Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2023 – 03:21 PM EDT

PDB ID	:	4H99
Title	:	Bacterial Photosynthetic Reaction Center from Rhodobacter sphaeroides with ILE M265 replaced with THR
Authors	:	Mattis, A.J.; Wraight, C.A.
Deposited on	:	2012-09-24
Resolution	:	2.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

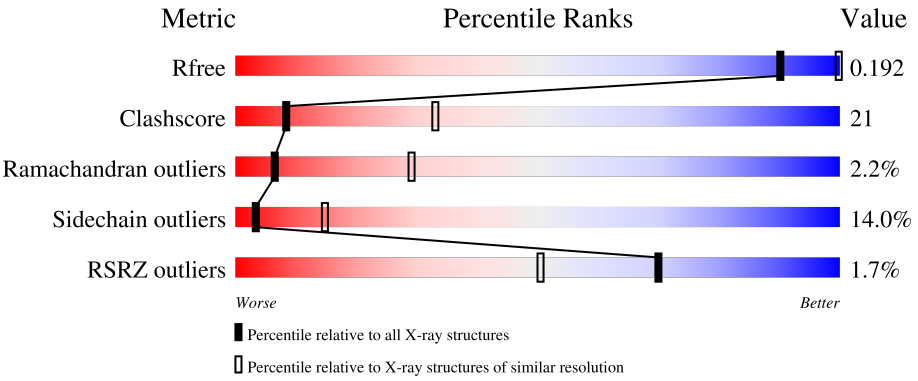
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	281	.% 60% 26% 11% ·
2	M	313	2% 52% 34% 8% · ·
3	H	260	2% 53% 28% 8% · 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BPH	L	303	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7005 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	0	0
			2230	1505	355	362	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	0	0
			2406	1604	394	398	10			

There are 12 discrepancies between the modelled and reference sequences:

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

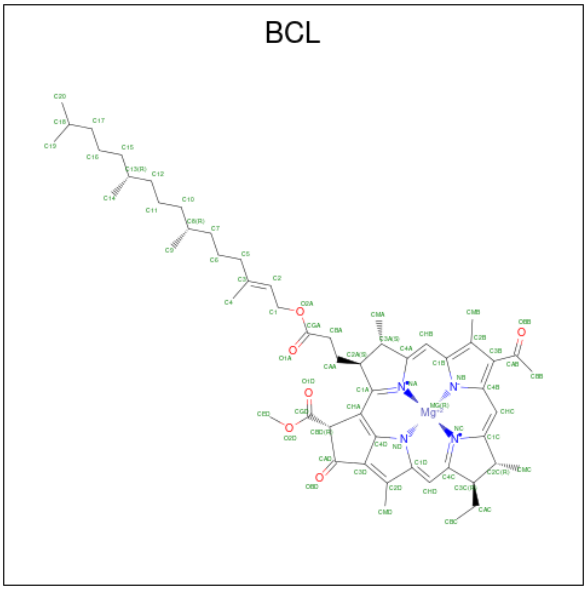
- Molecule 3 is a protein called Reaction center protein H chain.

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

There are 20 discrepancies between the modelled and reference sequences:

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

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



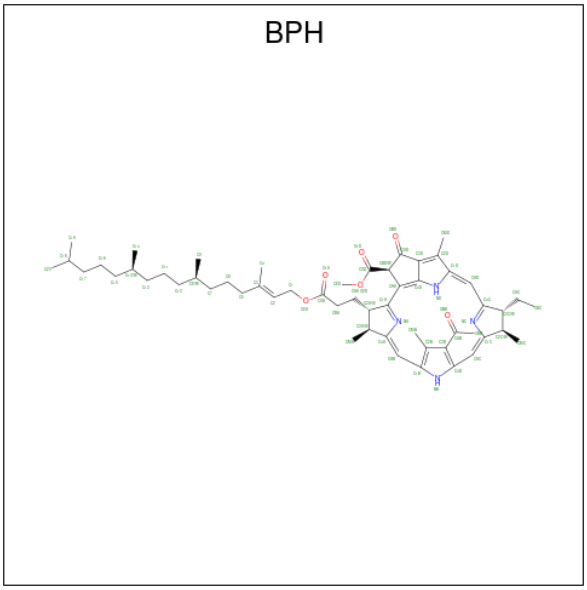
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

Continued on next page...

Continued from previous page...

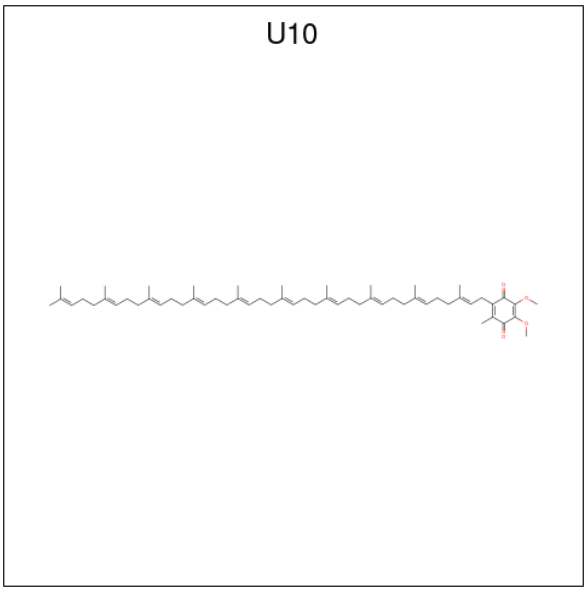
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	M	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			51	41	4	6		

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

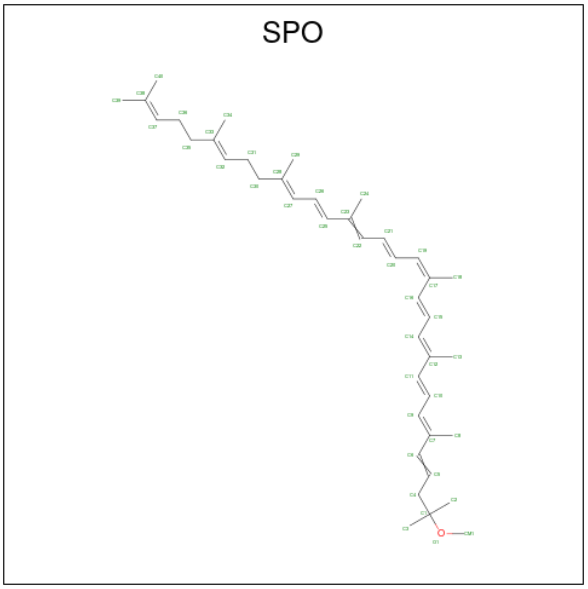


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C O 33 29 4	0	0
6	M	1	Total C O 48 44 4	0	0

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

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

- Molecule 8 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 9 is water.

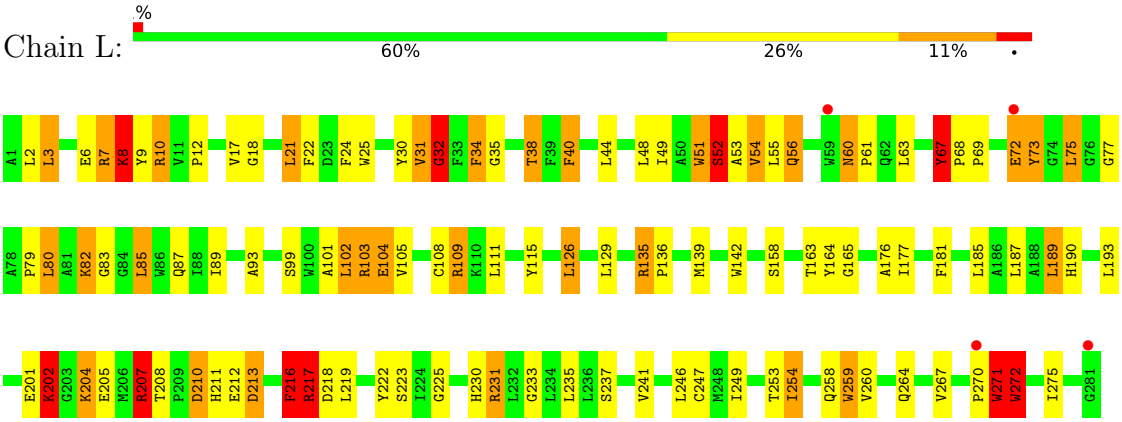
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	19	Total	O	0	0
			19	19		
9	M	18	Total	O	0	0
			18	18		
9	H	15	Total	O	0	0
			15	15		

3 Residue-property plots (i)

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

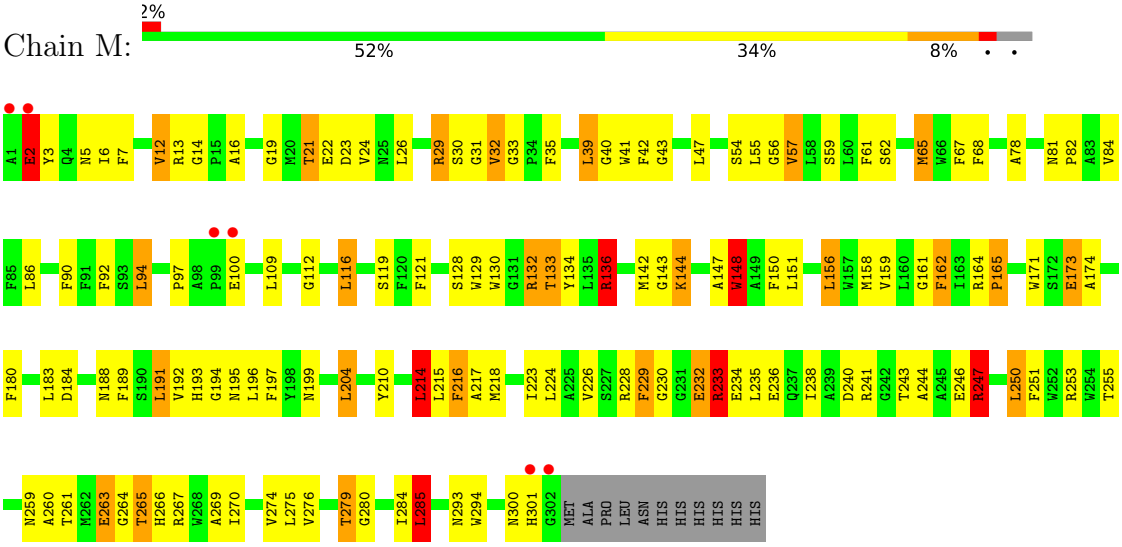
• Molecule 1: Reaction center protein L chain

Chain L:



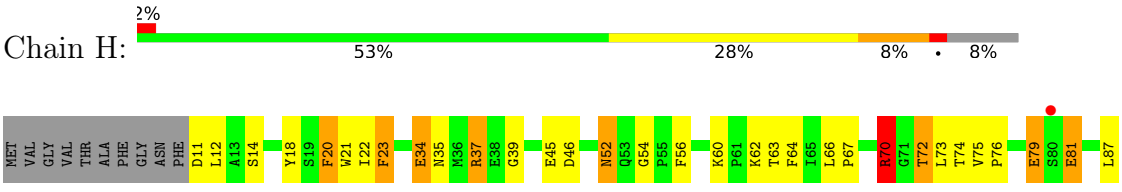
• Molecule 2: Reaction center protein M chain

Chain M:



• Molecule 3: Reaction center protein H chain

Chain H:




A88 R89 V92 S93 E94 G95 F96 P97 H98 G108 P111 A112 S113 R117 R118 D119 L120 P121 E122 L123 D124 G125 H128 N129 K130 M134 K135 F140 N147 P148 I149 G150 L151 P152 C156 E159 K163 D166 D170 I171 P172 E173 R177 F178 K184
D185 V196 S200 N201 R202 V205 N206 S210 D211 L212 F213 P217 T218 I219 K220 S221 E224 V225 T226 L227 L228 E229 E230 D231 K232 I233 G239 G240 L241 M242 P246 K247 R248 K249 S250 VAL VAL ALA ALA MET LEU ALA GLU TYR ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	138.87Å 138.87Å 185.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.77 – 2.97 19.77 – 2.97	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.77-2.97) 99.6 (19.77-2.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.5.0109, PHENIX	Depositor
R, R_{free}	0.174 , 0.194 0.184 , 0.192	Depositor DCC
R_{free} test set	2146 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	65.9	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7005	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, SPO, BPH, FE, 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	L	1.68	34/2318 (1.5%)	1.44	25/3172 (0.8%)
2	M	1.67	29/2498 (1.2%)	1.39	24/3410 (0.7%)
3	H	1.76	28/1877 (1.5%)	1.54	30/2553 (1.2%)
All	All	1.70	91/6693 (1.4%)	1.45	79/9135 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
3	H	0	2
All	All	0	3

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	94	GLU	CG-CD	11.30	1.69	1.51
1	L	72	GLU	CG-CD	10.89	1.68	1.51
1	L	82	LYS	CB-CG	10.31	1.80	1.52
1	L	67	TYR	CD2-CE2	10.06	1.54	1.39
3	H	94	GLU	CD-OE1	9.99	1.36	1.25
3	H	94	GLU	CB-CG	9.86	1.70	1.52
3	H	94	GLU	CD-OE2	8.86	1.35	1.25
3	H	173	GLU	CD-OE1	8.41	1.34	1.25
2	M	263	GLU	CD-OE1	8.39	1.34	1.25
1	L	82	LYS	CD-CE	8.26	1.71	1.51
1	L	67	TYR	CE2-CZ	8.12	1.49	1.38
1	L	67	TYR	CG-CD2	7.99	1.49	1.39
1	L	67	TYR	CE1-CZ	7.95	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	12	VAL	CB-CG2	-7.87	1.36	1.52
3	H	18	TYR	CD2-CE2	7.86	1.51	1.39
2	M	236	GLU	CG-CD	7.32	1.62	1.51
2	M	232	GLU	CD-OE1	7.17	1.33	1.25
3	H	184	LYS	CD-CE	7.01	1.68	1.51
3	H	20	PHE	CE1-CZ	6.99	1.50	1.37
3	H	200	SER	CB-OG	6.93	1.51	1.42
1	L	34	PHE	CD2-CE2	6.75	1.52	1.39
2	M	42	PHE	CE2-CZ	6.74	1.50	1.37
1	L	212	GLU	CD-OE1	6.71	1.33	1.25
2	M	100	GLU	CG-CD	6.69	1.61	1.51
3	H	18	TYR	CG-CD2	6.59	1.47	1.39
3	H	178	PHE	CE2-CZ	6.57	1.49	1.37
2	M	143	GLY	C-O	6.49	1.34	1.23
1	L	72	GLU	CB-CG	6.47	1.64	1.52
1	L	32	GLY	CA-C	6.45	1.62	1.51
3	H	45	GLU	CD-OE2	6.28	1.32	1.25
2	M	2	GLU	CD-OE2	6.27	1.32	1.25
3	H	56	PHE	CE1-CZ	6.26	1.49	1.37
3	H	18	TYR	CE1-CZ	6.26	1.46	1.38
3	H	219	ILE	CA-CB	-6.23	1.40	1.54
1	L	216	PHE	CE2-CZ	6.19	1.49	1.37
1	L	165	GLY	C-O	6.14	1.33	1.23
1	L	222	TYR	CE2-CZ	-6.12	1.30	1.38
3	H	163	LYS	CD-CE	6.12	1.66	1.51
3	H	224	GLU	CG-CD	6.08	1.61	1.51
2	M	217	ALA	CA-CB	-6.07	1.39	1.52
3	H	173	GLU	CD-OE2	5.98	1.32	1.25
2	M	68	PHE	CE1-CZ	5.96	1.48	1.37
2	M	57	VAL	CA-CB	5.94	1.67	1.54
3	H	72	THR	CB-CG2	5.94	1.72	1.52
1	L	67	TYR	CD1-CE1	5.93	1.48	1.39
1	L	164	TYR	C-O	5.92	1.34	1.23
1	L	82	LYS	CG-CD	5.91	1.72	1.52
2	M	7	PHE	CE2-CZ	5.90	1.48	1.37
2	M	162	PHE	CD2-CE2	5.90	1.51	1.39
3	H	18	TYR	CD1-CE1	5.88	1.48	1.39
3	H	135	LYS	CD-CE	5.84	1.65	1.51
3	H	23	PHE	CD2-CE2	5.83	1.50	1.39
3	H	118	ARG	CG-CD	5.79	1.66	1.51
1	L	82	LYS	CE-NZ	5.71	1.63	1.49
2	M	67	PHE	CE1-CZ	5.70	1.48	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	73	TYR	CB-CG	-5.68	1.43	1.51
3	H	96	PHE	CE1-CZ	5.67	1.48	1.37
2	M	41	TRP	CB-CG	-5.63	1.40	1.50
1	L	34	PHE	CE1-CZ	5.62	1.48	1.37
2	M	68	PHE	CG-CD2	5.61	1.47	1.38
2	M	236	GLU	CD-OE2	5.60	1.31	1.25
1	L	235	LEU	CG-CD2	5.59	1.72	1.51
1	L	259	TRP	CG-CD1	5.57	1.44	1.36
2	M	19	GLY	C-O	-5.53	1.14	1.23
3	H	46	ASP	CB-CG	5.45	1.63	1.51
3	H	18	TYR	CE2-CZ	5.43	1.45	1.38
3	H	213	PHE	CE1-CZ	5.40	1.47	1.37
1	L	3	LEU	C-O	5.40	1.33	1.23
1	L	67	TYR	CZ-OH	5.34	1.47	1.37
2	M	162	PHE	CD1-CE1	5.33	1.50	1.39
2	M	226	VAL	CB-CG2	-5.30	1.41	1.52
2	M	253	ARG	CZ-NH1	5.28	1.40	1.33
1	L	108	CYS	CB-SG	-5.27	1.73	1.81
2	M	61	PHE	CE2-CZ	5.23	1.47	1.37
1	L	34	PHE	CE2-CZ	5.22	1.47	1.37
2	M	233	ARG	CZ-NH1	5.20	1.39	1.33
3	H	135	LYS	CE-NZ	5.20	1.62	1.49
2	M	68	PHE	CD2-CE2	5.18	1.49	1.39
1	L	249	ILE	CA-CB	5.18	1.66	1.54
2	M	165	PRO	CA-C	5.17	1.63	1.52
2	M	68	PHE	CG-CD1	5.16	1.46	1.38
1	L	9	TYR	CE2-CZ	5.16	1.45	1.38
1	L	24	PHE	CE2-CZ	5.13	1.47	1.37
2	M	232	GLU	CD-OE2	5.12	1.31	1.25
2	M	148	TRP	CB-CG	5.12	1.59	1.50
1	L	231	ARG	CZ-NH1	5.12	1.39	1.33
1	L	104	GLU	CD-OE1	5.09	1.31	1.25
1	L	176	ALA	CA-CB	5.08	1.63	1.52
1	L	40	PHE	CG-CD2	5.05	1.46	1.38
1	L	258	GLN	C-O	5.02	1.32	1.23
2	M	92	PHE	CE1-CZ	5.02	1.46	1.37

