



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 07:23 am BST

PDB ID : 1PCR
Title : STRUCTURE OF THE PHOTOSYNTHETIC REACTION CENTRE FROM
RHODOBACTER SPHAEROIDES AT 2.65 ANGSTROMS RESOLUTION:
COFACTORS AND PROTEIN-COFACTOR INTERACTIONS
Authors : Ermler, U.; Fritzsche, G.; Michel, H.
Deposited on : 1994-11-10
Resolution : 2.65 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

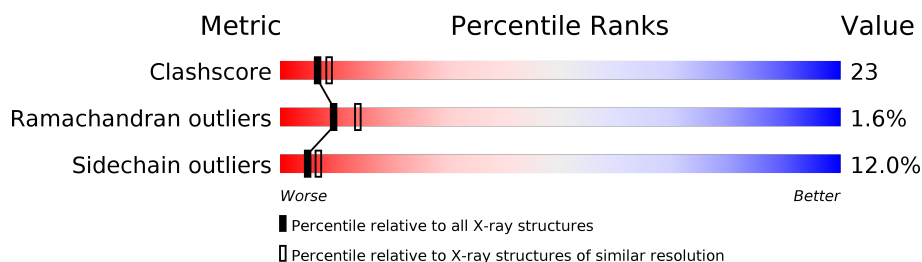
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)

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	281	
2	M	307	
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	301	X	-	-	-
4	BCL	L	304	X	-	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 7311 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.

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

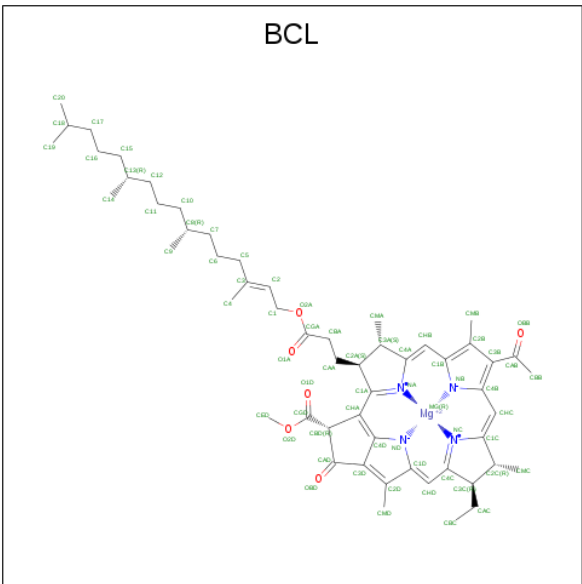
- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

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

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

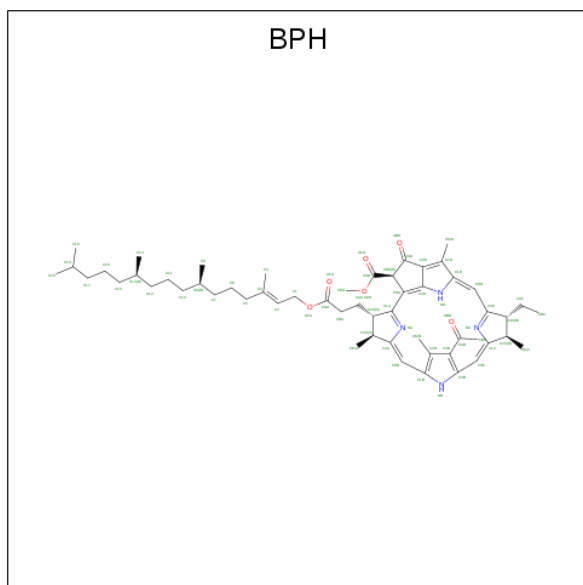
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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



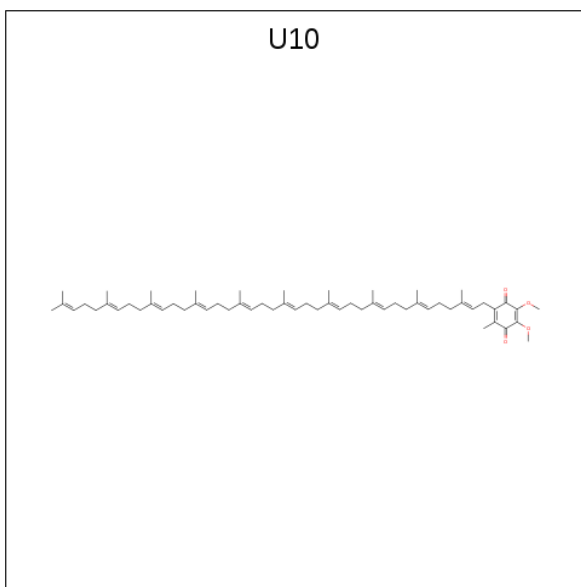
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



