



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:29 PM UTC

PDB ID : 3DU3 / pdb_00003du3
Title : E(L212)A, D(L213)A, A(M249)Y triple mutant structure of photosynthetic reaction center
Authors : Pokkuluri, P.R.; Schiffer, M.
Deposited on : 2008-07-16
Resolution : 2.80 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	:	9.0.010 (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

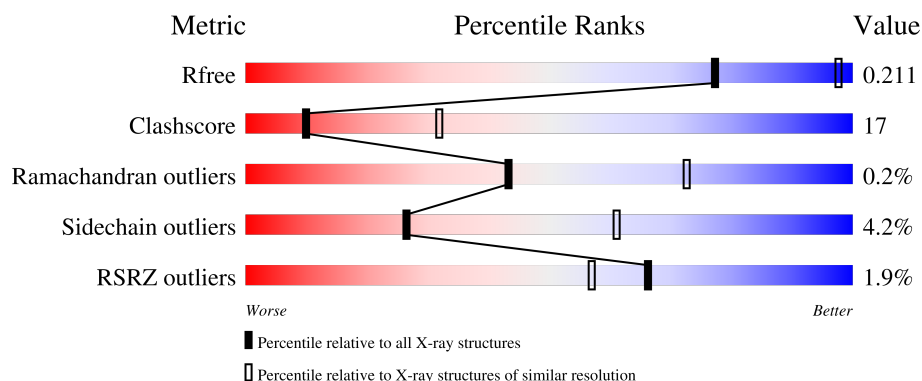
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	314	
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
10	LDA	H	703	-	-	X	-
4	BCL	L	501	X	-	-	-
4	BCL	M	501	X	-	-	-
5	BPH	M	503	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7288 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
			2225	1504	355	358	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	212	ALA	GLU	engineered mutation	UNP P0C0Y8
L	213	ALA	ASP	engineered mutation	UNP P0C0Y8

- 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
			2415	1613	394	398	10			

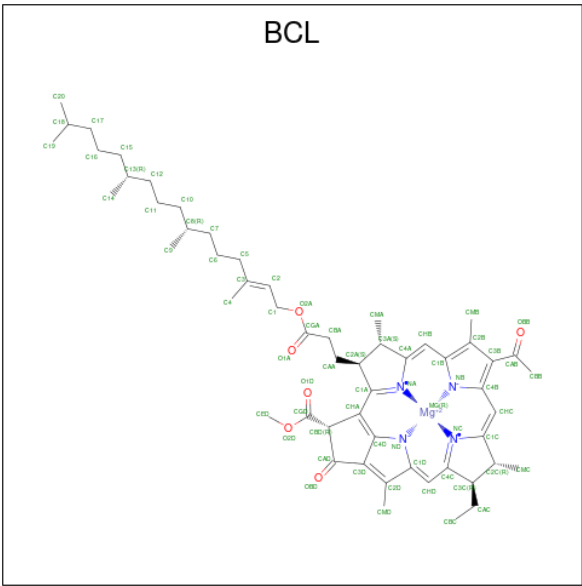
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	249	TYR	ALA	engineered mutation	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
M	314	HIS	-	expression tag	UNP P0C0Y9

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

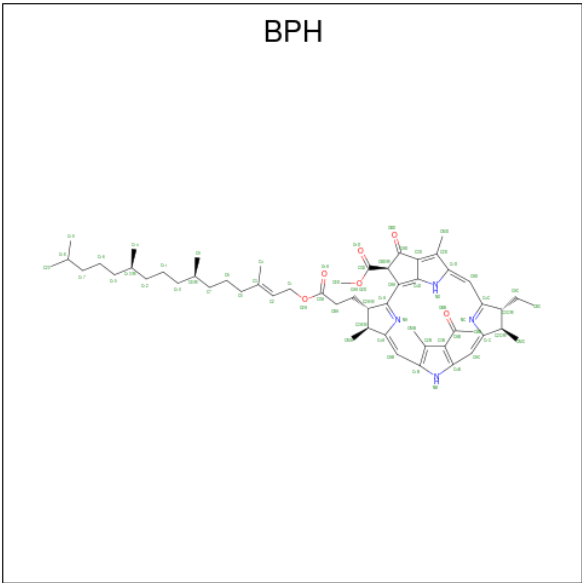
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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



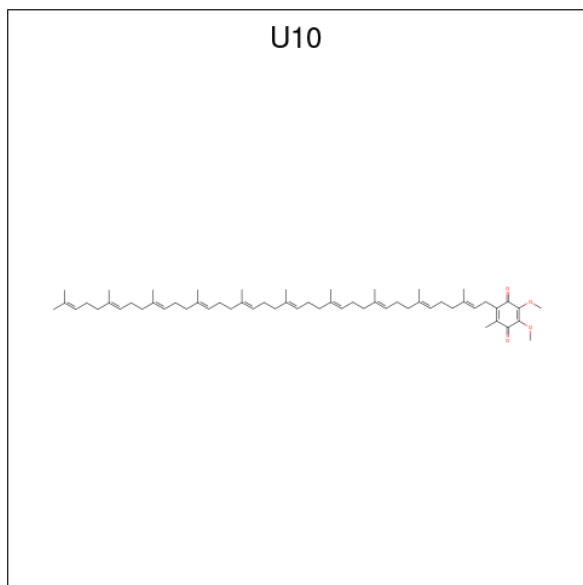
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



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
			55	45	4	6		

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

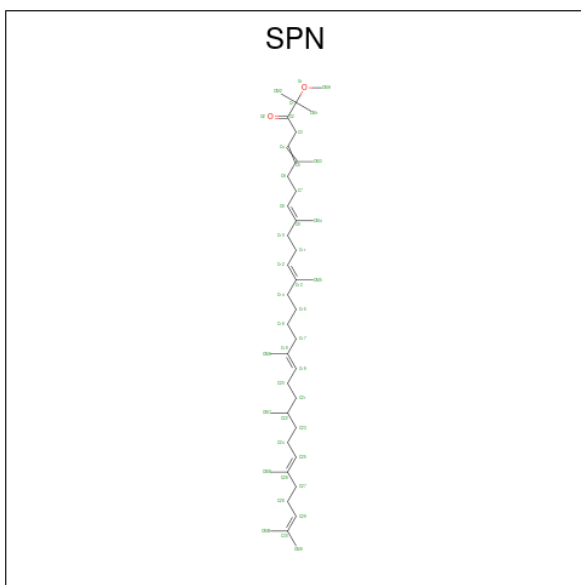


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			48	44	4		
6	M	1	Total	C	O	0	0
			48	44	4		

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

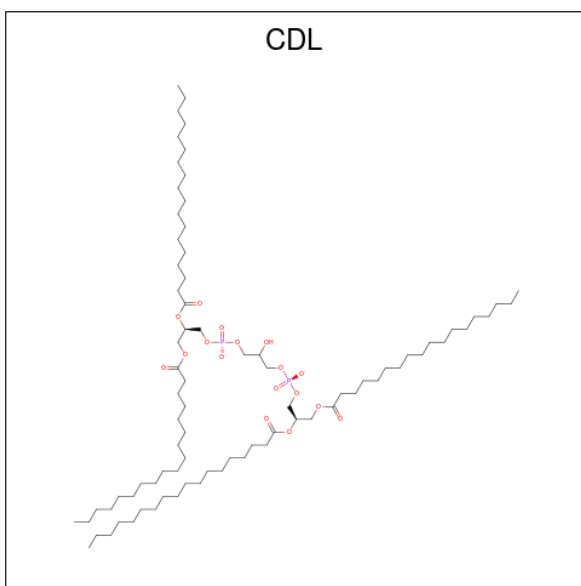
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Fe	0	0
			1	1		

- Molecule 8 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$).



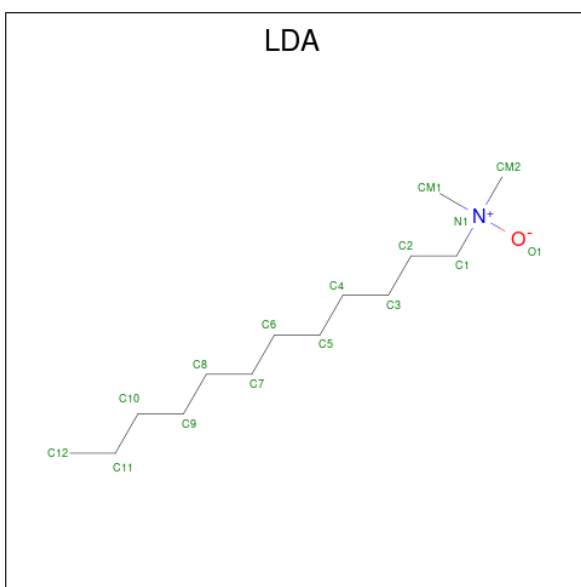
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			43	41	2		

- Molecule 9 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



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

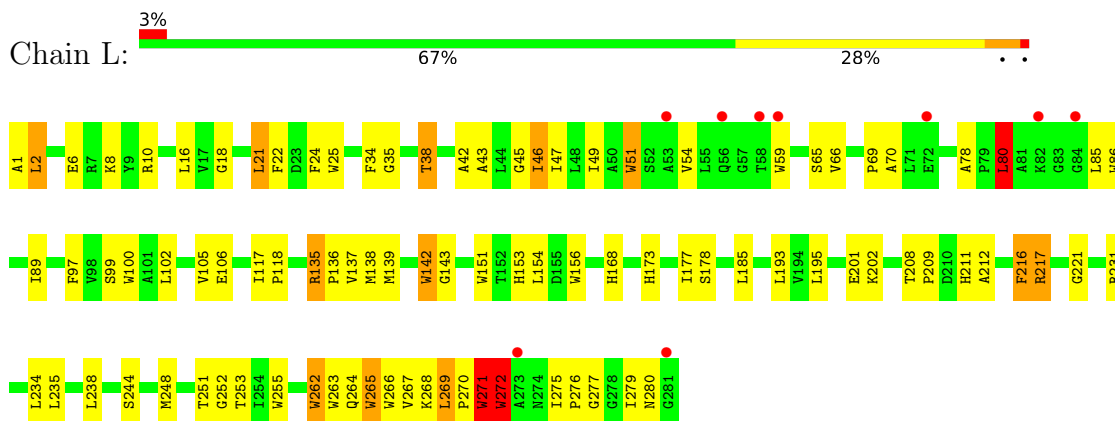
- Molecule 11 is water.

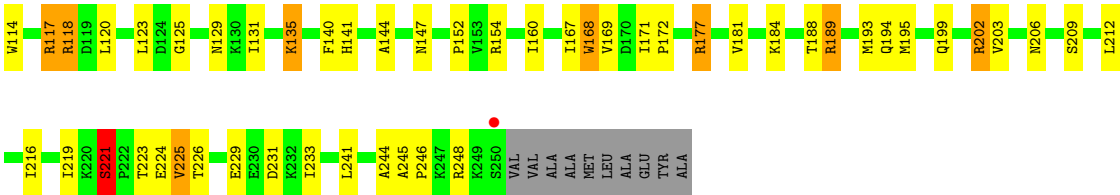
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	41	Total	O	0	0
			41	41		
11	M	55	Total	O	0	0
			55	55		
11	H	70	Total	O	0	0
			70	70		

3 Residue-property plots [i](#)

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

- Molecule 1: Reaction center protein L chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.10Å 141.10Å 187.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	84.0 (10.00-2.80) 90.0 (10.00-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.191 , 0.201 0.203 , 0.211	Depositor DCC
R_{free} test set	3488 reflections (7.05%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 76.8	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	7288	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: LDA, SPN, BCL, U10, CDL, BPH, FE

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	1.32	20/2313 (0.9%)	1.43	18/3166 (0.6%)
2	M	1.35	27/2508 (1.1%)	1.49	28/3424 (0.8%)
3	H	1.27	11/1877 (0.6%)	1.49	24/2553 (0.9%)
All	All	1.32	58/6698 (0.9%)	1.47	70/9143 (0.8%)

