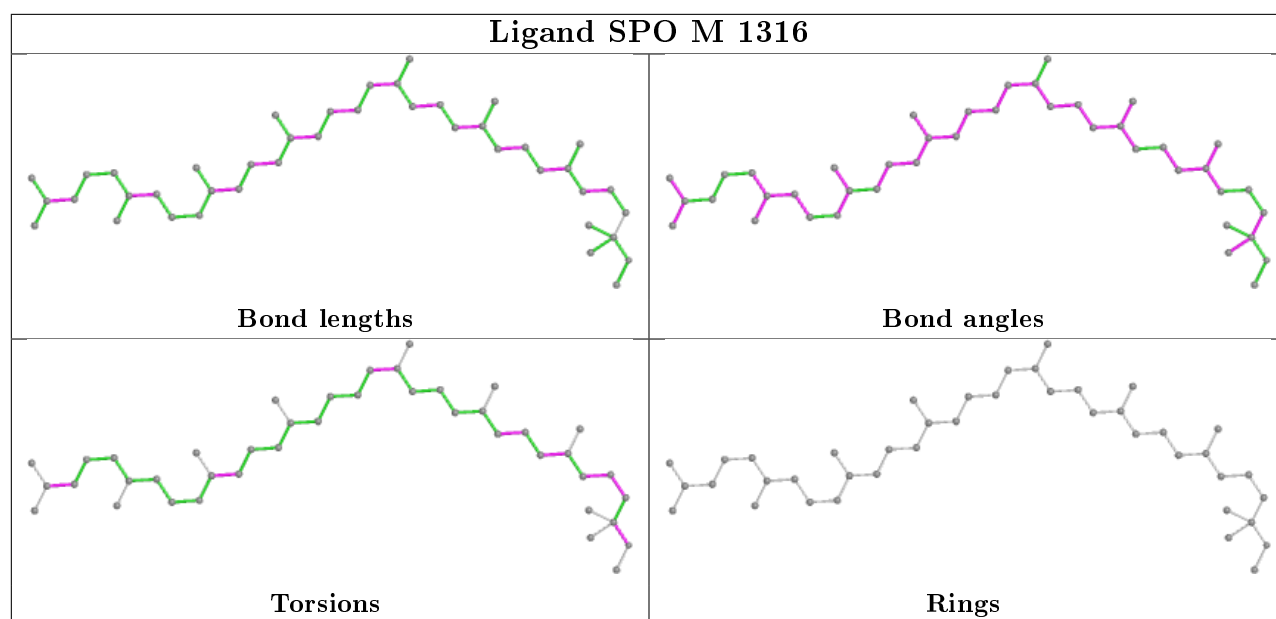
## Ligand UQ2 L 1286 (A)

