



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:39 AM UTC

PDB ID : 1K6L / pdb_00001k6l
Title : Photosynthetic Reaction Center from Rhodobacter sphaeroides
Authors : Pokkuluri, P.R.; Laible, P.D.; Deng, Y.-L.; Wong, T.N.; Hanson, D.K.; Schiffer, M.
Deposited on : 2001-10-16
Resolution : 3.10 Å(reported)

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

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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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

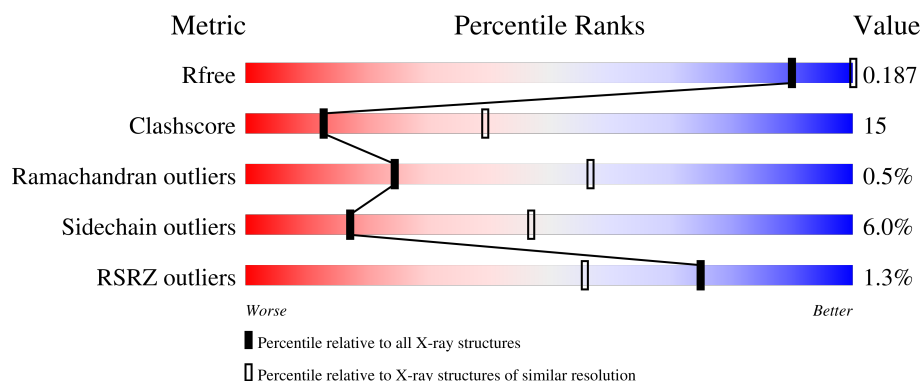
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	0.187 65% 29% 5%
2	M	314	2% 61% 29% 6%
3	H	260	0.187 63% 27% 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
4	BCL	L	304	X	-	-	-
4	BCL	M	501	X	-	-	-
5	BPH	M	401	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7285 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 PHOTOSYNTHETIC REACTION CENTER L SUBUNIT.

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

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER M SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	0	0
			2408	1607	394	397	10			

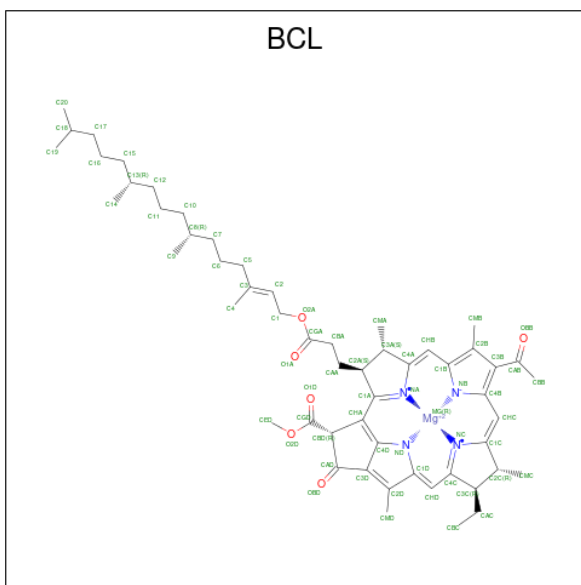
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	308	HIS	-	expression tag	UNP P02953
M	309	HIS	-	expression tag	UNP P02953
M	310	HIS	-	expression tag	UNP P02953
M	311	HIS	-	expression tag	UNP P02953
M	312	HIS	-	expression tag	UNP P02953
M	313	HIS	-	expression tag	UNP P02953
M	314	HIS	-	expression tag	UNP P02953

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER H SUBUNIT.

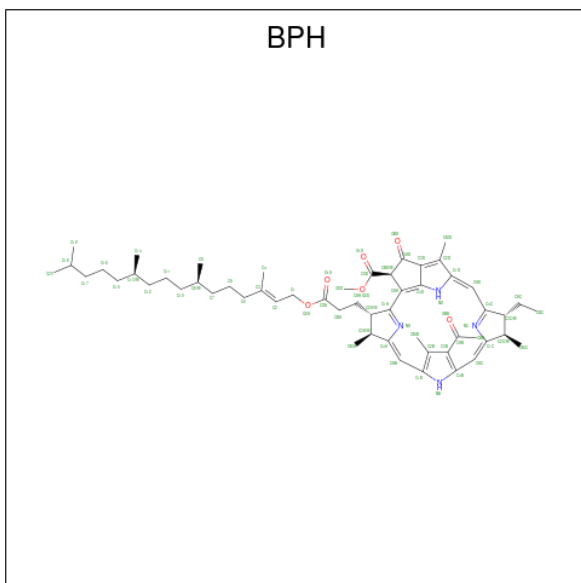
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



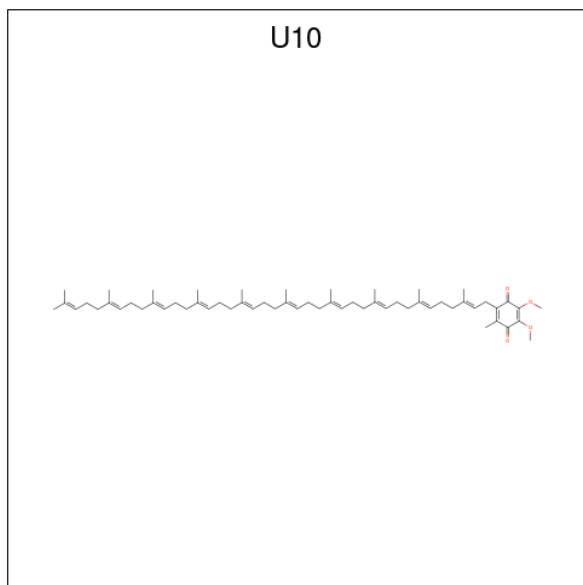
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



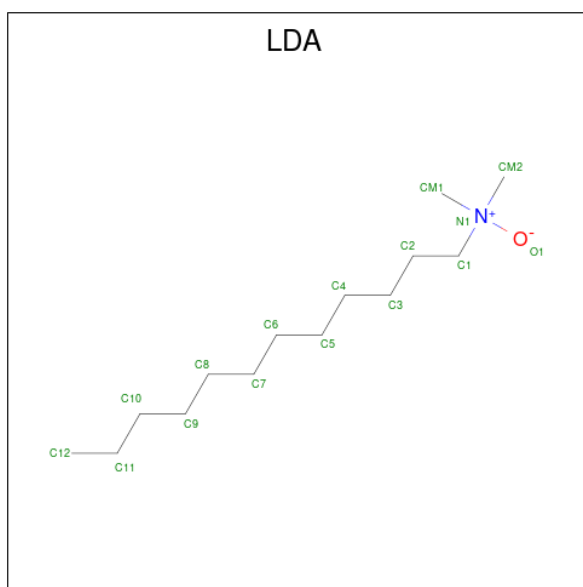
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	10	0
			65	55	4	6		

- 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
			48	44	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).

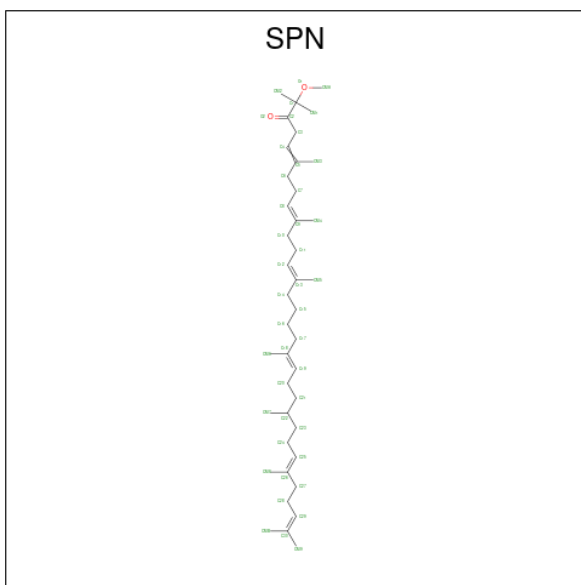


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

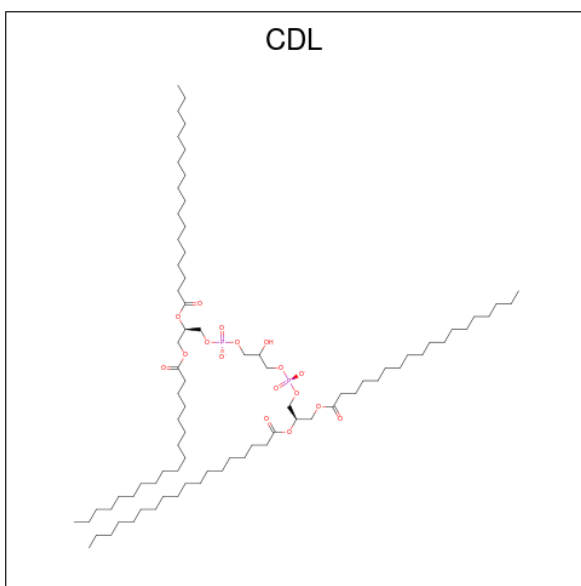
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is SPEROIDENONE (CCD ID: SPN) (formula: C₄₁H₇₀O₂).



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

- Molecule 10 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

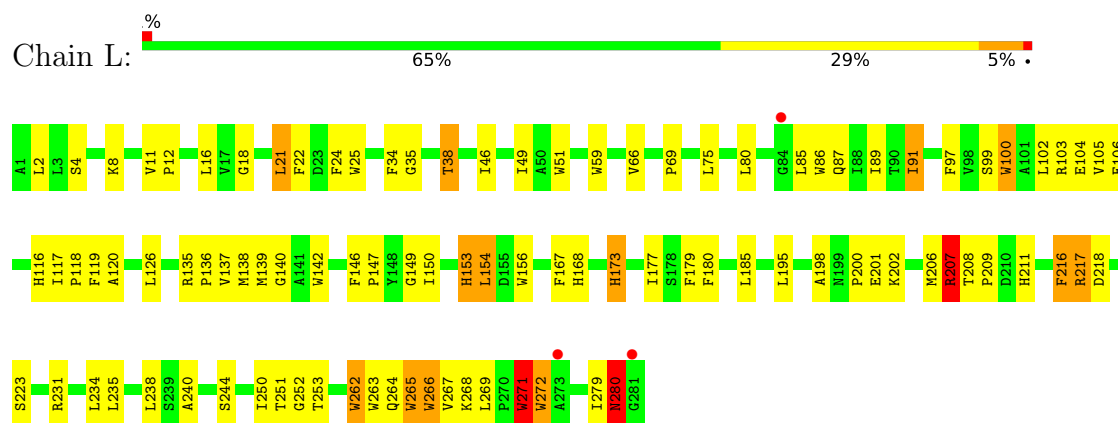
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	37	Total 37	O 37	0	0
11	M	40	Total 40	O 40	0	0
11	H	60	Total 60	O 60	0	0

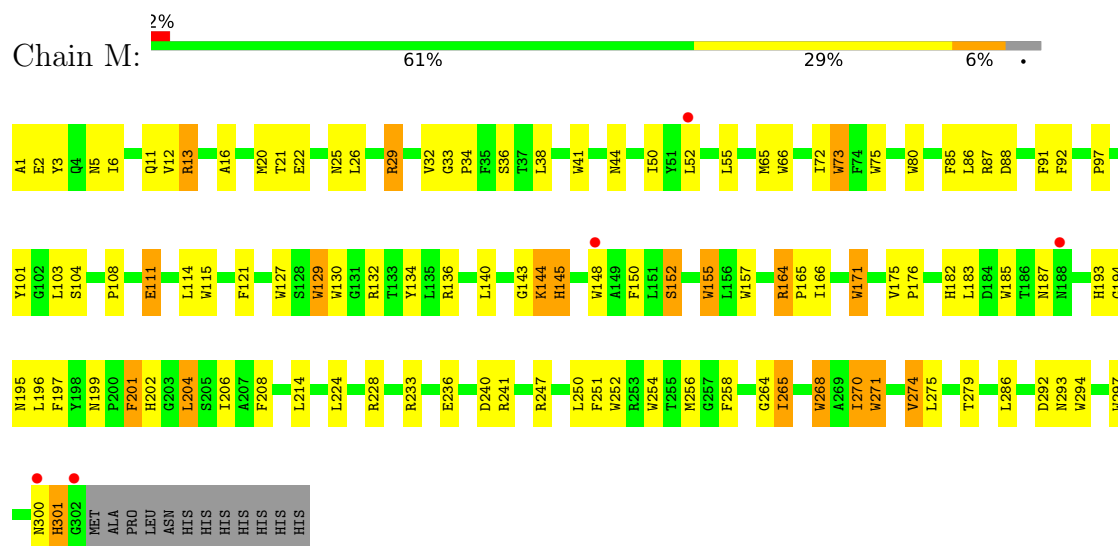
3 Residue-property plots [i](#)

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

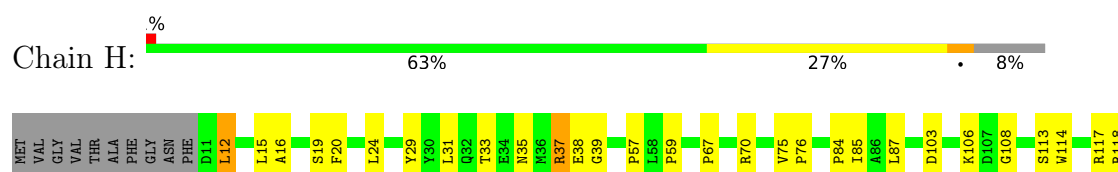
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER L SUBUNIT