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
2	M	0	1

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	272	TRP	C-N	14.74	1.53	1.33
2	M	301	HIS	CA-C	-9.87	1.39	1.52
3	H	77	GLY	C-N	9.04	1.43	1.33
2	M	89	LEU	N-CA	8.21	1.57	1.46
3	H	42	LEU	C-N	-7.25	1.23	1.33
3	H	221	SER	CA-C	7.19	1.58	1.52
3	H	75	VAL	C-N	6.89	1.47	1.34
2	M	88	ASP	CA-C	6.51	1.61	1.52
1	L	80	LEU	N-CA	6.33	1.54	1.46
2	M	49	PRO	C-N	5.89	1.41	1.33
3	H	63	THR	N-CA	-5.75	1.39	1.46
2	M	155	TRP	NE1-CE2	-5.74	1.31	1.37
2	M	66	TRP	NE1-CE2	-5.71	1.31	1.37
1	L	143	GLY	N-CA	5.69	1.54	1.45
2	M	301	HIS	CB-CG	5.69	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	265	TRP	NE1-CE2	-5.64	1.31	1.37
3	H	147	ASN	C-N	5.62	1.40	1.34
1	L	59	TRP	NE1-CE2	-5.61	1.31	1.37
2	M	171	TRP	NE1-CE2	-5.57	1.31	1.37
3	H	114	TRP	NE1-CE2	-5.57	1.31	1.37
1	L	100	TRP	NE1-CE2	-5.56	1.31	1.37
2	M	41	TRP	NE1-CE2	-5.54	1.31	1.37
2	M	73	TRP	NE1-CE2	-5.54	1.31	1.37
1	L	51	TRP	NE1-CE2	-5.52	1.31	1.37
1	L	266	TRP	NE1-CE2	-5.52	1.31	1.37
1	L	142	TRP	NE1-CE2	-5.51	1.31	1.37
2	M	297	TRP	NE1-CE2	-5.46	1.31	1.37
2	M	75	TRP	NE1-CE2	-5.46	1.31	1.37
2	M	185	TRP	NE1-CE2	-5.45	1.31	1.37
2	M	115	TRP	NE1-CE2	-5.44	1.31	1.37
2	M	268	TRP	NE1-CE2	-5.44	1.31	1.37
2	M	271	TRP	NE1-CE2	-5.44	1.31	1.37
2	M	252	TRP	NE1-CE2	-5.41	1.31	1.37
1	L	262	TRP	NE1-CE2	-5.40	1.31	1.37
2	M	254	TRP	NE1-CE2	-5.40	1.31	1.37
2	M	129	TRP	NE1-CE2	-5.40	1.31	1.37
2	M	294	TRP	NE1-CE2	-5.40	1.31	1.37
1	L	255	TRP	NE1-CE2	-5.40	1.31	1.37
1	L	156	TRP	NE1-CE2	-5.39	1.31	1.37
2	M	148	TRP	NE1-CE2	-5.39	1.31	1.37
2	M	23	ASP	N-CA	5.38	1.52	1.46
1	L	263	TRP	NE1-CE2	-5.36	1.31	1.37
3	H	223	THR	N-CA	5.34	1.53	1.45
1	L	272	TRP	NE1-CE2	-5.34	1.31	1.37
2	M	130	TRP	NE1-CE2	-5.34	1.31	1.37
1	L	25	TRP	NE1-CE2	-5.34	1.31	1.37
2	M	157	TRP	NE1-CE2	-5.33	1.31	1.37
1	L	86	TRP	NE1-CE2	-5.32	1.31	1.37
2	M	127	TRP	NE1-CE2	-5.31	1.31	1.37
3	H	168	TRP	NE1-CE2	-5.30	1.31	1.37
3	H	21	TRP	NE1-CE2	-5.27	1.31	1.37
1	L	271	TRP	NE1-CE2	-5.26	1.31	1.37
1	L	151	TRP	NE1-CE2	-5.25	1.31	1.37
2	M	80	TRP	NE1-CE2	-5.17	1.31	1.37
2	M	167	LEU	N-CA	5.15	1.53	1.46
1	L	2	LEU	N-CA	5.14	1.51	1.45
3	H	62	LYS	C-N	-5.11	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	142	TRP	CA-C	5.10	1.59	1.52

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	272	TRP	CA-C-N	11.76	136.99	120.29
1	L	272	TRP	C-N-CA	11.76	136.99	120.29
2	M	49	PRO	CA-C-N	-10.14	107.84	122.45
2	M	49	PRO	C-N-CA	-10.14	107.84	122.45
2	M	15	PRO	O-C-N	9.33	133.74	123.01
1	L	272	TRP	O-C-N	-9.27	110.52	122.20
3	H	75	VAL	O-C-N	-9.06	110.77	121.10
3	H	63	THR	O-C-N	8.32	133.20	123.30
3	H	75	VAL	C-N-CD	8.22	138.69	120.60
3	H	61	PRO	O-C-N	7.58	132.41	123.01
1	L	70	ALA	O-C-N	7.26	131.16	122.96
3	H	75	VAL	CA-C-N	-7.21	109.70	127.00
3	H	75	VAL	C-N-CA	-7.21	109.70	127.00
2	M	301	HIS	O-C-N	-7.14	113.09	122.59
2	M	49	PRO	O-C-N	7.09	134.58	121.10
1	L	276	PRO	O-C-N	6.98	131.52	123.00
2	M	52	LEU	CB-CA-C	6.57	120.60	109.50
2	M	199	ASN	O-C-N	-6.54	115.75	121.31
2	M	42	PHE	CA-CB-CG	6.50	120.30	113.80
1	L	35	GLY	N-CA-C	-6.04	105.50	112.50
1	L	43	ALA	O-C-N	5.96	128.21	122.07
3	H	62	LYS	O-C-N	5.95	130.56	123.24
3	H	147	ASN	CA-C-N	5.86	125.23	118.85
3	H	147	ASN	C-N-CA	5.86	125.23	118.85
1	L	65	SER	O-C-N	5.70	130.45	123.44
1	L	216	PHE	CA-CB-CG	-5.64	108.16	113.80
1	L	277	GLY	O-C-N	5.57	128.20	122.91
1	L	2	LEU	CB-CA-C	-5.55	99.21	109.37
2	M	143	GLY	N-CA-C	-5.49	106.29	112.33
2	M	249	TYR	CB-CA-C	-5.45	101.74	110.79
3	H	37	ARG	NE-CZ-NH2	5.45	124.11	119.20
2	M	38	LEU	O-C-N	5.42	128.39	122.11
2	M	164	ARG	NE-CZ-NH2	5.37	124.03	119.20
3	H	202	ARG	NE-CZ-NH2	5.34	124.01	119.20
3	H	221	SER	CA-C-N	5.33	126.51	119.84
3	H	221	SER	C-N-CA	5.33	126.51	119.84
2	M	278	LEU	O-C-N	5.32	127.83	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	240	ASP	O-C-N	5.32	129.66	122.59
2	M	136	ARG	NE-CZ-NH2	5.31	123.98	119.20
2	M	253	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	L	269	LEU	CB-CA-C	5.31	116.36	108.87
1	L	231	ARG	NE-CZ-NH2	5.30	123.97	119.20
3	H	154	ARG	NE-CZ-NH2	5.30	123.97	119.20
3	H	70	ARG	NE-CZ-NH2	5.30	123.97	119.20
3	H	117	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	M	279	THR	O-C-N	5.29	128.18	122.15
3	H	189	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	L	217	ARG	NE-CZ-NH2	5.28	123.96	119.20
1	L	135	ARG	NE-CZ-NH2	5.27	123.94	119.20
2	M	228	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	L	153	HIS	CA-CB-CG	5.25	119.05	113.80
2	M	13	ARG	NE-CZ-NH2	5.25	123.93	119.20
3	H	203	VAL	O-C-N	5.24	128.68	123.18
2	M	233	ARG	NE-CZ-NH2	5.24	123.91	119.20
3	H	64	PHE	O-C-N	5.22	129.17	123.27
3	H	177	ARG	NE-CZ-NH2	5.21	123.89	119.20
3	H	118	ARG	NE-CZ-NH2	5.19	123.87	119.20
3	H	83	ARG	NE-CZ-NH2	5.16	123.85	119.20
2	M	241	ARG	NE-CZ-NH2	5.14	123.82	119.20
2	M	81	ASN	CA-C-N	5.10	124.89	119.28
2	M	81	ASN	C-N-CA	5.10	124.89	119.28
3	H	44	ASN	N-CA-C	-5.08	103.97	110.53
2	M	15	PRO	CA-C-N	5.07	128.30	121.05
2	M	15	PRO	C-N-CA	5.07	128.30	121.05
1	L	10	ARG	NE-CZ-NH2	5.07	123.76	119.20
2	M	1	ALA	O-C-N	5.05	131.08	123.00
3	H	40	TYR	C-N-CD	5.02	131.65	120.60
2	M	247	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	L	276	PRO	N-CA-C	5.02	118.94	111.41
2	M	29	ARG	NE-CZ-NH2	5.02	123.72	119.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	301	HIS	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	2225	0	2187	65	0
2	M	2415	0	2325	104	0
3	H	1829	0	1836	75	0
4	L	132	0	148	16	0
4	M	132	0	148	17	0
5	L	65	0	76	3	0
5	M	55	0	53	1	0
6	L	48	0	62	5	0
6	M	48	0	63	15	0
7	M	1	0	0	0	0
8	M	43	0	69	4	0
9	M	81	0	106	3	0
10	H	16	0	31	10	0
10	M	32	0	62	8	0
11	H	70	0	0	2	0
11	L	41	0	0	1	0
11	M	55	0	0	0	0
All	All	7288	0	7166	248	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 17.