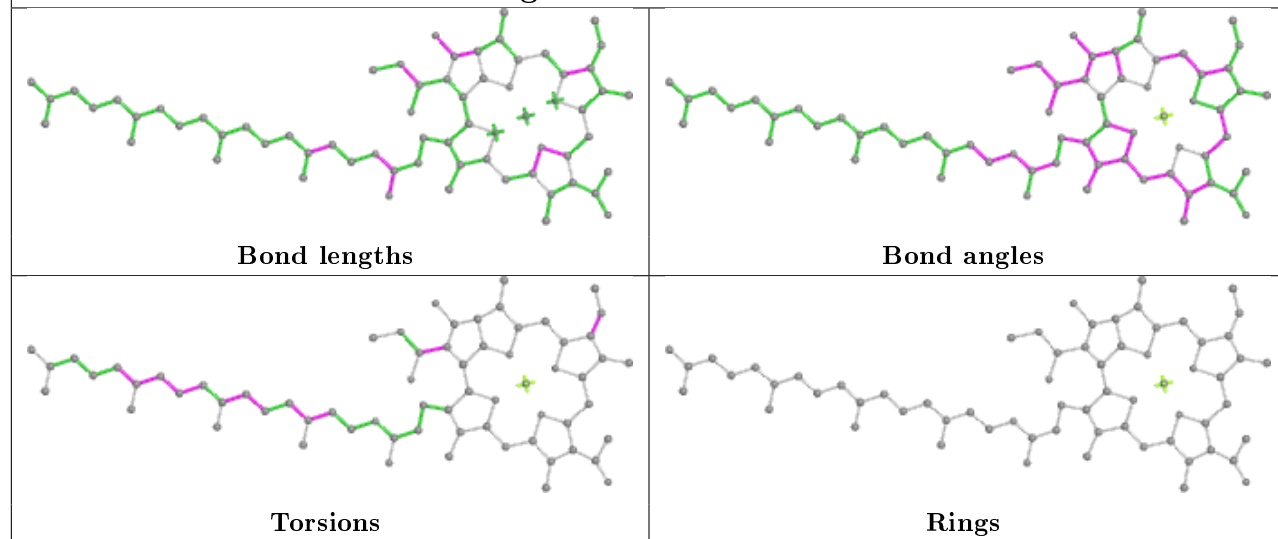
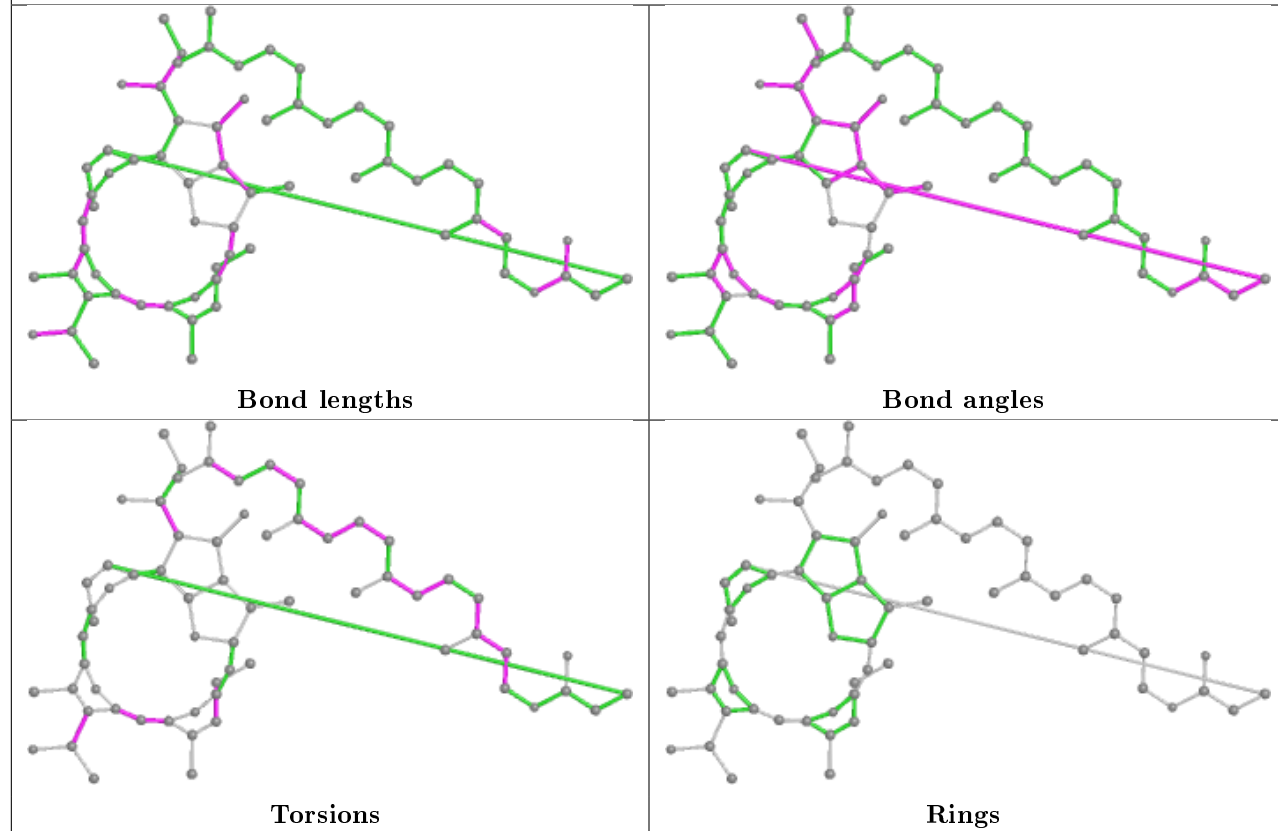


