



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:32 AM EDT

PDB ID : 4H9L / pdb_00004h9l
Title : Bacterial Photosynthetic Reaction Center from Rhodobacter sphaeroides with ILE M265 replaced with SER
Authors : Mattis, A.J.; Wraight, C.A.
Deposited on : 2012-09-24
Resolution : 2.77 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

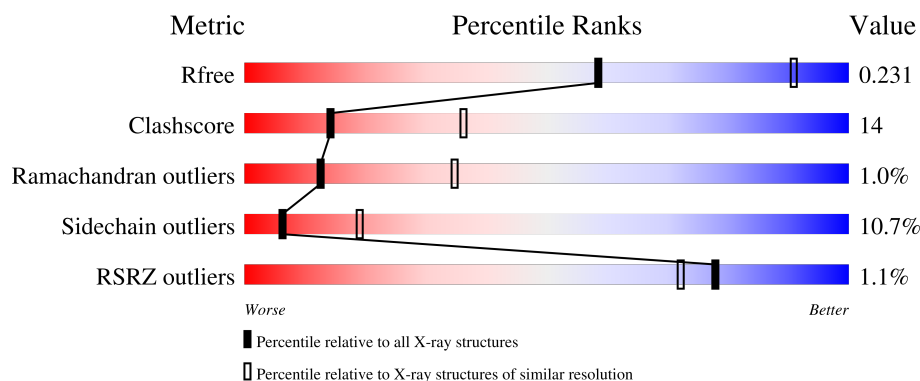
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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

Mol	Chain	Length	Quality of chain
1	L	281	 2% 62% 32% 5%
2	M	313	 67% 24% 5% 5%
3	H	260	 69% 17% 5% 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 6916 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	280	Total	C	N	O	S	0	0	0
			2195	1484	347	356	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	301	Total	C	N	O	S	0	0	0
			2375	1586	390	389	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	265	SER	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

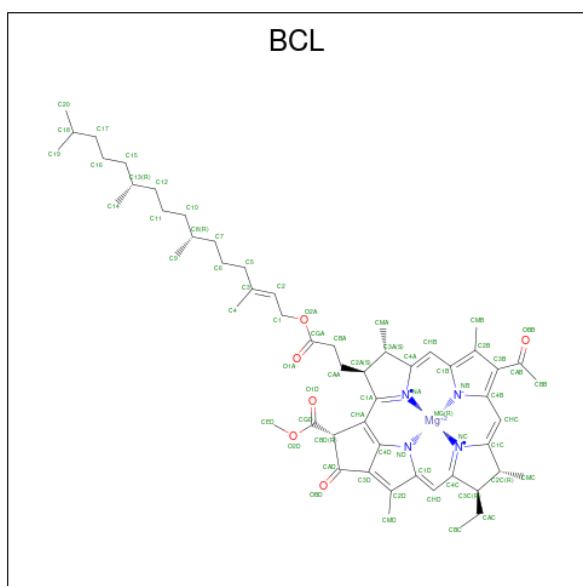
- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	238	Total	C	N	O	S	0	0	0
			1786	1143	303	331	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 (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



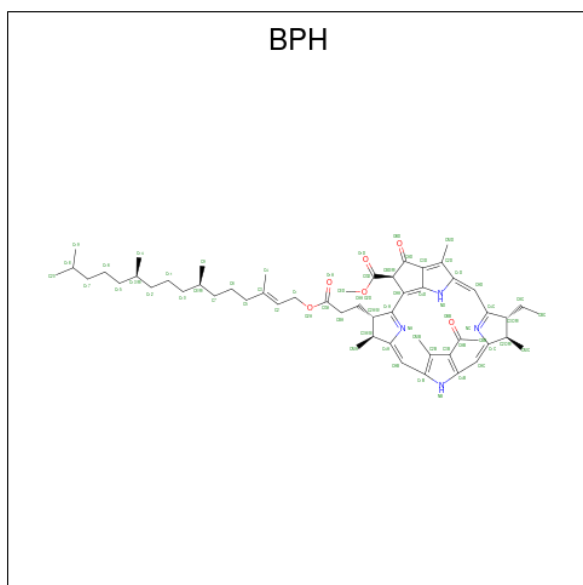
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

Continued on next page...

Continued from previous page...

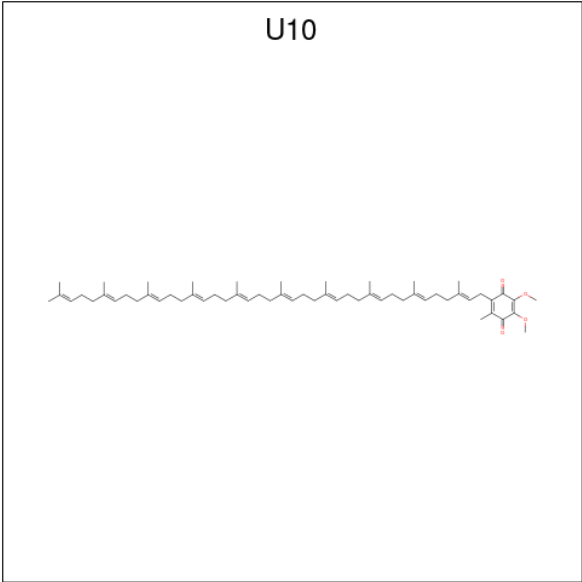
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	M	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: 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
			50	40	4	6		

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

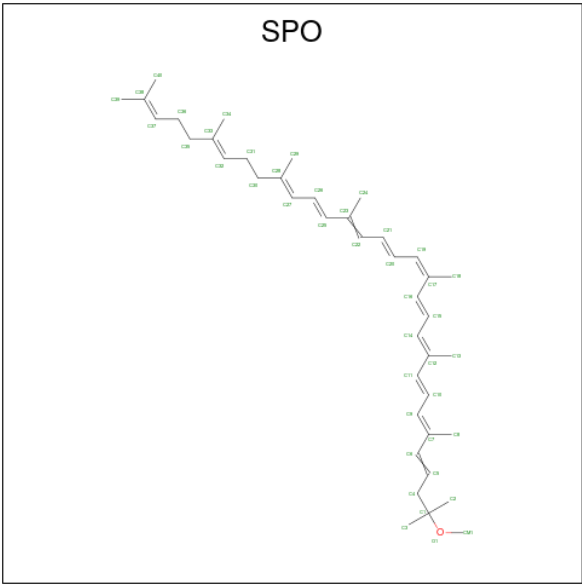


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			16	12	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 8 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			33	32	1		

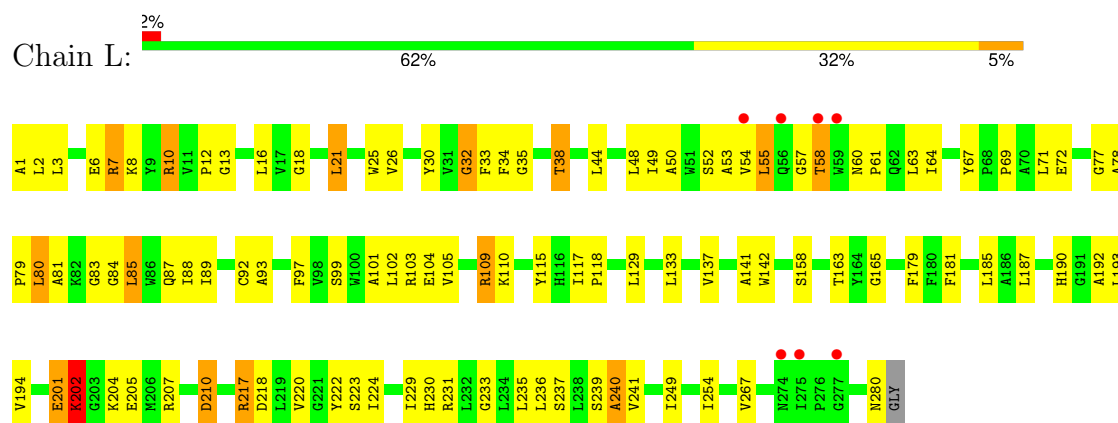
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	26	Total	O	0	0
			26	26		
9	M	30	Total	O	0	0
			30	30		
9	H	42	Total	O	0	0
			42	42		

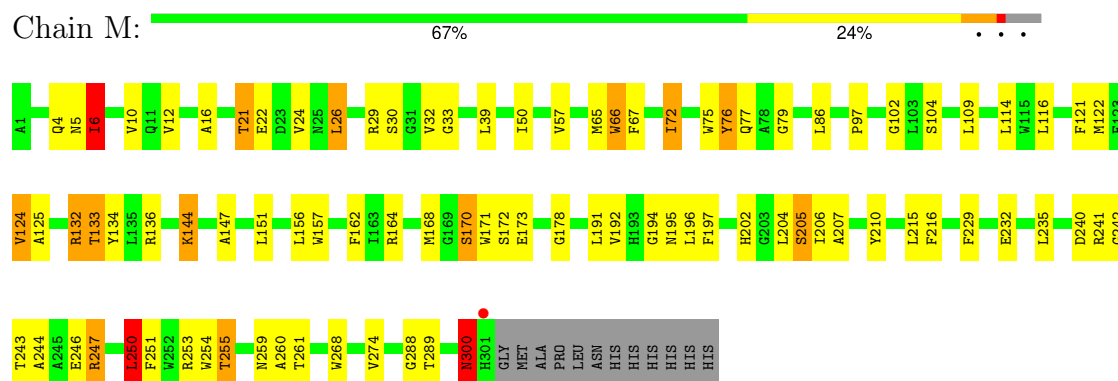
3 Residue-property plots

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

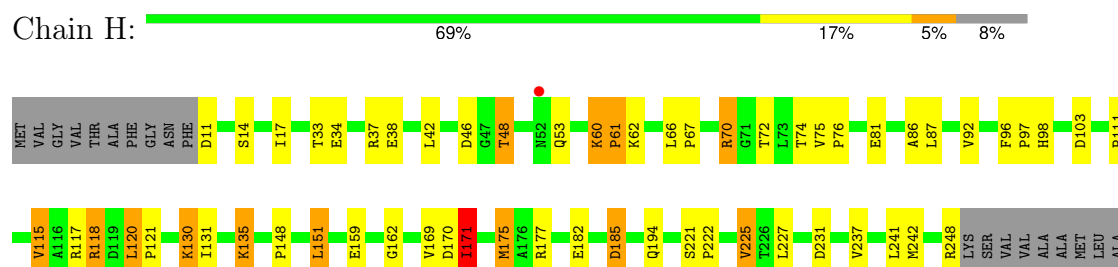
• Molecule 1: Reaction center protein L chain



• Molecule 2: Reaction center protein M chain



• Molecule 3: Reaction center protein H chain



GLU
TYR
ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.19Å 140.19Å 184.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 2.77 19.90 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.90-2.77) 99.5 (19.90-2.77)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109, PHENIX	Depositor
R, R_{free}	0.191 , 0.227 0.194 , 0.231	Depositor DCC
R_{free} test set	2682 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6916	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SPO, BPH, FE, BCL, 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	1.37	9/2281 (0.4%)	1.31	14/3125 (0.4%)
2	M	1.36	11/2466 (0.4%)	1.34	19/3369 (0.6%)
3	H	1.38	4/1834 (0.2%)	1.44	14/2504 (0.6%)
All	All	1.37	24/6581 (0.4%)	1.36	47/8998 (0.5%)