All (248) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:265:ILE:HG21	6:M:504:U10:H3M3	1.17	1.12
2:M:265:ILE:HG21	6:M:504:U10:C3M	1.88	1.03
2:M:204:LEU:HB3	2:M:279:THR:HG21	1.50	0.93
1:L:34:PHE:O	1:L:38:THR:HG23	1.69	0.91
6:M:504:U10:H202	10:H:703:LDA:H112	1.52	0.88
2:M:265:ILE:CG2	6:M:504:U10:H3M3	2.02	0.88
3:H:167:ILE:HG22	3:H:169:VAL:HG23	1.57	0.87
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.56	0.85
2:M:256:MET:HE3	2:M:258:PHE:CZ	2.13	0.84
3:H:135:LYS:HE2	11:H:1151:HOH:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:40:TYR:OH	10:H:703:LDA:HM23	1.79	0.81
3:H:33:THR:O	3:H:59:PRO:HG3	1.80	0.81
1:L:45:GLY:O	1:L:49:ILE:HG13	1.81	0.80
4:L:502:BCL:OBB	4:L:502:BCL:HHC	1.81	0.80
2:M:197:PHE:HZ	4:M:502:BCL:HBB2	1.48	0.79
1:L:264:GLN:O	1:L:267:VAL:HG12	1.83	0.78
2:M:155:TRP:CD2	9:M:800:CDL:H812	2.20	0.77
2:M:256:MET:HE3	2:M:258:PHE:CE1	2.19	0.76
1:L:38:THR:HG22	1:L:99:SER:HB3	1.67	0.76
1:L:212:ALA:HA	2:M:142:MET:HE1	1.66	0.76
2:M:197:PHE:CZ	4:M:502:BCL:HBB2	2.22	0.75
1:L:272:TRP:HA	1:L:275:ILE:HD12	1.68	0.74
2:M:98:ALA:HB1	2:M:100:GLU:OE1	1.87	0.74
1:L:272:TRP:O	2:M:87:ARG:NH1	2.20	0.74
3:H:37:ARG:HH11	3:H:37:ARG:HG2	1.52	0.73
10:M:701:LDA:H111	3:H:28:ILE:HD11	1.69	0.73
4:M:502:BCL:CBB	4:M:502:BCL:HHC	2.19	0.73
10:M:704:LDA:HM13	10:H:703:LDA:H11	1.71	0.72
2:M:152:SER:O	2:M:155:TRP:HB3	1.90	0.72
3:H:245:ALA:HB3	3:H:246:PRO:HD3	1.72	0.72
2:M:260:ALA:HB1	3:H:35:ASN:OD1	1.91	0.71
1:L:85:LEU:O	1:L:89:ILE:HG13	1.91	0.70
2:M:260:ALA:HA	3:H:35:ASN:OD1	1.90	0.70
2:M:260:ALA:CA	3:H:35:ASN:OD1	2.40	0.70
2:M:208:PHE:HE1	10:M:701:LDA:H91	1.55	0.70
4:M:501:BCL:H62	4:M:502:BCL:H193	1.74	0.69
1:L:262:TRP:O	1:L:265:TRP:HD1	1.76	0.69
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.73	0.69
2:M:260:ALA:CB	3:H:35:ASN:OD1	2.41	0.68
1:L:217:ARG:O	1:L:221:GLY:HA2	1.95	0.67
4:M:502:BCL:HHC	4:M:502:BCL:HBB3	1.77	0.67
2:M:245:ALA:O	2:M:249:TYR:CD1	2.48	0.66
6:M:504:U10:H202	10:H:703:LDA:C11	2.26	0.65
2:M:5:ASN:CG	3:H:194:GLN:NE2	2.54	0.65
4:L:501:BCL:HMB1	4:L:501:BCL:HBB2	1.79	0.65
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.32	0.64
2:M:65:MET:HB3	2:M:121:PHE:CD2	2.33	0.64
2:M:105:PHE:CD1	2:M:116:LEU:HD13	2.33	0.64
2:M:5:ASN:CG	3:H:194:GLN:HE22	2.05	0.64
1:L:8:LYS:HA	3:H:87:LEU:CD1	2.29	0.63
3:H:129:ASN:ND2	3:H:224:GLU:HG2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:167:ILE:HG22	3:H:169:VAL:CG2	2.26	0.63
1:L:38:THR:HG22	1:L:99:SER:CB	2.29	0.62
1:L:135:ARG:HB3	1:L:136:PRO:CD	2.30	0.62
2:M:13:ARG:O	3:H:140:PHE:HA	2.00	0.61
2:M:193:HIS:O	2:M:293:ASN:HA	2.00	0.61
2:M:39:LEU:HD12	2:M:47:LEU:HD21	1.82	0.61
3:H:241:LEU:O	3:H:248:ARG:NH2	2.33	0.61
4:L:501:BCL:H192	5:L:503:BPH:H7C2	1.83	0.60
1:L:16:LEU:N	1:L:106:GLU:OE2	2.31	0.60
2:M:215:LEU:HD11	2:M:265:ILE:HD11	1.83	0.60
3:H:40:TYR:OH	10:H:703:LDA:CM2	2.50	0.60
4:M:501:BCL:H121	4:M:502:BCL:H171	1.84	0.59
1:L:271:TRP:CD1	1:L:271:TRP:N	2.70	0.59
1:L:168:HIS:CD2	4:L:502:BCL:HMC2	2.37	0.59
5:L:503:BPH:HMB3	5:L:503:BPH:HBB3	1.83	0.59
2:M:208:PHE:CE1	10:M:701:LDA:H91	2.37	0.58
1:L:272:TRP:HA	1:L:275:ILE:CD1	2.32	0.58
2:M:162:PHE:O	2:M:166:ILE:HD12	2.04	0.58
1:L:8:LYS:HA	3:H:87:LEU:HD11	1.85	0.58
3:H:40:TYR:OH	10:H:703:LDA:HM12	2.04	0.57
1:L:193:LEU:HD23	6:L:504:U10:C2	2.34	0.57
1:L:244:SER:OG	4:L:502:BCL:HMA2	2.05	0.57
10:M:701:LDA:C11	3:H:28:ILE:HD11	2.34	0.56
3:H:24:LEU:O	3:H:28:ILE:HG12	2.05	0.56
1:L:117:ILE:HB	1:L:118:PRO:HD3	1.87	0.56
1:L:234:LEU:O	1:L:238:LEU:HG	2.05	0.56
2:M:75:TRP:HE1	8:M:600:SPN:HM13	1.69	0.56
2:M:187:ASN:HA	4:M:502:BCL:CBC	2.35	0.56
2:M:243:THR:O	2:M:247:ARG:HG3	2.06	0.56
2:M:65:MET:HB3	2:M:121:PHE:CE2	2.41	0.56
2:M:219:HIS:ND1	6:M:504:U10:H3M2	2.20	0.56
2:M:53:GLY:O	2:M:54:SER:C	2.48	0.56
4:M:501:BCL:HBB2	4:M:501:BCL:HMB3	1.88	0.55
2:M:155:TRP:CE3	9:M:800:CDL:H812	2.41	0.55
2:M:123:PHE:HE1	2:M:158:MET:HE1	1.72	0.55
2:M:187:ASN:HA	4:M:502:BCL:HBC3	1.88	0.55
2:M:235:LEU:HD23	2:M:238:ILE:HD12	1.87	0.55
3:H:229:GLU:O	3:H:233:ILE:HG13	2.07	0.55
3:H:206:ASN:ND2	3:H:248:ARG:HD2	2.22	0.54
3:H:184:LYS:HG3	3:H:184:LYS:O	2.07	0.54
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:279:ILE:HG21	2:M:91:PHE:HB3	1.89	0.54
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.89	0.53
2:M:219:HIS:CE1	6:M:504:U10:H3M2	2.43	0.53
2:M:3:TYR:CE2	3:H:194:GLN:NE2	2.76	0.53
1:L:6:GLU:OE1	2:M:253:ARG:NH1	2.42	0.53
2:M:136:ARG:NE	2:M:136:ARG:HA	2.23	0.53
3:H:219:ILE:HG21	3:H:225:VAL:HG13	1.91	0.53
10:M:701:LDA:H101	10:H:703:LDA:C12	2.39	0.52
4:L:502:BCL:H203	4:L:501:BCL:H102	1.91	0.52
3:H:199:GLN:HB2	3:H:202:ARG:O	2.09	0.52
1:L:208:THR:O	1:L:211:HIS:HB2	2.10	0.52
1:L:69:PRO:HB3	1:L:78:ALA:HB2	1.91	0.52
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.91	0.52
1:L:264:GLN:C	1:L:267:VAL:HG12	2.35	0.52
1:L:139:MET:HE3	1:L:252:GLY:HA3	1.91	0.51
2:M:251:PHE:CD1	2:M:251:PHE:C	2.89	0.51
3:H:70:ARG:HB3	3:H:118:ARG:HH12	1.75	0.51
2:M:157:TRP:HB2	4:M:502:BCL:H62	1.92	0.51
3:H:37:ARG:HG2	3:H:37:ARG:NH1	2.23	0.51
1:L:267:VAL:HG13	1:L:268:LYS:HG2	1.93	0.51
2:M:240:ASP:OD2	3:H:118:ARG:HG3	2.10	0.51
3:H:219:ILE:HD12	3:H:221:SER:O	2.11	0.51
3:H:199:GLN:HE22	3:H:202:ARG:HH11	1.57	0.50
2:M:219:HIS:HD1	6:M:504:U10:H3M2	1.76	0.50
3:H:68:HIS:CD2	3:H:123:LEU:HD12	2.46	0.50
3:H:189:ARG:HD2	3:H:216:ILE:HB	1.92	0.50
3:H:219:ILE:HA	3:H:229:GLU:OE2	2.10	0.50
3:H:68:HIS:CD2	3:H:123:LEU:HB2	2.46	0.50
1:L:51:TRP:CH2	1:L:80:LEU:CD1	2.95	0.50
3:H:244:ALA:C	3:H:246:PRO:HD2	2.36	0.50
4:L:502:BCL:HAA2	4:L:501:BCL:HAC1	1.93	0.50
10:M:704:LDA:H12	10:H:703:LDA:H31	1.94	0.50
2:M:300:ASN:O	2:M:301:HIS:HB2	2.11	0.49
3:H:131:ILE:HD11	3:H:177:ARG:HD2	1.94	0.49
2:M:3:TYR:HE2	3:H:194:GLN:NE2	2.09	0.49
2:M:20:MET:HE1	3:H:125:GLY:C	2.38	0.49
2:M:103:LEU:HD21	2:M:166:ILE:HA	1.94	0.49
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.47	0.49
1:L:193:LEU:HD23	6:L:504:U10:C3	2.42	0.49
3:H:12:LEU:O	3:H:15:LEU:HB3	2.12	0.49
3:H:131:ILE:CD1	3:H:177:ARG:HD2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:138:MET:HE2	1:L:253:THR:HG21	1.95	0.48
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.95	0.48
5:L:503:BPH:HMB3	5:L:503:BPH:CBB	2.43	0.48
2:M:175:VAL:HG11	8:M:600:SPN:H161	1.94	0.48
1:L:1:ALA:HB1	11:H:1141:HOH:O	2.13	0.48
1:L:271:TRP:CD1	1:L:271:TRP:H	2.31	0.48
1:L:66:VAL:HG11	1:L:89:ILE:HD12	1.96	0.48
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.94	0.48
2:M:5:ASN:OD1	3:H:194:GLN:NE2	2.41	0.48
4:M:501:BCL:H151	4:M:501:BCL:H112	1.54	0.48
3:H:206:ASN:HD21	3:H:248:ARG:HD2	1.79	0.48
2:M:264:GLY:O	2:M:267:ARG:N	2.42	0.47
3:H:181:VAL:O	3:H:188:THR:HA	2.13	0.47
1:L:51:TRP:O	1:L:54:VAL:HG22	2.14	0.47
2:M:164:ARG:N	2:M:165:PRO:HD2	2.28	0.47
3:H:40:TYR:HA	3:H:41:PRO:C	2.38	0.47
2:M:234:GLU:O	2:M:238:ILE:HG13	2.14	0.47
10:M:701:LDA:H101	10:H:703:LDA:H121	1.97	0.47
1:L:208:THR:HB	1:L:209:PRO:HD2	1.97	0.47
4:L:502:BCL:OBB	4:L:502:BCL:CHC	2.55	0.47
1:L:248:MET:CG	4:L:502:BCL:HED2	2.45	0.46
1:L:102:LEU:O	1:L:105:VAL:HB	2.15	0.46
3:H:118:ARG:C	3:H:120:LEU:H	2.23	0.46
1:L:34:PHE:HB2	11:L:1002:HOH:O	2.14	0.46
1:L:22:PHE:HA	1:L:24:PHE:HE2	1.79	0.46
2:M:75:TRP:HE1	8:M:600:SPN:CM1	2.29	0.45
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.97	0.45
2:M:17:ASP:C	2:M:19:GLY:H	2.24	0.45
2:M:20:MET:HE1	3:H:125:GLY:O	2.17	0.45
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.97	0.45
2:M:293:ASN:CG	2:M:296:VAL:HG23	2.41	0.45
4:M:501:BCL:C12	4:M:502:BCL:H171	2.46	0.45
4:L:501:BCL:H202	4:L:501:BCL:H162	1.84	0.45
6:M:504:U10:H28	6:M:504:U10:H322	1.47	0.45
2:M:98:ALA:C	2:M:100:GLU:H	2.24	0.45
2:M:194:GLY:O	2:M:195:ASN:HB3	2.16	0.45
1:L:42:ALA:O	1:L:46:ILE:HD12	2.17	0.44
2:M:265:ILE:HG12	6:M:504:U10:C2	2.47	0.44
2:M:271:TRP:CZ2	9:M:800:CDL:H722	2.52	0.44
1:L:280:ASN:HB2	2:M:88:ASP:OD1	2.17	0.44
2:M:30:SER:HB3	2:M:50:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:114:LEU:HD12	2:M:114:LEU:HA	1.83	0.44
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.52	0.44
4:M:501:BCL:C6	4:M:502:BCL:H193	2.44	0.44
4:M:502:BCL:HBB2	4:M:502:BCL:HHC	1.98	0.44
1:L:177:ILE:HG23	4:L:502:BCL:HMB3	1.99	0.44
3:H:68:HIS:HD2	3:H:123:LEU:HD12	1.82	0.44
2:M:252:TRP:CD1	6:M:504:U10:C6	3.01	0.44
2:M:20:MET:CE	3:H:125:GLY:HA3	2.48	0.43
2:M:30:SER:HG	2:M:31:GLY:N	2.16	0.43
3:H:12:LEU:HD12	3:H:12:LEU:HA	1.80	0.43
4:L:502:BCL:HBB3	4:L:502:BCL:HMB1	2.00	0.43
3:H:129:ASN:HD22	3:H:224:GLU:HG2	1.84	0.43
3:H:195:MET:HE1	3:H:241:LEU:HD11	1.99	0.43
3:H:209:SER:OG	3:H:212:LEU:HD12	2.19	0.43
2:M:53:GLY:O	2:M:56:GLY:N	2.52	0.43
1:L:272:TRP:CG	2:M:87:ARG:HB2	2.54	0.43
2:M:249:TYR:CE1	6:M:504:U10:H4M1	2.54	0.43
3:H:26:GLY:O	3:H:29:TYR:HB3	2.19	0.43
3:H:168:TRP:CZ3	3:H:225:VAL:HG22	2.54	0.43
1:L:117:ILE:HB	1:L:118:PRO:CD	2.48	0.43
3:H:40:TYR:CE2	3:H:42:LEU:HG	2.54	0.43
1:L:265:TRP:O	1:L:269:LEU:HG	2.18	0.43
2:M:211:GLY:HA2	2:M:214:LEU:HB3	2.01	0.42
2:M:268:TRP:CE3	6:M:504:U10:H122	2.53	0.42
3:H:245:ALA:HB3	3:H:246:PRO:CD	2.47	0.42
3:H:16:ALA:O	3:H:19:SER:HB2	2.20	0.42
3:H:70:ARG:NH2	3:H:120:LEU:HB3	2.33	0.42
1:L:97:PHE:CE1	4:L:502:BCL:H121	2.55	0.42
1:L:201:GLU:CG	2:M:144:LYS:NZ	2.82	0.42
2:M:74:PHE:CE2	2:M:92:PHE:HB2	2.54	0.42
2:M:215:LEU:HD23	2:M:269:ALA:HA	2.01	0.42
1:L:269:LEU:HA	1:L:270:PRO:HD3	1.92	0.42
2:M:142:MET:O	2:M:144:LYS:NZ	2.39	0.42
3:H:37:ARG:HH11	3:H:37:ARG:CG	2.26	0.42
3:H:40:TYR:OH	10:H:703:LDA:CM1	2.67	0.42
1:L:18:GLY:O	1:L:21:LEU:HB2	2.19	0.42
1:L:212:ALA:HA	2:M:142:MET:CE	2.42	0.42
2:M:98:ALA:C	2:M:100:GLU:N	2.78	0.42
2:M:219:HIS:HA	6:M:504:U10:O2	2.19	0.42
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.19	0.42
2:M:125:ALA:HB1	5:M:503:BPH:H2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:197:PHE:HD1	2:M:197:PHE:HA	1.72	0.42
2:M:249:TYR:CD1	6:M:504:U10:H4M1	2.55	0.42
3:H:65:ILE:HD13	3:H:65:ILE:HG21	1.84	0.42
3:H:36:MET:C	3:H:38:GLU:H	2.27	0.41
3:H:189:ARG:HD2	3:H:216:ILE:O	2.20	0.41
1:L:195:LEU:HD11	2:M:267:ARG:HG2	2.03	0.41
6:L:504:U10:H23	6:L:504:U10:H272	1.86	0.41
1:L:208:THR:HA	1:L:209:PRO:HD3	1.92	0.41
2:M:30:SER:OG	2:M:31:GLY:N	2.53	0.41
1:L:178:SER:HB3	6:L:504:U10:C25	2.50	0.41
2:M:68:PHE:CD1	8:M:600:SPN:O2	2.73	0.41
2:M:295:TYR:O	2:M:299:GLN:HG2	2.21	0.41
1:L:195:LEU:HD23	1:L:195:LEU:HA	1.93	0.41
4:M:501:BCL:HMB3	4:M:501:BCL:CBB	2.49	0.41
1:L:173:HIS:O	1:L:177:ILE:HG13	2.21	0.41
4:L:501:BCL:H161	4:L:501:BCL:H122	1.80	0.41
2:M:12:VAL:HA	3:H:141:HIS:O	2.21	0.41
2:M:74:PHE:O	2:M:77:GLN:HB2	2.20	0.41
2:M:164:ARG:N	2:M:165:PRO:CD	2.84	0.41
2:M:211:GLY:O	2:M:214:LEU:HB3	2.20	0.41
2:M:240:ASP:O	3:H:117:ARG:NH2	2.49	0.41
3:H:177:ARG:O	3:H:193:MET:HB2	2.21	0.41
3:H:245:ALA:N	3:H:246:PRO:HD2	2.36	0.41
1:L:135:ARG:N	1:L:136:PRO:HD2	2.35	0.41
2:M:11:GLN:HB2	3:H:144:ALA:HB3	2.01	0.41
3:H:152:PRO:HB2	3:H:160:ILE:HD12	2.03	0.41
2:M:129:TRP:O	2:M:132:ARG:HB3	2.21	0.40
4:L:502:BCL:H141	4:L:502:BCL:H162	1.90	0.40
1:L:97:PHE:CZ	4:L:502:BCL:H121	2.57	0.40
1:L:178:SER:HB3	6:L:504:U10:H251	2.03	0.40
4:M:501:BCL:C4A	4:M:501:BCL:HBA1	2.50	0.40
4:M:501:BCL:OB	4:M:501:BCL:HHC	2.21	0.40
2:M:235:LEU:O	2:M:238:ILE:HB	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	270 (97%)	9 (3%)	0	100	100
2	M	300/314 (96%)	290 (97%)	8 (3%)	2 (1%)	18	47
3	H	238/260 (92%)	227 (95%)	11 (5%)	0	100	100
All	All	817/855 (96%)	787 (96%)	28 (3%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	301	HIS
2	M	22	GLU