## Ligand BPH L 1285

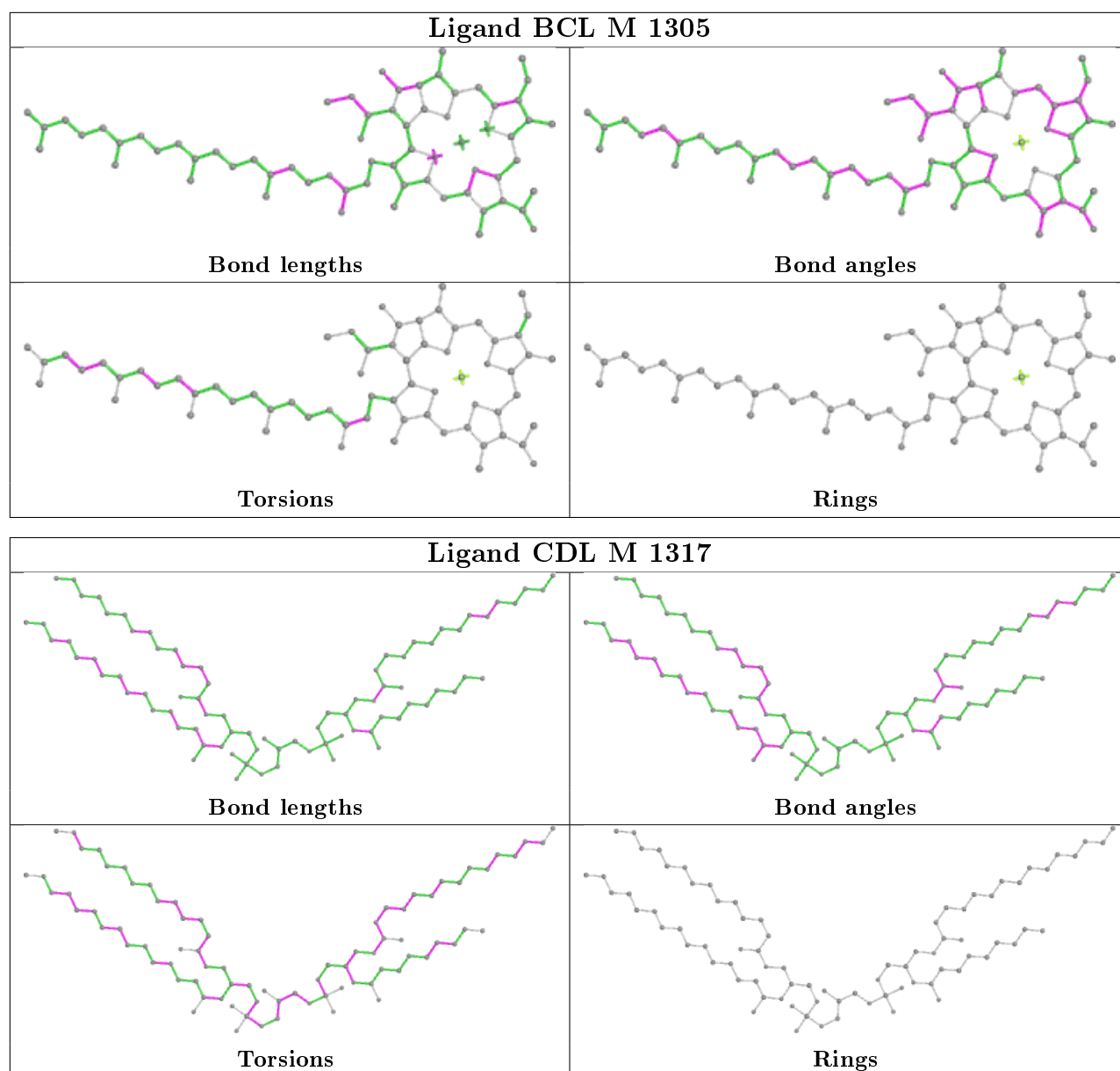


**Ligand UQ2 L 1286 (B)****Ligand BCL L 1287**



**Ligand BCL M 1304****Ligand BPH M 1314**





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	241/260 (92%)	-0.33	9 (3%) 41 39	29, 39, 51, 96	0
2	L	281/281 (100%)	-0.48	6 (2%) 63 61	27, 37, 61, 67	0
3	M	303/307 (98%)	-0.48	10 (3%) 46 44	24, 41, 63, 75	0
All	All	825/848 (97%)	-0.44	25 (3%) 50 48	24, 39, 61, 96	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	251	VAL	20.2
3	M	303	MET	8.9
3	M	1	ALA	8.8
1	H	250	SER	8.4
1	H	249	LYS	5.6