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

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	249	ILE	CA-CB	6.62	1.63	1.54
2	M	67	PHE	CA-C	6.59	1.61	1.52
2	M	72	ILE	CA-CB	6.55	1.62	1.54
2	M	67	PHE	N-CA	6.50	1.54	1.46
2	M	57	VAL	CA-CB	6.30	1.62	1.54
1	L	26	VAL	CA-CB	6.07	1.61	1.53
2	M	250	LEU	N-CA	-6.04	1.38	1.46
3	H	171	ILE	CA-CB	5.96	1.61	1.54
2	M	124	VAL	CA-CB	5.93	1.62	1.54
1	L	60	ASN	CA-C	5.81	1.57	1.52
2	M	21	THR	CA-C	-5.80	1.45	1.52
1	L	202	LYS	N-CA	5.74	1.53	1.46
1	L	165	GLY	C-O	5.72	1.31	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	103	ASP	CA-C	5.69	1.58	1.52
3	H	135	LYS	C-O	-5.63	1.16	1.24
2	M	125	ALA	CA-C	5.52	1.60	1.52
2	M	205	SER	N-CA	-5.47	1.39	1.46
1	L	202	LYS	CA-C	-5.13	1.45	1.52
1	L	54	VAL	CA-C	5.10	1.59	1.52
3	H	130	LYS	CA-C	-5.08	1.46	1.52
1	L	240	ALA	CA-CB	5.08	1.61	1.53
1	L	137	VAL	CA-CB	5.05	1.59	1.54
2	M	261	THR	N-CA	-5.03	1.39	1.45
2	M	50	ILE	C-O	-5.01	1.18	1.24

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	66	LEU	CA-C-N	-13.14	106.41	120.47
3	H	66	LEU	C-N-CA	-13.14	106.41	120.47
2	M	21	THR	CA-C-N	-9.81	102.81	121.54
2	M	21	THR	C-N-CA	-9.81	102.81	121.54
2	M	67	PHE	N-CA-C	8.55	121.74	111.82
1	L	201	GLU	N-CA-C	8.11	121.14	111.33
1	L	58	THR	N-CA-C	8.03	122.10	109.81
3	H	81	GLU	N-CA-C	-7.71	99.06	110.23
3	H	225	VAL	CB-CA-C	-7.64	98.73	110.50
2	M	66	TRP	CA-C-N	7.36	131.49	120.31
2	M	66	TRP	C-N-CA	7.36	131.49	120.31
2	M	289	THR	N-CA-C	-7.13	104.71	113.41
3	H	67	PRO	CA-C-N	-7.06	108.06	121.54
3	H	67	PRO	C-N-CA	-7.06	108.06	121.54
1	L	230	HIS	N-CA-C	-6.93	103.82	112.90
3	H	81	GLU	CA-C-N	-6.73	108.69	121.54
3	H	81	GLU	C-N-CA	-6.73	108.69	121.54
3	H	222	PRO	CA-C-N	-6.49	112.38	122.37
3	H	222	PRO	C-N-CA	-6.49	112.38	122.37
2	M	172	SER	N-CA-C	-6.22	105.17	112.89
1	L	236	LEU	N-CA-C	-6.18	103.86	111.40
1	L	57	GLY	N-CA-C	6.00	123.41	114.95
2	M	22	GLU	CB-CA-C	5.87	122.10	110.42
1	L	33	PHE	N-CA-C	-5.86	104.08	111.11
2	M	21	THR	N-CA-C	-5.83	98.91	108.41
1	L	192	ALA	N-CA-C	-5.81	104.91	112.23
3	H	60	LYS	CA-C-N	5.76	127.04	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	60	LYS	C-N-CA	5.76	127.04	119.84
2	M	6	ILE	CG1-CB-CG2	-5.68	93.67	110.70
1	L	141	ALA	N-CA-C	5.67	117.74	108.55
2	M	72	ILE	N-CA-CB	5.66	118.24	110.54
2	M	178	GLY	N-CA-C	-5.62	102.54	110.91
2	M	144	LYS	CD-CE-NZ	-5.60	93.97	111.90
2	M	10	VAL	CB-CA-C	-5.57	102.20	110.33
2	M	170	SER	N-CA-C	5.47	117.40	108.76
2	M	255	THR	N-CA-C	5.42	116.87	110.97
1	L	55	LEU	N-CA-C	5.36	117.88	111.71
1	L	7	ARG	CA-CB-CG	-5.34	103.42	114.10
2	M	207	ALA	N-CA-C	-5.20	105.69	111.36
1	L	239	SER	N-CA-C	-5.11	105.62	111.14
2	M	132	ARG	NE-CZ-NH1	-5.11	116.39	121.50
3	H	185	ASP	N-CA-C	5.10	121.66	110.80
3	H	131	ILE	N-CA-C	5.07	115.15	107.75
1	L	54	VAL	N-CA-C	5.03	116.35	110.62
2	M	4	GLN	N-CA-C	5.01	121.13	113.61
1	L	249	ILE	N-CA-C	-5.01	104.83	111.09
1	L	71	LEU	N-CA-C	5.00	118.15	111.75

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	32	GLY	Peptide
2	M	300	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2195	0	2125	67	0
2	M	2375	0	2270	67	0
3	H	1786	0	1747	43	0
4	L	132	0	148	10	0
4	M	117	0	115	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	65	0	76	8	0
5	M	50	0	43	5	0
6	L	16	0	12	8	0
6	M	48	0	63	7	0
7	M	1	0	0	0	0
8	M	33	0	43	6	0
9	H	42	0	0	1	0
9	L	26	0	0	1	0
9	M	30	0	0	1	0
All	All	6916	0	6642	191	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 14.