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	218/218 (100%)	203 (93%)	15 (7%)	14	41
2	M	237/248 (96%)	229 (97%)	8 (3%)	32	68
3	H	195/208 (94%)	191 (98%)	4 (2%)	47	79
All	All	650/674 (96%)	623 (96%)	27 (4%)	26	61

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	LEU

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Mol	Chain	Res	Type
1	L	21	LEU
1	L	38	THR
1	L	46	ILE
1	L	47	ILE
1	L	80	LEU
1	L	137	VAL
1	L	154	LEU
1	L	185	LEU
1	L	202	LYS
1	L	216	PHE
1	L	235	LEU
1	L	251	THR
1	L	271	TRP
1	L	272	TRP
2	M	30	SER
2	M	136	ARG
2	M	144	LYS
2	M	196	LEU
2	M	204	LEU
2	M	265	ILE
2	M	270	ILE
2	M	274	VAL
3	H	135	LYS
3	H	221	SER
3	H	225	VAL
3	H	231	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	4	GLN
2	M	44	ASN
3	H	68	HIS
3	H	199	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 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	LDA	H	703	-	13,15,15	2.75	2 (15%)	14,17,17	0.65	0
9	CDL	M	800	-	80,80,99	0.51	0	86,92,111	1.09	6 (6%)
5	BPH	M	503	-	49,60,70	2.19	12 (24%)	47,89,101	3.12	21 (44%)
4	BCL	L	501	1	69,74,74	1.31	8 (11%)	79,115,115	2.06	10 (12%)
8	SPN	M	600	-	42,42,42	3.78	17 (40%)	50,52,52	2.51	16 (32%)
6	U10	M	504	-	48,48,63	2.58	19 (39%)	60,61,79	1.73	12 (20%)
4	BCL	M	502	2	69,74,74	1.09	5 (7%)	79,115,115	1.80	11 (13%)
4	BCL	L	502	1	69,74,74	1.51	10 (14%)	79,115,115	2.16	12 (15%)
4	BCL	M	501	2	69,74,74	1.39	12 (17%)	79,115,115	2.26	23 (29%)
6	U10	L	504	-	48,48,63	1.83	13 (27%)	60,61,79	2.81	17 (28%)
10	LDA	M	701	-	13,15,15	2.43	2 (15%)	14,17,17	0.40	0
10	LDA	M	704	-	13,15,15	1.91	1 (7%)	14,17,17	0.52	0
5	BPH	L	503	-	59,70,70	2.06	17 (28%)	59,101,101	2.57	17 (28%)

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	LDA	H	703	-	-	5/13/13/13	-
9	CDL	M	800	-	-	29/91/91/110	-
5	BPH	M	503	-	1/1/16/22	6/25/93/105	0/5/6/6
4	BCL	L	501	1	1/1/21/25	10/41/137/137	-
8	SPN	M	600	-	-	18/50/51/51	-
6	U10	M	504	-	-	10/45/69/87	0/1/1/1
4	BCL	M	502	2	-	8/41/137/137	-
4	BCL	L	502	1	-	5/41/137/137	-
4	BCL	M	501	2	2/2/21/25	13/41/137/137	-
6	U10	L	504	-	-	11/45/69/87	0/1/1/1
10	LDA	M	701	-	-	8/13/13/13	-
10	LDA	M	704	-	-	4/13/13/13	-
5	BPH	L	503	-	-	4/37/105/105	0/5/6/6

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	600	SPN	C4-C5	9.28	1.54	1.33
8	M	600	SPN	C19-C18	9.14	1.54	1.33
8	M	600	SPN	C8-C9	8.79	1.53	1.33
8	M	600	SPN	C12-C13	8.51	1.52	1.33
10	M	701	LDA	O1-N1	-8.41	1.21	1.42
10	H	703	LDA	O1-N1	-8.00	1.22	1.42
5	M	503	BPH	C2C-C3C	-7.91	1.47	1.54
6	M	504	U10	C27-C28	-7.89	1.26	1.50
6	M	504	U10	O3-C3	7.41	1.54	1.36
10	M	704	LDA	O1-N1	-6.70	1.25	1.42
5	L	503	BPH	C2C-C3C	-6.29	1.49	1.54
5	L	503	BPH	C1D-C2D	6.16	1.46	1.39
8	M	600	SPN	C3-C4	-6.06	1.41	1.50
8	M	600	SPN	C17-C18	-6.01	1.38	1.51
5	M	503	BPH	C1D-C2D	5.93	1.46	1.39
8	M	600	SPN	C10-C9	-5.87	1.39	1.51
10	H	703	LDA	C1-N1	-5.81	1.45	1.51
5	L	503	BPH	C3A-C2A	-5.78	1.49	1.54
8	M	600	SPN	C14-C13	-5.43	1.40	1.51
4	L	502	BCL	O2D-CED	-5.39	1.33	1.45
8	M	600	SPN	C6-C5	-5.27	1.40	1.51
5	M	503	BPH	C1B-C2B	5.12	1.45	1.39
5	L	503	BPH	C1B-C2B	4.89	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	501	BCL	MG-ND	-4.83	1.96	2.05
4	M	501	BCL	O2D-CGD	4.76	1.44	1.33
6	L	504	U10	O4-C4	4.56	1.47	1.36
4	L	501	BCL	O2D-CGD	4.51	1.44	1.33
4	L	502	BCL	C1-C2	-4.51	1.36	1.49
4	M	501	BCL	MG-NA	4.49	2.16	2.06
4	L	502	BCL	O2A-CGA	4.22	1.45	1.33
4	L	502	BCL	MG-NA	4.20	2.16	2.06
6	M	504	U10	C17-C18	-4.09	1.38	1.50
4	L	501	BCL	MG-NA	4.07	2.15	2.06
4	M	502	BCL	MG-NA	4.06	2.15	2.06
5	M	503	BPH	O2A-CGA	3.88	1.44	1.33
5	M	503	BPH	O2D-CGD	3.85	1.42	1.33
5	L	503	BPH	O2D-CGD	3.83	1.42	1.33
6	M	504	U10	C11-C9	3.82	1.59	1.51
8	M	600	SPN	C20-C19	-3.80	1.39	1.50
4	M	501	BCL	O2A-CGA	3.77	1.44	1.33
6	M	504	U10	O4-C4	3.69	1.45	1.36
6	M	504	U10	C22-C23	-3.56	1.39	1.50
6	M	504	U10	C37-C38	-3.54	1.39	1.50
6	L	504	U10	C7-C8	-3.53	1.45	1.50
6	M	504	U10	C36-C34	3.52	1.58	1.51
6	L	504	U10	C13-C14	3.45	1.41	1.33
5	L	503	BPH	O2A-CGA	3.43	1.43	1.33
6	M	504	U10	C35-C34	3.36	1.58	1.50
8	M	600	SPN	C25-C26	3.36	1.40	1.33
8	M	600	SPN	C7-C8	-3.35	1.40	1.50
8	M	600	SPN	C11-C12	-3.34	1.40	1.50
6	L	504	U10	O3-C3	3.30	1.44	1.36
5	L	503	BPH	C3B-C2B	-3.27	1.34	1.39
6	L	504	U10	C23-C24	3.25	1.40	1.33
6	M	504	U10	C33-C34	3.21	1.40	1.33
6	L	504	U10	O3-C3M	-3.20	1.38	1.45
4	M	502	BCL	C3B-C4B	3.20	1.47	1.41
4	L	502	BCL	MG-NC	3.06	2.13	2.06
4	L	502	BCL	C3B-C4B	3.03	1.47	1.41
8	M	600	SPN	O1-CMA	3.00	1.52	1.43
5	M	503	BPH	O2D-CED	-2.99	1.38	1.45
6	L	504	U10	C32-C33	-2.95	1.41	1.50
5	L	503	BPH	CHA-CBD	2.93	1.55	1.51
6	M	504	U10	C8-C9	2.91	1.39	1.33
8	M	600	SPN	C29-C30	2.90	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	504	U10	C8-C9	2.87	1.39	1.33
4	L	501	BCL	C3B-C4B	2.85	1.46	1.41
4	M	502	BCL	C2-C3	2.80	1.39	1.33
8	M	600	SPN	C21-C22	-2.80	1.39	1.52
5	M	503	BPH	CHA-CBD	2.73	1.54	1.51
6	L	504	U10	C18-C19	2.69	1.39	1.33
4	L	501	BCL	C2-C3	2.69	1.39	1.33
5	M	503	BPH	C3B-C2B	-2.66	1.35	1.39
5	L	503	BPH	O2D-CED	-2.65	1.39	1.45
4	M	501	BCL	CAA-C2A	2.61	1.58	1.54
5	L	503	BPH	C2-C3	2.61	1.39	1.33
6	M	504	U10	O4-C4M	-2.59	1.39	1.45
6	M	504	U10	C38-C39	2.59	1.40	1.32
6	M	504	U10	C30-C29	2.56	1.57	1.50
6	M	504	U10	C15-C14	2.56	1.56	1.50
4	M	501	BCL	C3B-C4B	2.55	1.46	1.41
8	M	600	SPN	C16-C15	-2.52	1.39	1.51
5	M	503	BPH	C4D-ND	-2.52	1.34	1.38
6	L	504	U10	C38-C39	2.50	1.39	1.32
4	M	502	BCL	O2D-CED	-2.48	1.39	1.45
6	M	504	U10	C13-C14	2.46	1.38	1.33
4	L	501	BCL	O2A-CGA	2.46	1.40	1.33
6	M	504	U10	C18-C19	2.45	1.38	1.33
4	M	501	BCL	CMA-C3A	2.45	1.58	1.53
4	M	501	BCL	C2C-C3C	-2.45	1.47	1.54
6	M	504	U10	O3-C3M	-2.43	1.39	1.45
5	M	503	BPH	C2-C3	2.41	1.38	1.33
4	M	501	BCL	C2-C3	2.40	1.38	1.33
4	M	501	BCL	CMB-C2B	2.38	1.55	1.50
5	L	503	BPH	O1D-CGD	2.37	1.27	1.21
4	L	502	BCL	C4-C3	2.32	1.56	1.50
5	L	503	BPH	CAA-C2A	2.30	1.58	1.54
5	M	503	BPH	C3D-C2D	-2.24	1.35	1.39
6	M	504	U10	O2-C2	2.22	1.28	1.23
4	L	502	BCL	CMC-C2C	-2.21	1.48	1.53
4	L	502	BCL	MG-ND	-2.21	2.01	2.05
5	L	503	BPH	C3D-C4D	2.17	1.44	1.41
6	L	504	U10	C27-C28	-2.15	1.44	1.50
4	M	502	BCL	O2A-CGA	2.13	1.39	1.33
6	L	504	U10	C15-C14	2.12	1.55	1.50
4	L	502	BCL	O2D-CGD	2.11	1.38	1.33
4	M	501	BCL	C3B-C2B	-2.11	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	501	BCL	CMB-C2B	-2.10	1.46	1.50
6	L	504	U10	C28-C29	2.09	1.37	1.33
5	L	503	BPH	C5-C3	2.08	1.55	1.51
4	M	501	BCL	C4-C3	2.07	1.55	1.50
4	M	501	BCL	O2D-CED	-2.05	1.40	1.45
5	L	503	BPH	C3B-C4B	2.05	1.44	1.41
4	L	501	BCL	O2D-CED	-2.05	1.40	1.45
5	L	503	BPH	C4-C3	2.05	1.55	1.50
5	M	503	BPH	C1A-C2A	2.04	1.54	1.51
5	L	503	BPH	C3D-C2D	-2.02	1.36	1.39
10	M	701	LDA	C1-N1	-2.00	1.49	1.51

