



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:56 PM EDT

PDB ID : 4H99 / pdb_00004h99
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	:	4-5-2 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

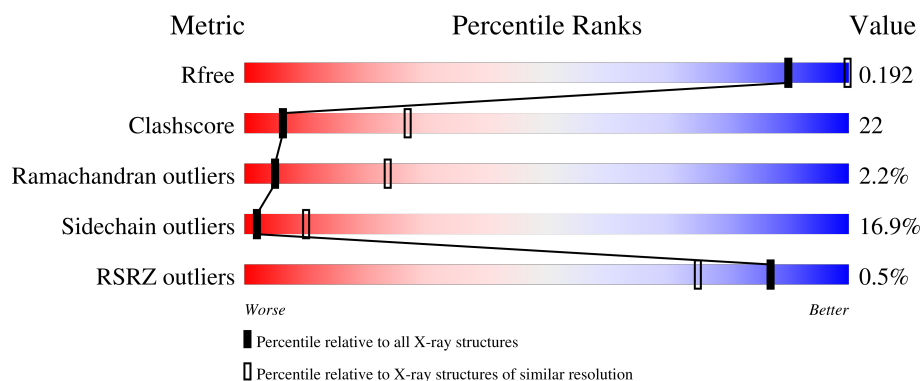
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (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 $\leq 5\%$. 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	M	313	
3	H	260	

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

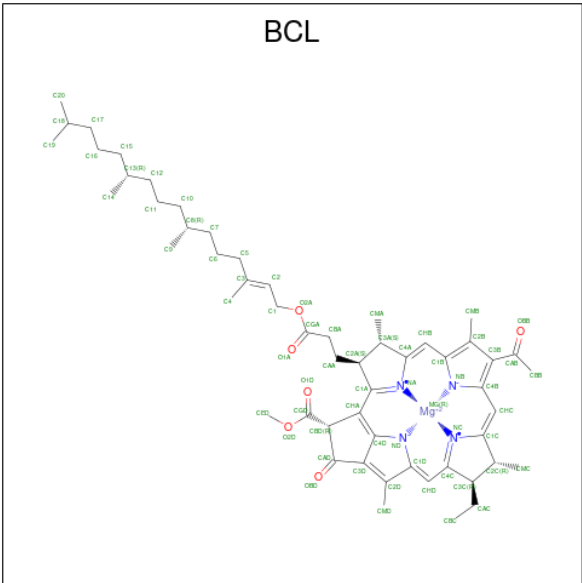
- Molecule 3 is a protein called Reaction center protein H chain.

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 (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



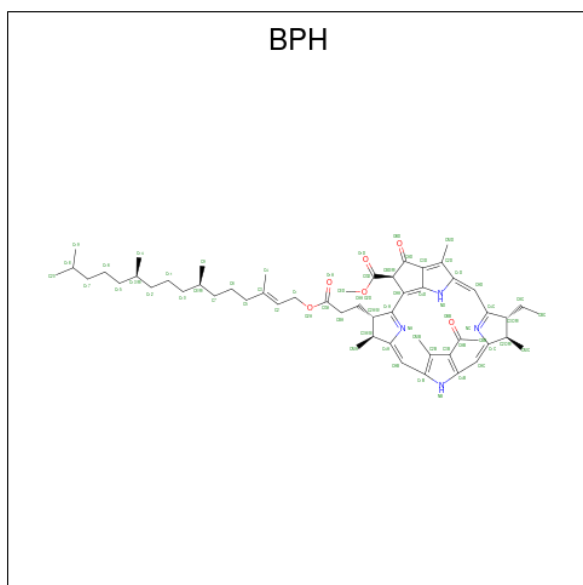
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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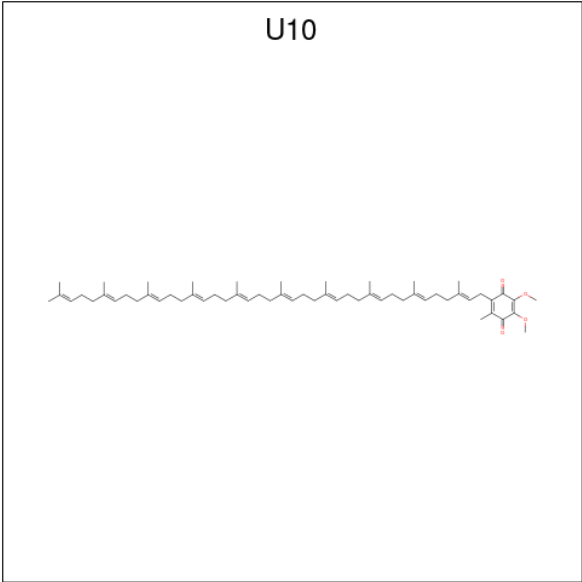
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	M	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (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
			51	41	4	6		

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

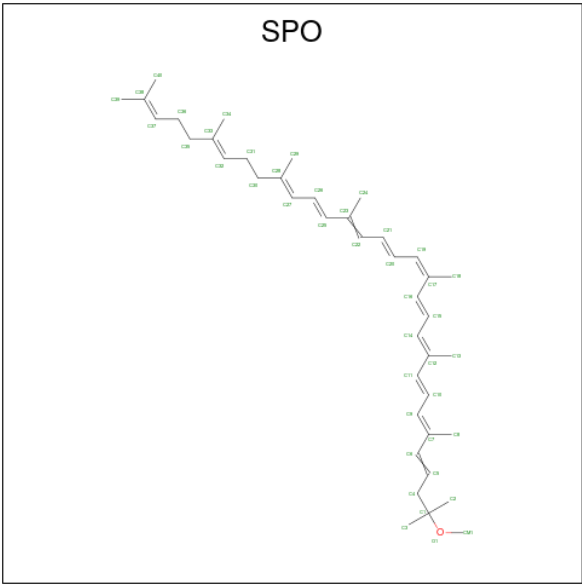


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			33	29	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- 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
			42	41	1		

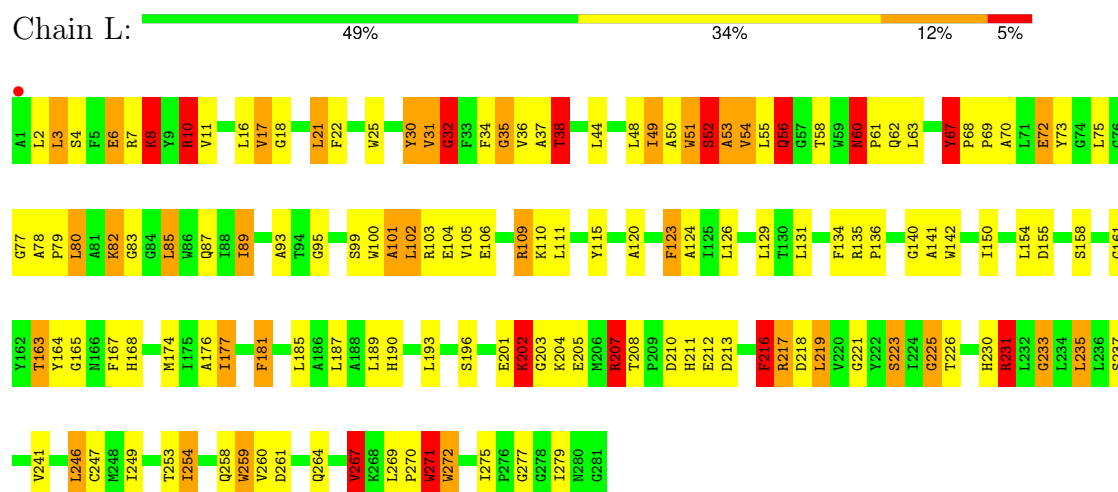
- Molecule 9 is water.

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		

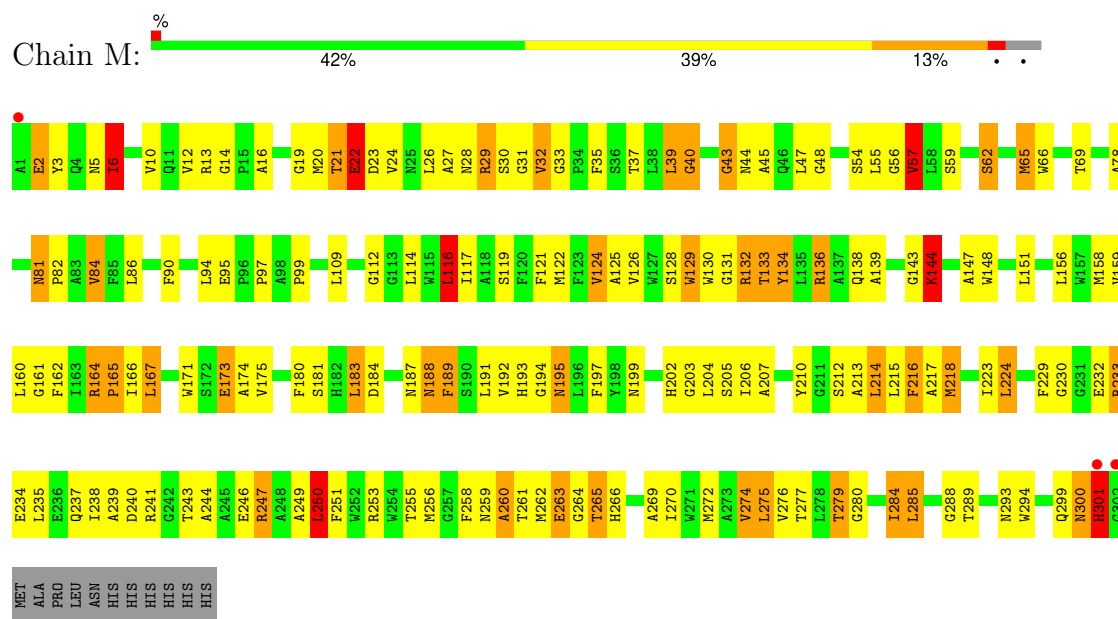
3 Residue-property plots

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

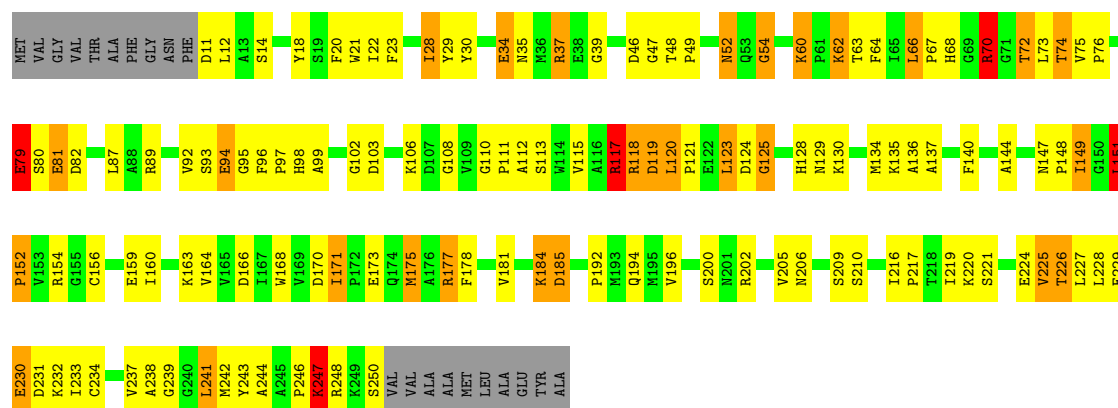


• Molecule 2: Reaction center protein M chain



• Molecule 3: Reaction center protein H chain

Chain H:



4 Data and refinement statistics

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) 99.2 (19.77-2.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.32 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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 ⓘ

5.1 Standard geometry ⓘ

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

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	1.90	46/2318 (2.0%)	1.72	45/3172 (1.4%)
2	M	1.88	39/2498 (1.6%)	1.71	48/3410 (1.4%)
3	H	2.03	42/1877 (2.2%)	1.89	49/2553 (1.9%)
All	All	1.93	127/6693 (1.9%)	1.77	142/9135 (1.6%)