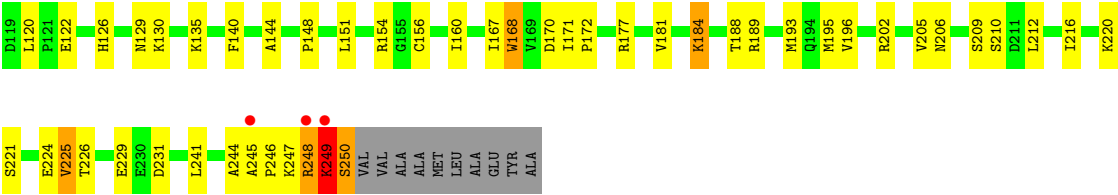


• Molecule 2: PHOTOSYNTHETIC REACTION CENTER M SUBUNIT



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER H SUBUNIT





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.50Å 141.50Å 187.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.10 10.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	81.4 (10.00-3.10) 89.4 (10.00-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 3.09Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.194 0.187 , 0.187	Depositor DCC
R_{free} test set	2565 reflections (7.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 87.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7285	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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, BPH, LDA, FE, SPN, BCL, CDL

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	1.11	13/2320 (0.6%)	1.25	8/3175 (0.3%)
2	M	1.16	20/2500 (0.8%)	1.28	13/3413 (0.4%)
3	H	1.11	3/1877 (0.2%)	1.32	11/2553 (0.4%)
All	All	1.13	36/6697 (0.5%)	1.28	32/9141 (0.4%)

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

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	145	HIS	C-N	-8.37	1.23	1.33
1	L	280	ASN	C-N	-5.98	1.25	1.33
2	M	155	TRP	NE1-CE2	-5.71	1.31	1.37
1	L	265	TRP	NE1-CE2	-5.64	1.31	1.37
1	L	59	TRP	NE1-CE2	-5.57	1.31	1.37
3	H	114	TRP	NE1-CE2	-5.54	1.31	1.37
2	M	75	TRP	NE1-CE2	-5.50	1.31	1.37
1	L	266	TRP	NE1-CE2	-5.48	1.31	1.37
2	M	66	TRP	NE1-CE2	-5.44	1.31	1.37
2	M	252	TRP	NE1-CE2	-5.43	1.31	1.37
2	M	73	TRP	NE1-CE2	-5.42	1.31	1.37
2	M	271	TRP	NE1-CE2	-5.38	1.31	1.37
1	L	137	VAL	C-N	-5.35	1.26	1.34
2	M	148	TRP	NE1-CE2	-5.35	1.31	1.37
3	H	168	TRP	NE1-CE2	-5.34	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	41	TRP	NE1-CE2	-5.33	1.31	1.37
2	M	268	TRP	NE1-CE2	-5.33	1.31	1.37
1	L	100	TRP	NE1-CE2	-5.30	1.31	1.37
2	M	297	TRP	NE1-CE2	-5.29	1.31	1.37
1	L	271	TRP	NE1-CE2	-5.27	1.31	1.37
2	M	294	TRP	NE1-CE2	-5.27	1.31	1.37
2	M	171	TRP	NE1-CE2	-5.27	1.31	1.37
1	L	272	TRP	NE1-CE2	-5.26	1.31	1.37
1	L	25	TRP	NE1-CE2	-5.24	1.31	1.37
2	M	254	TRP	NE1-CE2	-5.24	1.31	1.37
2	M	115	TRP	NE1-CE2	-5.24	1.31	1.37
1	L	262	TRP	NE1-CE2	-5.21	1.31	1.37
2	M	127	TRP	NE1-CE2	-5.20	1.31	1.37
1	L	156	TRP	NE1-CE2	-5.19	1.31	1.37
2	M	185	TRP	NE1-CE2	-5.16	1.31	1.37
2	M	129	TRP	NE1-CE2	-5.16	1.31	1.37
1	L	263	TRP	NE1-CE2	-5.16	1.31	1.37
3	H	250	SER	C-O	5.13	1.33	1.23
2	M	157	TRP	NE1-CE2	-5.06	1.31	1.37
1	L	51	TRP	NE1-CE2	-5.05	1.31	1.37
2	M	80	TRP	NE1-CE2	-5.00	1.31	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	280	ASN	O-C-N	-8.08	112.42	122.35
2	M	176	PRO	CB-CA-C	-6.14	102.93	110.98
3	H	120	LEU	O-C-N	-6.08	115.56	121.94
3	H	57	PRO	CB-CA-C	-6.07	103.00	110.95
1	L	217	ARG	NE-CZ-NH2	6.03	124.62	119.20
3	H	249	LYS	N-CA-C	6.02	120.38	112.13
1	L	35	GLY	N-CA-C	-6.02	105.52	112.50
2	M	201	PHE	CA-CB-CG	-5.99	107.81	113.80
1	L	217	ARG	NH1-CZ-NH2	-5.84	111.71	119.30
2	M	268	TRP	N-CA-C	-5.64	105.03	111.07
2	M	1	ALA	CB-CA-C	5.61	118.91	110.50
2	M	143	GLY	N-CA-C	-5.54	106.23	112.33
2	M	199	ASN	CA-C-N	-5.54	113.96	119.56
2	M	199	ASN	C-N-CA	-5.54	113.96	119.56
1	L	173	HIS	CA-CB-CG	5.41	119.21	113.80
2	M	145	HIS	O-C-N	5.40	127.86	122.08
1	L	103	ARG	NH1-CZ-NH2	-5.36	112.33	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	202	ARG	NE-CZ-NH2	5.34	124.01	119.20
3	H	154	ARG	NE-CZ-NH2	5.32	123.99	119.20
2	M	6	ILE	N-CA-C	-5.30	105.96	111.58
3	H	117	ARG	NE-CZ-NH2	5.29	123.96	119.20
3	H	70	ARG	NE-CZ-NH2	5.29	123.96	119.20
2	M	164	ARG	NE-CZ-NH2	5.29	123.96	119.20
2	M	247	ARG	NE-CZ-NH2	5.27	123.94	119.20
3	H	37	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	L	231	ARG	NE-CZ-NH2	5.26	123.93	119.20
2	M	13	ARG	NE-CZ-NH2	5.25	123.93	119.20
3	H	248	ARG	NE-CZ-NH2	5.22	123.90	119.20
3	H	29	TYR	N-CA-C	-5.08	105.83	111.36
3	H	126	HIS	CA-CB-CG	-5.07	108.73	113.80
2	M	286	LEU	N-CA-C	-5.02	107.11	113.18
1	L	207	ARG	NE-CZ-NH2	5.01	123.71	119.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	280	ASN	Mainchain

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	2232	0	2187	78	0
2	M	2408	0	2321	77	0
3	H	1829	0	1836	52	0
4	L	132	0	148	15	0
4	M	132	0	148	18	0
5	L	65	0	76	4	0
5	M	65	0	76	1	0
6	L	48	0	63	6	0
6	M	48	0	63	6	0
7	H	16	0	31	4	0
7	L	16	0	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	32	0	62	4	0
8	M	1	0	0	0	0
9	M	43	0	69	1	0
10	M	81	0	106	1	0
11	H	60	0	0	2	0
11	L	37	0	0	1	0
11	M	40	0	0	1	0
All	All	7285	0	7217	216	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 15.