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	231	ARG	NE-CZ-NH2	-13.09	113.76	120.30
1	L	231	ARG	NE-CZ-NH1	11.94	126.27	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	247	ARG	NE-CZ-NH1	11.91	126.26	120.30
1	L	217	ARG	NE-CZ-NH1	11.81	126.21	120.30
2	M	29	ARG	NE-CZ-NH2	-11.35	114.63	120.30
2	M	233	ARG	NE-CZ-NH1	-11.12	114.74	120.30
2	M	253	ARG	NE-CZ-NH2	-10.21	115.20	120.30
1	L	207	ARG	NE-CZ-NH1	9.95	125.28	120.30
1	L	103	ARG	NE-CZ-NH2	-9.64	115.48	120.30
3	H	170	ASP	CB-CG-OD1	9.34	126.71	118.30
1	L	103	ARG	NE-CZ-NH1	9.31	124.95	120.30
2	M	29	ARG	NE-CZ-NH1	9.15	124.88	120.30
3	H	37	ARG	NE-CZ-NH2	-9.04	115.78	120.30
3	H	70	ARG	NE-CZ-NH2	8.98	124.79	120.30
3	H	118	ARG	NE-CZ-NH1	8.75	124.67	120.30
2	M	132	ARG	NE-CZ-NH1	-8.62	115.99	120.30
3	H	119	ASP	CB-CG-OD1	8.46	125.92	118.30
3	H	117	ARG	NE-CZ-NH1	-8.44	116.08	120.30
3	H	248	ARG	NE-CZ-NH1	8.30	124.45	120.30
2	M	116	LEU	CA-CB-CG	7.90	133.48	115.30
1	L	207	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	L	210	ASP	CB-CG-OD1	7.71	125.24	118.30
3	H	37	ARG	NE-CZ-NH1	7.58	124.09	120.30
3	H	170	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	L	7	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	L	135	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	L	217	ARG	NE-CZ-NH2	-7.10	116.75	120.30
2	M	196	LEU	CB-CG-CD1	-7.03	99.06	111.00
3	H	89	ARG	NE-CZ-NH2	-7.02	116.79	120.30
3	H	118	ARG	NE-CZ-NH2	-6.99	116.80	120.30
2	M	21	THR	C-N-CA	-6.94	104.36	121.70
2	M	158	MET	CG-SD-CE	-6.93	89.11	100.20
1	L	75	LEU	CB-CG-CD1	6.88	122.70	111.00
2	M	267	ARG	NE-CZ-NH1	-6.84	116.88	120.30
3	H	117	ARG	NE-CZ-NH2	6.77	123.69	120.30
3	H	185	ASP	CB-CG-OD1	-6.70	112.27	118.30
3	H	89	ARG	NE-CZ-NH1	6.69	123.65	120.30
2	M	204	LEU	CB-CG-CD1	6.54	122.12	111.00
1	L	126	LEU	CB-CG-CD1	6.41	121.89	111.00
1	L	204	LYS	CD-CE-NZ	-6.34	97.12	111.70
3	H	67	PRO	C-N-CA	-6.33	105.88	121.70
3	H	221	SER	CB-CA-C	-6.32	98.09	110.10
1	L	235	LEU	CB-CG-CD2	6.22	121.58	111.00
3	H	46	ASP	CB-CG-OD1	6.19	123.87	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	177	ARG	NE-CZ-NH1	6.07	123.34	120.30
3	H	120	LEU	CA-CB-CG	6.03	129.17	115.30
2	M	136	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	L	213	ASP	CB-CG-OD1	5.93	123.64	118.30
1	L	31	VAL	C-N-CA	-5.92	109.86	122.30
2	M	23	ASP	CB-CG-OD1	5.89	123.60	118.30
1	L	82	LYS	CD-CE-NZ	5.79	125.00	111.70
1	L	108	CYS	CA-CB-SG	-5.78	103.60	114.00
3	H	37	ARG	CG-CD-NE	-5.73	99.77	111.80
1	L	109	ARG	CA-CB-CG	-5.68	100.91	113.40
2	M	285	LEU	CB-CG-CD2	-5.63	101.44	111.00
2	M	191	LEU	CB-CG-CD1	5.62	120.56	111.00
2	M	214	LEU	CB-CG-CD1	-5.58	101.51	111.00
3	H	81	GLU	C-N-CA	-5.58	107.75	121.70
1	L	139	MET	CG-SD-CE	5.51	109.02	100.20
1	L	67	TYR	CB-CG-CD1	-5.50	117.70	121.00
3	H	212	LEU	CB-CG-CD2	-5.48	101.68	111.00
3	H	185	ASP	CB-CG-OD2	5.43	123.19	118.30
3	H	211	ASP	CB-CG-OD2	-5.41	113.43	118.30
2	M	94	LEU	CB-CG-CD2	-5.40	101.83	111.00
2	M	142	MET	CA-CB-CG	-5.38	104.16	113.30
2	M	132	ARG	NE-CZ-NH2	5.37	122.99	120.30
2	M	31	GLY	N-CA-C	-5.36	99.70	113.10
3	H	173	GLU	OE1-CD-OE2	5.35	129.72	123.30
1	L	165	GLY	N-CA-C	-5.34	99.74	113.10
3	H	70	ARG	NH1-CZ-NH2	-5.34	113.53	119.40
3	H	227	LEU	CB-CG-CD2	-5.32	101.95	111.00
1	L	7	ARG	NE-CZ-NH2	-5.31	117.64	120.30
3	H	248	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	M	156	LEU	CA-CB-CG	5.15	127.14	115.30
3	H	18	TYR	CB-CA-C	5.14	120.69	110.40
2	M	228	ARG	NE-CZ-NH2	-5.12	117.74	120.30
3	H	117	ARG	CG-CD-NE	5.10	122.52	111.80
2	M	214	LEU	CB-CG-CD2	5.09	119.65	111.00
1	L	189	LEU	CB-CG-CD2	5.04	119.57	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	119	ASP	Peptide
3	H	79	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	L	32	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2230	0	2178	100	0
2	M	2406	0	2313	107	0
3	H	1829	0	1836	68	0
4	L	132	0	148	9	0
4	M	116	0	115	20	0
5	L	65	0	76	14	0
5	M	51	0	43	9	0
6	L	33	0	39	10	0
6	M	48	0	63	1	0
7	M	1	0	0	0	0
8	M	42	0	60	13	0
9	H	15	0	0	5	0
9	L	19	0	0	3	0
9	M	18	0	0	0	0
All	All	7005	0	6871	289	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 21.