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 (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	117	ARG	CA-C	9.42	1.65	1.52
2	M	57	VAL	CA-CB	9.38	1.67	1.54
1	L	82	LYS	CB-CG	9.31	1.80	1.52
1	L	249	ILE	CA-CB	8.87	1.66	1.54
3	H	219	ILE	CA-CB	-8.69	1.40	1.55
2	M	143	GLY	C-O	8.62	1.34	1.23
2	M	217	ALA	CA-CB	-8.54	1.39	1.53
3	H	152	PRO	CA-C	7.95	1.62	1.52
2	M	125	ALA	CA-C	7.56	1.62	1.52
2	M	165	PRO	CA-C	7.56	1.63	1.52
3	H	137	ALA	CA-CB	-7.50	1.42	1.53
1	L	258	GLN	C-O	7.31	1.32	1.24
3	H	89	ARG	C-O	-7.31	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	32	GLY	CA-C	7.30	1.62	1.51
2	M	19	GLY	C-O	-7.24	1.14	1.23
1	L	164	TYR	C-O	7.18	1.34	1.24
1	L	3	LEU	C-O	7.15	1.33	1.23
1	L	165	GLY	C-O	7.08	1.33	1.23
3	H	144	ALA	C-O	6.97	1.32	1.23
2	M	175	VAL	CA-CB	6.92	1.63	1.54
1	L	120	ALA	CA-CB	-6.88	1.42	1.53
1	L	259	TRP	N-CA	6.87	1.54	1.46
3	H	82	ASP	CA-C	-6.87	1.43	1.52
1	L	30	TYR	CA-C	6.78	1.61	1.52
1	L	31	VAL	CA-CB	6.78	1.61	1.53
2	M	126	VAL	CA-CB	6.77	1.61	1.54
3	H	94	GLU	CG-CD	6.74	1.69	1.52
2	M	114	LEU	CA-C	6.71	1.61	1.52
1	L	82	LYS	CG-CD	6.70	1.72	1.52
1	L	216	PHE	C-O	6.69	1.31	1.24
2	M	250	LEU	N-CA	-6.66	1.37	1.46
3	H	216	ILE	CA-CB	-6.62	1.45	1.54
3	H	28	ILE	CA-CB	6.58	1.61	1.54
3	H	168	TRP	N-CA	6.54	1.54	1.46
1	L	196	SER	C-O	6.54	1.32	1.24
1	L	82	LYS	CA-CB	6.51	1.61	1.53
1	L	120	ALA	N-CA	-6.51	1.38	1.46
1	L	72	GLU	CG-CD	6.49	1.68	1.52
1	L	82	LYS	CD-CE	6.48	1.71	1.52
2	M	189	PHE	C-O	6.40	1.31	1.24
1	L	70	ALA	CA-CB	-6.31	1.43	1.53
2	M	6	ILE	CA-CB	6.29	1.62	1.54
1	L	176	ALA	CA-CB	6.22	1.63	1.53
2	M	22	GLU	CA-C	-6.20	1.44	1.52
3	H	94	GLU	N-CA	6.20	1.53	1.46
2	M	301	HIS	CA-C	6.18	1.61	1.52
3	H	221	SER	CA-C	-6.16	1.45	1.53
3	H	94	GLU	CB-CG	6.15	1.70	1.52
1	L	267	VAL	CA-CB	6.09	1.63	1.54
3	H	209	SER	CA-C	6.09	1.60	1.52
3	H	238	ALA	C-O	6.08	1.31	1.24
1	L	235	LEU	CG-CD2	6.05	1.72	1.52
2	M	275	LEU	CA-C	6.04	1.61	1.52
1	L	279	ILE	CA-CB	6.03	1.62	1.54
2	M	195	ASN	C-O	6.00	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	94	GLU	CD-OE1	5.94	1.36	1.25
1	L	150	ILE	CA-C	-5.93	1.46	1.52
3	H	68	HIS	N-CA	5.93	1.53	1.46
1	L	223	SER	N-CA	-5.92	1.39	1.46
1	L	17	VAL	CA-CB	5.89	1.62	1.54
2	M	218	MET	C-O	5.89	1.30	1.24
3	H	72	THR	CB-CG2	5.88	1.72	1.52
1	L	202	LYS	N-CA	5.81	1.53	1.46
3	H	154	ARG	N-CA	5.78	1.53	1.46
1	L	235	LEU	CA-C	5.76	1.60	1.52
3	H	74	THR	CA-CB	5.76	1.62	1.53
1	L	131	LEU	C-O	5.75	1.30	1.24
1	L	154	LEU	C-O	5.74	1.30	1.24
1	L	155	ASP	CG-OD1	5.73	1.36	1.25
2	M	249	ALA	CA-CB	-5.72	1.44	1.53
3	H	192	PRO	N-CA	5.69	1.53	1.47
3	H	93	SER	CA-C	5.68	1.59	1.52
3	H	72	THR	C-O	5.67	1.31	1.23
2	M	144	LYS	CA-C	5.67	1.62	1.52
3	H	225	VAL	CA-CB	-5.62	1.47	1.54
1	L	36	VAL	C-O	-5.62	1.17	1.24
3	H	226	THR	CA-C	5.61	1.60	1.52
1	L	277	GLY	CA-C	5.55	1.57	1.52
2	M	116	LEU	N-CA	5.54	1.53	1.46
3	H	117	ARG	CD-NE	5.54	1.53	1.46
1	L	167	PHE	C-O	5.53	1.30	1.24
3	H	136	ALA	CA-CB	-5.53	1.45	1.53
3	H	62	LYS	C-O	5.49	1.30	1.23
2	M	212	SER	C-O	-5.48	1.17	1.24
2	M	217	ALA	CA-C	5.47	1.59	1.52
2	M	260	ALA	CA-C	5.46	1.59	1.52
2	M	224	LEU	C-O	5.45	1.30	1.24
3	H	184	LYS	CD-CE	5.44	1.68	1.52
3	H	152	PRO	C-O	5.43	1.29	1.23
3	H	244	ALA	CA-CB	-5.43	1.45	1.53
3	H	184	LYS	CG-CD	5.41	1.68	1.52
3	H	49	PRO	N-CA	5.39	1.54	1.47
2	M	134	TYR	CA-C	5.38	1.59	1.52
1	L	277	GLY	N-CA	5.34	1.51	1.45
2	M	124	VAL	CA-CB	5.31	1.61	1.54
2	M	129	TRP	N-CA	5.29	1.53	1.46
3	H	94	GLU	CD-OE2	5.29	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	212	SER	CA-C	-5.28	1.46	1.52
1	L	72	GLU	N-CA	5.28	1.52	1.46
2	M	48	GLY	CA-C	5.27	1.59	1.51
1	L	67	TYR	CD2-CE2	5.26	1.54	1.38
2	M	45	ALA	N-CA	5.26	1.53	1.46
3	H	28	ILE	C-O	-5.26	1.18	1.24
1	L	101	ALA	C-O	5.25	1.30	1.24
1	L	4	SER	C-O	-5.24	1.17	1.24
1	L	50	ALA	CA-CB	5.24	1.62	1.53
1	L	181	PHE	C-O	5.22	1.30	1.24
3	H	173	GLU	C-O	5.22	1.31	1.24
3	H	79	GLU	C-O	5.22	1.29	1.24
2	M	284	ILE	CA-CB	-5.21	1.47	1.54
3	H	81	GLU	CA-C	-5.20	1.46	1.52
2	M	183	LEU	C-O	5.19	1.30	1.24
2	M	117	ILE	CA-CB	5.17	1.60	1.54
2	M	131	GLY	CA-C	5.13	1.58	1.52
2	M	253	ARG	CZ-NH1	5.11	1.40	1.32
3	H	238	ALA	CA-C	5.10	1.59	1.52
2	M	95	GLU	N-CA	5.06	1.52	1.45
1	L	32	GLY	N-CA	5.05	1.52	1.45
1	L	100	TRP	CA-C	5.05	1.59	1.52
2	M	233	ARG	CZ-NH1	5.04	1.39	1.32
3	H	102	GLY	N-CA	5.04	1.50	1.45
2	M	213	ALA	CA-C	5.04	1.59	1.52
1	L	219	LEU	CA-CB	-5.03	1.45	1.53
1	L	134	PHE	CA-C	5.03	1.59	1.52
3	H	173	GLU	CD-OE1	5.03	1.34	1.25
2	M	263	GLU	CD-OE1	5.01	1.34	1.25
1	L	163	THR	C-O	-5.01	1.17	1.24