All (216) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:33:THR:O	3:H:59:PRO:HG3	1.69	0.91
1:L:34:PHE:O	1:L:38:THR:HG23	1.71	0.89
6:M:503:U10:H202	7:H:703:LDA:H112	1.54	0.88
2:M:204:LEU:HB3	2:M:279:THR:HG21	1.56	0.85
2:M:197:PHE:HZ	4:M:502:BCL:HBB2	1.47	0.80
4:L:302:BCL:HHC	4:L:302:BCL:OBB	1.81	0.79
1:L:179:PHE:CE1	6:L:502:U10:H18	2.21	0.76
2:M:21:THR:CG2	2:M:26:LEU:HD11	2.15	0.76
2:M:21:THR:HG23	2:M:26:LEU:HD21	1.67	0.76
2:M:197:PHE:CZ	4:M:502:BCL:HBB2	2.22	0.75
2:M:256:MET:HE3	2:M:258:PHE:CE1	2.22	0.74
4:M:502:BCL:CBB	4:M:502:BCL:HHC	2.19	0.73
2:M:270:ILE:HD13	10:M:800:CDL:H711	1.71	0.72
1:L:91:ILE:HG13	7:L:709:LDA:H91	1.71	0.72
2:M:152:SER:O	2:M:155:TRP:HB3	1.91	0.70
2:M:208:PHE:HE1	7:M:701:LDA:H91	1.55	0.70
1:L:91:ILE:CG1	7:L:709:LDA:H91	2.22	0.70
2:M:256:MET:HE3	2:M:258:PHE:CZ	2.28	0.68
1:L:208:THR:HB	1:L:209:PRO:HD2	1.76	0.68
2:M:21:THR:HG21	2:M:26:LEU:HD11	1.75	0.68
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.76	0.68
4:M:502:BCL:HHC	4:M:502:BCL:HBB3	1.77	0.67
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.76	0.67
2:M:130:TRP:HD1	2:M:150:PHE:CD2	2.13	0.67
4:M:501:BCL:C11	4:M:502:BCL:H203	2.26	0.66
4:L:304:BCL:HMB1	4:L:304:BCL:HBB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:249:LYS:O	3:H:250:SER:C	2.41	0.64
6:M:503:U10:H202	7:H:703:LDA:C11	2.27	0.64
3:H:241:LEU:O	3:H:248:ARG:NH2	2.30	0.64
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.34	0.63
1:L:216:PHE:CE2	6:L:502:U10:H4M2	2.34	0.63
2:M:13:ARG:O	3:H:140:PHE:HA	1.97	0.63
1:L:38:THR:HG22	1:L:99:SER:HB3	1.79	0.63
2:M:193:HIS:O	2:M:293:ASN:HA	1.98	0.63
4:M:501:BCL:H111	4:M:502:BCL:H203	1.81	0.61
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.83	0.61
2:M:134:TYR:CE2	2:M:144:LYS:HG2	2.36	0.61
4:L:304:BCL:H192	5:L:402:BPH:H7C2	1.83	0.60
3:H:37:ARG:HH11	3:H:37:ARG:HG2	1.67	0.60
1:L:16:LEU:N	1:L:106:GLU:OE2	2.31	0.60
1:L:168:HIS:CD2	4:M:501:BCL:HMD2	2.37	0.60
5:L:402:BPH:HBB3	5:L:402:BPH:HMB3	1.83	0.59
2:M:130:TRP:HD1	2:M:150:PHE:HD2	1.49	0.59
1:L:244:SER:OG	4:L:302:BCL:HMA2	2.02	0.59
1:L:8:LYS:HA	3:H:87:LEU:CD1	2.32	0.59
3:H:244:ALA:C	3:H:246:PRO:HD2	2.27	0.59
3:H:148:PRO:HA	3:H:151:LEU:HD12	1.84	0.59
2:M:194:GLY:O	2:M:195:ASN:HB3	2.03	0.58
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.85	0.58
2:M:208:PHE:CE1	7:M:701:LDA:H91	2.37	0.58
1:L:8:LYS:HA	3:H:87:LEU:HD11	1.85	0.58
1:L:116:HIS:O	1:L:119:PHE:HB3	2.04	0.58
3:H:177:ARG:O	3:H:193:MET:HB2	2.03	0.57
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.40	0.57
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.85	0.57
1:L:180:PHE:CE2	1:L:240:ALA:HB1	2.39	0.56
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.86	0.56
1:L:85:LEU:O	1:L:89:ILE:HG13	2.06	0.56
1:L:38:THR:HG22	1:L:99:SER:CB	2.35	0.56
4:M:501:BCL:HBB2	4:M:501:BCL:HMB3	1.88	0.56
3:H:129:ASN:ND2	3:H:224:GLU:HG2	2.22	0.55
1:L:201:GLU:OE2	2:M:144:LYS:NZ	2.39	0.55
1:L:87:GLN:HE21	1:L:142:TRP:CD1	2.25	0.55
1:L:269:LEU:HB2	1:L:272:TRP:NE1	2.22	0.54
1:L:4:SER:OG	3:H:39:GLY:HA2	2.07	0.54
1:L:218:ASP:OD1	2:M:29:ARG:HD3	2.08	0.54
1:L:271:TRP:H	1:L:271:TRP:CD1	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:72:ILE:HG13	2:M:73:TRP:N	2.22	0.54
2:M:85:PHE:HD2	2:M:86:LEU:HD12	1.73	0.54
2:M:130:TRP:CD1	2:M:150:PHE:HD2	2.25	0.54
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.90	0.53
1:L:250:ILE:HD12	6:L:502:U10:H402	1.90	0.53
1:L:267:VAL:HG21	1:L:280:ASN:ND2	2.24	0.53
3:H:84:PRO:C	3:H:85:ILE:HD13	2.34	0.53
4:L:302:BCL:H203	4:L:304:BCL:H102	1.91	0.53
1:L:271:TRP:CD1	1:L:271:TRP:N	2.77	0.52
3:H:20:PHE:HE2	3:H:24:LEU:HD22	1.74	0.52
1:L:142:TRP:CZ2	7:L:709:LDA:H51	2.44	0.52
7:M:701:LDA:H101	7:H:703:LDA:C12	2.39	0.52
1:L:223:SER:O	2:M:44:ASN:HB2	2.10	0.52
1:L:234:LEU:O	1:L:238:LEU:HG	2.09	0.52
2:M:32:VAL:HG12	2:M:33:GLY:O	2.10	0.52
2:M:44:ASN:HB3	11:M:809:HOH:O	2.10	0.52
2:M:101:TYR:O	2:M:104:SER:HB2	2.10	0.51
2:M:187:ASN:HA	4:M:502:BCL:CB	2.40	0.51
2:M:300:ASN:O	2:M:301:HIS:HB2	2.10	0.51
1:L:195:LEU:HB3	2:M:145:HIS:CD2	2.45	0.51
3:H:168:TRP:CZ3	3:H:225:VAL:HG22	2.44	0.51
5:L:402:BPH:ND	2:M:214:LEU:HD13	2.26	0.51
2:M:20:MET:O	2:M:29:ARG:NH2	2.44	0.50
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.10	0.50
3:H:84:PRO:O	3:H:85:ILE:HD13	2.11	0.50
2:M:250:LEU:O	2:M:251:PHE:C	2.53	0.50
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.47	0.50
2:M:175:VAL:HG11	9:M:600:SPN:H161	1.93	0.49
1:L:75:LEU:HD11	1:L:140:GLY:HA2	1.94	0.49
1:L:223:SER:OG	6:L:502:U10:H3M1	2.11	0.49
1:L:135:ARG:HB3	1:L:136:PRO:CD	2.42	0.49
2:M:241:ARG:NH1	3:H:38:GLU:OE1	2.41	0.49
1:L:262:TRP:O	1:L:265:TRP:HD1	1.95	0.49
1:L:11:VAL:HB	1:L:12:PRO:HD2	1.94	0.49
4:L:302:BCL:HAA2	4:L:304:BCL:HAC1	1.93	0.49
3:H:12:LEU:O	3:H:15:LEU:HB3	2.12	0.49
1:L:168:HIS:HB3	2:M:183:LEU:HD13	1.95	0.49
1:L:207:ARG:HG3	1:L:211:HIS:CG	2.47	0.49
2:M:88:ASP:HB2	2:M:92:PHE:CZ	2.48	0.48
2:M:251:PHE:C	2:M:251:PHE:CD1	2.91	0.48
5:L:402:BPH:HMB3	5:L:402:BPH:CBB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:184:LYS:O	3:H:184:LYS:HG3	2.10	0.48
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.95	0.48
2:M:101:TYR:O	2:M:104:SER:CB	2.62	0.48
4:L:302:BCL:OBB	4:L:302:BCL:CHC	2.55	0.48
1:L:104:GLU:HB3	1:L:118:PRO:HG3	1.96	0.47
3:H:20:PHE:CE2	3:H:24:LEU:HD22	2.48	0.47
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.82	0.47
1:L:139:MET:HE3	1:L:252:GLY:HA3	1.95	0.47
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.95	0.47
1:L:168:HIS:CD2	4:M:501:BCL:CMD	2.98	0.47
2:M:130:TRP:CD1	2:M:150:PHE:CD2	3.00	0.47
7:M:701:LDA:H101	7:H:703:LDA:H121	1.97	0.47
1:L:49:ILE:HG12	1:L:89:ILE:HD13	1.97	0.46
1:L:279:ILE:HG21	2:M:91:PHE:HB3	1.97	0.46
3:H:170:ASP:HB2	3:H:177:ARG:HG3	1.97	0.46
1:L:102:LEU:O	1:L:105:VAL:HB	2.15	0.46
1:L:22:PHE:HA	1:L:24:PHE:HE2	1.80	0.46
1:L:177:ILE:HG23	4:L:302:BCL:HMB3	1.97	0.46
1:L:34:PHE:HB2	11:L:712:HOH:O	2.15	0.45
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.98	0.45
1:L:138:MET:HE2	1:L:253:THR:HG21	1.98	0.45
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.52	0.45
6:L:502:U10:H372	6:L:502:U10:H351	1.70	0.45
2:M:240:ASP:HB2	3:H:118:ARG:HH21	1.82	0.45
3:H:12:LEU:HD12	3:H:12:LEU:HA	1.72	0.45
3:H:129:ASN:HD22	3:H:224:GLU:HG2	1.82	0.45
2:M:25:ASN:OD1	2:M:25:ASN:C	2.59	0.45
2:M:268:TRP:CD1	6:M:503:U10:H111	2.52	0.45
3:H:148:PRO:HD2	3:H:167:ILE:HD11	1.98	0.44
3:H:171:ILE:HB	3:H:172:PRO:CD	2.47	0.44
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.17	0.44
2:M:201:PHE:HD1	2:M:279:THR:HG23	1.83	0.44
1:L:207:ARG:NH1	2:M:140:LEU:O	2.47	0.44
6:L:502:U10:H271	6:L:502:U10:H251	1.79	0.44
3:H:209:SER:O	3:H:210:SER:C	2.61	0.44
1:L:217:ARG:O	2:M:50:ILE:HA	2.18	0.43
1:L:264:GLN:O	1:L:268:LYS:HB2	2.17	0.43
2:M:236:GLU:HB3	11:H:709:HOH:O	2.19	0.43
3:H:189:ARG:HD2	3:H:216:ILE:HB	1.99	0.43
6:M:503:U10:H322	6:M:503:U10:H28	1.48	0.43
4:L:302:BCL:HMB1	4:L:302:BCL:HBB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:2:GLU:OE2	2:M:228:ARG:NH2	2.51	0.43
4:M:502:BCL:HBB2	4:M:502:BCL:HHC	1.98	0.43
2:M:268:TRP:CE3	3:H:31:LEU:HD13	2.53	0.43
1:L:234:LEU:HD22	2:M:224:LEU:HD12	1.99	0.43
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.49	0.43
1:L:100:TRP:CH2	6:M:503:U10:H251	2.54	0.43
1:L:117:ILE:HB	1:L:118:PRO:HD3	2.01	0.43
2:M:11:GLN:HB2	3:H:144:ALA:HB3	1.99	0.43
3:H:37:ARG:HG2	3:H:37:ARG:NH1	2.32	0.43
2:M:12:VAL:CG1	3:H:140:PHE:HD2	2.32	0.43
1:L:85:LEU:HD23	1:L:85:LEU:HA	1.89	0.42
1:L:153:HIS:CE1	1:L:154:LEU:HD23	2.54	0.42
1:L:173:HIS:O	1:L:177:ILE:HG13	2.19	0.42
1:L:265:TRP:CG	1:L:266:TRP:N	2.87	0.42
4:M:502:BCL:H162	4:M:502:BCL:H121	1.85	0.42
3:H:16:ALA:O	3:H:19:SER:HB2	2.20	0.42
2:M:3:TYR:OH	2:M:5:ASN:HA	2.20	0.42
2:M:114:LEU:HD12	2:M:114:LEU:HA	1.84	0.42
2:M:129:TRP:CH2	2:M:132:ARG:NH1	2.88	0.42
3:H:209:SER:OG	3:H:212:LEU:HD12	2.20	0.42
3:H:181:VAL:O	3:H:188:THR:HA	2.19	0.42
2:M:36:SER:OG	2:M:38:LEU:HB3	2.19	0.42
3:H:249:LYS:O	3:H:250:SER:O	2.37	0.42
4:L:302:BCL:H141	4:L:302:BCL:H162	1.90	0.42
3:H:177:ARG:C	3:H:193:MET:HB2	2.44	0.42
1:L:167:PHE:HB3	4:L:302:BCL:HMC3	2.02	0.42
3:H:130:LYS:HD2	11:H:742:HOH:O	2.19	0.42
3:H:156:CYS:HB3	3:H:206:ASN:O	2.19	0.42
3:H:195:MET:HE1	3:H:241:LEU:HD11	2.01	0.42
3:H:245:ALA:HB3	3:H:246:PRO:HD3	2.02	0.42
1:L:149:GLY:O	1:L:153:HIS:HB3	2.20	0.41
2:M:197:PHE:HD1	2:M:197:PHE:HA	1.71	0.41
1:L:97:PHE:CE1	4:L:302:BCL:H121	2.55	0.41
2:M:2:GLU:HG2	2:M:3:TYR:N	2.35	0.41
2:M:65:MET:HB3	2:M:121:PHE:CD2	2.56	0.41
1:L:120:ALA:HB1	1:L:238:LEU:HD21	2.01	0.41
1:L:267:VAL:HG21	1:L:280:ASN:HD22	1.85	0.41
2:M:134:TYR:CD2	2:M:144:LYS:HG2	2.55	0.41
2:M:265:ILE:HG12	6:M:503:U10:C2	2.51	0.41
2:M:271:TRP:O	2:M:275:LEU:HG	2.20	0.41
3:H:103:ASP:HB3	3:H:106:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:304:BCL:H161	4:L:304:BCL:H122	1.80	0.41
4:M:501:BCL:HMB3	4:M:501:BCL:CBB	2.49	0.41
3:H:75:VAL:HA	3:H:76:PRO:C	2.46	0.41
3:H:247:LYS:O	3:H:249:LYS:NZ	2.53	0.41
1:L:18:GLY:O	1:L:21:LEU:HB2	2.21	0.41
4:M:501:BCL:C4A	4:M:501:BCL:HBA1	2.50	0.41
1:L:179:PHE:O	1:L:180:PHE:C	2.63	0.41
2:M:103:LEU:HD21	2:M:166:ILE:HA	2.03	0.41
3:H:148:PRO:O	3:H:151:LEU:HG	2.21	0.41
1:L:146:PHE:HA	1:L:147:PRO:HD3	1.94	0.41
1:L:267:VAL:HG23	2:M:87:ARG:HG2	2.03	0.41
4:L:304:BCL:H162	4:L:304:BCL:H202	1.85	0.41
1:L:21:LEU:HD13	1:L:22:PHE:CE1	2.56	0.40
1:L:198:ALA:C	1:L:200:PRO:HD3	2.46	0.40
1:L:206:MET:O	3:H:67:PRO:HG3	2.21	0.40
2:M:270:ILE:O	2:M:274:VAL:HB	2.20	0.40
2:M:187:ASN:HA	4:M:502:BCL:HBC3	2.03	0.40
4:M:502:BCL:CBB	4:M:502:BCL:CHC	2.92	0.40
4:M:502:BCL:H191	5:M:401:BPH:H8	2.04	0.40
1:L:66:VAL:HG12	1:L:86:TRP:HB2	2.03	0.40
4:M:501:BCL:OBB	4:M:501:BCL:HHC	2.21	0.40
1:L:208:THR:HB	1:L:209:PRO:CD	2.49	0.40
2:M:300:ASN:O	2:M:301:HIS:CB	2.70	0.40
1:L:97:PHE:CZ	4:L:302:BCL:H121	2.57	0.40
2:M:233:ARG:NH2	3:H:122:GLU:OE1	2.52	0.40
3:H:108:GLY:O	3:H:113:SER:HA	2.22	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%)	265 (95%)	14 (5%)	0	100	100
2	M	300/314 (96%)	285 (95%)	11 (4%)	4 (1%)	9	35
3	H	238/260 (92%)	229 (96%)	9 (4%)	0	100	100
All	All	817/855 (96%)	779 (95%)	34 (4%)	4 (0%)	24	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	22	GLU
2	M	301	HIS
2	M	52	LEU
2	M	34	PRO

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	220/220 (100%)	203 (92%)	17 (8%)	12	38
2	M	236/247 (96%)	223 (94%)	13 (6%)	19	50
3	H	195/208 (94%)	186 (95%)	9 (5%)	24	55
All	All	651/675 (96%)	612 (94%)	39 (6%)	17	47

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	LEU
1	L	21	LEU
1	L	38	THR
1	L	46	ILE
1	L	80	LEU
1	L	91	ILE
1	L	126	LEU
1	L	150	ILE
1	L	153	HIS

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Mol	Chain	Res	Type
1	L	154	LEU
1	L	185	LEU
1	L	202	LYS
1	L	207	ARG
1	L	216	PHE
1	L	235	LEU
1	L	251	THR
1	L	271	TRP
2	M	29	ARG
2	M	55	LEU
2	M	111	GLU
2	M	136	ARG
2	M	144	LYS
2	M	152	SER
2	M	182	HIS
2	M	196	LEU
2	M	204	LEU
2	M	265	ILE
2	M	270	ILE
2	M	274	VAL
2	M	292	ASP
3	H	12	LEU
3	H	135	LYS
3	H	160	ILE
3	H	184	LYS
3	H	220	LYS
3	H	221	SER
3	H	225	VAL
3	H	231	ASP
3	H	249	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	4	GLN
3	H	206	ASN

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 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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$
10	CDL	M	800	-	80,80,99	0.48	0	86,92,111	0.94	5 (5%)
4	BCL	M	501	2	69,74,74	1.39	12 (17%)	79,115,115	2.26	23 (29%)
7	LDA	H	703	-	13,15,15	2.73	2 (15%)	14,17,17	0.65	0
7	LDA	L	709	-	13,15,15	2.28	1 (7%)	14,17,17	0.49	0
6	U10	L	502	-	48,48,63	2.18	21 (43%)	60,61,79	1.03	4 (6%)
5	BPH	L	402	-	59,70,70	2.06	16 (27%)	59,101,101	2.57	17 (28%)
7	LDA	M	701	-	13,15,15	2.43	2 (15%)	14,17,17	0.40	0
6	U10	M	503	-	48,48,63	2.55	21 (43%)	60,61,79	1.28	8 (13%)
4	BCL	L	304	1	69,74,74	1.32	8 (11%)	79,115,115	2.05	10 (12%)
4	BCL	M	502	2	69,74,74	1.08	5 (7%)	79,115,115	1.80	11 (13%)
5	BPH	M	401	-	59,70,70	2.07	14 (23%)	59,101,101	2.95	27 (45%)
7	LDA	M	704	-	13,15,15	1.90	1 (7%)	14,17,17	0.51	0
4	BCL	L	302	1	69,74,74	1.52	10 (14%)	79,115,115	2.16	12 (15%)
9	SPN	M	600	-	42,42,42	4.05	18 (42%)	50,52,52	2.51	16 (32%)

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
10	CDL	M	800	-	-	30/91/91/110	-
4	BCL	M	501	2	2/2/21/25	13/41/137/137	-
7	LDA	H	703	-	-	5/13/13/13	-
7	LDA	L	709	-	-	4/13/13/13	-
6	U10	L	502	-	-	9/45/69/87	0/1/1/1
5	BPH	L	402	-	-	4/37/105/105	0/5/6/6
7	LDA	M	701	-	-	8/13/13/13	-
6	U10	M	503	-	-	10/45/69/87	0/1/1/1
4	BCL	L	304	1	1/1/21/25	10/41/137/137	-
4	BCL	M	502	2	-	7/41/137/137	-
5	BPH	M	401	-	1/1/18/22	10/37/105/105	0/5/6/6
7	LDA	M	704	-	-	2/13/13/13	-
4	BCL	L	302	1	-	5/41/137/137	-
9	SPN	M	600	-	-	19/50/51/51	-