All (289) 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:L:82:LYS:CG	1:L:82:LYS:CB	1.80	1.54
4:M:403:BCL:HHC	4:M:403:BCL:HBB3	1.27	1.14
6:L:304:U10:C8	6:L:304:U10:H1M1	1.79	1.12
1:L:38:THR:HG22	1:L:99:SER:HB2	1.20	1.11
1:L:7:ARG:HH11	3:H:98:HIS:CD2	1.69	1.10
6:L:304:U10:H1M1	6:L:304:U10:H8	1.10	1.10
1:L:38:THR:HG22	1:L:99:SER:CB	1.84	1.07
3:H:117:ARG:HG2	3:H:117:ARG:HH11	1.18	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:119:SER:HB2	8:M:406:SPO:C34	1.89	1.02
2:M:119:SER:HB2	8:M:406:SPO:H342	1.44	0.98
2:M:119:SER:CB	8:M:406:SPO:H342	1.93	0.97
5:L:303:BPH:HBB3	5:L:303:BPH:HHC	1.43	0.97
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.47	0.96
1:L:241:VAL:HG21	5:L:303:BPH:HAC2	1.47	0.95
1:L:32:GLY:HA3	9:L:416:HOH:O	1.64	0.95
1:L:49:ILE:HG13	1:L:89:ILE:HD13	1.47	0.95
2:M:197:PHE:CZ	4:M:403:BCL:HBB2	2.01	0.94
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.46	0.94
6:L:304:U10:H8	6:L:304:U10:C1M	1.99	0.92
2:M:32:VAL:HG13	2:M:33:GLY:O	1.69	0.92
4:M:403:BCL:HHC	4:M:403:BCL:CBB	2.00	0.92
3:H:129:ASN:ND2	3:H:224:GLU:HG2	1.86	0.89
2:M:197:PHE:HZ	4:M:403:BCL:CBB	1.84	0.89
2:M:240:ASP:O	3:H:117:ARG:NH1	2.04	0.89
1:L:201:GLU:O	1:L:202:LYS:CB	2.21	0.88
1:L:193:LEU:HD23	6:L:304:U10:H4M3	1.56	0.87
1:L:201:GLU:O	1:L:202:LYS:HB3	1.78	0.84
1:L:7:ARG:HH11	3:H:98:HIS:HD2	1.26	0.83
2:M:22:GLU:H	2:M:24:VAL:HG23	1.45	0.81
2:M:164:ARG:HH12	2:M:173:GLU:HG3	1.47	0.80
3:H:118:ARG:HG2	3:H:118:ARG:HH11	1.46	0.80
1:L:7:ARG:NH1	3:H:98:HIS:CD2	2.50	0.80
1:L:272:TRP:HA	1:L:275:ILE:HD12	1.64	0.79
2:M:59:SER:HB2	2:M:128:SER:OG	1.83	0.79
3:H:117:ARG:HG2	3:H:117:ARG:NH1	1.97	0.79
2:M:197:PHE:CZ	4:M:403:BCL:CBB	2.63	0.77
3:H:247:LYS:HB2	3:H:247:LYS:NZ	1.99	0.77
2:M:81:ASN:OD1	2:M:82:PRO:HD2	1.86	0.75
3:H:117:ARG:HH11	3:H:117:ARG:CG	1.92	0.75
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.69	0.74
2:M:119:SER:CB	8:M:406:SPO:C34	2.58	0.74
2:M:21:THR:CG2	2:M:26:LEU:HD11	2.15	0.74
2:M:189:PHE:O	2:M:193:HIS:HD2	1.71	0.74
2:M:65:MET:HB3	2:M:121:PHE:CD2	2.23	0.73
1:L:34:PHE:O	1:L:38:THR:HG23	1.87	0.73
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.70	0.73
5:L:303:BPH:HBB2	2:M:210:TYR:HB3	1.71	0.73
3:H:149:ILE:HD13	3:H:166:ASP:HA	1.71	0.73
2:M:197:PHE:CE1	4:M:403:BCL:HBB2	2.23	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:120:LEU:HB3	3:H:121:PRO:CD	2.20	0.72
1:L:7:ARG:NH1	3:H:98:HIS:HD2	1.86	0.71
3:H:70:ARG:O	3:H:118:ARG:NH2	2.23	0.71
4:L:302:BCL:CBB	4:L:302:BCL:HMB1	2.20	0.71
1:L:49:ILE:HG13	1:L:89:ILE:CD1	2.20	0.71
4:L:302:BCL:C19	5:L:303:BPH:H102	2.20	0.71
2:M:16:ALA:HB1	2:M:32:VAL:HG21	1.71	0.71
3:H:129:ASN:HD21	3:H:224:GLU:HG2	1.54	0.71
4:M:401:BCL:HHC	4:M:401:BCL:CBB	2.20	0.71
1:L:69:PRO:CG	1:L:142:TRP:HB2	2.19	0.70
3:H:62:LYS:HE3	3:H:64:PHE:CZ	2.27	0.69
3:H:170:ASP:OD2	3:H:177:ARG:NH1	2.20	0.69
2:M:184:ASP:O	2:M:188:ASN:HB2	1.93	0.68
3:H:152:PRO:HD2	3:H:202:ARG:HA	1.75	0.68
2:M:133:THR:HG22	2:M:147:ALA:HB2	1.75	0.67
2:M:238:ILE:HD13	2:M:263:GLU:HB2	1.76	0.67
2:M:275:LEU:O	2:M:279:THR:HB	1.94	0.66
4:L:302:BCL:HMB1	4:L:302:BCL:HBB2	1.78	0.66
1:L:190:HIS:HD1	6:L:304:U10:H4M1	1.61	0.65
2:M:164:ARG:NH1	2:M:173:GLU:HG3	2.10	0.65
3:H:241:LEU:O	3:H:248:ARG:NH2	2.30	0.65
1:L:38:THR:CG2	1:L:99:SER:CB	2.70	0.65
1:L:34:PHE:HB2	9:L:416:HOH:O	1.96	0.64
2:M:165:PRO:CG	2:M:174:ALA:HB2	2.26	0.64
5:M:404:BPH:HBC3	5:M:404:BPH:CHD	2.27	0.64
5:M:404:BPH:HBC3	5:M:404:BPH:HHD	1.79	0.64
1:L:187:LEU:HD13	2:M:216:PHE:CG	2.33	0.64
3:H:148:PRO:HA	3:H:151:LEU:HD22	1.80	0.64
2:M:133:THR:HG21	2:M:147:ALA:HA	1.80	0.63
4:L:302:BCL:H193	5:L:303:BPH:H102	1.80	0.63
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.80	0.63
5:L:303:BPH:HHC	5:L:303:BPH:CBB	2.21	0.62
5:M:404:BPH:HHD	5:M:404:BPH:CBC	2.30	0.62
4:M:401:BCL:HHC	4:M:401:BCL:HBB2	1.83	0.61
3:H:62:LYS:O	3:H:74:THR:HA	2.01	0.61
2:M:193:HIS:O	2:M:293:ASN:HA	2.01	0.61
3:H:70:ARG:NH2	3:H:121:PRO:O	2.34	0.60
1:L:271:TRP:H	1:L:271:TRP:HD1	1.49	0.60
2:M:119:SER:HB3	8:M:406:SPO:H342	1.80	0.60
1:L:38:THR:HG22	1:L:99:SER:HB3	1.79	0.60
2:M:133:THR:CG2	2:M:147:ALA:HB2	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.25	0.58
6:L:304:U10:C3M	6:L:304:U10:H4M2	2.33	0.58
1:L:181:PHE:CD2	5:M:404:BPH:HBB1	2.39	0.58
2:M:165:PRO:HG2	2:M:174:ALA:HB2	1.86	0.58
3:H:120:LEU:HB3	3:H:121:PRO:HD3	1.85	0.58
1:L:49:ILE:CG1	1:L:89:ILE:CD1	2.82	0.57
2:M:194:GLY:O	2:M:195:ASN:HB3	2.04	0.57
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.05	0.57
2:M:136:ARG:NE	2:M:136:ARG:HA	2.19	0.57
6:L:304:U10:H4M2	6:L:304:U10:H3M3	1.85	0.57
3:H:130:LYS:HE3	3:H:170:ASP:OD2	2.04	0.57
2:M:234:GLU:O	2:M:238:ILE:HG13	2.04	0.57
2:M:284:ILE:CD1	4:M:403:BCL:HED3	2.34	0.57
3:H:96:PHE:HB3	3:H:97:PRO:CD	2.34	0.57
2:M:130:TRP:O	2:M:133:THR:HB	2.05	0.56
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.88	0.56
3:H:247:LYS:HB2	3:H:247:LYS:HZ3	1.70	0.56
2:M:159:VAL:HG13	2:M:285:LEU:HD23	1.86	0.56
1:L:272:TRP:CA	1:L:275:ILE:HD12	2.33	0.56
2:M:243:THR:HG23	2:M:247:ARG:HD3	1.88	0.56
1:L:30:TYR:O	1:L:103:ARG:NH1	2.36	0.56
2:M:260:ALA:CB	2:M:265:THR:HG22	2.35	0.56
4:M:401:BCL:HMB1	4:M:401:BCL:OBB	2.06	0.56
5:L:303:BPH:HBC3	5:L:303:BPH:HHD	1.86	0.55
4:M:401:BCL:HBB3	4:M:403:BCL:H41	1.88	0.55
3:H:96:PHE:HB3	3:H:97:PRO:HD2	1.89	0.55
1:L:101:ALA:O	1:L:104:GLU:N	2.40	0.54
1:L:10:ARG:HG2	1:L:25:TRP:CH2	2.43	0.54
2:M:62:SER:HA	2:M:65:MET:HB2	1.89	0.54
1:L:231:ARG:HD2	2:M:6:ILE:O	2.08	0.54
2:M:133:THR:CG2	2:M:147:ALA:HA	2.38	0.54
2:M:214:LEU:HD22	2:M:218:MET:SD	2.48	0.54
1:L:202:LYS:O	1:L:202:LYS:HG3	2.01	0.53
2:M:243:THR:O	2:M:247:ARG:HG2	2.08	0.53
3:H:108:GLY:O	3:H:113:SER:HA	2.08	0.53
3:H:178:PHE:HZ	3:H:230:GLU:HG2	1.74	0.53
1:L:85:LEU:O	1:L:89:ILE:HG13	2.08	0.53
2:M:13:ARG:O	3:H:140:PHE:HA	2.08	0.53
1:L:103:ARG:NH2	2:M:255:THR:O	2.35	0.53
2:M:112:GLY:O	2:M:116:LEU:HD22	2.08	0.53
1:L:223:SER:HA	6:L:304:U10:O2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:304:U10:C8	6:L:304:U10:C1M	2.68	0.53
3:H:63:THR:HA	3:H:73:LEU:O	2.09	0.53
1:L:38:THR:CG2	1:L:99:SER:HB3	2.37	0.53
5:L:303:BPH:HBB3	5:L:303:BPH:CHC	2.29	0.53
2:M:189:PHE:O	2:M:193:HIS:CD2	2.59	0.53
2:M:2:GLU:HG3	2:M:3:TYR:N	2.24	0.52
1:L:54:VAL:O	1:L:56:GLN:N	2.42	0.52
4:L:301:BCL:CBB	4:L:301:BCL:HMB1	2.39	0.52
4:L:302:BCL:HHC	4:L:302:BCL:OBB	2.09	0.52
2:M:134:TYR:CE1	2:M:144:LYS:HD3	2.45	0.52
1:L:230:HIS:CD2	2:M:223:ILE:HG13	2.45	0.52
5:M:404:BPH:CHD	5:M:404:BPH:CBC	2.87	0.52
1:L:51:TRP:O	1:L:53:ALA:N	2.43	0.52
2:M:232:GLU:OE2	3:H:177:ARG:NH2	2.41	0.51
2:M:270:ILE:O	2:M:274:VAL:HB	2.10	0.51
5:L:303:BPH:CBB	2:M:210:TYR:HB3	2.40	0.51
2:M:13:ARG:HG2	2:M:14:GLY:N	2.23	0.51
3:H:117:ARG:O	3:H:228:LEU:HB2	2.10	0.51
2:M:162:PHE:HB2	8:M:406:SPO:C29	2.40	0.51
1:L:181:PHE:HB3	5:M:404:BPH:HBB2	1.92	0.51
1:L:187:LEU:HD13	2:M:216:PHE:CD2	2.45	0.51
3:H:75:VAL:HA	3:H:76:PRO:C	2.30	0.51
1:L:77:GLY:HA2	1:L:87:GLN:OE1	2.10	0.51
3:H:34:GLU:OE2	3:H:37:ARG:NH1	2.40	0.51
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.92	0.51
1:L:105:VAL:O	1:L:109:ARG:HG3	2.11	0.50
4:M:401:BCL:CBB	8:M:406:SPO:H243	2.41	0.50
2:M:269:ALA:O	2:M:270:ILE:C	2.50	0.50
2:M:234:GLU:OE2	2:M:266:HIS:CE1	2.65	0.50
1:L:272:TRP:HA	1:L:275:ILE:CD1	2.38	0.50
4:M:403:BCL:HAA2	4:M:403:BCL:HBD	1.94	0.50
1:L:181:PHE:HB3	5:M:404:BPH:CBB	2.42	0.50
2:M:165:PRO:HG3	2:M:174:ALA:HB2	1.93	0.49
2:M:180:PHE:O	2:M:183:LEU:HB2	2.12	0.49
2:M:284:ILE:HD11	4:M:403:BCL:HED3	1.92	0.49
1:L:32:GLY:CA	1:L:35:GLY:H	2.25	0.49
2:M:2:GLU:HG3	2:M:3:TYR:H	1.77	0.49
3:H:247:LYS:HB2	3:H:247:LYS:HZ2	1.77	0.49
3:H:52:ASN:ND2	3:H:54:GLY:H	2.10	0.49
1:L:60:ASN:HD22	1:L:61:PRO:N	2.11	0.49
3:H:148:PRO:HA	3:H:151:LEU:CD2	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:405:U10:H3M3	6:M:405:U10:H4M2	1.95	0.48
2:M:230:GLY:O	2:M:233:ARG:HG3	2.12	0.48
2:M:13:ARG:NH2	2:M:35:PHE:HB3	2.28	0.48
3:H:147:ASN:OD1	3:H:149:ILE:HG13	2.13	0.48
1:L:60:ASN:HD22	1:L:60:ASN:C	2.17	0.48
2:M:90:PHE:N	2:M:90:PHE:CD1	2.80	0.48
1:L:213:ASP:O	1:L:217:ARG:HG3	2.14	0.48
4:M:401:BCL:HBB2	8:M:406:SPO:H243	1.96	0.47
1:L:54:VAL:C	1:L:56:GLN:H	2.18	0.47
3:H:112:ALA:HB2	3:H:239:GLY:HA3	1.95	0.47
1:L:12:PRO:O	3:H:242:MET:HE3	2.14	0.47
2:M:40:GLY:HA2	2:M:43:GLY:O	2.14	0.47
3:H:128:HIS:O	3:H:129:ASN:C	2.52	0.47
2:M:39:LEU:HA	2:M:39:LEU:HD12	1.68	0.47
2:M:134:TYR:CZ	2:M:144:LYS:HD3	2.50	0.47
2:M:162:PHE:HD1	8:M:406:SPO:H32	1.79	0.47
2:M:241:ARG:NH1	2:M:246:GLU:OE2	2.37	0.47
3:H:159:GLU:HB3	3:H:210:SER:CB	2.44	0.47
1:L:219:LEU:HD12	2:M:132:ARG:NH1	2.29	0.47
2:M:133:THR:CG2	2:M:147:ALA:CB	2.93	0.47
3:H:148:PRO:O	3:H:151:LEU:HB2	2.15	0.47
5:L:303:BPH:HBB1	2:M:210:TYR:CD2	2.48	0.46
2:M:133:THR:HG22	2:M:147:ALA:CB	2.45	0.46
2:M:260:ALA:HB1	2:M:265:THR:HG22	1.96	0.46
1:L:93:ALA:HA	5:L:303:BPH:H9C2	1.96	0.46
2:M:78:ALA:HB1	2:M:84:VAL:HG12	1.97	0.46
4:M:403:BCL:H2	5:M:404:BPH:HHC	1.96	0.46
3:H:70:ARG:NH2	3:H:120:LEU:HB2	2.30	0.46
1:L:217:ARG:O	1:L:218:ASP:C	2.50	0.46
2:M:164:ARG:HD2	2:M:284:ILE:HG22	1.98	0.46
2:M:260:ALA:HB3	2:M:265:THR:HG22	1.97	0.46
1:L:69:PRO:HG2	1:L:142:TRP:CB	2.32	0.45
3:H:129:ASN:HD21	3:H:224:GLU:CG	2.25	0.45
1:L:8:LYS:HB3	9:L:411:HOH:O	2.15	0.45
1:L:272:TRP:CB	1:L:275:ILE:HD12	2.47	0.45
2:M:280:GLY:HA2	4:M:403:BCL:HED2	1.99	0.45
1:L:3:LEU:HD12	2:M:250:LEU:CD1	2.47	0.45
1:L:208:THR:HG21	3:H:125:GLY:HA2	1.99	0.45
2:M:192:VAL:HG12	2:M:192:VAL:O	2.17	0.45
3:H:70:ARG:NH1	3:H:123:LEU:HD11	2.31	0.45
3:H:159:GLU:HB3	3:H:210:SER:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:206:ASN:ND2	9:H:314:HOH:O	2.49	0.45
1:L:6:GLU:OE2	1:L:10:ARG:NH1	2.41	0.44
2:M:148:TRP:O	2:M:151:LEU:HB3	2.17	0.44
2:M:162:PHE:HB2	8:M:406:SPO:H291	1.99	0.44
1:L:163:THR:HG22	1:L:163:THR:O	2.18	0.44
1:L:233:GLY:HA3	2:M:216:PHE:CE1	2.52	0.44
2:M:193:HIS:O	2:M:294:TRP:N	2.42	0.44
2:M:276:VAL:O	2:M:279:THR:HG22	2.17	0.44
1:L:8:LYS:NZ	3:H:81:GLU:OE1	2.50	0.44
2:M:161:GLY:HA3	8:M:406:SPO:C26	2.48	0.44
2:M:197:PHE:CE1	4:M:403:BCL:HMC2	2.52	0.43
3:H:22:ILE:O	3:H:23:PHE:C	2.54	0.43
1:L:189:LEU:HD13	1:L:216:PHE:HZ	1.83	0.43
3:H:117:ARG:NE	9:H:306:HOH:O	2.41	0.43
2:M:55:LEU:HD12	2:M:55:LEU:HA	1.76	0.43
1:L:177:ILE:HD11	4:L:301:BCL:C1B	2.49	0.43
1:L:254:ILE:HG21	1:L:254:ILE:HD13	1.65	0.43
1:L:207:ARG:CG	1:L:211:HIS:CD2	3.02	0.43
1:L:79:PRO:O	1:L:80:LEU:C	2.56	0.43
1:L:101:ALA:O	1:L:104:GLU:HB2	2.19	0.43
1:L:111:LEU:HA	1:L:111:LEU:HD23	1.82	0.43
1:L:231:ARG:HD3	2:M:5:ASN:O	2.19	0.43
2:M:199:ASN:HB2	2:M:294:TRP:CG	2.54	0.43
4:M:401:BCL:HBC1	4:M:403:BCL:HBD	2.00	0.43
1:L:32:GLY:HA3	1:L:35:GLY:H	1.83	0.43
2:M:112:GLY:O	2:M:116:LEU:CD2	2.66	0.43
3:H:120:LEU:C	3:H:226:THR:HG22	2.40	0.43
2:M:150:PHE:N	5:M:404:BPH:HMD3	2.33	0.42
1:L:219:LEU:HD12	1:L:219:LEU:HA	1.82	0.42
1:L:190:HIS:CE1	1:L:230:HIS:CE1	3.06	0.42
2:M:223:ILE:O	2:M:224:LEU:C	2.54	0.42
1:L:10:ARG:HG2	1:L:25:TRP:CZ2	2.54	0.42
1:L:207:ARG:HG3	1:L:211:HIS:CD2	2.54	0.42
5:L:303:BPH:CBB	5:L:303:BPH:CHC	2.89	0.42
2:M:21:THR:HG23	2:M:26:LEU:CD1	2.34	0.42
2:M:133:THR:CG2	2:M:147:ALA:CA	2.98	0.42
2:M:162:PHE:HB2	8:M:406:SPO:H312	2.02	0.42
2:M:119:SER:HB2	8:M:406:SPO:H343	1.93	0.42
3:H:227:LEU:HA	3:H:227:LEU:HD23	1.76	0.42
1:L:18:GLY:O	1:L:21:LEU:HB2	2.20	0.42
1:L:73:TYR:OH	1:L:82:LYS:HE2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:31:VAL:O	1:L:32:GLY:C	2.58	0.42
4:L:301:BCL:HBB2	4:M:403:BCL:NA	2.35	0.42
3:H:229:GLU:O	3:H:233:ILE:HD12	2.19	0.42
1:L:48:LEU:O	1:L:52:SER:HB2	2.20	0.41
5:L:303:BPH:H162	5:L:303:BPH:H141	1.66	0.41
3:H:39:GLY:N	3:H:79:GLU:OE2	2.52	0.41
4:L:302:BCL:H142	4:L:302:BCL:H112	1.88	0.41
1:L:8:LYS:HA	3:H:87:LEU:HD11	2.02	0.41
1:L:253:THR:OG1	1:L:254:ILE:N	2.53	0.41
1:L:259:TRP:O	1:L:260:VAL:C	2.57	0.41
1:L:264:GLN:HA	1:L:267:VAL:CG1	2.51	0.41
2:M:251:PHE:CD1	2:M:251:PHE:C	2.93	0.41
1:L:202:LYS:C	1:L:204:LYS:N	2.74	0.41
5:L:303:BPH:H102	5:L:303:BPH:H6C1	1.92	0.41
3:H:120:LEU:HA	3:H:226:THR:HG22	2.01	0.41
3:H:149:ILE:CD1	3:H:166:ASP:HA	2.45	0.41
2:M:247:ARG:NH2	3:H:111:PRO:O	2.40	0.41
3:H:129:ASN:HD22	3:H:224:GLU:HG2	1.78	0.41
1:L:60:ASN:C	1:L:60:ASN:ND2	2.74	0.41
1:L:75:LEU:HA	1:L:75:LEU:HD23	1.66	0.41
2:M:261:THR:O	2:M:265:THR:HG22	2.21	0.41
3:H:156:CYS:HA	9:H:314:HOH:O	2.20	0.41
3:H:242:MET:N	9:H:313:HOH:O	2.52	0.41
1:L:109:ARG:HD2	1:L:115:TYR:OH	2.21	0.41
3:H:20:PHE:O	3:H:21:TRP:C	2.56	0.41
1:L:202:LYS:C	1:L:204:LYS:H	2.24	0.40
3:H:224:GLU:HA	9:H:302:HOH:O	2.21	0.40
1:L:67:TYR:HB3	1:L:68:PRO:HD2	2.02	0.40
1:L:102:LEU:HD12	1:L:102:LEU:HA	1.90	0.40
1:L:225:GLY:HA2	6:L:304:U10:H3M1	2.03	0.40
1:L:3:LEU:HD12	2:M:250:LEU:HD13	2.04	0.40
1:L:21:LEU:HD13	1:L:22:PHE:CE1	2.57	0.40
1:L:60:ASN:HD22	1:L:61:PRO:CD	2.35	0.40
1:L:83:GLY:O	1:L:87:GLN:HG3	2.21	0.40
1:L:2:LEU:HD21	1:L:10:ARG:CZ	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	279/281 (99%)	246 (88%)	22 (8%)	11 (4%)	3 15
2	M	300/313 (96%)	260 (87%)	35 (12%)	5 (2%)	9 36
3	H	238/260 (92%)	212 (89%)	24 (10%)	2 (1%)	19 55
All	All	817/854 (96%)	718 (88%)	81 (10%)	18 (2%)	6 29

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	52	SER
1	L	55	LEU
1	L	202	LYS
2	M	301	HIS
3	H	185	ASP
1	L	10	ARG
1	L	80	LEU
2	M	56	GLY
1	L	51	TRP
1	L	271	TRP
1	L	272	TRP
2	M	30	SER
1	L	8	LYS
2	M	57	VAL
3	H	124	ASP
1	L	270	PRO
2	M	129	TRP
1	L	32	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	L	219/220 (100%)	188 (86%)	31 (14%)	3	14
2	M	236/246 (96%)	204 (86%)	32 (14%)	3	15
3	H	195/208 (94%)	167 (86%)	28 (14%)	3	14
All	All	650/674 (96%)	559 (86%)	91 (14%)	3	15