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

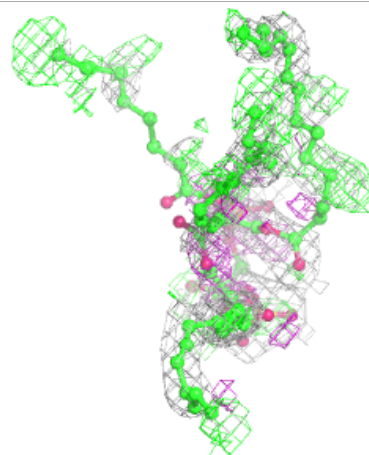
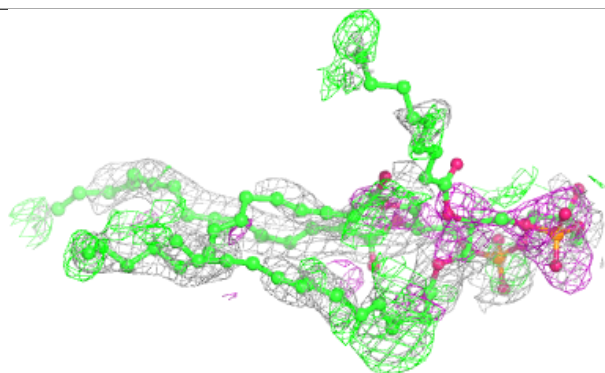
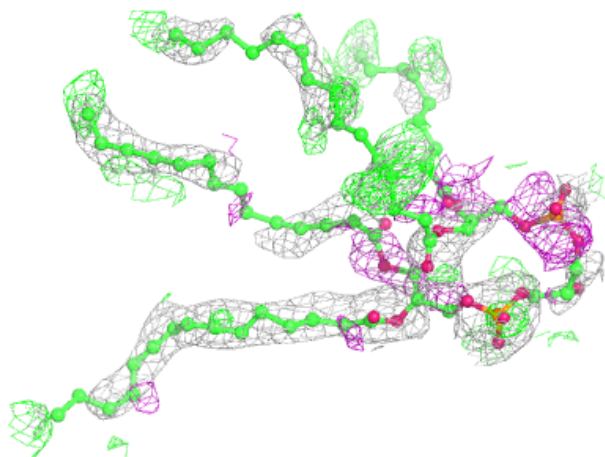
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	LDA	M	1312	16/16	0.13	0.30	78,90,101,101	0
6	LDA	L	1283	16/16	0.20	0.44	61,91,105,105	0
6	LDA	M	1311	16/16	0.25	0.44	95,104,112,113	0
4	GOL	H	1254	6/6	0.26	0.34	103,104,105,105	0
6	LDA	M	1309	16/16	0.32	0.35	98,102,109,110	0
6	LDA	M	1310	16/16	0.41	0.32	110,113,119,120	0
6	LDA	L	1284	16/16	0.47	0.33	109,110,114,114	0
14	CDL	M	1317	81/100	0.55	0.41	78,104,124,124	0
4	GOL	H	1253	6/6	0.61	0.26	74,77,77,80	0
6	LDA	M	1306	16/16	0.68	0.27	54,70,75,76	0
4	GOL	L	1291	6/6	0.69	0.23	94,95,96,96	0
10	HTO	L	1289	10/10	0.77	0.26	85,87,88,89	0
4	GOL	H	1255	6/6	0.79	0.31	101,101,102,102	0
6	LDA	M	1308	16/16	0.80	0.18	61,67,75,75	0
6	LDA	M	1307	16/16	0.80	0.19	66,69,80,80	0
4	GOL	H	1252	6/6	0.81	0.29	46,60,63,65	0
4	GOL	L	1290	6/6	0.83	0.18	49,57,57,61	0
13	SPO	M	1316	42/42	0.86	0.17	36,49,68,72	0
4	GOL	M	1318	6/6	0.89	0.08	83,84,84,85	0
8	UQ2	L	1286[B]	23/23	0.91	0.17	32,41,50,51	23
8	UQ2	L	1286[A]	23/23	0.91	0.17	36,41,50,52	23
12	U10	M	1315	48/63	0.92	0.13	26,45,73,75	0
9	PO4	L	1288	5/5	0.94	0.20	89,89,90,90	0
7	BPH	M	1314	65/65	0.94	0.11	26,41,98,101	0
5	BCL	M	1304	66/66	0.96	0.09	21,32,75,76	0
7	BPH	L	1285	65/65	0.97	0.10	23,31,44,48	0
5	BCL	M	1305	66/66	0.97	0.10	22,29,59,67	0
5	BCL	L	1287	66/66	0.97	0.12	19,30,50,57	0
5	BCL	L	1282	66/66	0.97	0.08	24,32,59,63	0
11	FE	M	1313	1/1	0.99	0.01	26,26,26,26	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.