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	504	U10	C32-C33-C34	15.42	162.91	127.62
5	M	503	BPH	O2D-CGD-CBD	13.68	125.97	110.95
5	L	503	BPH	O2D-CGD-CBD	13.07	125.31	110.95
4	L	502	BCL	OBb-CAB-C3B	9.12	136.56	120.43
4	L	501	BCL	C4A-NA-C1A	8.56	110.59	106.68
4	L	502	BCL	C4A-NA-C1A	8.26	110.45	106.68
4	M	501	BCL	C1-C2-C3	8.19	139.62	126.20
4	L	501	BCL	O2D-CGD-CBD	8.06	125.33	111.23
4	M	502	BCL	C4A-NA-C1A	7.94	110.30	106.68
8	M	600	SPN	CM6-C18-C17	6.86	127.13	115.23
6	L	504	U10	C27-C28-C29	6.75	143.08	127.62
6	L	504	U10	C3M-O3-C3	6.43	139.07	116.47
4	L	502	BCL	C1C-NC-C4C	6.40	109.60	106.68
8	M	600	SPN	CM5-C13-C14	6.25	126.08	115.23
5	M	503	BPH	C1-C2-C3	6.14	136.26	126.20
6	M	504	U10	C22-C23-C24	5.97	141.30	127.62
4	M	502	BCL	O2D-CGD-CBD	5.80	121.38	111.23
4	L	501	BCL	O1D-CGD-CBD	-5.79	113.09	124.52
4	M	501	BCL	C4-C3-C5	-5.71	105.32	115.23
4	M	501	BCL	OBb-CAB-C3B	5.63	130.39	120.43
4	M	502	BCL	C1C-NC-C4C	5.60	109.23	106.68
4	L	501	BCL	C1C-NC-C4C	5.55	109.21	106.68
5	L	503	BPH	O2A-CGA-O1A	-5.15	110.74	123.63
4	L	502	BCL	O2D-CGD-CBD	5.03	120.02	111.23
4	L	501	BCL	OBb-CAB-C3B	4.99	129.26	120.43
5	L	503	BPH	CMA-C3A-C4A	-4.98	103.88	114.61
5	M	503	BPH	C4D-CHA-CBD	-4.84	106.14	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	501	BCL	O2A-CGA-CBA	4.80	126.47	111.83
4	L	502	BCL	CAB-C3B-C2B	4.79	137.69	127.74
4	M	501	BCL	O2D-CGD-CBD	4.72	119.48	111.23
4	M	501	BCL	O2A-CGA-O1A	-4.71	111.85	123.63
8	M	600	SPN	C6-C5-C4	-4.68	110.66	121.17
5	L	503	BPH	O2D-CGD-O1D	-4.62	114.85	123.85
4	M	501	BCL	C4A-NA-C1A	4.54	108.75	106.68
8	M	600	SPN	C3-C4-C5	-4.47	119.13	126.83
8	M	600	SPN	C17-C18-C19	-4.45	111.17	121.17
5	M	503	BPH	O1D-CGD-CBD	-4.41	118.03	124.72
9	M	800	CDL	OB6-CB4-CB6	4.41	124.17	108.34
8	M	600	SPN	CM7-C22-C21	4.32	126.68	111.27
4	L	502	BCL	CBB-CAB-C3B	-4.28	111.39	120.40
6	M	504	U10	C10-C9-C11	-4.26	107.84	115.23
4	L	501	BCL	OB6-CAB-CBB	-4.20	110.37	119.77
8	M	600	SPN	C20-C19-C18	-4.16	118.11	127.62
6	L	504	U10	O5-C5-C6	-4.16	113.75	121.79
4	M	501	BCL	C1C-NC-C4C	4.13	108.56	106.68
6	M	504	U10	C12-C13-C14	4.09	136.99	127.62
5	M	503	BPH	CBC-CAC-C3C	4.07	121.78	113.78
4	M	501	BCL	CAA-C2A-C3A	-4.06	102.02	113.00
5	M	503	BPH	O2D-CGD-O1D	-4.05	115.96	123.85
6	M	504	U10	C26-C24-C23	4.05	130.26	121.17
8	M	600	SPN	C7-C8-C9	-3.98	118.52	127.62
4	L	502	BCL	OB6-CAB-CBB	-3.95	110.91	119.77
9	M	800	CDL	CB6-CB4-CB3	-3.95	102.57	111.78
5	M	503	BPH	CMA-C3A-C4A	-3.94	106.12	114.61
8	M	600	SPN	C11-C12-C13	-3.94	118.61	127.62
4	M	502	BCL	O1D-CGD-CBD	-3.92	116.79	124.52
8	M	600	SPN	CM4-C9-C10	3.80	121.83	115.23
5	M	503	BPH	CED-O2D-CGD	3.73	124.37	115.92
6	M	504	U10	C27-C28-C29	3.65	135.97	127.62
5	M	503	BPH	C1C-C2C-C3C	3.57	106.24	102.84
5	L	503	BPH	O2A-CGA-CBA	3.54	122.62	111.83
4	M	502	BCL	O2A-CGA-CBA	3.53	122.59	111.83
4	M	501	BCL	C5-C3-C2	3.50	129.02	121.17
8	M	600	SPN	C10-C9-C8	-3.50	113.32	121.17
5	L	503	BPH	OBD-CAD-CBD	-3.47	120.74	125.82
6	L	504	U10	C30-C29-C31	-3.45	109.24	115.23
5	M	503	BPH	C6-C5-C3	3.39	121.72	113.47
6	L	504	U10	O2-C2-C3	-3.39	113.85	121.03
5	M	503	BPH	CAA-C2A-C3A	-3.36	103.92	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	600	SPN	C14-C13-C12	-3.35	113.64	121.17
4	M	502	BCL	OBB-CAB-C3B	3.30	126.26	120.43
4	M	501	BCL	O2D-CGD-O1D	-3.29	117.44	123.85
8	M	600	SPN	C16-C17-C18	3.29	121.48	113.47
4	L	502	BCL	O2A-CGA-CBA	3.27	121.81	111.83
5	L	503	BPH	O1D-CGD-CBD	-3.24	119.80	124.72
5	L	503	BPH	CAA-C2A-C3A	-3.17	104.43	113.00
5	L	503	BPH	C4A-C3A-C2A	3.11	105.80	102.84
5	L	503	BPH	C1C-C2C-C3C	3.10	105.79	102.84
4	M	501	BCL	OBB-CAB-CBB	-3.07	112.90	119.77
4	M	501	BCL	C2C-C3C-C4C	2.99	105.82	101.34
4	L	502	BCL	O1D-CGD-CBD	-2.99	118.62	124.52
4	M	501	BCL	CMA-C3A-C2A	-2.95	102.57	113.98
5	M	503	BPH	O2A-CGA-O1A	-2.95	116.26	123.63
5	M	503	BPH	C1B-NB-C4B	-2.94	104.53	108.82
4	L	501	BCL	O2A-CGA-CBA	2.93	120.76	111.83
4	M	502	BCL	CED-O2D-CGD	2.92	122.54	115.92
6	L	504	U10	C16-C14-C13	2.91	127.69	121.17
5	M	503	BPH	C4C-C3C-C2C	2.87	105.57	102.84
5	L	503	BPH	C1B-NB-C4B	-2.77	104.77	108.82
6	L	504	U10	C20-C19-C21	-2.68	110.57	115.23
5	L	503	BPH	CED-O2D-CGD	2.68	122.00	115.92
6	M	504	U10	C7-C6-C1	-2.58	120.47	124.89
4	L	501	BCL	O2A-CGA-O1A	-2.56	117.23	123.63
9	M	800	CDL	OB8-CB6-CB4	2.55	115.75	108.40
4	M	501	BCL	C4D-CHA-C1A	2.53	124.26	121.24
4	M	502	BCL	C1-C2-C3	2.49	130.27	126.20
5	L	503	BPH	C4D-ND-C1D	-2.48	105.91	108.87
8	M	600	SPN	CM3-C5-C6	2.45	119.48	115.23
4	M	501	BCL	CHB-C1B-NB	2.44	127.72	124.05
4	L	502	BCL	C1-C2-C3	2.44	130.20	126.20
6	L	504	U10	C4-C3-C2	-2.39	116.30	120.69
5	L	503	BPH	C4-C3-C5	-2.38	111.10	115.23
6	L	504	U10	C1M-C1-C6	-2.38	120.54	124.45
5	M	503	BPH	CMB-C2B-C3B	2.36	129.41	124.68
4	L	501	BCL	C1D-ND-C4D	-2.36	104.66	106.31
4	L	501	BCL	CAC-C3C-C4C	-2.36	107.35	112.58
6	L	504	U10	C6-C1-C2	2.35	121.03	119.17
6	M	504	U10	C25-C24-C26	-2.34	111.17	115.23
4	M	501	BCL	CAB-C3B-C2B	2.34	132.60	127.74
6	L	504	U10	C17-C18-C19	2.33	132.95	127.62
4	L	502	BCL	CED-O2D-CGD	2.32	121.18	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	504	U10	C1-C6-C5	-2.31	117.38	119.62
6	M	504	U10	C7-C8-C9	2.30	130.80	126.83
6	L	504	U10	C7-C6-C5	-2.27	115.88	118.52
5	M	503	BPH	C5-C3-C2	-2.25	116.11	121.17
6	M	504	U10	C25-C24-C23	-2.25	117.84	123.63
9	M	800	CDL	OA8-CA7-OA9	-2.24	118.02	123.63
8	M	600	SPN	C15-C16-C17	2.24	121.35	113.13
5	M	503	BPH	CMD-C2D-C3D	2.24	129.16	124.68
4	M	501	BCL	CHA-C1A-NA	-2.23	121.35	126.39
6	M	504	U10	C3M-O3-C3	2.22	124.27	116.47
9	M	800	CDL	OB6-CB5-OB7	-2.18	118.61	123.70
6	M	504	U10	C26-C27-C28	-2.18	101.25	112.02
4	M	501	BCL	O1D-CGD-CBD	-2.17	120.24	124.52
4	M	502	BCL	C3A-C2A-C1A	2.15	104.56	101.34
5	M	503	BPH	OBD-CAD-CBD	-2.14	122.68	125.82
6	L	504	U10	O5-C5-C4	2.14	125.56	121.03
5	M	503	BPH	C7-C6-C5	-2.14	107.56	113.26
4	M	502	BCL	C1D-ND-C4D	-2.13	104.82	106.31
9	M	800	CDL	CA6-CA4-CA3	-2.11	106.86	111.78
8	M	600	SPN	C7-C6-C5	2.11	120.16	113.19
6	L	504	U10	C12-C13-C14	-2.09	122.85	127.62
6	L	504	U10	C31-C29-C28	2.08	125.85	121.17
4	M	502	BCL	O2A-CGA-O1A	-2.08	118.42	123.63
4	M	501	BCL	C3C-C2C-C1C	2.07	105.22	101.87
4	M	501	BCL	CMA-C3A-C4A	-2.06	106.22	111.77
5	L	503	BPH	CBC-CAC-C3C	2.05	117.80	113.78
5	M	503	BPH	CMA-C3A-C2A	-2.04	106.24	114.13
5	L	503	BPH	C3D-C4D-ND	2.04	110.32	107.71
4	M	501	BCL	C2B-C1B-NB	-2.04	108.22	110.33
6	M	504	U10	C4M-O4-C4	2.03	123.62	116.47
5	L	503	BPH	C4C-C3C-C2C	2.03	104.77	102.84
4	L	502	BCL	C2B-C1B-NB	-2.03	108.22	110.33
4	M	501	BCL	CAC-C3C-C4C	-2.01	108.11	112.58
5	M	503	BPH	C4-C3-C5	2.00	118.70	115.23

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	L	501	BCL	C13
4	M	501	BCL	C13
4	M	501	BCL	C8
5	M	503	BPH	C8

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	501	BCL	C2C-C3C-CAC-CBC
4	L	501	BCL	C4C-C3C-CAC-CBC
4	L	501	BCL	CHA-CBD-CGD-O1D
4	L	501	BCL	CHA-CBD-CGD-O2D
4	M	501	BCL	C1-C2-C3-C4
5	M	503	BPH	O2A-C1-C2-C3
5	M	503	BPH	C1-C2-C3-C5
6	L	504	U10	C12-C13-C14-C15
6	L	504	U10	C12-C13-C14-C16
8	M	600	SPN	C3-C4-C5-CM3
8	M	600	SPN	C11-C10-C9-CM4
9	M	800	CDL	CA3-OA5-PA1-OA2
9	M	800	CDL	CA3-OA5-PA1-OA3
9	M	800	CDL	CA3-OA5-PA1-OA4
10	M	701	LDA	C2-C1-N1-O1
10	M	701	LDA	C2-C1-N1-CM1
10	M	701	LDA	C2-C1-N1-CM2
10	H	703	LDA	C2-C1-N1-O1
10	H	703	LDA	C2-C1-N1-CM1
4	L	501	BCL	CBD-CGD-O2D-CED
4	L	501	BCL	O1D-CGD-O2D-CED
8	M	600	SPN	C16-C17-C18-CM6
8	M	600	SPN	C14-C15-C16-C17
8	M	600	SPN	C4-C5-C6-C7
8	M	600	SPN	C11-C10-C9-C8
8	M	600	SPN	C12-C13-C14-C15
8	M	600	SPN	C16-C17-C18-C19
6	L	504	U10	C14-C16-C17-C18
6	L	504	U10	C24-C26-C27-C28
6	L	504	U10	C29-C31-C32-C33
6	M	504	U10	C24-C26-C27-C28
5	M	503	BPH	C4-C3-C5-C6
8	M	600	SPN	CM5-C13-C14-C15
5	M	503	BPH	C2-C3-C5-C6
4	M	502	BCL	C3-C5-C6-C7
8	M	600	SPN	C20-C21-C22-CM7
4	M	501	BCL	C11-C12-C13-C15
6	M	504	U10	C29-C31-C32-C33
4	M	501	BCL	C15-C16-C17-C18
9	M	800	CDL	CB7-C71-C72-C73
4	L	502	BCL	C15-C16-C17-C18
4	M	502	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
4	M	501	BCL	C10-C11-C12-C13
9	M	800	CDL	C11-CA5-OA6-CA4
9	M	800	CDL	OA7-CA5-OA6-CA4
10	H	703	LDA	C7-C8-C9-C10
4	M	502	BCL	C12-C13-C15-C16
8	M	600	SPN	C24-C25-C26-CM8
9	M	800	CDL	C79-C80-C81-C82
10	H	703	LDA	C6-C7-C8-C9
6	M	504	U10	C30-C29-C31-C32
9	M	800	CDL	C39-C40-C41-C42
9	M	800	CDL	C78-C79-C80-C81
9	M	800	CDL	C54-C55-C56-C57
4	M	501	BCL	C4-C3-C5-C6
10	M	701	LDA	C7-C8-C9-C10
10	M	701	LDA	C1-C2-C3-C4
6	M	504	U10	C28-C29-C31-C32
5	L	503	BPH	C8-C10-C11-C12
4	L	501	BCL	C15-C16-C17-C18
10	M	704	LDA	C6-C7-C8-C9
9	M	800	CDL	OA5-CA3-CA4-OA6
9	M	800	CDL	C36-C37-C38-C39
9	M	800	CDL	C80-C81-C82-C83
4	M	501	BCL	C2-C3-C5-C6
6	L	504	U10	C23-C24-C26-C27
9	M	800	CDL	C21-C22-C23-C24
4	M	501	BCL	C3-C5-C6-C7
6	M	504	U10	C14-C16-C17-C18
10	H	703	LDA	C11-C10-C9-C8
5	L	503	BPH	C4-C3-C5-C6
6	L	504	U10	C15-C14-C16-C17
6	M	504	U10	C35-C34-C36-C37
8	M	600	SPN	CM3-C5-C6-C7
4	M	501	BCL	C11-C10-C8-C9
4	M	501	BCL	C11-C12-C13-C14
9	M	800	CDL	C55-C56-C57-C58
4	L	502	BCL	C11-C12-C13-C15
8	M	600	SPN	C21-C22-C23-C24
6	M	504	U10	C25-C24-C26-C27
5	L	503	BPH	C2-C3-C5-C6
10	M	701	LDA	C9-C10-C11-C12
9	M	800	CDL	C34-C35-C36-C37
5	M	503	BPH	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
6	L	504	U10	C25-C24-C26-C27
9	M	800	CDL	C51-C52-C53-C54
10	M	701	LDA	C4-C5-C6-C7
9	M	800	CDL	C40-C41-C42-C43
9	M	800	CDL	C13-C14-C15-C16
6	M	504	U10	C33-C34-C36-C37
9	M	800	CDL	C19-C20-C21-C22
8	M	600	SPN	C25-C26-C27-C28
6	L	504	U10	C13-C14-C16-C17
5	L	503	BPH	O2A-C1-C2-C3
9	M	800	CDL	C81-C82-C83-C84
9	M	800	CDL	OA5-CA3-CA4-CA6
4	L	501	BCL	C6-C7-C8-C10
4	M	501	BCL	C12-C13-C15-C16
4	L	502	BCL	C16-C17-C18-C20
4	L	501	BCL	C6-C7-C8-C9
5	M	503	BPH	C5-C6-C7-C8
9	M	800	CDL	CA3-CA4-CA6-OA8
4	M	501	BCL	CHA-CBD-CGD-O1D
10	M	701	LDA	C5-C6-C7-C8
4	L	502	BCL	C11-C12-C13-C14
6	L	504	U10	C30-C29-C31-C32
9	M	800	CDL	C33-C34-C35-C36
9	M	800	CDL	CA5-C11-C12-C13
9	M	800	CDL	C11-C12-C13-C14
10	M	704	LDA	C4-C5-C6-C7
9	M	800	CDL	C20-C21-C22-C23
4	M	502	BCL	C13-C15-C16-C17
6	L	504	U10	C28-C29-C31-C32
6	M	504	U10	C23-C24-C26-C27
4	L	501	BCL	C11-C10-C8-C9
4	M	502	BCL	C6-C7-C8-C9
10	M	704	LDA	C5-C6-C7-C8
4	M	501	BCL	C1-C2-C3-C5
8	M	600	SPN	CM8-C26-C27-C28
4	M	502	BCL	C14-C13-C15-C16
6	M	504	U10	C5-C4-O4-C4M
4	M	502	BCL	C6-C7-C8-C10
9	M	800	CDL	C72-C71-CB7-OB8
10	M	704	LDA	C3-C4-C5-C6
4	L	502	BCL	O1A-CGA-O2A-C1
9	M	800	CDL	C72-C71-CB7-OB9

