



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2020 – 11:45 pm BST

PDB ID : 1YST
Title : STRUCTURE OF THE PHOTOCHEMICAL REACTION CENTER OF A SPHEROIDENE CONTAINING PURPLE BACTERIUM, RHODOBACTER SPHAEROIDES Y, AT 3 ANGSTROMS RESOLUTION
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Deposited on : 1994-12-07
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

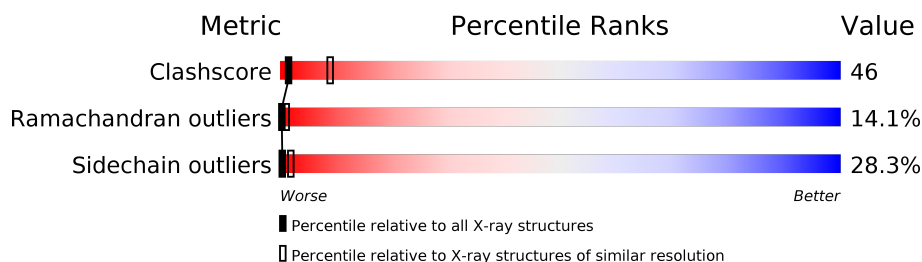
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	273	
2	M	305	
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
4	BCL	L	274	X	-	X	-
4	BCL	M	307	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BPH	L	276	X	-	X	-
5	BPH	M	309	X	-	-	-

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 7136 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	273	Total	C	N	O	S	0	0	0
			2181	1476	345	352	8			

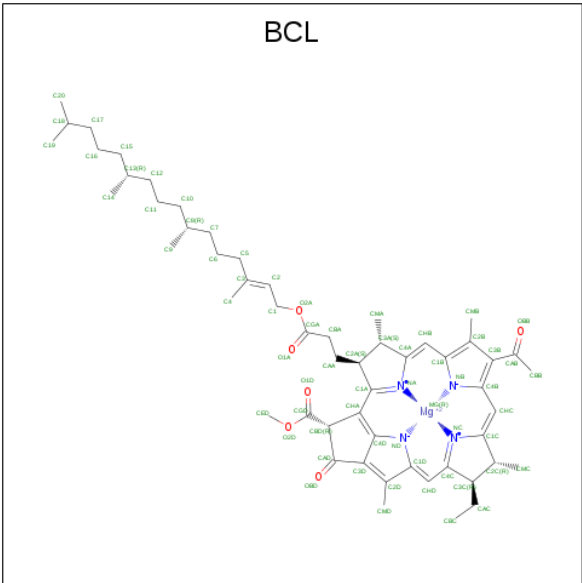
- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	305	Total	C	N	O	S	0	0	0
			2429	1619	397	401	12			

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

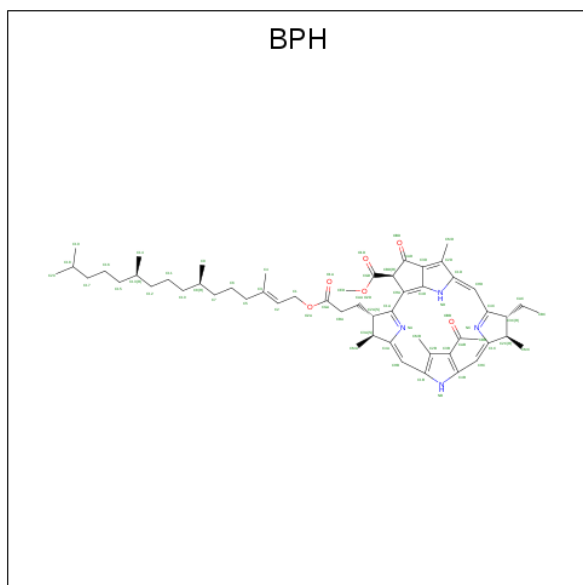
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	260	Total	C	N	O	S	0	0	0
			1973	1264	335	363	11			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



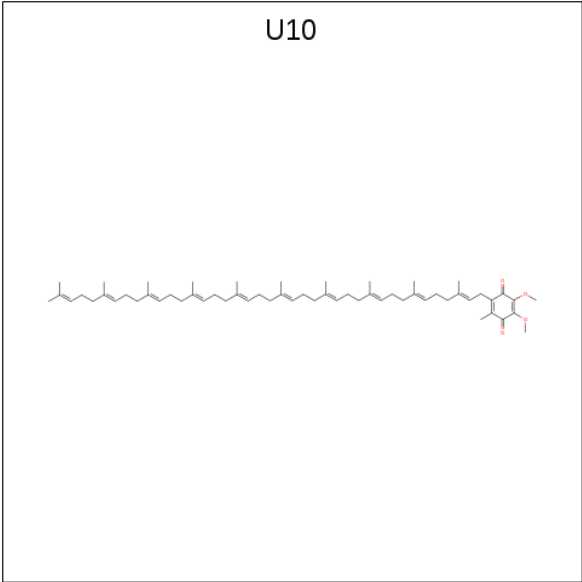
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



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

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

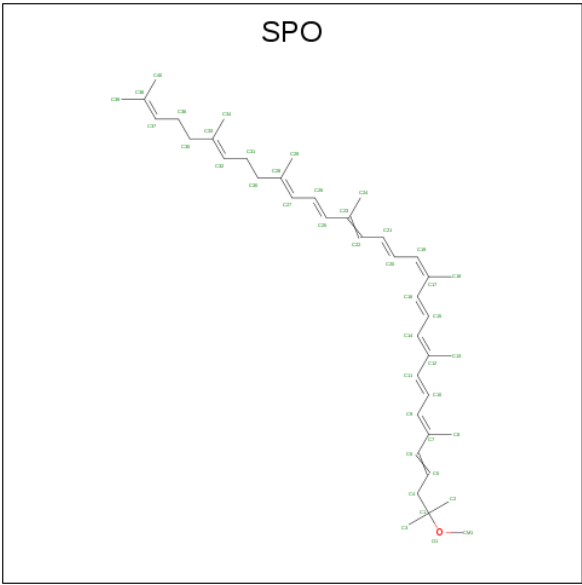


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			58	54	4		
6	M	1	Total	C	O	0	0
			58	54	4		

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 8 is SPHEROIDENE (three-letter code: SPO) (formula: C₄₁H₆₀O).



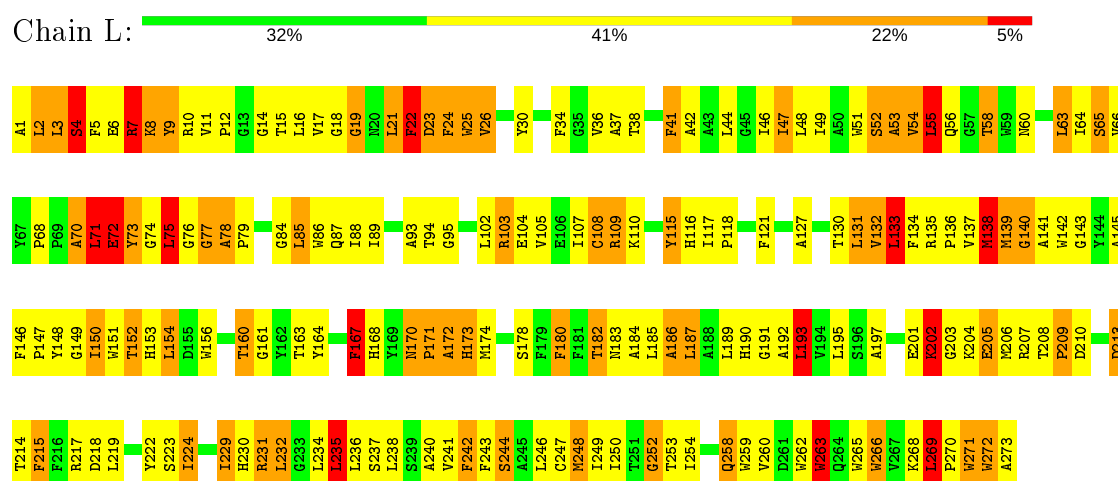
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			42	41	1		

3 Residue-property plots

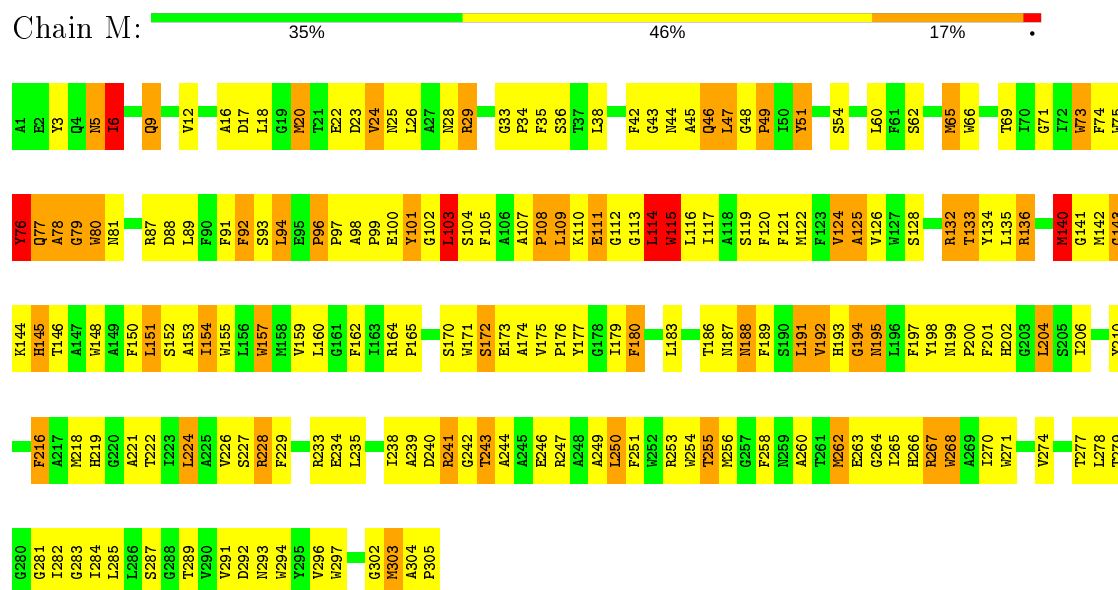
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

- Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)

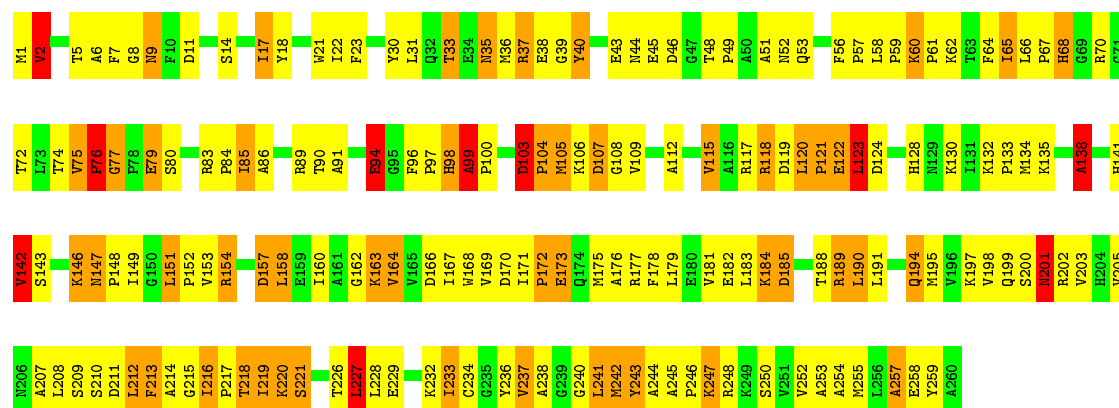


- Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)



- Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)

Frequency	Percentage
Daily	31%
Often	46%
Sometimes	20%
Not at all	3%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	143.70 Å 139.80 Å 78.65 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.234 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7136	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.87	1/2268 (0.0%)	1.04	11/3104 (0.4%)
2	M	0.85	4/2522 (0.2%)	1.41	10/3441 (0.3%)
3	H	0.92	2/2024 (0.1%)	1.16	8/2752 (0.3%)
All	All	0.87	7/6814 (0.1%)	1.22	29/9297 (0.3%)

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	3
3	H	0	4
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	76	PRO	C-N	18.97	1.67	1.33
1	L	252	GLY	C-N	-14.31	1.01	1.34
2	M	228	ARG	CD-NE	-11.97	1.26	1.46
2	M	228	ARG	NE-CZ	-9.37	1.20	1.33
3	H	99	ALA	C-N	6.71	1.47	1.34
2	M	228	ARG	CG-CD	5.94	1.66	1.51
2	M	93	SER	C-N	-5.83	1.20	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	228	ARG	NE-CZ-NH2	37.25	138.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	228	ARG	NE-CZ-NH1	-33.24	103.68	120.30
2	M	228	ARG	CD-NE-CZ	28.33	163.26	123.60
3	H	76	PRO	C-N-CA	9.99	143.28	122.30
1	L	133	LEU	CA-CB-CG	8.18	134.11	115.30
2	M	228	ARG	CG-CD-NE	-8.13	94.73	111.80
3	H	138	ALA	O-C-N	-7.40	110.62	123.20
2	M	103	LEU	CA-CB-CG	7.13	131.70	115.30
1	L	186	ALA	C-N-CA	-6.81	104.67	121.70
1	L	53	ALA	N-CA-CB	6.74	119.53	110.10
3	H	123	LEU	CA-CB-CG	6.66	130.62	115.30
1	L	193	LEU	CA-CB-CG	6.36	129.94	115.30
2	M	278	LEU	CA-CB-CG	6.34	129.89	115.30
1	L	252	GLY	CA-C-N	-6.26	103.42	117.20
2	M	46	GLN	CB-CA-C	6.19	122.78	110.40
3	H	120	LEU	CA-CB-CG	6.05	129.22	115.30
3	H	79	GLU	O-C-N	5.78	131.94	122.70
3	H	76	PRO	O-C-N	-5.69	113.52	123.20
2	M	241	ARG	NE-CZ-NH2	5.54	123.07	120.30
2	M	140	MET	CG-SD-CE	5.51	109.02	100.20
2	M	26	LEU	CA-CB-CG	5.51	127.98	115.30
1	L	75	LEU	CA-CB-CG	5.50	127.95	115.30
1	L	53	ALA	N-CA-C	-5.41	96.39	111.00
1	L	88	ILE	CG1-CB-CG2	-5.39	99.53	111.40
3	H	83	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	L	186	ALA	O-C-N	5.36	131.28	122.70
1	L	231	ARG	NE-CZ-NH2	-5.23	117.69	120.30
3	H	52	ASN	O-C-N	-5.19	114.40	122.70
1	L	252	GLY	C-N-CA	-5.03	109.13	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	138	ALA	Mainchain
3	H	142	VAL	Mainchain
3	H	147	ASN	Mainchain
3	H	99	ALA	Mainchain
1	L	153	HIS	Mainchain
1	L	252	GLY	Mainchain
1	L	263	TRP	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	2181	0	2136	239	0
2	M	2429	0	2339	202	0
3	H	1973	0	1981	197	0
4	L	132	0	145	28	0
4	M	132	0	148	36	0
5	L	65	0	76	23	0
5	M	65	0	76	11	0
6	L	58	0	79	16	0
6	M	58	0	79	19	0
7	M	1	0	0	0	0
8	M	42	0	60	13	0
All	All	7136	0	7119	661	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 46.