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	203	GLY	N-CA-C	-9.16	101.05	112.77
3	H	66	LEU	CA-C-N	-9.03	110.29	120.04
3	H	66	LEU	C-N-CA	-9.03	110.29	120.04
2	M	21	THR	CA-C-N	-8.99	104.36	121.54
2	M	21	THR	C-N-CA	-8.99	104.36	121.54
3	H	110	GLY	CA-C-N	-8.64	110.52	120.12
3	H	110	GLY	C-N-CA	-8.64	110.52	120.12
3	H	54	GLY	CA-C-N	-8.52	110.99	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	54	GLY	C-N-CA	-8.52	110.99	120.45
1	L	212	GLU	N-CA-C	-8.47	101.99	111.14
1	L	95	GLY	N-CA-C	-8.29	102.88	112.50
3	H	67	PRO	CA-C-N	-8.20	105.88	121.54
3	H	67	PRO	C-N-CA	-8.20	105.88	121.54
2	M	288	GLY	N-CA-C	-8.14	104.63	115.21
3	H	80	SER	N-CA-C	8.11	121.74	109.41
3	H	184	LYS	N-CA-C	-7.98	101.53	111.11
1	L	134	PHE	N-CA-C	7.91	120.60	111.11
3	H	81	GLU	N-CA-C	-7.78	98.95	110.23
3	H	230	GLU	N-CA-C	-7.74	102.44	111.03
1	L	131	LEU	N-CA-C	7.71	119.68	111.28
3	H	47	GLY	N-CA-C	7.70	125.22	115.21
2	M	188	ASN	N-CA-C	7.68	120.33	111.11
2	M	164	ARG	CA-C-N	-7.67	110.54	119.05
2	M	164	ARG	C-N-CA	-7.67	110.54	119.05
1	L	56	GLN	N-CA-C	-7.64	104.86	114.56
2	M	31	GLY	N-CA-C	-7.43	99.70	112.64
3	H	221	SER	CB-CA-C	-7.35	98.09	109.11
3	H	99	ALA	CA-C-N	7.34	127.61	119.90
3	H	99	ALA	C-N-CA	7.34	127.61	119.90
1	L	225	GLY	N-CA-C	7.28	122.11	112.65
3	H	81	GLU	CA-C-N	-7.22	107.75	121.54
3	H	81	GLU	C-N-CA	-7.22	107.75	121.54
1	L	203	GLY	N-CA-C	-7.14	106.16	115.59
1	L	141	ALA	N-CA-C	7.12	120.93	108.75
2	M	28	ASN	N-CA-C	7.12	121.72	112.89
3	H	194	GLN	N-CA-C	6.92	121.17	112.87
3	H	79	GLU	CA-C-N	-6.87	111.28	122.82
3	H	79	GLU	C-N-CA	-6.87	111.28	122.82
2	M	233	ARG	NE-CZ-NH1	-6.76	114.74	121.50
2	M	202	HIS	N-CA-C	-6.75	104.00	111.36
2	M	299	GLN	CA-C-N	-6.60	113.37	122.87
2	M	299	GLN	C-N-CA	-6.60	113.37	122.87
1	L	109	ARG	CA-CB-CG	-6.59	100.91	114.10
1	L	101	ALA	N-CA-C	-6.55	103.83	110.97
2	M	237	GLN	N-CA-C	-6.52	105.15	113.23
1	L	246	LEU	N-CA-C	-6.48	104.29	111.36
2	M	69	THR	CB-CA-C	-6.42	101.07	110.96
2	M	277	THR	CA-C-N	-6.39	111.93	120.63
2	M	277	THR	C-N-CA	-6.39	111.93	120.63
2	M	187	ASN	N-CA-C	-6.31	104.32	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	221	GLY	N-CA-C	-6.31	106.53	115.43
1	L	164	TYR	CA-C-O	6.31	127.10	119.78
1	L	226	THR	N-CA-C	6.28	118.93	111.71
2	M	289	THR	N-CA-C	-6.26	104.70	112.90
2	M	44	ASN	N-CA-C	6.21	119.24	110.23
3	H	70	ARG	NE-CZ-NH2	6.21	124.79	119.20
1	L	6	GLU	N-CA-C	6.20	120.04	112.23
3	H	192	PRO	CB-CA-C	-6.19	103.78	111.64
2	M	40	GLY	N-CA-C	6.19	121.27	114.40
1	L	49	ILE	N-CA-C	-6.16	105.72	111.45
2	M	259	ASN	N-CA-C	6.16	116.70	108.38
1	L	123	PHE	CA-C-N	-6.12	112.49	120.44
1	L	123	PHE	C-N-CA	-6.12	112.49	120.44
3	H	220	LYS	CA-C-O	-6.10	114.39	120.80
2	M	216	PHE	N-CA-C	-6.10	104.54	112.23
1	L	207	ARG	N-CA-C	6.07	117.71	110.19
1	L	231	ARG	NE-CZ-NH2	-6.05	113.76	119.20
3	H	171	ILE	CA-C-N	-6.04	113.54	119.64
3	H	171	ILE	C-N-CA	-6.04	113.54	119.64
1	L	233	GLY	N-CA-C	-5.95	105.44	112.64
1	L	140	GLY	N-CA-C	5.93	122.92	115.21
3	H	234	CYS	N-CA-C	-5.93	104.81	111.28
1	L	31	VAL	CA-C-N	-5.89	109.86	121.41
1	L	31	VAL	C-N-CA	-5.89	109.86	121.41
1	L	123	PHE	N-CA-C	-5.88	104.95	111.36
3	H	247	LYS	N-CA-C	5.88	120.45	113.28
1	L	37	ALA	N-CA-C	-5.87	104.79	111.07
1	L	82	LYS	N-CA-C	-5.84	103.64	111.87
2	M	250	LEU	N-CA-C	-5.83	105.66	112.89
2	M	300	ASN	N-CA-C	5.82	117.51	109.54
3	H	18	TYR	N-CA-C	-5.81	105.03	111.36
2	M	43	GLY	N-CA-C	-5.80	103.14	111.20
3	H	123	LEU	CA-C-O	-5.79	114.62	121.16
3	H	18	TYR	CB-CA-C	5.79	120.69	110.85
1	L	269	LEU	CA-C-N	5.77	127.06	119.84
1	L	269	LEU	C-N-CA	5.77	127.06	119.84
1	L	58	THR	N-CA-C	5.76	119.12	109.95
3	H	95	GLY	N-CA-C	5.76	122.70	114.64
3	H	119	ASP	N-CA-C	-5.73	104.93	112.72
1	L	165	GLY	N-CA-C	-5.67	99.74	113.18
2	M	99	PRO	CA-C-N	5.65	127.79	120.44
2	M	99	PRO	C-N-CA	5.65	127.79	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	261	ASP	N-CA-C	5.64	117.50	111.36
1	L	53	ALA	N-CA-C	-5.60	105.56	112.90
2	M	21	THR	N-CA-C	-5.58	100.59	109.96
2	M	126	VAL	CB-CA-C	5.58	119.06	111.87
1	L	168	HIS	CA-C-N	-5.57	112.30	122.38
1	L	168	HIS	C-N-CA	-5.57	112.30	122.38
3	H	37	ARG	CG-CD-NE	-5.56	99.77	112.00
2	M	132	ARG	NE-CZ-NH1	-5.51	115.99	121.50
3	H	241	LEU	N-CA-C	-5.49	105.29	111.28
3	H	151	LEU	N-CA-C	5.47	115.90	109.60
3	H	219	ILE	N-CA-C	5.47	117.60	109.17
2	M	81	ASN	N-CA-C	5.45	116.82	109.24
1	L	161	GLY	N-CA-C	-5.42	105.83	112.77
2	M	27	ALA	N-CA-C	-5.42	104.60	111.11
3	H	117	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	L	11	VAL	CA-C-N	-5.40	114.36	119.76
1	L	11	VAL	C-N-CA	-5.40	114.36	119.76
1	L	110	LYS	N-CA-C	-5.37	105.59	111.82
2	M	158	MET	CG-SD-CE	-5.36	89.11	100.90
1	L	174	MET	N-CA-C	-5.35	105.36	111.14
2	M	249	ALA	CA-C-O	5.35	126.22	120.55
3	H	221	SER	CA-C-N	-5.34	113.16	119.84
3	H	221	SER	C-N-CA	-5.34	113.16	119.84
2	M	247	ARG	CB-CA-C	5.31	119.88	110.85
2	M	160	LEU	N-CA-C	5.29	116.73	111.07
2	M	6	ILE	N-CA-CB	5.28	118.12	110.52
3	H	79	GLU	CB-CA-C	-5.28	102.65	110.62
1	L	35	GLY	N-CA-C	-5.26	106.04	112.77
2	M	10	VAL	N-CA-C	5.25	115.83	108.17
2	M	144	LYS	N-CA-C	5.22	118.77	112.93
2	M	239	ALA	N-CA-C	-5.18	106.80	113.23
3	H	125	GLY	N-CA-C	-5.16	108.99	114.67
2	M	272	MET	N-CA-C	-5.16	105.08	111.33
2	M	21	THR	CB-CA-C	-5.16	101.02	109.53
2	M	187	ASN	CA-C-O	5.14	126.00	120.70
1	L	38	THR	N-CA-CB	5.13	117.66	110.12
1	L	106	GLU	N-CA-C	-5.13	105.77	111.36
2	M	262	MET	CA-C-N	-5.12	113.47	120.44
2	M	262	MET	C-N-CA	-5.12	113.47	120.44
3	H	164	VAL	CB-CA-C	-5.12	104.47	111.33
3	H	72	THR	CA-CB-CG2	5.12	119.19	110.50
3	H	181	VAL	CB-CA-C	-5.11	103.01	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	23	ASP	N-CA-C	-5.11	104.67	111.87
1	L	78	ALA	N-CA-C	-5.11	98.53	109.81
2	M	29	ARG	NE-CZ-NH2	-5.08	114.63	119.20
3	H	185	ASP	N-CA-C	5.07	121.60	110.80
1	L	60	ASN	CB-CA-C	5.04	115.95	110.15
3	H	70	ARG	CB-CA-C	5.01	119.93	109.95
3	H	60	LYS	N-CA-C	-5.01	103.27	109.64
3	H	72	THR	CA-CB-OG1	-5.01	102.08	109.60

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
1	L	32	GLY	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	2230	0	2178	102	0
2	M	2406	0	2313	117	0
3	H	1829	0	1836	73	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	8	0
6	L	33	0	39	11	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	305	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 22.

All (305) 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
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
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
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
6:L:304:U10:H8	6:L:304:U10:H1M3	1.48	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
6:L:304:U10:H1M3	6:L:304:U10:C8	2.07	0.84
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
1:L:271:TRP:H	1:L:271:TRP:CD1	1.95	0.82
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:247:LYS:HB2	3:H:247:LYS:NZ	1.99	0.77
2:M:66:TRP:CZ2	2:M:122:MET:HE3	2.19	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
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
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
6:L:304:U10:C1M	6:L:304:U10:C8	2.68	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
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
4:L:302:BCL:HMB3	4:L:302:BCL:HBB2	1.80	0.64
1:L:187:LEU:HD13	2:M:216:PHE:CG	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:H:247:LYS:HB2	3:H:247:LYS:HZ2	1.67	0.59
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: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
2:M:194:GLY:O	2:M:195:ASN:HB3	2.04	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
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
3:H:75:VAL:HA	3:H:76:PRO:C	2.30	0.55
5:L:303:BPH:HBC3	5:L:303:BPH:HHD	1.86	0.55
6:L:304:U10:H8	6:L:304:U10:H1M2	1.85	0.55
2:M:269:ALA:O	2:M:270:ILE:C	2.50	0.55
4:M:401:BCL:HBB3	4:M:403:BCL:H41	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:96:PHE:HB3	3:H:97:PRO:HD2	1.89	0.55
2:M:256:MET:HE3	2:M:258:PHE:CZ	2.43	0.54
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
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
1:L:60:ASN:HD22	1:L:60:ASN:C	2.17	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
4:L:302:BCL:HMB3	4:L:302:BCL:CBB	2.38	0.52
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: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:54:VAL:C	1:L:56:GLN:H	2.18	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
3:H:128:HIS:O	3:H:129:ASN:C	2.52	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
1:L:77:GLY:HA2	1:L:87:GLN:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:217:ARG:O	1:L:218:ASP:C	2.50	0.50
2:M:205:SER:OG	4:M:403:BCL:HMA3	2.11	0.50
4:M:401:BCL:CBB	8:M:406:SPO:H243	2.41	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: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
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
3:H:22:ILE:O	3:H:23:PHE:C	2.54	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
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
1:L:79:PRO:O	1:L:80:LEU:C	2.56	0.47
4:M:401:BCL:HBB2	8:M:406:SPO:H243	1.96	0.47
3:H:112:ALA:HB2	3:H:239:GLY:HA3	1.95	0.47
2:M:40:GLY:HA2	2:M:43:GLY:O	2.14	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:223:ILE:O	2:M:224:LEU:C	2.54	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:120:LEU:C	3:H:226:THR:HG22	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:260:ALA:HB1	2:M:265:THR:HG22	1.96	0.46
2:M:256:MET:HE3	2:M:258:PHE:CE1	2.50	0.46
1:L:93:ALA:HA	5:L:303:BPH:H9C2	1.96	0.46
1:L:259:TRP:O	1:L:260:VAL:C	2.57	0.46
2:M:78:ALA:HB1	2:M:84:VAL:HG12	1.97	0.46
2:M:251:PHE:CD1	2:M:251:PHE:C	2.93	0.46
4:M:403:BCL:H2	5:M:404:BPH:HH C	1.96	0.46
3:H:70:ARG:NH2	3:H:120:LEU:HB2	2.30	0.46
2:M:164:ARG:HD2	2:M:284:ILE:HG22	1.98	0.46
3:H:247:LYS:HB2	3:H:247:LYS:HZ3	1.80	0.46
3:H:20:PHE:O	3:H:21:TRP:C	2.56	0.46
2:M:232:GLU:OE2	3:H:175:MET:HE1	2.16	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
1:L:202:LYS:C	1:L:204:LYS:H	2.24	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:31:VAL:O	1:L:32:GLY:C	2.58	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
3:H:242:MET:HE2	3:H:243:TYR:CE1	2.52	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
1:L:60:ASN:C	1:L:60:ASN:ND2	2.74	0.45
2:M:192:VAL:HG12	2:M:192:VAL:O	2.17	0.45
3:H:20:PHE:C	3:H:20:PHE:CD2	2.94	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
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: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:202:LYS:C	1:L:204:LYS:N	2.74	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:163:THR:O	1:L:163:THR:HG22	2.18	0.43
1:L:177:ILE:HD11	4:L:301:BCL:C1B	2.49	0.43
4:L:302:BCL:HMD2	2:M:206:ILE:HD13	1.99	0.43
1:L:254:ILE:HG21	1:L:254:ILE:HD13	1.65	0.43
2:M:284:ILE:O	2:M:285:LEU:C	2.61	0.43
1:L:207:ARG:CG	1:L:211:HIS:CD2	3.02	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
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
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
3:H:103:ASP:CG	3:H:106:LYS:HG3	2.44	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
2:M:138:GLN:O	2:M:139:ALA:C	2.61	0.42
3:H:29:TYR:O	3:H:30:TYR:C	2.62	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:264:GLN:HA	1:L:267:VAL:CG1	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:129:ASN:HD22	3:H:224:GLU:HG2	1.78	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
1:L:8:LYS:NZ	3:H:81:GLU:OE1	2.50	0.40
2:M:166:ILE:O	2:M:167:LEU:C	2.64	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
2:M:20:MET:HE3	2:M:20:MET:HB3	1.53	0.40
3:H:46:ASP:OD1	3:H:48:THR:OG1	2.33	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:51:TRP:C	1:L:53:ALA:H	2.30	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:123:PHE:O	1:L:124:ALA:C	2.64	0.40
1:L:2:LEU:HD21	1:L:10:ARG:CZ	2.51	0.40
2:M:206:ILE:O	2:M:207:ALA:C	2.65	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%)	2	12
2	M	300/313 (96%)	260 (87%)	35 (12%)	5 (2%)	7	30
3	H	238/260 (92%)	212 (89%)	24 (10%)	2 (1%)	16	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	817/854 (96%)	718 (88%)	81 (10%)	18 (2%)	5	24

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 ⓘ

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%)	182 (83%)	37 (17%)	2	10
2	M	236/246 (96%)	198 (84%)	38 (16%)	2	11
3	H	195/208 (94%)	160 (82%)	35 (18%)	2	9
All	All	650/674 (96%)	540 (83%)	110 (17%)	2	10

