



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2020 – 09:16 am GMT

PDB ID : 6Z1J  
Title : Photosynthetic Reaction Center From Rhodobacter Sphaeroides strain RV  
LSP co-crystallization with spheroidene  
Authors : Gabdulkhakov, A.G.; Fufina, T.Y.; Vasilieva, L.G.; Betzel, C.; Selikhanov,  
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Deposited on : 2020-05-13  
Resolution : 2.10 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 : 2.14.6  
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) : 2.14.6

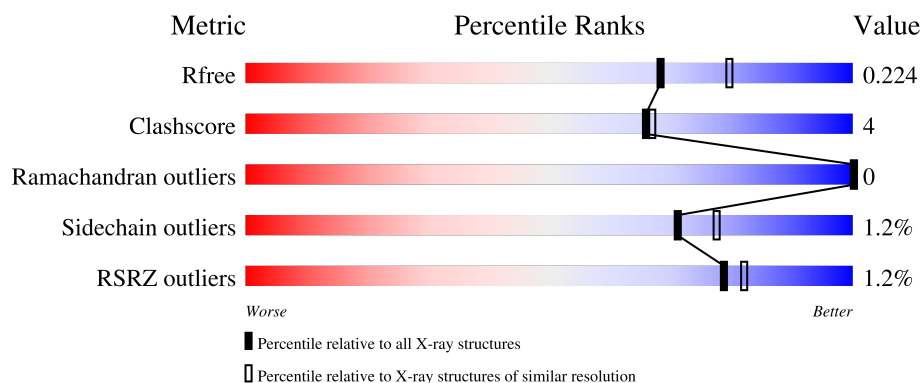
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	241	
2	L	281	
3	M	302	

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 7643 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	7	0
			1894	1210	324	350	10			

- 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	21	0
			2422	1639	386	389	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	conflict	UNP P0C0Y8

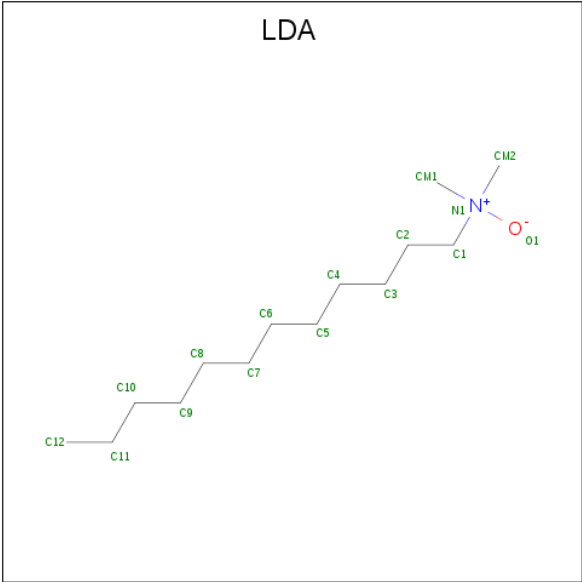
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	301	Total	C	N	O	S	0	5	0
			2441	1631	398	401	11			

There is a discrepancy between the modelled and reference sequences:

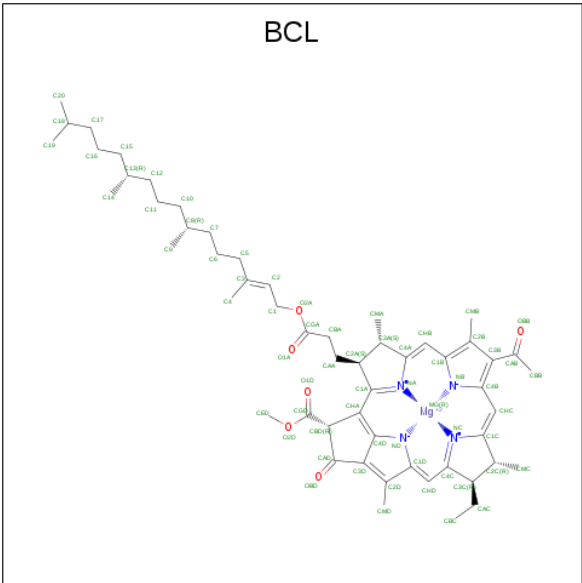
Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	conflict	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



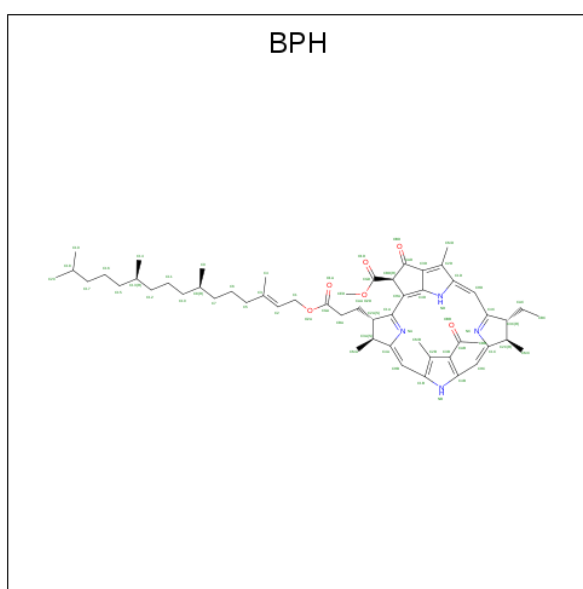
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- 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>) (labeled as "Ligand of Interest" by author).



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

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ) (labeled as "Ligand of Interest" by author).



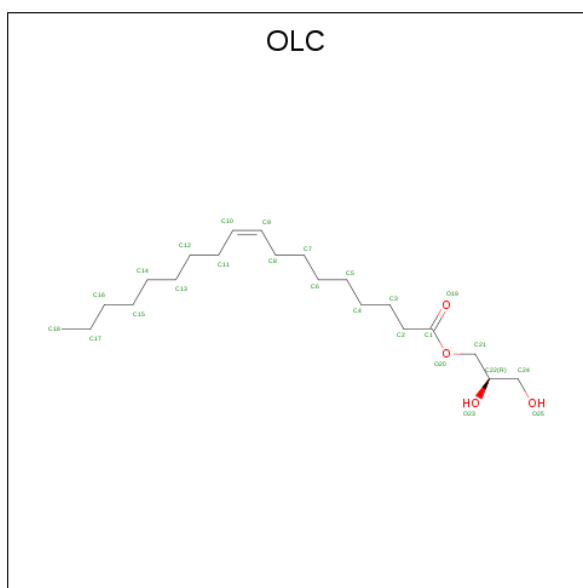
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O		
			65	55	4	6		
6	M	1	Total	C	N	O		
			65	55	4	6		

- Molecule 7 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	2	Total	C		
			27	27	0	0
7	M	3	Total	C		
			36	36	0	0

- Molecule 8 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC)

(formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).

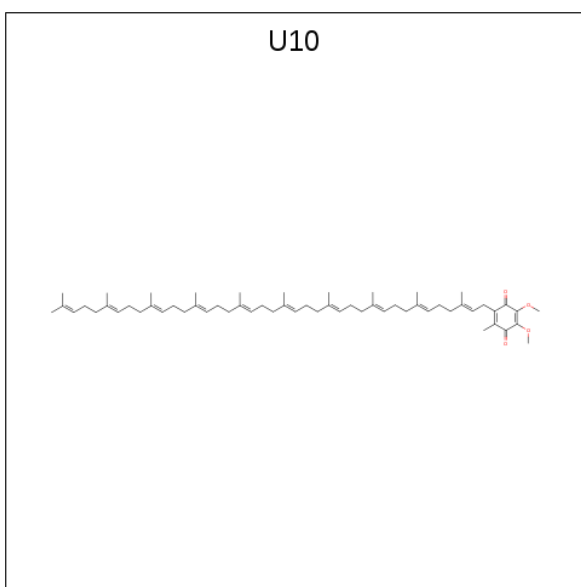


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			25	21	4		

- Molecule 9 is FE (III) ION (three-letter code: FE) (formula: Fe).

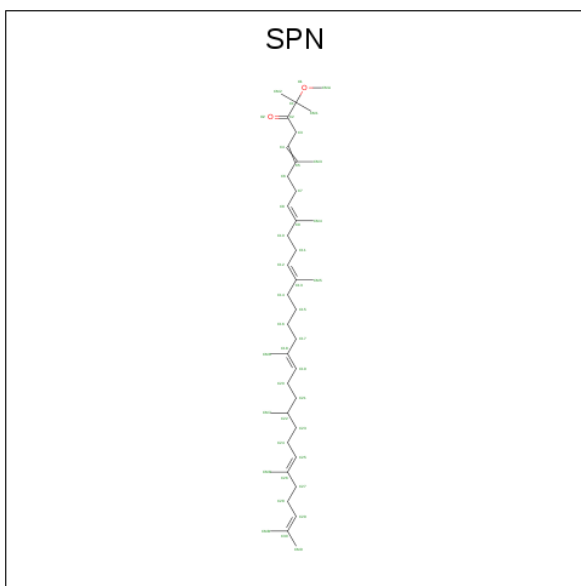
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total	Fe	0	0
			1	1		

- Molecule 10 is UBIQUINONE-10 (three-letter code: U10) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by author).



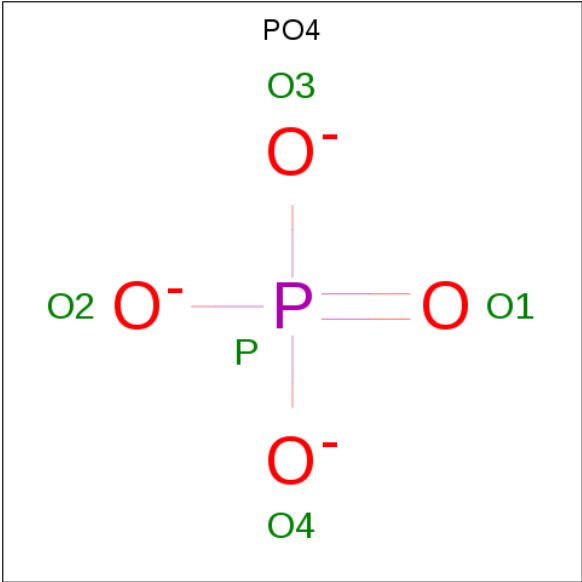
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 11 is SPEROIDENONE (three-letter code: SPN) (formula:  $C_{41}H_{70}O_2$ ) (labeled as "Ligand of Interest" by author).