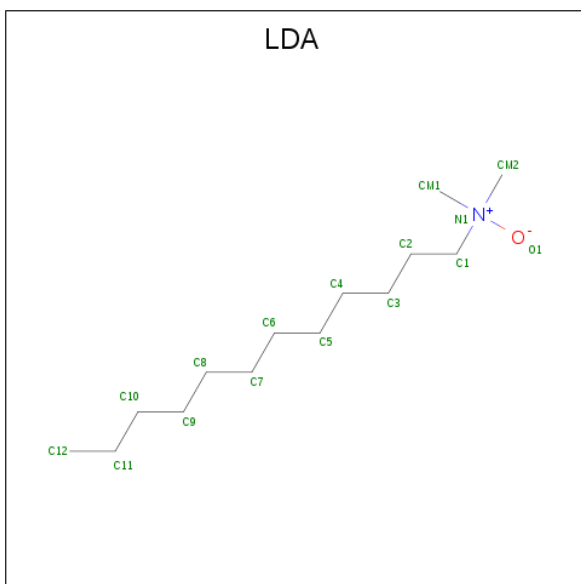
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

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

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



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

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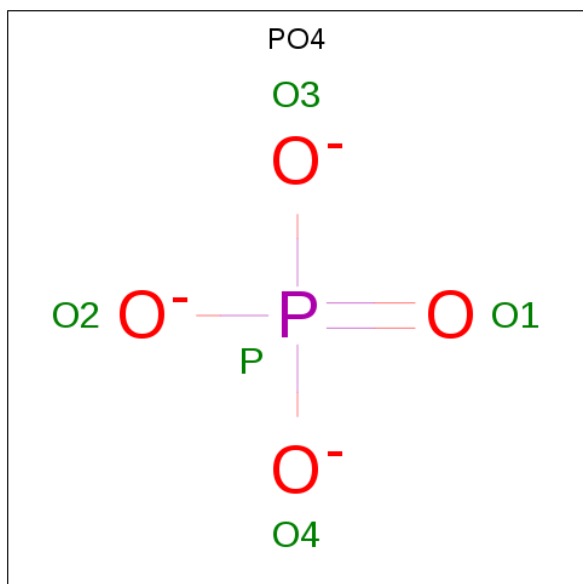
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0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

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

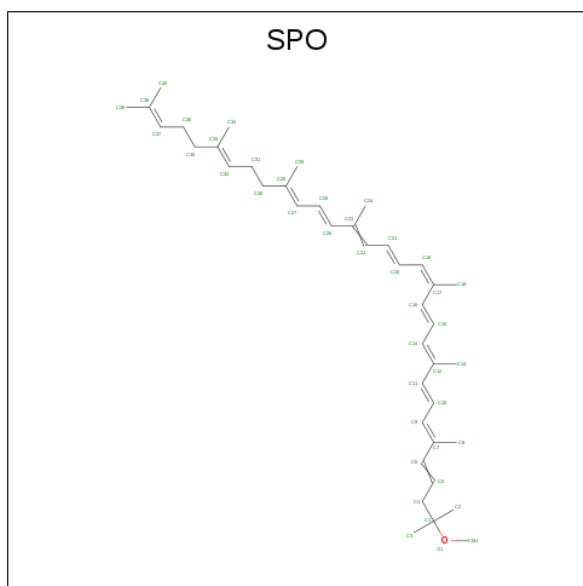
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 10 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	40	Total	O	0	0
			40	40		
11	M	50	Total	O	0	0
			50	50		
11	H	70	Total	O	0	0
			70	70		

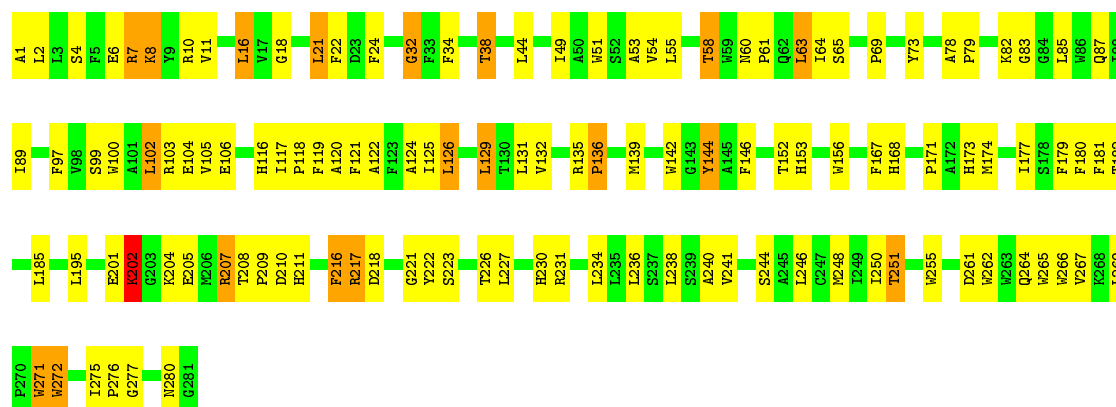
3 Residue-property plots

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.