All (191) 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)
2:M:197:PHE:CZ	4:M:403:BCL:HBB2	1.94	1.03
1:L:38:THR:HG22	1:L:99:SER:CB	1.89	1.02
1:L:49:ILE:HG13	1:L:89:ILE:HD13	1.41	1.02
1:L:38:THR:HG22	1:L:99:SER:HB2	1.06	1.02
2:M:197:PHE:HZ	4:M:403:BCL:HBB2	1.24	1.02
1:L:7:ARG:HH11	3:H:98:HIS:CD2	1.77	1.01
6:M:405:U10:H322	6:M:405:U10:H272	1.42	1.00
5:M:404:BPH:HHC	5:M:404:BPH:HBB3	1.45	0.98
5:L:303:BPH:HBB3	5:L:303:BPH:HHC	1.51	0.90
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.53	0.90
2:M:164:ARG:HH12	2:M:173:GLU:HG3	1.41	0.86
4:M:403:BCL:HBB3	4:M:403:BCL:HHC	1.59	0.84
2:M:242:GLY:CA	3:H:117:ARG:HD2	2.07	0.84
1:L:12:PRO:O	3:H:242:MET:HE1	1.78	0.84
1:L:7:ARG:HH11	3:H:98:HIS:HD2	1.26	0.83
2:M:197:PHE:HZ	4:M:403:BCL:CBB	1.90	0.83
4:M:403:BCL:HHC	4:M:403:BCL:CBB	2.08	0.83
2:M:242:GLY:HA2	3:H:117:ARG:HD2	1.63	0.78
6:M:405:U10:H272	6:M:405:U10:C32	2.13	0.78
6:L:304:U10:C8	6:L:304:U10:C1M	2.61	0.78
4:M:401:BCL:CBB	8:M:406:SPO:H243	2.13	0.78
5:M:404:BPH:HHC	5:M:404:BPH:CBB	2.13	0.78
1:L:38:THR:CG2	1:L:99:SER:HB2	2.02	0.78
2:M:32:VAL:HG12	2:M:33:GLY:O	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:303:BPH:HBB2	2:M:210:TYR:HB3	1.69	0.74
1:L:34:PHE:O	1:L:38:THR:HG23	1.86	0.74
1:L:201:GLU:O	1:L:202:LYS:CB	2.34	0.74
4:M:401:BCL:HBB2	8:M:406:SPO:H243	1.69	0.74
3:H:70:ARG:NH2	3:H:121:PRO:O	2.21	0.73
5:L:303:BPH:HHC	5:L:303:BPH:CBB	2.19	0.72
2:M:133:THR:HG22	2:M:147:ALA:HB2	1.73	0.71
4:L:302:BCL:HMB3	4:L:302:BCL:HBB2	1.73	0.71
2:M:164:ARG:HH12	2:M:173:GLU:CG	2.03	0.70
1:L:231:ARG:HD3	2:M:5:ASN:O	1.90	0.70
1:L:218:ASP:OD1	2:M:29:ARG:HD3	1.92	0.69
2:M:240:ASP:O	3:H:117:ARG:NH1	2.24	0.69
2:M:133:THR:HG21	2:M:147:ALA:HA	1.76	0.68
1:L:49:ILE:HG13	1:L:89:ILE:CD1	2.19	0.67
3:H:148:PRO:HA	3:H:151:LEU:HD22	1.76	0.66
1:L:181:PHE:HB3	5:M:404:BPH:HBB2	1.79	0.65
2:M:66:TRP:CZ2	2:M:122:MET:HE3	2.33	0.64
4:M:401:BCL:CBB	4:M:401:BCL:HHC	2.27	0.64
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.79	0.63
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.80	0.63
1:L:7:ARG:NH1	3:H:98:HIS:HD2	1.96	0.63
2:M:132:ARG:HH11	2:M:132:ARG:HG2	1.63	0.63
6:L:304:U10:C8	6:L:304:U10:H1M1	2.27	0.63
1:L:69:PRO:CG	1:L:142:TRP:HB2	2.30	0.61
1:L:79:PRO:O	1:L:80:LEU:C	2.44	0.61
3:H:96:PHE:HB3	3:H:97:PRO:CD	2.31	0.61
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.69	0.61
2:M:164:ARG:NH1	2:M:173:GLU:CG	2.64	0.60
1:L:69:PRO:HD3	1:L:83:GLY:O	2.00	0.60
2:M:197:PHE:CE1	4:M:403:BCL:HBB2	2.35	0.60
2:M:164:ARG:NH1	2:M:173:GLU:HG3	2.14	0.60
2:M:133:THR:CG2	2:M:147:ALA:HA	2.32	0.60
1:L:85:LEU:O	1:L:89:ILE:HG13	2.03	0.59
4:M:401:BCL:HBB1	8:M:406:SPO:H243	1.83	0.59
2:M:134:TYR:CE2	2:M:144:LYS:HG2	2.37	0.59
2:M:300:ASN:N	2:M:300:ASN:OD1	2.36	0.58
2:M:76:TYR:C	2:M:76:TYR:CD1	2.82	0.58
1:L:103:ARG:NH2	2:M:255:THR:O	2.35	0.58
2:M:242:GLY:HA3	3:H:117:ARG:HD2	1.87	0.57
4:L:302:BCL:HMB3	4:L:302:BCL:CBB	2.35	0.56
4:M:401:BCL:HHC	4:M:401:BCL:HBB3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:251:PHE:CD1	2:M:251:PHE:C	2.84	0.56
1:L:210:ASP:N	1:L:210:ASP:OD1	2.39	0.56
3:H:96:PHE:HB3	3:H:97:PRO:HD2	1.88	0.56
1:L:224:ILE:H	6:L:304:U10:H72	1.71	0.56
1:L:280:ASN:C	9:L:421:HOH:O	2.49	0.56
1:L:187:LEU:HD13	2:M:216:PHE:CG	2.41	0.55
3:H:70:ARG:O	3:H:118:ARG:NH2	2.40	0.55
1:L:48:LEU:CD1	1:L:88:ILE:HG22	2.37	0.55
3:H:98:HIS:HE1	9:H:325:HOH:O	1.90	0.55
1:L:7:ARG:HD2	3:H:98:HIS:CD2	2.42	0.54
2:M:16:ALA:HB1	2:M:32:VAL:HG21	1.88	0.54
4:M:403:BCL:H11	5:M:404:BPH:HBB3	1.90	0.54
6:L:304:U10:C8	6:L:304:U10:H1M2	2.38	0.53
3:H:37:ARG:O	3:H:38:GLU:HG2	2.09	0.53
2:M:232:GLU:OE1	2:M:232:GLU:N	2.36	0.53
3:H:170:ASP:HB2	3:H:177:ARG:HD2	1.91	0.53
2:M:232:GLU:OE2	3:H:177:ARG:NH2	2.42	0.53
4:M:403:BCL:HBB3	4:M:403:BCL:CHC	2.35	0.52
1:L:52:SER:HB2	1:L:85:LEU:HD13	1.91	0.52
4:M:403:BCL:H11	5:M:404:BPH:CBB	2.39	0.52
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.28	0.52
2:M:194:GLY:O	2:M:195:ASN:HB3	2.08	0.52
4:M:403:BCL:HAA2	4:M:403:BCL:HBD	1.90	0.52
1:L:8:LYS:HA	3:H:87:LEU:HD11	1.92	0.52
2:M:136:ARG:NE	2:M:136:ARG:HA	2.25	0.51
1:L:55:LEU:HD13	1:L:81:ALA:HB2	1.91	0.51
4:M:401:BCL:HBB3	4:M:403:BCL:H41	1.91	0.51
2:M:241:ARG:HD3	2:M:246:GLU:HG2	1.91	0.51
3:H:70:ARG:NH2	3:H:120:LEU:HB3	2.25	0.51
1:L:3:LEU:HD12	2:M:250:LEU:HD13	1.92	0.51
2:M:133:THR:HG22	2:M:147:ALA:CB	2.40	0.50
3:H:175:MET:HE1	3:H:177:ARG:NH2	2.26	0.50
1:L:50:ALA:O	1:L:53:ALA:HB3	2.12	0.50
3:H:117:ARG:NH2	3:H:227:LEU:HD22	2.27	0.50
1:L:18:GLY:O	1:L:21:LEU:HB2	2.12	0.50
2:M:24:VAL:HG11	2:M:29:ARG:NH1	2.27	0.50
3:H:241:LEU:O	3:H:248:ARG:NH2	2.45	0.49
4:L:302:BCL:H191	5:L:303:BPH:H6C1	1.95	0.49
3:H:62:LYS:O	3:H:74:THR:HA	2.12	0.49
2:M:102:GLY:HA2	2:M:170:SER:HB2	1.95	0.49
3:H:75:VAL:HA	3:H:76:PRO:C	2.36	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:130:LYS:HZ2	3:H:170:ASP:CG	2.20	0.49
4:L:302:BCL:H193	5:L:303:BPH:H112	1.95	0.49
3:H:37:ARG:NH2	3:H:60:LYS:O	2.46	0.49
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.47	0.49
2:M:268:TRP:CD1	6:M:405:U10:H111	2.47	0.49
1:L:179:PHE:HB3	1:L:240:ALA:HB2	1.94	0.48
3:H:14:SER:HA	3:H:17:ILE:HG22	1.94	0.48
2:M:164:ARG:NH1	2:M:173:GLU:HG2	2.28	0.48
3:H:175:MET:CE	3:H:177:ARG:NH2	2.76	0.48
1:L:101:ALA:O	1:L:104:GLU:N	2.46	0.48
1:L:6:GLU:OE2	1:L:10:ARG:HD2	2.13	0.48
2:M:260:ALA:O	6:M:405:U10:H4M3	2.14	0.48
1:L:105:VAL:O	1:L:109:ARG:HG3	2.13	0.47
6:M:405:U10:H322	6:M:405:U10:C27	2.23	0.47
6:L:304:U10:H3M3	6:L:304:U10:H4M3	1.96	0.47
2:M:132:ARG:HG2	2:M:132:ARG:NH1	2.26	0.47
1:L:115:TYR:O	1:L:118:PRO:HG2	2.15	0.47
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.96	0.47
1:L:193:LEU:HD23	6:L:304:U10:H3M3	1.97	0.46
5:L:303:BPH:HBB1	2:M:210:TYR:CD2	2.50	0.46
3:H:46:ASP:OD1	3:H:48:THR:OG1	2.33	0.46
1:L:222:TYR:CG	1:L:223:SER:N	2.83	0.46
4:L:301:BCL:HBB2	4:M:403:BCL:NA	2.31	0.46
2:M:205:SER:OG	4:M:403:BCL:HMA3	2.16	0.46
2:M:76:TYR:O	2:M:79:GLY:N	2.32	0.45
2:M:133:THR:CG2	2:M:147:ALA:CA	2.94	0.45
2:M:157:TRP:CD1	8:M:406:SPO:H26	2.51	0.45
2:M:253:ARG:HB2	2:M:259:ASN:OD1	2.16	0.45
2:M:247:ARG:NH2	3:H:111:PRO:O	2.47	0.45
4:L:301:BCL:HMB3	4:L:301:BCL:CBB	2.47	0.44
2:M:260:ALA:C	6:M:405:U10:H4M3	2.42	0.44
3:H:148:PRO:O	3:H:151:LEU:HB2	2.16	0.44
2:M:157:TRP:NE1	8:M:406:SPO:H26	2.33	0.44
1:L:77:GLY:HA2	1:L:87:GLN:OE1	2.18	0.44
1:L:193:LEU:O	1:L:194:VAL:C	2.59	0.44
1:L:241:VAL:HG21	5:L:303:BPH:H2C	1.98	0.44
3:H:42:LEU:N	3:H:53:GLN:OE1	2.51	0.44
1:L:78:ALA:O	1:L:79:PRO:C	2.61	0.44
3:H:60:LYS:HA	3:H:61:PRO:HD2	1.71	0.44
3:H:148:PRO:HA	3:H:151:LEU:CD2	2.46	0.44
4:L:301:BCL:H202	4:L:301:BCL:H161	1.85	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:52:SER:HB2	1:L:85:LEU:CD1	2.48	0.43
1:L:1:ALA:C	1:L:2:LEU:HD23	2.43	0.43
9:M:504:HOH:O	3:H:175:MET:HE1	2.17	0.43
1:L:84:GLY:HA2	1:L:87:GLN:HG3	2.00	0.43
1:L:217:ARG:O	1:L:218:ASP:C	2.60	0.43
3:H:34:GLU:CD	3:H:37:ARG:HH11	2.27	0.43
1:L:117:ILE:HB	1:L:118:PRO:CD	2.48	0.43
2:M:243:THR:N	3:H:115:VAL:HG13	2.34	0.43
1:L:163:THR:HG22	1:L:163:THR:O	2.19	0.43
4:L:302:BCL:CBB	4:L:302:BCL:CMB	2.97	0.43
1:L:6:GLU:OE2	1:L:10:ARG:NH1	2.43	0.42
1:L:30:TYR:O	1:L:103:ARG:NH1	2.52	0.42
1:L:101:ALA:O	1:L:104:GLU:HB2	2.19	0.42
6:L:304:U10:H1M2	6:L:304:U10:H8	2.00	0.42
3:H:162:GLY:HA3	3:H:182:GLU:O	2.19	0.42
3:H:194:GLN:H	3:H:194:GLN:CD	2.28	0.42
3:H:151:LEU:HD12	3:H:151:LEU:HA	1.80	0.42
1:L:30:TYR:HB2	2:M:254:TRP:HB3	2.01	0.42
2:M:133:THR:CG2	2:M:147:ALA:HB2	2.47	0.42
3:H:33:THR:O	3:H:34:GLU:C	2.60	0.42
1:L:97:PHE:CE1	4:L:301:BCL:H121	2.54	0.42
4:M:403:BCL:HBC2	4:M:403:BCL:H2C	1.82	0.42
1:L:13:GLY:O	1:L:110:LYS:NZ	2.46	0.41
1:L:93:ALA:HA	5:L:303:BPH:H9C2	2.02	0.41
2:M:21:THR:HG23	2:M:26:LEU:CD1	2.47	0.41
2:M:114:LEU:HD23	2:M:114:LEU:HA	1.87	0.41
4:M:403:BCL:HBB2	4:M:403:BCL:HHC	1.98	0.41
2:M:168:MET:SD	2:M:288:GLY:O	2.79	0.41
1:L:25:TRP:CD1	1:L:30:TYR:HA	2.56	0.41
1:L:83:GLY:O	1:L:87:GLN:HG3	2.20	0.41
2:M:76:TYR:C	2:M:76:TYR:HD1	2.26	0.41
2:M:162:PHE:HB2	8:M:406:SPO:C31	2.50	0.41
2:M:65:MET:HB3	2:M:121:PHE:CE2	2.56	0.41
6:M:405:U10:C32	6:M:405:U10:C27	2.90	0.41
1:L:32:GLY:CA	1:L:35:GLY:H	2.33	0.41
4:L:301:BCL:CGA	4:L:302:BCL:HBC1	2.51	0.41
1:L:44:LEU:HD23	1:L:92:CYS:SG	2.60	0.41
1:L:61:PRO:HA	1:L:64:ILE:HD12	2.03	0.41
1:L:231:ARG:CD	2:M:5:ASN:O	2.65	0.41
1:L:231:ARG:HD2	2:M:6:ILE:O	2.21	0.41
3:H:169:VAL:HG23	3:H:171:ILE:CD1	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:190:HIS:HD1	6:L:304:U10:H3M1	1.85	0.40
1:L:233:GLY:HA3	2:M:216:PHE:CE1	2.56	0.40
2:M:197:PHE:CZ	4:M:403:BCL:CBB	2.75	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	278/281 (99%)	244 (88%)	32 (12%)	2 (1%)	18	44
2	M	299/313 (96%)	276 (92%)	21 (7%)	2 (1%)	18	44
3	H	236/260 (91%)	220 (93%)	12 (5%)	4 (2%)	7	22
All	All	813/854 (95%)	740 (91%)	65 (8%)	8 (1%)	12	35

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	202	LYS
2	M	77	GLN
1	L	80	LEU
2	M	30	SER
3	H	61	PRO
3	H	135	LYS
3	H	185	ASP
3	H	86	ALA

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	213/220 (97%)	187 (88%)	26 (12%)	5	14
2	M	228/246 (93%)	203 (89%)	25 (11%)	6	18
3	H	184/208 (88%)	168 (91%)	16 (9%)	9	27
All	All	625/674 (93%)	558 (89%)	67 (11%)	6	19