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	8	LYS
1	L	10	ARG
1	L	16	LEU
1	L	17	VAL
1	L	21	LEU
1	L	38	THR
1	L	44	LEU
1	L	52	SER
1	L	54	VAL
1	L	56	GLN
1	L	60	ASN
1	L	62	GLN
1	L	63	LEU
1	L	67	TYR
1	L	72	GLU
1	L	85	LEU
1	L	89	ILE
1	L	102	LEU
1	L	126	LEU
1	L	129	LEU
1	L	158	SER
1	L	177	ILE
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	231	ARG
1	L	235	LEU
1	L	237	SER
1	L	246	LEU
1	L	247	CYS
1	L	254	ILE
1	L	267	VAL
1	L	271	TRP
2	M	2	GLU
2	M	6	ILE
2	M	12	VAL
2	M	22	GLU
2	M	29	ARG
2	M	32	VAL

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Mol	Chain	Res	Type
2	M	37	THR
2	M	39	LEU
2	M	47	LEU
2	M	54	SER
2	M	57	VAL
2	M	62	SER
2	M	65	MET
2	M	84	VAL
2	M	86	LEU
2	M	94	LEU
2	M	109	LEU
2	M	116	LEU
2	M	124	VAL
2	M	133	THR
2	M	136	ARG
2	M	144	LYS
2	M	156	LEU
2	M	167	LEU
2	M	173	GLU
2	M	181	SER
2	M	191	LEU
2	M	204	LEU
2	M	214	LEU
2	M	215	LEU
2	M	235	LEU
2	M	250	LEU
2	M	265	THR
2	M	274	VAL
2	M	279	THR
2	M	285	LEU
2	M	300	ASN
2	M	301	HIS
3	H	11	ASP
3	H	12	LEU
3	H	14	SER
3	H	28	ILE
3	H	34	GLU
3	H	52	ASN
3	H	60	LYS
3	H	66	LEU
3	H	70	ARG
3	H	72	THR

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Mol	Chain	Res	Type
3	H	92	VAL
3	H	94	GLU
3	H	115	VAL
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	160	ILE
3	H	163	LYS
3	H	171	ILE
3	H	175	MET
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	237	VAL
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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	60	ASN
1	L	258	GLN
2	M	193	HIS
3	H	52	ASN
3	H	68	HIS
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
6	U10	L	304	-	33,33,63	3.58	11 (33%)	42,43,79	3.59	21 (50%)
4	BCL	L	301	1	69,74,74	1.25	7 (10%)	79,115,115	1.87	18 (22%)
8	SPO	M	406	-	41,41,41	1.68	9 (21%)	47,50,50	2.89	19 (40%)
4	BCL	M	401	2	53,58,74	2.04	9 (16%)	58,95,115	3.04	23 (39%)
6	U10	M	405	-	48,48,63	2.96	18 (37%)	60,61,79	2.35	20 (33%)
5	BPH	M	404	-	44,55,70	2.04	9 (20%)	41,83,101	2.99	19 (46%)
4	BCL	L	302	1	69,74,74	1.29	6 (8%)	79,115,115	2.45	26 (32%)
5	BPH	L	303	-	59,70,70	1.92	9 (15%)	59,101,101	2.22	21 (35%)
4	BCL	M	403	2	69,74,74	1.28	8 (11%)	79,115,115	2.03	21 (26%)

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	-	-	13/27/51/87	0/1/1/1
4	BCL	L	301	1	-	0/41/137/137	-
8	SPO	M	406	-	-	9/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	M	401	2	-	3/22/118/137	-
6	U10	M	405	-	-	16/45/69/87	0/1/1/1
5	BPH	M	404	-	-	4/19/87/105	0/5/6/6
4	BCL	L	302	1	-	5/41/137/137	-
5	BPH	L	303	-	2/2/18/22	13/37/105/105	0/5/6/6
4	BCL	M	403	2	-	10/41/137/137	-

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	303	BPH	C1D-C2D	9.91	1.50	1.39
6	L	304	U10	C13-C14	9.78	1.55	1.33
6	L	304	U10	C8-C9	9.33	1.54	1.33
5	M	404	BPH	C1D-C2D	9.14	1.49	1.39
4	M	401	BCL	C1B-NB	8.32	1.48	1.37
6	L	304	U10	C18-C19	7.97	1.51	1.33
6	M	405	U10	C33-C34	7.69	1.50	1.33
6	M	405	U10	C13-C14	7.34	1.49	1.33
6	M	405	U10	C28-C29	7.19	1.49	1.33
6	L	304	U10	C23-C24	6.74	1.52	1.32
6	M	405	U10	C8-C9	6.51	1.48	1.33
6	M	405	U10	C38-C39	6.11	1.50	1.32
6	M	405	U10	C18-C19	6.09	1.47	1.33
6	L	304	U10	C7-C6	5.99	1.62	1.51
4	M	401	BCL	C1D-ND	4.88	1.44	1.37
4	L	302	BCL	MG-ND	-4.81	1.96	2.05
6	M	405	U10	C23-C24	4.69	1.43	1.33
6	M	405	U10	C6-C1	4.60	1.43	1.35
4	M	401	BCL	MG-ND	-4.37	1.97	2.05
6	L	304	U10	C7-C8	4.22	1.57	1.50
4	M	401	BCL	CAA-C2A	4.07	1.61	1.54
8	M	406	SPO	C25-C23	4.05	1.54	1.46
4	M	401	BCL	MG-NB	-4.00	1.97	2.05
4	M	403	BCL	MG-ND	-3.84	1.98	2.05
4	M	401	BCL	C4B-NB	3.77	1.42	1.37
4	M	403	BCL	MG-NB	-3.72	1.98	2.05
4	L	301	BCL	MG-ND	-3.71	1.98	2.05
5	L	303	BPH	CHA-CBD	-3.71	1.47	1.51
4	M	403	BCL	C1B-NB	3.48	1.42	1.37
5	L	303	BPH	O2A-CGA	3.46	1.43	1.33
8	M	406	SPO	C26-C27	3.46	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	301	BCL	C1D-C2D	-3.39	1.38	1.45
4	M	401	BCL	O2A-CGA	3.35	1.43	1.33
4	L	302	BCL	CHD-C1D	3.25	1.44	1.38
6	M	405	U10	O3-C3	-3.18	1.29	1.36
5	M	404	BPH	C1A-C2A	3.16	1.55	1.51
6	L	304	U10	C12-C13	3.15	1.60	1.50
4	L	302	BCL	MG-NB	-3.11	1.99	2.05
6	L	304	U10	C16-C14	3.06	1.57	1.51
5	L	303	BPH	C3D-C2D	-3.04	1.34	1.39
6	M	405	U10	O4-C4	-3.00	1.29	1.36
4	L	301	BCL	MG-NB	-2.98	1.99	2.05
8	M	406	SPO	C4-C5	2.93	1.54	1.50
4	L	302	BCL	C4B-NB	2.93	1.41	1.37
5	L	303	BPH	C1B-C2B	2.87	1.42	1.39
5	M	404	BPH	CMB-C2B	-2.83	1.46	1.51
8	M	406	SPO	C6-C7	2.76	1.51	1.46
5	M	404	BPH	C5-C3	2.69	1.57	1.50
8	M	406	SPO	C27-C28	2.68	1.43	1.35
6	L	304	U10	C21-C19	2.66	1.56	1.51
5	M	404	BPH	O2A-CGA	2.66	1.41	1.33
6	L	304	U10	C26-C24	2.65	1.57	1.50
5	M	404	BPH	C4D-CHA	-2.63	1.35	1.39
5	M	404	BPH	C3B-C2B	2.63	1.44	1.39
4	M	401	BCL	C3C-C4C	2.60	1.54	1.51
6	M	405	U10	O2-C2	2.49	1.29	1.23
6	M	405	U10	C30-C29	2.48	1.56	1.50
4	M	403	BCL	C1-C2	2.48	1.56	1.49
5	L	303	BPH	C4D-CHA	-2.46	1.35	1.39
4	M	403	BCL	CHD-C1D	2.44	1.43	1.38
5	L	303	BPH	C3B-C4B	-2.43	1.37	1.41
6	M	405	U10	O5-C5	2.42	1.28	1.23
6	M	405	U10	C35-C34	2.38	1.56	1.50
6	M	405	U10	C32-C33	2.37	1.57	1.50
8	M	406	SPO	C37-C38	2.36	1.39	1.32
4	M	401	BCL	CBD-CGD	-2.33	1.45	1.52
4	M	403	BCL	C1D-ND	2.29	1.40	1.37
8	M	406	SPO	C8-C7	2.27	1.55	1.50
8	M	406	SPO	C10-C9	2.27	1.50	1.43
8	M	406	SPO	C4-C1	2.25	1.56	1.52
4	L	301	BCL	C1B-NB	2.25	1.40	1.37
4	L	301	BCL	O2D-CGD	2.24	1.38	1.33
6	L	304	U10	C22-C23	2.18	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	301	BCL	C1B-C2B	-2.17	1.38	1.43
6	M	405	U10	C36-C34	2.15	1.55	1.51
5	L	303	BPH	OBD-CAD	2.13	1.25	1.22
5	L	303	BPH	C3D-C4D	2.10	1.44	1.41
6	M	405	U10	C4-C3	2.09	1.44	1.36
4	L	301	BCL	CHD-C1D	2.09	1.42	1.38
4	L	302	BCL	CAC-C3C	2.09	1.58	1.54
4	M	403	BCL	MG-NA	2.07	2.11	2.06
6	M	405	U10	C31-C32	2.06	1.60	1.53
4	M	403	BCL	C1D-C2D	-2.04	1.41	1.45
4	L	302	BCL	CBB-CAB	2.04	1.54	1.50
5	M	404	BPH	CBA-CGA	2.02	1.56	1.50
5	M	404	BPH	O1A-CGA	2.00	1.28	1.22