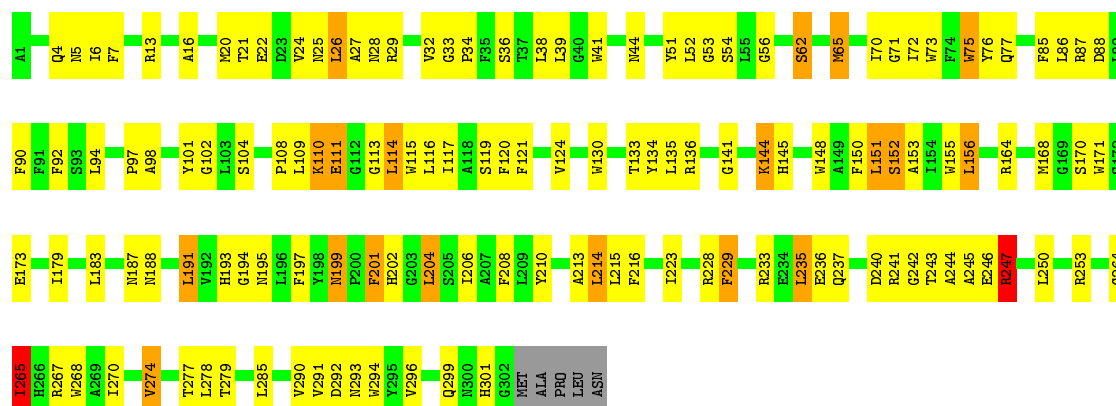
- Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain L: 57% 36% 7%



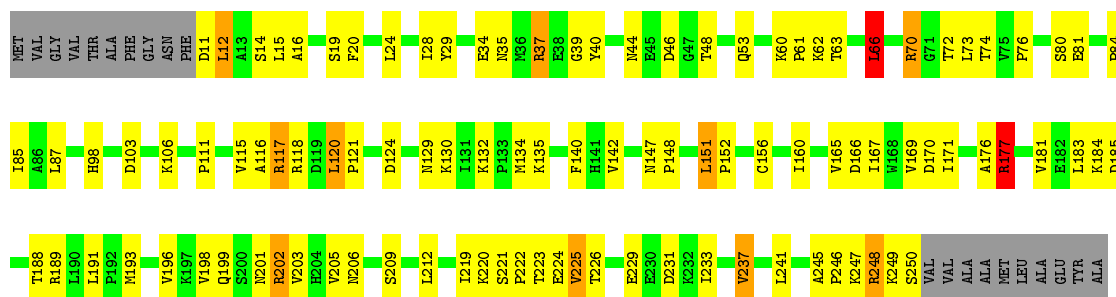
- Molecule 2: PHOTOSYNTHETIC REACTION CENTER

Chain M: 54% 38% 6%



- Molecule 3: PHOTOSYNTHETIC REACTION CENTER

Chain H:  53% 35% 8%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.30 Å 141.30 Å 187.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.65	Depositor
% Data completeness (in resolution range)	88.9 (10.00-2.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7311	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LDA, BPH, PO4, FE, SPO, U10

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L	0.64	0/2320	0.71	0/3175
2	M	0.61	0/2500	0.69	1/3413 (0.0%)
3	H	0.63	0/1877	0.74	0/2553
All	All	0.63	0/6697	0.71	1/9141 (0.0%)

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	6
2	M	0	4
3	H	0	4
All	All	0	14

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	M	156	LEU	CA-CB-CG	5.59	128.16	115.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	177	ARG	Sidechain
3	H	29	TYR	Sidechain
3	H	37	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	H	66	LEU	Peptide
1	L	103	ARG	Sidechain
1	L	144	TYR	Sidechain
1	L	167	PHE	Sidechain
1	L	216	PHE	Sidechain
1	L	32	GLY	Peptide
1	L	73	TYR	Sidechain
2	M	201	PHE	Sidechain
2	M	247	ARG	Sidechain
2	M	265	ILE	Mainchain
2	M	76	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2187	105	0
2	M	2408	0	2321	142	0
3	H	1829	0	1836	73	0
4	L	198	0	222	21	0
4	M	66	0	74	14	0
5	L	65	0	76	12	0
5	M	65	0	76	8	0
6	L	48	0	63	8	0
6	M	48	0	63	8	0
7	L	48	0	93	2	0
7	M	96	0	186	25	0
8	M	1	0	0	0	0
9	M	5	0	0	0	0
10	M	42	0	60	7	0
11	H	70	0	0	7	0
11	L	40	0	0	2	0
11	M	50	0	0	3	0
All	All	7311	0	7257	338	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 23.