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	8	LYS
1	L	17	VAL
1	L	21	LEU
1	L	38	THR
1	L	40	PHE
1	L	44	LEU
1	L	52	SER
1	L	54	VAL
1	L	56	GLN
1	L	60	ASN
1	L	63	LEU
1	L	67	TYR
1	L	72	GLU
1	L	85	LEU
1	L	102	LEU
1	L	126	LEU
1	L	129	LEU
1	L	158	SER
1	L	185	LEU
1	L	202	LYS
1	L	205	GLU
1	L	207	ARG
1	L	210	ASP
1	L	216	PHE
1	L	217	ARG
1	L	237	SER
1	L	246	LEU
1	L	247	CYS
1	L	254	ILE
1	L	271	TRP
1	L	272	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	2	GLU
2	M	12	VAL
2	M	29	ARG
2	M	32	VAL
2	M	39	LEU
2	M	47	LEU
2	M	54	SER
2	M	65	MET
2	M	86	LEU
2	M	94	LEU
2	M	109	LEU
2	M	133	THR
2	M	136	ARG
2	M	144	LYS
2	M	148	TRP
2	M	156	LEU
2	M	173	GLU
2	M	191	LEU
2	M	204	LEU
2	M	214	LEU
2	M	215	LEU
2	M	216	PHE
2	M	229	PHE
2	M	233	ARG
2	M	235	LEU
2	M	247	ARG
2	M	250	LEU
2	M	259	ASN
2	M	265	THR
2	M	279	THR
2	M	285	LEU
2	M	300	ASN
3	H	11	ASP
3	H	12	LEU
3	H	14	SER
3	H	34	GLU
3	H	52	ASN
3	H	60	LYS
3	H	66	LEU
3	H	70	ARG
3	H	72	THR
3	H	92	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	117	ARG
3	H	118	ARG
3	H	120	LEU
3	H	134	MET
3	H	135	LYS
3	H	149	ILE
3	H	151	LEU
3	H	171	ILE
3	H	177	ARG
3	H	184	LYS
3	H	200	SER
3	H	217	PRO
3	H	225	VAL
3	H	231	ASP
3	H	232	LYS
3	H	246	PRO
3	H	247	LYS
3	H	250	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	60	ASN
2	M	193	HIS
3	H	52	ASN
3	H	98	HIS

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 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BCL	L	302	-	58,74,74	1.54	5 (8%)	69,115,115	2.37	26 (37%)
4	BCL	L	301	-	58,74,74	1.44	5 (8%)	69,115,115	1.64	12 (17%)
5	BPH	L	303	-	51,70,70	1.31	3 (5%)	52,101,101	2.05	18 (34%)
8	SPO	M	406	-	40,41,41	2.18	8 (20%)	47,50,50	2.93	20 (42%)
5	BPH	M	404	-	36,55,70	1.47	7 (19%)	34,83,101	2.77	14 (41%)
4	BCL	M	401	-	42,58,74	2.99	7 (16%)	48,95,115	2.90	20 (41%)
4	BCL	M	403	-	58,74,74	1.47	4 (6%)	69,115,115	1.71	18 (26%)
6	U10	M	405	-	48,48,63	2.89	17 (35%)	58,61,79	2.44	19 (32%)
6	U10	L	304	-	33,33,63	3.55	11 (33%)	40,43,79	3.44	21 (52%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	L	302	-	-	6/37/137/137	-
4	BCL	L	301	-	-	1/37/137/137	-
5	BPH	L	303	-	2/2/18/22	15/37/105/105	0/5/6/6
8	SPO	M	406	-	-	9/47/47/47	-
5	BPH	M	404	-	-	5/19/87/105	0/5/6/6
4	BCL	M	401	-	-	4/18/118/137	-
4	BCL	M	403	-	-	7/37/137/137	-
6	U10	M	405	-	-	16/45/69/87	0/1/1/1
6	U10	L	304	-	-	13/27/51/87	0/1/1/1

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	401	BCL	C1B-NB	15.23	1.48	1.35
6	L	304	U10	C13-C14	9.42	1.55	1.33
8	M	406	SPO	C27-C28	9.22	1.43	1.34
6	L	304	U10	C8-C9	8.99	1.54	1.33
4	M	401	BCL	C4B-NB	8.52	1.42	1.35
4	M	403	BCL	C1B-NB	8.10	1.42	1.35
6	L	304	U10	C18-C19	7.68	1.51	1.33
6	M	405	U10	C33-C34	7.42	1.50	1.33
4	L	302	BCL	C4B-NB	7.29	1.41	1.35
6	M	405	U10	C13-C14	7.07	1.49	1.33
6	L	304	U10	C23-C24	7.03	1.52	1.32
6	M	405	U10	C28-C29	6.93	1.49	1.33
6	L	304	U10	C7-C6	6.74	1.62	1.51
6	M	405	U10	C38-C39	6.39	1.50	1.32
6	M	405	U10	C8-C9	6.28	1.48	1.33
4	L	301	BCL	C1B-NB	6.28	1.40	1.35
6	M	405	U10	C18-C19	5.88	1.47	1.33
4	L	302	BCL	C1B-NB	5.33	1.40	1.35
4	L	301	BCL	C4B-NB	5.15	1.39	1.35
6	M	405	U10	C23-C24	4.53	1.43	1.33
6	L	304	U10	C7-C8	4.52	1.57	1.50
6	M	405	U10	C6-C1	4.52	1.43	1.35
5	L	303	BPH	CHA-CBD	-4.27	1.47	1.52
8	M	406	SPO	C25-C23	4.04	1.54	1.45
4	M	401	BCL	CAA-C2A	3.98	1.61	1.54
4	M	403	BCL	C4B-NB	3.66	1.38	1.35
5	L	303	BPH	O2A-CGA	3.46	1.43	1.33
8	M	406	SPO	C26-C27	3.38	1.53	1.43
4	M	401	BCL	O2A-CGA	3.35	1.43	1.33
6	M	405	U10	O3-C3	-3.16	1.29	1.36
5	M	404	BPH	C1A-C2A	3.16	1.55	1.51
6	L	304	U10	C16-C14	3.04	1.57	1.51
6	M	405	U10	O4-C4	-2.99	1.29	1.36
6	L	304	U10	C12-C13	2.94	1.60	1.50
4	L	302	BCL	C3D-C2D	-2.92	1.34	1.39
5	L	303	BPH	C3D-C2D	-2.77	1.34	1.39
8	M	406	SPO	C6-C7	2.75	1.51	1.45
8	M	406	SPO	C4-C5	2.72	1.54	1.50
5	M	404	BPH	C5-C3	2.68	1.57	1.50
5	M	404	BPH	O2A-CGA	2.66	1.41	1.33
6	L	304	U10	C26-C24	2.65	1.57	1.50
6	L	304	U10	C21-C19	2.64	1.56	1.51
5	M	404	BPH	C3B-C2B	2.62	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	401	BCL	C3C-C4C	2.60	1.54	1.51
6	M	405	U10	O2-C2	2.57	1.29	1.23
4	L	301	BCL	OBD-CAD	2.53	1.25	1.22
6	M	405	U10	O5-C5	2.50	1.28	1.23
8	M	406	SPO	C37-C38	2.49	1.39	1.32
4	M	403	BCL	C1-C2	2.38	1.56	1.49
6	M	405	U10	C30-C29	2.37	1.56	1.50
5	M	404	BPH	CMB-C2B	-2.35	1.46	1.51
6	M	405	U10	C35-C34	2.27	1.56	1.50
4	L	301	BCL	O2D-CGD	2.26	1.38	1.33
4	M	401	BCL	CBD-CGD	-2.24	1.45	1.52
6	M	405	U10	C32-C33	2.21	1.57	1.50
8	M	406	SPO	C8-C7	2.20	1.55	1.50
8	M	406	SPO	C10-C9	2.18	1.50	1.43
6	M	405	U10	C36-C34	2.13	1.55	1.51
4	M	401	BCL	C3B-C2B	2.08	1.43	1.39
4	M	403	BCL	MG-NA	2.07	2.11	2.06
4	L	301	BCL	CHD-C4C	-2.07	1.35	1.41
4	L	302	BCL	CAC-C3C	2.04	1.58	1.54
4	L	302	BCL	C4B-CHC	-2.04	1.35	1.41
6	L	304	U10	C22-C23	2.04	1.57	1.50
6	M	405	U10	C31-C32	2.02	1.60	1.53
5	M	404	BPH	CBA-CGA	2.01	1.56	1.50
5	M	404	BPH	O1A-CGA	2.00	1.28	1.22

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	401	BCL	O2A-C1-C2	9.77	131.82	108.97
8	M	406	SPO	C16-C17-C19	8.76	132.38	118.94
6	L	304	U10	O5-C5-C4	-7.94	104.08	120.93
4	M	401	BCL	O2D-CGD-CBD	7.52	124.64	111.27
5	M	404	BPH	O2D-CGD-CBD	7.44	120.43	111.00
4	L	302	BCL	O2D-CGD-CBD	7.15	123.97	111.27
6	L	304	U10	C6-C1-C2	-6.94	113.70	119.18
6	L	304	U10	O2-C2-C3	-6.75	106.59	120.93
4	L	302	BCL	C16-C15-C13	-6.70	94.25	115.92
6	L	304	U10	C4M-O4-C4	6.59	139.82	116.47
6	M	405	U10	C35-C34-C36	6.54	126.27	115.27
8	M	406	SPO	C20-C21-C22	-6.24	110.69	123.47
6	L	304	U10	C1-C6-C5	-6.22	113.73	119.58
6	M	405	U10	C22-C23-C24	-6.12	112.93	127.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	406	SPO	C24-C23-C22	-5.98	114.54	122.92
4	M	401	BCL	O1D-CGD-CBD	-5.91	112.40	124.48
6	L	304	U10	C7-C6-C5	5.82	125.48	118.48
6	L	304	U10	C3M-O3-C3	5.78	136.94	116.47
6	M	405	U10	C31-C29-C28	-5.70	109.57	121.12
6	M	405	U10	C30-C29-C31	5.68	124.82	115.27
6	M	405	U10	C17-C18-C19	-5.59	114.19	127.66
4	M	401	BCL	O2A-CGA-CBA	5.53	129.26	111.91
4	L	302	BCL	C4A-NA-C1A	-5.40	104.28	106.71
4	M	403	BCL	O2D-CGD-O1D	-5.34	113.41	123.84
5	M	404	BPH	C1-O2A-CGA	5.31	130.37	116.44
5	L	303	BPH	CAC-C3C-C2C	-5.15	101.38	114.26
8	M	406	SPO	C24-C23-C25	5.10	126.11	118.08
5	L	303	BPH	CAC-C3C-C4C	-4.96	102.64	113.73
8	M	406	SPO	C29-C28-C30	-4.92	107.00	115.27
4	M	401	BCL	C1B-CHB-C4A	-4.91	120.39	130.12
8	M	406	SPO	C18-C17-C19	-4.82	116.18	122.92
5	M	404	BPH	C1A-C2A-C3A	-4.80	98.27	102.84
5	M	404	BPH	CAC-C3C-C2C	-4.69	102.54	114.26
5	M	404	BPH	OBD-CAD-CBD	-4.64	119.02	125.82
5	L	303	BPH	C4C-C3C-C2C	-4.60	98.47	102.84
6	L	304	U10	C8-C7-C6	4.58	124.39	112.05
4	L	301	BCL	C1-O2A-CGA	4.46	128.16	116.44
6	L	304	U10	C26-C24-C25	4.38	124.27	114.60
8	M	406	SPO	C6-C7-C9	-4.38	112.23	118.94
6	M	405	U10	C26-C27-C28	-4.30	97.76	111.88
8	M	406	SPO	C18-C17-C16	-4.23	111.41	118.08
4	L	301	BCL	C4-C3-C5	4.18	122.30	115.27
5	M	404	BPH	C4C-C3C-C2C	-4.11	98.93	102.84
6	L	304	U10	C11-C12-C13	4.07	125.26	111.88
4	L	301	BCL	C2C-C3C-C4C	4.00	107.32	101.34
5	M	404	BPH	O2A-C1-C2	-4.00	98.13	108.64
4	L	302	BCL	C5-C3-C2	-3.98	113.07	121.12
6	L	304	U10	C3-C4-C5	-3.95	112.92	120.68
6	M	405	U10	C15-C14-C16	3.90	121.83	115.27
4	L	302	BCL	C11-C12-C13	-3.89	103.33	115.92
4	L	302	BCL	O2A-CGA-CBA	3.89	124.11	111.91
4	L	302	BCL	C6-C7-C8	-3.89	103.36	115.92
5	M	404	BPH	OBB-CAB-CBB	-3.74	111.76	120.17
6	L	304	U10	C1M-C1-C6	-3.67	118.41	124.40
4	M	401	BCL	C1C-NC-C4C	3.64	108.34	106.71
4	M	401	BCL	CHD-C4C-NC	3.61	129.08	125.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	401	BCL	CAC-C3C-C4C	3.60	120.57	112.58
4	M	403	BCL	O2A-CGA-CBA	3.59	123.18	111.91
8	M	406	SPO	C21-C22-C23	3.58	132.42	127.31
8	M	406	SPO	C10-C9-C7	3.57	132.41	127.31
4	M	401	BCL	O1A-CGA-CBA	-3.57	109.81	123.73
4	M	401	BCL	CHB-C4A-NA	3.52	129.39	124.51
4	M	401	BCL	C4C-CHD-C1D	-3.49	120.73	125.88
6	L	304	U10	C4-C3-C2	-3.47	113.86	120.68
8	M	406	SPO	C8-C7-C6	3.45	123.52	118.08
4	L	302	BCL	O1D-CGD-CBD	-3.43	117.46	124.48
5	L	303	BPH	OBB-CAB-CBB	-3.41	112.50	120.17
6	M	405	U10	C25-C24-C23	-3.33	115.14	123.68
6	M	405	U10	C7-C8-C9	-3.33	121.25	126.79
4	M	403	BCL	C4B-C3B-CAB	-3.32	120.71	127.13
6	M	405	U10	C27-C28-C29	-3.32	119.67	127.66
5	L	303	BPH	C11-C10-C8	3.29	126.56	115.92
4	L	302	BCL	C2A-C1A-CHA	-3.29	118.11	123.86
4	M	403	BCL	O2D-CGD-CBD	3.28	117.09	111.27
5	L	303	BPH	C6-C5-C3	3.28	122.05	113.45
4	L	301	BCL	O2A-CGA-CBA	3.26	122.14	111.91
8	M	406	SPO	C36-C35-C33	3.25	123.67	112.98
4	L	302	BCL	CAA-CBA-CGA	3.22	122.66	113.25
5	L	303	BPH	CMA-C3A-C4A	-3.20	107.37	114.38
4	L	302	BCL	OBD-CAD-CBD	3.19	130.45	125.89
5	M	404	BPH	CMD-C2D-C3D	3.13	130.54	124.68
4	L	302	BCL	O2A-CGA-O1A	-3.08	115.83	123.59
4	M	403	BCL	CMC-C2C-C1C	-3.06	103.54	111.77
4	L	302	BCL	C1-C2-C3	3.06	131.33	126.04
8	M	406	SPO	C21-C20-C19	3.04	129.69	123.47
6	M	405	U10	C36-C34-C33	-3.03	114.98	121.12
4	M	401	BCL	CAC-C3C-C2C	-3.03	106.70	114.26
6	L	304	U10	C1M-C1-C2	3.01	127.88	116.99
5	M	404	BPH	O2D-CGD-O1D	-2.99	117.99	123.84
8	M	406	SPO	C11-C12-C14	2.99	123.53	118.94
5	L	303	BPH	CBA-CAA-C2A	-2.98	105.11	113.81
5	L	303	BPH	C1-C2-C3	-2.98	120.89	126.04
8	M	406	SPO	C15-C16-C17	-2.94	118.17	126.42
4	L	301	BCL	O2A-C1-C2	-2.91	100.99	108.64
4	L	302	BCL	CAC-C3C-C2C	-2.86	107.12	114.26
4	L	302	BCL	C4C-CHD-C1D	-2.84	121.69	125.88
4	L	301	BCL	C4-C3-C2	-2.83	116.41	123.68
4	L	302	BCL	C1C-NC-C4C	2.80	107.97	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	303	BPH	C12-C11-C10	2.79	126.04	113.24
6	M	405	U10	C25-C24-C26	2.78	119.95	115.27
4	L	301	BCL	C4C-CHD-C1D	-2.77	121.79	125.88
8	M	406	SPO	C26-C25-C23	2.77	134.19	126.42
5	L	303	BPH	C1C-C2C-C3C	2.73	105.44	102.84
8	M	406	SPO	C2-C1-C4	-2.71	106.69	110.86
5	L	303	BPH	CBC-CAC-C3C	-2.71	108.31	113.77
4	L	302	BCL	O2D-CGD-O1D	-2.71	118.55	123.84
4	L	302	BCL	C6-C5-C3	-2.68	106.43	113.45
4	M	401	BCL	C3A-C2A-C1A	-2.67	97.33	101.34
8	M	406	SPO	C13-C12-C11	-2.65	113.91	118.08
4	M	403	BCL	C4A-NA-C1A	-2.59	105.54	106.71
4	M	403	BCL	CAD-C3D-C4D	-2.58	107.03	108.47
8	M	406	SPO	C3-C1-C4	-2.58	106.90	110.86
4	L	302	BCL	CHD-C4C-NC	2.57	127.93	125.08
5	M	404	BPH	CMA-C3A-C4A	-2.54	108.82	114.38
4	M	401	BCL	C3D-CAD-CBD	-2.53	104.28	107.61
4	L	302	BCL	OBD-CAD-C3D	-2.52	123.79	127.98
4	M	403	BCL	CAC-C3C-C4C	-2.49	107.06	112.58
4	L	301	BCL	CMB-C2B-C1B	-2.48	124.65	128.46
4	L	302	BCL	C4-C3-C5	2.47	119.43	115.27
8	M	406	SPO	C30-C31-C32	2.47	120.00	111.88
4	L	302	BCL	C16-C17-C18	-2.47	104.35	115.98
4	L	301	BCL	C6-C5-C3	-2.45	107.04	113.45
4	M	403	BCL	C1-C2-C3	2.44	130.27	126.04
5	M	404	BPH	C3D-CAD-CBD	2.43	110.81	107.61
5	M	404	BPH	CBC-CAC-C3C	-2.42	108.88	113.77
4	M	403	BCL	O1D-CGD-CBD	2.41	129.41	124.48
6	M	405	U10	C37-C36-C34	2.40	120.87	112.98
4	M	403	BCL	CMA-C3A-C4A	2.39	118.19	111.77
4	L	301	BCL	C3D-CAD-CBD	-2.39	104.46	107.61
6	L	304	U10	O2-C2-C1	-2.38	113.71	120.73
4	M	403	BCL	C2A-C3A-C4A	2.37	105.70	101.87
6	L	304	U10	C11-C9-C8	2.36	125.90	121.12
4	M	403	BCL	C14-C13-C12	-2.36	102.75	111.29
5	L	303	BPH	C6-C7-C8	2.34	123.49	115.92
6	M	405	U10	C4M-O4-C4	2.32	124.70	116.47
6	L	304	U10	C22-C23-C24	2.31	135.65	127.75
6	M	405	U10	C10-C9-C8	-2.30	117.77	123.68
6	L	304	U10	C20-C19-C18	-2.30	117.78	123.68
4	M	403	BCL	O2A-CGA-O1A	-2.30	117.80	123.59
4	M	403	BCL	CHC-C1C-NC	-2.29	121.34	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	303	BPH	CAA-C2A-C3A	-2.28	106.53	112.78
4	L	302	BCL	C1-O2A-CGA	2.24	122.32	116.44
4	M	401	BCL	CBA-CAA-C2A	2.24	120.46	113.86
4	M	401	BCL	CMD-C2D-C3D	-2.23	120.50	124.68
5	L	303	BPH	C1A-C2A-C3A	-2.22	100.73	102.84
4	L	302	BCL	CMB-C2B-C1B	-2.20	125.08	128.46
4	L	302	BCL	O2A-C1-C2	-2.20	102.86	108.64
6	M	405	U10	C10-C9-C11	2.19	118.95	115.27
4	L	302	BCL	C3A-C2A-C1A	-2.18	98.08	101.34
4	M	401	BCL	CAA-C2A-C1A	2.17	119.08	111.97
4	M	403	BCL	CAA-C2A-C3A	-2.16	106.85	112.78
4	M	401	BCL	CMC-C2C-C3C	-2.16	105.11	113.83
6	M	405	U10	C20-C19-C21	2.16	118.91	115.27
4	M	401	BCL	CED-O2D-CGD	-2.16	111.05	115.94
5	L	303	BPH	CED-O2D-CGD	-2.15	111.08	115.94
6	L	304	U10	C16-C17-C18	2.15	118.93	111.88
6	L	304	U10	C10-C9-C11	-2.13	111.69	115.27
5	L	303	BPH	O2A-CGA-O1A	2.11	128.92	123.59
6	M	405	U10	C20-C19-C18	-2.11	118.28	123.68
6	L	304	U10	C16-C14-C13	2.10	125.37	121.12
5	L	303	BPH	C14-C13-C12	2.10	118.89	111.29
4	M	403	BCL	C2A-C1A-CHA	-2.08	120.23	123.86
4	L	301	BCL	CHD-C4C-NC	2.02	127.33	125.08
4	M	401	BCL	C4-C3-C2	-2.01	109.76	126.37
4	M	403	BCL	CED-O2D-CGD	-2.01	111.40	115.94
6	M	405	U10	C3M-O3-C3	2.01	123.58	116.47
5	M	404	BPH	CAC-C3C-C4C	2.00	118.21	113.73
4	L	301	BCL	C14-C13-C12	-2.00	104.04	111.29