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	401	BCL	C1D-ND-C4D	-10.48	98.96	106.31
4	M	401	BCL	O2A-C1-C2	9.59	131.82	108.99
4	M	403	BCL	C1D-ND-C4D	-9.44	99.69	106.31
4	L	302	BCL	C1D-ND-C4D	-8.85	100.10	106.31
5	M	404	BPH	O2D-CGD-CBD	8.63	120.43	110.95
8	M	406	SPO	C16-C17-C19	8.50	132.38	119.01
6	L	304	U10	O5-C5-C4	-8.00	104.08	121.03
4	M	401	BCL	O2D-CGD-CBD	7.67	124.64	111.23
4	L	301	BCL	C1D-ND-C4D	-7.65	100.94	106.31
6	L	304	U10	C3-C2-C1	7.50	132.94	118.10
4	L	302	BCL	O2D-CGD-CBD	7.29	123.97	111.23
5	M	404	BPH	C2D-C1D-ND	-7.18	104.24	109.43
6	L	304	U10	C6-C1-C2	-6.94	113.70	119.17
6	L	304	U10	O2-C2-C3	-6.82	106.59	121.03
6	L	304	U10	C4M-O4-C4	6.64	139.82	116.47
4	L	302	BCL	C16-C15-C13	-6.53	94.25	115.97
6	M	405	U10	C22-C23-C24	-6.42	112.93	127.62
6	M	405	U10	C35-C34-C36	6.36	126.27	115.23
8	M	406	SPO	C20-C21-C22	-6.27	110.69	123.52
4	M	401	BCL	O1D-CGD-CBD	-6.14	112.40	124.52
5	L	303	BPH	C2B-C1B-NB	-6.08	105.04	109.43
6	L	304	U10	C1-C6-C5	-6.06	113.73	119.62
6	L	304	U10	C7-C6-C5	5.99	125.48	118.52
5	L	303	BPH	C2D-C1D-ND	-5.90	105.16	109.43
6	M	405	U10	C17-C18-C19	-5.87	114.19	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	304	U10	C3M-O3-C3	5.82	136.94	116.47
4	M	401	BCL	O2A-CGA-CBA	5.71	129.26	111.83
5	M	404	BPH	C1-O2A-CGA	5.67	130.37	116.65
6	M	405	U10	C30-C29-C31	5.53	124.82	115.23
4	M	403	BCL	O2D-CGD-O1D	-5.37	113.41	123.85
4	L	302	BCL	C4A-NA-C1A	-5.26	104.28	106.68
8	M	406	SPO	C24-C23-C25	5.25	126.11	118.09
6	M	405	U10	C31-C29-C28	-5.16	109.57	121.17
8	M	406	SPO	C24-C23-C22	-5.11	114.54	122.82
6	L	304	U10	C8-C7-C6	5.00	124.39	112.08
5	M	404	BPH	C1A-C2A-C3A	-4.80	98.27	102.84
5	L	303	BPH	OB B-CAB-C3B	4.75	127.93	119.99
4	L	301	BCL	C1-O2A-CGA	4.75	128.16	116.65
8	M	406	SPO	C29-C28-C30	-4.74	107.00	115.23
5	M	404	BPH	C4D-CHA-CBD	4.69	110.70	108.45
5	M	404	BPH	OB D-CAD-CBD	-4.64	119.02	125.82
5	L	303	BPH	C4C-C3C-C2C	-4.60	98.47	102.84
8	M	406	SPO	C26-C27-C28	4.59	134.15	127.69
4	M	401	BCL	CMD-C2D-C1D	4.43	132.53	124.73
8	M	406	SPO	C18-C17-C16	-4.37	111.41	118.09
8	M	406	SPO	C6-C7-C9	-4.31	112.23	119.01
6	L	304	U10	C3-C4-C5	-4.23	112.92	120.69
6	L	304	U10	C26-C24-C25	4.21	124.27	114.59
6	L	304	U10	C7-C6-C1	-4.14	117.79	124.89
5	M	404	BPH	C4C-C3C-C2C	-4.11	98.93	102.84
8	M	406	SPO	C18-C17-C19	-4.10	116.18	122.82
5	L	303	BPH	C4D-CHA-CBD	4.08	110.41	108.45
4	L	301	BCL	C4-C3-C5	4.07	122.30	115.23
4	L	302	BCL	O2A-CGA-CBA	4.03	124.11	111.83
4	L	301	BCL	C2C-C3C-C4C	4.00	107.32	101.34
5	M	404	BPH	OB B-CAB-CBB	-3.96	111.76	120.19
5	M	404	BPH	C4D-ND-C1D	3.94	113.60	108.87
6	M	405	U10	C15-C14-C16	3.81	121.83	115.23
4	L	302	BCL	C11-C12-C13	-3.80	103.33	115.97
4	L	302	BCL	C6-C7-C8	-3.79	103.36	115.97
4	M	403	BCL	O2A-CGA-CBA	3.72	123.18	111.83
6	L	304	U10	C4-C3-C2	-3.72	113.86	120.69
6	L	304	U10	C1M-C1-C6	-3.67	118.41	124.45
8	M	406	SPO	C21-C22-C23	3.67	132.42	127.28
8	M	406	SPO	C10-C9-C7	3.66	132.41	127.28
4	M	401	BCL	C1C-NC-C4C	3.65	108.34	106.68
4	M	401	BCL	CHD-C1D-ND	-3.64	119.68	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	303	BPH	OBB-CAB-CBB	-3.61	112.50	120.19
4	L	302	BCL	C5-C3-C2	-3.61	113.07	121.17
4	M	401	BCL	CAC-C3C-C4C	3.60	120.57	112.58
4	L	302	BCL	O1D-CGD-CBD	-3.58	117.46	124.52
4	M	401	BCL	O1A-CGA-CBA	-3.57	109.81	123.78
5	M	404	BPH	C2B-C1B-NB	-3.57	106.85	109.43
8	M	406	SPO	C8-C7-C6	3.55	123.52	118.09
5	L	303	BPH	C6-C5-C3	3.52	122.05	113.47
4	L	302	BCL	CMD-C2D-C1D	3.49	130.87	124.73
4	L	302	BCL	C3D-C4D-ND	3.48	115.64	109.99
6	M	405	U10	C27-C28-C29	-3.47	119.67	127.62
4	M	401	BCL	CHB-C4A-NA	3.45	129.39	124.40
4	M	403	BCL	C3D-C4D-ND	3.40	115.51	109.99
4	L	301	BCL	O2A-CGA-CBA	3.38	122.14	111.83
5	L	303	BPH	CMA-C3A-C4A	-3.36	107.37	114.61
4	M	403	BCL	O2D-CGD-CBD	3.35	117.09	111.23
4	L	302	BCL	CAA-CBA-CGA	3.33	122.66	113.21
4	L	302	BCL	C2A-C1A-CHA	-3.32	118.11	123.87
6	M	405	U10	C25-C24-C23	-3.31	115.14	123.63
6	M	405	U10	C7-C8-C9	-3.24	121.25	126.83
5	L	303	BPH	C1-C2-C3	-3.24	120.89	126.20
6	L	304	U10	C1M-C1-C2	3.20	127.88	116.93
5	L	303	BPH	C11-C10-C8	3.19	126.56	115.97
8	M	406	SPO	C36-C35-C33	3.17	123.67	113.19
4	M	401	BCL	CMD-C2D-C3D	-3.14	120.50	127.69
4	L	302	BCL	C1-C2-C3	3.13	131.33	126.20
4	M	403	BCL	C2D-C1D-ND	3.13	113.22	110.13
4	L	302	BCL	O2A-CGA-O1A	-3.12	115.83	123.63
4	M	401	BCL	C3D-C4D-ND	3.11	115.04	109.99
4	M	401	BCL	C2D-C1D-ND	3.07	113.17	110.13
4	M	403	BCL	CMC-C2C-C1C	-3.06	103.54	111.77
8	M	406	SPO	C21-C20-C19	3.02	129.69	123.52
5	M	404	BPH	O2D-CGD-O1D	-3.01	117.99	123.85
4	M	403	BCL	CMB-C2B-C1B	3.00	129.98	125.42
8	M	406	SPO	C15-C16-C17	-2.99	118.17	126.36
5	L	303	BPH	CBA-CAA-C2A	-2.94	105.11	113.78
5	M	404	BPH	CMD-C2D-C3D	2.93	130.54	124.68
4	L	301	BCL	CHD-C1D-ND	-2.93	120.68	124.80
4	L	302	BCL	C6-C5-C3	-2.89	106.43	113.47
6	M	405	U10	C26-C27-C28	-2.88	97.76	112.02
8	M	406	SPO	C11-C12-C14	2.87	123.53	119.01
8	M	406	SPO	C26-C25-C23	2.85	134.19	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	303	BPH	C12-C11-C10	2.85	126.04	113.28
4	L	302	BCL	C1C-NC-C4C	2.82	107.97	106.68
4	L	301	BCL	C4-C3-C2	-2.81	116.41	123.63
5	L	303	BPH	CBC-CAC-C3C	-2.78	108.31	113.78
6	M	405	U10	C36-C34-C33	-2.76	114.98	121.17
8	M	406	SPO	C13-C12-C11	-2.74	113.91	118.09
5	L	303	BPH	C1C-C2C-C3C	2.73	105.44	102.84
4	L	302	BCL	O2D-CGD-O1D	-2.72	118.55	123.85
6	M	405	U10	C25-C24-C26	2.72	119.95	115.23
5	M	404	BPH	CMA-C3A-C4A	-2.69	108.82	114.61
6	L	304	U10	C11-C12-C13	2.68	125.26	112.02
4	M	401	BCL	C3A-C2A-C1A	-2.67	97.33	101.34
4	L	301	BCL	C3D-C4D-ND	2.66	114.32	109.99
4	L	302	BCL	C4D-CHA-C1A	-2.66	118.08	121.24
4	L	302	BCL	CMD-C2D-C3D	-2.66	121.60	127.69
4	L	301	BCL	CHB-C1B-NB	-2.66	120.07	124.05
4	L	301	BCL	C6-C5-C3	-2.64	107.04	113.47
4	L	301	BCL	C3D-C2D-C1D	2.60	109.38	105.83
4	L	302	BCL	C16-C17-C18	-2.60	104.35	115.94
5	M	404	BPH	O2A-C1-C2	-2.59	98.13	108.11
4	M	401	BCL	CMB-C2B-C1B	2.58	129.35	125.42
4	L	302	BCL	C2D-C1D-ND	2.56	112.66	110.13
4	L	301	BCL	CHC-C4B-NB	-2.55	120.23	124.05
4	M	403	BCL	CHD-C1D-ND	-2.53	121.23	124.80
6	L	304	U10	O2-C2-C1	-2.51	113.71	120.73
4	M	403	BCL	C4A-NA-C1A	-2.49	105.54	106.68
4	M	403	BCL	CAC-C3C-C4C	-2.49	107.06	112.58
5	M	404	BPH	CBC-CAC-C3C	-2.49	108.88	113.78
4	M	403	BCL	C1-C2-C3	2.48	130.27	126.20
4	M	403	BCL	O1D-CGD-CBD	2.48	129.41	124.52
6	M	405	U10	C7-C6-C1	-2.48	120.64	124.89
5	M	404	BPH	C3D-C4D-ND	-2.46	104.55	107.71
4	M	401	BCL	C1D-CHD-C4C	-2.44	120.73	126.62
5	M	404	BPH	C3D-CAD-CBD	2.43	110.81	107.61
4	L	302	BCL	C4-C3-C5	2.42	119.43	115.23
6	L	304	U10	C22-C23-C24	2.40	135.65	127.64
5	L	303	BPH	CAA-C2A-C3A	-2.39	106.53	113.00
4	M	403	BCL	C14-C13-C12	-2.39	102.75	111.27
4	M	403	BCL	CMA-C3A-C4A	2.39	118.19	111.77
4	M	403	BCL	C2A-C3A-C4A	2.37	105.70	101.87
4	M	403	BCL	CHB-C1B-NB	-2.37	120.50	124.05
4	L	302	BCL	C1-O2A-CGA	2.34	122.32	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	405	U10	C4M-O4-C4	2.34	124.70	116.47
4	M	403	BCL	O2A-CGA-O1A	-2.33	117.80	123.63
4	L	301	BCL	C3B-C4B-NB	2.33	112.83	109.76
6	M	405	U10	C37-C36-C34	2.32	120.87	113.19
4	M	401	BCL	CMC-C2C-C3C	-2.30	105.11	113.98
6	M	405	U10	C10-C9-C8	-2.28	117.77	123.63
6	L	304	U10	C20-C19-C18	-2.28	117.78	123.63
4	M	403	BCL	CAA-C2A-C3A	-2.27	106.85	113.00
5	L	303	BPH	C6-C7-C8	2.26	123.49	115.97
8	M	406	SPO	C4-C5-C6	-2.25	121.75	124.91
4	M	401	BCL	C2B-C1B-NB	-2.25	108.00	110.33
4	M	401	BCL	CBA-CAA-C2A	2.24	120.46	113.79
5	L	303	BPH	C1A-C2A-C3A	-2.22	100.73	102.84
4	L	301	BCL	CMD-C2D-C3D	-2.21	122.63	127.69
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
6	M	405	U10	C10-C9-C11	2.15	118.95	115.23
4	M	401	BCL	CED-O2D-CGD	-2.14	111.05	115.92
5	L	303	BPH	C14-C13-C12	2.14	118.89	111.27
4	M	401	BCL	C4-C3-C2	-2.13	109.76	126.43
5	L	303	BPH	CED-O2D-CGD	-2.13	111.08	115.92
6	M	405	U10	C20-C19-C21	2.12	118.91	115.23
5	L	303	BPH	O2A-CGA-O1A	2.12	128.92	123.63
4	M	403	BCL	CHC-C1C-NC	-2.12	121.34	124.40
5	L	303	BPH	C4D-ND-C1D	2.11	111.41	108.87
6	L	304	U10	C11-C9-C8	2.11	125.90	121.17
4	M	403	BCL	C2A-C1A-CHA	-2.10	120.23	123.87
6	M	405	U10	C20-C19-C18	-2.08	118.28	123.63
5	M	404	BPH	O1D-CGD-CBD	-2.07	121.58	124.72
5	M	404	BPH	OBB-CAB-C3B	2.07	123.44	119.99
4	L	302	BCL	C1D-CHD-C4C	-2.04	121.69	126.62
6	L	304	U10	C10-C9-C11	-2.04	111.69	115.23
4	L	301	BCL	C14-C13-C12	-2.03	104.04	111.27
6	M	405	U10	C3M-O3-C3	2.02	123.58	116.47
4	L	301	BCL	C4D-CHA-C1A	-2.02	118.83	121.24
4	L	301	BCL	C1D-CHD-C4C	-2.00	121.79	126.62
4	L	301	BCL	CBC-CAC-C3C	-2.00	109.17	113.41

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	303	BPH	C8

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Mol	Chain	Res	Type	Atom
5	L	303	BPH	C13