All (338) 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)
4:M:801:BCL:HBB3	4:M:801:BCL:HHC	1.35	1.09
1:L:272:TRP:HA	1:L:275:ILE:HD13	1.39	1.01
2:M:119:SER:HB2	10:M:600:SPO:H342	1.47	0.93
3:H:44:ASN:HD22	3:H:48:THR:HB	1.36	0.89
1:L:182:THR:HG22	1:L:236:LEU:HD13	1.54	0.88
1:L:32:GLY:HA3	11:L:712:HOH:O	1.74	0.87
3:H:148:PRO:HA	3:H:151:LEU:HD22	1.56	0.86
2:M:204:LEU:HB3	2:M:279:THR:HG21	1.57	0.86
6:M:501:U10:H202	7:M:703:LDA:H112	1.58	0.86
4:L:301:BCL:HHC	4:L:301:BCL:HBB2	1.55	0.85
2:M:242:GLY:HA2	3:H:117:ARG:HD2	1.60	0.83
4:L:302:BCL:HBB2	4:M:801:BCL:NB	1.93	0.82
1:L:34:PHE:O	1:L:38:THR:HG23	1.80	0.80
5:L:402:BPH:HHC	5:L:402:BPH:HBB3	1.64	0.80
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.62	0.79
11:L:718:HOH:O	2:M:253:ARG:HD3	1.82	0.78
3:H:198:VAL:HA	3:H:203:VAL:HG22	1.64	0.77
4:L:301:BCL:HBB3	4:M:801:BCL:H41	1.67	0.76
1:L:179:PHE:CE1	6:L:502:U10:H18	2.21	0.76
2:M:197:PHE:CZ	4:M:801:BCL:HBB2	2.20	0.76
4:M:801:BCL:HHC	4:M:801:BCL:CBB	2.14	0.76
3:H:61:PRO:HA	3:H:76:PRO:HD2	1.69	0.74
1:L:7:ARG:HH11	3:H:98:HIS:CD2	2.06	0.74
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.69	0.73
4:L:301:BCL:HHC	4:L:301:BCL:CBB	2.18	0.73
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.70	0.72
7:M:706:LDA:H71	7:M:706:LDA:HM21	1.71	0.72
1:L:231:ARG:HD3	2:M:5:ASN:O	1.90	0.71
2:M:197:PHE:HZ	4:M:801:BCL:HBB2	1.53	0.71
2:M:72:ILE:HG13	2:M:73:TRP:N	2.05	0.70
2:M:153:ALA:HB2	5:M:401:BPH:HAC1	1.73	0.70
3:H:103:ASP:HB3	3:H:106:LYS:HB2	1.73	0.69
1:L:8:LYS:HA	3:H:87:LEU:HD11	1.73	0.69
3:H:169:VAL:HG23	3:H:171:ILE:HD12	1.73	0.69
7:M:706:LDA:HM21	7:M:706:LDA:H52	1.73	0.69
5:L:402:BPH:HBB2	2:M:210:TYR:HB3	1.75	0.69
2:M:243:THR:O	2:M:247:ARG:HG2	1.92	0.69
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.75	0.67
3:H:156:CYS:SG	3:H:248:ARG:HA	2.34	0.67
2:M:130:TRP:HD1	2:M:150:PHE:CD2	2.12	0.67
2:M:197:PHE:HZ	4:M:801:BCL:CBB	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:62:SER:HA	2:M:65:MET:HB2	1.77	0.66
4:L:301:BCL:HMD2	4:L:302:BCL:OBB	1.95	0.66
1:L:182:THR:HG22	1:L:236:LEU:CD1	2.26	0.65
1:L:51:TRP:O	1:L:54:VAL:HG22	1.97	0.65
2:M:13:ARG:O	3:H:140:PHE:HA	1.98	0.64
10:M:600:SPO:H5	10:M:600:SPO:HM13	1.79	0.64
1:L:38:THR:HG22	1:L:99:SER:HB3	1.79	0.63
2:M:193:HIS:O	2:M:293:ASN:HA	1.97	0.63
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.34	0.63
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.81	0.63
1:L:208:THR:HB	1:L:209:PRO:HD2	1.80	0.63
5:L:402:BPH:CBB	2:M:210:TYR:HB3	2.29	0.62
1:L:7:ARG:NH1	3:H:98:HIS:CD2	2.66	0.62
1:L:69:PRO:HB3	1:L:78:ALA:HB2	1.80	0.62
2:M:90:PHE:HD1	2:M:179:ILE:HD13	1.65	0.62