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	600	SPN	C3-C2	9.77	1.60	1.52
9	M	600	SPN	C4-C5	9.25	1.54	1.33
9	M	600	SPN	C19-C18	9.13	1.54	1.33
9	M	600	SPN	C8-C9	8.76	1.53	1.33
9	M	600	SPN	C12-C13	8.51	1.52	1.33
7	M	701	LDA	O1-N1	-8.37	1.21	1.42
7	H	703	LDA	O1-N1	-7.96	1.22	1.42
7	L	709	LDA	O1-N1	-7.91	1.22	1.42
6	M	503	U10	C27-C28	-7.90	1.26	1.50
5	M	401	BPH	C2C-C3C	-7.84	1.47	1.54
6	M	503	U10	O3-C3	7.40	1.54	1.36
7	M	704	LDA	O1-N1	-6.66	1.25	1.42
5	L	402	BPH	C2C-C3C	-6.31	1.49	1.54
5	L	402	BPH	C1D-C2D	6.17	1.46	1.39
9	M	600	SPN	C3-C4	-5.98	1.41	1.50
9	M	600	SPN	C17-C18	-5.96	1.39	1.51
5	M	401	BPH	C1D-C2D	5.89	1.46	1.39
9	M	600	SPN	C10-C9	-5.86	1.39	1.51
5	L	402	BPH	C3A-C2A	-5.77	1.49	1.54
7	H	703	LDA	C1-N1	-5.76	1.45	1.51
9	M	600	SPN	C14-C13	-5.44	1.40	1.51
4	L	302	BCL	O2D-CED	-5.36	1.33	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	600	SPN	C6-C5	-5.24	1.40	1.51
5	M	401	BPH	C1B-C2B	5.12	1.45	1.39
5	L	402	BPH	C1B-C2B	4.87	1.44	1.39
4	L	304	BCL	MG-ND	-4.86	1.96	2.05
4	M	501	BCL	O2D-CGD	4.73	1.44	1.33
6	L	502	U10	O3-C3	4.63	1.47	1.36
4	L	304	BCL	O2D-CGD	4.55	1.44	1.33
4	L	302	BCL	C1-C2	-4.53	1.36	1.49
4	M	501	BCL	MG-NA	4.49	2.16	2.06
4	L	302	BCL	MG-NA	4.20	2.16	2.06
4	L	302	BCL	O2A-CGA	4.18	1.45	1.33
6	M	503	U10	C17-C18	-4.11	1.38	1.50
6	L	502	U10	O4-C4	4.09	1.46	1.36
4	L	304	BCL	MG-NA	4.04	2.15	2.06
4	M	502	BCL	MG-NA	4.01	2.15	2.06
5	M	401	BPH	O2A-CGA	3.87	1.44	1.33
5	L	402	BPH	O2D-CGD	3.81	1.42	1.33
5	M	401	BPH	O2D-CGD	3.79	1.42	1.33
9	M	600	SPN	C20-C19	-3.78	1.39	1.50
4	M	501	BCL	O2A-CGA	3.75	1.44	1.33
6	M	503	U10	O4-C4	3.71	1.45	1.36
6	M	503	U10	C37-C38	-3.54	1.39	1.50
6	M	503	U10	C36-C34	3.53	1.58	1.51
6	L	502	U10	C33-C34	3.50	1.41	1.33
6	M	503	U10	C22-C23	-3.50	1.39	1.50
6	L	502	U10	C28-C29	3.49	1.41	1.33
6	L	502	U10	C7-C6	3.49	1.57	1.51
9	M	600	SPN	C25-C26	3.45	1.41	1.33
5	L	402	BPH	O2A-CGA	3.45	1.43	1.33
6	M	503	U10	C35-C34	3.36	1.58	1.50
6	L	502	U10	C17-C18	-3.35	1.40	1.50
9	M	600	SPN	C7-C8	-3.32	1.40	1.50
9	M	600	SPN	C11-C12	-3.31	1.40	1.50
5	L	402	BPH	C3B-C2B	-3.28	1.34	1.39
6	L	502	U10	C36-C34	3.25	1.58	1.51
6	L	502	U10	C23-C24	3.24	1.40	1.33
6	M	503	U10	C33-C34	3.24	1.40	1.33
4	M	502	BCL	C3B-C4B	3.18	1.47	1.41
6	L	502	U10	O4-C4M	-3.14	1.38	1.45
4	L	302	BCL	C3B-C4B	3.12	1.47	1.41
4	L	302	BCL	MG-NC	3.06	2.13	2.06
6	L	502	U10	C13-C14	3.05	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	502	U10	C8-C9	3.04	1.40	1.33
5	M	401	BPH	O2D-CED	-3.01	1.38	1.45
6	L	502	U10	C31-C29	2.98	1.57	1.51
9	M	600	SPN	O1-CMA	2.94	1.52	1.43
6	M	503	U10	C8-C9	2.93	1.39	1.33
5	L	402	BPH	CHA-CBD	2.90	1.55	1.51
9	M	600	SPN	C29-C30	2.88	1.41	1.32
6	M	503	U10	C23-C24	2.88	1.39	1.33
4	L	304	BCL	C3B-C4B	2.85	1.46	1.41
5	M	401	BPH	CHA-CBD	2.80	1.54	1.51
9	M	600	SPN	C21-C22	-2.80	1.39	1.52
4	M	502	BCL	C2-C3	2.79	1.39	1.33
6	L	502	U10	C21-C19	2.78	1.57	1.51
6	L	502	U10	C38-C39	2.75	1.40	1.32
4	M	501	BCL	CAA-C2A	2.71	1.59	1.54
4	L	304	BCL	C2-C3	2.70	1.39	1.33
5	M	401	BPH	C3B-C2B	-2.65	1.35	1.39
6	M	503	U10	O4-C4M	-2.64	1.39	1.45
5	M	401	BPH	C15-C13	2.63	1.65	1.52
5	L	402	BPH	O2D-CED	-2.58	1.39	1.45
5	L	402	BPH	C2-C3	2.58	1.39	1.33
6	M	503	U10	C38-C39	2.56	1.40	1.32
6	M	503	U10	C30-C29	2.56	1.56	1.50
4	M	501	BCL	C3B-C4B	2.53	1.46	1.41
6	M	503	U10	C13-C14	2.52	1.38	1.33
9	M	600	SPN	C16-C15	-2.50	1.39	1.51
6	M	503	U10	C15-C14	2.50	1.56	1.50
4	L	304	BCL	O2A-CGA	2.50	1.40	1.33
6	L	502	U10	C18-C19	2.47	1.38	1.33
5	M	401	BPH	C4D-ND	-2.47	1.34	1.38
6	M	503	U10	C18-C19	2.46	1.38	1.33
4	M	501	BCL	CMA-C3A	2.45	1.58	1.53
4	M	502	BCL	O2D-CED	-2.45	1.39	1.45
5	M	401	BPH	C2-C3	2.45	1.38	1.33
4	M	501	BCL	C2C-C3C	-2.43	1.47	1.54
6	M	503	U10	O3-C3M	-2.42	1.39	1.45
6	L	502	U10	C10-C9	2.40	1.56	1.50
6	L	502	U10	C15-C14	2.38	1.56	1.50
4	M	501	BCL	C2-C3	2.37	1.38	1.33
5	L	402	BPH	O1D-CGD	2.36	1.27	1.21
4	L	302	BCL	C4-C3	2.35	1.56	1.50
4	M	501	BCL	CMB-C2B	2.33	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	402	BPH	CAA-C2A	2.33	1.58	1.54
6	L	502	U10	C16-C14	2.29	1.56	1.51
6	M	503	U10	O2-C2	2.27	1.28	1.23
4	L	302	BCL	MG-ND	-2.25	2.01	2.05
4	L	302	BCL	CMC-C2C	-2.25	1.48	1.53
6	L	502	U10	C35-C34	2.24	1.56	1.50
5	M	401	BPH	C3D-C2D	-2.21	1.35	1.39
6	L	502	U10	C7-C8	-2.16	1.47	1.50
4	M	502	BCL	O2A-CGA	2.14	1.39	1.33
5	L	402	BPH	C3D-C4D	2.14	1.44	1.41
4	L	304	BCL	CMB-C2B	-2.11	1.46	1.50
4	L	302	BCL	O2D-CGD	2.10	1.38	1.33
4	L	304	BCL	O2D-CED	-2.09	1.40	1.45
4	M	501	BCL	C3B-C2B	-2.09	1.35	1.42
6	L	502	U10	C25-C24	2.08	1.55	1.50
7	M	701	LDA	C1-N1	-2.08	1.49	1.51
4	M	501	BCL	C4-C3	2.07	1.55	1.50
5	L	402	BPH	C5-C3	2.06	1.55	1.51
6	M	503	U10	C40-C39	2.06	1.55	1.50
5	L	402	BPH	C3B-C4B	2.05	1.44	1.41
5	M	401	BPH	C1A-C2A	2.05	1.54	1.51
5	M	401	BPH	CAA-C2A	2.03	1.58	1.54
5	L	402	BPH	C4-C3	2.03	1.55	1.50
4	M	501	BCL	O2D-CED	-2.03	1.40	1.45
6	M	503	U10	C7-C8	-2.00	1.47	1.50