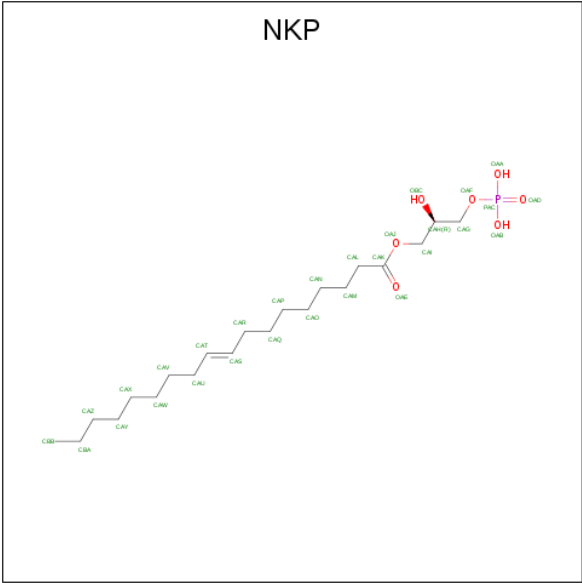
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	M	1	Total	C	O	0	0
			43	41	2		

- Molecule 12 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 13 is (2R)-2-hydroxy-3-(phosphonoxy)propyl (9E)-octadec-9-enoate (three-letter code: NKP) (formula: C<sub>21</sub>H<sub>41</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	O	P	0	0
			29	21	7	1		
13	M	1	Total	C	O	P	0	0
			29	21	7	1		



- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	78	Total 78	O 78	0	0
14	L	50	Total 50	O 50	0	0
14	M	57	Total 57	O 57	0	0

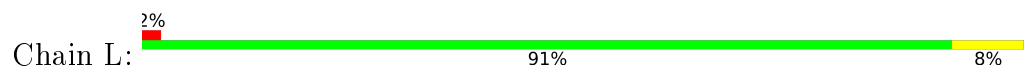
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

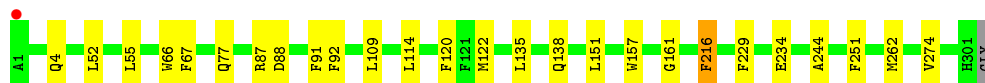
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.89Å 99.89Å 238.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.07 – 2.10 48.88 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.07-2.10) 100.0 (48.88-2.10)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18_3861, PHENIX 1.18_3861	Depositor
R, $R_{free}$	0.188 , 0.224 0.188 , 0.224	Depositor DCC
$R_{free}$ test set	3567 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7643	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LDA, OLC, BPH, PO4, NKP, FE, SPN, U10, UNL

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	0.42	0/1946	0.56	0/2646
2	L	0.41	0/2523	0.49	0/3457
3	M	0.41	0/2533	0.50	0/3458
All	All	0.41	0/7002	0.51	0/9561

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1894	0	1895	13	0
2	L	2422	0	2356	17	0
3	M	2441	0	2361	25	0
4	H	16	0	31	1	0
4	M	48	0	93	2	0
5	L	132	0	148	3	0
5	M	132	0	148	2	0
6	L	65	0	76	0	0
6	M	65	0	76	2	0
7	L	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	36	0	0	0	0
8	L	25	0	40	0	0
9	M	1	0	0	0	0
10	M	48	0	63	0	0
11	M	43	0	70	10	0
12	M	5	0	0	1	0
13	M	58	0	78	3	0
14	H	78	0	0	0	0
14	L	50	0	0	0	0
14	M	57	0	0	1	0
All	All	7643	0	7435	59	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (59) 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)
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.74	0.69
2:L:267[A]:VAL:HG13	2:L:280[A]:ASN:HB3	1.76	0.68
2:L:277[B]:GLY:O	3:M:87:ARG:NH2	2.28	0.66
2:L:201:GLU:OE2	3:M:138:GLN:HG3	2.01	0.61
5:L:301:BCL:CAB	11:M:406:SPN:H162	2.32	0.60
3:M:161:GLY:HA3	11:M:406:SPN:H201	1.83	0.60
1:H:26:GLY:HA3	13:M:415:NKP:HAT	1.85	0.59
1:H:70:ARG:O	1:H:118[A]:ARG:NH2	2.35	0.58
3:M:274:VAL:HG11	13:M:414:NKP:HAP	1.85	0.58
2:L:138:MET:HE1	2:L:249:ILE:HG13	1.85	0.57
3:M:4:GLN:HB2	12:M:413:PO4:O3	2.06	0.55
1:H:87:LEU:HD23	1:H:100:PRO:HA	1.89	0.54
3:M:120:PHE:HD1	11:M:406:SPN:HMB2	1.74	0.53
6:M:403:BPH:HHD	6:M:403:BPH:HBC3	1.91	0.52
3:M:157:TRP:CD1	11:M:406:SPN:H202	2.46	0.51
3:M:120:PHE:CD1	11:M:406:SPN:HMB2	2.46	0.50
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.94	0.49
2:L:138:MET:HE3	2:L:253:THR:HG21	1.95	0.49
1:H:59:PRO:HG2	1:H:76:PRO:HG3	1.93	0.49
1:H:21:TRP:HZ2	4:M:407:LDA:HM13	1.78	0.48
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.94	0.48
3:M:157:TRP:CZ2	11:M:406:SPN:H22	2.49	0.48
1:H:171:ILE:HB	1:H:172:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:234:GLU:HG2	3:M:262[A]:MET:SD	2.54	0.47
3:M:109:LEU:HG	3:M:114[B]:LEU:HG	1.96	0.47
5:M:402:BCL:HBB2	5:M:402:BCL:HMB1	1.96	0.47
3:M:55:LEU:HD12	3:M:135:LEU:HD12	1.97	0.46
4:M:408:LDA:HM11	4:M:408:LDA:H22	1.69	0.45
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.52	0.45
3:M:67:PHE:CE1	11:M:406:SPN:H61	2.52	0.45
2:L:209:PRO:HG3	14:M:557:HOH:O	2.16	0.45
11:M:406:SPN:HM51	11:M:406:SPN:H152	1.89	0.45
3:M:88:ASP:HB2	3:M:92:PHE:CZ	2.53	0.44
1:H:157:ASP:N	1:H:157:ASP:OD1	2.51	0.44
2:L:278[A]:GLY:HA2	3:M:77:GLN:O	2.17	0.44
3:M:55:LEU:HD23	3:M:55:LEU:HA	1.90	0.44
1:H:132:LYS:NZ	1:H:136:ALA:O	2.51	0.43
3:M:157:TRP:CE2	11:M:406:SPN:H22	2.53	0.43
1:H:63[B]:THR:HG22	1:H:74:THR:OG1	2.18	0.43
2:L:272[A]:TRP:CD2	3:M:87:ARG:HB2	2.54	0.43
2:L:52:SER:HB2	2:L:85:LEU:HD13	2.01	0.43
3:M:151[A]:LEU:HD23	13:M:414:NKP:HAS	2.00	0.43
2:L:265[A]:TRP:O	2:L:269[A]:LEU:HD13	2.19	0.42
6:M:403:BPH:H141	6:M:403:BPH:H161	1.81	0.42
1:H:135:LYS:HG3	1:H:166:ASP:OD2	2.20	0.42
2:L:279[A]:ILE:HG21	3:M:91:PHE:HB3	2.02	0.41
2:L:233:GLY:HA3	3:M:216:PHE:CE1	2.56	0.41
4:H:301:LDA:HM11	4:H:301:LDA:H22	1.78	0.41
2:L:170:ASN:O	2:L:173:HIS:HB3	2.19	0.41
5:L:301:BCL:OBB	5:L:301:BCL:HHC	2.20	0.41
2:L:135:ARG:HB3	2:L:136:PRO:HD3	2.03	0.41
5:L:302:BCL:HMB1	5:L:302:BCL:CBB	2.50	0.41
5:M:401:BCL:HBB3	5:M:402:BCL:HMD2	2.02	0.41
3:M:251:PHE:CD1	3:M:251:PHE:C	2.94	0.41
2:L:234:LEU:O	2:L:238:LEU:HG	2.21	0.41
1:H:157:ASP:OD2	1:H:210:SER:OG	2.35	0.40
2:L:266[B]:TRP:HA	2:L:269[B]:LEU:HD23	2.02	0.40
3:M:157:TRP:NE1	11:M:406:SPN:H202	2.36	0.40
2:L:268[A]:LYS:HD3	2:L:268[A]:LYS:HA	1.91	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	246/241 (102%)	240 (98%)	6 (2%)	0	100	100
2	L	299/281 (106%)	291 (97%)	8 (3%)	0	100	100
3	M	304/302 (101%)	294 (97%)	10 (3%)	0	100	100
All	All	849/824 (103%)	825 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	203/196 (104%)	202 (100%)	1 (0%)	88	92
2	L	237/220 (108%)	229 (97%)	8 (3%)	37	39
3	M	240/236 (102%)	237 (99%)	3 (1%)	69	75
All	All	680/652 (104%)	668 (98%)	12 (2%)	71	65

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	231	ASP
2	L	216	PHE
2	L	247	CYS
2	L	265[A]	TRP
2	L	265[B]	TRP