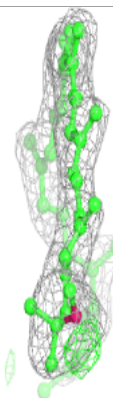
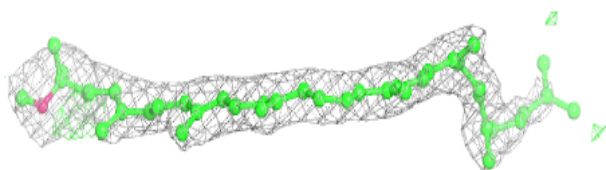
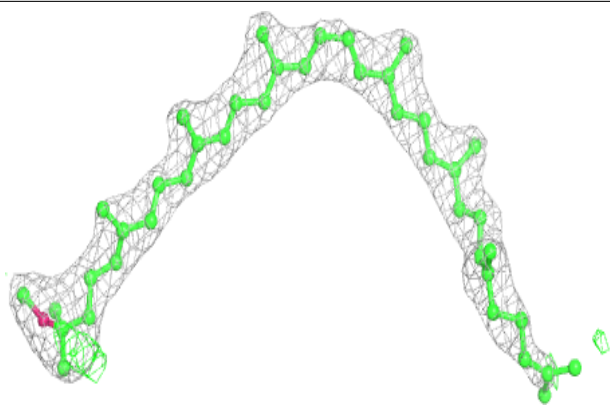
**Electron density around CDL M 1317:**

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

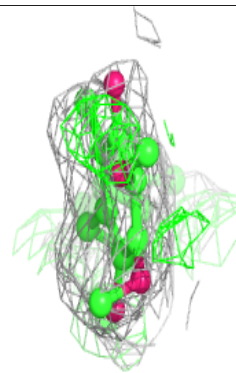
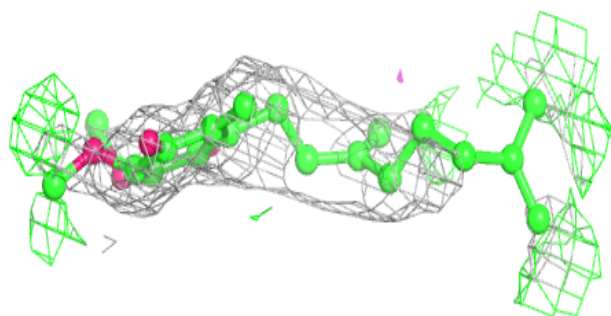
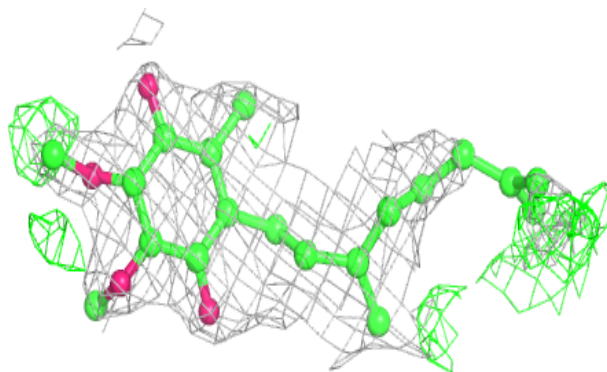


**Electron density around SPO M 1316:**

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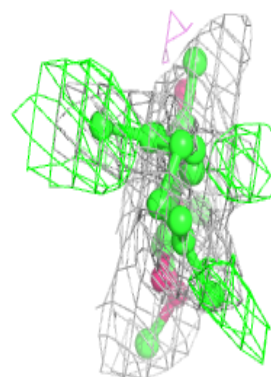
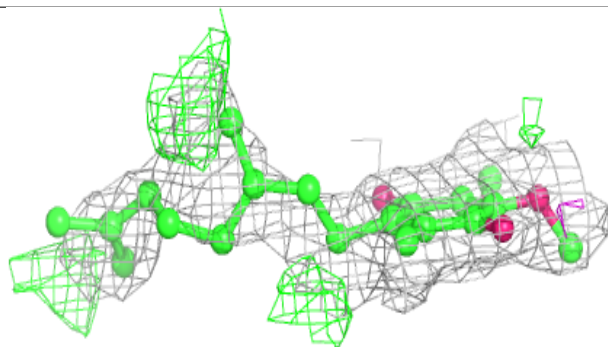
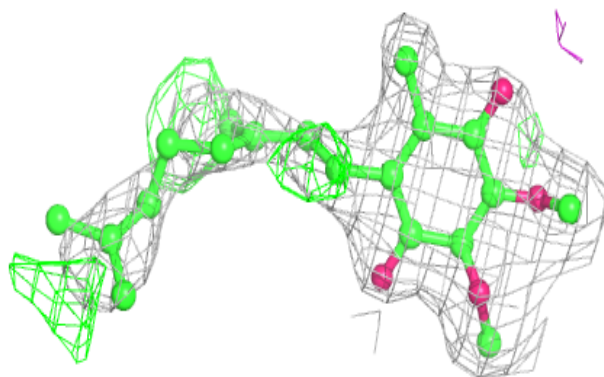
**Electron density around UQ2 L 1286 (B):**