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	401	BPH	O2D-CGD-CBD	13.75	126.06	110.95
5	L	402	BPH	O2D-CGD-CBD	13.05	125.29	110.95
4	L	302	BCL	OBB-CAB-C3B	9.10	136.53	120.43
4	L	304	BCL	C4A-NA-C1A	8.38	110.50	106.68
4	L	302	BCL	C4A-NA-C1A	8.23	110.43	106.68
4	M	501	BCL	C1-C2-C3	8.18	139.60	126.20
4	L	304	BCL	O2D-CGD-CBD	8.06	125.32	111.23
4	M	502	BCL	C4A-NA-C1A	7.75	110.21	106.68
9	M	600	SPN	CM6-C18-C17	6.81	127.05	115.23
4	L	302	BCL	C1C-NC-C4C	6.29	109.55	106.68
9	M	600	SPN	CM5-C13-C14	6.27	126.10	115.23
5	M	401	BPH	C1-C2-C3	6.13	136.23	126.20
4	M	502	BCL	O2D-CGD-CBD	5.79	121.35	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	304	BCL	O1D-CGD-CBD	-5.74	113.20	124.52
4	M	501	BCL	C4-C3-C5	-5.74	105.27	115.23
4	M	502	BCL	C1C-NC-C4C	5.68	109.27	106.68
4	M	501	BCL	OBB-CAB-C3B	5.64	130.40	120.43
4	L	304	BCL	C1C-NC-C4C	5.46	109.17	106.68
5	L	402	BPH	O2A-CGA-O1A	-5.18	110.68	123.63
4	L	302	BCL	O2D-CGD-CBD	5.04	120.05	111.23
4	L	304	BCL	OBB-CAB-C3B	5.04	129.35	120.43
5	L	402	BPH	CMA-C3A-C4A	-4.96	103.93	114.61
5	M	401	BPH	C4D-CHA-CBD	-4.93	106.09	108.45
4	M	501	BCL	O2A-CGA-CBA	4.79	126.45	111.83
4	L	302	BCL	CAB-C3B-C2B	4.79	137.69	127.74
4	M	501	BCL	O2A-CGA-O1A	-4.72	111.83	123.63
4	M	501	BCL	O2D-CGD-CBD	4.70	119.44	111.23
9	M	600	SPN	C6-C5-C4	-4.67	110.68	121.17
5	L	402	BPH	O2D-CGD-O1D	-4.57	114.95	123.85
9	M	600	SPN	C3-C4-C5	-4.50	119.08	126.83
4	M	501	BCL	C4A-NA-C1A	4.49	108.73	106.68
5	M	401	BPH	O1D-CGD-CBD	-4.47	117.94	124.72
9	M	600	SPN	C17-C18-C19	-4.42	111.24	121.17
9	M	600	SPN	CM7-C22-C21	4.32	126.69	111.27
4	L	302	BCL	CBB-CAB-C3B	-4.29	111.36	120.40
4	L	304	BCL	OBB-CAB-CBB	-4.23	110.29	119.77
5	M	401	BPH	C16-C15-C13	4.22	130.00	115.97
9	M	600	SPN	C20-C19-C18	-4.15	118.11	127.62
4	M	501	BCL	C1C-NC-C4C	4.11	108.55	106.68
4	M	501	BCL	CAA-C2A-C3A	-4.07	102.00	113.00
5	M	401	BPH	O2D-CGD-O1D	-4.05	115.96	123.85
5	M	401	BPH	CBC-CAC-C3C	4.04	121.72	113.78
9	M	600	SPN	C7-C8-C9	-3.97	118.53	127.62
5	M	401	BPH	CMA-C3A-C4A	-3.95	106.09	114.61
4	L	302	BCL	OBB-CAB-CBB	-3.94	110.95	119.77
9	M	600	SPN	C11-C12-C13	-3.93	118.63	127.62
4	M	502	BCL	O1D-CGD-CBD	-3.91	116.80	124.52
9	M	600	SPN	CM4-C9-C10	3.78	121.80	115.23
5	M	401	BPH	CED-O2D-CGD	3.77	124.47	115.92
6	M	503	U10	C27-C28-C29	3.65	135.98	127.62
5	L	402	BPH	O2A-CGA-CBA	3.56	122.69	111.83
5	L	402	BPH	OBD-CAD-CBD	-3.56	120.60	125.82
5	M	401	BPH	C1C-C2C-C3C	3.54	106.21	102.84
4	M	502	BCL	O2A-CGA-CBA	3.52	122.58	111.83
4	M	501	BCL	C5-C3-C2	3.50	129.03	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	600	SPN	C10-C9-C8	-3.50	113.31	121.17
5	M	401	BPH	C6-C5-C3	3.41	121.77	113.47
9	M	600	SPN	C14-C13-C12	-3.36	113.63	121.17
5	M	401	BPH	CAA-C2A-C3A	-3.35	103.94	113.00
5	L	402	BPH	O1D-CGD-CBD	-3.30	119.71	124.72
9	M	600	SPN	C16-C17-C18	3.30	121.50	113.47
4	L	302	BCL	O2A-CGA-CBA	3.29	121.88	111.83
4	M	502	BCL	OBB-CAB-C3B	3.28	126.24	120.43
4	M	501	BCL	O2D-CGD-O1D	-3.24	117.54	123.85
5	L	402	BPH	CAA-C2A-C3A	-3.17	104.44	113.00
5	L	402	BPH	C4A-C3A-C2A	3.12	105.81	102.84
5	M	401	BPH	C17-C16-C15	3.11	127.23	113.28
4	M	501	BCL	OBB-CAB-CBB	-3.05	112.93	119.77
5	L	402	BPH	C1C-C2C-C3C	3.04	105.73	102.84
4	M	501	BCL	C2C-C3C-C4C	3.00	105.83	101.34
5	M	401	BPH	C11-C12-C13	-2.99	106.02	115.97
4	L	302	BCL	O1D-CGD-CBD	-2.99	118.61	124.52
4	M	501	BCL	CMA-C3A-C2A	-2.97	102.52	113.98
5	M	401	BPH	C1B-NB-C4B	-2.95	104.52	108.82
5	M	401	BPH	O2A-CGA-O1A	-2.94	116.28	123.63
4	M	502	BCL	CED-O2D-CGD	2.92	122.55	115.92
10	M	800	CDL	OB8-CB6-CB4	2.91	116.78	108.40
4	L	304	BCL	O2A-CGA-CBA	2.91	120.70	111.83
5	M	401	BPH	C4C-C3C-C2C	2.87	105.57	102.84
5	L	402	BPH	C1B-NB-C4B	-2.73	104.84	108.82
6	L	502	U10	C7-C8-C9	2.67	131.44	126.83
5	L	402	BPH	CED-O2D-CGD	2.66	121.94	115.92
10	M	800	CDL	CB6-CB4-CB3	-2.64	105.62	111.78
6	M	503	U10	C7-C6-C1	-2.60	120.43	124.89
4	L	304	BCL	C1D-ND-C4D	-2.54	104.53	106.31
4	L	304	BCL	O2A-CGA-O1A	-2.54	117.28	123.63
4	M	501	BCL	C4D-CHA-C1A	2.53	124.27	121.24
4	M	501	BCL	CHB-C1B-NB	2.49	127.79	124.05
4	M	502	BCL	C1-C2-C3	2.45	130.22	126.20
5	L	402	BPH	C4D-ND-C1D	-2.45	105.94	108.87
4	L	302	BCL	C1-C2-C3	2.43	130.18	126.20
9	M	600	SPN	CM3-C5-C6	2.43	119.44	115.23
5	L	402	BPH	C4-C3-C5	-2.40	111.05	115.23
4	L	304	BCL	CAC-C3C-C4C	-2.38	107.31	112.58
5	M	401	BPH	C14-C13-C12	2.37	119.71	111.27
5	M	401	BPH	CMB-C2B-C3B	2.36	129.40	124.68
4	M	501	BCL	CAB-C3B-C2B	2.35	132.62	127.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	302	BCL	CED-O2D-CGD	2.32	121.18	115.92
6	M	503	U10	C25-C24-C26	-2.31	111.21	115.23
6	L	502	U10	C7-C6-C1	-2.31	120.93	124.89
6	M	503	U10	C7-C8-C9	2.28	130.76	126.83
10	M	800	CDL	OA8-CA7-OA9	-2.26	117.97	123.63
6	L	502	U10	C3M-O3-C3	2.25	124.37	116.47
5	M	401	BPH	CMD-C2D-C3D	2.24	129.17	124.68
4	M	501	BCL	CHA-C1A-NA	-2.24	121.32	126.39
5	M	401	BPH	C5-C3-C2	-2.24	116.14	121.17
9	M	600	SPN	C15-C16-C17	2.22	121.28	113.13
6	M	503	U10	C3M-O3-C3	2.22	124.25	116.47
10	M	800	CDL	OB6-CB5-OB7	-2.21	118.54	123.70
4	M	502	BCL	C1D-ND-C4D	-2.20	104.77	106.31
4	M	501	BCL	O1D-CGD-CBD	-2.20	120.19	124.52
6	M	503	U10	C26-C27-C28	-2.18	101.23	112.02
4	M	502	BCL	C3A-C2A-C1A	2.18	104.60	101.34
6	L	502	U10	C4M-O4-C4	2.18	124.13	116.47
5	M	401	BPH	OBD-CAD-CBD	-2.17	122.65	125.82
5	M	401	BPH	C7-C6-C5	-2.14	107.56	113.26
9	M	600	SPN	C7-C6-C5	2.11	120.18	113.19
5	L	402	BPH	C4C-C3C-C2C	2.11	104.85	102.84
10	M	800	CDL	CA6-CA4-CA3	-2.09	106.91	111.78
4	M	502	BCL	O2A-CGA-O1A	-2.09	118.40	123.63
5	M	401	BPH	C11-C10-C8	2.09	122.90	115.97
4	M	501	BCL	C2B-C1B-NB	-2.06	108.19	110.33
4	M	501	BCL	CMA-C3A-C4A	-2.06	106.23	111.77
5	M	401	BPH	CMA-C3A-C2A	-2.05	106.20	114.13
4	L	302	BCL	C2B-C1B-NB	-2.05	108.20	110.33
4	M	501	BCL	C3C-C2C-C1C	2.04	105.17	101.87
4	M	501	BCL	CHD-C1D-ND	-2.04	121.93	124.80
6	M	503	U10	C4M-O4-C4	2.04	123.62	116.47
5	L	402	BPH	CBC-CAC-C3C	2.03	117.77	113.78
5	L	402	BPH	C3D-C4D-ND	2.02	110.30	107.71
6	M	503	U10	C22-C23-C24	2.02	132.24	127.62
5	M	401	BPH	C4-C3-C5	2.02	118.73	115.23
5	M	401	BPH	C6-C7-C8	-2.01	109.27	115.97

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	L	304	BCL	C13
4	M	501	BCL	C13

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Mol	Chain	Res	Type	Atom
4	M	501	BCL	C8
5	M	401	BPH	C8

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	304	BCL	C2C-C3C-CAC-CBC
4	L	304	BCL	C4C-C3C-CAC-CBC
4	L	304	BCL	CHA-CBD-CGD-O1D
4	L	304	BCL	CHA-CBD-CGD-O2D
4	M	501	BCL	C1-C2-C3-C4
5	M	401	BPH	O2A-C1-C2-C3
5	M	401	BPH	C1-C2-C3-C5
6	L	502	U10	C23-C24-C26-C27
6	L	502	U10	C25-C24-C26-C27
7	L	709	LDA	N1-C1-C2-C3
7	M	701	LDA	C2-C1-N1-O1
7	M	701	LDA	C2-C1-N1-CM1
7	M	701	LDA	C2-C1-N1-CM2
7	H	703	LDA	C2-C1-N1-O1
7	H	703	LDA	C2-C1-N1-CM1
9	M	600	SPN	C3-C4-C5-CM3
10	M	800	CDL	CA3-OA5-PA1-OA2
10	M	800	CDL	CA3-OA5-PA1-OA3
10	M	800	CDL	CA3-OA5-PA1-OA4
4	L	304	BCL	CBD-CGD-O2D-CED
4	L	304	BCL	O1D-CGD-O2D-CED
6	L	502	U10	C35-C34-C36-C37
9	M	600	SPN	C11-C10-C9-CM4
9	M	600	SPN	C16-C17-C18-CM6
9	M	600	SPN	C14-C15-C16-C17
6	L	502	U10	C33-C34-C36-C37
9	M	600	SPN	C4-C5-C6-C7
9	M	600	SPN	C11-C10-C9-C8
9	M	600	SPN	C12-C13-C14-C15
9	M	600	SPN	C16-C17-C18-C19
6	M	503	U10	C24-C26-C27-C28
7	L	709	LDA	C6-C7-C8-C9
5	M	401	BPH	C4-C3-C5-C6
9	M	600	SPN	CM5-C13-C14-C15
5	M	401	BPH	C2-C3-C5-C6
4	M	502	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
9	M	600	SPN	C20-C21-C22-CM7
4	M	501	BCL	C11-C12-C13-C15
6	L	502	U10	C29-C31-C32-C33
6	M	503	U10	C29-C31-C32-C33
4	M	502	BCL	C13-C15-C16-C17
4	M	501	BCL	C15-C16-C17-C18
10	M	800	CDL	CB7-C71-C72-C73
4	M	502	BCL	C15-C16-C17-C18
4	L	302	BCL	C15-C16-C17-C18
4	M	501	BCL	C10-C11-C12-C13
10	M	800	CDL	C11-CA5-OA6-CA4
10	M	800	CDL	OA7-CA5-OA6-CA4
7	H	703	LDA	C7-C8-C9-C10
9	M	600	SPN	C24-C25-C26-CM8
10	M	800	CDL	C54-C55-C56-C57
7	H	703	LDA	C6-C7-C8-C9
10	M	800	CDL	C79-C80-C81-C82
6	M	503	U10	C30-C29-C31-C32
10	M	800	CDL	C39-C40-C41-C42
10	M	800	CDL	C78-C79-C80-C81
4	M	501	BCL	C4-C3-C5-C6
7	L	709	LDA	C2-C3-C4-C5
10	M	800	CDL	C34-C35-C36-C37
7	M	701	LDA	C7-C8-C9-C10
6	M	503	U10	C28-C29-C31-C32
7	M	701	LDA	C1-C2-C3-C4
5	L	402	BPH	C8-C10-C11-C12
4	L	304	BCL	C15-C16-C17-C18
10	M	800	CDL	OA5-CA3-CA4-OA6
10	M	800	CDL	C36-C37-C38-C39
10	M	800	CDL	C80-C81-C82-C83
4	M	501	BCL	C2-C3-C5-C6
10	M	800	CDL	C52-C53-C54-C55
10	M	800	CDL	C21-C22-C23-C24
4	M	501	BCL	C3-C5-C6-C7
6	M	503	U10	C14-C16-C17-C18
7	H	703	LDA	C11-C10-C9-C8
5	L	402	BPH	C4-C3-C5-C6
6	M	503	U10	C35-C34-C36-C37
9	M	600	SPN	CM3-C5-C6-C7
4	M	501	BCL	C11-C10-C8-C9
4	M	501	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
5	M	401	BPH	C11-C12-C13-C14
4	L	302	BCL	C11-C12-C13-C15
5	M	401	BPH	C11-C12-C13-C15
9	M	600	SPN	C21-C22-C23-C24
6	M	503	U10	C25-C24-C26-C27
5	L	402	BPH	C2-C3-C5-C6
7	M	701	LDA	C9-C10-C11-C12
5	M	401	BPH	C1-C2-C3-C4
6	M	503	U10	C23-C24-C26-C27
10	M	800	CDL	C40-C41-C42-C43
7	M	701	LDA	C4-C5-C6-C7
10	M	800	CDL	C11-C12-C13-C14
10	M	800	CDL	C13-C14-C15-C16
6	M	503	U10	C33-C34-C36-C37
10	M	800	CDL	C19-C20-C21-C22
6	L	502	U10	C14-C16-C17-C18
9	M	600	SPN	C25-C26-C27-C28
5	L	402	BPH	O2A-C1-C2-C3
10	M	800	CDL	C81-C82-C83-C84
5	M	401	BPH	C13-C15-C16-C17
10	M	800	CDL	OA5-CA3-CA4-CA6
4	L	304	BCL	C6-C7-C8-C10
4	M	501	BCL	C12-C13-C15-C16
4	L	302	BCL	C16-C17-C18-C20
4	L	304	BCL	C6-C7-C8-C9
5	M	401	BPH	C5-C6-C7-C8
10	M	800	CDL	CA3-CA4-CA6-OA8
7	M	704	LDA	C3-C4-C5-C6
10	M	800	CDL	C55-C56-C57-C58
4	M	501	BCL	CHA-CBD-CGD-O1D
7	M	704	LDA	C5-C6-C7-C8
7	M	701	LDA	C5-C6-C7-C8
4	L	302	BCL	C11-C12-C13-C14
10	M	800	CDL	C33-C34-C35-C36
10	M	800	CDL	CA5-C11-C12-C13
10	M	800	CDL	C20-C21-C22-C23
4	M	502	BCL	C10-C11-C12-C13
7	L	709	LDA	C4-C5-C6-C7
4	L	304	BCL	C11-C10-C8-C9
4	M	502	BCL	C6-C7-C8-C9
5	M	401	BPH	C8-C10-C11-C12
6	L	502	U10	C2-C3-O3-C3M

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Mol	Chain	Res	Type	Atoms
6	L	502	U10	C26-C27-C28-C29
4	M	501	BCL	C1-C2-C3-C5
9	M	600	SPN	CM8-C26-C27-C28
9	M	600	SPN	C2-C3-C4-C5
6	L	502	U10	C12-C11-C9-C10
6	M	503	U10	C5-C4-O4-C4M
4	M	502	BCL	C6-C7-C8-C10
10	M	800	CDL	C72-C71-CB7-OB8
4	M	501	BCL	C14-C13-C15-C16
10	M	800	CDL	C51-C52-C53-C54
4	L	302	BCL	O1A-CGA-O2A-C1
10	M	800	CDL	C72-C71-CB7-OB9
9	M	600	SPN	C10-C11-C12-C13
9	M	600	SPN	C18-C19-C20-C21
9	M	600	SPN	C6-C7-C8-C9
4	M	502	BCL	CAA-CBA-CGA-O2A