All (2) chirality outliers are listed below:

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

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	303	BPH	C4C-C3C-CAC-CBC
5	L	303	BPH	O2A-C1-C2-C3
5	L	303	BPH	C14-C13-C15-C16
5	M	404	BPH	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	L	304	U10	C1-C6-C7-C8
6	L	304	U10	C5-C6-C7-C8
6	L	304	U10	C7-C8-C9-C10
6	L	304	U10	C7-C8-C9-C11
6	L	304	U10	C14-C16-C17-C18
6	L	304	U10	C17-C18-C19-C21
6	M	405	U10	C12-C13-C14-C15
6	M	405	U10	C14-C16-C17-C18
6	M	405	U10	C27-C28-C29-C30
6	M	405	U10	C27-C28-C29-C31
6	M	405	U10	C32-C33-C34-C35
6	M	405	U10	C32-C33-C34-C36
6	M	405	U10	C37-C38-C39-C41
8	M	406	SPO	C1-C4-C5-C6
8	M	406	SPO	C33-C35-C36-C37
6	M	405	U10	C37-C38-C39-C40
6	L	304	U10	C17-C18-C19-C20
6	M	405	U10	C12-C13-C14-C16
4	M	403	BCL	CBD-CGD-O2D-CED
6	L	304	U10	C22-C23-C24-C26
6	L	304	U10	C9-C11-C12-C13
4	L	302	BCL	CBD-CGD-O2D-CED
6	L	304	U10	C15-C14-C16-C17
5	L	303	BPH	C11-C10-C8-C9
6	L	304	U10	C22-C23-C24-C25
4	L	302	BCL	C15-C16-C17-C18
5	L	303	BPH	C5-C6-C7-C8
5	L	303	BPH	C6-C7-C8-C10
6	L	304	U10	C19-C21-C22-C23
5	L	303	BPH	C6-C7-C8-C9
4	L	302	BCL	O1D-CGD-O2D-CED
5	L	303	BPH	C3-C5-C6-C7
5	L	303	BPH	C4-C3-C5-C6
6	M	405	U10	C25-C24-C26-C27
5	L	303	BPH	C2-C3-C5-C6
6	M	405	U10	C23-C24-C26-C27
4	M	401	BCL	CBA-CGA-O2A-C1
6	L	304	U10	C13-C14-C16-C17
8	M	406	SPO	C24-C23-C25-C26
4	M	401	BCL	O1A-CGA-O2A-C1
4	M	403	BCL	O1D-CGD-O2D-CED
6	M	405	U10	C24-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	M	406	SPO	C4-C1-O1-CM1
8	M	406	SPO	C2-C1-O1-CM1
5	L	303	BPH	C11-C10-C8-C7
5	L	303	BPH	C8-C10-C11-C12
4	M	401	BCL	O2A-C1-C2-C3
5	L	303	BPH	CAD-CBD-CGD-O2D
6	M	405	U10	C5-C4-O4-C4M
5	L	303	BPH	C12-C13-C15-C16
4	L	302	BCL	C16-C17-C18-C20
4	M	403	BCL	C16-C17-C18-C20
4	L	302	BCL	C16-C17-C18-C19
8	M	406	SPO	C3-C1-O1-CM1
8	M	406	SPO	C18-C17-C19-C20
8	M	406	SPO	C16-C17-C19-C20
8	M	406	SPO	C22-C23-C25-C26
6	M	405	U10	C20-C19-C21-C22
5	M	404	BPH	CBA-CGA-O2A-C1
6	M	405	U10	C3-C4-O4-C4M
4	L	301	BCL	CAD-CBD-CGD-O2D
4	L	302	BCL	CAD-CBD-CGD-O2D
4	M	401	BCL	CAD-CBD-CGD-O2D
4	M	403	BCL	CAD-CBD-CGD-O2D
5	M	404	BPH	CAD-CBD-CGD-O2D
5	M	404	BPH	CHA-CBD-CGD-O1D
4	M	403	BCL	C5-C6-C7-C8
4	M	403	BCL	CAA-CBA-CGA-O2A
6	M	405	U10	C21-C22-C23-C24
5	L	303	BPH	C2C-C3C-CAC-CBC
5	M	404	BPH	O1A-CGA-O2A-C1
4	M	403	BCL	C11-C10-C8-C9

There are no ring outliers.

9 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	302	BCL	6	0
4	L	301	BCL	3	0
5	L	303	BPH	14	0
8	M	406	SPO	13	0
5	M	404	BPH	9	0
4	M	401	BCL	7	0
4	M	403	BCL	15	0

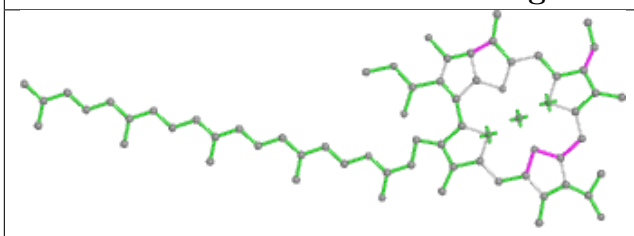
Continued on next page...

Continued from previous page...

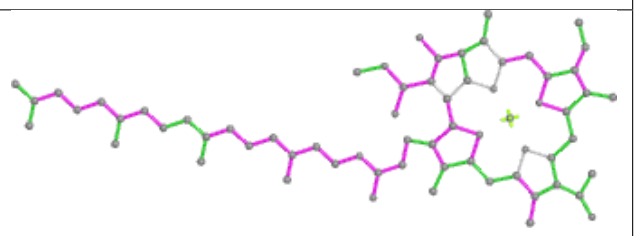
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	405	U10	1	0
6	L	304	U10	10	0

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 then 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.