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

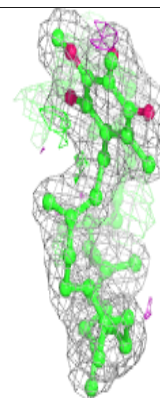
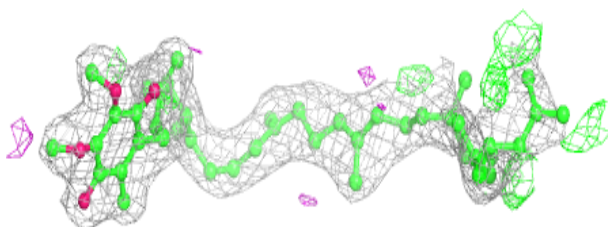
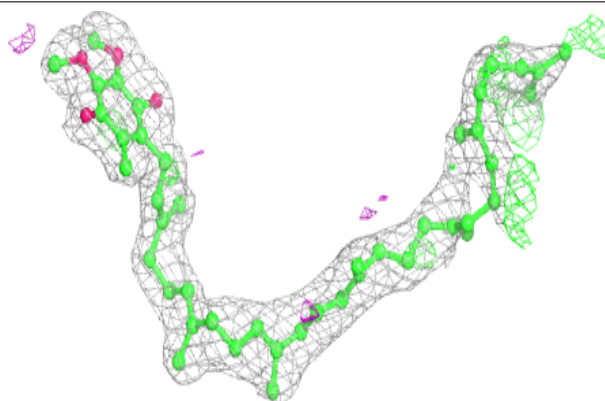


**Electron density around UQ2 L 1286 (A):**

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and green (positive)

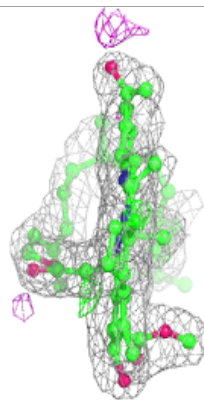
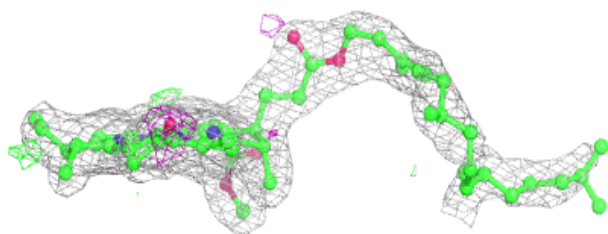
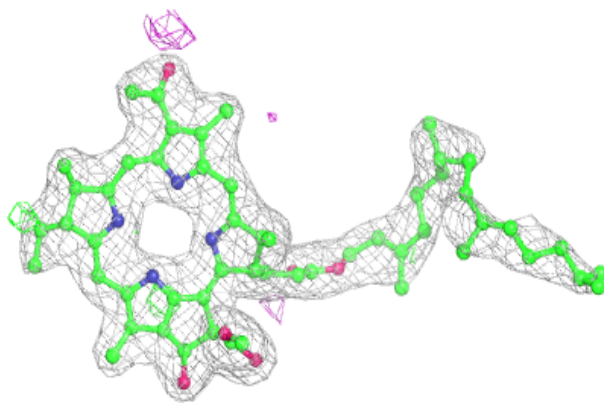
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and green (positive)



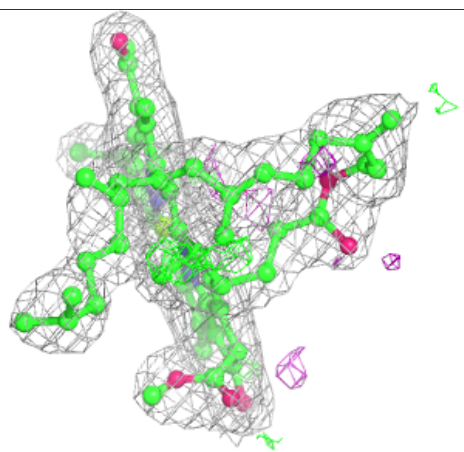
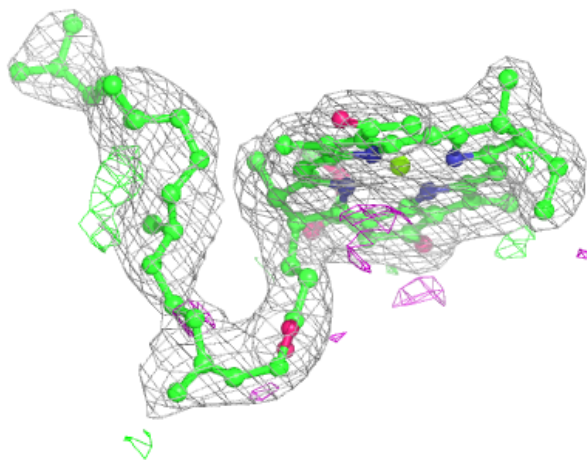
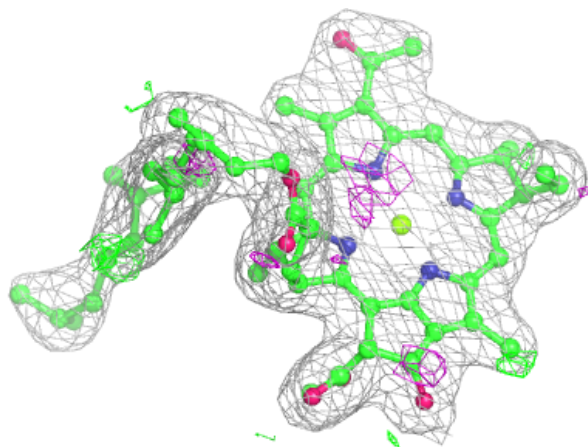
**Electron density around BPH M 1314:**