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	303	BPH	C4C-C3C-CAC-CBC
5	L	303	BPH	C14-C13-C15-C16
5	M	404	BPH	C2C-C3C-CAC-CBC
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	C17-C18-C19-C21
6	M	405	U10	C12-C13-C14-C15
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
6	M	405	U10	C37-C38-C39-C40
6	L	304	U10	C17-C18-C19-C20
6	M	405	U10	C12-C13-C14-C16
6	L	304	U10	C9-C11-C12-C13
6	L	304	U10	C14-C16-C17-C18
6	M	405	U10	C14-C16-C17-C18
8	M	406	SPO	C33-C35-C36-C37
4	M	403	BCL	CBD-CGD-O2D-CED
6	L	304	U10	C22-C23-C24-C26
5	L	303	BPH	C11-C10-C8-C9
4	L	302	BCL	CBD-CGD-O2D-CED
5	L	303	BPH	C6-C7-C8-C10
6	L	304	U10	C15-C14-C16-C17
6	L	304	U10	C19-C21-C22-C23
4	L	302	BCL	C15-C16-C17-C18
5	L	303	BPH	C5-C6-C7-C8
6	L	304	U10	C22-C23-C24-C25
5	L	303	BPH	C3-C5-C6-C7
4	M	401	BCL	CBA-CGA-O2A-C1
4	L	302	BCL	O1D-CGD-O2D-CED
6	L	304	U10	C13-C14-C16-C17
4	M	401	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
6	M	405	U10	C23-C24-C26-C27
5	L	303	BPH	C11-C10-C8-C7
5	L	303	BPH	C4-C3-C5-C6
5	L	303	BPH	C2-C3-C5-C6
8	M	406	SPO	C4-C1-O1-CM1
6	M	405	U10	C25-C24-C26-C27
5	L	303	BPH	O2A-C1-C2-C3
4	M	403	BCL	O1D-CGD-O2D-CED
6	M	405	U10	C24-C26-C27-C28
8	M	406	SPO	C2-C1-O1-CM1
5	L	303	BPH	C8-C10-C11-C12
8	M	406	SPO	C24-C23-C25-C26
4	M	401	BCL	O2A-C1-C2-C3
4	M	403	BCL	C2B-C3B-CAB-OBB
4	M	403	BCL	C2B-C3B-CAB-CBB
5	L	303	BPH	C12-C13-C15-C16
4	L	302	BCL	C16-C17-C18-C20
6	M	405	U10	C5-C4-O4-C4M
4	M	403	BCL	CHA-CBD-CGD-O1D
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
6	M	405	U10	C20-C19-C21-C22
4	M	403	BCL	C4B-C3B-CAB-OBB
5	L	303	BPH	C6-C7-C8-C9
5	M	404	BPH	CHA-CBD-CGD-O1D
5	M	404	BPH	CBA-CGA-O2A-C1
4	M	403	BCL	C4B-C3B-CAB-CBB
8	M	406	SPO	C22-C23-C25-C26
6	M	405	U10	C3-C4-O4-C4M
4	M	403	BCL	CAA-CBA-CGA-O2A
4	M	403	BCL	C5-C6-C7-C8
6	M	405	U10	C21-C22-C23-C24
5	M	404	BPH	O1A-CGA-O2A-C1

There are no ring outliers.

9 monomers are involved in 70 short contacts:

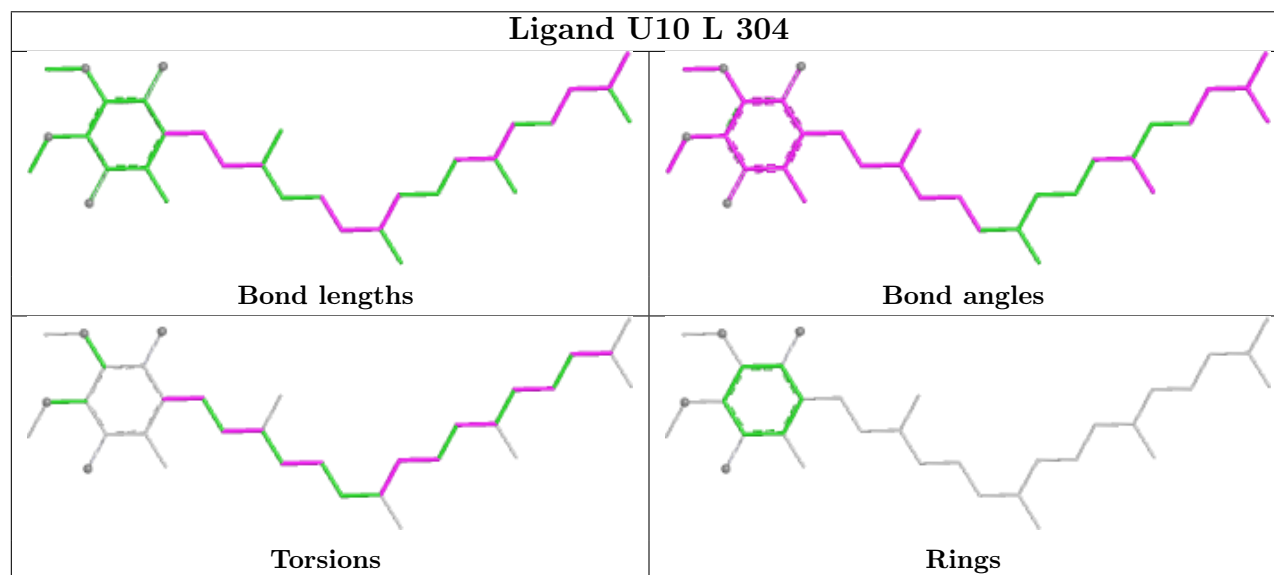
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	304	U10	11	0

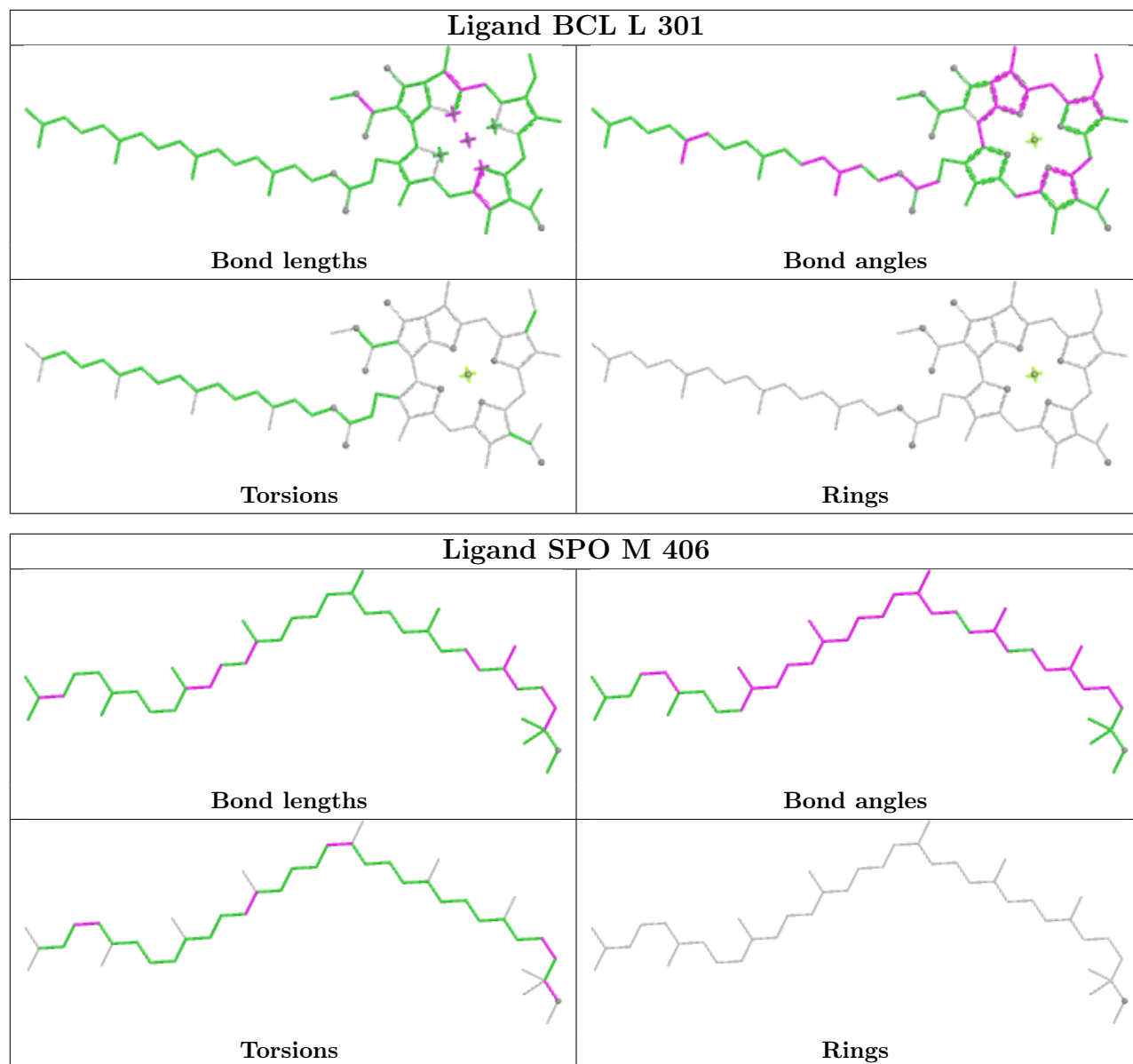
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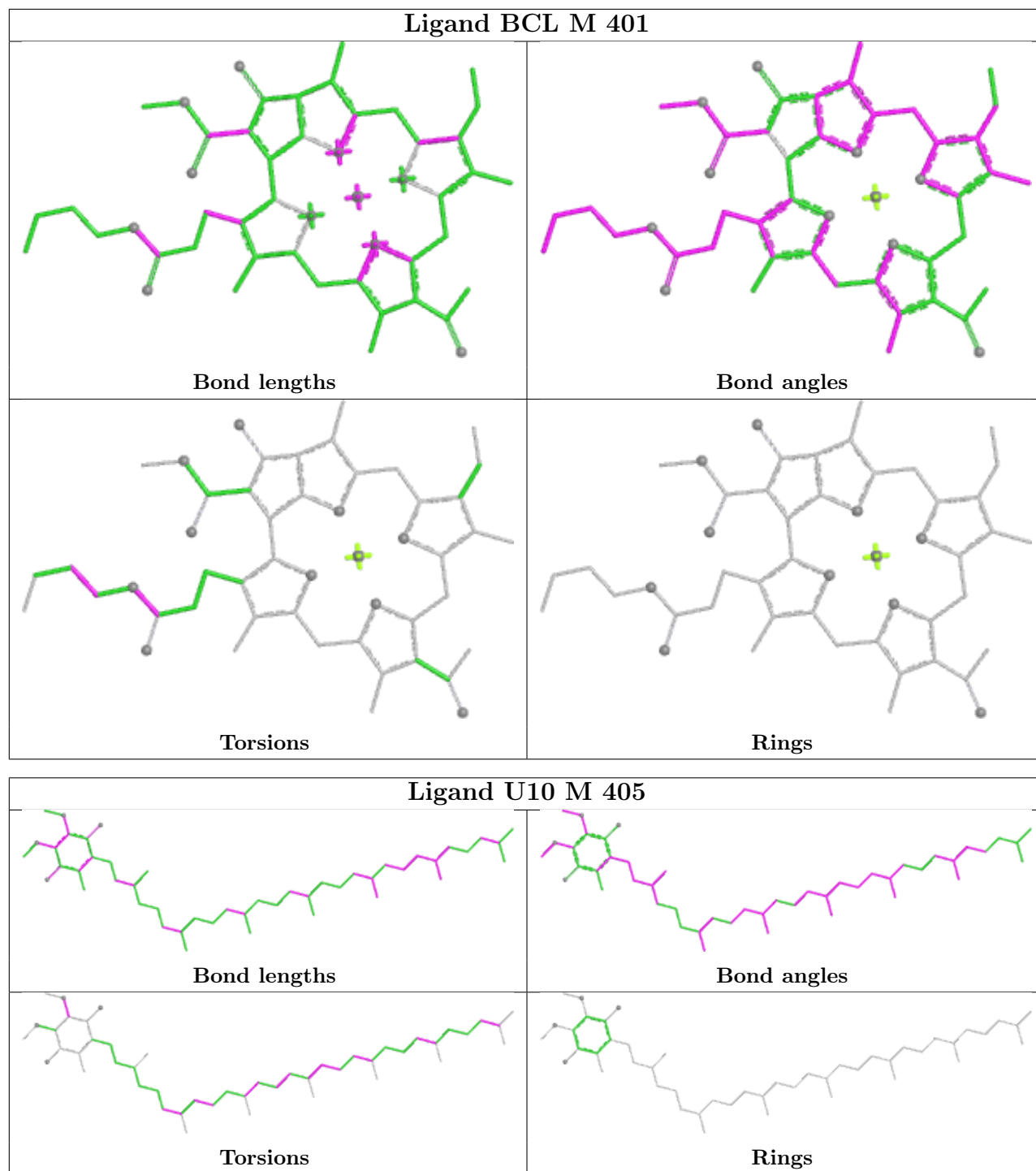
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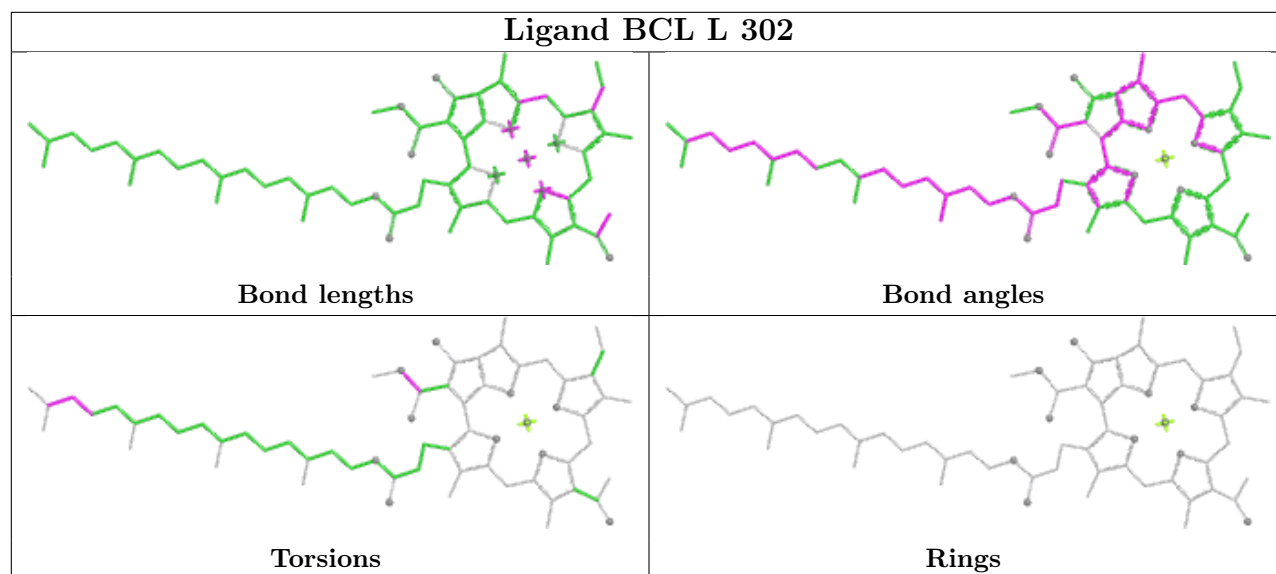
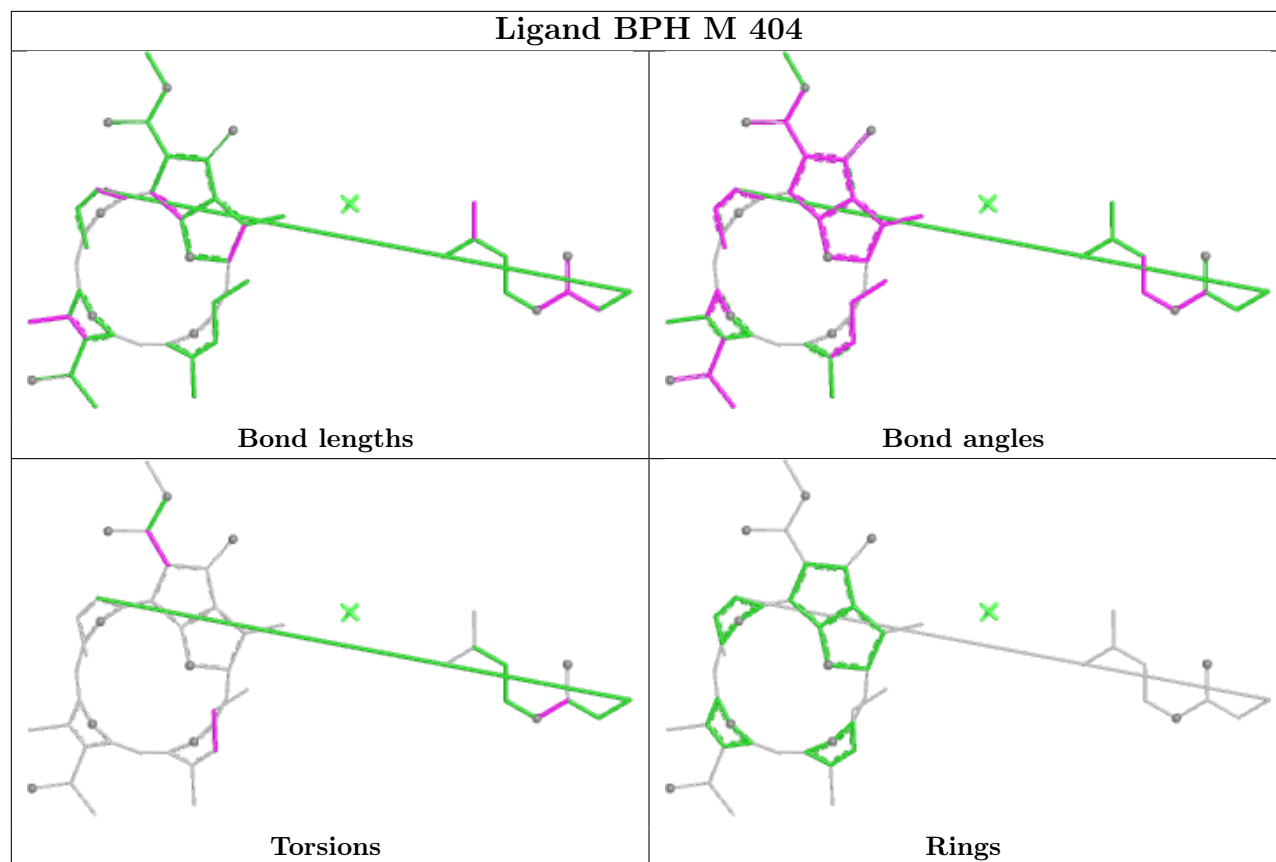
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	301	BCL	2	0
8	M	406	SPO	13	0
4	M	401	BCL	6	0
6	M	405	U10	1	0
5	M	404	BPH	8	0
4	L	302	BCL	7	0
5	L	303	BPH	14	0
4	M	403	BCL	16	0