All (661) 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)
6:L:277:U10:C27	6:L:277:U10:C28	1.79	1.56
5:L:276:BPH:C2A	5:L:276:BPH:CAA	1.75	1.54
1:L:78:ALA:HB1	1:L:79:PRO:CD	1.69	1.21
1:L:78:ALA:CB	1:L:79:PRO:HD3	1.74	1.15
1:L:78:ALA:CB	1:L:79:PRO:CD	2.25	1.15
1:L:53:ALA:HB1	1:L:64:ILE:CD1	1.84	1.08
2:M:98:ALA:HB3	2:M:99:PRO:HD3	1.37	1.03
1:L:205:GLU:HB3	3:H:67:PRO:HG3	1.40	1.00
2:M:96:PRO:HD3	2:M:176:PRO:HG2	1.43	1.00
1:L:53:ALA:HB1	1:L:64:ILE:HD12	1.41	1.00
3:H:211:ASP:O	3:H:212:LEU:HB2	1.62	0.97
2:M:96:PRO:HD3	2:M:176:PRO:CG	1.95	0.96
5:M:309:BPH:HHC	5:M:309:BPH:HBB2	1.47	0.95
1:L:64:ILE:HG22	1:L:65:SER:H	1.30	0.95
3:H:37:ARG:HH21	3:H:59:PRO:HB2	1.31	0.95
2:M:222:THR:O	2:M:226:VAL:HG23	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:SER:CB	1:L:149:GLY:HA3	1.98	0.92
5:M:309:BPH:HHB	5:M:309:BPH:HBC2	1.50	0.92
2:M:186:THR:HG21	4:M:307:BCL:H3C	1.52	0.91
1:L:246:LEU:O	1:L:250:ILE:HG22	1.71	0.91
1:L:54:VAL:HG12	1:L:54:VAL:O	1.69	0.90
1:L:78:ALA:HB1	1:L:79:PRO:HD3	0.89	0.88
3:H:217:PRO:HG2	3:H:232:LYS:HG2	1.56	0.88
1:L:66:VAL:O	1:L:147:PRO:HA	1.73	0.88
2:M:238:ILE:HG12	2:M:262:MET:HB3	1.56	0.88
3:H:68:HIS:HE1	3:H:124:ASP:H	1.19	0.87
4:M:307:BCL:HHB	4:M:307:BCL:CBB	2.02	0.87
1:L:55:LEU:HD12	1:L:56:GLN:HE21	1.39	0.87
5:L:276:BPH:C1A	5:L:276:BPH:CAA	2.53	0.85
3:H:240:GLY:HA2	3:H:244:ALA:HB2	1.59	0.85
4:L:275:BCL:HMB1	4:L:275:BCL:HBB3	1.59	0.85
1:L:54:VAL:CG1	1:L:54:VAL:O	2.24	0.84
1:L:65:SER:HB3	1:L:149:GLY:HA3	1.61	0.82
5:M:309:BPH:H13	5:M:309:BPH:C19	2.09	0.82
4:L:274:BCL:CBB	4:L:274:BCL:HMB1	2.08	0.82
3:H:122:GLU:HG2	3:H:130:LYS:HD2	1.60	0.81
2:M:46:GLN:HE21	2:M:48:GLY:HA2	1.43	0.81
1:L:248:MET:SD	4:L:274:BCL:OBD	2.38	0.80
3:H:104:PRO:HG3	3:H:243:TYR:CD2	2.16	0.80
1:L:127:ALA:HB1	4:L:274:BCL:H11	1.64	0.80
3:H:154:ARG:HE	3:H:202:ARG:HD3	1.47	0.79
3:H:65:ILE:HD13	3:H:65:ILE:H	1.46	0.79
1:L:232:LEU:HD23	1:L:236:LEU:HD22	1.65	0.79
3:H:158:LEU:HD12	3:H:210:SER:HB2	1.65	0.78
2:M:165:PRO:HG3	2:M:173:GLU:O	1.83	0.78
2:M:260:ALA:HB1	3:H:35:ASN:HD21	1.47	0.78
3:H:168:TRP:HB3	3:H:178:PHE:HB2	1.66	0.78
3:H:77:GLY:C	3:H:79:GLU:H	1.87	0.78
6:M:311:U10:H43	6:M:311:U10:H38	1.64	0.78
2:M:136:ARG:NE	2:M:136:ARG:HA	1.99	0.78
1:L:53:ALA:CB	1:L:64:ILE:HD12	2.14	0.78
1:L:65:SER:HA	1:L:148:TYR:O	1.84	0.77
1:L:52:SER:HA	1:L:55:LEU:HD21	1.66	0.77
3:H:56:PHE:HA	3:H:58:LEU:HG	1.65	0.77
1:L:65:SER:HB2	1:L:149:GLY:HA3	1.65	0.77
3:H:149:ILE:O	3:H:164:VAL:HG23	1.85	0.77
3:H:195:MET:CE	3:H:241:LEU:HD21	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:311:U10:C33	6:M:311:U10:H301	2.15	0.76
3:H:158:LEU:HD12	3:H:210:SER:CB	2.15	0.76
3:H:66:LEU:CB	3:H:70:ARG:CB	2.63	0.76
3:H:66:LEU:HB3	3:H:70:ARG:CB	2.16	0.76
1:L:241:VAL:HG21	5:L:276:BPH:HAC2	1.68	0.76
1:L:66:VAL:HG12	1:L:86:TRP:HD1	1.49	0.76
2:M:296:VAL:HG11	3:H:2:VAL:HB	1.68	0.76
3:H:5:THR:HG22	3:H:6:ALA:O	1.86	0.76
3:H:68:HIS:HE1	3:H:124:ASP:N	1.83	0.76
4:M:307:BCL:HBB2	4:M:307:BCL:HHC	1.68	0.75
1:L:250:ILE:HG13	1:L:254:ILE:HB	1.69	0.75
3:H:219:ILE:HD13	3:H:221:SER:O	1.89	0.73
1:L:79:PRO:O	1:L:84:GLY:HA3	1.88	0.72
1:L:205:GLU:HB3	3:H:67:PRO:CG	2.18	0.72
1:L:78:ALA:HB3	1:L:79:PRO:CD	2.19	0.72
3:H:5:THR:HG21	3:H:9:ASN:HA	1.71	0.72
4:M:307:BCL:HBC1	4:M:308:BCL:HBA2	1.70	0.72
4:M:307:BCL:HBB3	4:M:307:BCL:HHC	1.72	0.72
4:L:274:BCL:H172	4:L:275:BCL:C9	2.19	0.72
2:M:65:MET:SD	2:M:121:PHE:CG	2.83	0.71
3:H:117:ARG:NH1	3:H:227:LEU:HB3	2.05	0.71
1:L:121:PHE:HE1	5:L:276:BPH:HAA1	1.55	0.71
5:L:276:BPH:HBB1	2:M:210:TYR:HD2	1.55	0.71
6:M:311:U10:H4M3	6:M:311:U10:O3	1.91	0.70
2:M:33:GLY:HA3	2:M:47:LEU:HB3	1.72	0.70
1:L:170:ASN:C	1:L:170:ASN:HD22	1.94	0.70
2:M:71:GLY:O	2:M:75:TRP:HD1	1.74	0.70
2:M:200:PRO:CG	2:M:297:TRP:HZ3	2.04	0.70
2:M:105:PHE:HD1	2:M:116:LEU:HD22	1.56	0.70
3:H:66:LEU:HB2	3:H:70:ARG:HB3	1.72	0.69
5:M:309:BPH:H13	5:M:309:BPH:H193	1.72	0.69
1:L:272:TRP:HB3	2:M:87:ARG:HD3	1.75	0.69
2:M:200:PRO:HG2	2:M:297:TRP:CZ3	2.26	0.69
1:L:217:ARG:HD3	2:M:49:PRO:HD2	1.74	0.69
3:H:201:ASN:HD22	3:H:202:ARG:HG2	1.58	0.69
3:H:118:ARG:HH11	3:H:118:ARG:HB2	1.59	0.68
1:L:66:VAL:HG12	1:L:86:TRP:CD1	2.28	0.68
1:L:183:ASN:ND2	1:L:237:SER:HB3	2.08	0.68
4:M:308:BCL:CBB	4:M:308:BCL:HMB1	2.23	0.68
3:H:195:MET:HE1	3:H:241:LEU:HD21	1.74	0.68
4:L:274:BCL:H172	4:L:275:BCL:H92	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:66:LEU:HB2	3:H:70:ARG:CB	2.24	0.67
3:H:158:LEU:CD1	3:H:210:SER:HB2	2.25	0.67
3:H:163:LYS:HB2	3:H:182:GLU:O	1.95	0.67
2:M:171:TRP:O	2:M:174:ALA:HB2	1.95	0.67
3:H:74:THR:HG22	3:H:76:PRO:HD2	1.76	0.67
1:L:248:MET:SD	4:L:274:BCL:CAD	2.82	0.67
1:L:107:ILE:HG23	2:M:254:TRP:HE3	1.59	0.67
4:M:307:BCL:HBB1	8:M:310:SPO:H243	1.75	0.67
4:L:275:BCL:HMB1	4:L:275:BCL:CBB	2.24	0.67
2:M:279:THR:O	2:M:282:ILE:HG22	1.95	0.67
1:L:64:ILE:O	1:L:65:SER:HB3	1.94	0.67
1:L:167:PHE:HD1	1:L:173:HIS:HD1	1.41	0.66
3:H:66:LEU:CB	3:H:70:ARG:HB3	2.24	0.66
3:H:74:THR:CG2	3:H:76:PRO:HD2	2.26	0.66
1:L:55:LEU:HD12	1:L:56:GLN:NE2	2.10	0.66
1:L:266:TRP:HE1	2:M:87:ARG:HA	1.59	0.66
3:H:175:MET:HE3	3:H:177:ARG:HH12	1.61	0.66
3:H:66:LEU:CB	3:H:70:ARG:HB2	2.23	0.66
3:H:177:ARG:HH11	3:H:177:ARG:HG3	1.61	0.66
1:L:138:MET:SD	1:L:139:MET:HG3	2.36	0.66
1:L:187:LEU:HG	2:M:216:PHE:CD1	2.31	0.66
2:M:270:ILE:O	2:M:274:VAL:HG12	1.94	0.66
3:H:66:LEU:HB3	3:H:70:ARG:HB2	1.77	0.66
2:M:115:TRP:CZ2	2:M:174:ALA:HB1	2.31	0.66
3:H:211:ASP:O	3:H:212:LEU:CB	2.42	0.66
3:H:190:LEU:HD23	3:H:190:LEU:H	1.61	0.65
3:H:189:ARG:HH11	3:H:218:THR:HG23	1.61	0.65
2:M:33:GLY:HA3	2:M:47:LEU:CB	2.27	0.65
3:H:227:LEU:HD13	3:H:227:LEU:H	1.61	0.65
3:H:56:PHE:C	3:H:58:LEU:H	2.00	0.65
1:L:65:SER:CA	1:L:148:TYR:O	2.44	0.65
2:M:175:VAL:HG13	8:M:310:SPO:H242	1.77	0.65
2:M:268:TRP:CD1	6:M:311:U10:H111	2.32	0.65
1:L:164:TYR:HD2	1:L:167:PHE:HE2	1.45	0.64
2:M:243:THR:O	2:M:247:ARG:HB2	1.97	0.64
3:H:190:LEU:N	3:H:190:LEU:HD23	2.11	0.64
2:M:98:ALA:HB3	2:M:99:PRO:CD	2.19	0.64
3:H:37:ARG:O	3:H:76:PRO:HA	1.97	0.64
2:M:103:LEU:HD13	2:M:103:LEU:H	1.62	0.64
2:M:98:ALA:CB	2:M:99:PRO:HD3	2.21	0.64
3:H:163:LYS:HB3	3:H:163:LYS:NZ	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:153:VAL:HG13	3:H:164:VAL:HG13	1.80	0.64
1:L:130:THR:HA	1:L:134:PHE:HB2	1.80	0.64
1:L:78:ALA:HB3	1:L:79:PRO:HD2	1.80	0.64
2:M:153:ALA:HA	2:M:277:THR:HG21	1.79	0.64
1:L:108:CYS:HB2	2:M:251:PHE:HE2	1.63	0.64
2:M:94:LEU:HB3	2:M:114:LEU:HD13	1.78	0.64
2:M:249:ALA:HA	6:M:311:U10:C4M	2.26	0.64
2:M:34:PRO:HD2	2:M:47:LEU:HG	1.79	0.64
3:H:213:PHE:O	3:H:216:ILE:HG12	1.98	0.64
1:L:75:LEU:HD23	1:L:142:TRP:HE1	1.63	0.64
5:M:309:BPH:CB	5:M:309:BPH:HHD	2.26	0.64
3:H:65:ILE:HG12	3:H:65:ILE:O	1.95	0.63
1:L:34:PHE:O	1:L:38:THR:HG23	1.98	0.63
1:L:78:ALA:CB	1:L:79:PRO:HD2	2.27	0.63
2:M:110:LYS:HG3	2:M:111:GLU:H	1.63	0.63
2:M:101:TYR:HD1	2:M:101:TYR:N	1.95	0.63
5:M:309:BPH:H13	5:M:309:BPH:H192	1.81	0.63
1:L:75:LEU:HG	1:L:140:GLY:O	1.98	0.63
3:H:190:LEU:HG	3:H:233:ILE:HD12	1.80	0.63
3:H:37:ARG:HH21	3:H:59:PRO:CB	2.08	0.63
1:L:219:LEU:HD12	2:M:132:ARG:HH11	1.64	0.63
1:L:272:TRP:CD1	1:L:272:TRP:N	2.67	0.63
6:M:311:U10:C33	6:M:311:U10:C30	2.78	0.62
3:H:104:PRO:HG3	3:H:243:TYR:CE2	2.34	0.62
1:L:152:THR:HB	2:M:305:PRO:O	2.00	0.62
2:M:200:PRO:CG	2:M:297:TRP:CZ3	2.81	0.62
5:M:309:BPH:H171	5:M:309:BPH:H141	1.81	0.62
6:L:277:U10:H3M2	6:L:277:U10:O2	2.00	0.62
3:H:242:MET:HB3	3:H:243:TYR:HD1	1.63	0.62
3:H:36:MET:SD	3:H:40:TYR:HD2	2.21	0.62
1:L:21:LEU:O	1:L:22:PHE:HB2	2.00	0.62
1:L:171:PRO:O	1:L:172:ALA:C	2.37	0.62
4:M:307:BCL:C2	4:M:307:BCL:H72	2.29	0.61
3:H:195:MET:HE3	3:H:241:LEU:HD21	1.81	0.61
3:H:120:LEU:O	3:H:227:LEU:HD21	2.00	0.61
2:M:51:TYR:O	2:M:51:TYR:CD1	2.53	0.61
2:M:175:VAL:N	2:M:176:PRO:HD3	2.15	0.61
2:M:24:VAL:HG23	2:M:51:TYR:HE2	1.66	0.61
1:L:263:TRP:HE3	2:M:180:PHE:CZ	2.19	0.61
3:H:31:LEU:O	3:H:35:ASN:HB2	2.00	0.61
3:H:240:GLY:CA	3:H:244:ALA:HB2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:260:ALA:CB	3:H:35:ASN:HD21	2.13	0.61
1:L:65:SER:CB	1:L:149:GLY:CA	2.77	0.61
1:L:9:TYR:H	1:L:9:TYR:HD1	1.48	0.61
6:L:277:U10:H251	6:L:277:U10:C28	2.30	0.61
3:H:61:PRO:HG3	3:H:76:PRO:HG2	1.82	0.60
5:L:276:BPH:C3A	5:L:276:BPH:CAA	2.75	0.60
3:H:151:LEU:CD1	3:H:203:VAL:HG23	2.31	0.60
1:L:127:ALA:HB1	4:L:274:BCL:C1	2.31	0.60
2:M:101:TYR:CD1	2:M:101:TYR:N	2.67	0.60
1:L:214:THR:HG21	2:M:20:MET:HB2	1.82	0.60
3:H:153:VAL:HG22	3:H:162:GLY:HA2	1.83	0.60
1:L:197:ALA:HB1	1:L:207:ARG:O	2.01	0.60
6:M:311:U10:H103	6:M:311:U10:O5	2.01	0.60
3:H:142:VAL:HG21	3:H:147:ASN:HB3	1.83	0.60
3:H:135:LYS:O	3:H:135:LYS:HG2	2.01	0.60
1:L:105:VAL:O	1:L:109:ARG:HB2	2.01	0.60
2:M:175:VAL:CG1	8:M:310:SPO:H242	2.32	0.60
2:M:73:TRP:CH2	2:M:114:LEU:HA	2.36	0.60
1:L:6:GLU:HG2	1:L:10:ARG:HD3	1.83	0.60
4:M:308:BCL:HMB1	4:M:308:BCL:HBB3	1.83	0.60
2:M:229:PHE:HB3	3:H:234:CYS:CB	2.32	0.59
2:M:28:ASN:HB2	2:M:51:TYR:CE1	2.36	0.59
1:L:51:TRP:C	1:L:53:ALA:H	2.05	0.59
1:L:64:ILE:HG22	1:L:65:SER:N	2.08	0.59
2:M:122:MET:SD	2:M:157:TRP:CH2	2.95	0.59
2:M:228:ARG:HB2	2:M:229:PHE:CD1	2.37	0.59
2:M:234:GLU:CD	2:M:266:HIS:CE1	2.75	0.59
1:L:131:LEU:CD2	4:L:274:BCL:HED3	2.32	0.59
1:L:131:LEU:HD21	4:L:274:BCL:HED3	1.83	0.59
1:L:222:TYR:HE1	1:L:224:ILE:HG23	1.68	0.59
1:L:68:PRO:HG3	1:L:86:TRP:NE1	2.18	0.59
4:M:307:BCL:CB	4:M:308:BCL:HBA2	2.32	0.58
1:L:52:SER:OG	1:L:85:LEU:HG	2.04	0.58
1:L:51:TRP:O	1:L:53:ALA:N	2.37	0.58
2:M:197:PHE:CE2	4:M:308:BCL:HMC2	2.38	0.58
2:M:260:ALA:HA	3:H:35:ASN:ND2	2.18	0.58
1:L:151:TRP:HB3	2:M:304:ALA:O	2.04	0.58
1:L:244:SER:OG	4:L:274:BCL:H2A	2.03	0.58
4:L:274:BCL:HBD	4:L:275:BCL:HBC1	1.85	0.58
2:M:206:ILE:HG13	4:M:308:BCL:HMB3	1.84	0.58
2:M:177:TYR:HE1	8:M:310:SPO:H25	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:302:GLY:O	2:M:304:ALA:N	2.37	0.58
3:H:183:LEU:O	3:H:185:ASP:N	2.37	0.58
3:H:168:TRP:HB3	3:H:178:PHE:CB	2.34	0.58
2:M:99:PRO:HB2	2:M:101:TYR:HE1	1.67	0.57
3:H:198:VAL:HG23	3:H:198:VAL:O	2.04	0.57
2:M:256:MET:HE3	6:M:311:U10:H211	1.87	0.57
3:H:147:ASN:ND2	3:H:149:ILE:HB	2.19	0.57
1:L:262:TRP:O	1:L:265:TRP:HD1	1.86	0.57
5:L:276:BPH:HBB1	2:M:210:TYR:CD2	2.39	0.57
1:L:167:PHE:O	1:L:170:ASN:HB3	2.04	0.57
5:L:276:BPH:OBB	5:L:276:BPH:HHC	2.04	0.57
1:L:104:GLU:HB2	1:L:118:PRO:HG3	1.87	0.57
2:M:239:ALA:HB1	3:H:66:LEU:HD21	1.86	0.57
1:L:170:ASN:HD22	1:L:171:PRO:N	2.03	0.57
4:M:307:BCL:CBB	8:M:310:SPO:H243	2.34	0.57
3:H:134:MET:HB3	3:H:166:ASP:OD1	2.05	0.57
1:L:164:TYR:HD2	1:L:167:PHE:CE2	2.22	0.57
2:M:122:MET:SD	2:M:157:TRP:HH2	2.28	0.57
3:H:158:LEU:HB2	3:H:160:ILE:HG12	1.87	0.56
1:L:24:PHE:N	1:L:24:PHE:CD1	2.73	0.56
1:L:174:MET:HB3	4:M:307:BCL:O1D	2.05	0.56
1:L:241:VAL:HG21	5:L:276:BPH:CAC	2.35	0.56
1:L:37:ALA:O	1:L:41:PHE:HB2	2.05	0.56
4:L:274:BCL:HMC3	4:M:308:BCL:HBC3	1.88	0.56
3:H:154:ARG:NE	3:H:202:ARG:HH11	2.04	0.56
1:L:65:SER:HB2	1:L:149:GLY:CA	2.34	0.56
3:H:209:SER:O	3:H:210:SER:C	2.43	0.56
1:L:109:ARG:HG3	1:L:109:ARG:NH1	2.21	0.56
1:L:218:ASP:OD1	2:M:51:TYR:HD2	1.89	0.56
2:M:24:VAL:HG23	2:M:51:TYR:CE2	2.40	0.56
3:H:228:LEU:O	3:H:232:LYS:HB2	2.05	0.56
1:L:30:TYR:O	1:L:103:ARG:NH1	2.39	0.56
2:M:142:MET:O	2:M:143:GLY:C	2.43	0.56
2:M:22:GLU:HG2	2:M:140:MET:HA	1.88	0.56
2:M:24:VAL:HG21	2:M:29:ARG:HH11	1.71	0.56
3:H:65:ILE:HG22	3:H:72:THR:HG22	1.86	0.56
2:M:229:PHE:HB3	3:H:234:CYS:SG	2.46	0.56
3:H:37:ARG:NH2	3:H:59:PRO:HB2	2.12	0.56
1:L:156:TRP:HE1	1:L:160:THR:HG21	1.71	0.55
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.41	0.55
2:M:200:PRO:HG3	2:M:297:TRP:HZ3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:SER:O	1:L:66:VAL:HG23	2.06	0.55
2:M:201:PHE:HD2	2:M:283:GLY:HA2	1.72	0.55
6:L:277:U10:H321	4:M:307:BCL:C19	2.36	0.55
6:L:277:U10:H251	6:L:277:U10:H28	1.89	0.55
4:L:274:BCL:H121	5:L:276:BPH:HBA1	1.88	0.55
1:L:51:TRP:O	1:L:54:VAL:N	2.39	0.55
2:M:186:THR:CG2	4:M:307:BCL:H3C	2.32	0.55
2:M:97:PRO:HA	2:M:112:GLY:HA3	1.88	0.55
3:H:67:PRO:O	3:H:68:HIS:CB	2.55	0.55
1:L:18:GLY:O	1:L:19:GLY:C	2.46	0.55
3:H:158:LEU:CD1	3:H:210:SER:CB	2.83	0.55
2:M:119:SER:HB3	8:M:310:SPO:H342	1.89	0.54
2:M:287:SER:HG	2:M:294:TRP:HE1	1.53	0.54
1:L:187:LEU:O	1:L:191:GLY:N	2.39	0.54
2:M:256:MET:HE1	6:M:311:U10:H18	1.88	0.54
1:L:185:LEU:O	1:L:189:LEU:HD23	2.07	0.54
1:L:271:TRP:HD1	1:L:271:TRP:H	1.53	0.54
2:M:162:PHE:HB2	8:M:310:SPO:H312	1.90	0.54
2:M:3:TYR:OH	3:H:241:LEU:HD11	2.07	0.54
1:L:14:GLY:HA2	1:L:109:ARG:HD2	1.88	0.54
2:M:9:GLN:HA	2:M:9:GLN:HE21	1.73	0.54
1:L:66:VAL:O	1:L:147:PRO:CA	2.49	0.54
1:L:154:LEU:HD12	2:M:197:PHE:HB3	1.90	0.54
2:M:186:THR:CG2	4:M:307:BCL:HMC3	2.38	0.54
2:M:65:MET:SD	2:M:121:PHE:CD2	3.01	0.54
2:M:162:PHE:CE1	8:M:310:SPO:H361	2.43	0.54
1:L:202:LYS:O	1:L:204:LYS:N	2.41	0.54
2:M:155:TRP:O	2:M:159:VAL:HG23	2.08	0.54
2:M:16:ALA:HB2	2:M:35:PHE:CE1	2.42	0.54
1:L:214:THR:O	1:L:217:ARG:N	2.42	0.53
3:H:68:HIS:CE1	3:H:124:ASP:H	2.11	0.53
2:M:224:LEU:HD13	2:M:224:LEU:H	1.73	0.53
3:H:160:ILE:HG22	3:H:184:LYS:HE2	1.91	0.53
2:M:281:GLY:O	2:M:284:ILE:HG22	2.09	0.53
1:L:217:ARG:CD	2:M:49:PRO:HD2	2.39	0.53
3:H:77:GLY:C	3:H:79:GLU:N	2.59	0.53
1:L:7:ARG:HH11	1:L:7:ARG:HG3	1.73	0.53
3:H:194:GLN:H	3:H:194:GLN:NE2	2.07	0.53
6:L:277:U10:H4M3	6:L:277:U10:O3	2.09	0.53
1:L:197:ALA:HB1	2:M:235:LEU:HD21	1.91	0.53
3:H:205:VAL:C	3:H:207:ALA:H	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:219:ILE:O	3:H:221:SER:N	2.42	0.52
1:L:230:HIS:CE1	2:M:234:GLU:CD	2.82	0.52
3:H:118:ARG:HB2	3:H:118:ARG:NH1	2.24	0.52
1:L:170:ASN:O	1:L:174:MET:HE2	2.09	0.52
3:H:68:HIS:CE1	3:H:124:ASP:N	2.71	0.52
3:H:61:PRO:CG	3:H:76:PRO:HG2	2.39	0.52
3:H:75:VAL:N	3:H:76:PRO:CD	2.72	0.52
1:L:109:ARG:HH11	1:L:109:ARG:HG3	1.73	0.52
1:L:132:VAL:O	1:L:136:PRO:HG3	2.09	0.52
1:L:25:TRP:CZ2	1:L:110:LYS:NZ	2.76	0.52
3:H:67:PRO:O	3:H:68:HIS:CG	2.63	0.52
1:L:52:SER:OG	1:L:85:LEU:HD11	2.10	0.52
3:H:153:VAL:HG11	3:H:181:VAL:HG12	1.91	0.52
1:L:171:PRO:O	1:L:173:HIS:N	2.42	0.52
1:L:10:ARG:HH21	1:L:25:TRP:HB2	1.74	0.52
3:H:75:VAL:O	3:H:77:GLY:N	2.42	0.52
1:L:172:ALA:O	1:L:173:HIS:C	2.46	0.52
2:M:78:ALA:O	2:M:79:GLY:C	2.48	0.52
1:L:104:GLU:O	1:L:108:CYS:HB3	2.10	0.51
2:M:117:ILE:H	2:M:117:ILE:HD12	1.75	0.51
6:M:311:U10:H33	6:M:311:U10:H301	1.91	0.51
3:H:219:ILE:HG12	3:H:219:ILE:O	2.10	0.51
2:M:192:VAL:HG12	2:M:193:HIS:HD1	1.76	0.51
4:L:275:BCL:OBB	4:L:275:BCL:HHC	2.09	0.51
3:H:212:LEU:O	3:H:236:TYR:HE2	1.94	0.51
5:L:276:BPH:HBB2	5:L:276:BPH:CMB	2.41	0.51
2:M:152:SER:CB	2:M:274:VAL:HG23	2.41	0.51
6:M:311:U10:C4M	6:M:311:U10:O3	2.58	0.51