3:H:233:ILE:O	3:H:237:VAL:HG13	1.99	0.62
2:M:102:GLY:HA2	2:M:170:SER:CB	2.30	0.62
2:M:130:TRP:HD1	2:M:150:PHE:HD2	1.46	0.62
1:L:230:HIS:CD2	2:M:223:ILE:HG13	2.35	0.62
1:L:201:GLU:O	1:L:202:LYS:HB2	2.00	0.61
1:L:265:TRP:CH2	1:L:266:TRP:HE3	2.18	0.61
1:L:269:LEU:HB2	1:L:272:TRP:NE1	2.15	0.61
1:L:181:PHE:CD2	5:M:401:BPH:HBB1	2.35	0.61
1:L:168:HIS:HB3	2:M:183:LEU:HD13	1.80	0.61
1:L:244:SER:OG	4:L:302:BCL:HMA2	2.01	0.60
2:M:253:ARG:NH2	7:M:703:LDA:HM12	2.15	0.60
2:M:119:SER:HB3	10:M:600:SPO:H311	1.84	0.60
1:L:135:ARG:NH1	1:L:251:THR:HG22	2.17	0.59
2:M:120:PHE:O	2:M:124:VAL:HG13	2.03	0.59
1:L:38:THR:HG22	1:L:99:SER:CB	2.32	0.59
7:L:708:LDA:H92	7:L:708:LDA:H51	1.85	0.59
3:H:156:CYS:HB3	3:H:206:ASN:O	2.02	0.58
2:M:242:GLY:CA	3:H:117:ARG:HD2	2.31	0.58
1:L:202:LYS:C	1:L:204:LYS:H	2.05	0.58
2:M:152:SER:O	2:M:155:TRP:HB3	2.04	0.58
2:M:208:PHE:HE1	7:M:701:LDA:H91	1.68	0.58
1:L:116:HIS:O	1:L:119:PHE:HB3	2.04	0.58
3:H:129:ASN:ND2	3:H:224:GLU:HG3	2.19	0.58
1:L:8:LYS:HA	3:H:87:LEU:CD1	2.33	0.57
3:H:132:LYS:HB2	3:H:171:ILE:HD11	1.86	0.57
2:M:270:ILE:O	2:M:274:VAL:HB	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:269:LEU:HD12	1:L:272:TRP:CZ2	2.39	0.57
2:M:114:LEU:HD21	7:M:706:LDA:HM13	1.86	0.57
2:M:301:HIS:N	2:M:301:HIS:CD2	2.73	0.57
3:H:70:ARG:NH2	3:H:121:PRO:O	2.37	0.57
1:L:231:ARG:HD2	2:M:6:ILE:O	2.05	0.57
3:H:66:LEU:HD12	3:H:118:ARG:NH2	2.20	0.56
2:M:90:PHE:CD1	2:M:179:ILE:HD13	2.40	0.56
1:L:180:PHE:CE2	1:L:240:ALA:HB1	2.40	0.56
5:M:401:BPH:HBB3	5:M:401:BPH:HHC	1.85	0.56
1:L:241:VAL:HG21	5:L:402:BPH:HAC2	1.87	0.56
7:M:706:LDA:H72	7:M:706:LDA:HM11	1.87	0.56
3:H:202:ARG:HG2	3:H:203:VAL:N	2.19	0.56
1:L:85:LEU:O	1:L:89:ILE:HG13	2.06	0.56
2:M:164:ARG:NH1	2:M:173:GLU:HG3	2.20	0.56
4:L:301:BCL:H51	5:M:401:BPH:HMB2	1.88	0.56
3:H:66:LEU:N	3:H:66:LEU:HD23	2.21	0.55
2:M:130:TRP:CD1	2:M:150:PHE:HD2	2.23	0.55
7:M:703:LDA:HM12	3:H:40:TYR:OH	2.06	0.55
2:M:24:VAL:HG11	2:M:29:ARG:NH1	2.21	0.55
2:M:65:MET:HB3	2:M:121:PHE:CD2	2.42	0.54
6:M:501:U10:H202	7:M:703:LDA:C11	2.33	0.54
5:L:402:BPH:HMC3	2:M:213:ALA:HB3	1.90	0.54
3:H:118:ARG:HD2	11:H:311:HOH:O	2.07	0.54
1:L:181:PHE:HB3	5:M:401:BPH:CBB	2.38	0.54
4:L:301:BCL:H72	4:M:801:BCL:H203	1.89	0.54
3:H:148:PRO:HA	3:H:151:LEU:CD2	2.34	0.53
7:M:706:LDA:H12	7:M:706:LDA:H52	1.90	0.53
3:H:11:ASP:HB2	11:H:323:HOH:O	2.08	0.53
2:M:24:VAL:HG21	2:M:29:ARG:HH12	1.74	0.53
4:L:302:BCL:H203	4:L:304:BCL:H102	1.91	0.53
5:L:402:BPH:CHC	5:L:402:BPH:HBB3	2.36	0.53
2:M:85:PHE:HD2	2:M:86:LEU:HD12	1.74	0.53
3:H:20:PHE:HE2	3:H:24:LEU:HD22	1.74	0.52
1:L:250:ILE:HD12	6:L:502:U10:H402	1.91	0.52
1:L:269:LEU:HD12	1:L:272:TRP:HZ2	1.74	0.52