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Mol	Chain	Res	Type
2	L	269[A]	LEU
2	L	269[B]	LEU
2	L	272[A]	TRP
2	L	272[B]	TRP
3	M	52[A]	LEU
3	M	52[B]	LEU
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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 5 are unknown and 1 is monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	BCL	M	402	-	58,74,74	1.18	3 (5%)	69,115,115	1.30	8 (11%)
6	BPH	M	403	-	64,70,70	0.93	3 (4%)	76,101,101	1.12	8 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	PO4	M	413	-	4,4,4	0.95	0	6,6,6	0.30	0
4	LDA	M	408	-	12,15,15	2.04	1 (8%)	14,17,17	0.55	0
5	BCL	L	301	-	58,74,74	1.31	4 (6%)	69,115,115	1.47	15 (21%)
10	U10	M	405	-	48,48,63	2.59	13 (27%)	58,61,79	1.77	15 (25%)
8	OLC	L	306	-	24,24,24	0.95	1 (4%)	25,25,25	0.79	2 (8%)
4	LDA	M	409	-	12,15,15	2.11	1 (8%)	14,17,17	0.62	0
13	NKP	M	415	-	28,28,28	0.35	0	31,32,32	0.47	0
5	BCL	L	302	-	58,74,74	1.33	6 (10%)	69,115,115	1.30	9 (13%)
4	LDA	H	301	-	12,15,15	2.01	1 (8%)	14,17,17	0.60	0
5	BCL	M	401	-	58,74,74	1.26	4 (6%)	69,115,115	1.38	10 (14%)
13	NKP	M	414	-	28,28,28	0.37	0	31,32,32	0.40	0
6	BPH	L	303	-	64,70,70	1.05	5 (7%)	76,101,101	0.99	3 (3%)
4	LDA	M	407	-	12,15,15	2.00	1 (8%)	14,17,17	0.41	0
11	SPN	M	406	-	40,42,42	0.32	0	50,52,52	0.37	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
5	BCL	M	402	-	-	1/37/137/137	-
6	BPH	M	403	-	-	14/54/105/105	0/5/6/6
4	LDA	M	408	-	-	6/13/13/13	-
5	BCL	L	301	-	-	1/37/137/137	-
10	U10	M	405	-	-	9/45/69/87	0/1/1/1
8	OLC	L	306	-	-	11/24/24/24	-
4	LDA	M	409	-	-	8/13/13/13	-
13	NKP	M	415	-	-	6/28/28/28	-
5	BCL	L	302	-	-	1/37/137/137	-
4	LDA	H	301	-	-	3/13/13/13	-
5	BCL	M	401	-	-	1/37/137/137	-
13	NKP	M	414	-	-	6/28/28/28	-
6	BPH	L	303	-	-	3/54/105/105	0/5/6/6
4	LDA	M	407	-	-	6/13/13/13	-
11	SPN	M	406	-	-	19/50/51/51	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	409	LDA	O1-N1	-7.25	1.25	1.42
4	M	408	LDA	O1-N1	-7.01	1.25	1.42
4	H	301	LDA	O1-N1	-6.89	1.26	1.42
4	M	407	LDA	O1-N1	-6.77	1.26	1.42
10	M	405	U10	C8-C9	6.20	1.47	1.33
10	M	405	U10	C33-C34	5.96	1.47	1.33
10	M	405	U10	C13-C14	5.94	1.47	1.33
10	M	405	U10	C28-C29	5.82	1.46	1.33
10	M	405	U10	C18-C19	5.71	1.46	1.33
10	M	405	U10	C23-C24	5.60	1.46	1.33
5	L	301	BCL	C1B-NB	5.30	1.39	1.35
5	M	401	BCL	C1B-NB	5.02	1.39	1.35
10	M	405	U10	O3-C3	-4.92	1.24	1.36
5	L	302	BCL	C1B-NB	4.90	1.39	1.35
5	M	401	BCL	MG-NA	4.81	2.17	2.06
5	L	301	BCL	MG-NA	4.80	2.17	2.06
10	M	405	U10	C38-C39	4.79	1.46	1.32
10	M	405	U10	O4-C4	-4.77	1.25	1.36
5	L	302	BCL	MG-NA	4.72	2.17	2.06
5	M	402	BCL	C1B-NB	4.48	1.39	1.35
8	L	306	OLC	O20-C1	4.23	1.45	1.33
5	M	402	BCL	MG-NA	3.99	2.15	2.06
5	M	401	BCL	MG-NC	3.41	2.14	2.06
5	L	301	BCL	MG-NC	3.38	2.14	2.06
5	L	302	BCL	MG-NC	3.31	2.14	2.06
10	M	405	U10	C6-C1	3.09	1.40	1.35
10	M	405	U10	C3-C2	-3.04	1.40	1.48
6	M	403	BPH	C3D-CAD	-3.01	1.41	1.47
6	L	303	BPH	C1B-C2B	-2.76	1.39	1.45
5	M	402	BCL	MG-NC	2.69	2.12	2.06
6	L	303	BPH	OBD-CAD	2.66	1.26	1.22
6	L	303	BPH	C3D-CAD	-2.64	1.42	1.47
10	M	405	U10	C4-C5	-2.58	1.41	1.48
6	L	303	BPH	CHC-C1C	2.42	1.41	1.36
6	M	403	BPH	C1B-C2B	-2.30	1.40	1.45
5	L	301	BCL	O1A-CGA	-2.25	1.15	1.22
10	M	405	U10	C6-C5	-2.15	1.40	1.46
6	M	403	BPH	OBD-CAD	2.14	1.25	1.22
6	L	303	BPH	CAC-C3C	2.13	1.58	1.54
5	L	302	BCL	C1-C2	2.11	1.55	1.49
5	L	302	BCL	C4B-NB	2.09	1.37	1.35
5	L	302	BCL	OBD-CAD	2.01	1.25	1.22
5	M	401	BCL	CBD-CGD	-2.00	1.46	1.52

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	301	BCL	CMB-C2B-C1B	-4.25	121.93	128.46
10	M	405	U10	C30-C29-C31	4.23	122.39	115.27
5	L	302	BCL	CMB-C2B-C1B	-4.12	122.14	128.46
5	M	401	BCL	CMB-C2B-C1B	-4.09	122.18	128.46
5	M	402	BCL	OBD-CAD-CBD	-3.88	120.36	125.89
5	M	401	BCL	C4A-NA-C1A	3.79	108.41	106.71
10	M	405	U10	C32-C33-C34	-3.69	118.76	127.66
5	M	402	BCL	CMB-C2B-C1B	-3.63	122.88	128.46
5	M	401	BCL	CHA-C1A-NA	-3.33	118.76	126.40
5	L	302	BCL	C4D-C3D-CAD	-3.27	106.64	108.47
10	M	405	U10	C22-C23-C24	-3.26	119.80	127.66
5	M	401	BCL	C4D-C3D-CAD	-3.24	106.66	108.47
10	M	405	U10	C35-C34-C36	3.18	120.61	115.27
6	L	303	BPH	C1C-NC-C4C	-3.18	107.75	110.54
5	L	301	BCL	OBD-CAD-CBD	-3.12	121.43	125.89
5	M	401	BCL	OBD-CAD-CBD	-3.12	121.44	125.89
10	M	405	U10	C37-C38-C39	-3.12	117.09	127.75
5	M	401	BCL	CMB-C2B-C3B	3.11	130.50	124.68
5	L	301	BCL	CMB-C2B-C3B	3.09	130.46	124.68
5	M	402	BCL	CHA-C1A-NA	-3.08	119.35	126.40
10	M	405	U10	C41-C39-C40	3.07	121.39	114.60
5	L	302	BCL	CMB-C2B-C3B	3.07	130.42	124.68
10	M	405	U10	C25-C24-C26	3.07	120.43	115.27
5	L	301	BCL	CHA-C1A-NA	-3.06	119.39	126.40
5	L	302	BCL	CHA-C1A-NA	-3.02	119.49	126.40
10	M	405	U10	C27-C28-C29	-3.02	120.40	127.66
6	L	303	BPH	OBD-CAD-CBD	-3.01	121.59	125.89
6	M	403	BPH	OBD-CAD-CBD	-3.01	121.60	125.89
5	M	402	BCL	C4D-C3D-CAD	-2.96	106.82	108.47
5	L	302	BCL	OBD-CAD-CBD	-2.95	121.68	125.89
5	M	402	BCL	CMB-C2B-C3B	2.90	130.10	124.68
5	M	401	BCL	C2A-C1A-CHA	2.76	128.69	123.86
5	L	301	BCL	C4D-C3D-CAD	-2.76	106.93	108.47
5	L	302	BCL	C2A-C1A-CHA	2.75	128.67	123.86
10	M	405	U10	C17-C18-C19	-2.72	121.12	127.66
6	M	403	BPH	CHC-C1C-NC	-2.70	122.00	125.20
5	L	301	BCL	C2A-C1A-CHA	2.69	128.55	123.86
6	M	403	BPH	C1C-NC-C4C	-2.67	108.19	110.54
5	L	301	BCL	OBB-CAB-CBB	-2.65	114.21	120.17
5	L	301	BCL	O2D-CGD-O1D	-2.61	118.73	123.84
5	M	402	BCL	C2A-C1A-CHA	2.60	128.40	123.86
5	L	301	BCL	C1-O2A-CGA	2.59	123.25	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	405	U10	C4M-O4-C4	2.53	125.44	116.47
5	L	302	BCL	CMD-C2D-C3D	2.49	129.33	124.68
10	M	405	U10	C15-C14-C16	2.47	119.43	115.27
5	L	301	BCL	O2A-C1-C2	-2.44	102.23	108.64
8	L	306	OLC	O20-C1-C2	2.42	119.51	111.91
10	M	405	U10	C10-C9-C11	2.41	119.33	115.27
5	L	301	BCL	C4B-C3B-CAB	-2.37	122.54	127.13
5	L	301	BCL	C4A-NA-C1A	2.36	107.77	106.71
5	M	402	BCL	CMD-C2D-C3D	2.34	129.05	124.68
5	M	401	BCL	CMD-C2D-C3D	2.31	129.00	124.68
8	L	306	OLC	O20-C1-O19	-2.31	117.77	123.59
5	L	301	BCL	CMD-C2D-C3D	2.31	128.99	124.68
6	M	403	BPH	C3A-C4A-CHB	2.27	125.75	121.83
5	L	301	BCL	O2D-CGD-CBD	2.25	115.27	111.27
5	M	402	BCL	C4B-C3B-CAB	-2.23	122.82	127.13
6	M	403	BPH	CMD-C2D-C3D	2.22	128.83	124.68
10	M	405	U10	C31-C29-C28	-2.21	116.65	121.12
10	M	405	U10	C22-C21-C19	-2.18	105.81	112.98
10	M	405	U10	C32-C31-C29	-2.16	105.88	112.98
5	M	401	BCL	OBB-CAB-CBB	-2.07	115.51	120.17
6	M	403	BPH	O2A-C1-C2	-2.06	103.21	108.64
5	M	401	BCL	C4B-C3B-CAB	-2.06	123.14	127.13
5	L	302	BCL	OBB-CAB-CBB	-2.05	115.56	120.17
6	M	403	BPH	C1-C2-C3	-2.02	122.54	126.04
5	L	301	BCL	C16-C15-C13	2.02	122.46	115.92
6	L	303	BPH	C3A-C4A-CHB	2.02	125.31	121.83
6	M	403	BPH	C17-C16-C15	2.02	122.51	113.24
5	L	302	BCL	C1D-CHD-C4C	2.01	128.86	125.88