3:H:170:ASP:OD1	3:H:172:PRO:HD2	2.11	0.51
3:H:61:PRO:HG3	3:H:76:PRO:CG	2.40	0.51
2:M:186:THR:HG21	4:M:307:BCL:C3C	2.34	0.51
1:L:164:TYR:CD2	1:L:167:PHE:HE2	2.27	0.51
1:L:214:THR:OG1	2:M:20:MET:HG2	2.11	0.51
2:M:71:GLY:O	2:M:75:TRP:CD1	2.60	0.51
1:L:170:ASN:C	1:L:170:ASN:ND2	2.63	0.50
2:M:234:GLU:OE2	2:M:266:HIS:CE1	2.63	0.50
2:M:180:PHE:O	2:M:183:LEU:HB3	2.11	0.50
2:M:260:ALA:CB	3:H:35:ASN:ND2	2.74	0.50
3:H:163:LYS:HZ3	3:H:163:LYS:HB3	1.76	0.50
3:H:36:MET:SD	3:H:40:TYR:CD2	3.05	0.50
2:M:253:ARG:NH2	3:H:40:TYR:CE1	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:307:BCL:H93	4:M:307:BCL:H42	1.92	0.50
2:M:51:TYR:C	2:M:51:TYR:CD1	2.85	0.50
1:L:148:TYR:CD1	5:L:276:BPH:H162	2.47	0.50
1:L:52:SER:OG	1:L:85:LEU:CD1	2.59	0.50
2:M:229:PHE:HZ	2:M:247:ARG:HE	1.59	0.50
1:L:79:PRO:O	1:L:84:GLY:CA	2.58	0.50
2:M:105:PHE:CD1	2:M:116:LEU:HD22	2.42	0.50
1:L:182:THR:HG22	1:L:236:LEU:HD21	1.93	0.50
3:H:68:HIS:CE1	3:H:124:ASP:O	2.65	0.50
2:M:5:ASN:HD22	2:M:227:SER:HB2	1.76	0.50
6:L:277:U10:H321	4:M:307:BCL:H191	1.93	0.50
2:M:46:GLN:NE2	2:M:48:GLY:HA2	2.18	0.50
1:L:121:PHE:HE1	5:L:276:BPH:CAA	2.24	0.50
1:L:272:TRP:HD1	1:L:272:TRP:N	2.08	0.50
2:M:247:ARG:HA	2:M:250:LEU:HD22	1.94	0.50
3:H:215:GLY:O	3:H:216:ILE:C	2.48	0.49
4:L:274:BCL:HBC3	4:L:274:BCL:HMC2	1.92	0.49
1:L:60:ASN:HD22	1:L:63:LEU:HB2	1.76	0.49
2:M:74:PHE:O	2:M:78:ALA:HB2	2.12	0.49
3:H:121:PRO:HA	3:H:226:THR:OG1	2.13	0.49
3:H:169:VAL:HG12	3:H:176:ALA:HA	1.94	0.49
1:L:223:SER:HB2	6:L:277:U10:C4M	2.42	0.49
5:L:276:BPH:CED	2:M:218:MET:SD	3.00	0.49
5:M:309:BPH:CHC	5:M:309:BPH:HBB2	2.28	0.49
3:H:94:GLU:HA	3:H:94:GLU:OE1	2.12	0.49
3:H:98:HIS:N	3:H:98:HIS:CD2	2.80	0.49
1:L:186:ALA:O	1:L:187:LEU:C	2.49	0.49
1:L:23:ASP:CG	1:L:23:ASP:O	2.50	0.49
1:L:167:PHE:HD1	1:L:173:HIS:ND1	2.09	0.49
1:L:52:SER:HG	1:L:85:LEU:HD11	1.78	0.48
1:L:60:ASN:HD22	1:L:63:LEU:N	2.10	0.48
1:L:217:ARG:HD3	2:M:49:PRO:CD	2.43	0.48
1:L:52:SER:OG	1:L:85:LEU:CG	2.61	0.48
2:M:5:ASN:ND2	3:H:194:GLN:HG2	2.29	0.48
1:L:72:GLU:C	1:L:74:GLY:H	2.17	0.48
3:H:219:ILE:O	3:H:220:LYS:C	2.51	0.48
1:L:46:ILE:HG13	5:L:276:BPH:H9C1	1.95	0.48
4:M:307:BCL:HBC1	4:M:308:BCL:CBA	2.43	0.48
3:H:5:THR:HG21	3:H:9:ASN:CA	2.40	0.48
1:L:164:TYR:CD2	1:L:167:PHE:CE2	3.02	0.48
1:L:180:PHE:HE2	4:L:274:BCL:HBA2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:142:VAL:HG11	3:H:147:ASN:HB3	1.96	0.48
3:H:158:LEU:HD12	3:H:210:SER:HB3	1.93	0.48
3:H:56:PHE:CA	3:H:58:LEU:HG	2.41	0.48
1:L:10:ARG:HG3	1:L:10:ARG:HH11	1.78	0.48
2:M:51:TYR:C	2:M:51:TYR:HD1	2.17	0.48
1:L:192:ALA:HB1	2:M:145:HIS:HB3	1.96	0.48
3:H:149:ILE:O	3:H:164:VAL:CG2	2.59	0.47
3:H:117:ARG:O	3:H:118:ARG:C	2.51	0.47
1:L:131:LEU:O	1:L:132:VAL:HG23	2.14	0.47
2:M:151:LEU:O	2:M:154:ILE:HG22	2.14	0.47
2:M:164:ARG:HH11	2:M:164:ARG:HG2	1.79	0.47
3:H:168:TRP:HH2	3:H:219:ILE:HD12	1.79	0.47
1:L:170:ASN:OD1	1:L:259:TRP:NE1	2.47	0.47
1:L:171:PRO:O	1:L:174:MET:N	2.44	0.47
3:H:104:PRO:HG2	3:H:105:MET:H	1.80	0.47
1:L:93:ALA:HB2	5:L:276:BPH:H121	1.96	0.47
2:M:179:ILE:HG22	2:M:180:PHE:N	2.29	0.47
1:L:172:ALA:HB3	1:L:247:CYS:HA	1.97	0.47
1:L:85:LEU:O	1:L:89:ILE:HG12	2.14	0.47
4:M:308:BCL:HMB1	4:M:308:BCL:HBB2	1.94	0.47
1:L:108:CYS:HB2	2:M:251:PHE:CE2	2.47	0.47
2:M:16:ALA:HB2	2:M:35:PHE:HE1	1.79	0.47
3:H:153:VAL:HG13	3:H:164:VAL:CG1	2.45	0.47
4:L:274:BCL:HMC2	4:M:308:BCL:H2C	1.96	0.47
6:M:311:U10:C48	6:M:311:U10:H451	2.44	0.47
2:M:80:TRP:O	2:M:81:ASN:C	2.53	0.47
3:H:167:ILE:HG22	3:H:168:TRP:N	2.30	0.47
3:H:98:HIS:H	3:H:98:HIS:CD2	2.33	0.47
1:L:171:PRO:HG3	1:L:262:TRP:CE3	2.50	0.47
3:H:207:ALA:O	3:H:240:GLY:HA3	2.14	0.47
3:H:56:PHE:C	3:H:58:LEU:N	2.67	0.47
2:M:136:ARG:HE	2:M:136:ARG:HA	1.74	0.47
3:H:118:ARG:O	3:H:120:LEU:N	2.48	0.46
3:H:141:HIS:CG	3:H:141:HIS:O	2.68	0.46
1:L:271:TRP:N	1:L:271:TRP:CD1	2.83	0.46
1:L:170:ASN:ND2	1:L:171:PRO:HD2	2.30	0.46
1:L:3:LEU:HD12	2:M:253:ARG:HG2	1.97	0.46
2:M:12:VAL:HG21	3:H:169:VAL:HG11	1.96	0.46
1:L:184:ALA:O	1:L:185:LEU:C	2.51	0.46
3:H:151:LEU:HD12	3:H:203:VAL:HG23	1.97	0.46
1:L:187:LEU:HG	2:M:216:PHE:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:201:PHE:CD2	2:M:283:GLY:HA2	2.49	0.46
3:H:132:LYS:HA	3:H:133:PRO:HD3	1.81	0.46
3:H:33:THR:O	3:H:36:MET:HG2	2.15	0.46
1:L:205:GLU:CD	1:L:205:GLU:N	2.68	0.46
1:L:47:ILE:HG22	1:L:48:LEU:N	2.30	0.46
1:L:51:TRP:C	1:L:53:ALA:N	2.69	0.46
1:L:5:PHE:O	1:L:8:LYS:HG3	2.15	0.46
2:M:73:TRP:HH2	2:M:117:ILE:HD13	1.81	0.46
2:M:96:PRO:HD3	2:M:176:PRO:HG3	1.89	0.46
1:L:173:HIS:CE1	4:L:274:BCL:NC	2.82	0.46
1:L:265:TRP:CG	1:L:266:TRP:N	2.83	0.46
1:L:34:PHE:HA	1:L:37:ALA:HB3	1.97	0.46
1:L:117:ILE:HD12	2:M:251:PHE:CE1	2.51	0.46
2:M:297:TRP:HZ2	3:H:14:SER:HA	1.80	0.46
3:H:85:ILE:HG22	3:H:109:VAL:HG12	1.96	0.46
2:M:271:TRP:HA	2:M:274:VAL:CG1	2.46	0.46
3:H:86:ALA:O	3:H:100:PRO:HA	2.16	0.46
1:L:151:TRP:CH2	2:M:198:TYR:HA	2.51	0.46
2:M:119:SER:CB	8:M:310:SPO:H342	2.45	0.46
2:M:253:ARG:HH22	3:H:40:TYR:HE1	1.64	0.46
2:M:78:ALA:HB1	2:M:92:PHE:CZ	2.51	0.46
1:L:272:TRP:O	1:L:273:ALA:C	2.53	0.46
2:M:175:VAL:HG13	2:M:175:VAL:O	2.16	0.46
2:M:204:LEU:HD23	2:M:204:LEU:HA	1.81	0.46
3:H:181:VAL:HG22	3:H:189:ARG:O	2.16	0.45
1:L:11:VAL:HG12	1:L:12:PRO:HD2	1.96	0.45
1:L:170:ASN:ND2	1:L:171:PRO:N	2.64	0.45
1:L:49:ILE:HG13	1:L:89:ILE:HD12	1.98	0.45
2:M:117:ILE:O	2:M:120:PHE:HB3	2.17	0.45
1:L:42:ALA:HB1	5:L:276:BPH:H9C3	1.96	0.45
1:L:77:GLY:HA2	1:L:87:GLN:NE2	2.32	0.45
5:L:276:BPH:H141	5:L:276:BPH:H161	1.81	0.45
2:M:154:ILE:HD13	2:M:157:TRP:HD1	1.82	0.45
3:H:205:VAL:C	3:H:207:ALA:N	2.70	0.45
3:H:98:HIS:H	3:H:98:HIS:HD2	1.64	0.45
6:L:277:U10:H451	6:L:277:U10:C48	2.46	0.45
3:H:152:PRO:HA	3:H:162:GLY:O	2.17	0.45
3:H:154:ARG:HE	3:H:202:ARG:HH11	1.64	0.45
1:L:161:GLY:HA2	1:L:167:PHE:CD2	2.52	0.45
1:L:263:TRP:HD1	1:L:263:TRP:HA	1.67	0.45
6:M:311:U10:H43	6:M:311:U10:C38	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:107:ASP:N	3:H:107:ASP:OD1	2.49	0.45
3:H:163:LYS:HB2	3:H:182:GLU:HB3	1.98	0.45
3:H:70:ARG:HA	3:H:70:ARG:HD3	1.59	0.45
1:L:237:SER:O	1:L:240:ALA:HB3	2.16	0.45
1:L:73:TYR:OH	1:L:79:PRO:CG	2.64	0.45
2:M:171:TRP:O	2:M:172:SER:C	2.55	0.45
3:H:65:ILE:H	3:H:65:ILE:CD1	2.23	0.45
1:L:68:PRO:HB2	1:L:142:TRP:O	2.16	0.45
1:L:171:PRO:HG3	1:L:262:TRP:CZ3	2.52	0.45
2:M:115:TRP:O	2:M:116:LEU:C	2.54	0.45
5:M:309:BPH:CHD	5:M:309:BPH:HBC2	2.35	0.45
1:L:17:VAL:C	1:L:19:GLY:H	2.20	0.45
2:M:97:PRO:CA	2:M:112:GLY:HA3	2.47	0.45
1:L:190:HIS:HD1	1:L:193:LEU:HD12	1.82	0.44
4:L:275:BCL:H93	4:L:275:BCL:H61	1.80	0.44
5:L:276:BPH:H2	5:L:276:BPH:H6C1	1.71	0.44
1:L:174:MET:HG2	4:M:307:BCL:OBD	2.17	0.44
6:M:311:U10:C48	6:M:311:U10:C45	2.95	0.44
1:L:214:THR:O	1:L:215:PHE:C	2.54	0.44
6:L:277:U10:H461	6:L:277:U10:C50	2.47	0.44
2:M:159:VAL:HG13	2:M:285:LEU:HD13	1.99	0.44
2:M:271:TRP:HA	2:M:274:VAL:HG12	1.99	0.44
6:M:311:U10:H151	6:M:311:U10:H171	1.74	0.44
3:H:68:HIS:NE2	3:H:124:ASP:O	2.50	0.44
3:H:17:ILE:O	3:H:21:TRP:HD1	1.99	0.44
3:H:212:LEU:HD12	3:H:236:TYR:OH	2.17	0.44
3:H:208:LEU:HD11	3:H:237:VAL:HG22	1.98	0.44
4:M:308:BCL:H41	4:M:308:BCL:H61	1.68	0.44
2:M:76:TYR:HD1	2:M:76:TYR:O	2.01	0.44
3:H:103:ASP:OD2	3:H:106:LYS:HB2	2.17	0.44
3:H:60:LYS:HE2	3:H:60:LYS:HB2	1.82	0.44
1:L:148:TYR:HB3	5:L:276:BPH:H171	1.98	0.44
1:L:269:LEU:O	1:L:272:TRP:O	2.36	0.44
1:L:244:SER:OG	4:L:274:BCL:HBA1	2.17	0.44
2:M:171:TRP:O	2:M:173:GLU:N	2.51	0.44
1:L:135:ARG:HG2	1:L:135:ARG:HH11	1.82	0.44
1:L:266:TRP:CD1	1:L:266:TRP:C	2.91	0.44
6:M:311:U10:H251	6:M:311:U10:H272	1.28	0.44
2:M:260:ALA:O	6:M:311:U10:H4M1	2.17	0.44
2:M:96:PRO:HB2	2:M:97:PRO:HD2	2.00	0.44
3:H:219:ILE:HG12	3:H:229:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:228:ARG:HB2	2:M:229:PHE:CE1	2.52	0.44
3:H:17:ILE:HG13	3:H:18:TYR:N	2.33	0.44
1:L:160:THR:HA	1:L:163:THR:OG1	2.18	0.44
1:L:121:PHE:CE1	5:L:276:BPH:HAA1	2.44	0.44
1:L:2:LEU:HB2	3:H:43:GLU:HB2	2.00	0.44
2:M:253:ARG:NH2	3:H:40:TYR:HE1	2.16	0.43
1:L:68:PRO:HG3	1:L:86:TRP:CE2	2.52	0.43
2:M:98:ALA:CB	2:M:99:PRO:CD	2.89	0.43
1:L:201:GLU:O	1:L:202:LYS:O	2.35	0.43
1:L:208:THR:HB	1:L:209:PRO:HD2	2.00	0.43
1:L:64:ILE:CG2	1:L:65:SER:H	2.08	0.43
2:M:51:TYR:O	2:M:51:TYR:HD1	2.01	0.43
3:H:227:LEU:O	3:H:228:LEU:C	2.56	0.43
1:L:21:LEU:HG	1:L:21:LEU:H	1.53	0.43
3:H:38:GLU:O	3:H:40:TYR:N	2.51	0.43
1:L:16:LEU:HD13	1:L:102:LEU:HD21	2.00	0.43
1:L:263:TRP:HE3	2:M:180:PHE:HZ	1.62	0.43
4:L:275:BCL:H143	4:L:275:BCL:H111	1.67	0.43
1:L:93:ALA:HB1	5:L:276:BPH:H143	1.99	0.43
2:M:33:GLY:HA3	2:M:47:LEU:CG	2.48	0.43
2:M:97:PRO:HA	2:M:112:GLY:CA	2.49	0.43
1:L:215:PHE:CZ	2:M:146:THR:HG21	2.54	0.43
1:L:167:PHE:HB2	4:L:274:BCL:H3C	2.00	0.43
1:L:71:LEU:C	1:L:73:TYR:H	2.21	0.43
1:L:168:HIS:CE1	4:M:308:BCL:HBC1	2.53	0.43
3:H:33:THR:HG22	3:H:57:PRO:O	2.19	0.43
1:L:60:ASN:ND2	1:L:63:LEU:HB2	2.33	0.43
1:L:85:LEU:HD22	1:L:85:LEU:HA	1.62	0.43
3:H:175:MET:CE	3:H:177:ARG:HH12	2.29	0.43
3:H:238:ALA:C	3:H:240:GLY:H	2.22	0.43
2:M:263:GLU:HG3	2:M:264:GLY:N	2.34	0.43
1:L:174:MET:CB	4:M:307:BCL:O1D	2.67	0.43
1:L:213:ASP:O	1:L:217:ARG:HG3	2.18	0.43
1:L:242:PHE:CD1	1:L:243:PHE:N	2.87	0.43
4:L:274:BCL:CMC	4:M:308:BCL:HBC3	2.47	0.43
3:H:153:VAL:HG21	3:H:181:VAL:HG11	2.01	0.43
2:M:194:GLY:O	2:M:195:ASN:C	2.57	0.43
4:M:307:BCL:HBB3	4:M:308:BCL:H43	2.01	0.43
3:H:173:GLU:H	3:H:173:GLU:HG3	1.58	0.42
3:H:79:GLU:O	3:H:79:GLU:HG2	2.19	0.42
1:L:204:LYS:HG3	1:L:207:ARG:HH12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:234:LEU:HB2	1:L:235:LEU:H	1.60	0.42
1:L:268:LYS:O	1:L:269:LEU:C	2.58	0.42
2:M:304:ALA:HB1	2:M:305:PRO:CD	2.49	0.42
3:H:105:MET:HB3	3:H:236:TYR:CE1	2.54	0.42
2:M:3:TYR:OH	3:H:241:LEU:CD1	2.67	0.42
3:H:60:LYS:HA	3:H:61:PRO:HD3	1.79	0.42
3:H:74:THR:C	3:H:76:PRO:HD2	2.40	0.42
3:H:151:LEU:HD11	3:H:203:VAL:HG23	2.01	0.42
1:L:10:ARG:NH1	1:L:10:ARG:HG3	2.34	0.42
1:L:70:ALA:H	1:L:73:TYR:HD2	1.67	0.42
3:H:56:PHE:N	3:H:57:PRO:HD3	2.34	0.42
2:M:108:PRO:O	2:M:113:GLY:HA3	2.18	0.42
2:M:260:ALA:CA	3:H:35:ASN:ND2	2.81	0.42
5:M:309:BPH:HHC	5:M:309:BPH:CBB	2.33	0.42
2:M:34:PRO:CD	2:M:47:LEU:HG	2.45	0.42
3:H:257:ALA:C	3:H:259:TYR:H	2.23	0.42
1:L:213:ASP:HA	6:L:277:U10:H4M1	2.01	0.42
2:M:162:PHE:CE1	8:M:310:SPO:C36	3.03	0.42
3:H:151:LEU:HA	3:H:152:PRO:HD3	1.82	0.42
3:H:189:ARG:NH1	3:H:218:THR:HG23	2.32	0.42
3:H:86:ALA:H	3:H:109:VAL:HG11	1.85	0.42
2:M:199:ASN:HA	2:M:200:PRO:HD3	1.90	0.42
2:M:224:LEU:HA	2:M:227:SER:OG	2.19	0.42
2:M:249:ALA:HA	6:M:311:U10:H4M2	2.00	0.42
5:M:309:BPH:CBB	5:M:309:BPH:CHC	2.96	0.42
3:H:153:VAL:CG1	3:H:164:VAL:CG1	2.97	0.42
3:H:153:VAL:HG21	3:H:181:VAL:CG1	2.49	0.42
1:L:204:LYS:HG3	1:L:207:ARG:NH1	2.35	0.42
1:L:222:TYR:CE1	1:L:224:ILE:HG23	2.53	0.42
6:L:277:U10:H71	6:L:277:U10:H1M1	1.34	0.42
2:M:270:ILE:HG23	2:M:271:TRP:N	2.35	0.42
3:H:122:GLU:HG3	3:H:123:LEU:N	2.34	0.42
3:H:151:LEU:O	3:H:164:VAL:CG2	2.68	0.42
3:H:247:LYS:HB2	3:H:247:LYS:HE3	1.75	0.42
2:M:284:ILE:HA	2:M:284:ILE:HD12	1.90	0.42
3:H:142:VAL:HG11	3:H:147:ASN:CB	2.50	0.42
3:H:58:LEU:HA	3:H:59:PRO:HD3	1.66	0.42
1:L:161:GLY:O	1:L:167:PHE:HD2	2.02	0.42
1:L:237:SER:OG	1:L:238:LEU:N	2.51	0.42
2:M:24:VAL:HG21	2:M:29:ARG:NH1	2.35	0.42
2:M:189:PHE:CE1	2:M:284:ILE:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:36:SER:H	2:M:45:ALA:HB1	1.84	0.42
3:H:213:PHE:C	3:H:215:GLY:H	2.23	0.42
1:L:41:PHE:CE2	1:L:95:GLY:HA3	2.55	0.42
2:M:188:ASN:HA	2:M:191:LEU:HB2	2.00	0.42
2:M:201:PHE:CB	2:M:283:GLY:HA3	2.50	0.42
1:L:3:LEU:O	1:L:4:SER:C	2.57	0.41
1:L:53:ALA:HB1	1:L:64:ILE:HD11	1.91	0.41
2:M:102:GLY:O	2:M:104:SER:N	2.53	0.41
1:L:53:ALA:CB	1:L:64:ILE:CD1	2.73	0.41
2:M:115:TRP:CD2	2:M:119:SER:OG	2.72	0.41
3:H:68:HIS:CE1	3:H:123:LEU:HA	2.55	0.41
1:L:231:ARG:CZ	2:M:6:ILE:O	2.69	0.41
1:L:241:VAL:HG11	5:L:276:BPH:HAC2	2.01	0.41
2:M:226:VAL:CG1	2:M:244:ALA:HA	2.51	0.41
8:M:310:SPO:H81	8:M:310:SPO:H10	1.77	0.41
3:H:74:THR:HG23	3:H:76:PRO:HD2	2.00	0.41
1:L:244:SER:O	1:L:247:CYS:CB	2.69	0.41
2:M:107:ALA:HA	2:M:108:PRO:HD3	1.89	0.41
8:M:310:SPO:H131	8:M:310:SPO:H15	1.69	0.41
1:L:195:LEU:HD22	2:M:267:ARG:HD2	2.02	0.41
2:M:126:VAL:HG13	2:M:150:PHE:HZ	1.86	0.41
4:M:307:BCL:HBB2	4:M:307:BCL:CHC	2.45	0.41
2:M:206:ILE:CG1	4:M:308:BCL:HMB3	2.50	0.41
2:M:71:GLY:O	2:M:74:PHE:HB2	2.21	0.41
3:H:90:THR:OG1	3:H:98:HIS:HA	2.21	0.41
1:L:136:PRO:O	1:L:137:VAL:C	2.59	0.41
1:L:242:PHE:HD1	1:L:243:PHE:N	2.18	0.41
1:L:229:ILE:HG13	6:L:277:U10:C1	2.50	0.41
6:L:277:U10:H321	4:M:307:BCL:H192	2.01	0.41
2:M:77:GLN:O	2:M:79:GLY:N	2.51	0.41
2:M:99:PRO:HB2	2:M:101:TYR:CE1	2.51	0.41
3:H:168:TRP:CH2	3:H:219:ILE:HD12	2.55	0.41
3:H:64:PHE:CE2	3:H:75:VAL:HG21	2.55	0.41
1:L:8:LYS:HB3	3:H:85:ILE:HG21	2.02	0.41
1:L:110:LYS:HE2	1:L:110:LYS:HB3	1.93	0.41
1:L:133:LEU:O	1:L:133:LEU:HD12	2.21	0.41
1:L:66:VAL:O	1:L:66:VAL:HG12	2.21	0.41
2:M:254:TRP:O	2:M:255:THR:C	2.58	0.41
1:L:151:TRP:CZ2	2:M:303:MET:SD	3.14	0.41
1:L:22:PHE:HE2	1:L:36:VAL:HG21	1.86	0.41
1:L:223:SER:HB2	6:L:277:U10:H4M1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:38:THR:O	1:L:42:ALA:N	2.51	0.41
1:L:141:ALA:O	1:L:143:GLY:N	2.45	0.41
1:L:205:GLU:O	1:L:207:ARG:N	2.54	0.41
6:L:277:U10:H222	4:M:308:BCL:H201	2.03	0.41
1:L:3:LEU:HB2	1:L:6:GLU:OE1	2.20	0.41
8:M:310:SPO:H26	8:M:310:SPO:H241	1.96	0.41
3:H:67:PRO:O	3:H:68:HIS:HB2	2.20	0.40
1:L:218:ASP:OD1	2:M:51:TYR:CD2	2.72	0.40
4:M:307:BCL:CHC	4:M:307:BCL:CBB	2.78	0.40
3:H:245:ALA:HA	3:H:246:PRO:HD2	1.83	0.40
3:H:66:LEU:O	3:H:70:ARG:HB2	2.21	0.40
1:L:12:PRO:HG3	3:H:97:PRO:HB2	2.03	0.40
3:H:96:PHE:HA	3:H:97:PRO:HD3	1.87	0.40
1:L:234:LEU:HD21	2:M:221:ALA:HA	2.02	0.40
4:L:274:BCL:HED2	4:L:274:BCL:HBD	1.51	0.40
1:L:48:LEU:HA	1:L:48:LEU:HD12	1.90	0.40
2:M:202:HIS:NE2	4:M:308:BCL:NB	2.70	0.40
3:H:37:ARG:NH2	3:H:59:PRO:CB	2.78	0.40
1:L:219:LEU:HD12	2:M:132:ARG:NH1	2.34	0.40
4:L:275:BCL:CMB	4:L:275:BCL:CBB	2.98	0.40
2:M:124:VAL:O	2:M:125:ALA:C	2.59	0.40
2:M:242:GLY:HA2	3:H:115:VAL:HG12	2.03	0.40
6:M:311:U10:C43	6:M:311:U10:C38	2.99	0.40
3:H:33:THR:HB	3:H:59:PRO:HG3	2.03	0.40
1:L:150:ILE:HG22	1:L:151:TRP:N	2.36	0.40
4:L:274:BCL:HHC	4:L:274:BCL:OBB	2.21	0.40
2:M:116:LEU:HG	2:M:116:LEU:H	1.61	0.40
1:L:263:TRP:CE3	2:M:180:PHE:CZ	3.04	0.40
1:L:1:ALA:N	2:M:253:ARG:CG	2.85	0.40
2:M:79:GLY:O	2:M:81:ASN:N	2.55	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	271/273 (99%)	166 (61%)	63 (23%)	42 (16%)	0	1
2	M	303/305 (99%)	201 (66%)	70 (23%)	32 (11%)	0	2
3	H	258/260 (99%)	151 (58%)	64 (25%)	43 (17%)	0	0
All	All	832/838 (99%)	518 (62%)	197 (24%)	117 (14%)	0	1