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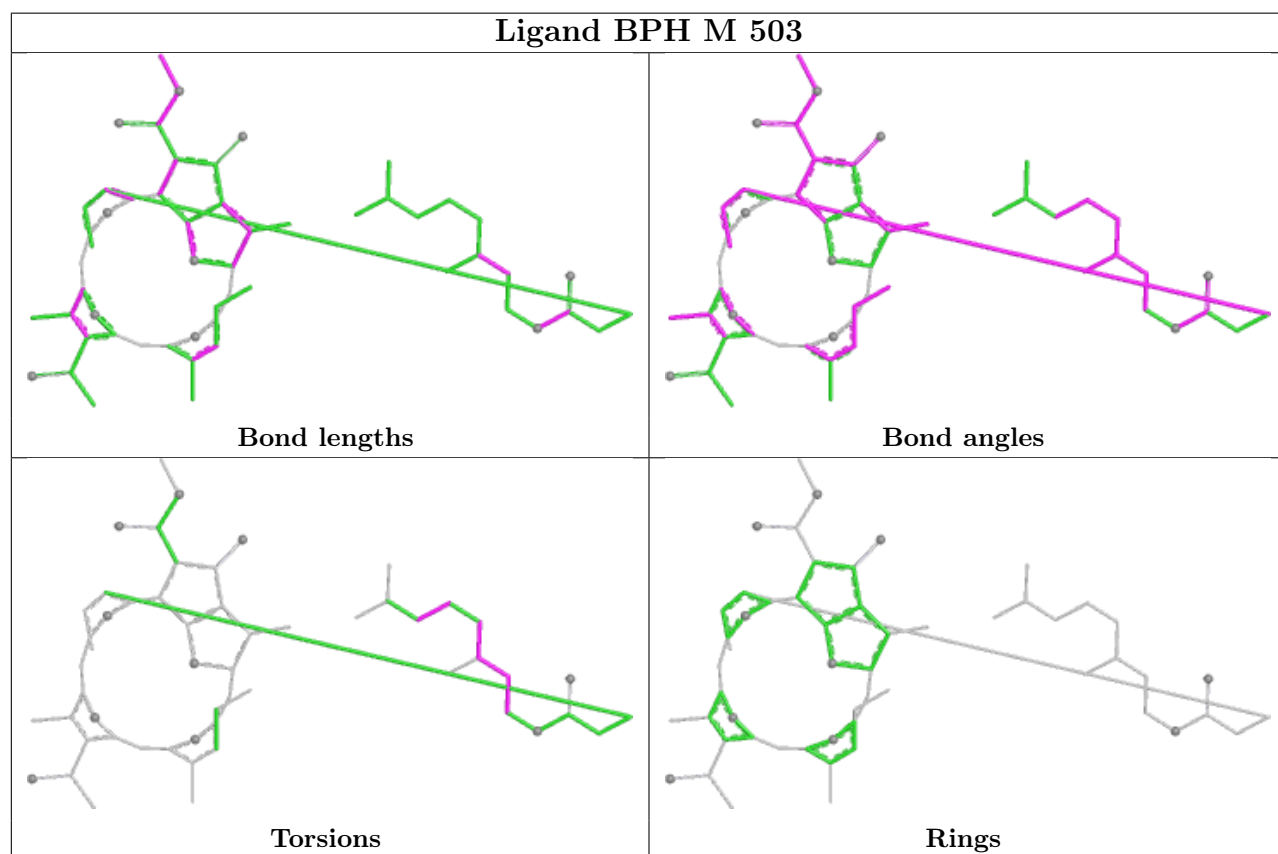
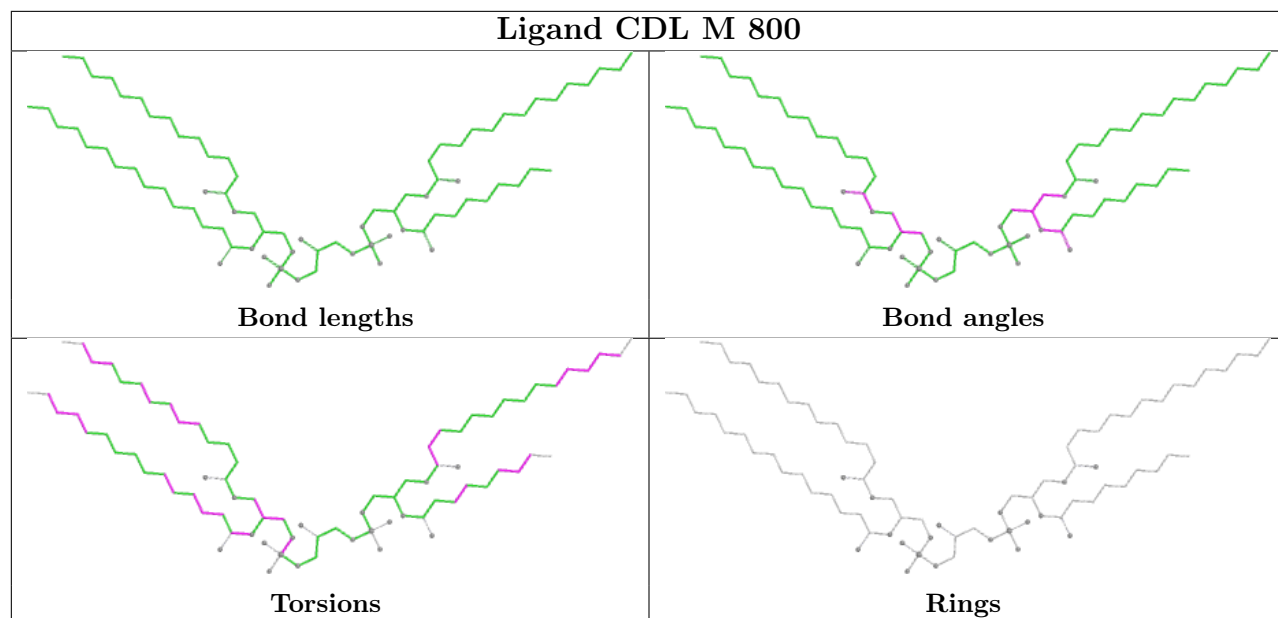
Mol	Chain	Res	Type	Atoms
8	M	600	SPN	C10-C11-C12-C13
8	M	600	SPN	C18-C19-C20-C21
4	M	501	BCL	C14-C13-C15-C16
8	M	600	SPN	C6-C7-C8-C9
4	M	502	BCL	CAA-CBA-CGA-O2A

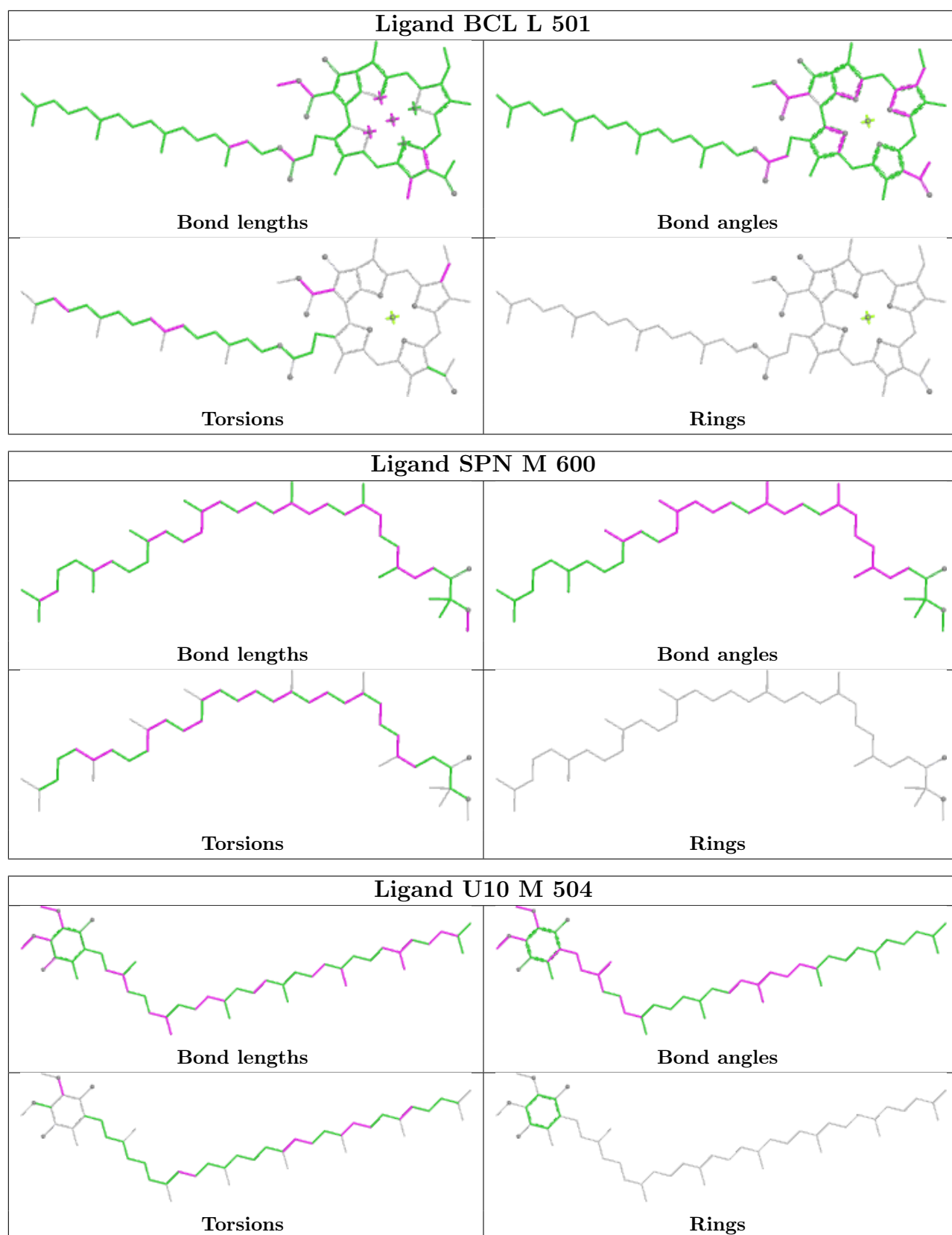
There are no ring outliers.