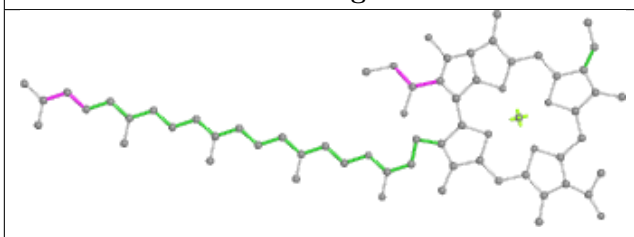
Ligand BCL L 302



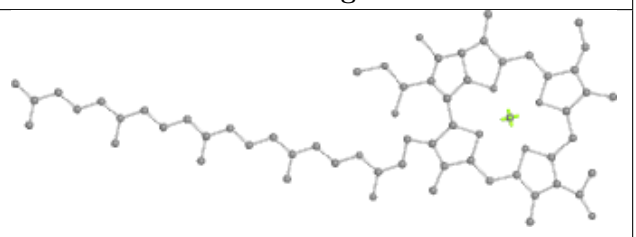
Bond lengths



Bond angles

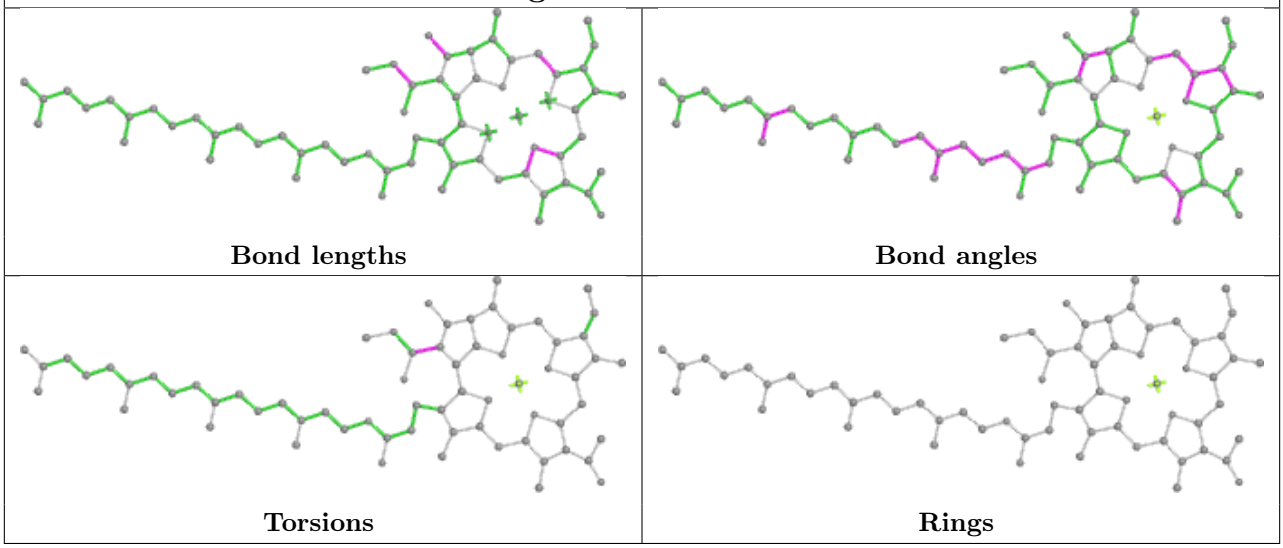


Torsions

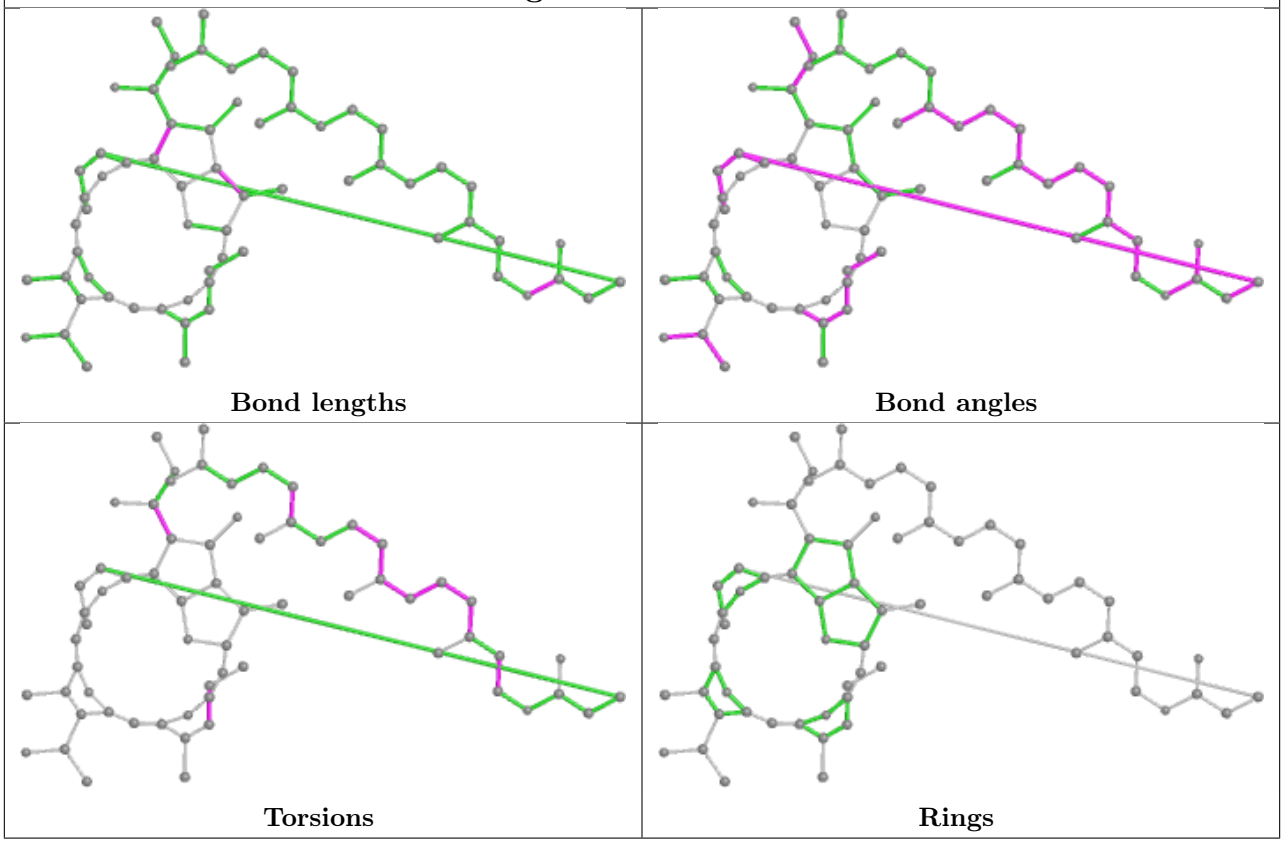


Rings

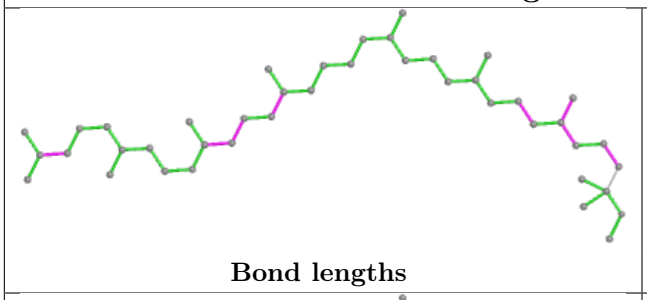
Ligand BCL L 301



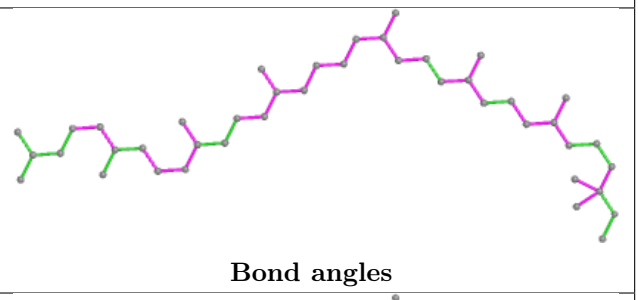
Ligand BPH L 303



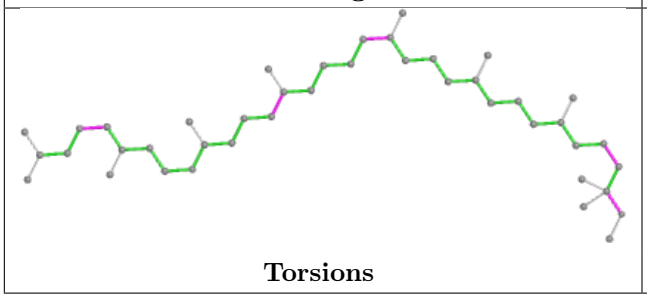
Ligand SPO M 406



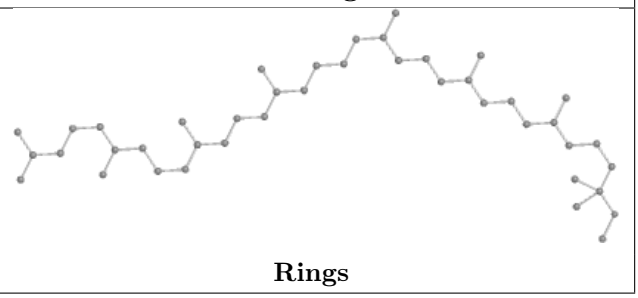
Bond lengths



Bond angles

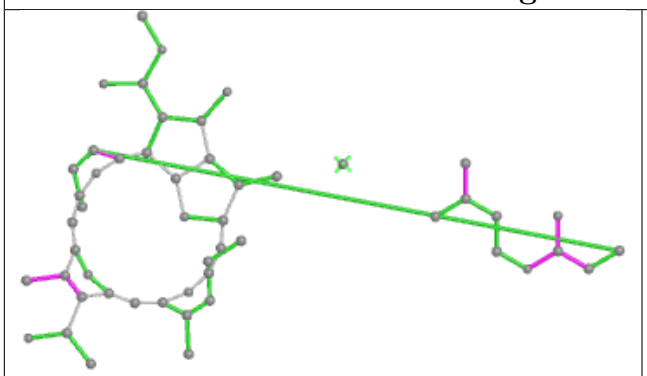


Torsions

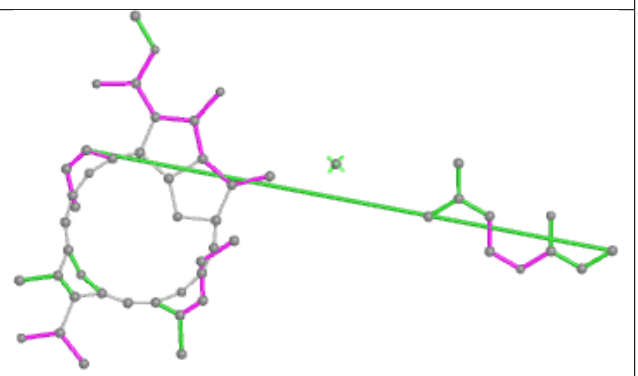


Rings

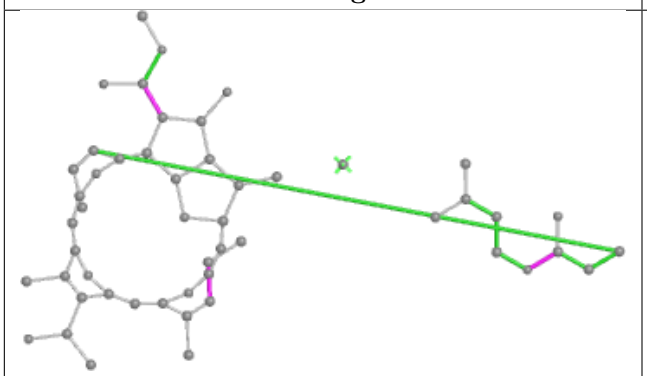
Ligand BPH M 404



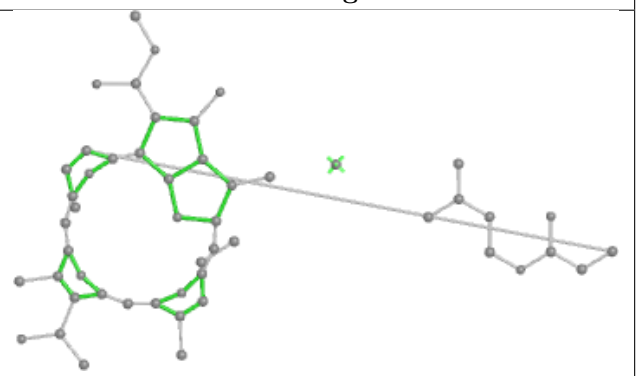
Bond lengths



Bond angles

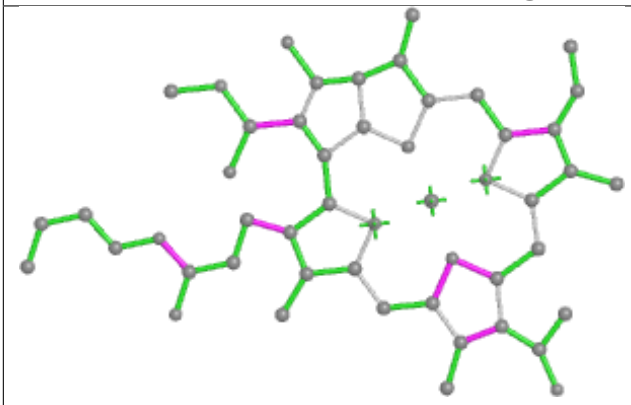


Torsions

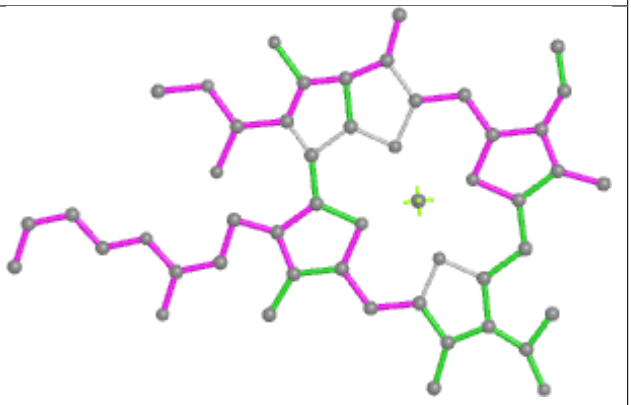


Rings

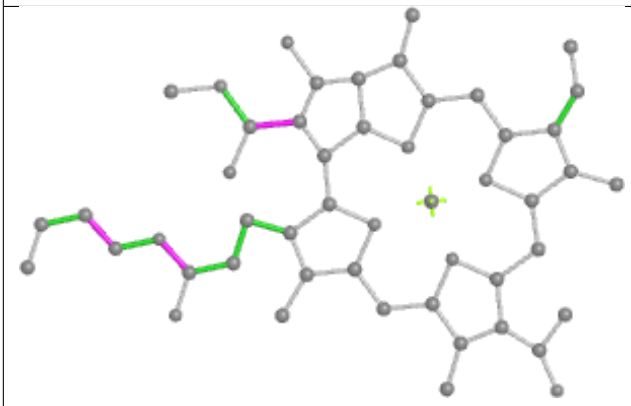
Ligand BCL M 401



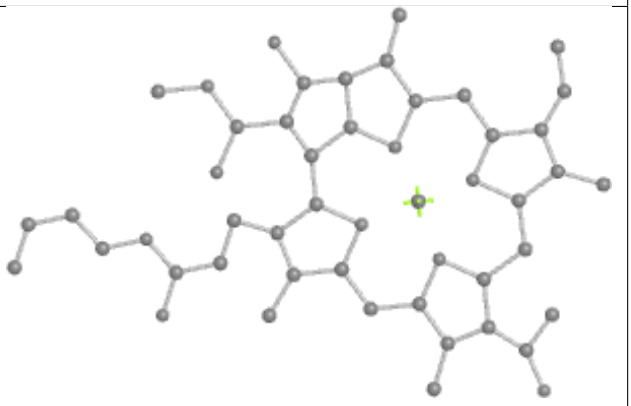
Bond lengths



Bond angles

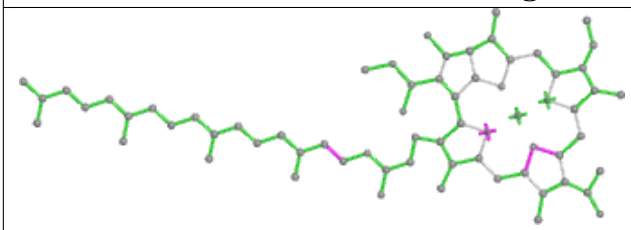


Torsions

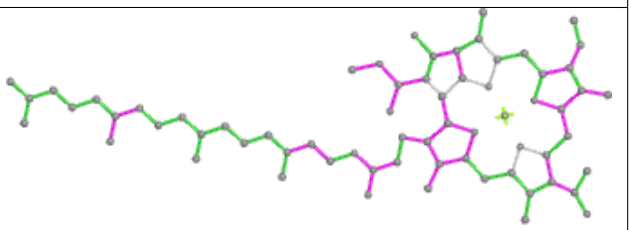


Rings

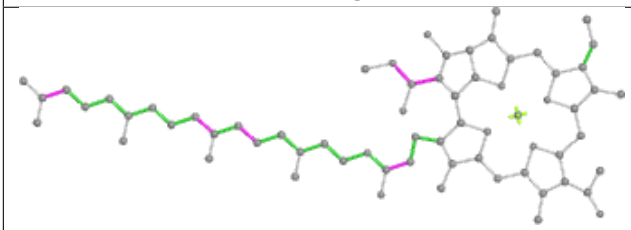
Ligand BCL M 403



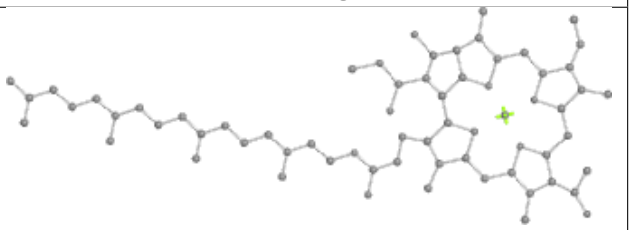
Bond lengths



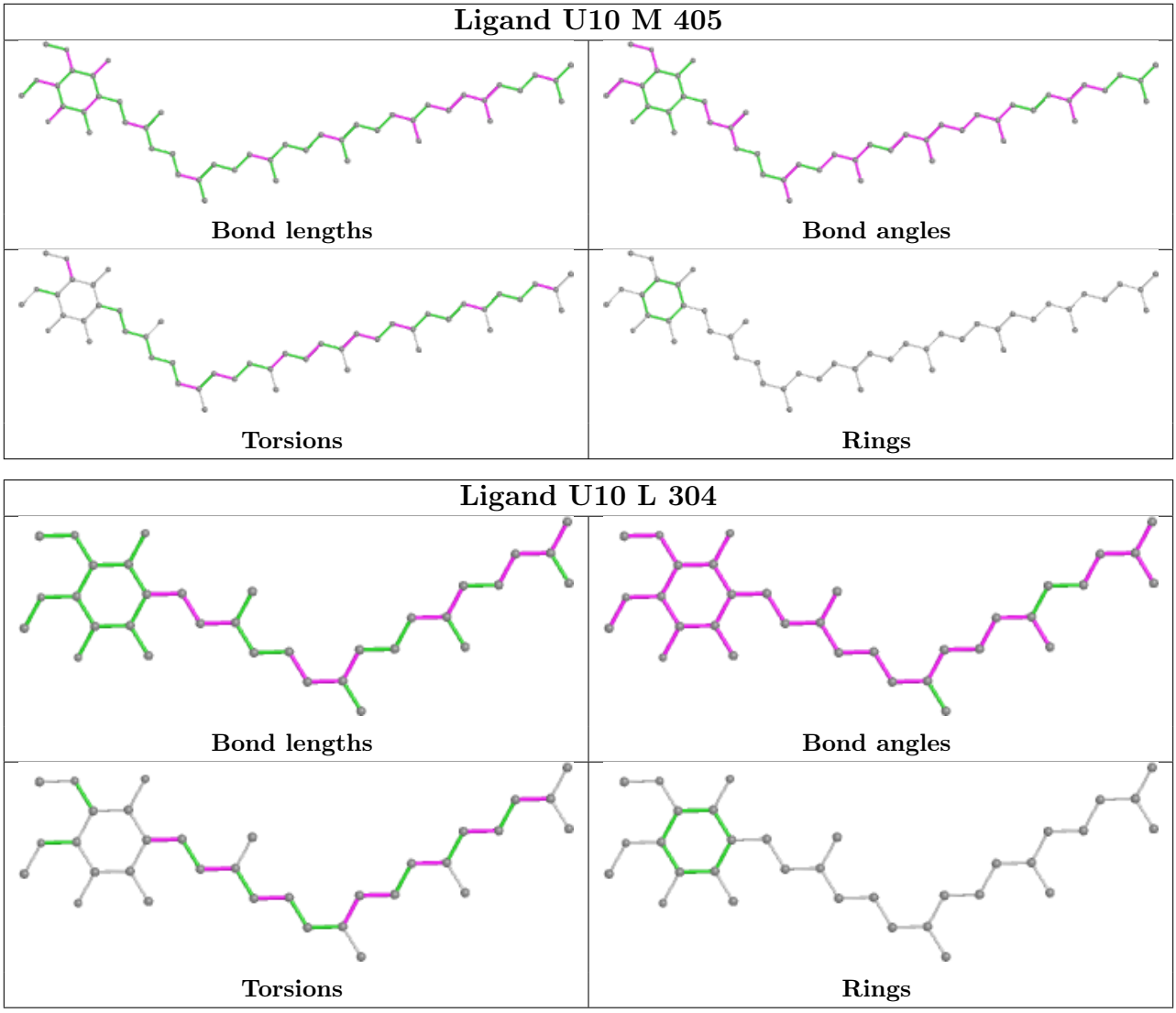
Bond angles



Torsions



Rings



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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	L	281/281 (100%)	-0.66	4 (1%)	75	57	35, 48, 83, 98	0
2	M	302/313 (96%)	-0.67	6 (1%)	65	45	34, 52, 82, 108	0
3	H	240/260 (92%)	-0.48	4 (1%)	70	50	38, 52, 69, 96	0
All	All	823/854 (96%)	-0.61	14 (1%)	70	50	34, 50, 81, 108	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	6.3
3	H	250	SER	4.5
3	H	80	SER	3.2
2	M	301	HIS	2.9
2	M	302	GLY	2.9
3	H	246	PRO	2.8
1	L	59	TRP	2.8
1	L	270	PRO	2.4
2	M	100	GLU	2.2
1	L	72	GLU	2.2
1	L	281	GLY	2.1
2	M	99	PRO	2.1
2	M	2	GLU	2.1
3	H	249	LYS	2.1