All (117) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	3	LEU
1	L	4	SER
1	L	65	SER
1	L	70	ALA
1	L	71	LEU
1	L	78	ALA
1	L	140	GLY
1	L	171	PRO
1	L	172	ALA
1	L	202	LYS
1	L	258	GLN
1	L	260	VAL
2	M	5	ASN
2	M	6	ILE
2	M	54	SER
2	M	78	ALA
2	M	80	TRP
2	M	133	THR
2	M	145	HIS
2	M	303	MET
3	H	2	VAL
3	H	68	HIS
3	H	77	GLY
3	H	94	GLU
3	H	99	ALA
3	H	103	ASP
3	H	104	PRO
3	H	105	MET
3	H	112	ALA
3	H	119	ASP
3	H	138	ALA

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Mol	Chain	Res	Type
3	H	146	LYS
3	H	184	LYS
3	H	185	ASP
3	H	220	LYS
3	H	221	SER
3	H	227	LEU
3	H	241	LEU
3	H	254	ALA
3	H	255	MET
1	L	15	THR
1	L	19	GLY
1	L	25	TRP
1	L	55	LEU
1	L	58	THR
1	L	76	GLY
1	L	77	GLY
1	L	115	TYR
1	L	132	VAL
1	L	145	ALA
1	L	150	ILE
1	L	203	GLY
1	L	206	MET
1	L	270	PRO
2	M	23	ASP
2	M	76	TYR
2	M	103	LEU
2	M	111	GLU
2	M	114	LEU
2	M	143	GLY
2	M	192	VAL
2	M	195	ASN
2	M	289	THR
2	M	291	VAL
3	H	8	GLY
3	H	39	GLY
3	H	91	ALA
3	H	108	GLY
3	H	118	ARG
3	H	143	SER
3	H	157	ASP
3	H	247	LYS
3	H	250	SER