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	M	405	U10	C32-C33-C34-C35
10	M	405	U10	C32-C33-C34-C36
4	M	409	LDA	C2-C1-N1-O1
4	M	409	LDA	C2-C1-N1-CM1
4	M	409	LDA	C2-C1-N1-CM2
11	M	406	SPN	CM2-C1-C2-O2
11	M	406	SPN	CM2-C1-C2-C3
8	L	306	OLC	O20-C21-C22-O23
6	M	403	BPH	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
6	M	403	BPH	C4B-C3B-CAB-OBB
6	M	403	BPH	C2B-C3B-CAB-CBB
4	M	407	LDA	C2-C1-N1-CM1
4	M	407	LDA	C2-C1-N1-CM2
13	M	415	NKP	OAF-CAG-CAH-OBC
10	M	405	U10	C37-C38-C39-C40
11	M	406	SPN	CM3-C5-C6-C7
11	M	406	SPN	C11-C10-C9-CM4
11	M	406	SPN	CM5-C13-C14-C15
11	M	406	SPN	C16-C17-C18-CM6
11	M	406	SPN	C4-C5-C6-C7
11	M	406	SPN	C11-C10-C9-C8
11	M	406	SPN	C16-C17-C18-C19
13	M	415	NKP	OAF-CAG-CAH-CAI
6	M	403	BPH	C13-C15-C16-C17
10	M	405	U10	C37-C38-C39-C41
6	M	403	BPH	C5-C6-C7-C8
10	M	405	U10	C24-C26-C27-C28
8	L	306	OLC	C11-C12-C13-C14
6	M	403	BPH	C2B-C3B-CAB-OBB
13	M	414	NKP	CAN-CAO-CAP-CAQ
8	L	306	OLC	O20-C21-C22-C24
4	M	408	LDA	C5-C6-C7-C8
4	M	408	LDA	C11-C10-C9-C8
4	M	409	LDA	C2-C3-C4-C5
13	M	415	NKP	CAM-CAN-CAO-CAP
11	M	406	SPN	C26-C27-C28-C29
13	M	414	NKP	CAO-CAP-CAQ-CAR
13	M	415	NKP	CAL-CAM-CAN-CAO
11	M	406	SPN	C12-C13-C14-C15
10	M	405	U10	C30-C29-C31-C32
10	M	405	U10	C28-C29-C31-C32
8	L	306	OLC	C10-C11-C12-C13
4	M	409	LDA	C7-C8-C9-C10
4	M	408	LDA	C6-C7-C8-C9
4	M	409	LDA	C1-C2-C3-C4
4	M	407	LDA	C1-C2-C3-C4
5	M	402	BCL	C13-C15-C16-C17
4	M	408	LDA	C1-C2-C3-C4
13	M	415	NKP	CAK-CAL-CAM-CAN
4	M	408	LDA	C9-C10-C11-C12
4	H	301	LDA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
4	H	301	LDA	C7-C8-C9-C10
8	L	306	OLC	C1-C2-C3-C4
11	M	406	SPN	CM1-C1-O1-CMA
4	M	409	LDA	C4-C5-C6-C7
6	M	403	BPH	C11-C12-C13-C14
4	H	301	LDA	C1-C2-C3-C4
4	M	409	LDA	C5-C6-C7-C8
11	M	406	SPN	C14-C15-C16-C17
6	M	403	BPH	C11-C12-C13-C15
11	M	406	SPN	C19-C20-C21-C22
13	M	414	NKP	CAM-CAN-CAO-CAP
11	M	406	SPN	CM2-C1-O1-CMA
11	M	406	SPN	O1-C1-C2-O2
4	M	407	LDA	C2-C1-N1-O1
6	M	403	BPH	C11-C10-C8-C7
6	L	303	BPH	O2A-C1-C2-C3
13	M	414	NKP	CAL-CAM-CAN-CAO
6	M	403	BPH	C10-C11-C12-C13
5	L	301	BCL	C2-C1-O2A-CGA
6	M	403	BPH	C11-C10-C8-C9
13	M	414	NKP	CAH-CAG-OAF-PAC
13	M	414	NKP	CAS-CAT-CAU-CAV
8	L	306	OLC	C9-C10-C11-C12
4	M	407	LDA	C3-C4-C5-C6
8	L	306	OLC	C3-C4-C5-C6
8	L	306	OLC	C5-C6-C7-C8
6	M	403	BPH	C4C-C3C-CAC-CBC
8	L	306	OLC	C7-C8-C9-C10
10	M	405	U10	C5-C4-O4-C4M
6	L	303	BPH	CAD-CBD-CGD-O2D
5	L	302	BCL	CAD-CBD-CGD-O2D
6	M	403	BPH	CAD-CBD-CGD-O2D
5	M	401	BCL	CAA-CBA-CGA-O2A
8	L	306	OLC	O20-C1-C2-C3
11	M	406	SPN	C2-C1-O1-CMA
6	M	403	BPH	C2-C3-C5-C6
13	M	415	NKP	CAS-CAT-CAU-CAV
11	M	406	SPN	C18-C19-C20-C21
11	M	406	SPN	C2-C3-C4-C5
6	L	303	BPH	C2B-C3B-CAB-OBB
10	M	405	U10	C25-C24-C26-C27
8	L	306	OLC	O19-C1-C2-C3

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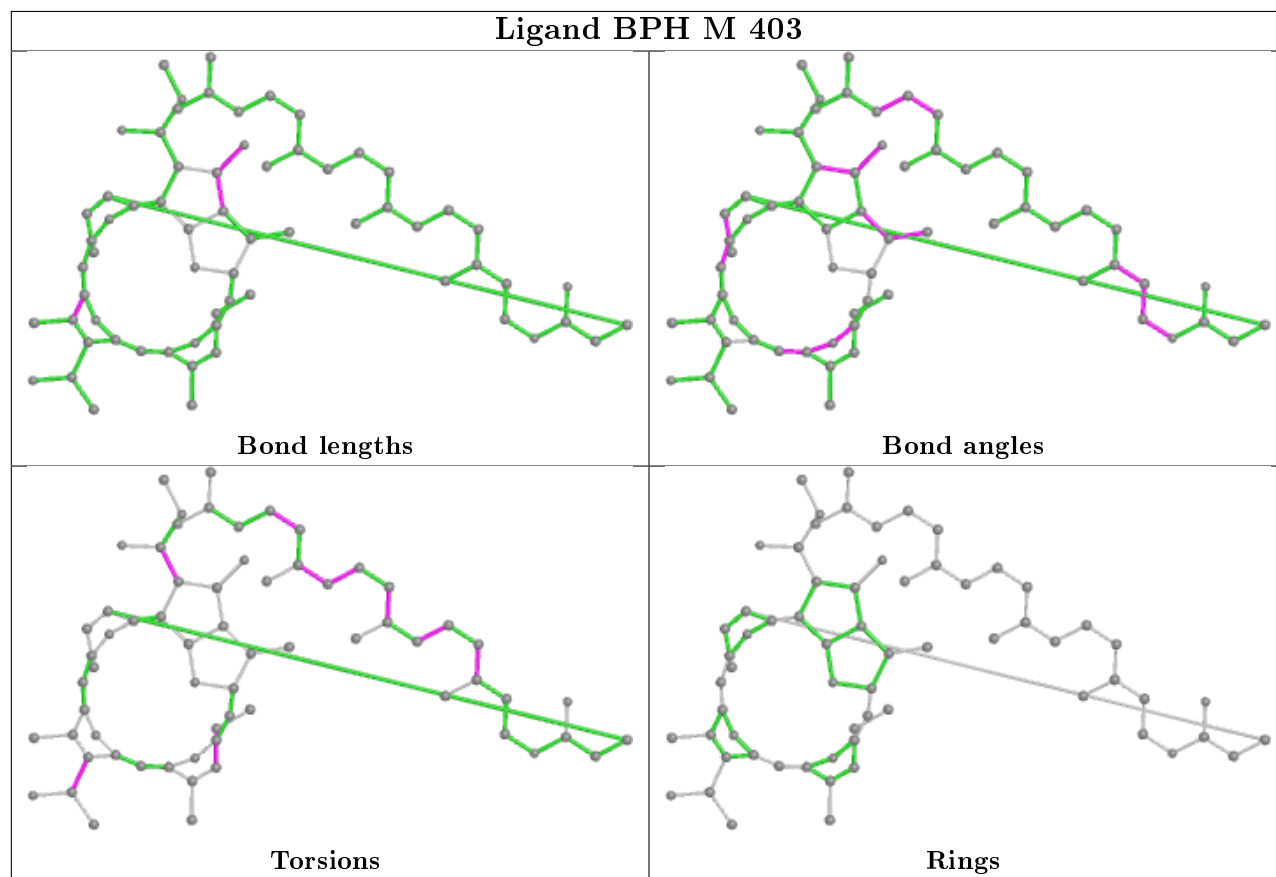
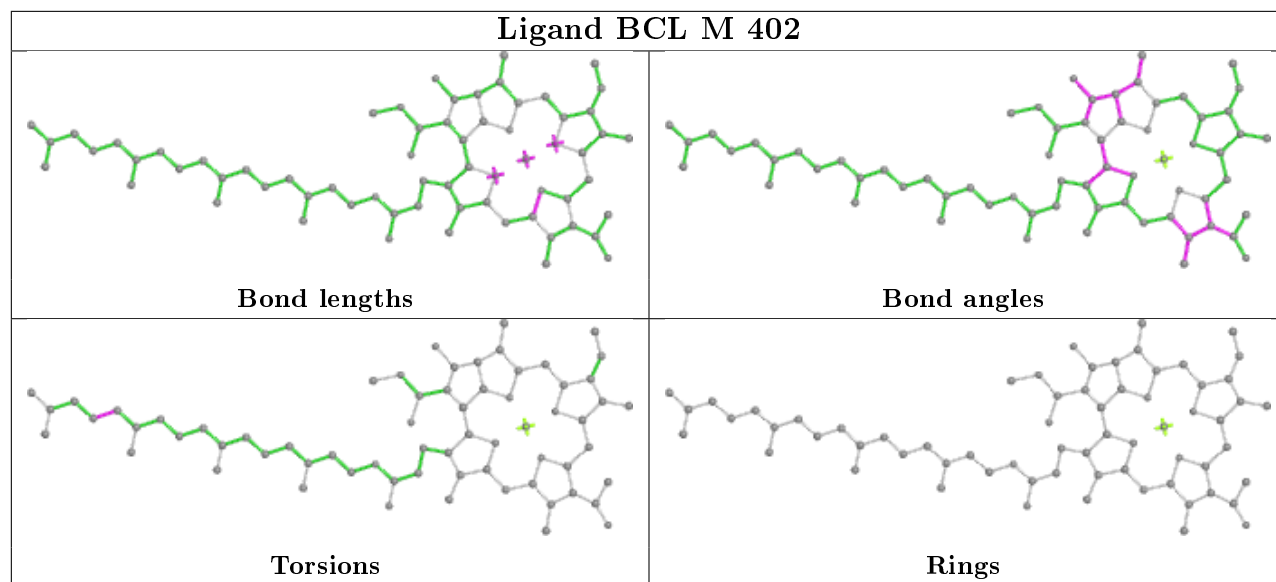
Mol	Chain	Res	Type	Atoms
4	M	408	LDA	C2-C3-C4-C5
4	M	407	LDA	C11-C10-C9-C8

There are no ring outliers.