1:L:4:SER:OG	3:H:39:GLY:HA2	2.09	0.52
2:M:102:GLY:HA2	2:M:170:SER:HB2	1.91	0.52
7:M:701:LDA:H101	7:M:703:LDA:C12	2.39	0.52
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.09	0.52
4:L:301:BCL:H72	4:M:801:BCL:C20	2.40	0.52
1:L:195:LEU:HB3	2:M:145:HIS:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:108:PRO:HG2	2:M:111:GLU:CB	2.40	0.52
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.44	0.52
2:M:32:VAL:HG12	2:M:33:GLY:O	2.10	0.52
3:H:245:ALA:N	3:H:246:PRO:HD2	2.25	0.52
1:L:202:LYS:C	1:L:204:LYS:N	2.63	0.52
1:L:201:GLU:HG3	2:M:141:GLY:C	2.30	0.52
6:L:502:U10:H122	7:M:702:LDA:H92	1.92	0.52
4:L:301:BCL:HBB3	4:M:801:BCL:C4	2.38	0.51
2:M:152:SER:HB2	2:M:274:VAL:HG22	1.91	0.51
2:M:77:GLN:NE2	2:M:92:PHE:CD1	2.77	0.51
1:L:267:VAL:HG23	2:M:87:ARG:HG2	1.92	0.51
2:M:21:THR:HG23	2:M:26:LEU:CD1	2.40	0.51
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.45	0.51
2:M:25:ASN:OD1	2:M:27:ALA:HB3	2.10	0.51
1:L:271:TRP:CD1	1:L:271:TRP:N	2.79	0.51
2:M:41:TRP:CB	7:M:702:LDA:HM21	2.39	0.51
2:M:134:TYR:CE2	2:M:144:LYS:HG2	2.46	0.51
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.46	0.51
3:H:63:THR:HA	3:H:73:LEU:O	2.10	0.51
2:M:119:SER:CB	10:M:600:SPO:H342	2.31	0.50
1:L:135:ARG:NH1	1:L:251:THR:O	2.45	0.50
2:M:199:ASN:HD22	2:M:199:ASN:C	2.15	0.50
2:M:237:GLN:HE22	2:M:242:GLY:HA3	1.77	0.50
5:L:402:BPH:HMC3	2:M:213:ALA:CB	2.42	0.50
2:M:241:ARG:HD3	2:M:246:GLU:HG2	1.94	0.49
1:L:16:LEU:N	1:L:106:GLU:OE2	2.44	0.49
2:M:236:GLU:HB3	11:H:270:HOH:O	2.11	0.49
2:M:301:HIS:H	2:M:301:HIS:CD2	2.30	0.49
2:M:247:ARG:NH2	3:H:111:PRO:O	2.46	0.49
2:M:75:TRP:HZ3	10:M:600:SPO:O1	1.95	0.49
2:M:197:PHE:CZ	4:M:801:BCL:CBB	2.89	0.49
4:L:302:BCL:HAA2	4:L:304:BCL:HAC1	1.93	0.49
2:M:113:GLY:HA2	2:M:116:LEU:HD23	1.95	0.49
2:M:253:ARG:HH22	7:M:703:LDA:HM12	1.78	0.49
2:M:77:GLN:HE22	2:M:92:PHE:HA	1.76	0.49
1:L:264:GLN:O	1:L:267:VAL:HG12	2.13	0.49
1:L:280:ASN:HD22	2:M:88:ASP:CG	2.16	0.49
1:L:102:LEU:O	1:L:105:VAL:HB	2.13	0.48
3:H:44:ASN:HB2	3:H:46:ASP:OD1	2.12	0.48
2:M:88:ASP:HB2	2:M:92:PHE:CZ	2.48	0.48
1:L:135:ARG:HB3	1:L:136:PRO:CD	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:227:LEU:O	1:L:231:ARG:HG3	2.13	0.48
3:H:170:ASP:OD2	3:H:177:ARG:NH1	2.46	0.48
1:L:234:LEU:O	1:L:238:LEU:HG	2.13	0.48
1:L:201:GLU:O	1:L:202:LYS:CB	2.62	0.48
6:M:501:U10:H322	6:M:501:U10:H28	1.64	0.48
2:M:164:ARG:NH1	2:M:173:GLU:CG	2.77	0.48
2:M:241:ARG:HD3	2:M:246:GLU:CG	2.43	0.48
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.14	0.48
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.95	0.48
2:M:278:LEU:HD13	7:M:705:LDA:H102	1.96	0.48