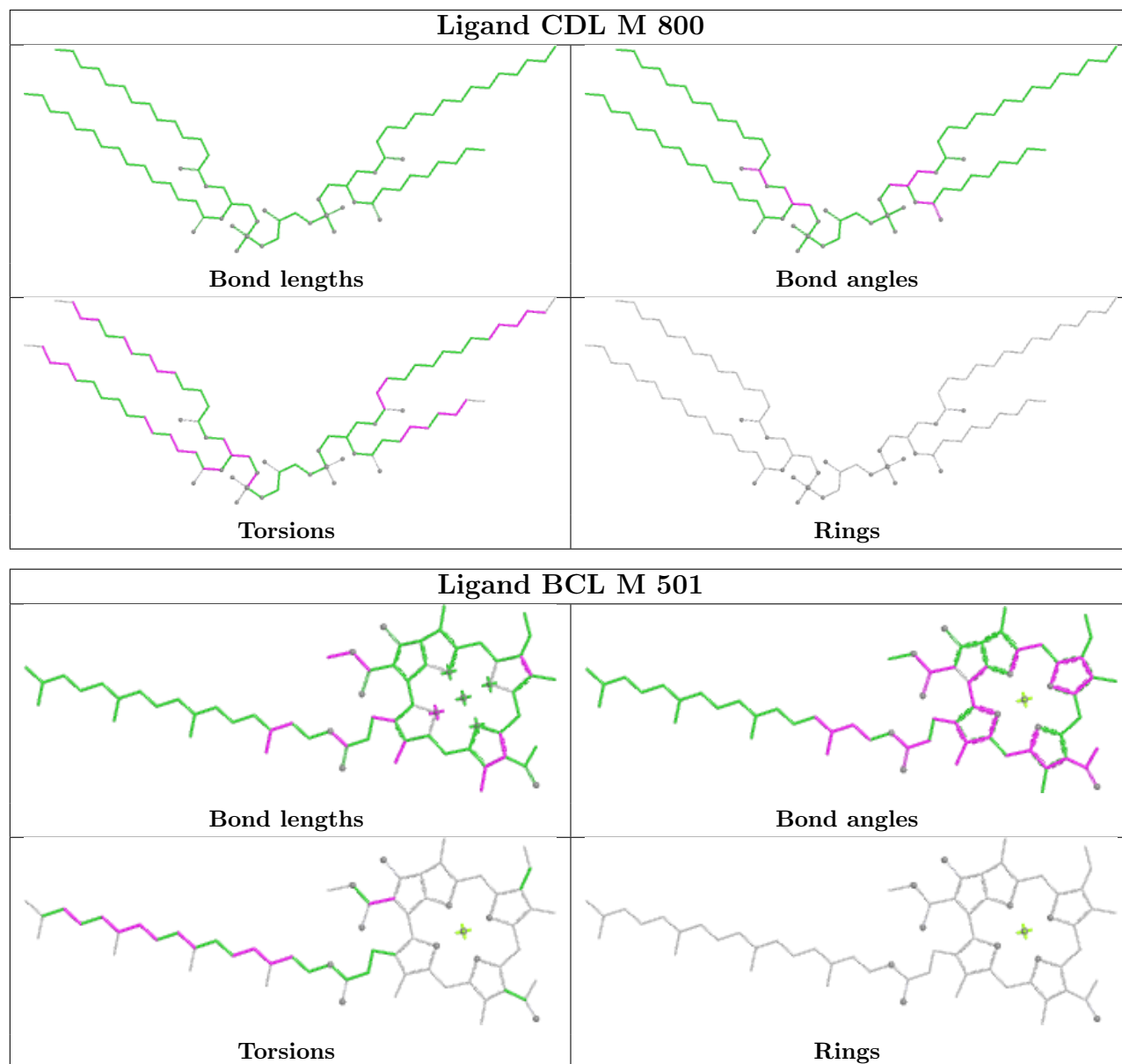
There are no ring outliers.

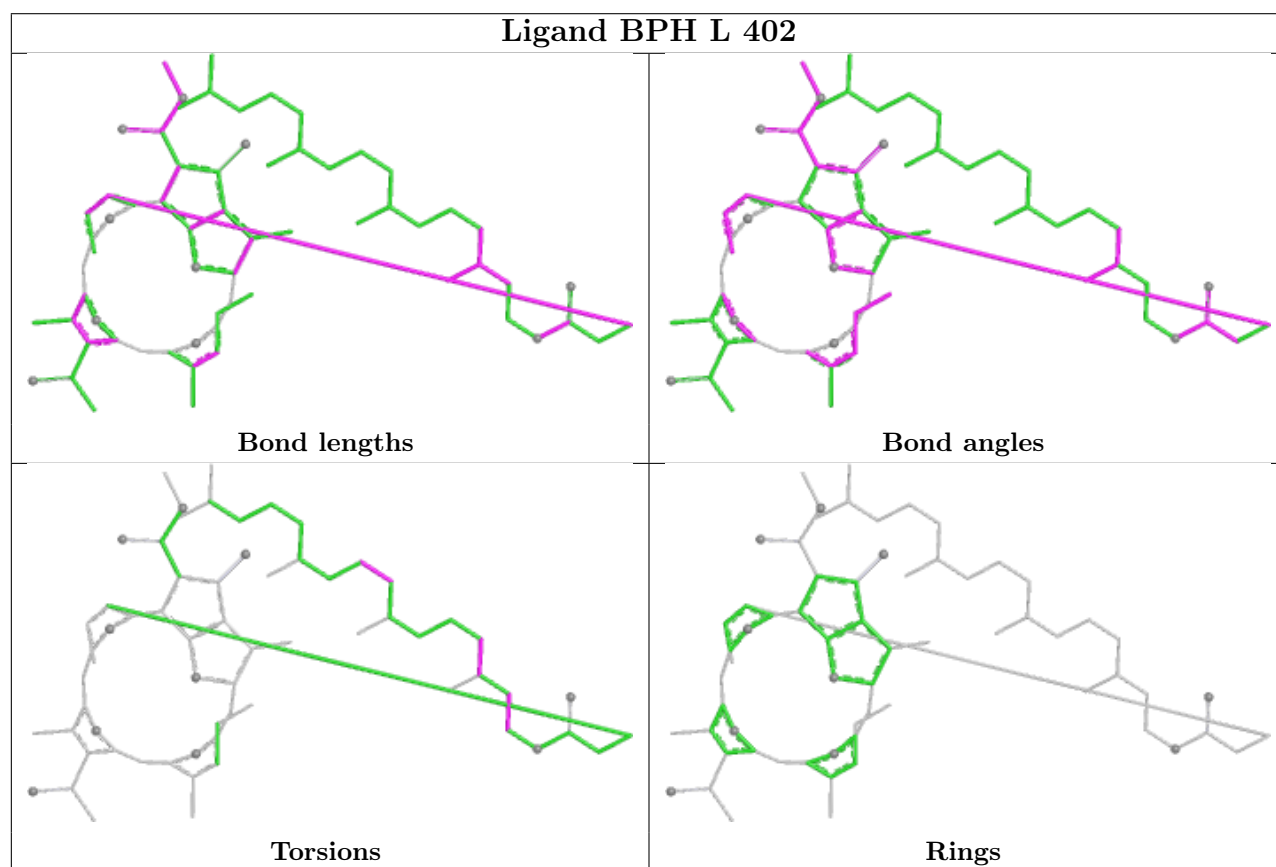
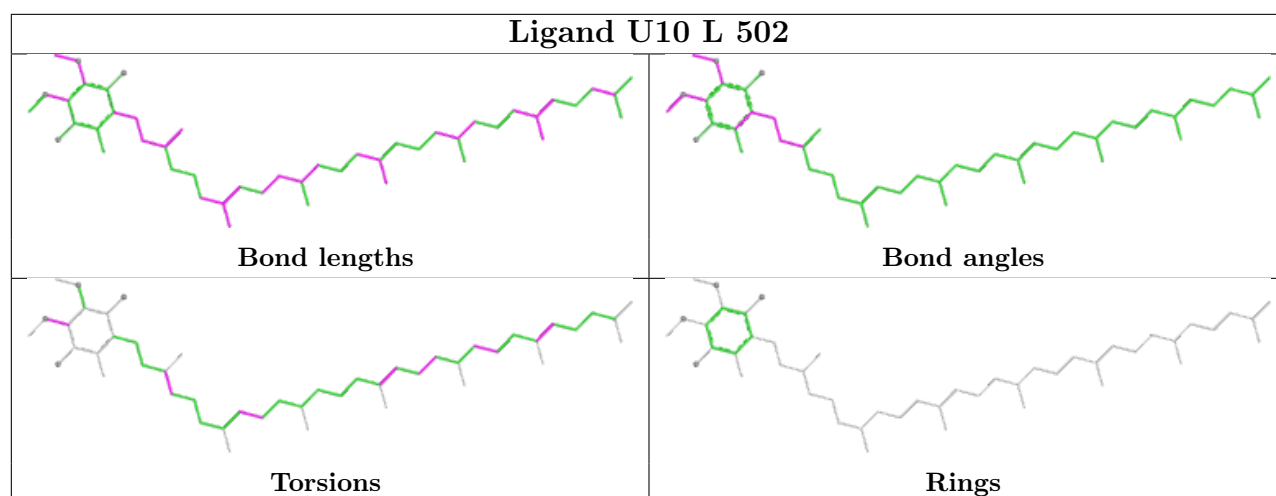
13 monomers are involved in 57 short contacts:

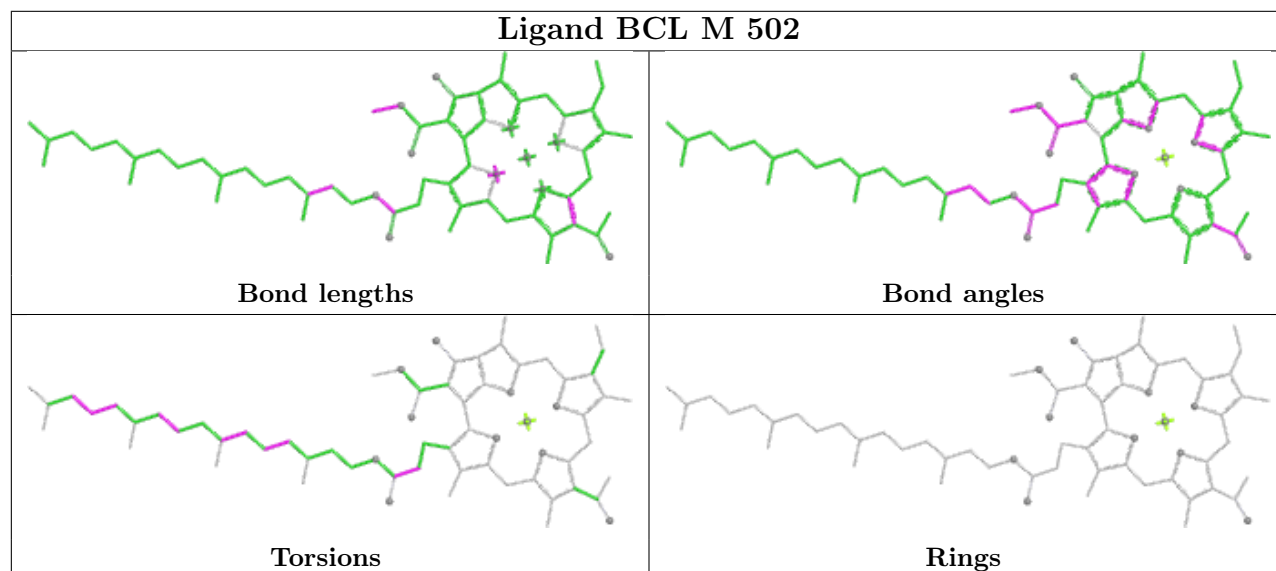
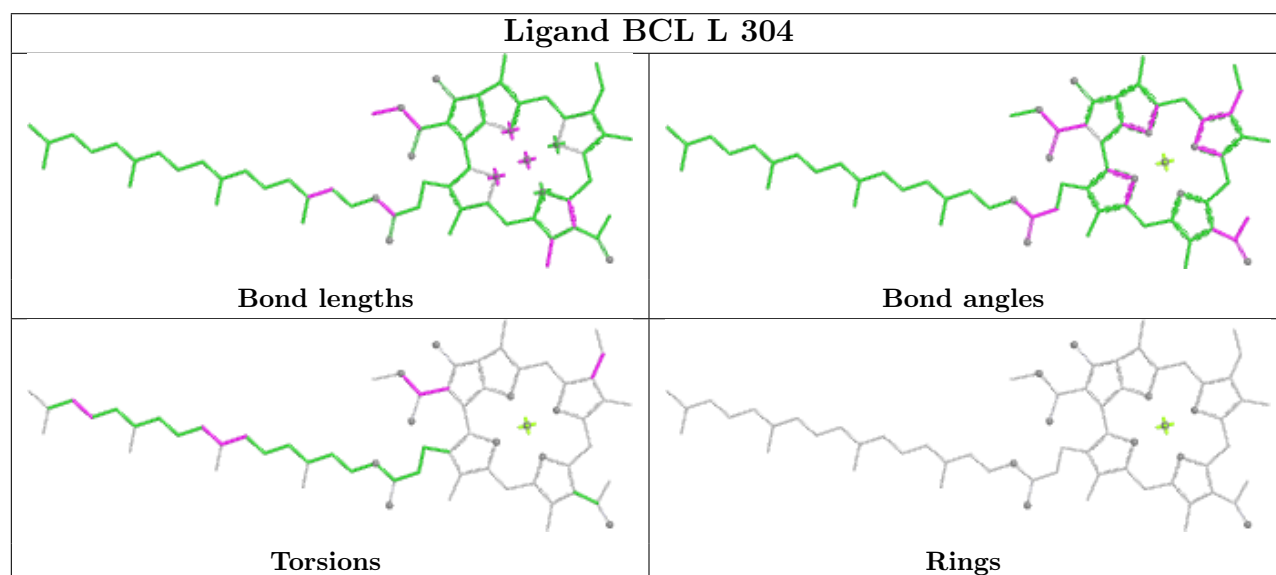
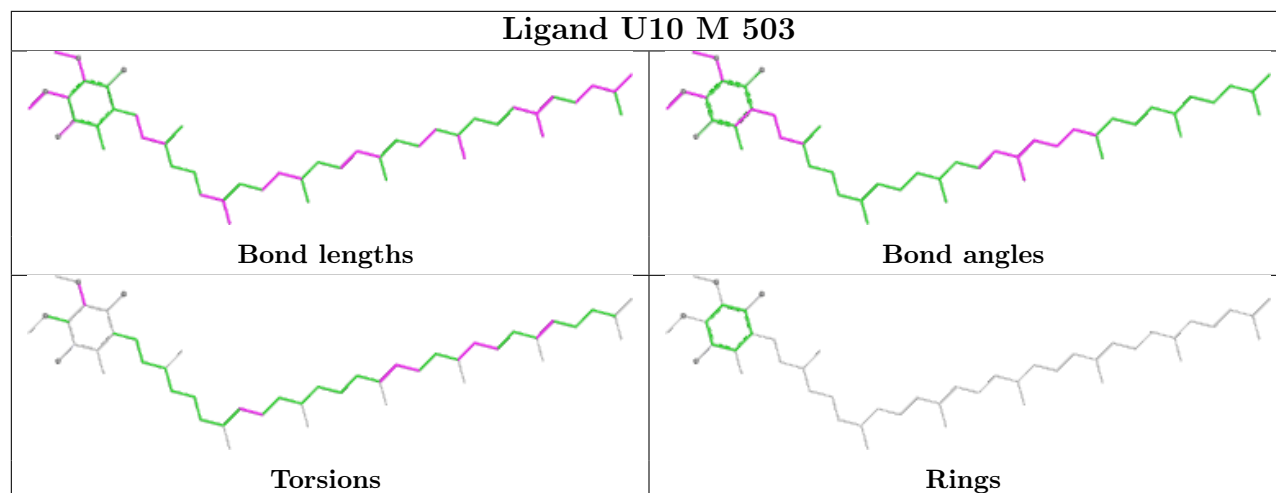
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	M	800	CDL	1	0
4	M	501	BCL	8	0
7	H	703	LDA	4	0
7	L	709	LDA	3	0
6	L	502	U10	6	0
5	L	402	BPH	4	0
7	M	701	LDA	4	0
6	M	503	U10	6	0
4	L	304	BCL	6	0
4	M	502	BCL	12	0
5	M	401	BPH	1	0
4	L	302	BCL	11	0
9	M	600	SPN	1	0