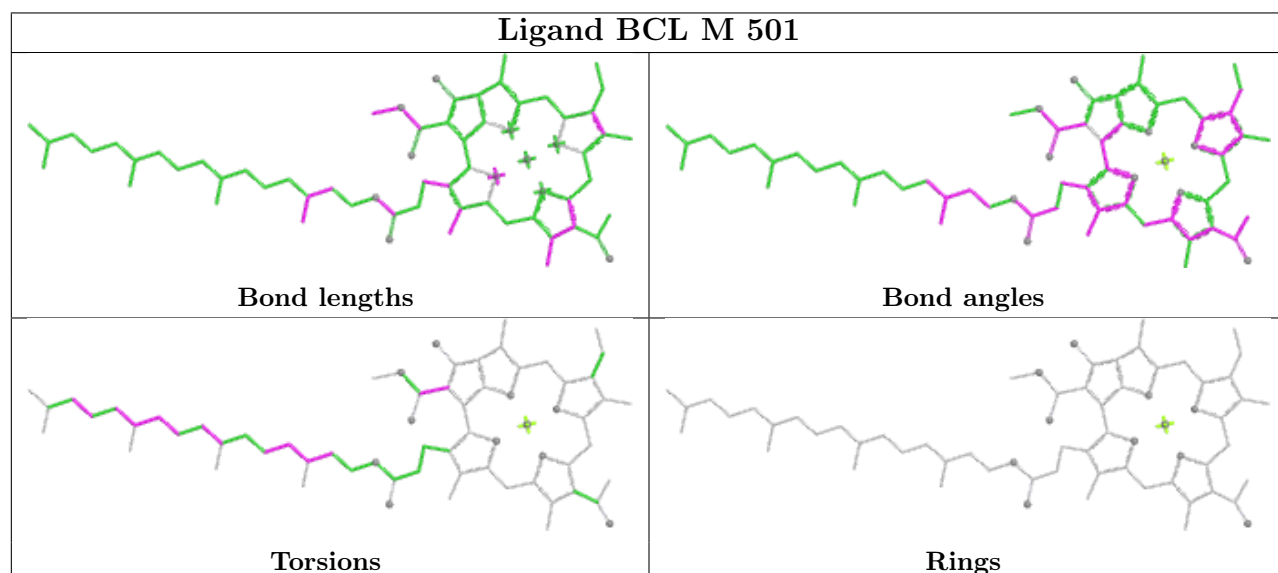
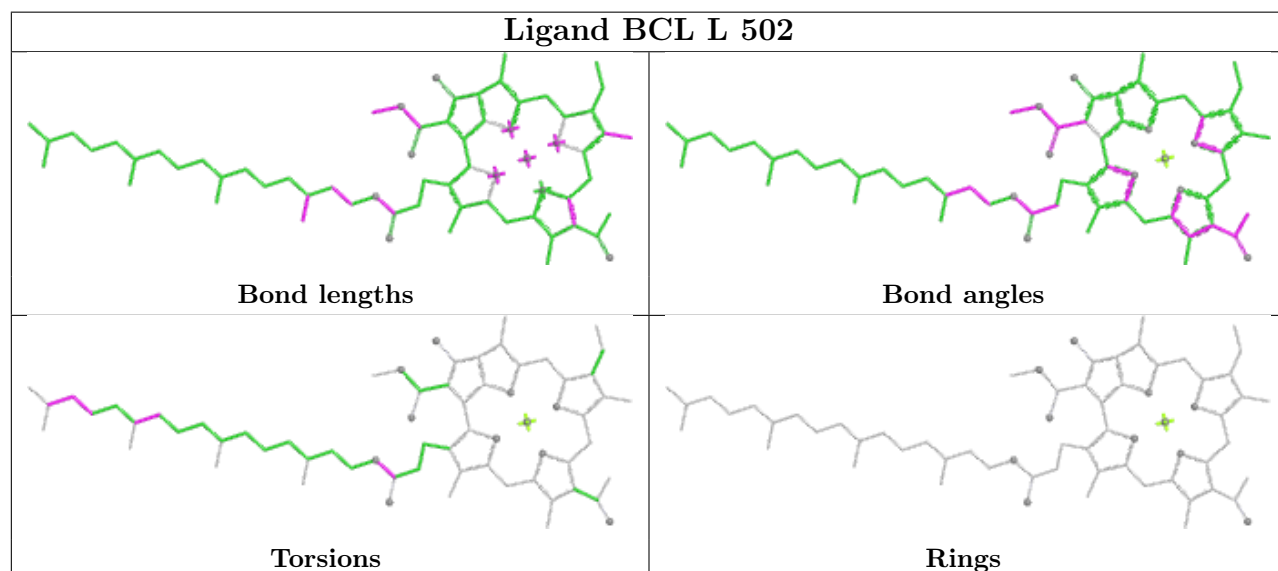
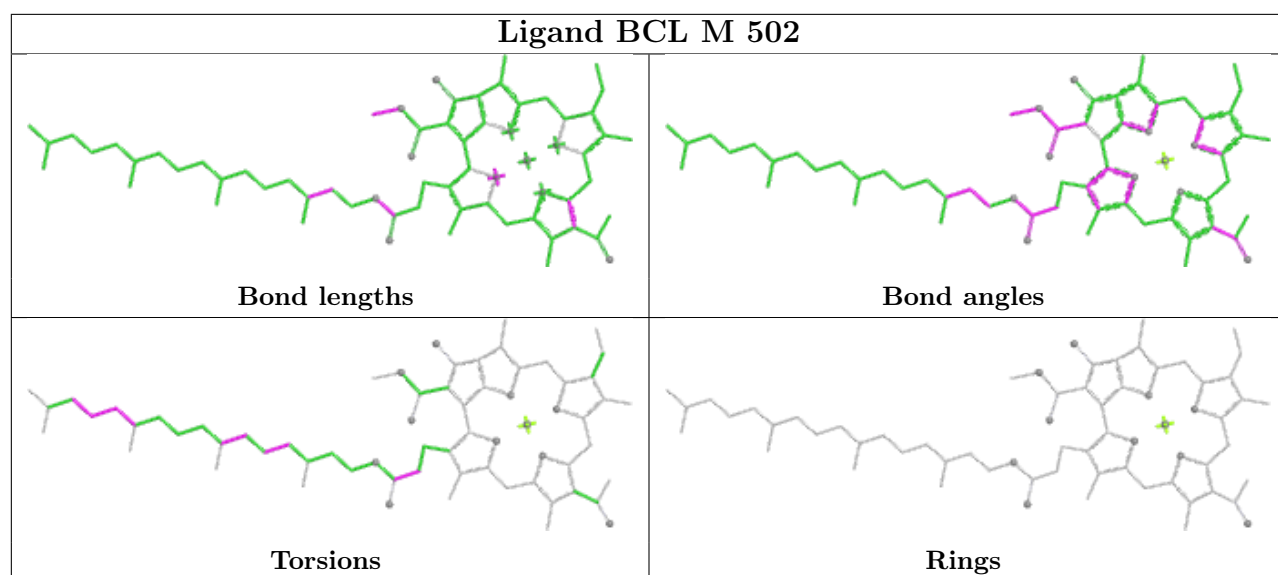
13 monomers are involved in 75 short contacts:

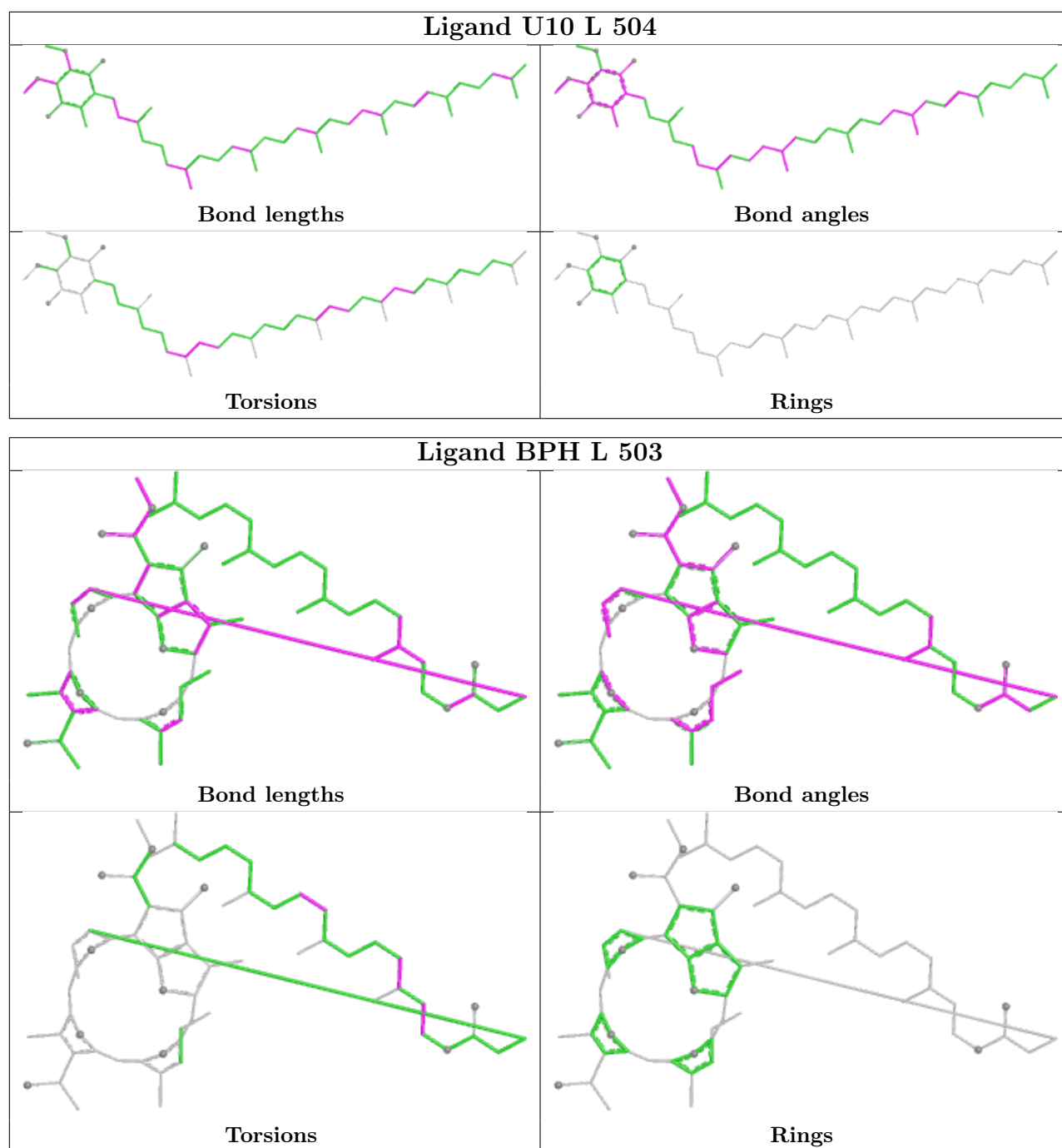
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	703	LDA	10	0
9	M	800	CDL	3	0
5	M	503	BPH	1	0
4	L	501	BCL	6	0
8	M	600	SPN	4	0
6	M	504	U10	15	0
4	M	502	BCL	12	0
4	L	502	BCL	12	0
4	M	501	BCL	9	0
6	L	504	U10	5	0
10	M	701	LDA	6	0
10	M	704	LDA	2	0
5	L	503	BPH	3	0

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%)	-0.08	9 (3%)	50	40	19, 34, 76, 89	0
2	M	302/314 (96%)	-0.13	6 (1%)	65	56	16, 38, 75, 101	0
3	H	240/260 (92%)	-0.23	1 (0%)	88	84	24, 37, 62, 94	0
All	All	823/855 (96%)	-0.14	16 (1%)	66	57	16, 37, 73, 101	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	281	GLY	4.1
1	L	53	ALA	3.6
2	M	301	HIS	3.2
2	M	300	ASN	2.9
1	L	59	TRP	2.9
1	L	273	ALA	2.8
3	H	250	SER	2.7
1	L	56	GLN	2.6
1	L	58	THR	2.5
1	L	84	GLY	2.3
2	M	4	GLN	2.3
1	L	72	GLU	2.2
2	M	76	TYR	2.2
2	M	53	GLY	2.2
1	L	82	LYS	2.1
2	M	113	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

There are no oligosaccharides in this entry.

6.4 Ligands

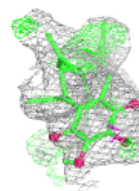
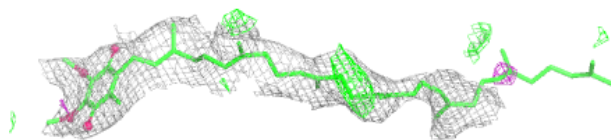
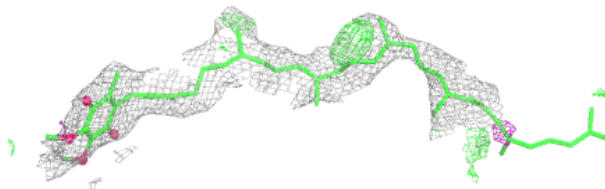
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	LDA	M	704	16/16	0.53	0.21	81,95,110,111	0
10	LDA	H	703	16/16	0.67	0.15	64,71,83,85	0
6	U10	L	504	48/63	0.83	0.16	56,81,114,115	0
9	CDL	M	800	81/100	0.84	0.14	49,73,88,91	0
10	LDA	M	701	16/16	0.84	0.11	40,61,80,80	0
6	U10	M	504	48/63	0.89	0.10	31,48,77,80	0
8	SPN	M	600	43/43	0.93	0.10	30,53,76,79	0
7	FE	M	500	1/1	0.94	0.03	24,24,24,24	0
4	BCL	M	501	66/66	0.94	0.09	19,25,101,104	0
5	BPH	M	503	55/65	0.95	0.07	20,35,74,82	0
4	BCL	L	501	66/66	0.95	0.07	16,25,53,61	0
4	BCL	M	502	66/66	0.95	0.07	21,31,64,66	0
5	BPH	L	503	65/65	0.96	0.06	15,24,43,47	0
4	BCL	L	502	66/66	0.96	0.07	17,30,49,58	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.