3:H:206:ASN:O	3:H:248:ARG:NH1	2.47	0.48
6:L:502:U10:H122	7:M:702:LDA:C9	2.44	0.48
1:L:277:GLY:O	2:M:87:ARG:NH2	2.47	0.47
3:H:20:PHE:CE2	3:H:24:LEU:HD22	2.48	0.47
3:H:177:ARG:O	3:H:193:MET:HB2	2.14	0.47
3:H:199:GLN:OE1	3:H:202:ARG:HD2	2.14	0.47
1:L:171:PRO:HA	1:L:174:MET:HG3	1.96	0.47
5:L:402:BPH:H6C2	5:L:402:BPH:H2	1.66	0.47
4:L:302:BCL:HBB2	4:M:801:BCL:C1B	2.43	0.47
1:L:65:SER:CB	1:L:152:THR:HG21	2.44	0.47
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.82	0.47
2:M:21:THR:HG22	2:M:21:THR:O	2.13	0.47
5:L:402:BPH:CMC	2:M:213:ALA:HB3	2.45	0.47
3:H:117:ARG:HA	11:H:290:HOH:O	2.13	0.47
4:L:304:BCL:HMD1	2:M:206:ILE:HD13	1.96	0.47
1:L:6:GLU:OE2	1:L:10:ARG:NH1	2.44	0.47
2:M:268:TRP:CD1	6:M:501:U10:H111	2.50	0.47
7:M:701:LDA:H101	7:M:703:LDA:H121	1.97	0.47
2:M:75:TRP:CZ3	10:M:600:SPO:O1	2.67	0.47
2:M:20:MET:O	2:M:29:ARG:NH2	2.48	0.47
2:M:265:ILE:HG21	6:M:501:U10:H3M3	1.97	0.46
3:H:70:ARG:NH2	3:H:120:LEU:CB	2.79	0.46
1:L:146:PHE:HA	1:L:156:TRP:CD1	2.50	0.46
2:M:187:ASN:HA	4:M:801:BCL:CB	2.45	0.46
1:L:58:THR:HG21	1:L:63:LEU:HD23	1.97	0.46
2:M:44:ASN:HB3	11:M:812:HOH:O	2.14	0.46
3:H:183:LEU:HD11	3:H:189:ARG:HG2	1.98	0.46
2:M:70:ILE:O	2:M:73:TRP:HB3	2.15	0.46
2:M:267:ARG:HD2	3:H:34:GLU:HG2	1.98	0.46
2:M:242:GLY:HA2	3:H:117:ARG:CD	2.38	0.46
1:L:53:ALA:HB2	1:L:64:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:60:ASN:HA	1:L:61:PRO:HD3	1.75	0.46
3:H:142:VAL:HG21	3:H:147:ASN:ND2	2.31	0.46
3:H:148:PRO:HG2	3:H:167:ILE:HD11	1.98	0.46
3:H:16:ALA:O	3:H:19:SER:HB2	2.16	0.46
3:H:241:LEU:O	3:H:248:ARG:NH2	2.49	0.46
1:L:124:ALA:HB2	5:L:402:BPH:HAC1	1.97	0.46
1:L:22:PHE:HA	1:L:24:PHE:HE2	1.80	0.46
2:M:194:GLY:O	2:M:195:ASN:HB3	2.14	0.46
2:M:199:ASN:HD22	2:M:201:PHE:H	1.62	0.46
2:M:130:TRP:NE1	2:M:151:LEU:HD22	2.30	0.46
1:L:11:VAL:HB	11:H:286:HOH:O	2.16	0.45
1:L:177:ILE:HG23	4:L:302:BCL:HMB3	1.98	0.45
5:L:402:BPH:HMC2	2:M:214:LEU:N	2.30	0.45
2:M:114:LEU:HD23	2:M:117:ILE:HD12	1.97	0.45
2:M:240:ASP:O	3:H:117:ARG:NH1	2.50	0.45
3:H:219:ILE:HG21	3:H:225:VAL:HG13	1.99	0.45
2:M:29:ARG:HA	2:M:51:TYR:HA	1.98	0.45
1:L:100:TRP:CH2	6:M:501:U10:H251	2.52	0.45
6:L:502:U10:H372	6:L:502:U10:H351	1.70	0.45
1:L:79:PRO:HD2	1:L:82:LYS:HB2	1.97	0.45
1:L:8:LYS:NZ	3:H:81:GLU:OE1	2.47	0.45
1:L:217:ARG:O	1:L:221:GLY:HA2	2.17	0.45
1:L:222:TYR:CG	1:L:223:SER:N	2.84	0.45
1:L:135:ARG:HH12	1:L:251:THR:HG22	1.80	0.45
5:M:401:BPH:HBB3	5:M:401:BPH:CHC	2.47	0.45
2:M:24:VAL:HG13	2:M:51:TYR:CD2	2.51	0.45
5:L:402:BPH:HBB1	2:M:210:TYR:CD2	2.52	0.45
2:M:4:GLN:HB3	2:M:6:ILE:CD1	2.47	0.45
1:L:129:LEU:HD12	1:L:129:LEU:HA	1.67	0.45
3:H:241:LEU:HA	3:H:248:ARG:NH2	2.33	0.44