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and green (positive)



**Electron density around BCL M 1304:**

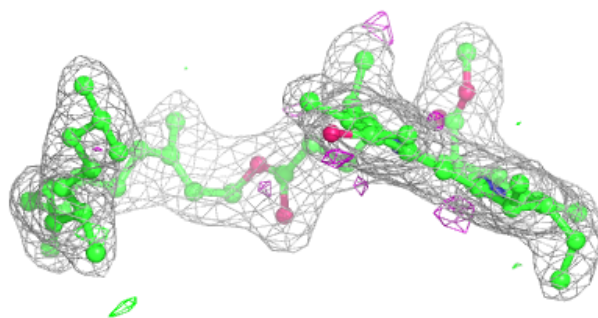
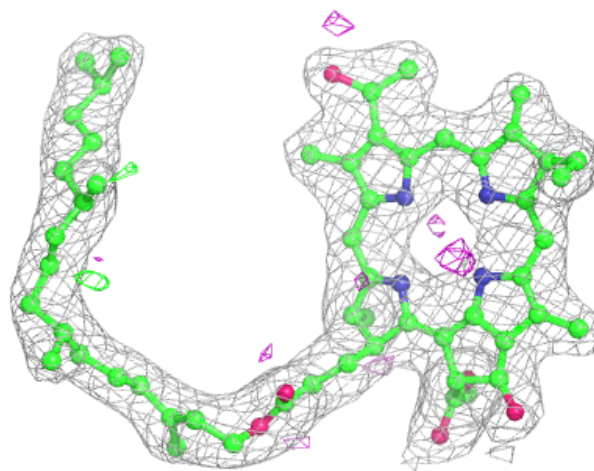
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and green (positive)





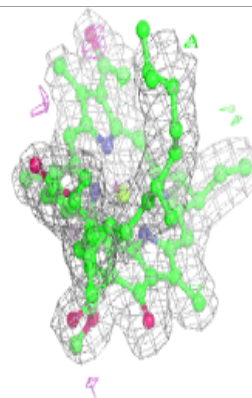
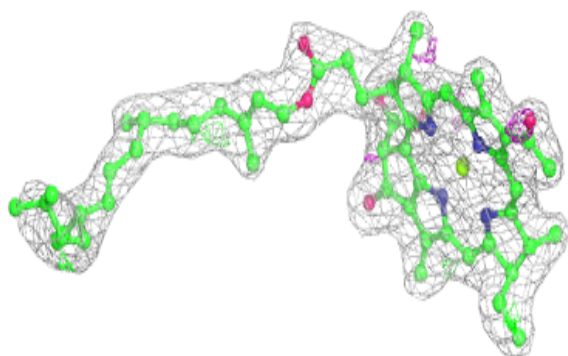
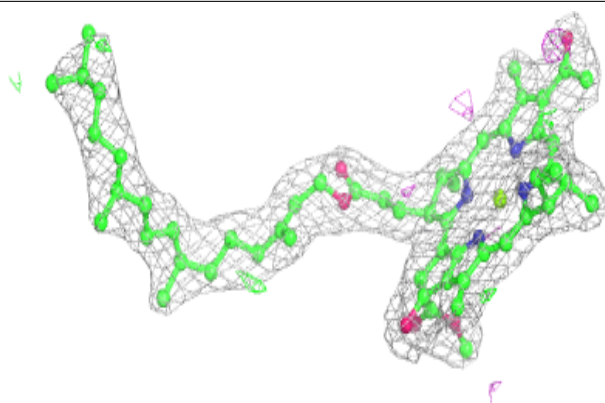
**Electron density around BPH L 1285:**