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Mol	Chain	Res	Type
3	H	257	ALA
1	L	7	ARG
1	L	22	PHE
1	L	52	SER
1	L	75	LEU
1	L	138	MET
1	L	182	THR
1	L	193	LEU
2	M	43	GLY
2	M	91	PHE
2	M	109	LEU
2	M	172	SER
3	H	49	PRO
3	H	84	PRO
3	H	172	PRO
3	H	201	ASN
3	H	248	ARG
3	H	253	ALA
1	L	167	PHE
1	L	215	PHE
1	L	235	LEU
1	L	263	TRP
2	M	25	ASN
2	M	132	ARG
2	M	293	ASN
3	H	128	HIS
1	L	72	GLU
1	L	242	PHE
2	M	49	PRO
2	M	79	GLY
2	M	115	TRP
2	M	125	ALA
3	H	46	ASP
3	H	51	ALA
3	H	76	PRO
3	H	148	PRO
3	H	214	ALA
2	M	108	PRO
2	M	194	GLY
3	H	252	VAL
1	L	26	VAL
1	L	249	ILE

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Mol	Chain	Res	Type
1	L	269	LEU
2	M	141	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	215/215 (100%)	156 (73%)	59 (27%)	0	2
2	M	238/238 (100%)	173 (73%)	65 (27%)	0	2
3	H	208/208 (100%)	145 (70%)	63 (30%)	0	1
All	All	661/661 (100%)	474 (72%)	187 (28%)	0	2

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	LEU
1	L	4	SER
1	L	7	ARG
1	L	8	LYS
1	L	9	TYR
1	L	21	LEU
1	L	22	PHE
1	L	23	ASP
1	L	24	PHE
1	L	26	VAL
1	L	41	PHE
1	L	44	LEU
1	L	47	ILE
1	L	54	VAL
1	L	55	LEU
1	L	58	THR
1	L	63	LEU
1	L	71	LEU
1	L	72	GLU
1	L	73	TYR

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Mol	Chain	Res	Type
1	L	75	LEU
1	L	85	LEU
1	L	94	THR
1	L	103	ARG
1	L	108	CYS
1	L	109	ARG
1	L	115	TYR
1	L	116	HIS
1	L	131	LEU
1	L	133	LEU
1	L	138	MET
1	L	139	MET
1	L	146	PHE
1	L	152	THR
1	L	154	LEU
1	L	160	THR
1	L	167	PHE
1	L	170	ASN
1	L	173	HIS
1	L	178	SER
1	L	180	PHE
1	L	187	LEU
1	L	202	LYS
1	L	205	GLU
1	L	209	PRO
1	L	210	ASP
1	L	213	ASP
1	L	224	ILE
1	L	229	ILE
1	L	232	LEU
1	L	235	LEU
1	L	244	SER
1	L	248	MET
1	L	253	THR
1	L	258	GLN
1	L	266	TRP
1	L	269	LEU
1	L	271	TRP
1	L	272	TRP
2	M	6	ILE
2	M	9	GLN
2	M	17	ASP

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Mol	Chain	Res	Type
2	M	18	LEU
2	M	20	MET
2	M	24	VAL
2	M	29	ARG
2	M	38	LEU
2	M	42	PHE
2	M	44	ASN
2	M	47	LEU
2	M	51	TYR
2	M	60	LEU
2	M	62	SER
2	M	65	MET
2	M	69	THR
2	M	73	TRP
2	M	76	TYR
2	M	77	GLN
2	M	88	ASP
2	M	89	LEU
2	M	92	PHE
2	M	94	LEU
2	M	96	PRO
2	M	100	GLU
2	M	101	TYR
2	M	103	LEU
2	M	109	LEU
2	M	114	LEU
2	M	115	TRP
2	M	124	VAL
2	M	128	SER
2	M	133	THR
2	M	134	TYR
2	M	135	LEU
2	M	136	ARG
2	M	140	MET
2	M	144	LYS
2	M	148	TRP
2	M	151	LEU
2	M	154	ILE
2	M	157	TRP
2	M	160	LEU
2	M	170	SER
2	M	180	PHE

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Mol	Chain	Res	Type
2	M	187	ASN
2	M	188	ASN
2	M	191	LEU
2	M	204	LEU
2	M	216	PHE
2	M	219	HIS
2	M	224	LEU
2	M	233	ARG
2	M	240	ASP
2	M	241	ARG
2	M	243	THR
2	M	246	GLU
2	M	250	LEU
2	M	255	THR
2	M	258	PHE
2	M	262	MET
2	M	265	ILE
2	M	267	ARG
2	M	268	TRP
2	M	292	ASP
3	H	1	MET
3	H	2	VAL
3	H	7	PHE
3	H	9	ASN
3	H	11	ASP
3	H	17	ILE
3	H	22	ILE
3	H	23	PHE
3	H	30	TYR
3	H	33	THR
3	H	35	ASN
3	H	37	ARG
3	H	40	TYR
3	H	44	ASN
3	H	45	GLU
3	H	48	THR
3	H	53	GLN
3	H	60	LYS
3	H	62	LYS
3	H	65	ILE
3	H	75	VAL
3	H	80	SER

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Mol	Chain	Res	Type
3	H	85	ILE
3	H	89	ARG
3	H	94	GLU
3	H	98	HIS
3	H	103	ASP
3	H	107	ASP
3	H	115	VAL
3	H	121	PRO
3	H	122	GLU
3	H	123	LEU
3	H	142	VAL
3	H	146	LYS
3	H	151	LEU
3	H	154	ARG
3	H	157	ASP
3	H	158	LEU
3	H	163	LYS
3	H	164	VAL
3	H	171	ILE
3	H	173	GLU
3	H	179	LEU
3	H	188	THR
3	H	189	ARG
3	H	190	LEU
3	H	191	LEU
3	H	194	GLN
3	H	197	LYS
3	H	199	GLN
3	H	200	SER
3	H	201	ASN
3	H	212	LEU
3	H	213	PHE
3	H	216	ILE
3	H	218	THR
3	H	219	ILE
3	H	227	LEU
3	H	233	ILE
3	H	237	VAL
3	H	242	MET
3	H	243	TYR
3	H	258	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such

sidechains are listed below:

Mol	Chain	Res	Type
1	L	56	GLN
1	L	60	ASN
1	L	116	HIS
1	L	170	ASN
1	L	183	ASN
1	L	211	HIS
1	L	258	GLN
2	M	5	ASN
2	M	9	GLN
2	M	25	ASN
2	M	46	GLN
2	M	81	ASN
2	M	145	HIS
2	M	188	ASN
2	M	300	ASN
3	H	32	GLN
3	H	35	ASN
3	H	68	HIS
3	H	98	HIS
3	H	128	HIS
3	H	129	ASN
3	H	147	ASN
3	H	194	GLN
3	H	201	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BCL	M	307	2	58,74,74	2.53	18 (31%)	69,115,115	1.99	15 (21%)
5	BPH	L	276	-	64,70,70	2.32	16 (25%)	76,101,101	1.39	12 (15%)
4	BCL	L	274	1	58,74,74	4.19	24 (41%)	69,115,115	1.83	14 (20%)
4	BCL	M	308	2	58,74,74	3.58	23 (39%)	69,115,115	1.78	15 (21%)
6	U10	L	277	-	58,58,63	3.69	36 (62%)	70,73,79	1.80	14 (20%)
8	SPO	M	310	-	40,41,41	2.99	22 (55%)	47,50,50	1.93	12 (25%)
4	BCL	L	275	1	58,74,74	3.13	27 (46%)	69,115,115	1.70	15 (21%)
5	BPH	M	309	-	64,70,70	2.63	20 (31%)	76,101,101	1.40	12 (15%)
6	U10	M	311	-	58,58,63	3.02	31 (53%)	70,73,79	1.44	11 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	M	307	2	2/2/21/25	10/37/137/137	-
5	BPH	L	276	-	1/1/18/22	17/54/105/105	0/5/6/6
4	BCL	L	274	1	1/1/21/25	9/37/137/137	-
4	BCL	M	308	2	-	12/37/137/137	-
6	U10	L	277	-	-	13/57/81/87	0/1/1/1
8	SPO	M	310	-	-	6/47/47/47	-
4	BCL	L	275	1	-	15/37/137/137	-
5	BPH	M	309	-	1/1/18/22	16/54/105/105	0/5/6/6
6	U10	M	311	-	-	20/57/81/87	0/1/1/1