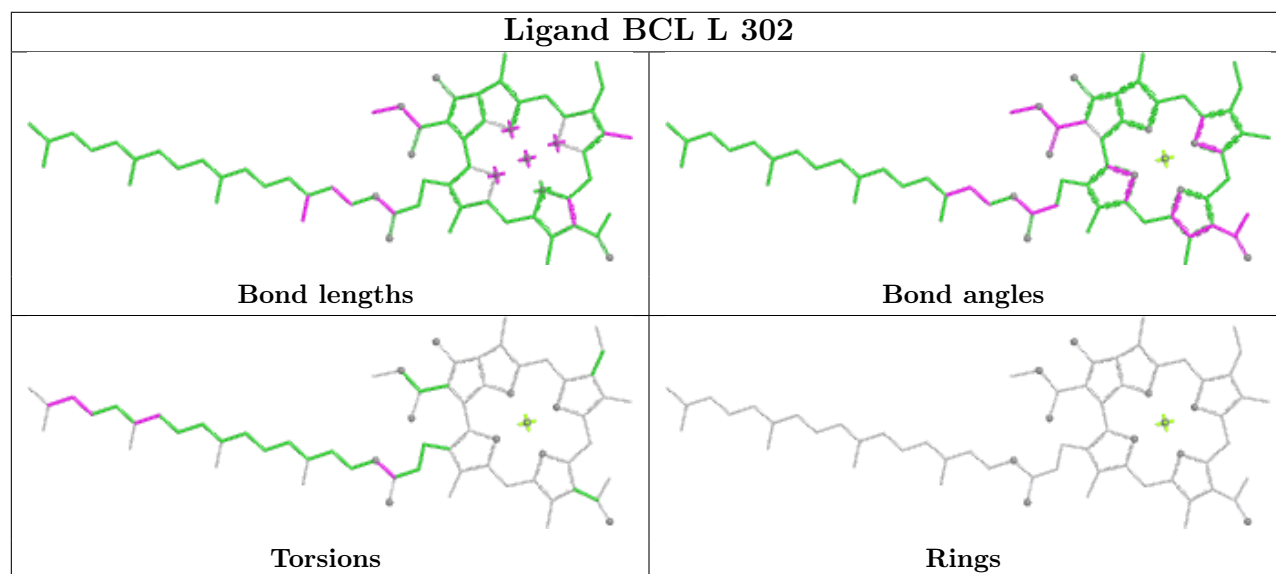
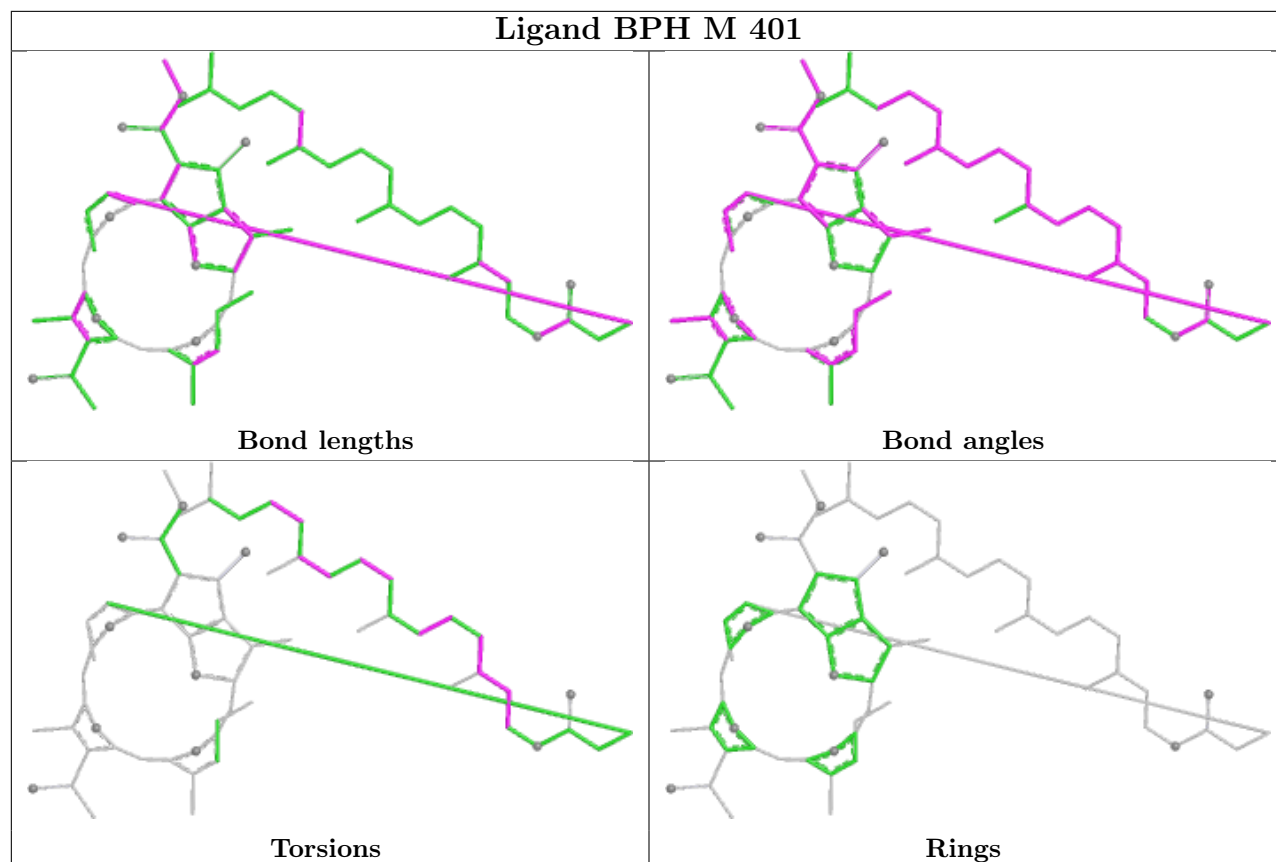
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

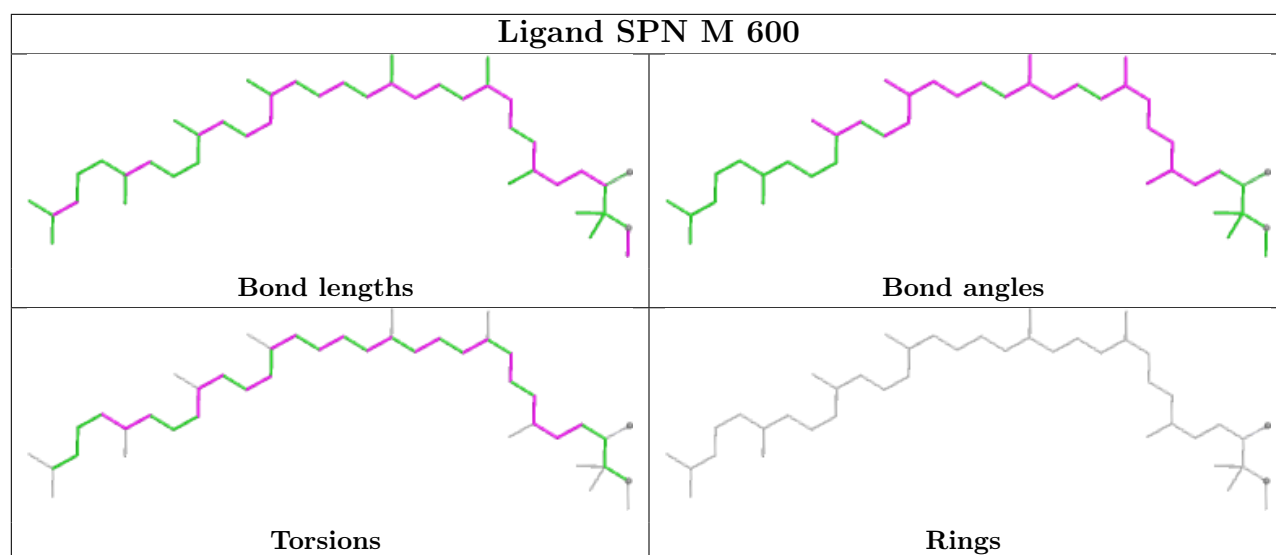
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers 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 [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.52	3 (1%) 78 59	10, 26, 66, 94	0
2	M	302/314 (96%)	-0.40	5 (1%) 69 48	11, 32, 68, 97	0
3	H	240/260 (92%)	-0.45	3 (1%) 75 56	13, 29, 58, 95	0
All	All	823/855 (96%)	-0.46	11 (1%) 75 56	10, 29, 66, 97	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	302	GLY	3.9
2	M	300	ASN	3.3
2	M	52	LEU	3.0
3	H	249	LYS	2.9
1	L	281	GLY	2.8
2	M	148	TRP	2.7
3	H	245	ALA	2.6
3	H	248	ARG	2.3
1	L	273	ALA	2.3
2	M	188	ASN	2.3
1	L	84	GLY	2.1

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 ⓘ

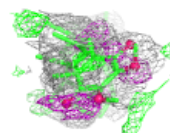
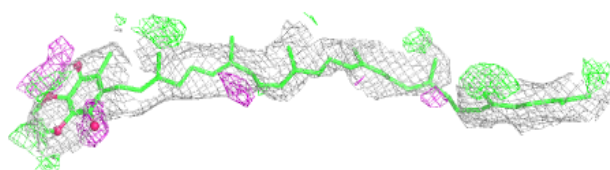
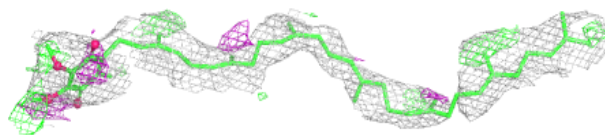
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	LDA	L	709	16/16	0.72	0.17	67,85,95,97	0
7	LDA	M	704	16/16	0.75	0.14	48,75,109,109	0
6	U10	L	502	48/63	0.76	0.14	61,76,89,90	0
10	CDL	M	800	81/100	0.78	0.27	41,62,76,77	81
7	LDA	H	703	16/16	0.80	0.14	34,50,64,67	0
7	LDA	M	701	16/16	0.90	0.09	29,44,52,58	0
4	BCL	M	501	66/66	0.92	0.10	27,32,92,94	0
6	U10	M	503	48/63	0.93	0.08	15,29,60,62	0
9	SPN	M	600	43/43	0.94	0.09	36,47,64,67	0
5	BPH	M	401	65/65	0.94	0.09	29,33,63,67	10
5	BPH	L	402	65/65	0.95	0.09	23,27,38,40	0
4	BCL	L	302	66/66	0.97	0.06	5,17,40,54	0
4	BCL	M	502	66/66	0.97	0.06	10,19,52,68	0
4	BCL	L	304	66/66	0.97	0.06	2,14,40,49	0
8	FE	M	500	1/1	1.00	0.02	18,18,18,18	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.