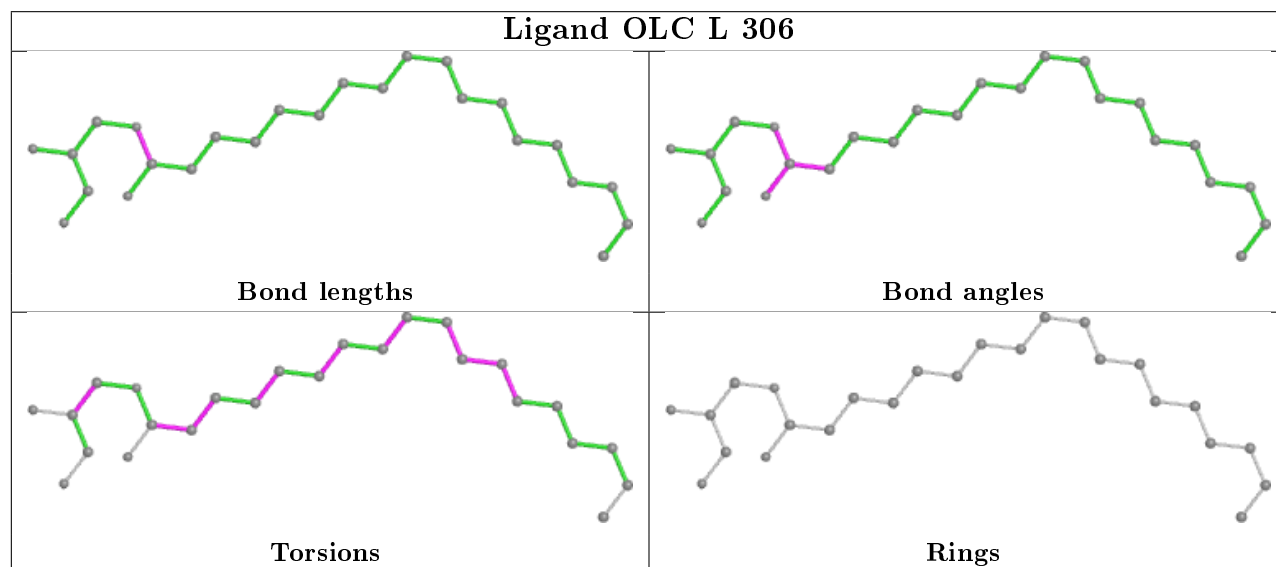
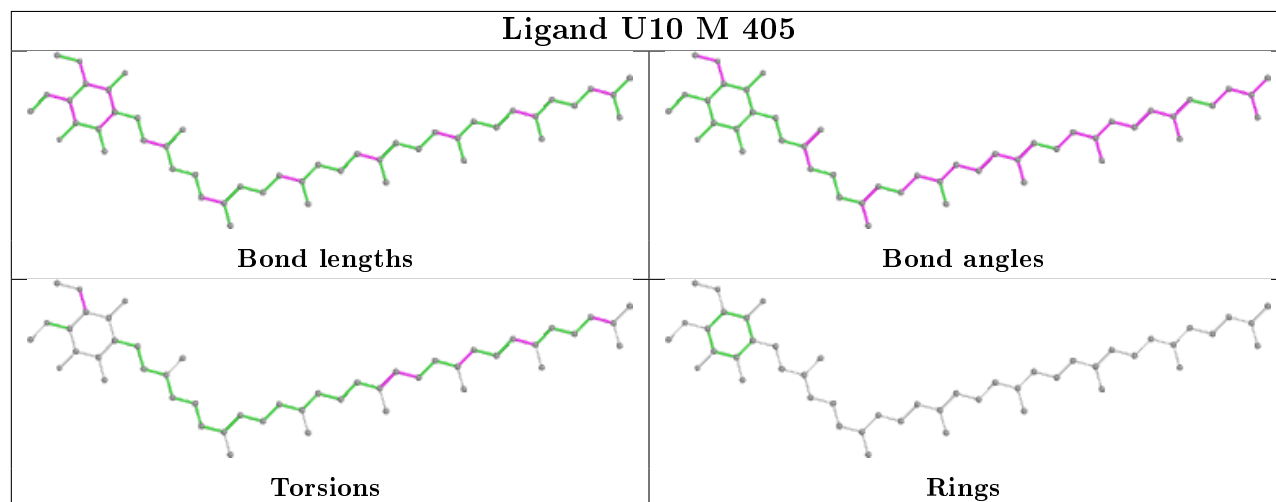
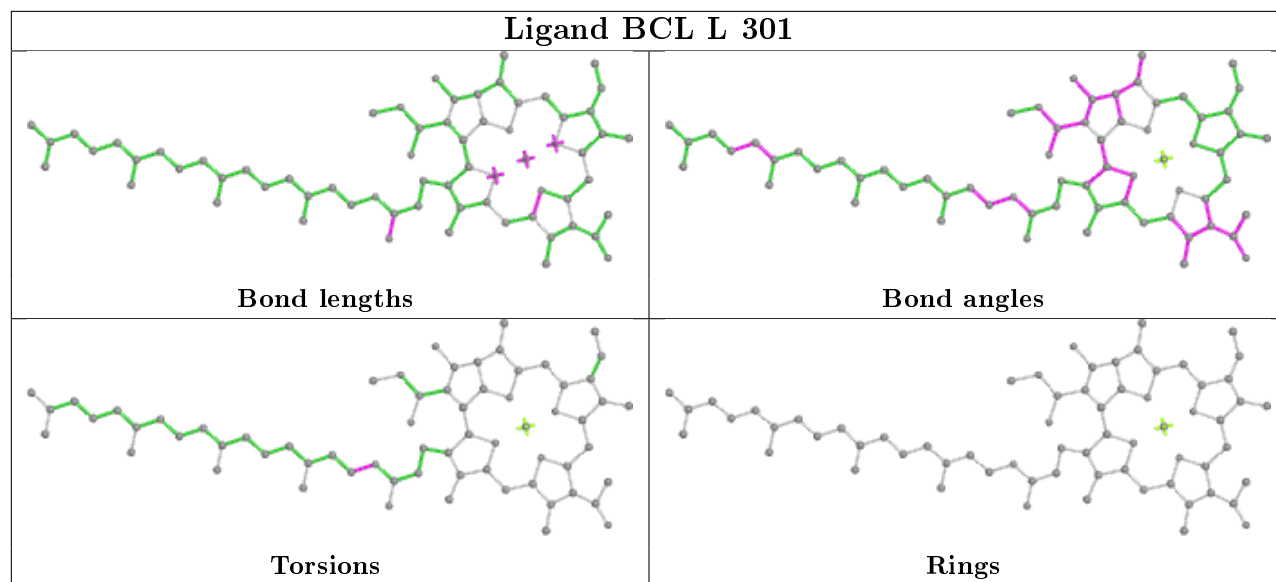
12 monomers are involved in 23 short contacts:

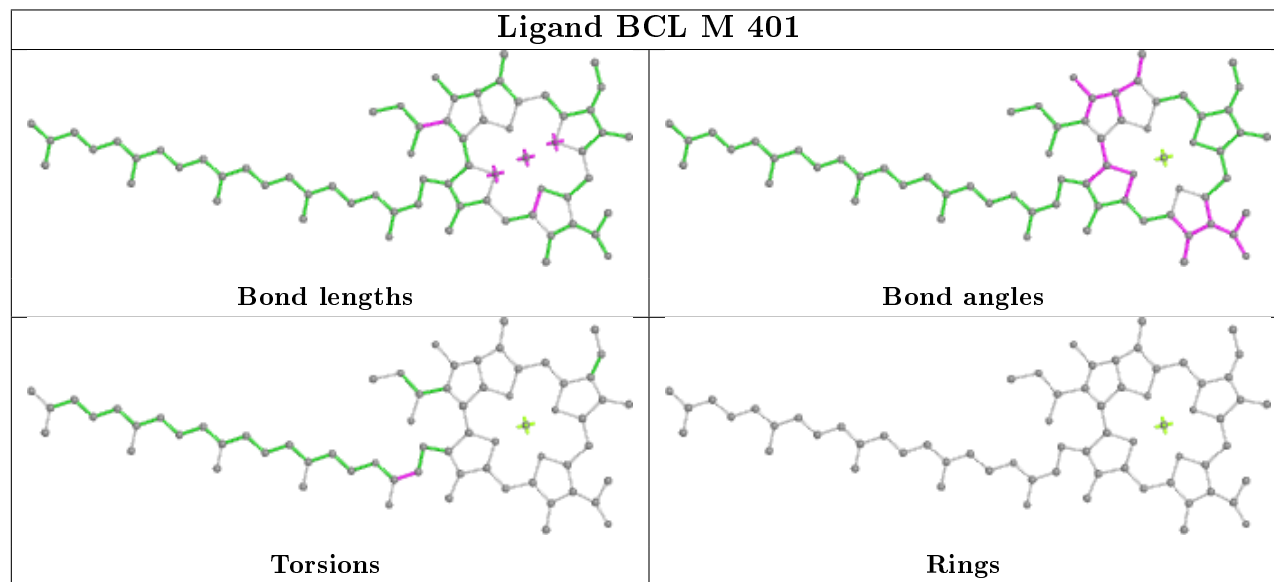
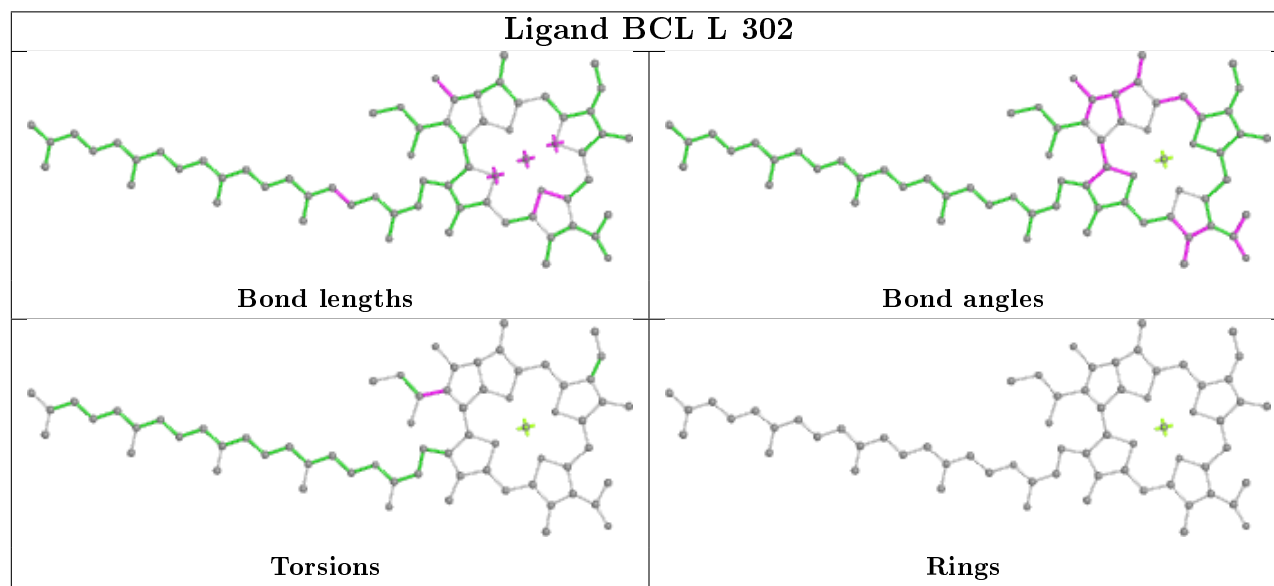
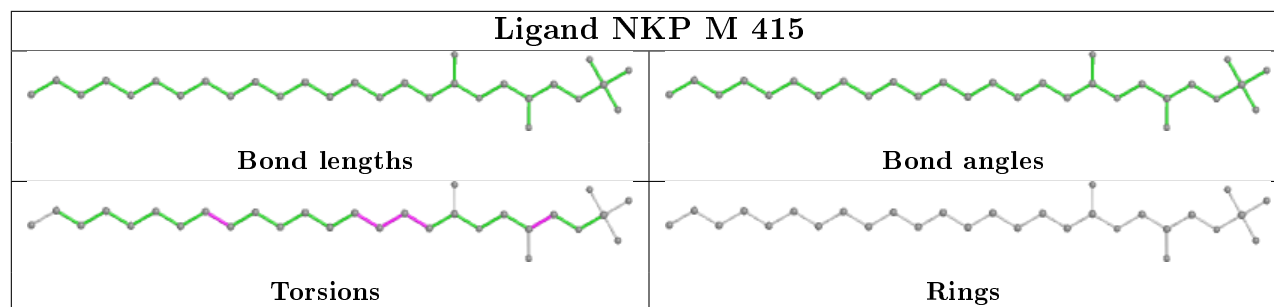
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	402	BCL	2	0
6	M	403	BPH	2	0
12	M	413	PO4	1	0
4	M	408	LDA	1	0
5	L	301	BCL	2	0
13	M	415	NKP	1	0
5	L	302	BCL	1	0
4	H	301	LDA	1	0
5	M	401	BCL	1	0
13	M	414	NKP	2	0
4	M	407	LDA	1	0
11	M	406	SPN	10	0