All (217) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	274	BCL	C3C-C4C	17.85	1.74	1.51
4	M	308	BCL	C4B-NB	15.87	1.49	1.35
5	L	276	BPH	CAA-C2A	11.61	1.75	1.54
4	L	274	BCL	CAA-C2A	10.51	1.73	1.54
4	L	274	BCL	OBB-CAB	10.16	1.54	1.22
6	L	277	U10	C28-C29	9.75	1.56	1.33
4	L	274	BCL	CBB-CAB	-9.65	1.21	1.49
8	M	310	SPO	C4-C5	9.49	1.65	1.50
4	L	274	BCL	CAC-C3C	9.21	1.72	1.54
5	M	309	BPH	CHB-C1B	9.03	1.56	1.38
6	L	277	U10	C27-C28	8.98	1.79	1.50
4	M	308	BCL	C3C-C4C	-8.94	1.40	1.51
5	M	309	BPH	CAA-C2A	8.59	1.70	1.54
4	L	275	BCL	CAA-C2A	8.35	1.69	1.54
4	M	308	BCL	MG-NA	8.18	2.25	2.06
6	M	311	U10	C18-C19	-7.83	1.14	1.33
6	L	277	U10	C23-C24	7.56	1.51	1.33
4	L	275	BCL	MG-NC	-7.40	1.88	2.06
4	M	308	BCL	C2C-C3C	-7.38	1.33	1.54
4	M	307	BCL	CAA-C2A	7.09	1.67	1.54
4	L	275	BCL	MG-NA	7.08	2.23	2.06
4	L	275	BCL	CAC-C3C	-6.88	1.40	1.54
6	L	277	U10	C22-C23	6.87	1.72	1.50
4	L	275	BCL	C4B-NB	6.70	1.41	1.35
4	M	307	BCL	C2A-C1A	6.45	1.66	1.52
4	M	307	BCL	C1B-NB	6.39	1.40	1.35
6	L	277	U10	C13-C14	6.38	1.48	1.33
6	L	277	U10	C26-C24	6.35	1.64	1.51
5	L	276	BPH	CMB-C2B	6.22	1.64	1.50
6	M	311	U10	C33-C34	6.19	1.47	1.33
4	L	274	BCL	C2A-C1A	6.17	1.66	1.52
4	L	275	BCL	CMD-C2D	-6.11	1.37	1.51
6	L	277	U10	C33-C34	6.07	1.47	1.33
4	M	307	BCL	CHD-C4C	-6.03	1.24	1.41
5	M	309	BPH	C2A-C1A	6.00	1.61	1.51
4	M	308	BCL	C3A-C2A	-5.95	1.37	1.54
6	M	311	U10	C17-C18	5.91	1.69	1.50
4	L	274	BCL	CBD-CGD	-5.81	1.34	1.52
4	L	274	BCL	CHD-C4C	-5.73	1.24	1.41
6	M	311	U10	C28-C29	5.72	1.46	1.33
4	M	307	BCL	C3C-C4C	5.72	1.58	1.51
4	M	308	BCL	C1D-C2D	-5.66	1.29	1.42
6	M	311	U10	C22-C23	5.63	1.68	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	275	BCL	C5-C3	5.44	1.62	1.51
6	L	277	U10	C38-C39	5.34	1.45	1.33
6	L	277	U10	C17-C18	5.32	1.67	1.50
4	M	308	BCL	C5-C3	5.27	1.62	1.51
5	M	309	BPH	C1-C2	5.26	1.64	1.49
8	M	310	SPO	C22-C23	5.20	1.42	1.35
6	L	277	U10	C18-C19	5.19	1.45	1.33
4	L	274	BCL	C4B-NB	5.18	1.39	1.35
8	M	310	SPO	C27-C28	5.16	1.39	1.34
8	M	310	SPO	C9-C7	5.14	1.42	1.35
4	L	275	BCL	C2-C3	5.14	1.45	1.33
4	L	275	BCL	OBD-CAD	5.04	1.29	1.22
4	M	308	BCL	CAA-C2A	4.91	1.63	1.54
5	M	309	BPH	C3A-C2A	-4.87	1.40	1.54
5	M	309	BPH	CHB-C4A	4.85	1.52	1.40
6	M	311	U10	C38-C39	4.85	1.44	1.33
4	M	307	BCL	C3B-C2B	4.81	1.48	1.39
6	M	311	U10	C21-C19	4.78	1.61	1.51
6	M	311	U10	C23-C24	4.77	1.44	1.33
4	L	275	BCL	CBD-CGD	-4.75	1.37	1.52
6	L	277	U10	C32-C33	4.70	1.65	1.50
4	L	275	BCL	CMC-C2C	-4.69	1.43	1.53
6	L	277	U10	C48-C49	4.63	1.45	1.32
6	M	311	U10	C7-C8	-4.61	1.44	1.50
4	M	308	BCL	CAC-C3C	4.56	1.63	1.54
6	L	277	U10	C16-C14	4.56	1.60	1.51
4	L	274	BCL	C4B-CHC	-4.50	1.28	1.41
4	M	308	BCL	MG-NC	-4.48	1.95	2.06
4	M	307	BCL	C1B-CHB	-4.45	1.28	1.41
5	L	276	BPH	C2A-C1A	-4.44	1.44	1.51
8	M	310	SPO	C32-C33	4.40	1.43	1.33
4	M	307	BCL	CMA-C3A	-4.38	1.43	1.53
6	M	311	U10	C43-C44	4.37	1.43	1.33
4	L	274	BCL	C1D-C2D	4.34	1.52	1.42
6	L	277	U10	C6-C5	4.25	1.58	1.46
6	L	277	U10	C43-C44	4.25	1.43	1.33
6	L	277	U10	C31-C29	4.19	1.60	1.51
5	M	309	BPH	CMA-C3A	-4.17	1.44	1.53
5	L	276	BPH	C1B-C2B	-4.16	1.36	1.45
6	M	311	U10	C32-C33	4.12	1.63	1.50
4	L	274	BCL	CMD-C2D	4.11	1.61	1.51
4	M	308	BCL	CBD-CGD	4.11	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	274	BCL	C2C-C3C	-4.10	1.43	1.54
5	M	309	BPH	C4A-NA	-4.09	1.25	1.35
6	M	311	U10	C42-C43	4.08	1.63	1.50
6	L	277	U10	O2-C2	4.04	1.32	1.23
5	M	309	BPH	C3C-C4C	4.01	1.56	1.50
4	M	307	BCL	C3A-C4A	-3.91	1.39	1.51
8	M	310	SPO	C8-C7	3.89	1.58	1.50
6	M	311	U10	C8-C9	-3.87	1.23	1.33
6	M	311	U10	C6-C1	3.86	1.42	1.35
4	L	275	BCL	C3C-C4C	3.82	1.56	1.51
4	L	274	BCL	C1B-NB	-3.80	1.31	1.35
6	M	311	U10	C48-C49	3.79	1.43	1.32
5	L	276	BPH	C3B-C4B	-3.75	1.31	1.43
8	M	310	SPO	C15-C14	-3.74	1.31	1.43
4	L	275	BCL	C3A-C4A	-3.74	1.39	1.51
8	M	310	SPO	C37-C38	3.68	1.42	1.32
8	M	310	SPO	C14-C12	-3.68	1.30	1.35
4	L	274	BCL	O2D-CGD	-3.67	1.24	1.33
4	M	308	BCL	CMA-C3A	-3.63	1.45	1.53
8	M	310	SPO	C21-C22	-3.60	1.32	1.43
6	L	277	U10	O3-C3M	-3.58	1.36	1.45
5	L	276	BPH	CHA-C1A	-3.55	1.30	1.38
5	M	309	BPH	CMB-C2B	-3.55	1.43	1.50
4	L	275	BCL	C1A-CHA	-3.50	1.28	1.43
6	M	311	U10	C36-C34	3.49	1.58	1.51
6	L	277	U10	C37-C38	3.44	1.61	1.50
8	M	310	SPO	C36-C37	3.41	1.61	1.50
6	M	311	U10	C51-C49	3.31	1.59	1.50
6	L	277	U10	C40-C39	3.30	1.59	1.50
5	M	309	BPH	C3D-C2D	-3.29	1.33	1.39
4	M	308	BCL	CMC-C2C	-3.23	1.46	1.53
4	M	307	BCL	C5-C3	-3.21	1.44	1.51
6	L	277	U10	C12-C13	3.17	1.60	1.50
4	L	274	BCL	C3B-C2B	-3.15	1.33	1.39
4	M	308	BCL	C2A-C1A	3.14	1.59	1.52
8	M	310	SPO	C31-C32	3.14	1.60	1.50
6	L	277	U10	C45-C44	3.10	1.58	1.50
5	L	276	BPH	C4A-NA	-3.09	1.27	1.35
6	M	311	U10	C45-C44	3.06	1.58	1.50
4	L	275	BCL	C2C-C3C	-3.05	1.45	1.54
5	L	276	BPH	C1-C2	-3.02	1.40	1.49
4	M	308	BCL	CMB-C2B	2.98	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	276	BPH	C2-C3	2.96	1.40	1.33
5	M	309	BPH	C4C-NC	-2.96	1.31	1.37
6	M	311	U10	C7-C6	-2.94	1.46	1.51
5	M	309	BPH	CBD-CGD	-2.92	1.43	1.52
8	M	310	SPO	C20-C19	-2.92	1.34	1.43
5	M	309	BPH	C3D-CAD	-2.90	1.41	1.47
6	L	277	U10	C4-C5	2.90	1.57	1.48
6	L	277	U10	C6-C1	-2.87	1.29	1.35
8	M	310	SPO	C10-C9	-2.86	1.34	1.43
4	M	307	BCL	O2D-CGD	-2.85	1.26	1.33
6	M	311	U10	C35-C34	2.82	1.57	1.50
5	L	276	BPH	C3B-C2B	2.82	1.46	1.39
4	M	308	BCL	C3B-CAB	2.81	1.56	1.49
8	M	310	SPO	C40-C38	2.80	1.57	1.50
4	L	274	BCL	O2A-CGA	-2.75	1.25	1.33
4	M	308	BCL	O2A-C1	-2.74	1.38	1.46
6	L	277	U10	C25-C24	2.73	1.57	1.50
6	L	277	U10	C50-C49	2.73	1.57	1.50
6	L	277	U10	C36-C34	2.72	1.56	1.51
4	M	308	BCL	O2A-CGA	-2.72	1.25	1.33
4	L	275	BCL	C4B-CHC	-2.72	1.33	1.41
6	M	311	U10	C15-C14	2.68	1.57	1.50
4	M	308	BCL	CMD-C2D	-2.68	1.45	1.51
4	L	274	BCL	O2A-C1	-2.67	1.38	1.46
5	L	276	BPH	O2A-C1	-2.67	1.38	1.46
5	L	276	BPH	CAC-C3C	-2.66	1.48	1.54
5	M	309	BPH	C5-C3	2.66	1.56	1.51
4	L	274	BCL	C3D-CAD	2.64	1.52	1.46
4	M	308	BCL	OBD-CAD	2.61	1.26	1.22
4	M	307	BCL	C2-C3	2.61	1.39	1.33
6	M	311	U10	C16-C14	2.61	1.56	1.51
6	L	277	U10	O5-C5	2.60	1.29	1.23
6	M	311	U10	C50-C49	2.57	1.57	1.50
6	M	311	U10	C31-C29	2.56	1.56	1.51
6	L	277	U10	C15-C14	2.56	1.57	1.50
4	L	275	BCL	O2A-CGA	-2.55	1.25	1.33
5	L	276	BPH	C3A-C4A	-2.55	1.44	1.51
8	M	310	SPO	C6-C5	2.54	1.38	1.32
6	M	311	U10	C27-C28	2.53	1.58	1.50
6	L	277	U10	C1M-C1	-2.53	1.45	1.50
4	L	275	BCL	CAA-CBA	2.53	1.60	1.52
6	M	311	U10	C13-C14	2.50	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	277	U10	C42-C43	2.49	1.58	1.50
6	L	277	U10	C47-C48	2.49	1.58	1.50
4	L	275	BCL	C4-C3	2.48	1.57	1.50
4	M	308	BCL	C3B-C2B	2.47	1.43	1.39
5	M	309	BPH	C3B-C2B	-2.46	1.32	1.39
5	M	309	BPH	CAA-CBA	2.46	1.60	1.52
6	L	277	U10	C1-C2	2.45	1.55	1.47
4	L	275	BCL	O2A-C1	-2.45	1.39	1.46
6	L	277	U10	C21-C19	2.44	1.56	1.51
5	L	276	BPH	C4C-NC	-2.43	1.32	1.37
4	L	274	BCL	CAA-CBA	2.39	1.60	1.52
4	M	307	BCL	O2A-C1	-2.37	1.39	1.46
4	M	308	BCL	CHD-C4C	-2.34	1.34	1.41
4	L	274	BCL	C1-C2	2.33	1.56	1.49
5	M	309	BPH	O2A-C1	-2.32	1.39	1.46
4	L	275	BCL	C3B-C2B	2.32	1.43	1.39
8	M	310	SPO	C30-C28	2.31	1.56	1.51
5	M	309	BPH	CBA-CGA	2.31	1.57	1.50
4	L	275	BCL	C1-C2	2.30	1.56	1.49
4	M	307	BCL	C1A-CHA	-2.27	1.33	1.43
5	L	276	BPH	O2A-CGA	-2.27	1.26	1.33
4	L	274	BCL	CBA-CGA	2.24	1.57	1.50
8	M	310	SPO	C19-C17	2.24	1.38	1.35
5	M	309	BPH	CMC-C2C	-2.23	1.48	1.53
6	L	277	U10	C20-C19	2.22	1.56	1.50
4	L	275	BCL	C16-C15	2.21	1.61	1.52
6	M	311	U10	C37-C38	2.21	1.57	1.50
8	M	310	SPO	C11-C12	-2.20	1.41	1.45
4	M	307	BCL	OBD-CAD	2.18	1.25	1.22
4	L	275	BCL	C16-C17	2.15	1.61	1.52
4	L	275	BCL	C6-C5	2.11	1.60	1.52
4	L	274	BCL	C3A-C4A	-2.11	1.45	1.51
6	M	311	U10	C26-C24	2.10	1.55	1.51
4	M	307	BCL	C2C-C3C	-2.10	1.48	1.54
6	L	277	U10	C46-C44	2.10	1.55	1.51
6	M	311	U10	C25-C24	2.10	1.56	1.50
4	M	307	BCL	C4B-NB	2.10	1.37	1.35
4	M	308	BCL	C4B-CHC	-2.05	1.35	1.41
8	M	310	SPO	C26-C27	-2.05	1.37	1.43
6	M	311	U10	O4-C4	-2.05	1.31	1.36
4	L	275	BCL	C1B-NB	-2.03	1.33	1.35
5	L	276	BPH	CMA-C3A	-2.03	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	275	BCL	C3D-CAD	2.02	1.51	1.46
8	M	310	SPO	C13-C12	2.02	1.55	1.50
4	M	307	BCL	CMC-C2C	2.01	1.57	1.53
6	M	311	U10	C46-C44	2.01	1.55	1.51
4	L	274	BCL	C1A-CHA	-2.01	1.34	1.43
8	M	310	SPO	C21-C20	-2.00	1.30	1.36