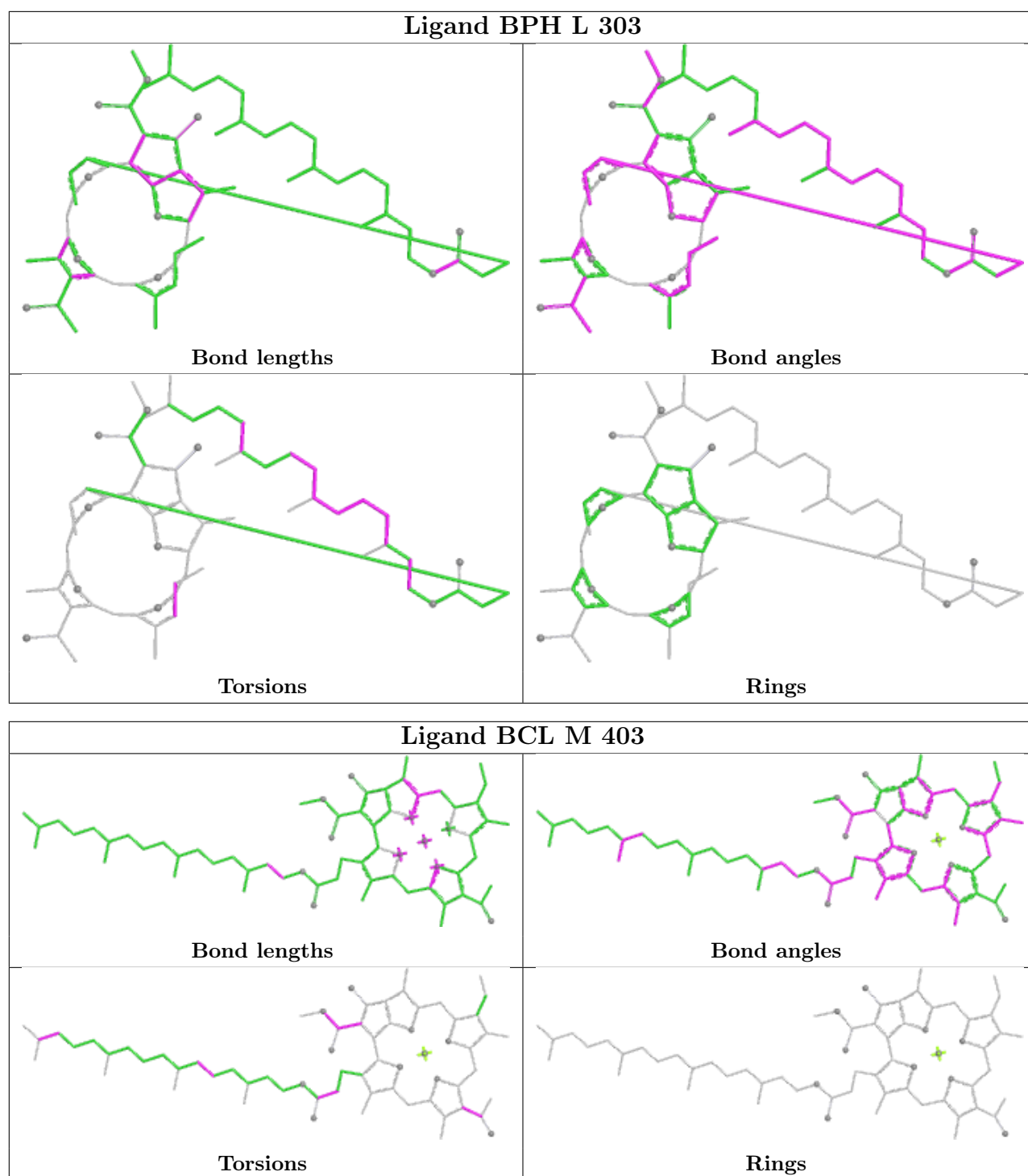
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	281/281 (100%)	-0.71	1 (0%) 88 79	35, 48, 83, 98	0
2	M	302/313 (96%)	-0.62	3 (0%) 79 63	34, 52, 82, 108	0
3	H	240/260 (92%)	-0.69	0 100 100	38, 52, 69, 96	0
All	All	823/854 (96%)	-0.67	4 (0%) 87 75	34, 50, 81, 108	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	1	ALA	2.6
2	M	302	GLY	2.4
2	M	301	HIS	2.4
2	M	1	ALA	2.2

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 [i](#)

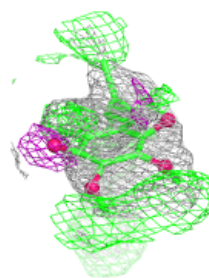
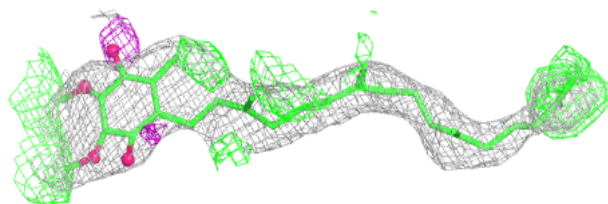
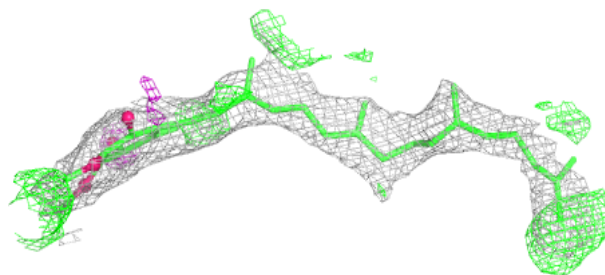
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	U10	L	304	33/63	0.71	0.25	64,85,99,101	0
8	SPO	M	406	42/42	0.92	0.18	64,87,114,116	0
5	BPH	M	404	51/65	0.94	0.09	36,54,66,101	0
6	U10	M	405	48/63	0.96	0.09	31,50,76,82	0
4	BCL	M	401	50/66	0.96	0.08	35,43,80,100	0
4	BCL	L	302	66/66	0.97	0.06	24,34,54,64	0
4	BCL	M	403	66/66	0.98	0.06	30,51,61,77	0
5	BPH	L	303	65/65	0.98	0.05	27,38,50,54	0
4	BCL	L	301	66/66	0.98	0.06	34,48,55,58	0
7	FE	M	402	1/1	1.00	0.01	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.