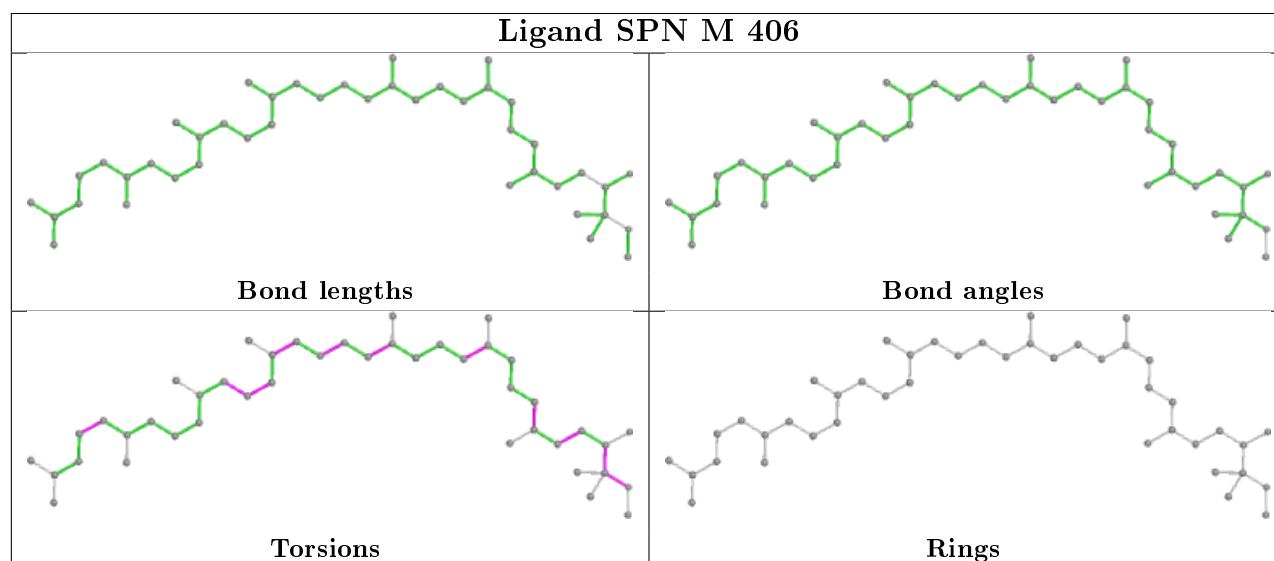
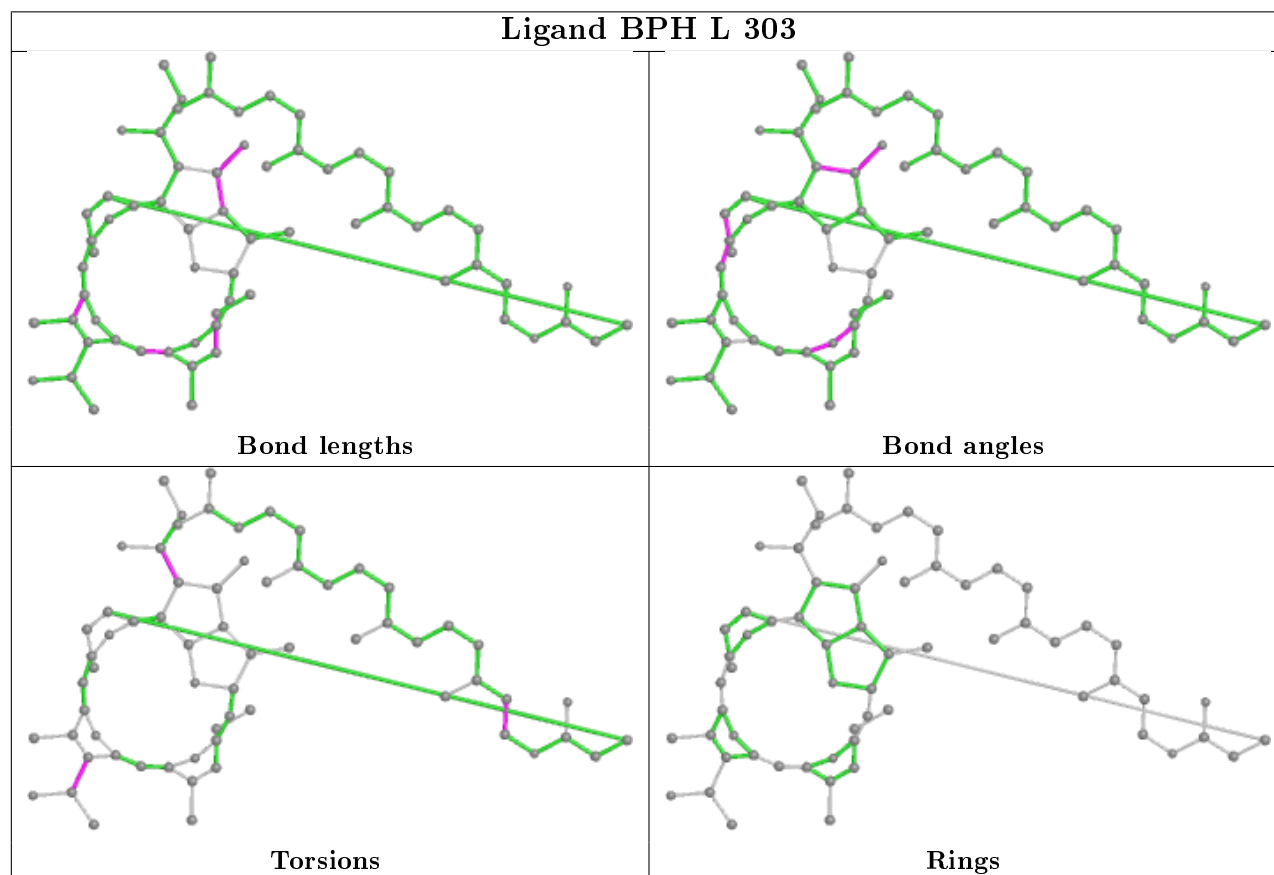
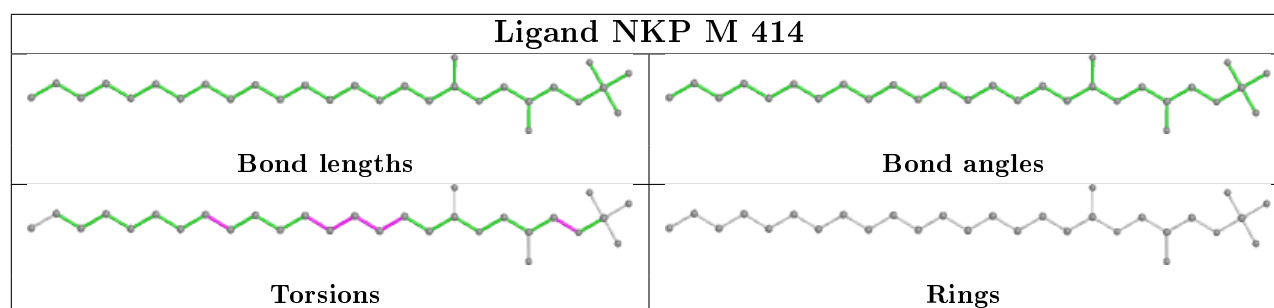
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	241/241 (100%)	-0.37	2 (0%) 86 88	26, 36, 49, 95	0
2	L	281/281 (100%)	-0.34	7 (2%) 57 62	23, 32, 45, 66	0
3	M	301/302 (99%)	-0.30	1 (0%) 94 94	23, 33, 55, 104	0
All	All	823/824 (99%)	-0.33	10 (1%) 79 82	23, 34, 51, 104	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	6.7
1	H	250	SER	5.3
1	H	249	LYS	5.0
2	L	59	TRP	4.2
2	L	266[A]	TRP	3.9
2	L	51	TRP	3.6
2	L	265[A]	TRP	3.2
2	L	276[A]	PRO	2.7
2	L	281[A]	GLY	2.1
2	L	277[A]	GLY	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 monosaccharides in this entry.