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	307	BCL	CHD-C4C-NC	7.89	133.84	125.08
6	L	277	U10	C8-C7-C6	6.91	130.67	112.05
4	L	274	BCL	CHC-C1C-NC	-6.47	115.56	124.51
8	M	310	SPO	C3-C1-C4	-6.36	101.09	110.86
6	L	277	U10	C6-C1-C2	5.64	123.64	119.18
5	L	276	BPH	CBB-CAB-C3B	-5.51	108.66	120.43
4	L	275	BCL	C1-C2-C3	5.00	134.70	126.04
4	M	308	BCL	C2C-C3C-C4C	4.98	108.80	101.34
4	M	307	BCL	C2A-C1A-CHA	4.97	132.55	123.86
4	L	274	BCL	CHD-C4C-NC	4.92	130.54	125.08
4	L	274	BCL	OBB-CAB-C3B	-4.82	111.44	119.99
5	M	309	BPH	CBB-CAB-C3B	-4.81	110.15	120.43
6	L	277	U10	C32-C33-C34	4.66	138.89	127.66
4	L	274	BCL	C4D-C3D-CAD	-4.59	105.91	108.47
6	M	311	U10	C17-C18-C19	-4.57	116.65	127.66
4	M	307	BCL	CHB-C4A-NA	-4.53	118.25	124.51
6	M	311	U10	C21-C19-C18	-4.50	112.02	121.12
4	M	307	BCL	C4D-C3D-CAD	-4.34	106.05	108.47
4	M	308	BCL	CMC-C2C-C1C	4.27	123.26	111.77
4	M	307	BCL	C1-C2-C3	4.22	133.34	126.04
4	L	274	BCL	C4A-NA-C1A	4.18	108.59	106.71
4	M	308	BCL	CHA-C1A-NA	-4.15	116.89	126.40
4	M	307	BCL	C1C-NC-C4C	4.09	108.54	106.71
5	L	276	BPH	C1-C2-C3	3.99	132.94	126.04
4	M	308	BCL	C1C-NC-C4C	-3.91	104.95	106.71
4	L	275	BCL	CHD-C4C-NC	3.71	129.20	125.08
5	M	309	BPH	C4D-C3D-CAD	3.70	110.21	107.87
4	L	275	BCL	C4B-C3B-CAB	-3.68	120.03	127.13
4	L	275	BCL	C1C-NC-C4C	-3.62	105.08	106.71
8	M	310	SPO	C10-C9-C7	-3.59	122.19	127.31
8	M	310	SPO	C13-C12-C14	-3.57	117.92	122.92
4	L	274	BCL	C1C-NC-C4C	-3.50	105.13	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	308	BCL	C1-C2-C3	3.48	132.07	126.04
4	M	307	BCL	CHC-C1C-NC	-3.46	119.72	124.51
8	M	310	SPO	C18-C17-C19	-3.46	118.08	122.92
6	L	277	U10	C7-C8-C9	3.41	132.48	126.79
4	M	308	BCL	O2A-CGA-CBA	3.40	122.56	111.91
8	M	310	SPO	C2-C1-C4	-3.37	105.69	110.86
4	M	307	BCL	C2C-C3C-C4C	3.35	106.36	101.34
5	L	276	BPH	C1B-NB-C4B	3.17	112.49	106.51
5	M	309	BPH	C2A-C3A-C4A	3.16	107.58	101.34
4	M	308	BCL	CHD-C4C-NC	-3.10	121.64	125.08
4	L	275	BCL	C3D-CAD-CBD	-3.09	103.54	107.61
4	L	275	BCL	CBB-CAB-C3B	-3.07	111.23	120.34
6	M	311	U10	C20-C19-C18	3.05	131.50	123.68
4	M	308	BCL	CMB-C2B-C1B	-3.04	123.80	128.46
4	L	275	BCL	C2C-C3C-C4C	3.04	105.89	101.34
8	M	310	SPO	C1-C4-C5	2.98	120.95	113.06
5	L	276	BPH	CAA-C2A-C1A	-2.96	104.67	112.33
5	L	276	BPH	C1C-NC-C4C	-2.92	107.97	110.54
6	L	277	U10	C1M-C1-C6	-2.90	119.67	124.40
8	M	310	SPO	C3-C1-C2	-2.89	104.94	110.37
4	M	308	BCL	C2A-C1A-CHA	2.86	128.86	123.86
5	M	309	BPH	C2B-C1B-NB	-2.85	105.50	109.79
6	L	277	U10	C37-C38-C39	2.84	134.50	127.66
4	M	307	BCL	CBB-CAB-C3B	-2.81	111.99	120.34
4	L	275	BCL	C2A-C3A-C4A	2.79	106.38	101.87
5	M	309	BPH	C3A-C2A-C1A	-2.79	98.31	101.64
4	M	308	BCL	CAA-C2A-C1A	2.79	121.11	111.97
4	L	275	BCL	O2A-CGA-CBA	2.78	120.64	111.91
4	M	308	BCL	C3D-CAD-CBD	-2.77	103.96	107.61
6	L	277	U10	C1-C6-C5	2.77	122.19	119.58
4	M	308	BCL	CBB-CAB-C3B	-2.74	112.21	120.34
6	L	277	U10	C27-C28-C29	2.72	134.21	127.66
4	L	275	BCL	OBD-CAD-C3D	2.69	132.45	127.98
4	M	307	BCL	CAC-C3C-C4C	-2.66	106.68	112.58
6	M	311	U10	C7-C6-C5	-2.64	115.30	118.48
6	L	277	U10	C11-C12-C13	2.63	120.54	111.88
4	L	275	BCL	OBB-CAB-C3B	2.62	124.64	119.99
4	M	307	BCL	C3A-C2A-C1A	2.59	105.22	101.34
8	M	310	SPO	C8-C7-C9	-2.59	119.29	122.92
8	M	310	SPO	C34-C33-C35	-2.56	110.97	115.27
5	M	309	BPH	C4-C3-C5	-2.52	111.03	115.27
4	L	275	BCL	CMA-C3A-C4A	2.52	118.53	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	276	BPH	OBD-CAD-C3D	2.48	132.10	127.98
4	L	275	BCL	CAA-C2A-C1A	-2.43	104.01	111.97
4	M	308	BCL	OBB-CAB-C3B	2.43	124.31	119.99
4	L	274	BCL	OBD-CAD-CBD	-2.42	122.44	125.89
4	L	274	BCL	C4B-CHC-C1C	-2.40	125.36	130.12
5	M	309	BPH	C4D-CHA-C1A	-2.40	124.59	130.51
8	M	310	SPO	C21-C22-C23	2.39	130.73	127.31
4	L	275	BCL	CHC-C1C-NC	-2.39	121.20	124.51
4	M	308	BCL	CMB-C2B-C3B	2.38	129.13	124.68
4	M	307	BCL	OBB-CAB-C3B	2.37	124.20	119.99
5	M	309	BPH	C1B-NB-C4B	2.35	110.93	106.51
4	L	274	BCL	O2A-CGA-CBA	2.34	119.26	111.91
5	M	309	BPH	OBB-CAB-C3B	2.34	124.74	120.41
4	L	274	BCL	CHB-C4A-NA	-2.29	121.35	124.51
4	M	308	BCL	O2A-CGA-O1A	-2.29	117.82	123.59
6	M	311	U10	C30-C29-C31	-2.28	111.43	115.27
6	M	311	U10	C16-C17-C18	2.28	119.38	111.88
4	L	274	BCL	CGD-CBD-CAD	-2.27	103.38	110.73
6	M	311	U10	C21-C22-C23	2.27	119.34	111.88
5	L	276	BPH	C2B-C1B-NB	-2.26	106.39	109.79
4	L	275	BCL	CAA-C2A-C3A	-2.24	106.65	112.78
5	L	276	BPH	O2A-CGA-CBA	2.23	118.90	111.91
5	M	309	BPH	C3B-C2B-C1B	2.22	109.11	105.87
4	L	274	BCL	C1-C2-C3	2.22	129.88	126.04
4	L	274	BCL	C2A-C1A-CHA	2.20	127.70	123.86
4	L	274	BCL	O2A-CGA-O1A	-2.20	118.04	123.59
5	L	276	BPH	CBA-CAA-C2A	2.20	120.35	113.86
8	M	310	SPO	C5-C6-C7	-2.20	122.58	125.89
6	L	277	U10	C42-C43-C44	2.18	132.92	127.66
6	M	311	U10	C32-C33-C34	2.18	132.90	127.66
4	M	307	BCL	CAA-C2A-C3A	-2.17	106.84	112.78
4	M	307	BCL	C3D-CAD-CBD	-2.17	104.75	107.61
6	M	311	U10	C42-C43-C44	2.16	132.87	127.66
6	M	311	U10	C7-C8-C9	2.14	130.35	126.79
4	M	307	BCL	C4-C3-C5	-2.12	111.70	115.27
6	L	277	U10	C31-C32-C33	-2.12	104.91	111.88
8	M	310	SPO	C9-C10-C11	2.11	129.80	123.22
5	M	309	BPH	C1C-NC-C4C	-2.10	108.70	110.54
5	L	276	BPH	C3D-CAD-CBD	-2.08	104.87	107.61
6	L	277	U10	C12-C13-C14	2.07	132.64	127.66
6	L	277	U10	C35-C34-C36	-2.06	111.81	115.27
5	L	276	BPH	OBB-CAB-C3B	2.06	124.21	120.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	276	BPH	OBD-CAD-CBD	-2.05	122.96	125.89
6	L	277	U10	C7-C6-C5	2.05	120.94	118.48
6	M	311	U10	C25-C24-C26	-2.03	111.86	115.27
5	M	309	BPH	C5-C3-C2	2.02	125.20	121.12

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	307	BCL	C8
4	M	307	BCL	C13
5	L	276	BPH	C8
4	L	274	BCL	C2C
5	M	309	BPH	C3C

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	276	BPH	CBD-CGD-O2D-CED
5	L	276	BPH	C4C-C3C-CAC-CBC
5	L	276	BPH	C2C-C3C-CAC-CBC
5	L	276	BPH	C4B-C3B-CAB-CBB
4	L	274	BCL	CBD-CGD-O2D-CED
4	M	308	BCL	CBD-CGD-O2D-CED
6	L	277	U10	C23-C24-C26-C27
6	L	277	U10	C25-C24-C26-C27
6	L	277	U10	C46-C47-C48-C49
8	M	310	SPO	C1-C4-C5-C6
8	M	310	SPO	C35-C36-C37-C38
4	L	275	BCL	C6-C7-C8-C9
5	M	309	BPH	CBD-CGD-O2D-CED
5	M	309	BPH	C4B-C3B-CAB-CBB
5	M	309	BPH	C1A-C2A-CAA-CBA
5	M	309	BPH	O2A-C1-C2-C3
6	M	311	U10	C17-C18-C19-C20
6	M	311	U10	C21-C22-C23-C24
6	M	311	U10	C24-C26-C27-C28
6	M	311	U10	C30-C29-C31-C32
6	M	311	U10	C43-C44-C46-C47
6	M	311	U10	C45-C44-C46-C47
4	L	274	BCL	O1D-CGD-O2D-CED
5	L	276	BPH	O1D-CGD-O2D-CED
4	L	275	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
5	M	309	BPH	O1D-CGD-O2D-CED
4	L	275	BCL	CBD-CGD-O2D-CED
4	M	308	BCL	O1A-CGA-O2A-C1
4	M	308	BCL	CBA-CGA-O2A-C1
4	M	308	BCL	O1D-CGD-O2D-CED
5	L	276	BPH	C3-C5-C6-C7
6	M	311	U10	C28-C29-C31-C32
4	L	275	BCL	CBA-CGA-O2A-C1
4	M	307	BCL	CBD-CGD-O2D-CED
4	M	308	BCL	C3-C5-C6-C7
4	M	308	BCL	C4-C3-C5-C6
6	M	311	U10	C25-C24-C26-C27
4	M	308	BCL	C2-C3-C5-C6
6	M	311	U10	C23-C24-C26-C27
4	L	275	BCL	O1A-CGA-O2A-C1
6	L	277	U10	C9-C11-C12-C13
6	M	311	U10	C34-C36-C37-C38
5	M	309	BPH	C13-C15-C16-C17
5	M	309	BPH	C8-C10-C11-C12
4	M	307	BCL	C5-C6-C7-C8
4	L	275	BCL	C5-C6-C7-C8
4	L	275	BCL	C6-C7-C8-C10
4	L	275	BCL	C11-C12-C13-C15
4	M	308	BCL	C13-C15-C16-C17
4	L	275	BCL	C11-C12-C13-C14
5	M	309	BPH	C5-C6-C7-C8
5	M	309	BPH	C15-C16-C17-C18
6	L	277	U10	C29-C31-C32-C33
5	M	309	BPH	C3A-C2A-CAA-CBA
5	L	276	BPH	C4-C3-C5-C6
5	L	276	BPH	C2-C3-C5-C6
8	M	310	SPO	C27-C28-C30-C31
4	M	307	BCL	O1D-CGD-O2D-CED
6	M	311	U10	C15-C14-C16-C17
6	M	311	U10	C13-C14-C16-C17
5	L	276	BPH	C1A-C2A-CAA-CBA
4	L	274	BCL	C13-C15-C16-C17
6	L	277	U10	C1-C6-C7-C8
5	L	276	BPH	C2B-C3B-CAB-CBB
6	L	277	U10	C35-C34-C36-C37
6	L	277	U10	C5-C6-C7-C8
8	M	310	SPO	C34-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
6	L	277	U10	C33-C34-C36-C37
5	M	309	BPH	C3-C5-C6-C7
5	L	276	BPH	C3A-C2A-CAA-CBA
4	L	275	BCL	C3A-C2A-CAA-CBA
4	L	274	BCL	CBA-CGA-O2A-C1
8	M	310	SPO	C32-C33-C35-C36
5	L	276	BPH	C2-C1-O2A-CGA
4	M	308	BCL	C2-C1-O2A-CGA
5	L	276	BPH	C5-C6-C7-C8
4	M	308	BCL	C2A-CAA-CBA-CGA
6	M	311	U10	C35-C34-C36-C37
6	L	277	U10	C5-C4-O4-C4M
4	M	307	BCL	CHA-CBD-CGD-O1D
8	M	310	SPO	C29-C28-C30-C31
5	L	276	BPH	C13-C15-C16-C17
4	L	275	BCL	C13-C15-C16-C17
5	M	309	BPH	C12-C13-C15-C16
6	M	311	U10	C33-C34-C36-C37
4	M	307	BCL	O1A-CGA-O2A-C1
6	M	311	U10	C5-C4-O4-C4M
4	M	307	BCL	CBA-CGA-O2A-C1
6	M	311	U10	C31-C32-C33-C34
4	L	274	BCL	O1A-CGA-O2A-C1
4	L	274	BCL	C15-C16-C17-C18
4	L	275	BCL	C3-C5-C6-C7
6	M	311	U10	C40-C39-C41-C42
5	M	309	BPH	C11-C10-C8-C7
4	L	275	BCL	C2A-CAA-CBA-CGA
6	M	311	U10	C14-C16-C17-C18
6	M	311	U10	C38-C39-C41-C42
6	L	277	U10	C40-C39-C41-C42
4	M	307	BCL	C3-C5-C6-C7
6	L	277	U10	C20-C19-C21-C22
4	M	307	BCL	C3A-C2A-CAA-CBA
5	L	276	BPH	C10-C11-C12-C13
4	M	307	BCL	CHA-CBD-CGD-O2D
5	L	276	BPH	CHA-CBD-CGD-O1D
5	L	276	BPH	CHA-CBD-CGD-O2D
4	L	274	BCL	CHA-CBD-CGD-O1D
4	L	274	BCL	CHA-CBD-CGD-O2D
4	M	308	BCL	CHA-CBD-CGD-O2D
5	M	309	BPH	CHA-CBD-CGD-O1D