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	10	ARG
1	L	16	LEU
1	L	21	LEU
1	L	38	THR
1	L	58	THR
1	L	63	LEU
1	L	67	TYR
1	L	72	GLU
1	L	85	LEU
1	L	102	LEU
1	L	109	ARG
1	L	129	LEU
1	L	133	LEU
1	L	158	SER
1	L	185	LEU
1	L	204	LYS
1	L	205	GLU
1	L	207	ARG
1	L	210	ASP
1	L	217	ARG
1	L	220	VAL
1	L	229	ILE
1	L	235	LEU
1	L	237	SER
1	L	254	ILE
1	L	267	VAL
2	M	6	ILE
2	M	12	VAL
2	M	26	LEU
2	M	39	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	72	ILE
2	M	75	TRP
2	M	76	TYR
2	M	86	LEU
2	M	104	SER
2	M	109	LEU
2	M	116	LEU
2	M	124	VAL
2	M	133	THR
2	M	151	LEU
2	M	156	LEU
2	M	191	LEU
2	M	192	VAL
2	M	196	LEU
2	M	204	LEU
2	M	215	LEU
2	M	235	LEU
2	M	247	ARG
2	M	250	LEU
2	M	274	VAL
2	M	300	ASN
3	H	11	ASP
3	H	48	THR
3	H	70	ARG
3	H	72	THR
3	H	92	VAL
3	H	115	VAL
3	H	118	ARG
3	H	120	LEU
3	H	151	LEU
3	H	159	GLU
3	H	171	ILE
3	H	175	MET
3	H	221	SER
3	H	225	VAL
3	H	231	ASP
3	H	237	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	258	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	280	ASN
2	M	4	GLN
3	H	32	GLN
3	H	44	ASN
3	H	98	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
6	U10	L	304	-	16,16,63	1.91	7 (43%)	21,22,79	3.24	11 (52%)
4	BCL	M	403	2	69,74,74	1.19	5 (7%)	79,115,115	1.95	20 (25%)
8	SPO	M	406	-	32,32,41	1.28	3 (9%)	35,39,50	2.57	12 (34%)
5	BPH	M	404	-	44,55,70	2.02	10 (22%)	41,83,101	2.99	16 (39%)
5	BPH	L	303	-	59,70,70	1.67	4 (6%)	59,101,101	2.12	14 (23%)
6	U10	M	405	-	48,48,63	3.05	12 (25%)	60,61,79	1.78	12 (20%)
4	BCL	L	301	1	69,74,74	1.29	6 (8%)	79,115,115	1.90	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BCL	M	401	2	54,59,74	1.55	7 (12%)	61,97,115	2.48	15 (24%)
4	BCL	L	302	1	69,74,74	1.24	6 (8%)	79,115,115	2.15	15 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	U10	L	304	-	-	5/7/31/87	0/1/1/1
4	BCL	M	403	2	-	4/41/137/137	-
8	SPO	M	406	-	-	14/37/37/47	-
5	BPH	M	404	-	-	3/19/87/105	0/5/6/6
5	BPH	L	303	-	2/2/18/22	10/37/105/105	0/5/6/6
6	U10	M	405	-	-	14/45/69/87	0/1/1/1
4	BCL	L	301	1	-	2/41/137/137	-
4	BCL	M	401	2	-	2/23/119/137	-
4	BCL	L	302	1	-	6/41/137/137	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	404	BPH	C1D-C2D	8.97	1.49	1.39
5	L	303	BPH	C1D-C2D	8.93	1.49	1.39
6	M	405	U10	C13-C14	8.25	1.52	1.33
6	M	405	U10	C33-C34	7.91	1.51	1.33
6	M	405	U10	C18-C19	7.81	1.51	1.33
6	M	405	U10	C28-C29	7.00	1.49	1.33
6	M	405	U10	C8-C9	6.50	1.48	1.33
6	M	405	U10	C38-C39	6.12	1.50	1.32
6	M	405	U10	C23-C24	6.00	1.46	1.33
4	L	302	BCL	MG-ND	-5.12	1.95	2.05
4	M	401	BCL	MG-ND	-5.04	1.95	2.05
4	M	401	BCL	C1B-NB	5.02	1.44	1.37
4	L	301	BCL	MG-ND	-4.91	1.96	2.05
6	M	405	U10	O3-C3	-4.52	1.25	1.36
4	M	401	BCL	MG-NB	-4.49	1.96	2.05
4	M	403	BCL	MG-NB	-4.31	1.97	2.05
5	L	303	BPH	C4D-CHA	-4.31	1.33	1.39
4	L	301	BCL	C4B-NB	4.10	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	403	BCL	MG-ND	-4.01	1.97	2.05
4	L	302	BCL	C1D-C2D	-3.83	1.37	1.45
4	L	301	BCL	C1D-C2D	-3.81	1.37	1.45
6	M	405	U10	O4-C4	-3.78	1.27	1.36
4	M	401	BCL	C1D-C2D	-3.61	1.38	1.45
6	L	304	U10	C9-C8	3.42	1.51	1.29
4	L	302	BCL	C1B-NB	3.39	1.42	1.37
4	L	301	BCL	MG-NB	-3.24	1.99	2.05
8	M	406	SPO	C25-C23	3.23	1.52	1.46
6	M	405	U10	C6-C1	3.18	1.40	1.35
6	L	304	U10	C7-C6	3.14	1.57	1.51
5	M	404	BPH	C4D-ND	-3.00	1.34	1.38
4	L	302	BCL	MG-NB	-2.98	1.99	2.05
6	L	304	U10	O3-C3	-2.85	1.29	1.36
5	M	404	BPH	C2-C3	2.84	1.41	1.32
4	M	403	BCL	C1D-C2D	-2.81	1.39	1.45
5	M	404	BPH	OBD-CAD	-2.78	1.18	1.22
5	L	303	BPH	C3D-C4D	2.74	1.45	1.41
6	L	304	U10	C4-C3	2.70	1.46	1.36
5	L	303	BPH	C3B-CAB	-2.63	1.42	1.49
5	M	404	BPH	C5-C3	2.62	1.57	1.50
5	M	404	BPH	C4C-C3C	2.57	1.56	1.51
4	M	401	BCL	C1D-ND	2.56	1.41	1.37
8	M	406	SPO	C26-C27	2.49	1.50	1.43
4	M	403	BCL	C4B-NB	2.48	1.41	1.37
6	L	304	U10	C3-C2	-2.42	1.41	1.48
6	L	304	U10	O4-C4	-2.39	1.31	1.36
6	M	405	U10	C3-C2	-2.39	1.41	1.48
4	M	403	BCL	C1B-NB	2.29	1.40	1.37
4	L	302	BCL	C4B-NB	2.29	1.40	1.37
5	M	404	BPH	C4D-CHA	-2.25	1.36	1.39
4	L	301	BCL	CHB-C4A	-2.23	1.32	1.37
4	M	401	BCL	C4B-NB	2.23	1.40	1.37
4	L	301	BCL	C1B-NB	2.22	1.40	1.37
5	M	404	BPH	C3D-C2D	-2.21	1.35	1.39
6	M	405	U10	C4-C5	-2.19	1.42	1.48
8	M	406	SPO	C16-C17	2.17	1.50	1.46
5	M	404	BPH	C3B-C4B	-2.14	1.38	1.41
4	M	401	BCL	O2A-CGA	2.14	1.39	1.33
4	L	302	BCL	CMA-C3A	2.10	1.57	1.53
6	L	304	U10	C6-C1	2.02	1.38	1.35
5	M	404	BPH	O2A-CGA	2.01	1.39	1.33

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	302	BCL	C1D-ND-C4D	-10.20	99.16	106.31
4	M	401	BCL	C1-C2-C3	9.62	142.34	126.76
4	M	401	BCL	C1D-ND-C4D	-9.23	99.84	106.31
4	L	301	BCL	C1D-ND-C4D	-8.29	100.49	106.31
4	M	403	BCL	C1D-ND-C4D	-8.04	100.67	106.31
5	M	404	BPH	C4D-CHA-CBD	8.00	112.29	108.45
8	M	406	SPO	C16-C17-C19	7.93	131.48	119.01
6	L	304	U10	C7-C6-C5	7.64	127.39	118.52
5	L	303	BPH	C6-C5-C3	7.39	131.48	113.47
5	M	404	BPH	C2D-C1D-ND	-7.25	104.19	109.43
4	L	302	BCL	O2D-CGD-CBD	6.66	122.87	111.23
5	L	303	BPH	C2D-C1D-ND	-6.41	104.80	109.43
8	M	406	SPO	C18-C17-C19	-6.15	112.85	122.82
4	M	401	BCL	O2D-CGD-CBD	6.03	121.78	111.23
5	M	404	BPH	O2D-CGD-CBD	6.00	117.54	110.95
8	M	406	SPO	C20-C21-C22	-5.87	111.51	123.52
6	L	304	U10	C1-C6-C5	-5.83	113.95	119.62
4	L	302	BCL	O1D-CGD-CBD	-5.75	113.17	124.52
5	L	303	BPH	C4D-CHA-CBD	5.74	111.21	108.45
4	L	301	BCL	C1-O2A-CGA	5.48	129.91	116.65
4	L	302	BCL	C1C-NC-C4C	5.25	109.07	106.68
5	M	404	BPH	OBD-CAD-CBD	-5.07	118.39	125.82
5	M	404	BPH	C1-C2-C3	4.97	134.81	126.76
4	L	301	BCL	C1C-NC-C4C	4.89	108.91	106.68
5	M	404	BPH	C2B-C1B-NB	-4.86	105.92	109.43
6	M	405	U10	C17-C18-C19	-4.86	116.50	127.62
4	M	403	BCL	O2D-CGD-CBD	4.81	119.64	111.23
4	L	301	BCL	C4A-NA-C1A	-4.81	104.49	106.68
5	M	404	BPH	C1-O2A-CGA	4.72	128.08	116.65
4	M	401	BCL	O2A-C1-C2	4.66	126.04	108.11
6	L	304	U10	C6-C1-C2	4.61	122.81	119.17
8	M	406	SPO	C4-C5-C6	-4.55	118.52	124.91
6	M	405	U10	C35-C34-C36	4.48	123.00	115.23
5	M	404	BPH	C1A-C2A-C3A	-4.23	98.82	102.84
5	M	404	BPH	C5-C3-C4	-4.10	105.15	114.59
4	M	403	BCL	C2D-C1D-ND	4.09	114.17	110.13
6	L	304	U10	C1M-C1-C6	-4.08	117.73	124.45
8	M	406	SPO	C21-C22-C23	4.07	132.98	127.28
6	L	304	U10	C7-C6-C1	-4.04	117.97	124.89
6	L	304	U10	O5-C5-C4	-3.97	112.62	121.03
4	M	401	BCL	C1C-NC-C4C	3.91	108.47	106.68
5	L	303	BPH	C1-O2A-CGA	-3.87	107.28	116.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	401	BCL	O2D-CGD-O1D	-3.81	116.43	123.85
5	M	404	BPH	C3D-CAD-CBD	3.68	112.45	107.61
6	M	405	U10	C30-C29-C31	3.66	121.58	115.23
4	L	302	BCL	C3D-C4D-ND	3.65	115.92	109.99
4	L	302	BCL	C2D-C1D-ND	3.64	113.72	110.13
6	M	405	U10	C10-C9-C11	3.57	121.42	115.23
4	M	403	BCL	CHD-C1D-ND	-3.56	119.79	124.80
4	M	401	BCL	C2D-C1D-ND	3.56	113.65	110.13
5	M	404	BPH	C4D-ND-C1D	3.52	113.09	108.87
4	L	302	BCL	C4A-NA-C1A	3.51	108.28	106.68
6	M	405	U10	C7-C8-C9	-3.51	120.79	126.83
6	L	304	U10	C4M-O4-C4	3.49	128.74	116.47
6	L	304	U10	O2-C2-C3	-3.47	113.68	121.03
4	L	301	BCL	C2D-C1D-ND	3.46	113.55	110.13
4	L	302	BCL	C1D-CHD-C4C	-3.35	118.54	126.62
5	L	303	BPH	C2B-C1B-NB	-3.29	107.05	109.43
6	M	405	U10	C27-C28-C29	-3.26	120.17	127.62
4	M	403	BCL	O2D-CGD-O1D	-3.15	117.71	123.85
5	M	404	BPH	CMD-C2D-C3D	3.15	130.98	124.68
4	L	301	BCL	O2A-CGA-CBA	3.10	121.27	111.83
4	M	403	BCL	CED-O2D-CGD	3.09	122.92	115.92
6	L	304	U10	C3-C2-C1	3.08	124.19	118.10
4	M	403	BCL	C1-O2A-CGA	3.03	123.99	116.65
4	M	401	BCL	O2A-CGA-CBA	3.02	121.05	111.83
4	L	301	BCL	C4D-CHA-C1A	-3.01	117.65	121.24
6	M	405	U10	C1M-C1-C6	-3.00	119.52	124.45
4	M	403	BCL	O2A-CGA-CBA	2.97	120.88	111.83
4	L	301	BCL	CHD-C1D-ND	-2.96	120.64	124.80
4	L	301	BCL	O2D-CGD-CBD	2.93	116.35	111.23
5	L	303	BPH	C4-C3-C5	-2.89	110.21	115.23
6	L	304	U10	C3M-O3-C3	2.88	126.59	116.47
4	M	403	BCL	O2A-CGA-O1A	-2.88	116.43	123.63
5	L	303	BPH	CMA-C3A-C4A	-2.84	108.48	114.61
4	M	403	BCL	C4D-C3D-CAD	-2.77	105.10	108.11
4	M	401	BCL	C1D-CHD-C4C	-2.76	119.97	126.62
5	L	303	BPH	C1A-C2A-C3A	-2.74	100.23	102.84
4	L	301	BCL	CAA-CBA-CGA	2.72	120.93	113.21
6	M	405	U10	C25-C24-C26	2.67	119.86	115.23
4	L	302	BCL	C5-C3-C2	-2.67	115.17	121.17
6	M	405	U10	C15-C14-C16	2.66	119.85	115.23
5	L	303	BPH	CMC-C2C-C1C	-2.66	108.88	114.61
8	M	406	SPO	C24-C23-C25	2.65	122.13	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	401	BCL	C3D-C4D-ND	2.64	114.28	109.99
5	M	404	BPH	O1D-CGD-CBD	-2.64	120.72	124.72
4	M	403	BCL	OBb-CAB-C3B	2.64	125.09	120.43
5	L	303	BPH	C4D-ND-C1D	2.59	111.97	108.87
4	M	403	BCL	C6-C5-C3	-2.56	107.24	113.47
4	L	302	BCL	O2A-CGA-CBA	2.55	119.61	111.83
4	M	401	BCL	CBC-CAC-C3C	-2.54	108.03	113.41
4	M	401	BCL	O1A-CGA-CBA	-2.53	113.87	123.78
4	L	302	BCL	CHB-C4A-NA	2.52	128.04	124.40
5	L	303	BPH	C11-C10-C8	2.51	124.32	115.97
4	M	403	BCL	CGD-CBD-CAD	-2.51	102.72	110.85
4	L	302	BCL	C3C-C4C-CHD	-2.49	118.14	123.39
5	L	303	BPH	CMD-C2D-C3D	2.49	129.65	124.68
5	L	303	BPH	OBb-CAB-C3B	2.48	124.14	119.99
4	L	302	BCL	C4-C3-C5	2.48	119.53	115.23
6	M	405	U10	C7-C6-C1	-2.46	120.67	124.89
6	L	304	U10	C4-C3-C2	-2.45	116.19	120.69
4	L	302	BCL	CHC-C1C-NC	2.42	127.89	124.40
8	M	406	SPO	C10-C9-C7	2.42	130.67	127.28
4	M	403	BCL	C3D-C4D-ND	2.40	113.90	109.99
4	M	403	BCL	C7-C6-C5	-2.39	106.89	113.26
4	M	403	BCL	O2A-C1-C2	2.39	117.29	108.11
6	M	405	U10	C4M-O4-C4	2.35	124.73	116.47
5	L	303	BPH	OBb-CAB-CBB	-2.33	115.21	120.19
4	L	301	BCL	C3D-C4D-ND	2.33	113.77	109.99
4	M	403	BCL	CAA-C2A-C3A	-2.30	106.78	113.00
8	M	406	SPO	C20-C19-C17	2.29	130.49	127.28
4	L	301	BCL	O2A-CGA-O1A	-2.27	117.94	123.63
4	M	403	BCL	C11-C10-C8	-2.27	108.42	115.97
4	L	301	BCL	C14-C13-C15	-2.25	103.27	111.27
4	L	301	BCL	O2A-C1-C2	-2.21	99.60	108.11
4	M	403	BCL	CHB-C1B-NB	-2.20	120.74	124.05
4	M	401	BCL	CHB-C4A-NA	2.19	127.57	124.40
8	M	406	SPO	C29-C28-C30	2.17	118.68	116.13
4	M	403	BCL	CHB-C4A-NA	2.17	127.53	124.40
8	M	406	SPO	C21-C20-C19	2.13	127.88	123.52
4	L	302	BCL	CHB-C1B-NB	-2.12	120.87	124.05
4	M	401	BCL	CAA-C2A-C1A	2.09	118.84	111.97
5	M	404	BPH	C5-C3-C2	2.08	128.90	122.66
6	M	405	U10	C22-C23-C24	-2.07	122.88	127.62
8	M	406	SPO	C15-C16-C17	-2.07	120.68	126.36
8	M	406	SPO	C26-C25-C23	2.07	132.04	126.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	404	BPH	C4C-C3C-C2C	-2.06	100.88	102.84
4	M	401	BCL	C4-C3-C2	-2.06	116.47	122.66
5	M	404	BPH	C4A-C3A-C2A	-2.06	100.88	102.84