## 6.4 Ligands ⓘ

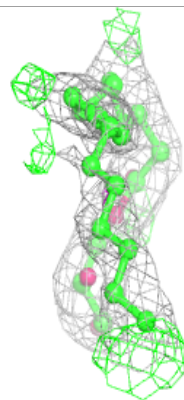
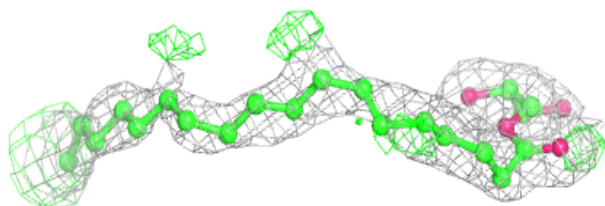
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	LDA	M	407	16/16	0.62	0.30	27,55,72,79	0
4	LDA	M	409	16/16	0.73	0.34	56,68,95,96	0
7	UNL	M	411	12/-	0.75	0.23	34,50,59,61	0
7	UNL	M	412	12/-	0.75	0.19	55,64,71,77	0
4	LDA	M	408	16/16	0.78	0.26	63,71,87,94	0
8	OLC	L	306	25/25	0.80	0.18	33,44,60,63	0
7	UNL	L	305	15/-	0.82	0.24	43,51,68,74	0
7	UNL	L	304	12/-	0.86	0.11	37,43,63,66	0
13	NKP	M	415	29/29	0.87	0.20	33,56,76,82	0
7	UNL	M	410	12/-	0.89	0.20	37,46,50,51	0
12	PO4	M	413	5/5	0.90	0.28	57,66,79,80	0
11	SPN	M	406	43/43	0.90	0.16	30,41,60,74	0
13	NKP	M	414	29/29	0.91	0.14	29,52,59,75	0
4	LDA	H	301	16/16	0.91	0.16	38,46,58,66	0
10	U10	M	405	48/63	0.92	0.17	21,30,55,60	0
6	BPH	M	403	65/65	0.94	0.12	22,30,81,93	0
5	BCL	M	401	66/66	0.94	0.11	21,29,41,56	0
5	BCL	L	301	66/66	0.95	0.10	24,30,59,67	0
5	BCL	L	302	66/66	0.95	0.11	21,29,34,38	0
6	BPH	L	303	65/65	0.96	0.14	20,26,34,36	0
5	BCL	M	402	66/66	0.97	0.12	20,27,38,49	0
9	FE	M	404	1/1	1.00	0.10	26,26,26,26	0

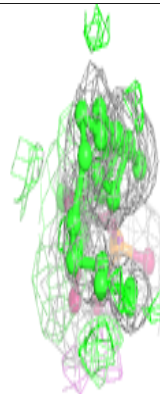
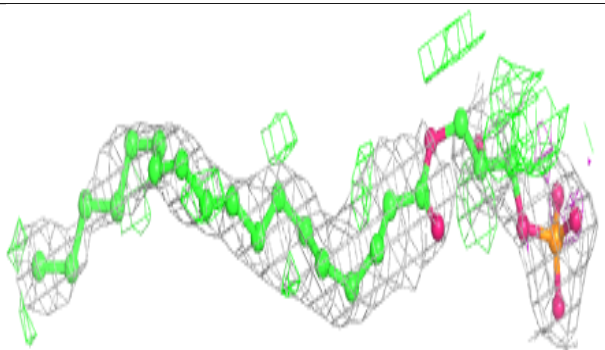
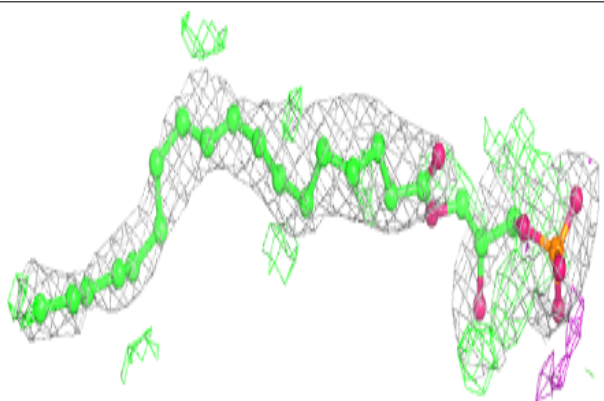
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OLC L 306:**

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

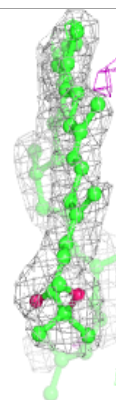
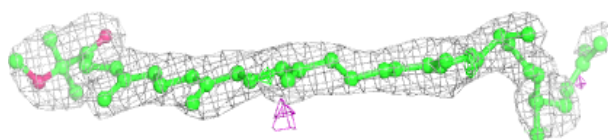
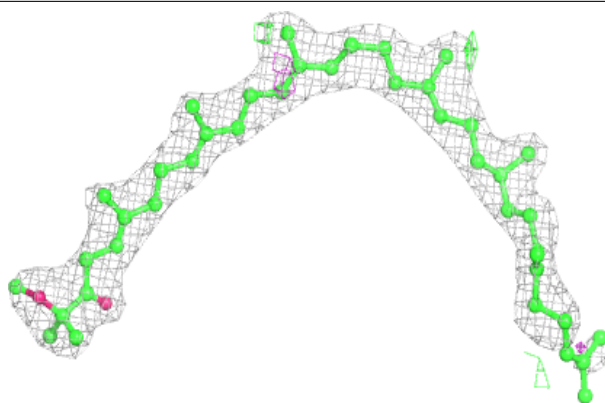
**Electron density around NKP M 415:**

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

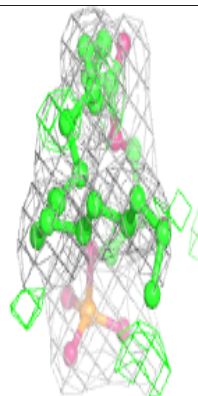
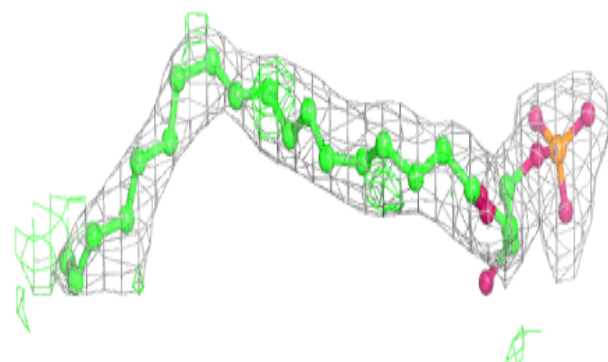
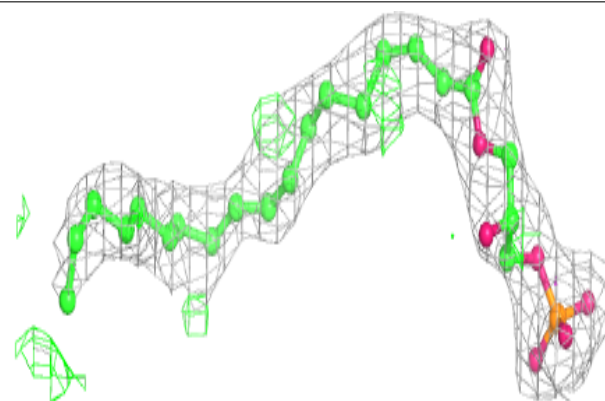


**Electron density around SPN M 406:**

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

**Electron density around NKP M 414:**

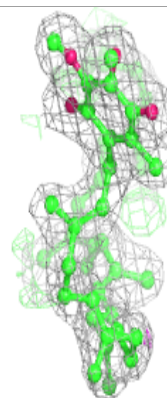
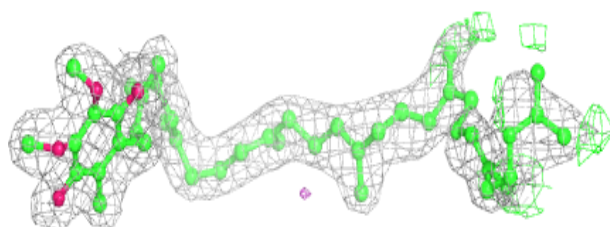
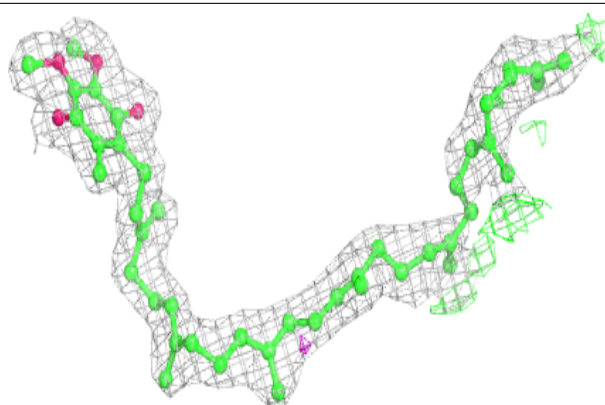
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



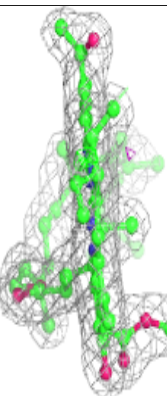
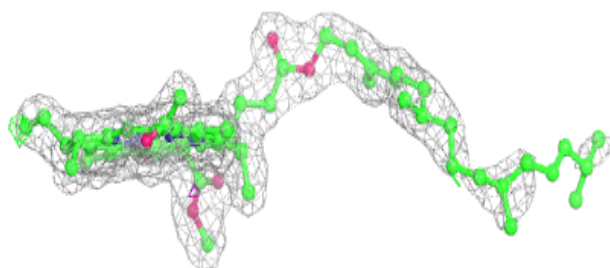
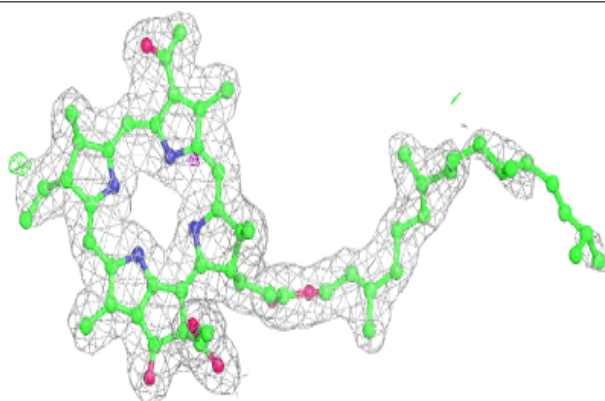