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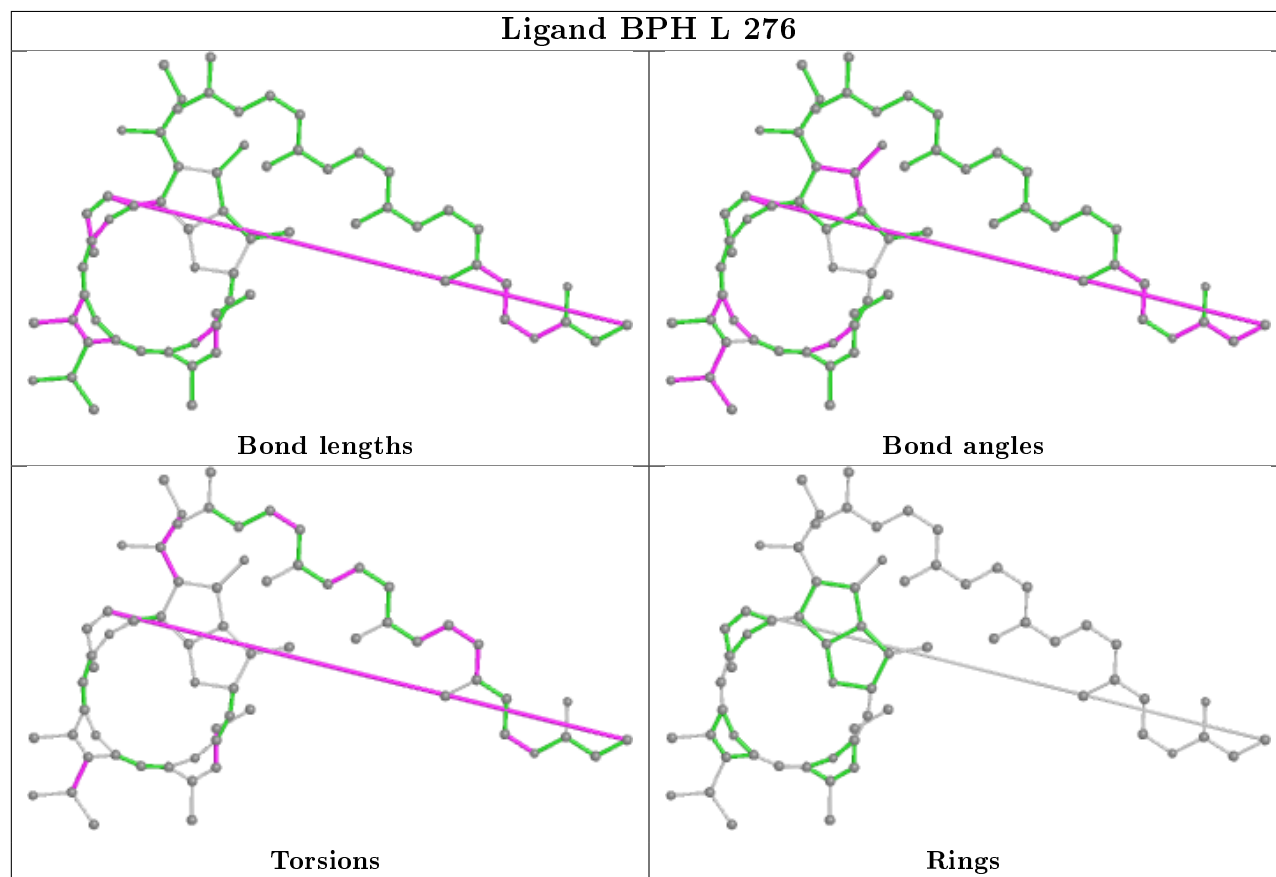
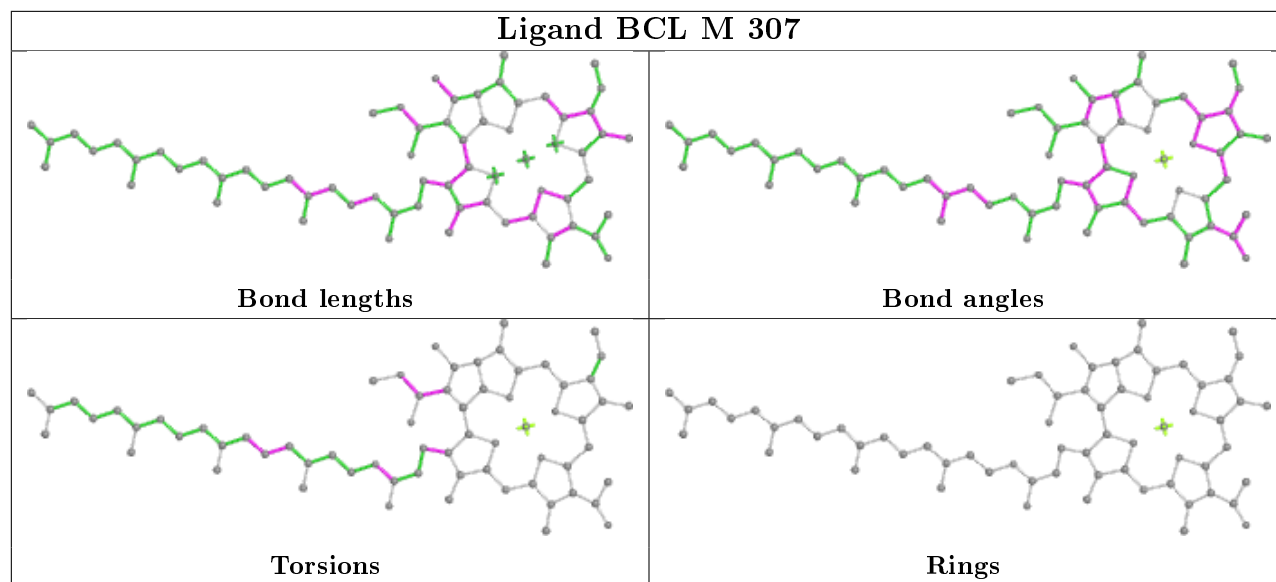
Mol	Chain	Res	Type	Atoms
5	M	309	BPH	C14-C13-C15-C16
6	L	277	U10	C21-C22-C23-C24
4	L	275	BCL	CAA-CBA-CGA-O2A
4	M	307	BCL	C1A-C2A-CAA-CBA
4	L	275	BCL	C1A-C2A-CAA-CBA
6	M	311	U10	C41-C42-C43-C44
5	M	309	BPH	C11-C10-C8-C9
4	L	274	BCL	CAA-CBA-CGA-O2A
4	M	308	BCL	CAA-CBA-CGA-O1A

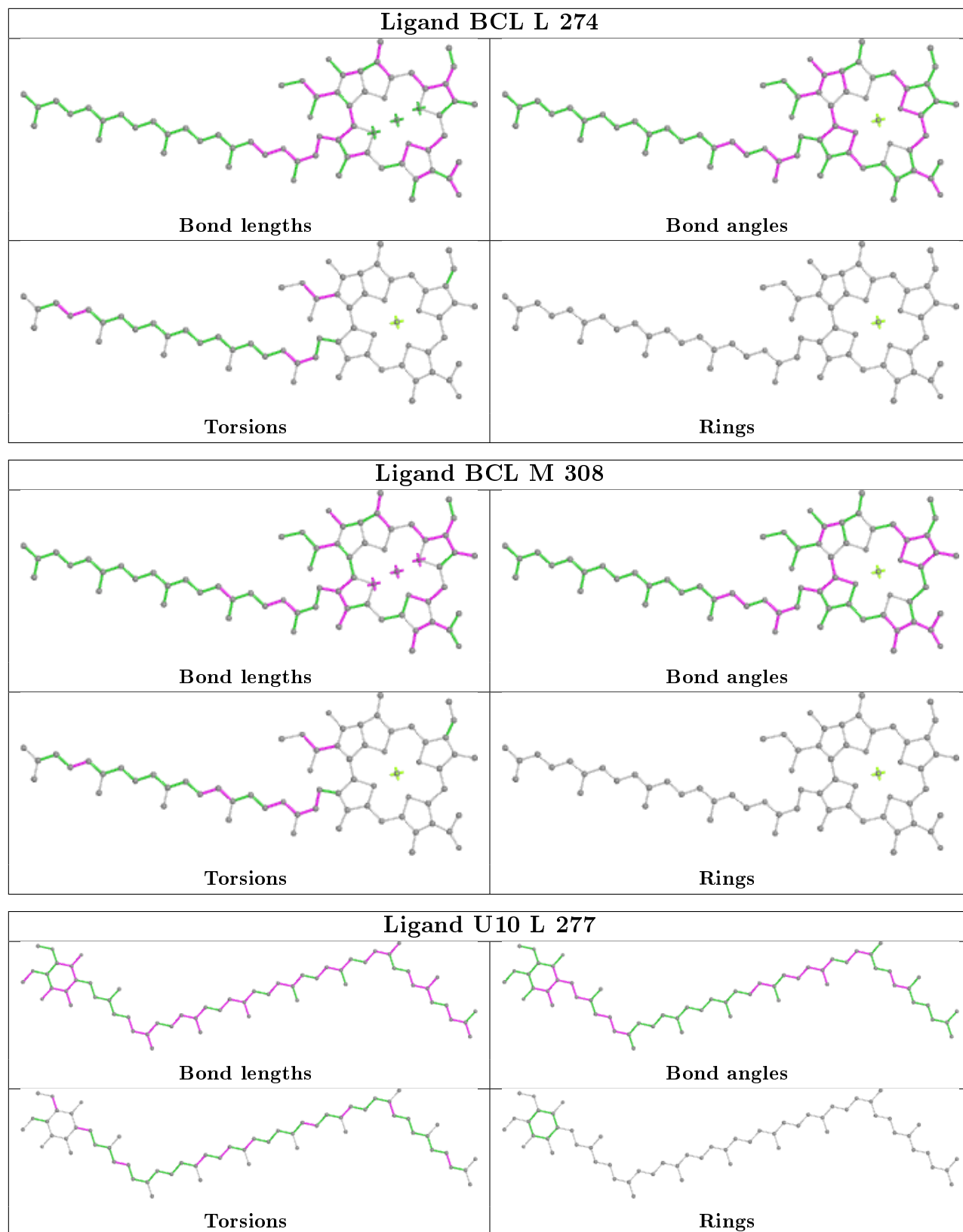
There are no ring outliers.

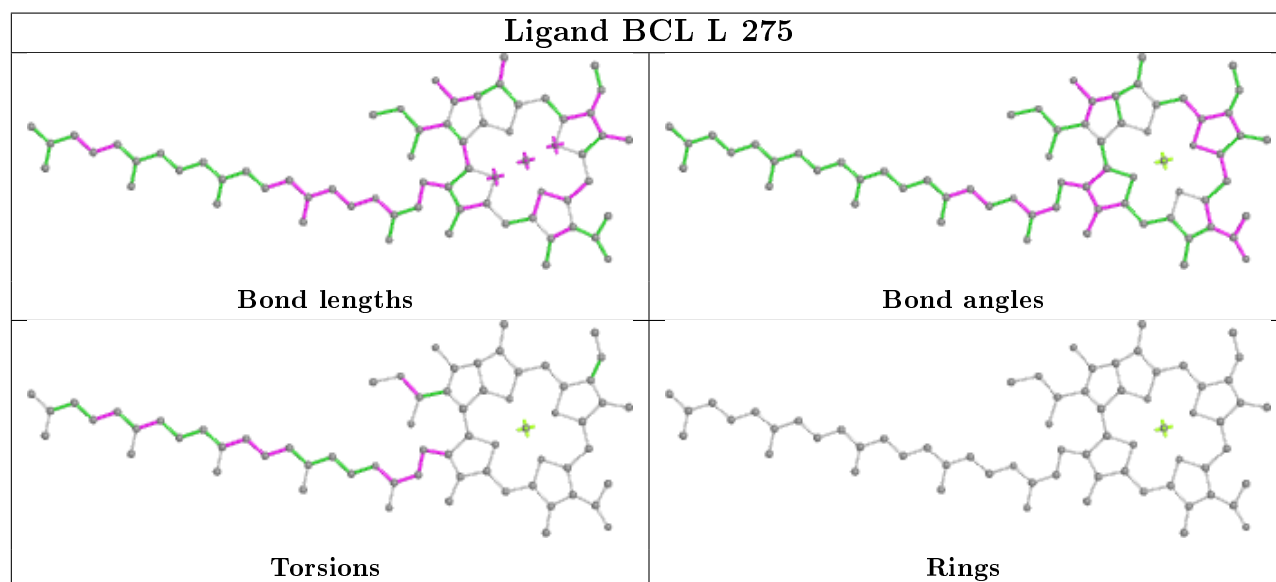
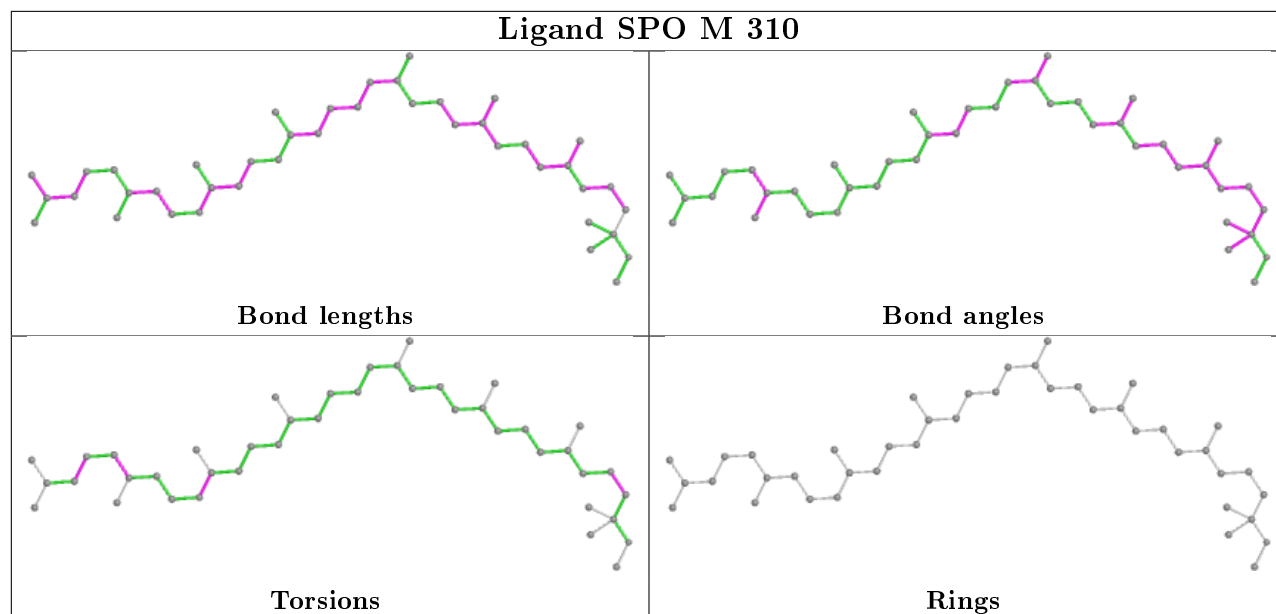
9 monomers are involved in 136 short contacts:

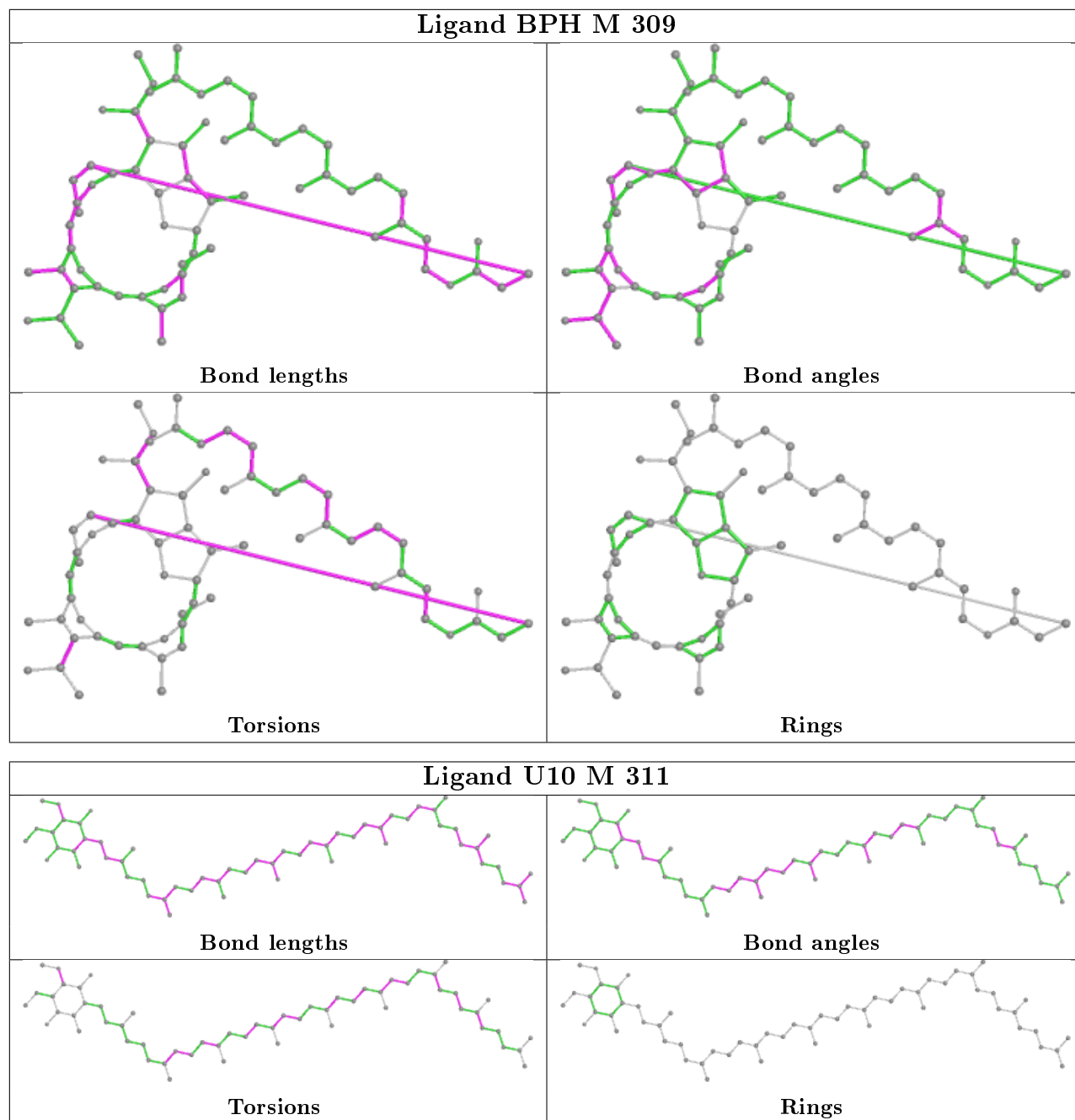
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	307	BCL	23	0
5	L	276	BPH	23	0
4	L	274	BCL	22	0
4	M	308	BCL	17	0
6	L	277	U10	16	0
8	M	310	SPO	13	0
4	L	275	BCL	9	0
5	M	309	BPH	11	0
6	M	311	U10	19	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	H	1
1	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	76:PRO	C	77:GLY	N	1.67
1	L	252:GLY	C	253:THR	N	1.01

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.