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

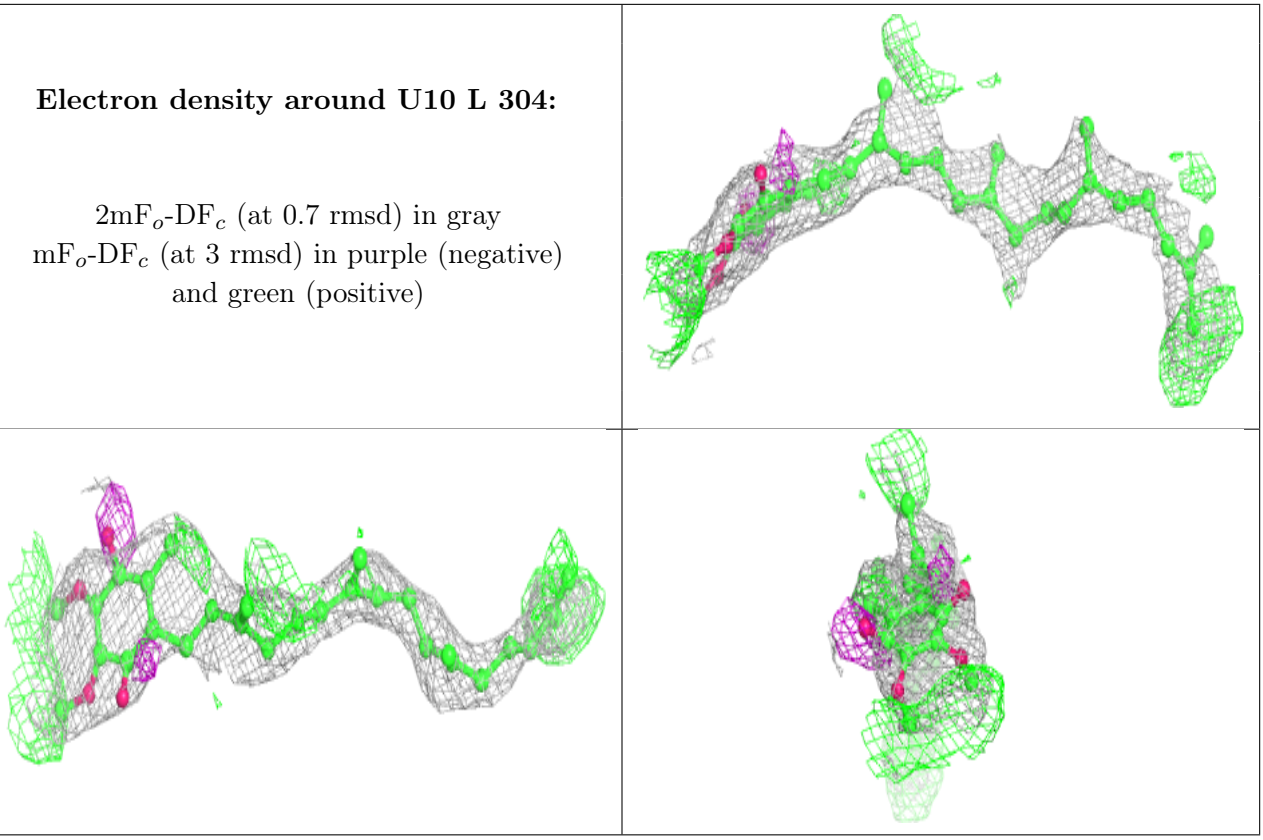
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	U10	L	304	33/63	0.75	0.35	64,85,99,101	0
8	SPO	M	406	42/42	0.87	0.28	64,87,114,116	0
6	U10	M	405	48/63	0.94	0.15	31,50,76,82	0
4	BCL	M	403	66/66	0.96	0.15	30,51,61,77	0
4	BCL	L	301	66/66	0.97	0.16	34,48,55,58	0
5	BPH	M	404	51/65	0.98	0.11	36,54,66,101	0
4	BCL	M	401	50/66	0.98	0.10	35,43,80,100	0
4	BCL	L	302	66/66	0.98	0.09	24,34,54,64	0
5	BPH	L	303	65/65	0.98	0.12	27,38,50,54	0
7	FE	M	402	1/1	1.00	0.07	41,41,41,41	0

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

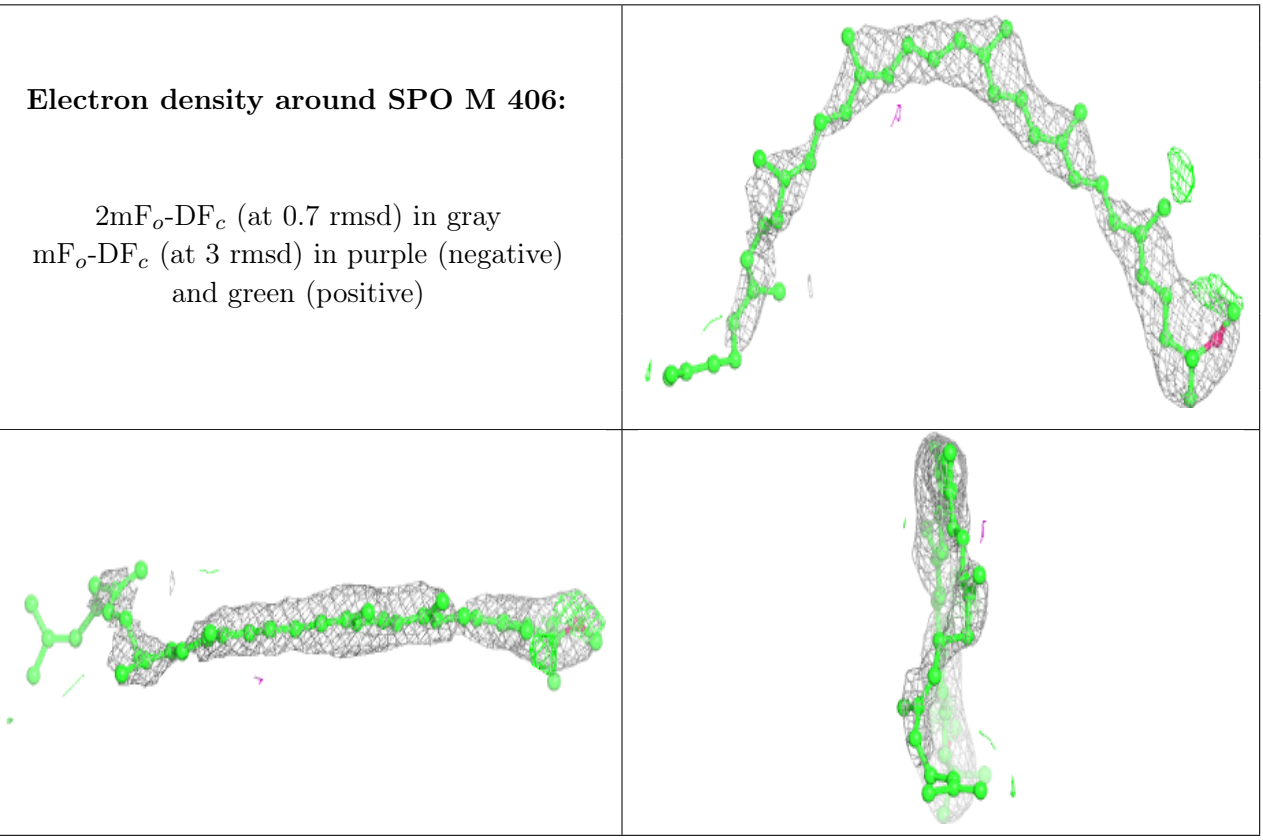
Electron density around U10 L 304:

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



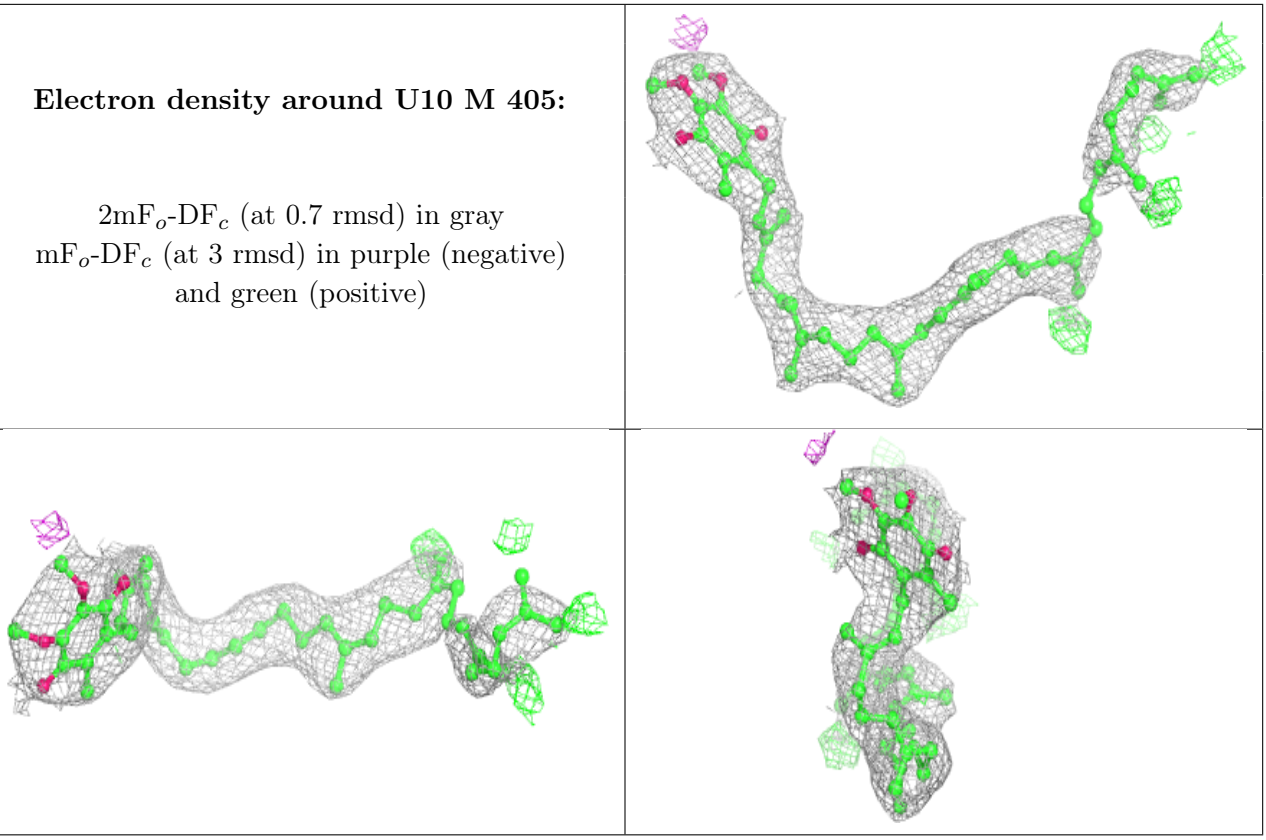
Electron density around SPO M 406:

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



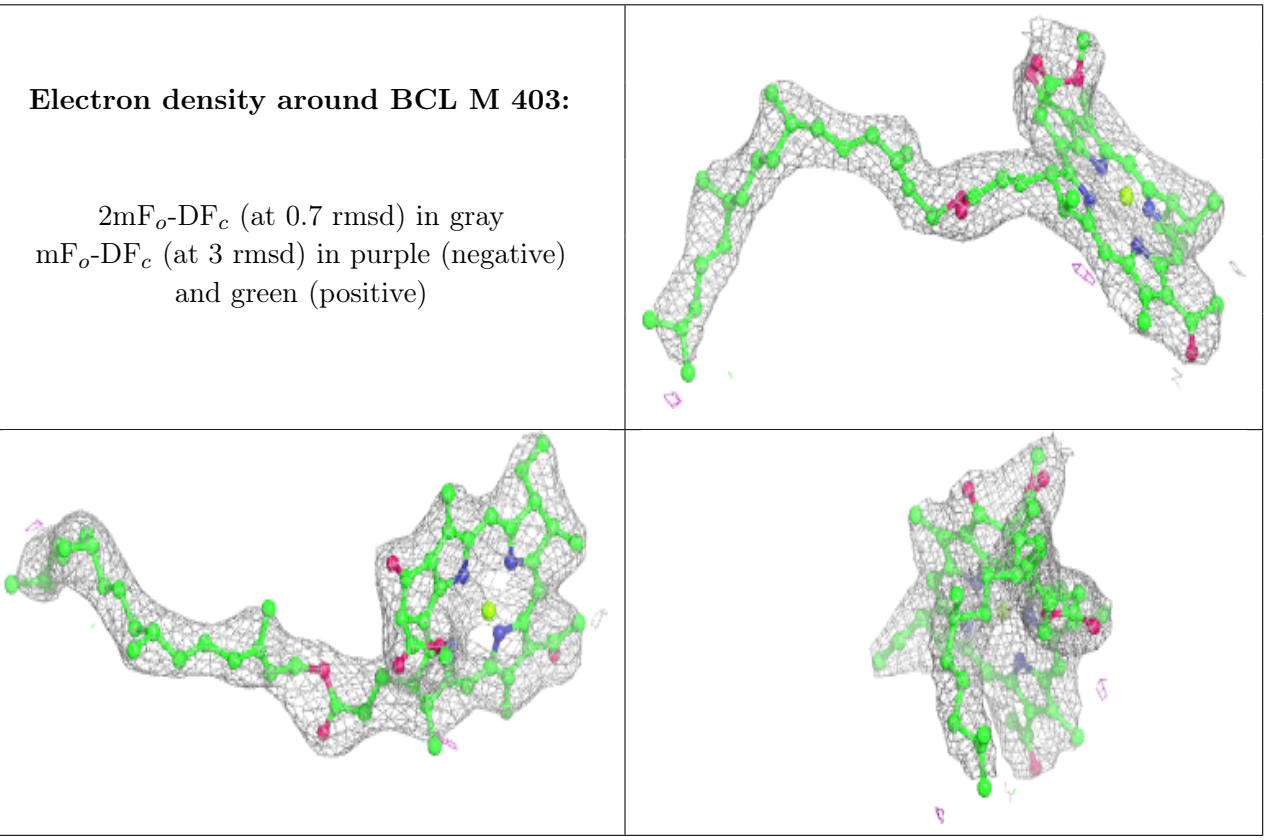
Electron density around U10 M 405:

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



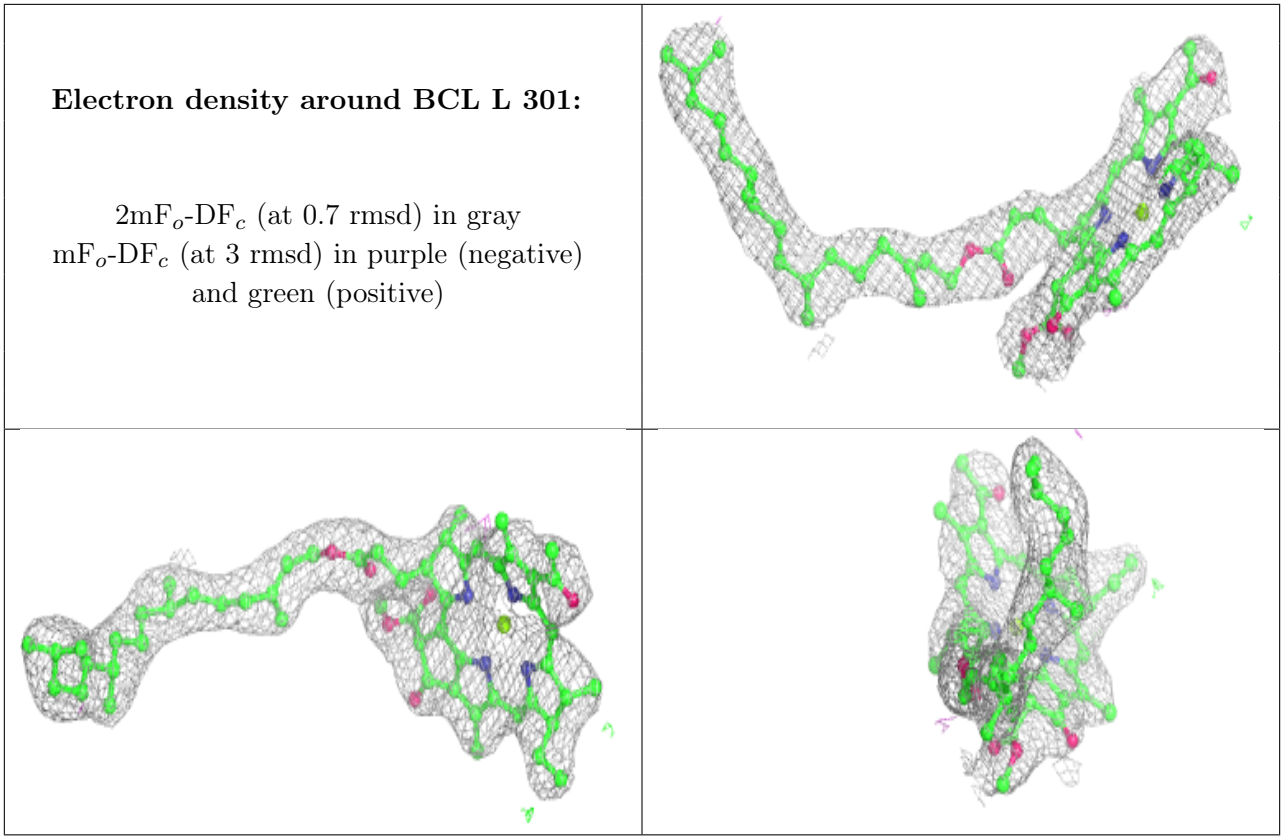
Electron density around BCL M 403:

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



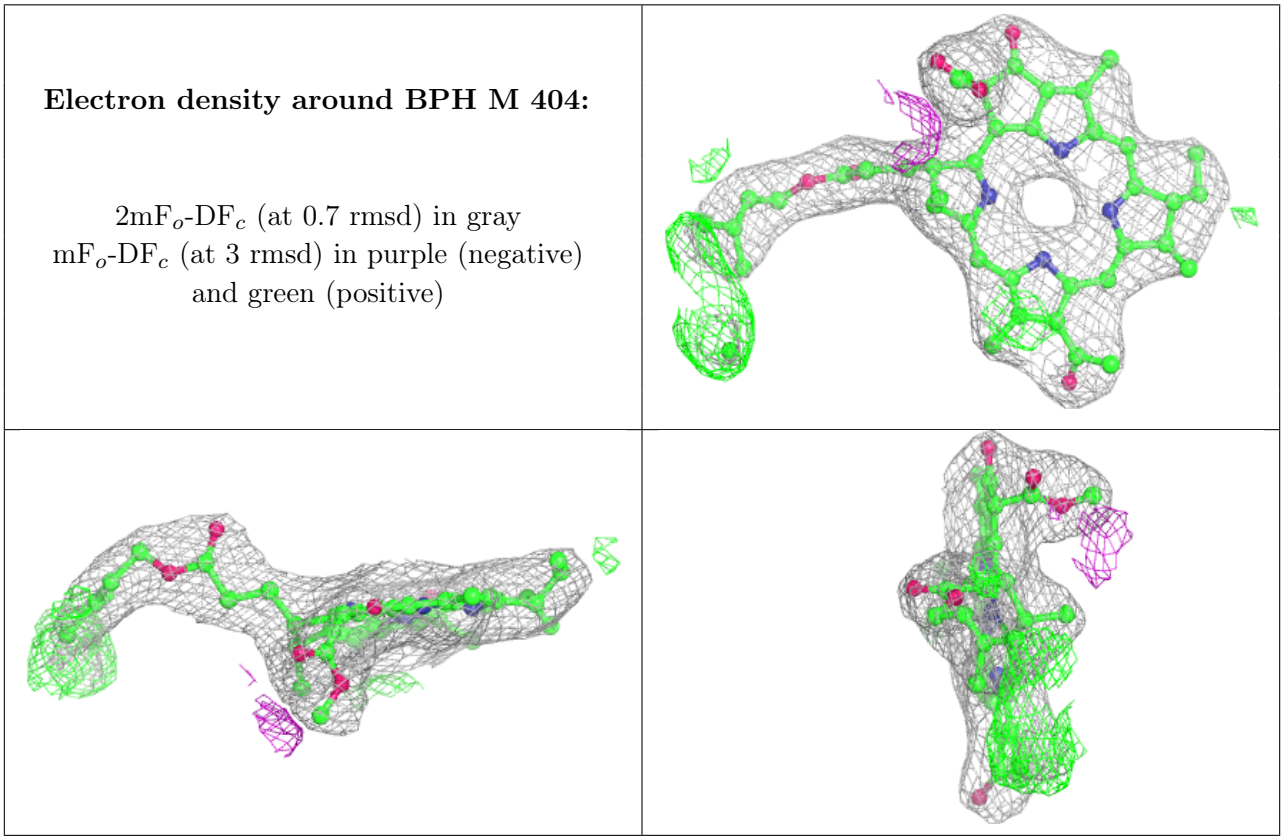
Electron density around BCL L 301:

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



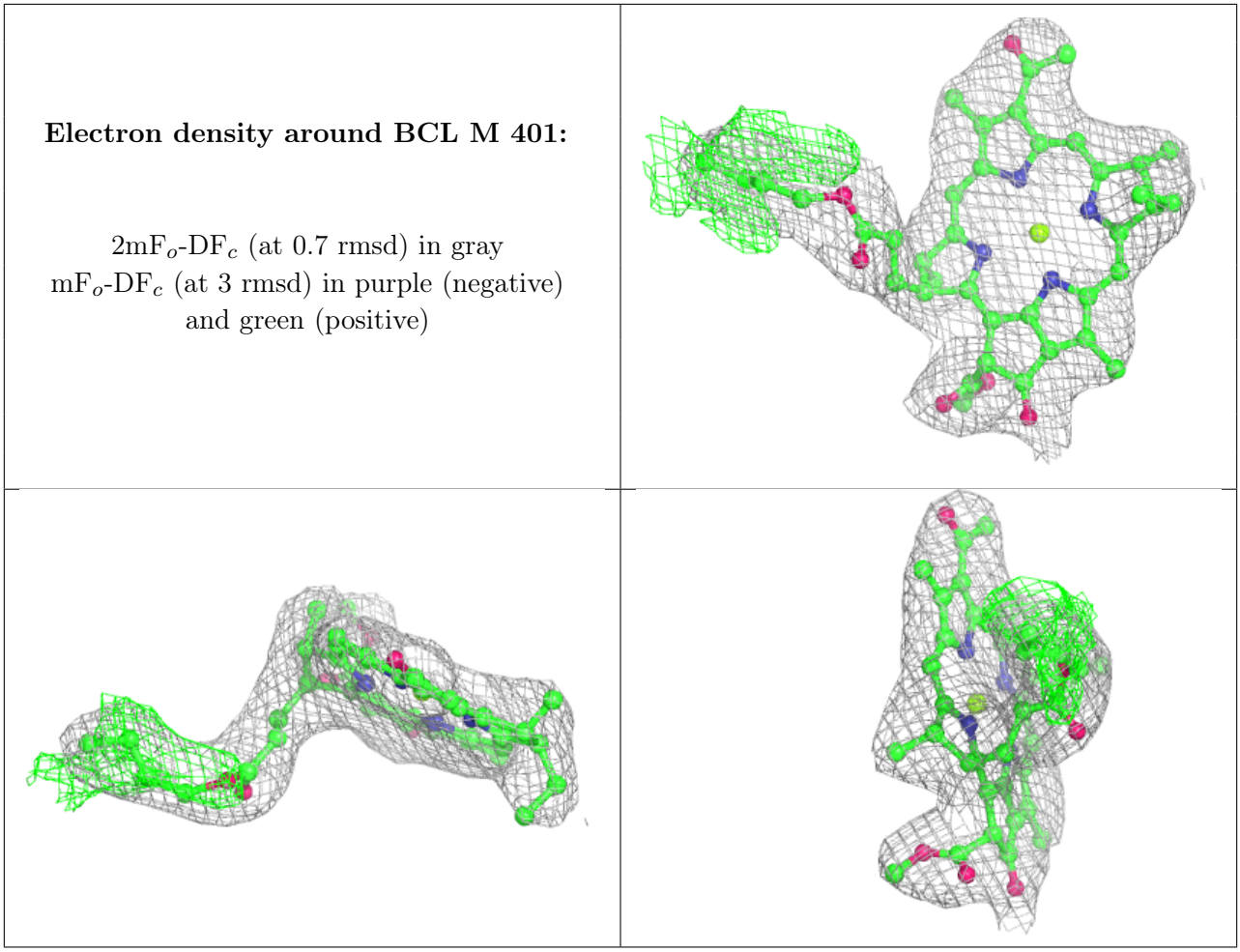
Electron density around BPH M 404:

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



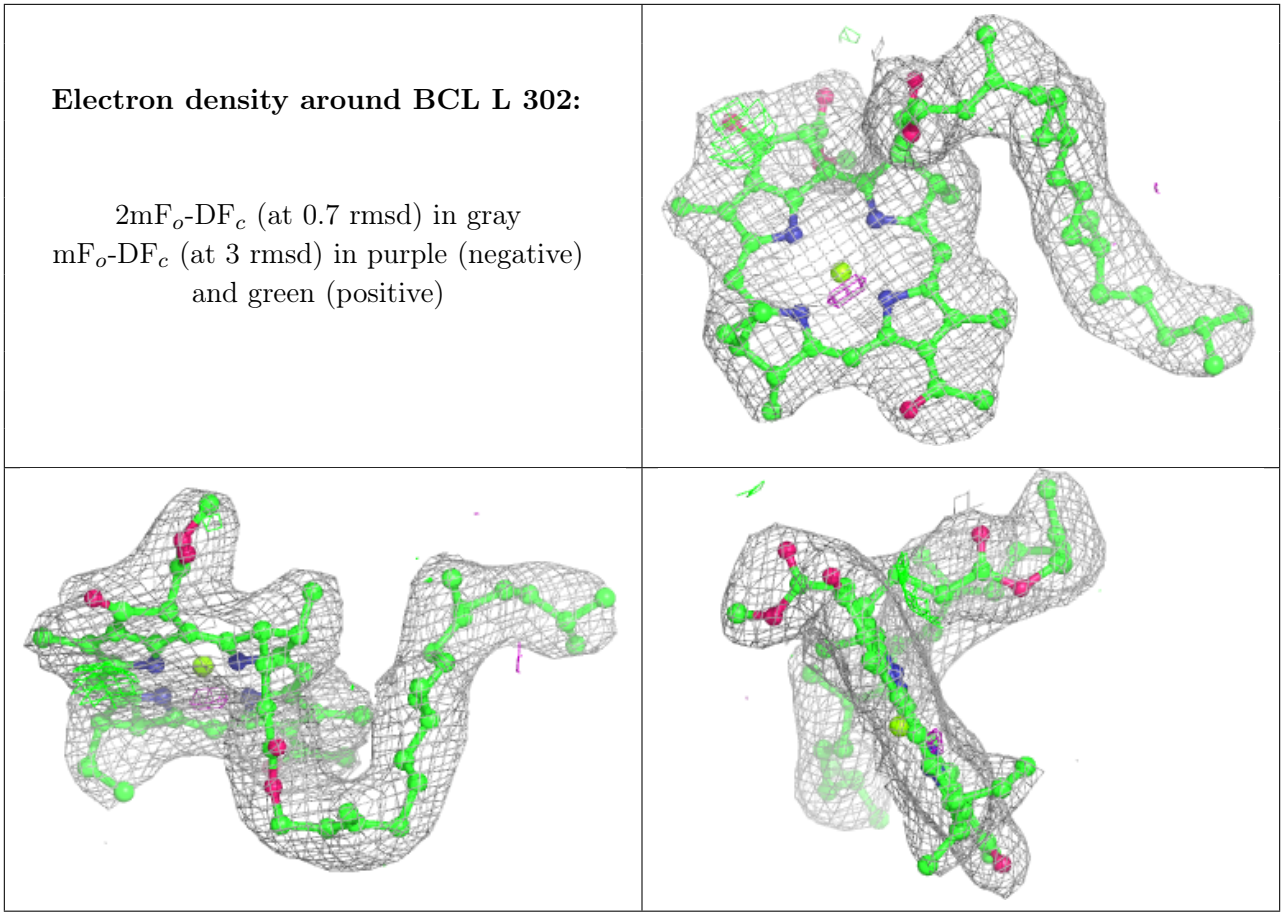
Electron density around BCL M 401:

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



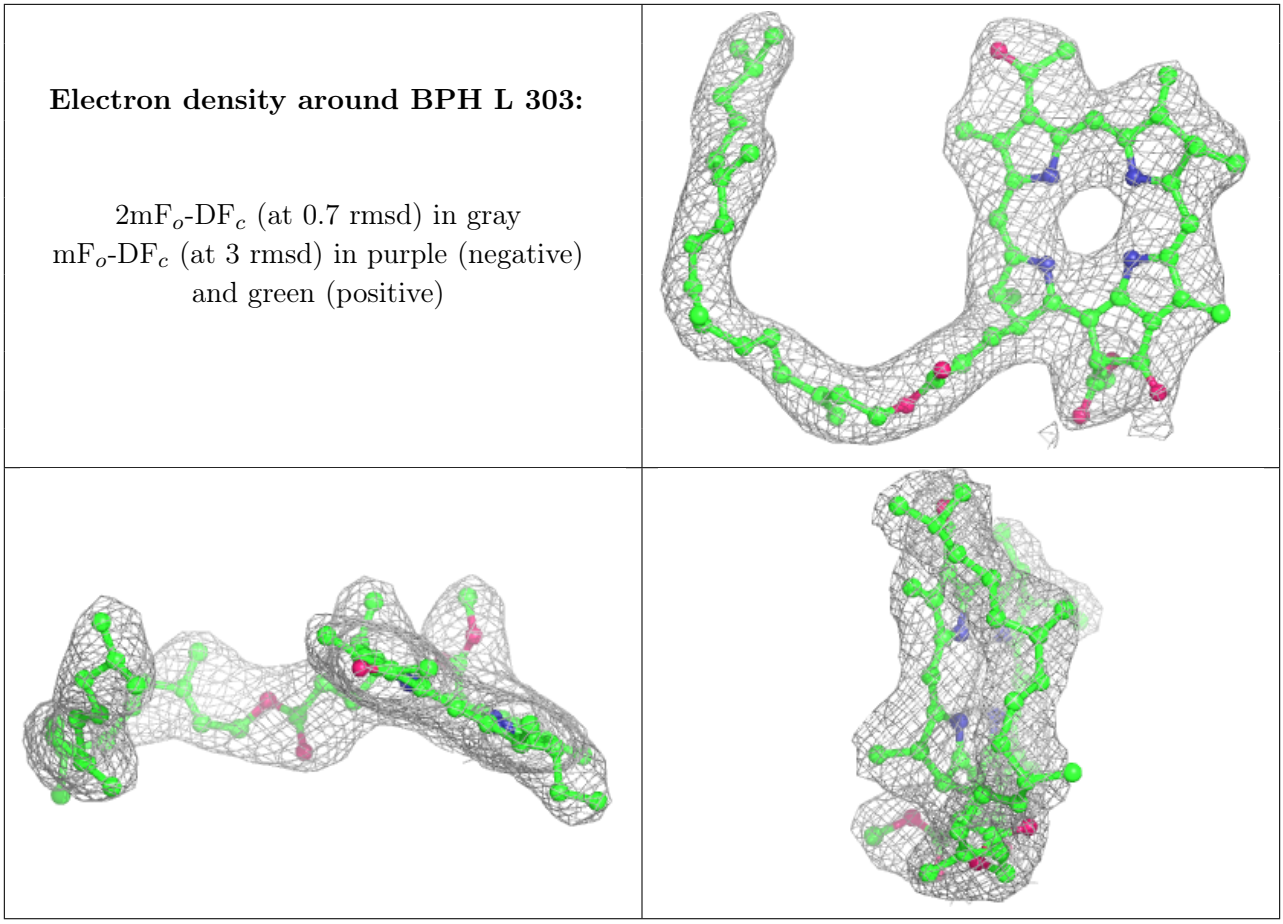
Electron density around BCL L 302:

$2mF_o$-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)



6.5 Other polymers (i)

There are no such residues in this entry.