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and green (positive)

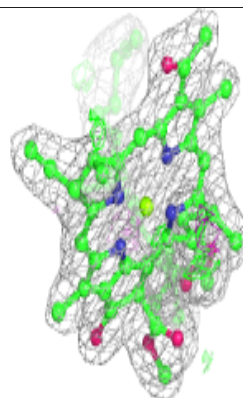
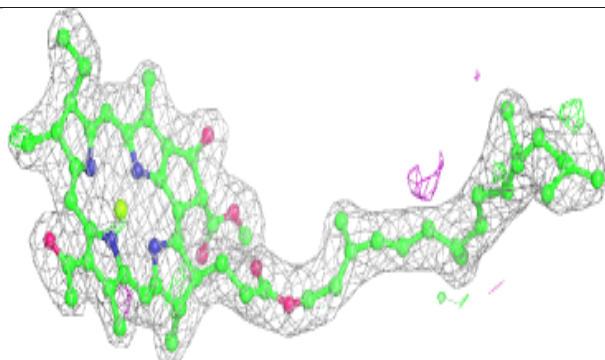
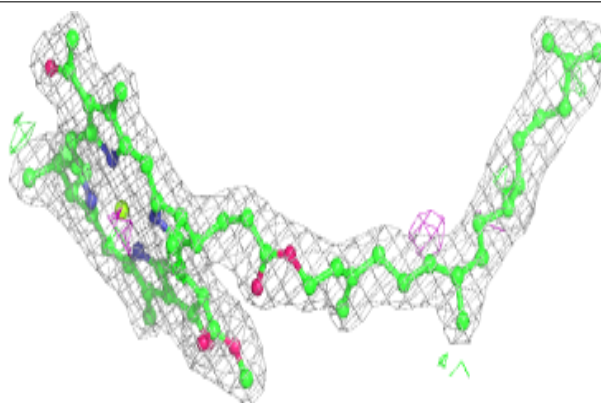


**Electron density around BCL M 1305:**

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

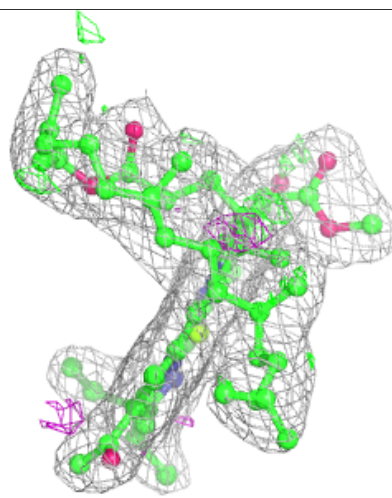
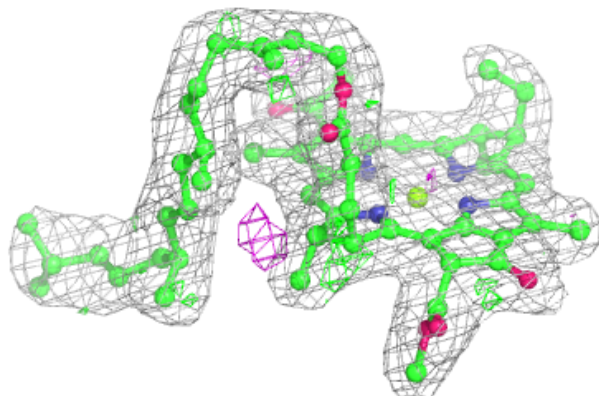
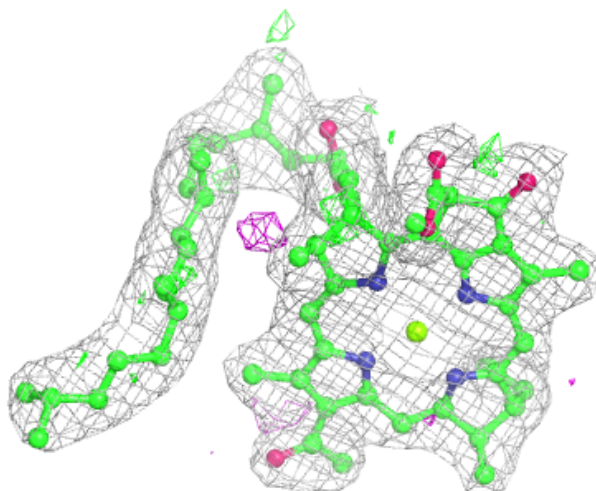
**Electron density around BCL L 1287:**

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



**Electron density around BCL L 1282:**

$2mF_o-DF_c$  (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.