All (2) chirality outliers are listed below:

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

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	401	BCL	O2A-C1-C2-C3
6	L	304	U10	C1-C6-C7-C8
6	M	405	U10	C24-C26-C27-C28
6	M	405	U10	C27-C28-C29-C30
6	M	405	U10	C27-C28-C29-C31
6	M	405	U10	C32-C33-C34-C36
8	M	406	SPO	O1-C1-C4-C5
8	M	406	SPO	C2-C1-C4-C5
8	M	406	SPO	C3-C1-C4-C5
8	M	406	SPO	C22-C23-C25-C26
8	M	406	SPO	C24-C23-C25-C26
6	M	405	U10	C37-C38-C39-C40
6	M	405	U10	C37-C38-C39-C41
6	M	405	U10	C32-C33-C34-C35
5	M	404	BPH	CBA-CGA-O2A-C1
5	L	303	BPH	C14-C13-C15-C16
5	L	303	BPH	C11-C12-C13-C15
5	L	303	BPH	C5-C6-C7-C8
5	M	404	BPH	O1A-CGA-O2A-C1
5	L	303	BPH	O2A-C1-C2-C3
4	M	403	BCL	C16-C17-C18-C20
5	L	303	BPH	C11-C10-C8-C7
4	M	403	BCL	C16-C17-C18-C19
4	L	301	BCL	C15-C16-C17-C18
4	M	403	BCL	C13-C15-C16-C17
4	L	302	BCL	C13-C15-C16-C17
6	M	405	U10	C28-C29-C31-C32
6	M	405	U10	C30-C29-C31-C32
5	L	303	BPH	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	M	405	U10	C14-C16-C17-C18
5	L	303	BPH	C2-C3-C5-C6
8	M	406	SPO	C1-C4-C5-C6
6	L	304	U10	C5-C6-C7-C8
4	L	302	BCL	C3-C5-C6-C7
8	M	406	SPO	C27-C28-C30-C31
4	L	302	BCL	CHA-CBD-CGD-O1D
4	L	302	BCL	CHA-CBD-CGD-O2D
4	L	302	BCL	C15-C16-C17-C18
8	M	406	SPO	C25-C26-C27-C28
6	M	405	U10	C20-C19-C21-C22
6	M	405	U10	C29-C31-C32-C33
6	L	304	U10	C6-C7-C8-C9
8	M	406	SPO	C2-C1-O1-CM1
5	L	303	BPH	C11-C10-C8-C9
6	M	405	U10	C5-C4-O4-C4M
8	M	406	SPO	C18-C17-C19-C20
8	M	406	SPO	C29-C28-C30-C31
6	M	405	U10	C18-C19-C21-C22
4	L	302	BCL	C16-C17-C18-C19
8	M	406	SPO	C4-C1-O1-CM1
4	L	301	BCL	C16-C17-C18-C20
6	L	304	U10	C5-C4-O4-C4M
8	M	406	SPO	C16-C17-C19-C20
5	L	303	BPH	C10-C11-C12-C13
4	M	403	BCL	CAA-CBA-CGA-O2A
5	M	404	BPH	C2C-C3C-CAC-CBC
8	M	406	SPO	C3-C1-O1-CM1
6	L	304	U10	C2-C3-O3-C3M
5	L	303	BPH	C12-C13-C15-C16
4	M	401	BCL	CAD-CBD-CGD-O2D

There are no ring outliers.

9 monomers are involved in 57 short contacts:

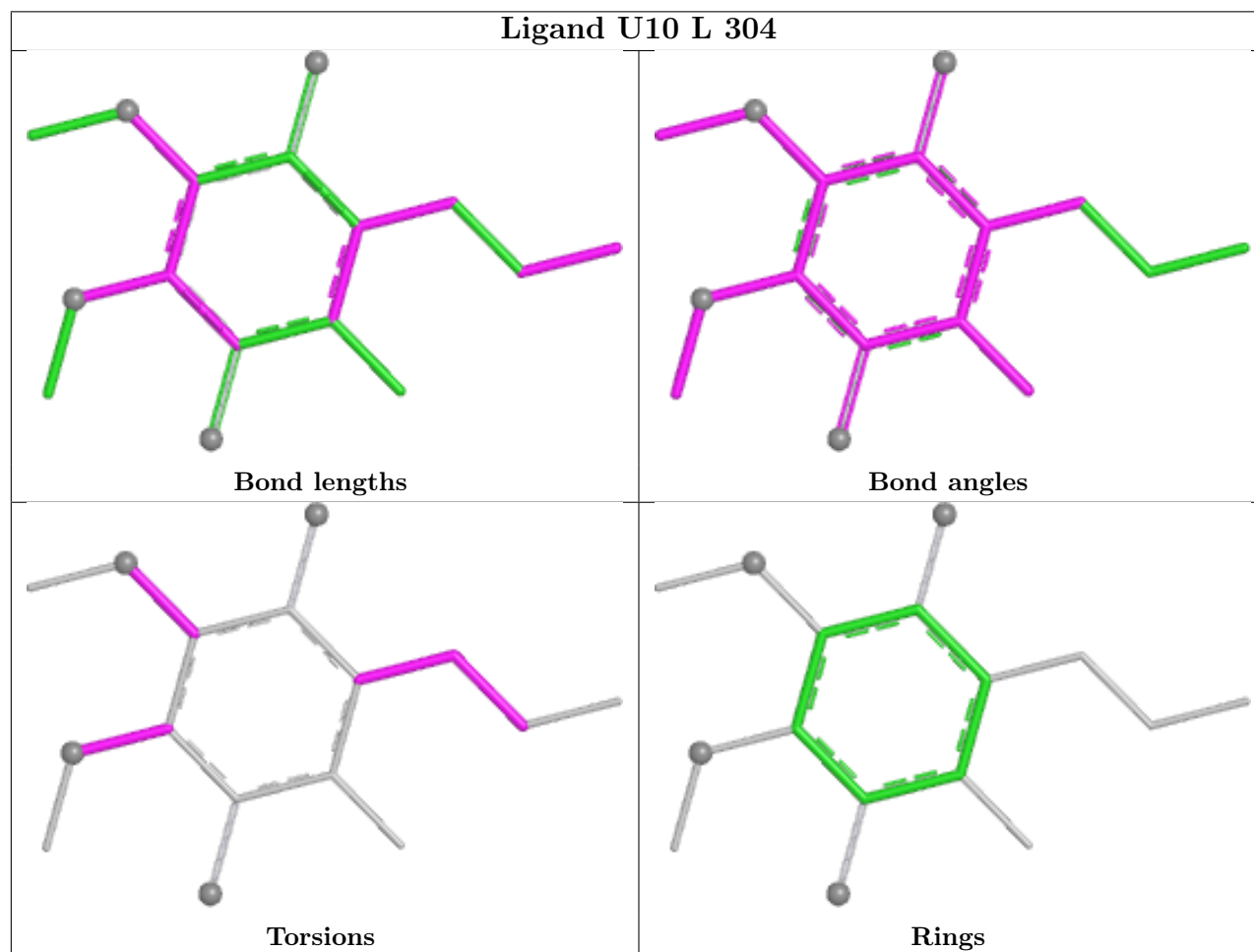
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	304	U10	8	0
4	M	403	BCL	16	0
8	M	406	SPO	6	0
5	M	404	BPH	5	0
5	L	303	BPH	8	0
6	M	405	U10	7	0