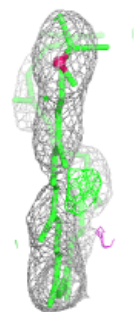
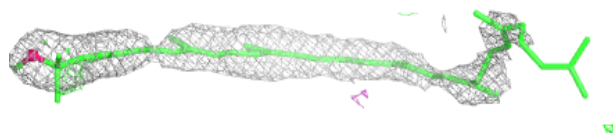
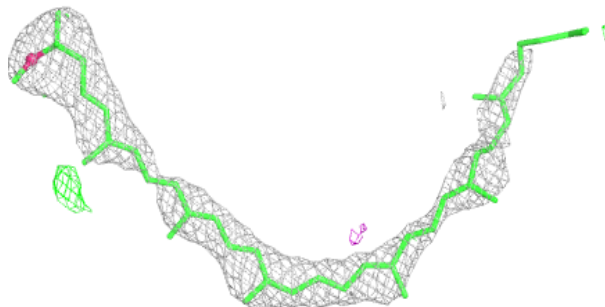
Electron density around U10 L 304:

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

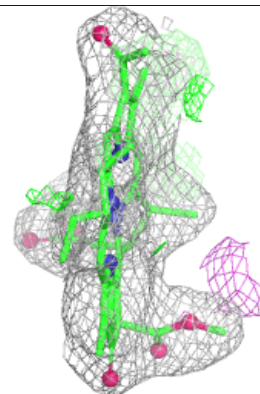
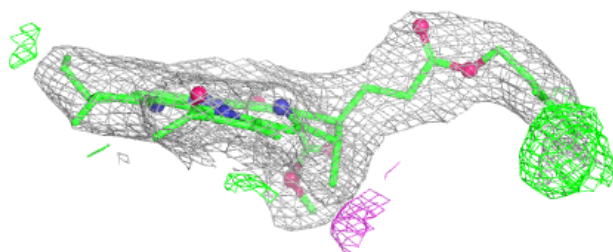
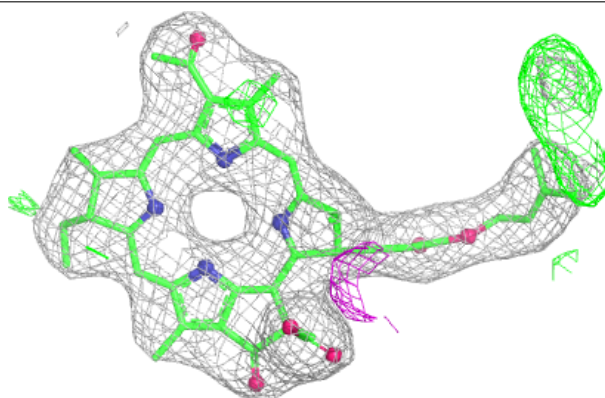


Electron density around SPO M 406:

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

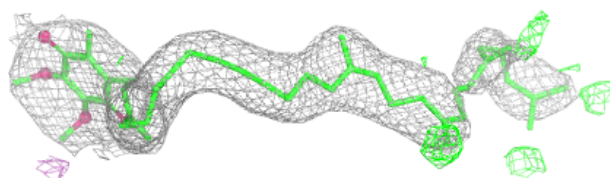
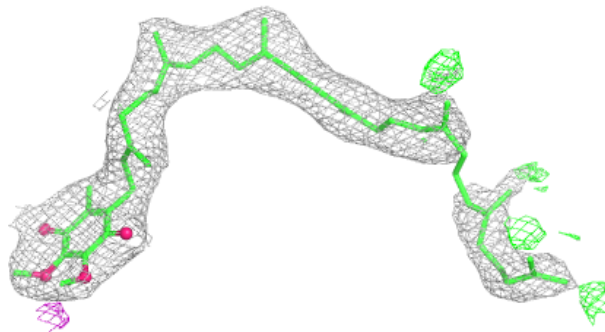
**Electron density around BPH M 404:**

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



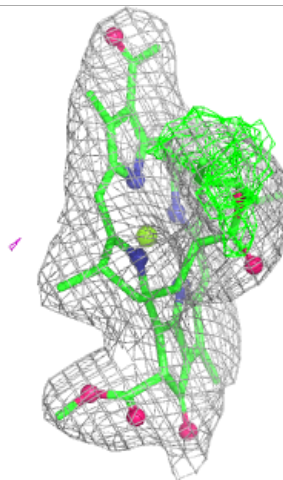
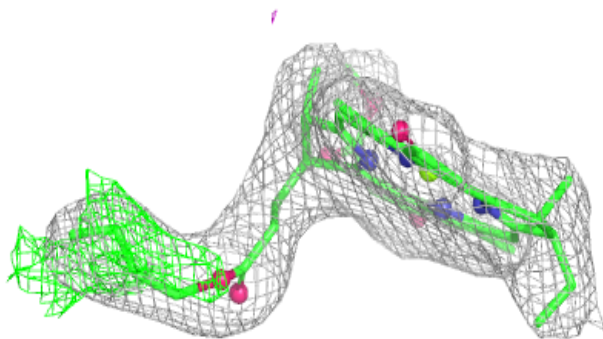
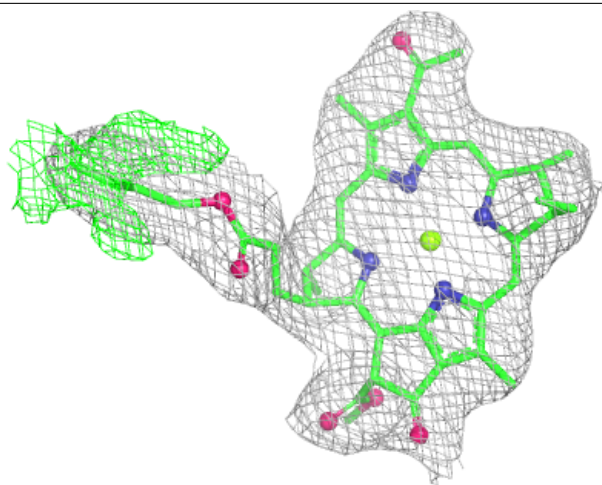
Electron density around U10 M 405:

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



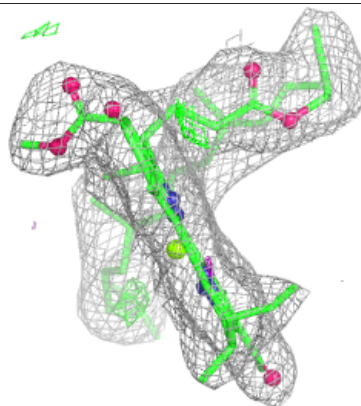
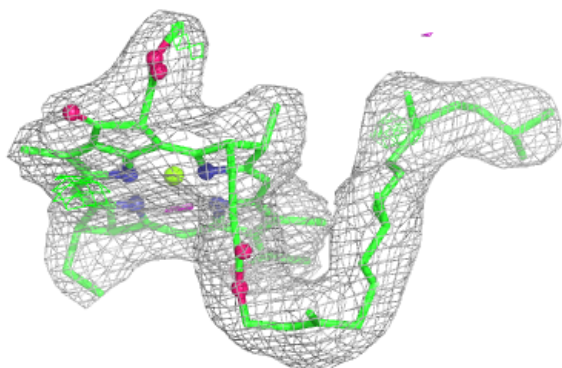
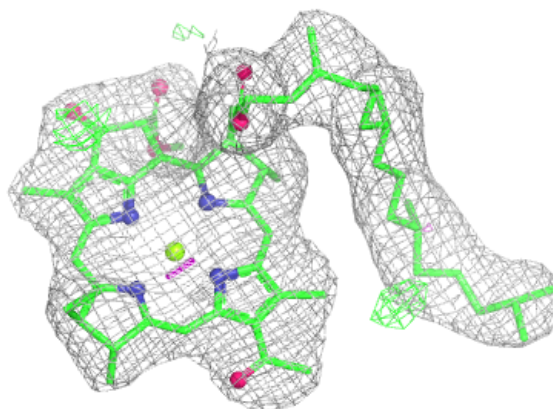
Electron density around BCL M 401:

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

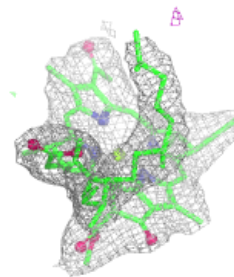
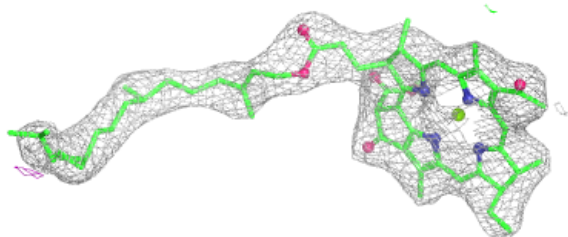
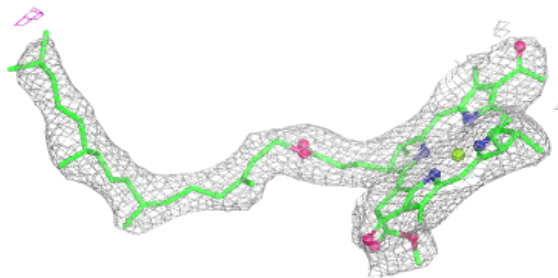


Electron density around BCL L 302:

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

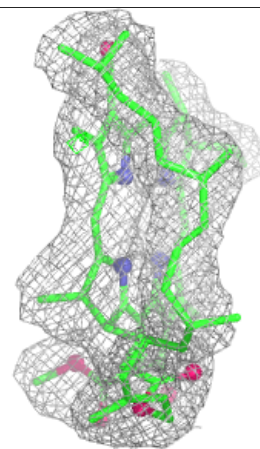
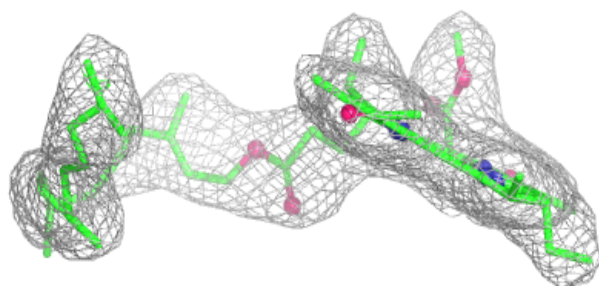
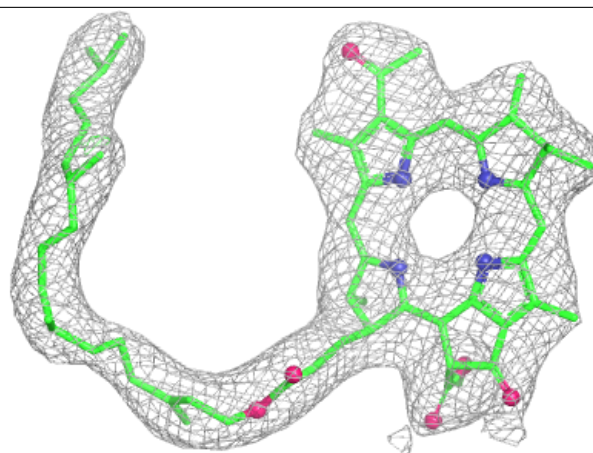
**Electron density around BCL M 403:**

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



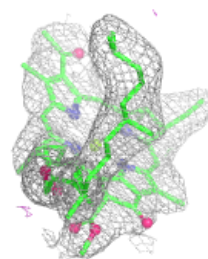
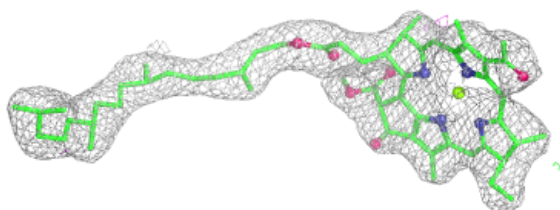
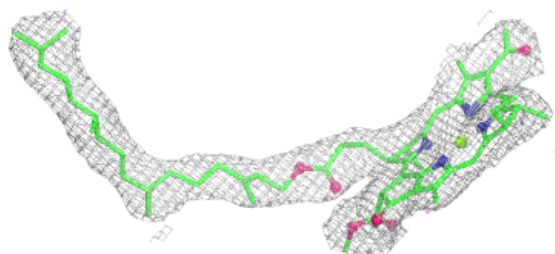
Electron density around BPH L 303:

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



Electron density around BCL 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.