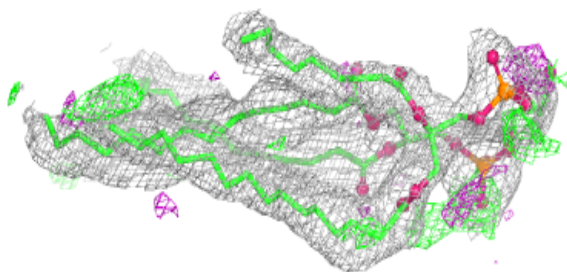
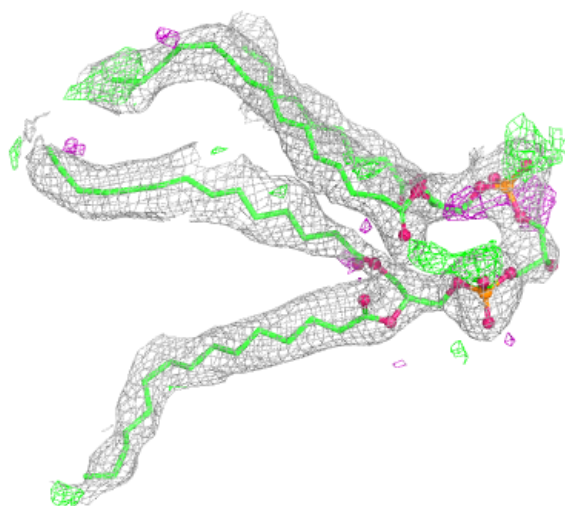
Electron density around U10 L 504:

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



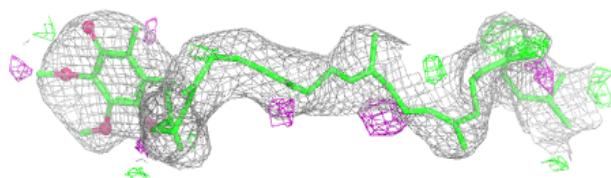
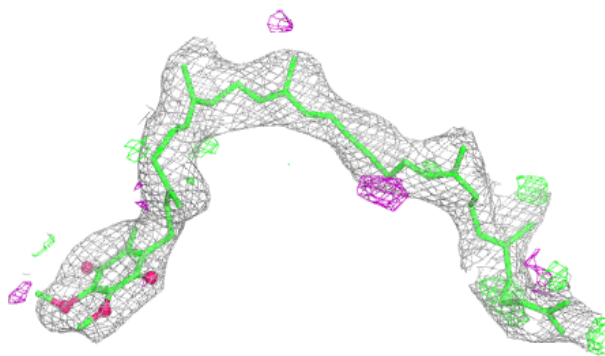
Electron density around CDL M 800:

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

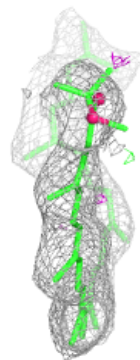
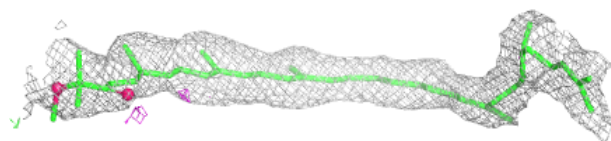
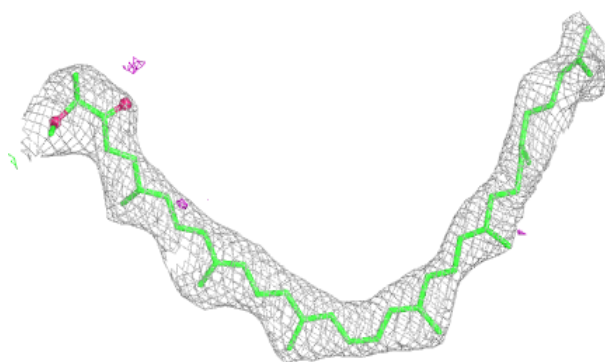


Electron density around U10 M 504:

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

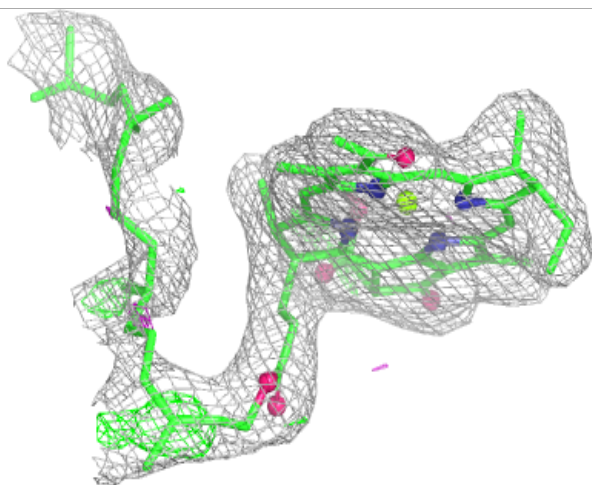
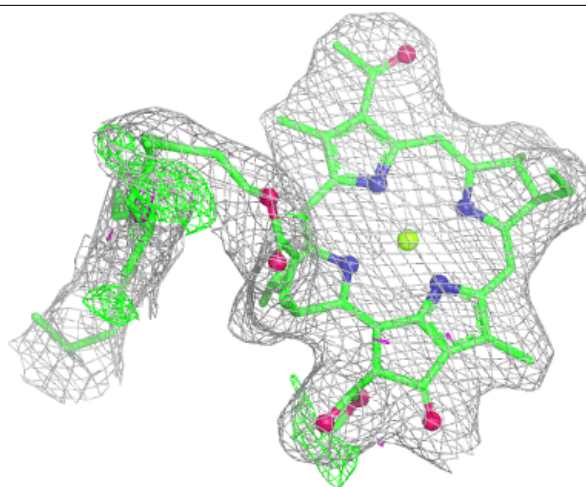
**Electron density around SPN M 600:**

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



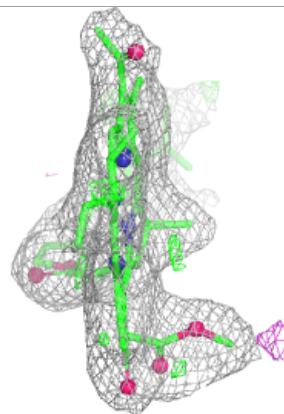
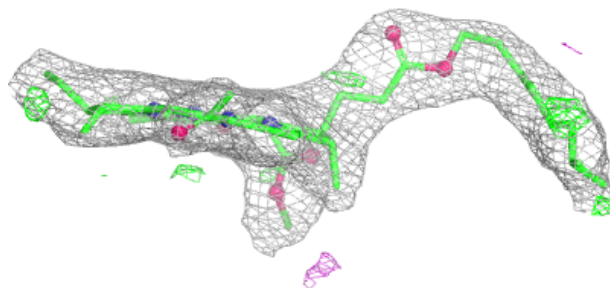
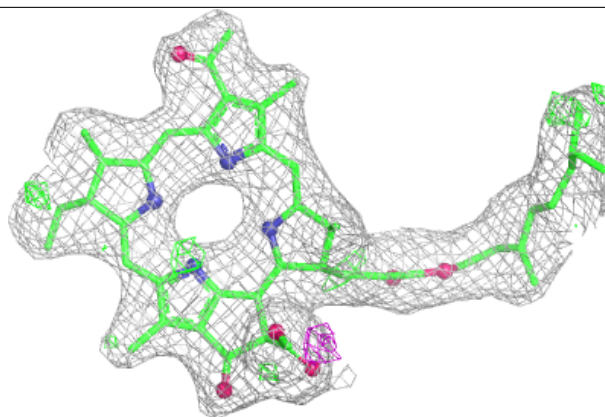
Electron density around BCL M 501:

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

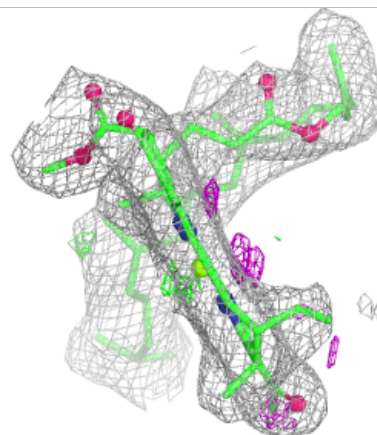
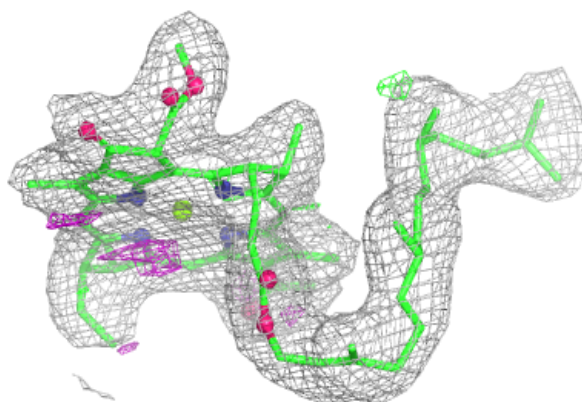
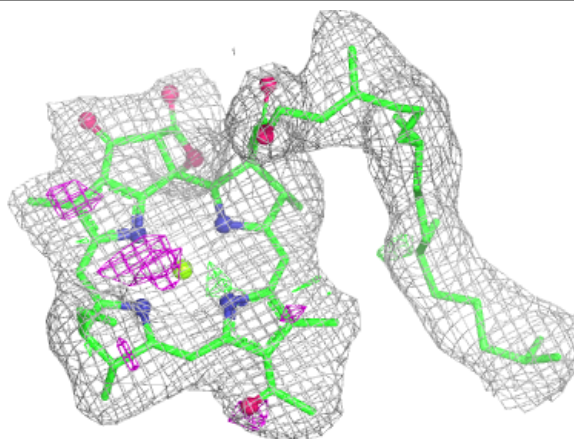


Electron density around BPH M 503:

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

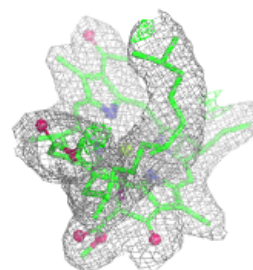
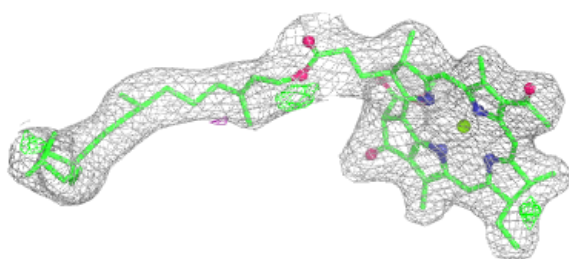
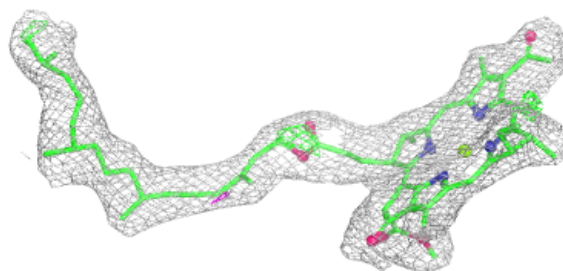
**Electron density around BCL L 501:**

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

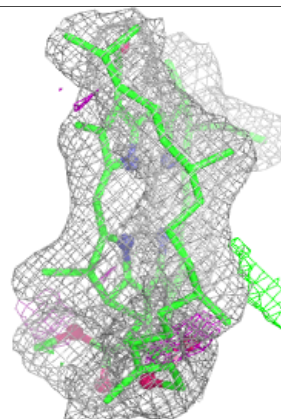
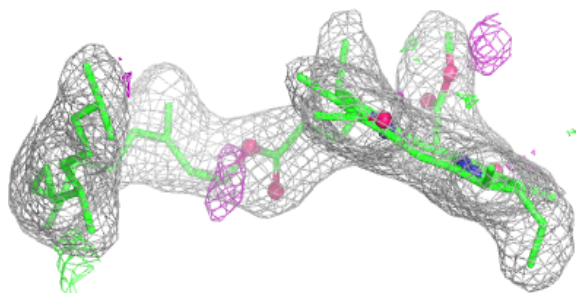
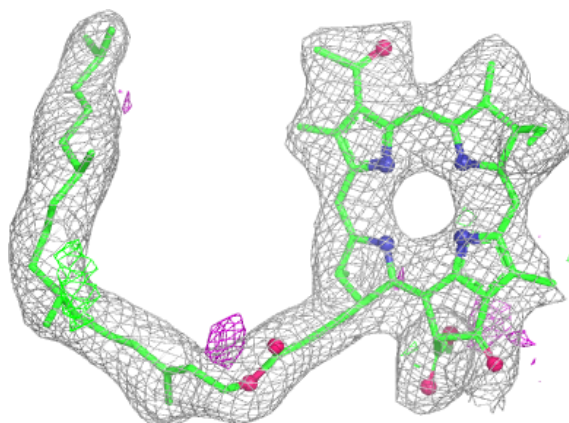


Electron density around BCL M 502:

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

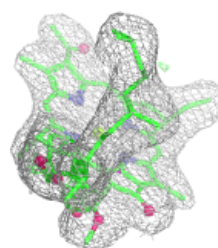
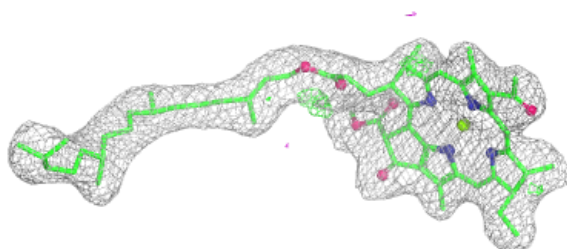
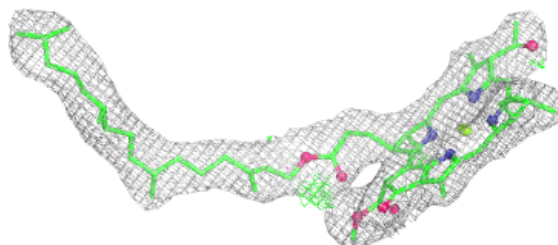
**Electron density around BPH L 503:**

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



Electron density around BCL 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.