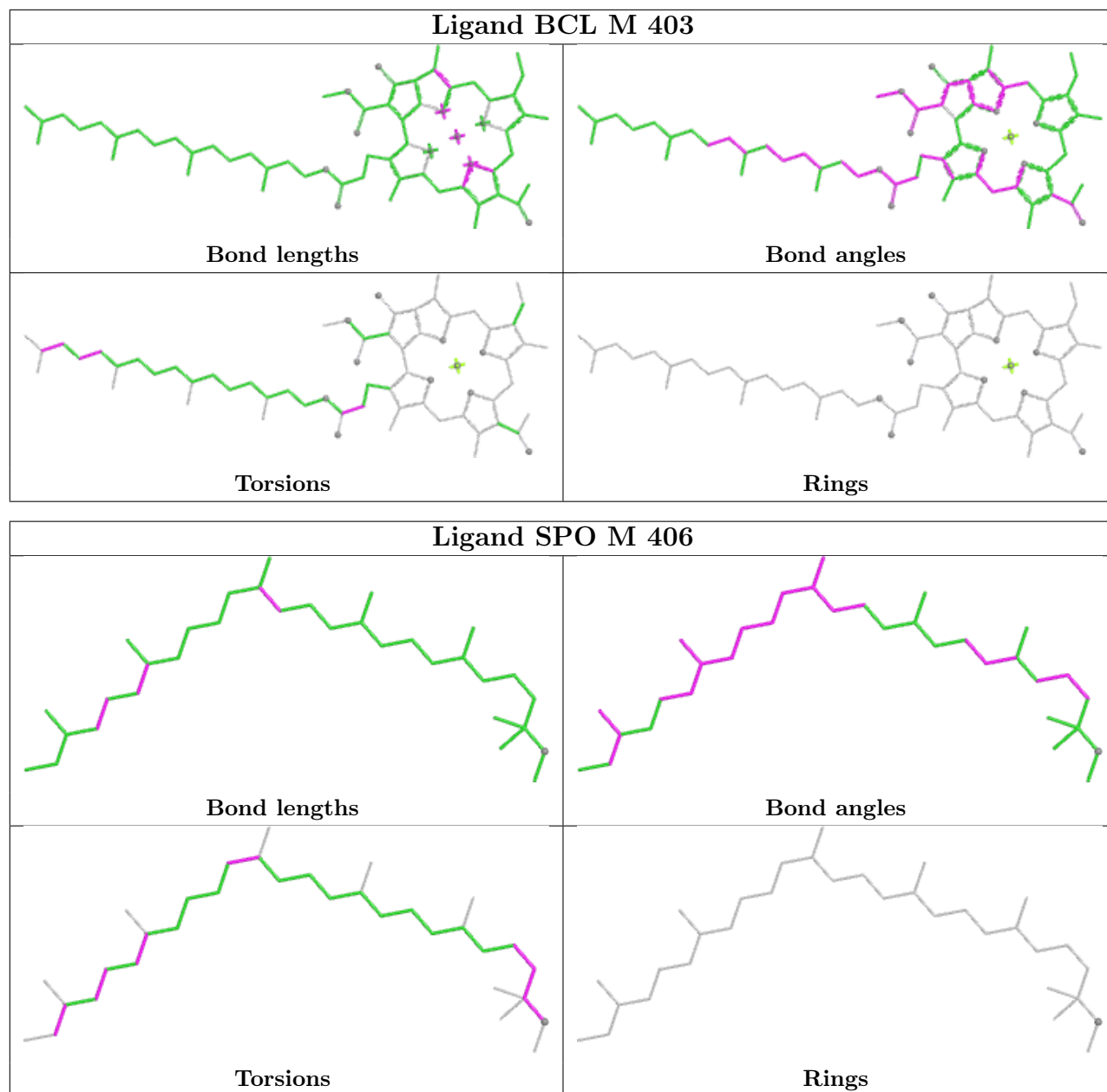
Continued on next page...

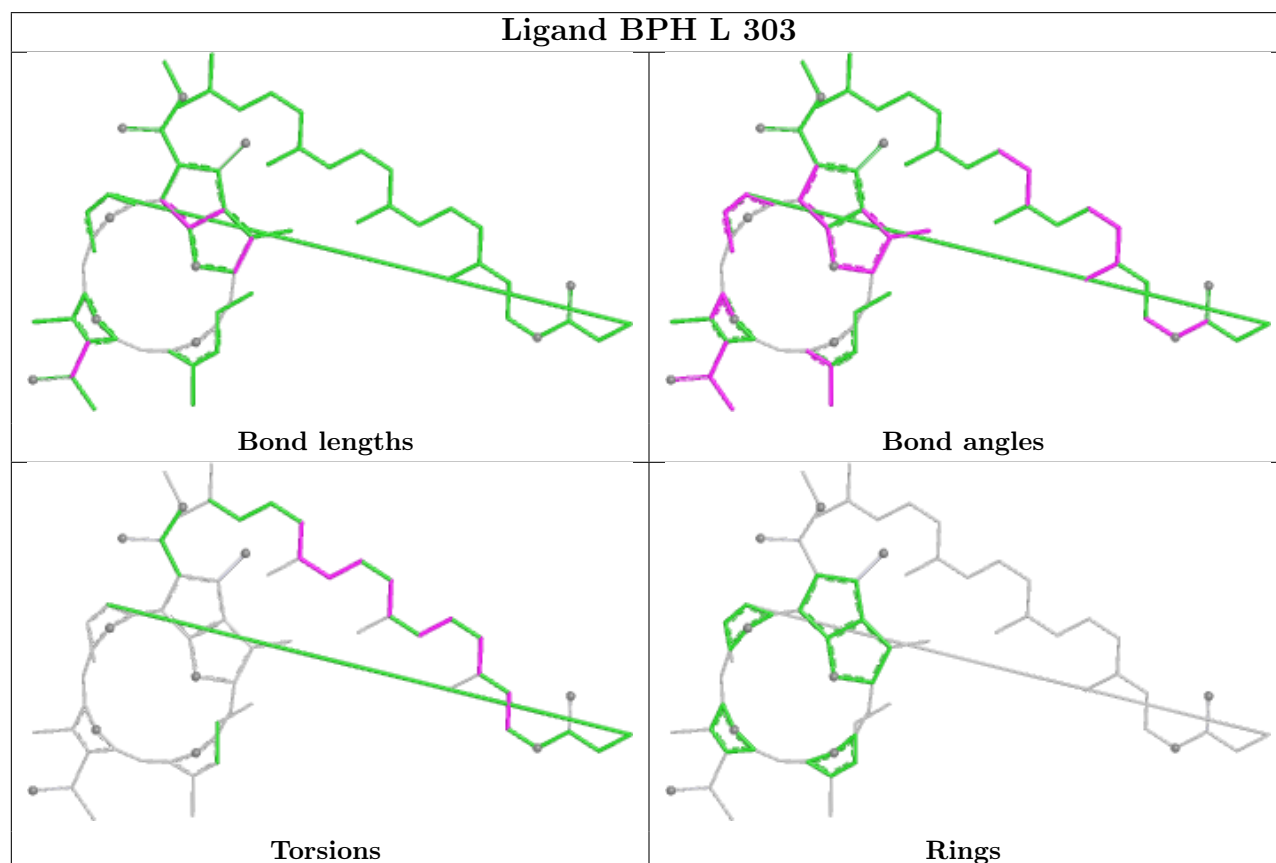
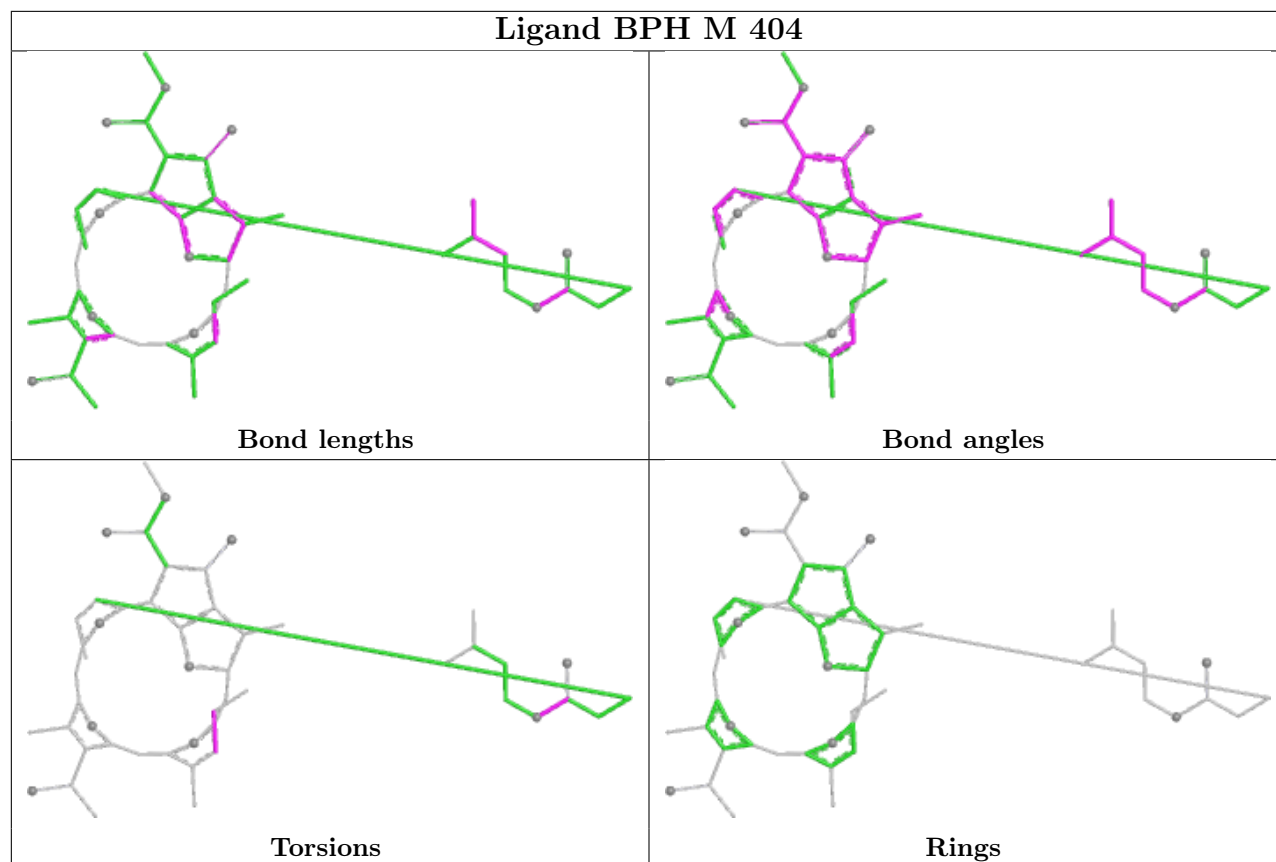
Continued from previous page...

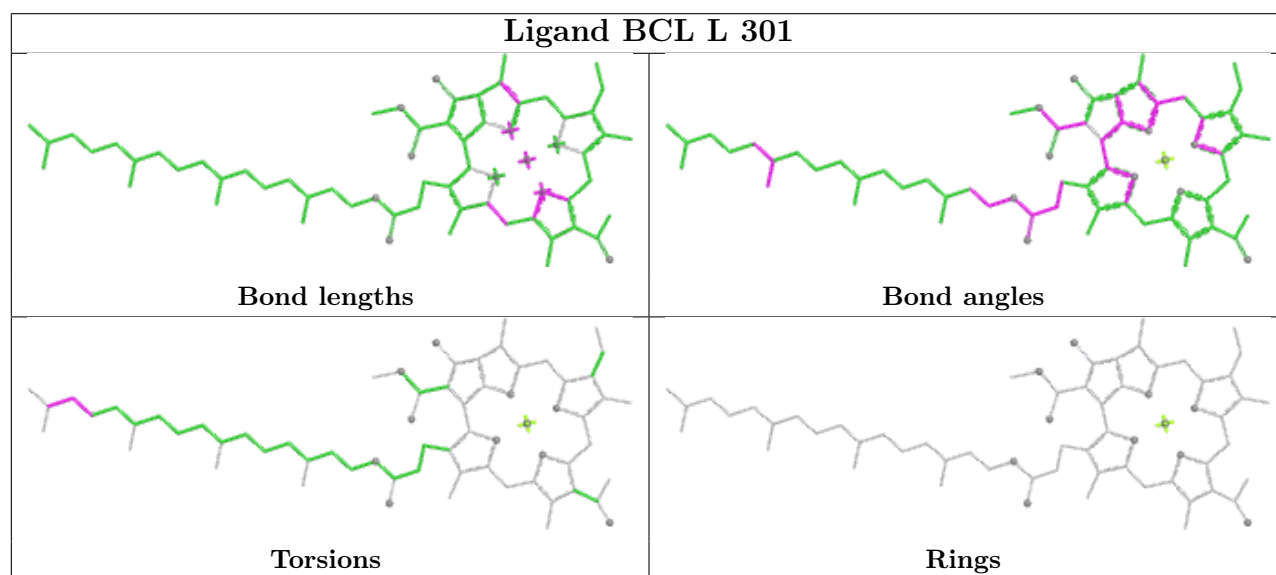
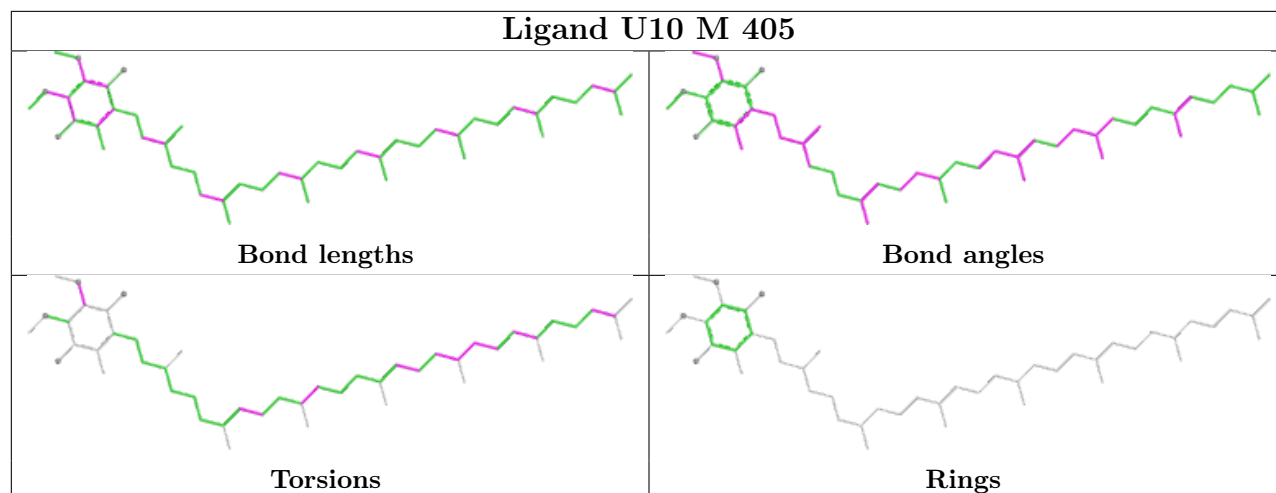
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	301	BCL	5	0
4	M	401	BCL	6	0
4	L	302	BCL	6	0