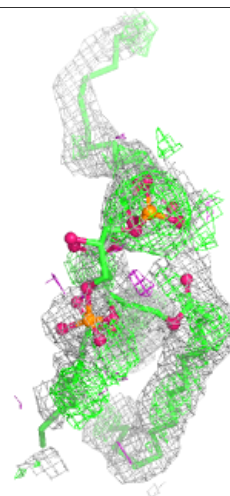
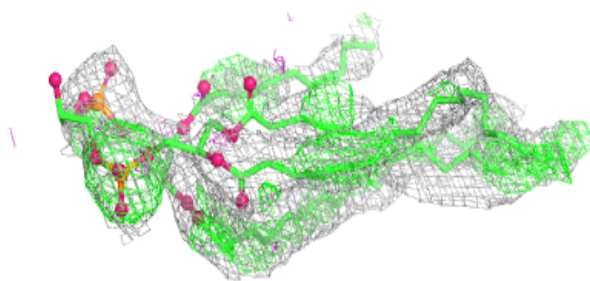
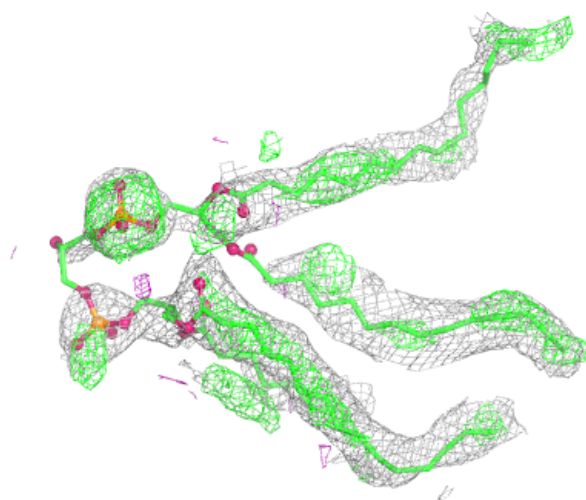
Electron density around U10 L 502:

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



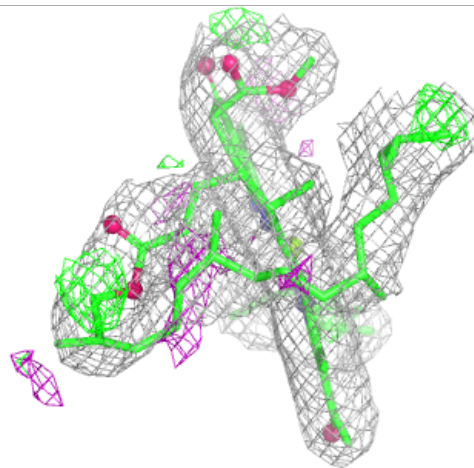
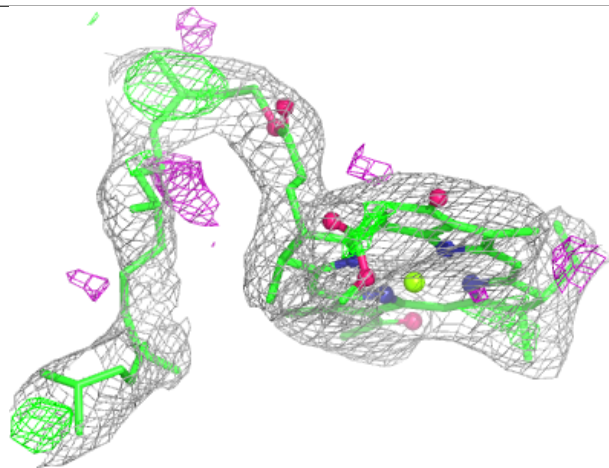
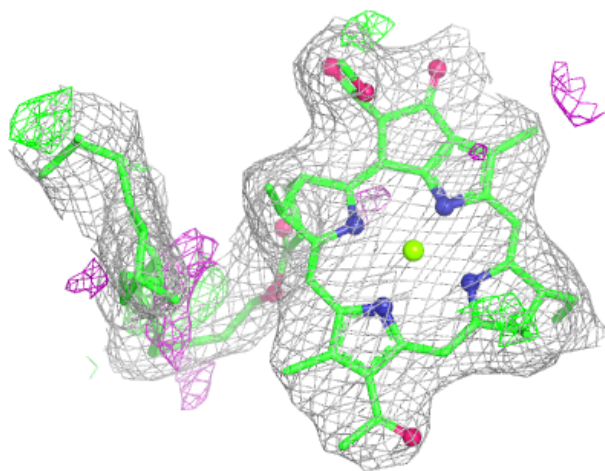
Electron density around CDL M 800:

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



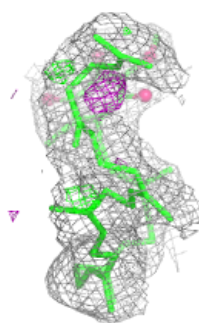
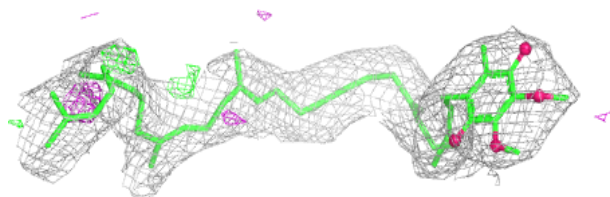
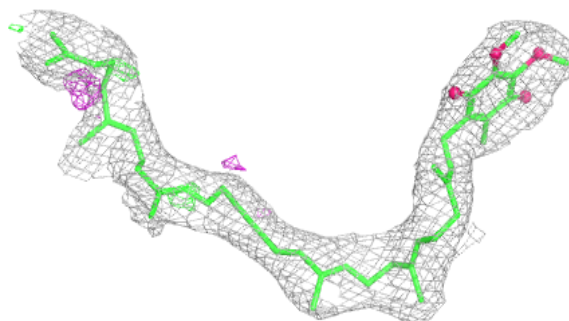
Electron density around BCL M 501:

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

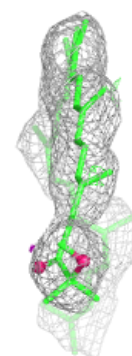
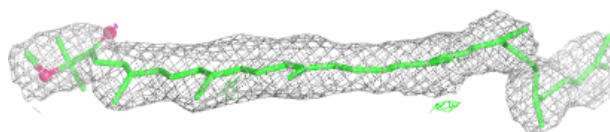
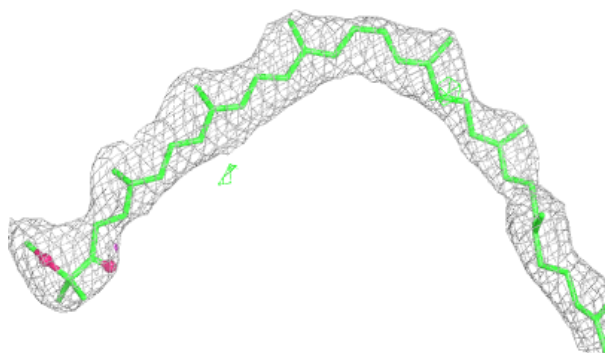


Electron density around U10 M 503:

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

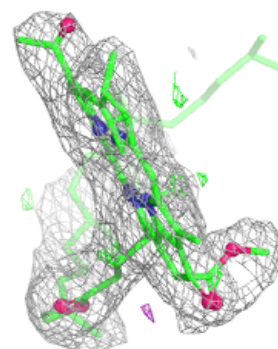
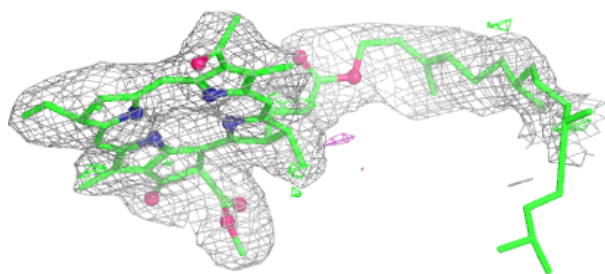
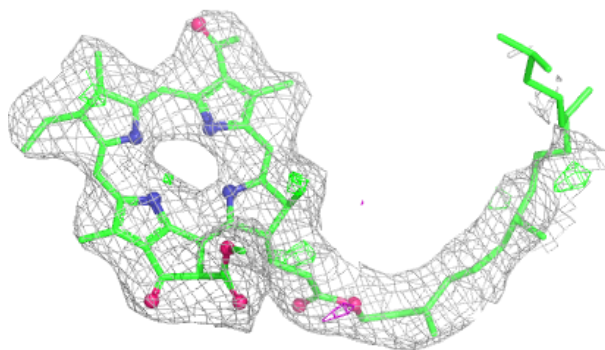
**Electron density around SPN M 600:**

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

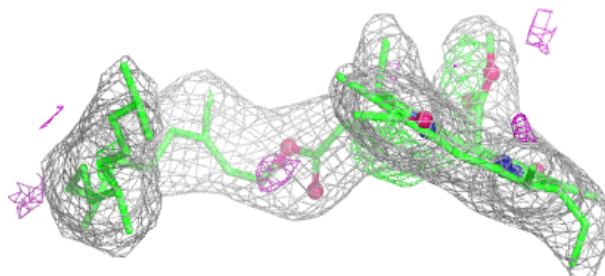
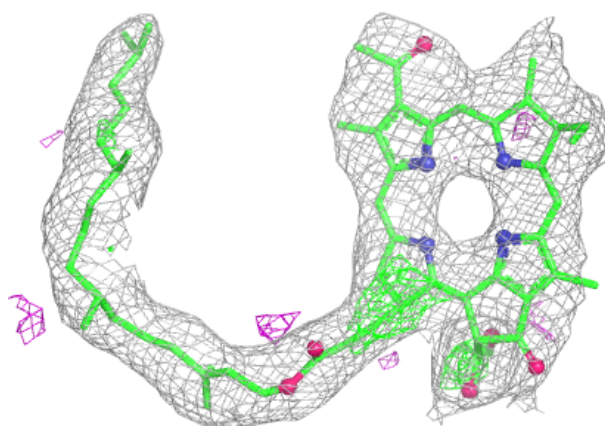


Electron density around BPH M 401:

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

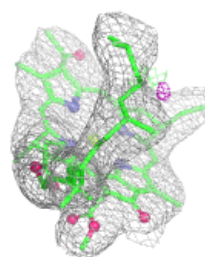
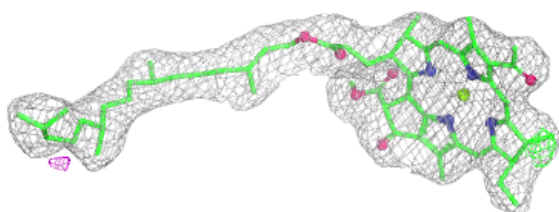
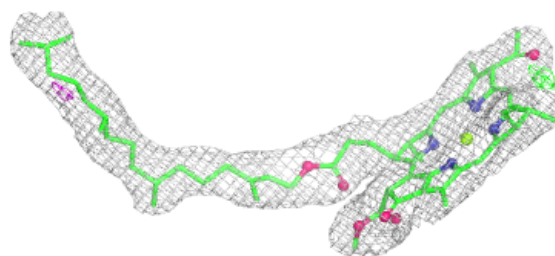
**Electron density around BPH L 402:**

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

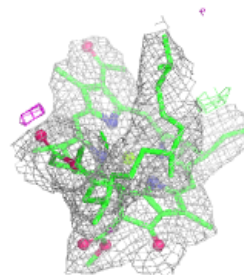
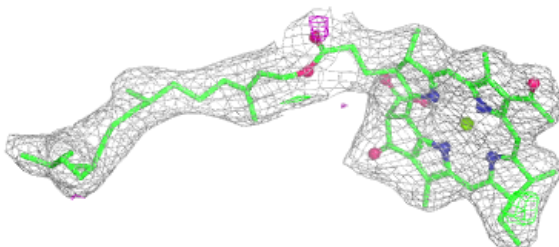
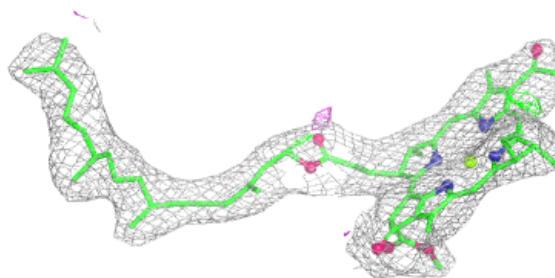


Electron density around BCL L 302:

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

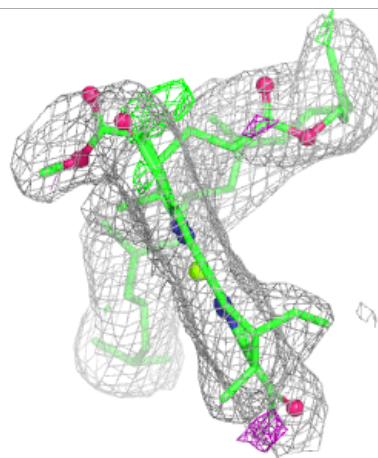
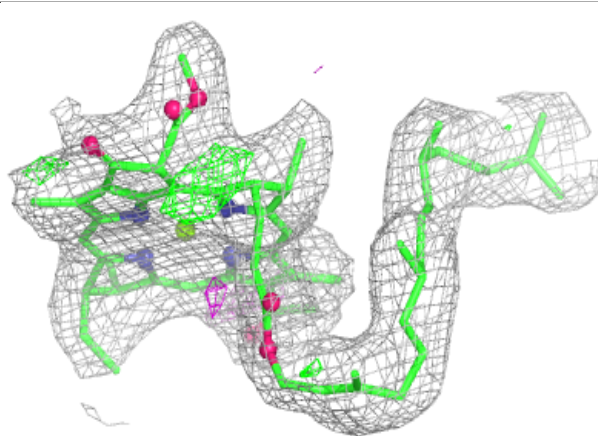
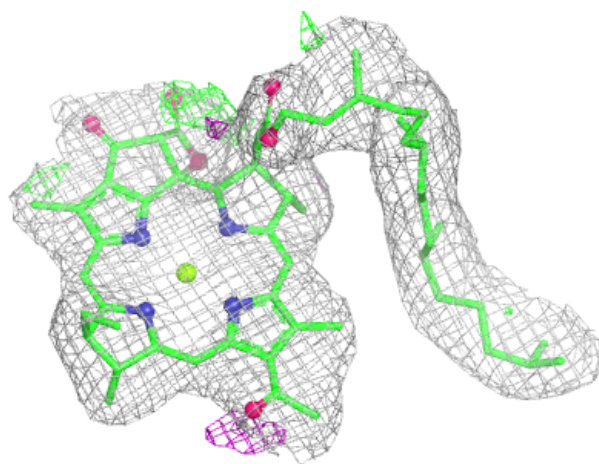
**Electron density around BCL M 502:**

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



Electron density around BCL L 304:

$2mF_o-DF_c$ (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.