**Electron density around U10 M 405:**

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

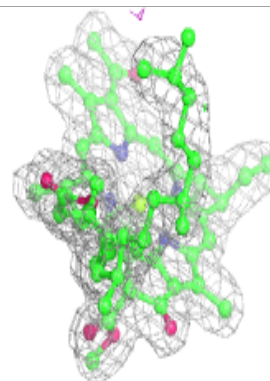
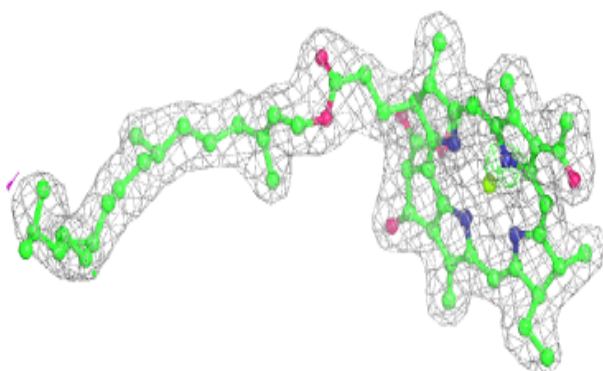
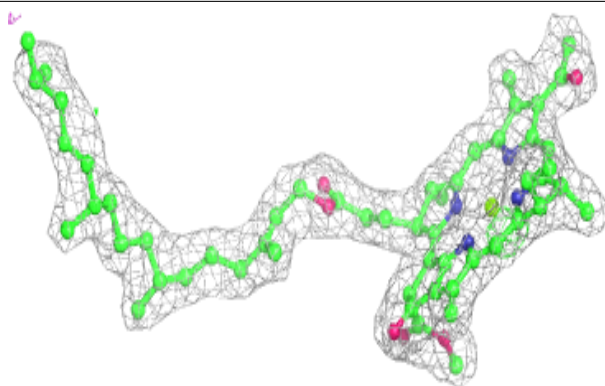
**Electron density around BPH M 403:**

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

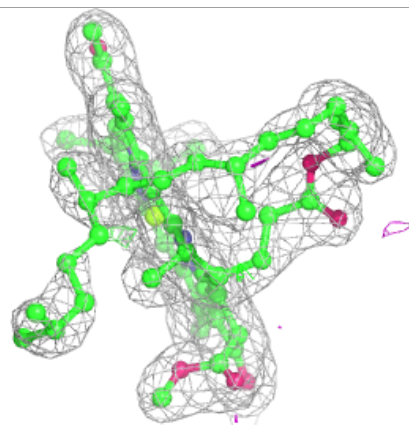
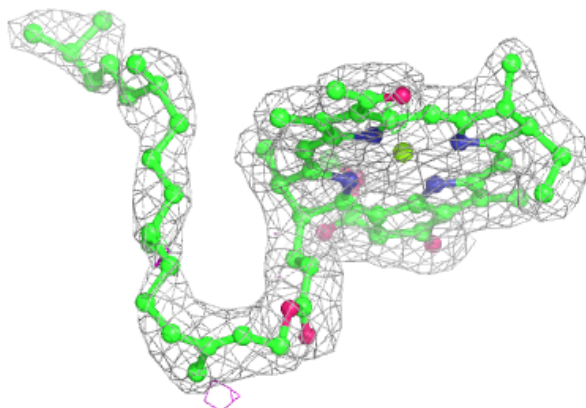
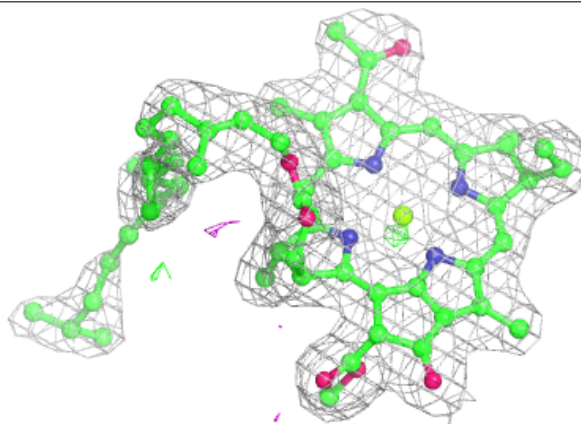


**Electron density around BCL M 401:**

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

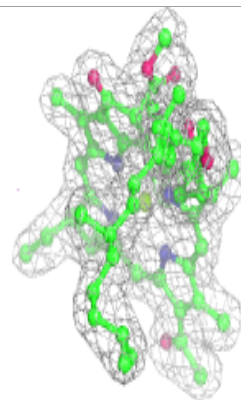
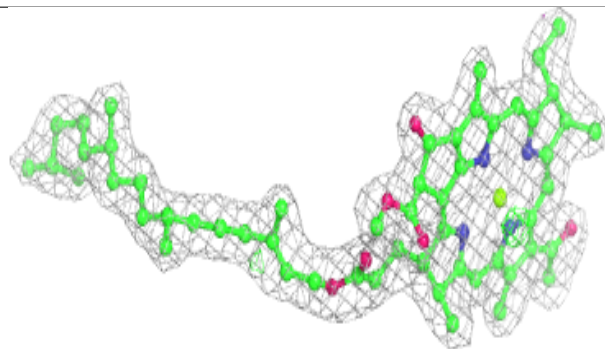
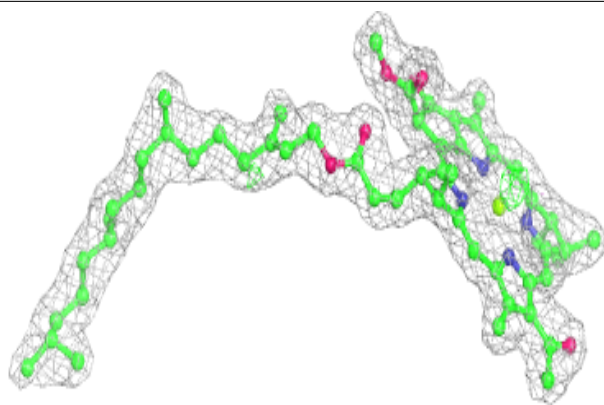
**Electron density around BCL L 301:**

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



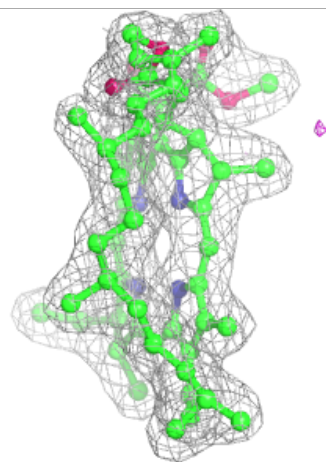
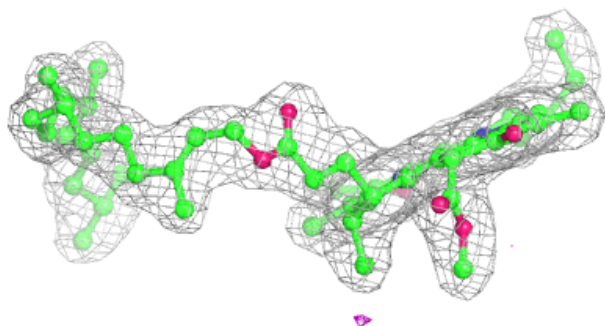
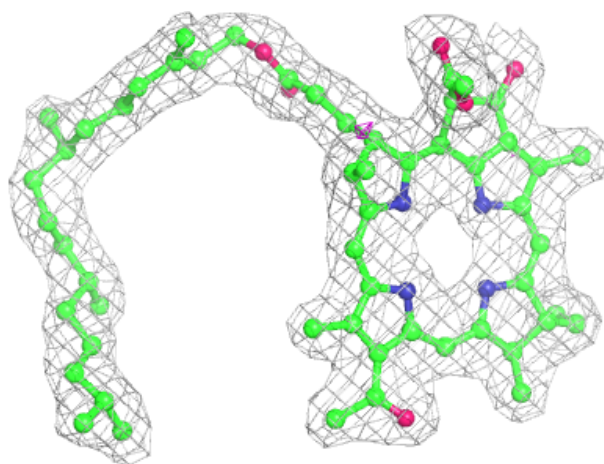
**Electron density around BCL L 302:**

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



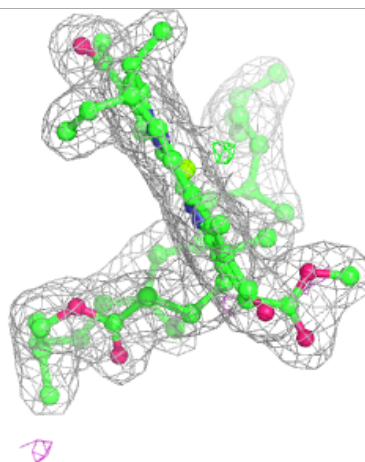
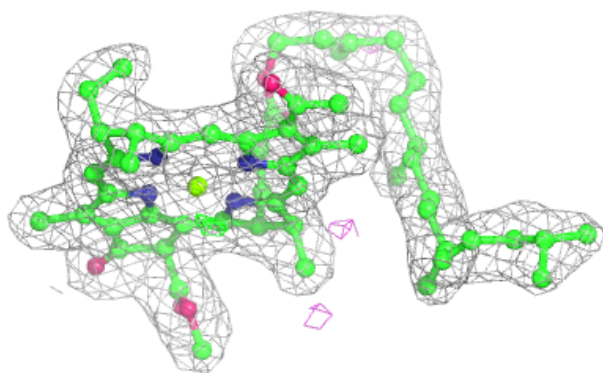
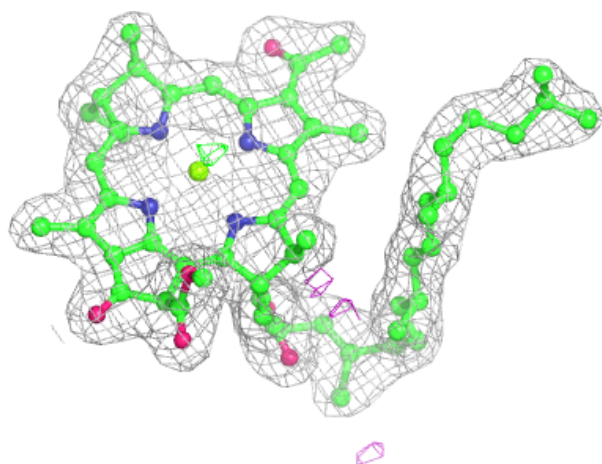
**Electron density around BPH L 303:**

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



**Electron density around BCL M 402:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.