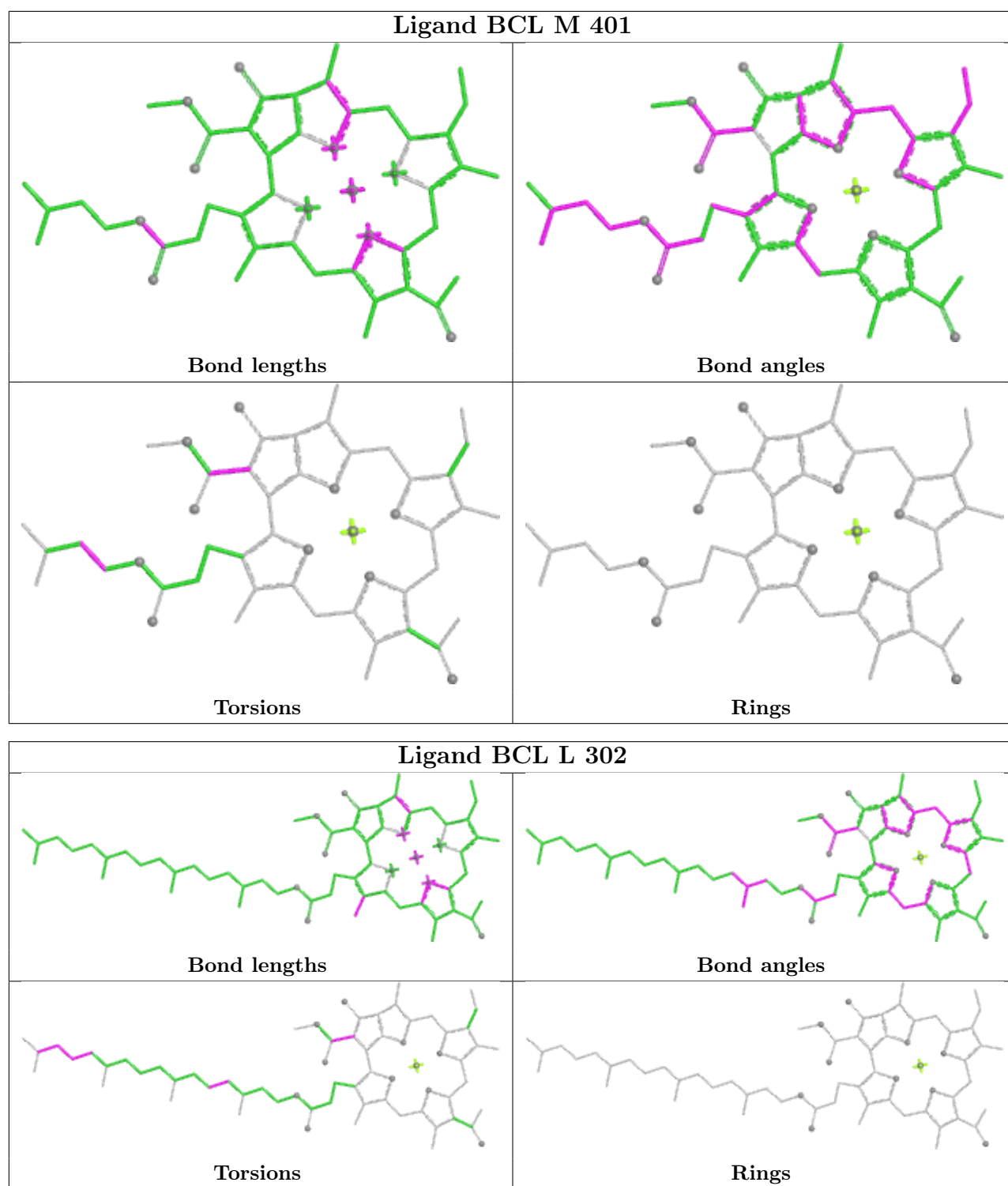
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	280/281 (99%)	-0.32	7 (2%) 58 50	33, 47, 84, 90	0
2	M	301/313 (96%)	-0.44	1 (0%) 90 88	33, 47, 77, 86	0
3	H	238/260 (91%)	-0.59	1 (0%) 88 85	35, 47, 62, 77	0
All	All	819/854 (95%)	-0.44	9 (1%) 78 72	33, 47, 77, 90	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	59	TRP	4.3
2	M	301	HIS	4.2
1	L	56	GLN	4.1
1	L	58	THR	3.0
1	L	274	ASN	2.6
1	L	277	GLY	2.5
1	L	275	ILE	2.1
3	H	52	ASN	2.0
1	L	54	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

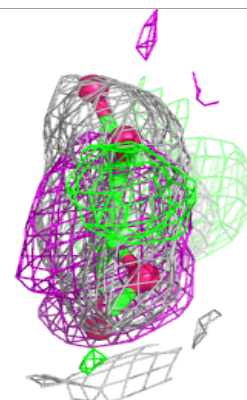
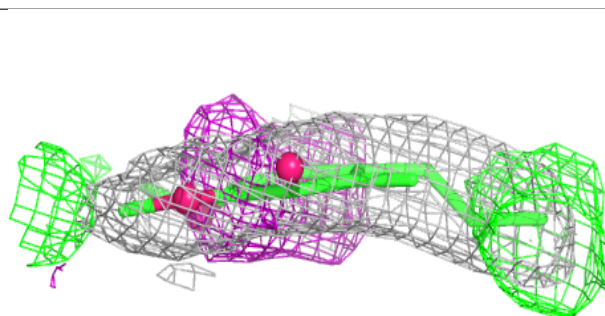
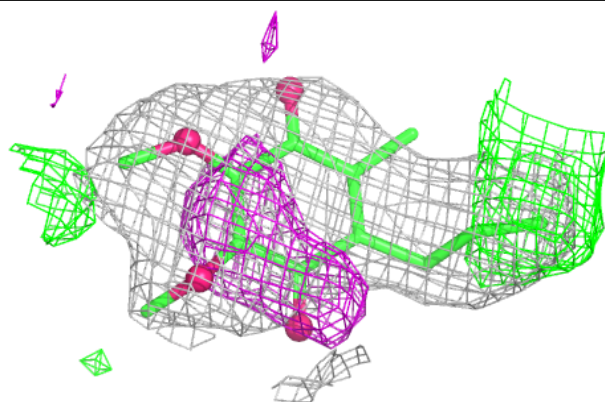
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	U10	L	304	16/63	0.68	0.28	57,71,81,90	0
8	SPO	M	406	33/42	0.89	0.19	54,63,94,95	0
6	U10	M	405	48/63	0.94	0.12	36,46,80,82	0
5	BPH	M	404	50/65	0.94	0.08	35,45,59,68	0
4	BCL	M	401	51/66	0.96	0.07	34,40,57,65	0
4	BCL	L	302	66/66	0.97	0.07	23,33,58,66	0
4	BCL	L	301	66/66	0.97	0.07	35,45,51,56	0
4	BCL	M	403	66/66	0.97	0.07	34,45,63,69	0
5	BPH	L	303	65/65	0.97	0.06	24,37,47,51	0
7	FE	M	402	1/1	1.00	0.01	40,40,40,40	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.

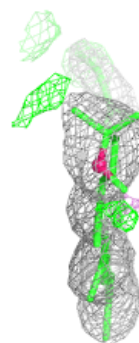
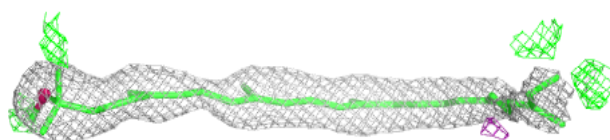
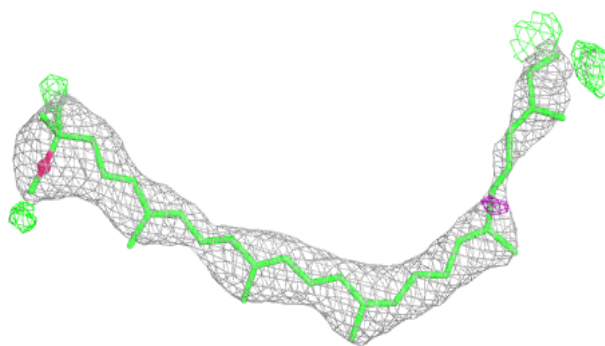
Electron density around U10 L 304:

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

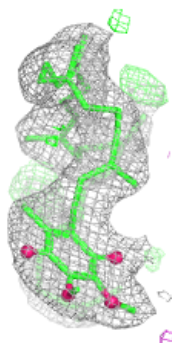
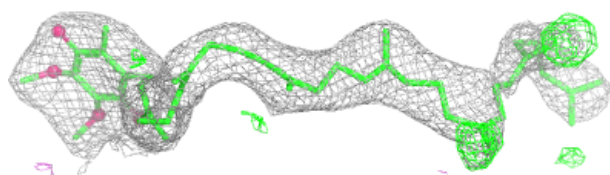
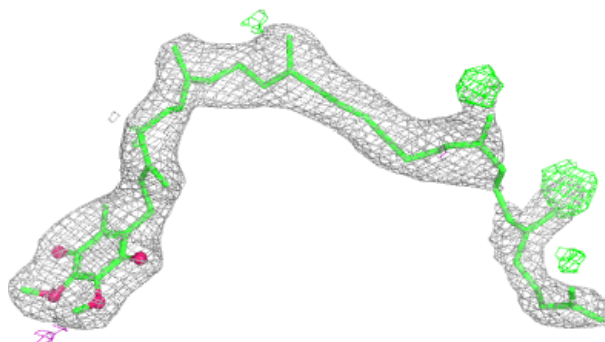


Electron density around SPO M 406:

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

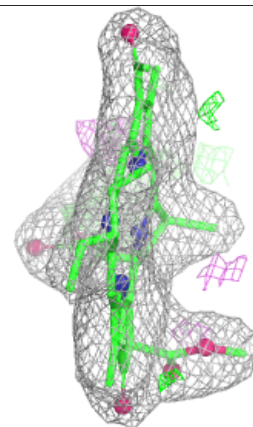
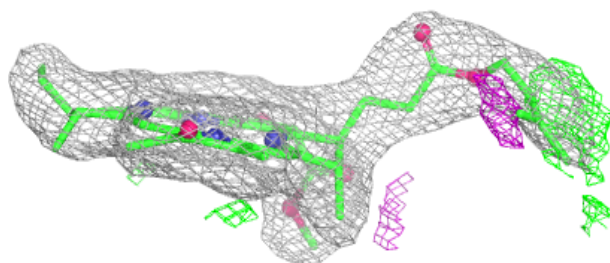
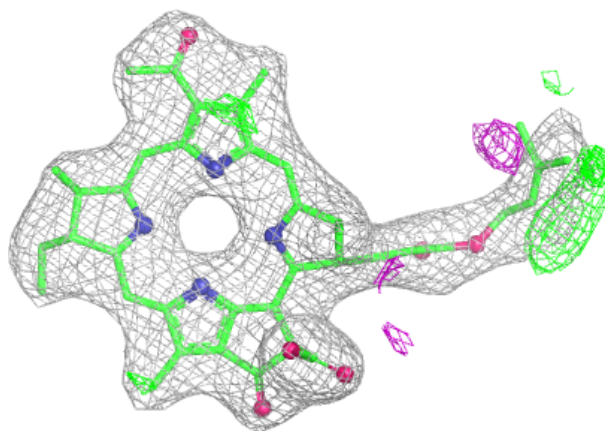
**Electron density around U10 M 405:**

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



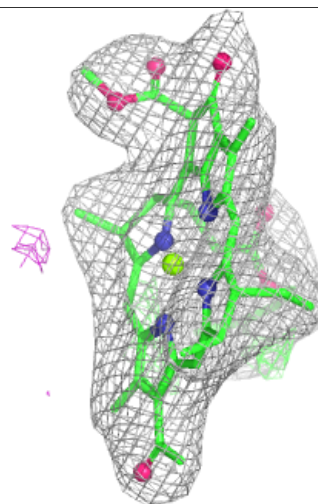
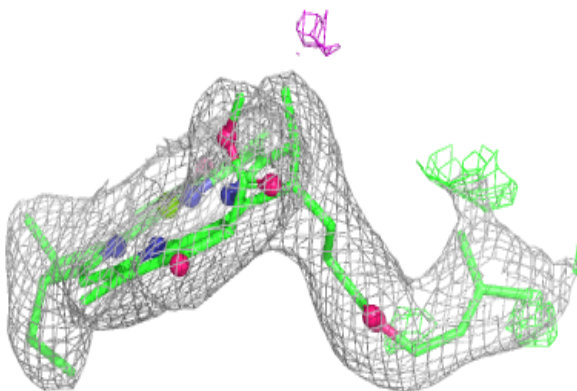
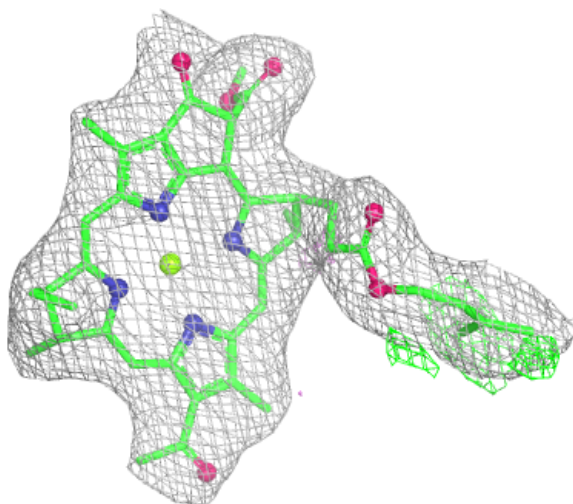
Electron density around BPH M 404:

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



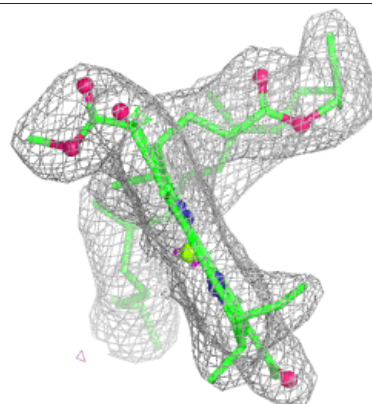
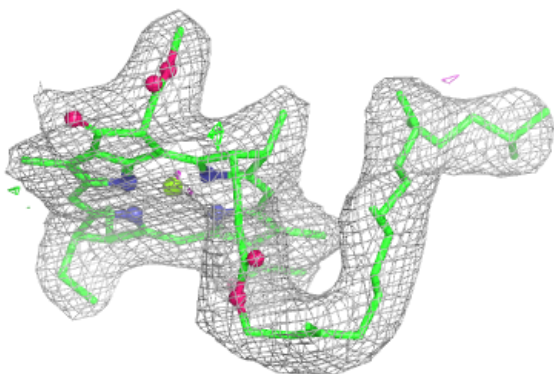
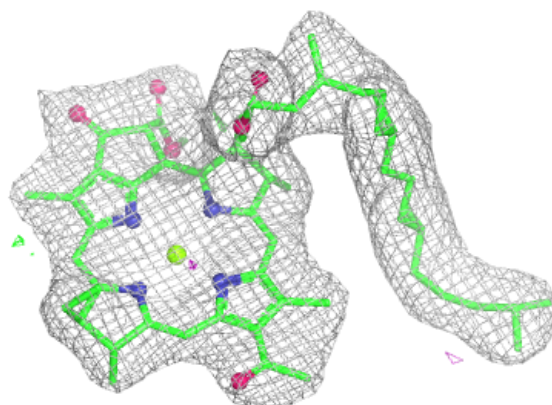
Electron density around BCL M 401:

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

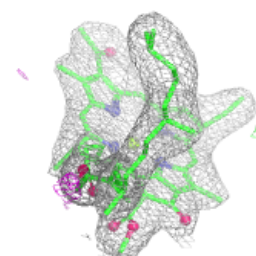
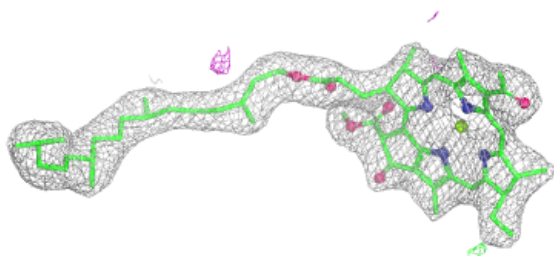
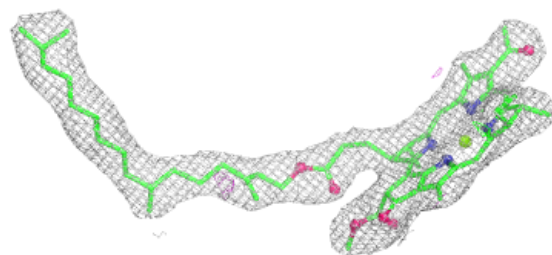


Electron density around BCL L 302:

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

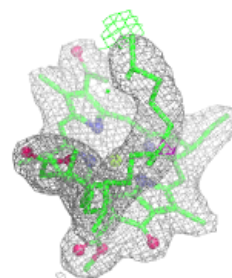
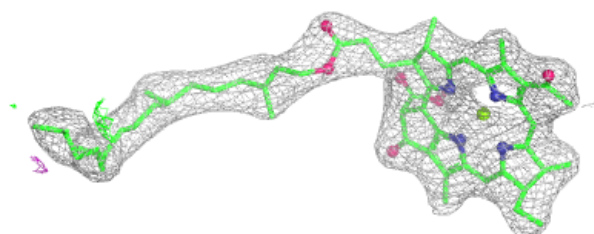
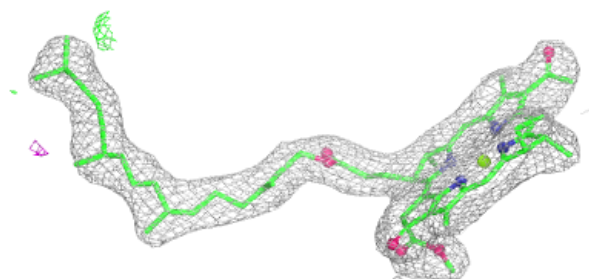
**Electron density around BCL L 301:**

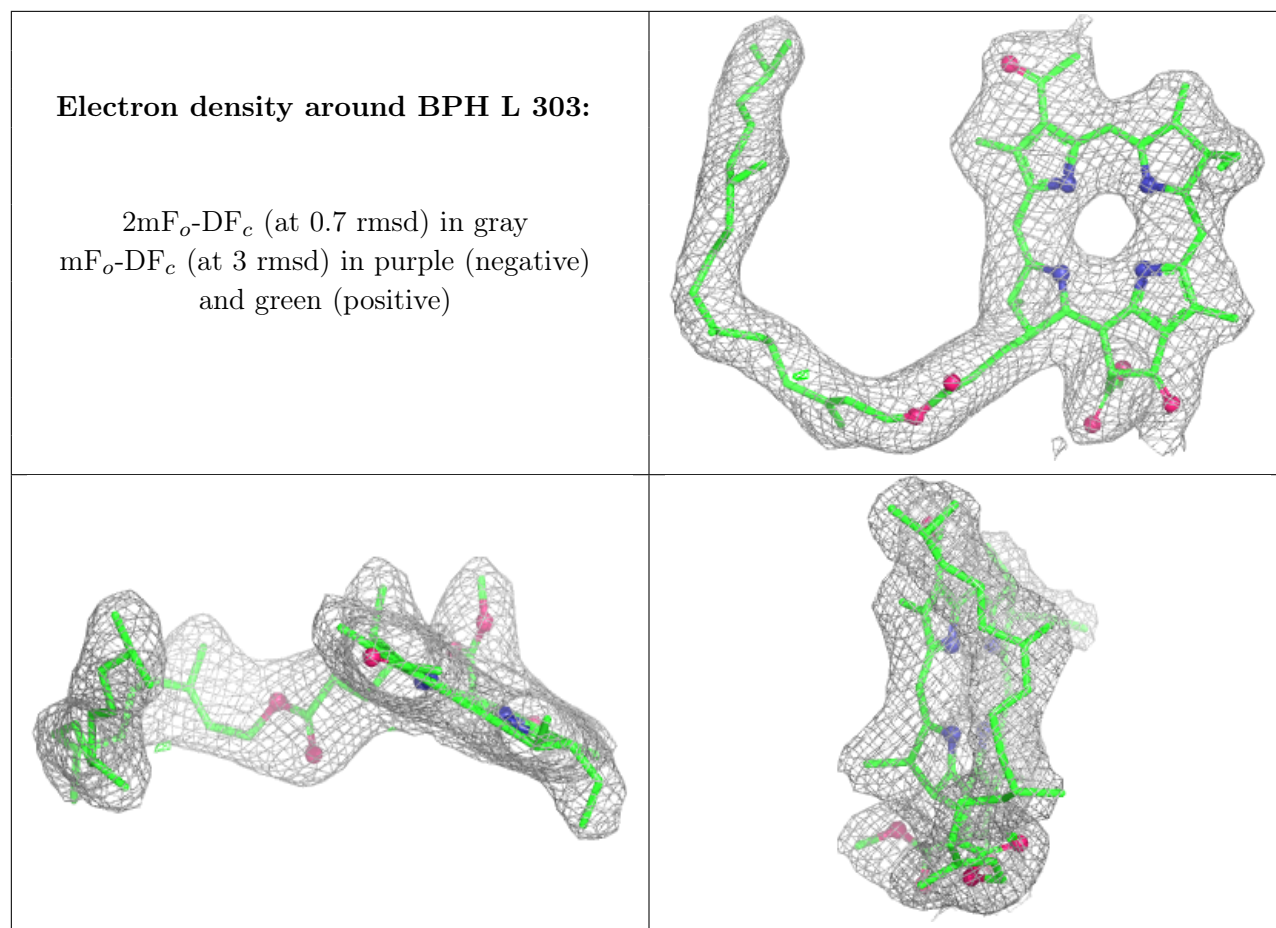
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCL 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.