1:L:218:ASP:OD1	2:M:29:ARG:HD3	2.17	0.44
3:H:62:LYS:O	3:H:74:THR:HA	2.17	0.44
1:L:2:LEU:N	1:L:2:LEU:HD23	2.32	0.44
1:L:54:VAL:HG23	1:L:55:LEU:N	2.33	0.44
2:M:151:LEU:HA	2:M:151:LEU:HD13	1.65	0.44
2:M:24:VAL:HG11	2:M:29:ARG:CZ	2.47	0.44
2:M:152:SER:CB	2:M:274:VAL:HG22	2.47	0.44
3:H:70:ARG:NH2	3:H:120:LEU:HB2	2.32	0.44
6:L:502:U10:H271	6:L:502:U10:H251	1.79	0.44
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.99	0.44
3:H:181:VAL:O	3:H:188:THR:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.48	0.44
2:M:228:ARG:HG3	2:M:229:PHE:CE1	2.53	0.44
2:M:41:TRP:CD1	7:M:702:LDA:HM11	2.53	0.44
2:M:98:ALA:HB3	2:M:101:TYR:CE1	2.52	0.44
2:M:148:TRP:HB3	7:M:705:LDA:H61	2.00	0.44
2:M:53:GLY:O	2:M:56:GLY:N	2.51	0.44
3:H:209:SER:OG	3:H:212:LEU:HD12	2.17	0.43
2:M:135:LEU:HD23	2:M:135:LEU:HA	1.83	0.43
2:M:41:TRP:HA	2:M:41:TRP:CE3	2.53	0.43
1:L:122:ALA:O	1:L:126:LEU:HB2	2.18	0.43
1:L:131:LEU:HD21	1:L:248:MET:HG3	2.00	0.43
2:M:134:TYR:CD1	2:M:134:TYR:C	2.91	0.43
3:H:176:ALA:O	3:H:193:MET:HG2	2.18	0.43
3:H:148:PRO:CG	3:H:167:ILE:HD11	2.48	0.43
1:L:131:LEU:HB2	1:L:146:PHE:HE1	1.83	0.43
2:M:4:GLN:HB3	2:M:6:ILE:HD12	1.99	0.43
7:M:705:LDA:H31	7:M:705:LDA:H61	1.83	0.43
3:H:130:LYS:HD2	11:H:284:HOH:O	2.18	0.43
1:L:117:ILE:HB	1:L:118:PRO:HD3	2.01	0.43
2:M:164:ARG:O	2:M:168:MET:HG2	2.18	0.43
2:M:235:LEU:HD12	2:M:235:LEU:HA	1.62	0.43
2:M:245:ALA:HB1	11:M:807:HOH:O	2.18	0.43
3:H:60:LYS:HA	3:H:61:PRO:HD3	1.78	0.43
1:L:264:GLN:HA	1:L:267:VAL:HG12	2.00	0.43
1:L:261:ASP:O	1:L:264:GLN:HB2	2.19	0.43
2:M:94:LEU:HD21	2:M:115:TRP:HA	2.00	0.43
2:M:130:TRP:CZ2	2:M:151:LEU:HD21	2.53	0.43
2:M:197:PHE:CE1	4:M:801:BCL:HBB2	2.53	0.43
1:L:223:SER:OG	6:L:502:U10:H3M1	2.19	0.42
1:L:85:LEU:HD23	1:L:85:LEU:HA	1.89	0.42
2:M:265:ILE:HG21	6:M:501:U10:C3M	2.49	0.42
3:H:84:PRO:C	3:H:85:ILE:HD13	2.39	0.42
7:L:707:LDA:H42	7:L:707:LDA:H71	1.88	0.42
2:M:110:LYS:HE3	2:M:110:LYS:HB2	1.69	0.42
2:M:130:TRP:HE1	2:M:151:LEU:HD22	1.84	0.42
3:H:152:PRO:HB2	3:H:160:ILE:HD13	2.00	0.42
2:M:191:LEU:HD13	2:M:191:LEU:HA	1.59	0.42
3:H:37:ARG:HH21	3:H:61:PRO:HA	1.84	0.42
1:L:121:PHE:CE2	1:L:125:ILE:HD11	2.55	0.42
1:L:223:SER:O	2:M:44:ASN:HB2	2.20	0.42
4:L:302:BCL:H162	4:L:302:BCL:H141	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:16:ALA:HB1	2:M:32:VAL:HG21	2.02	0.42
2:M:41:TRP:HB3	7:M:702:LDA:HM21	2.02	0.42
1:L:132:VAL:HG13	1:L:146:PHE:CE1	2.55	0.42
2:M:134:TYR:CD2	2:M:144:LYS:HG2	2.55	0.42
3:H:248:ARG:HB2	3:H:248:ARG:CZ	2.49	0.42
1:L:255:TRP:CZ2	1:L:262:TRP:HB2	2.55	0.42
1:L:265:TRP:CE3	1:L:266:TRP:HA	2.54	0.42
1:L:49:ILE:HG12	1:L:89:ILE:HD13	2.02	0.42
3:H:134:MET:HB2	3:H:167:ILE:O	2.19	0.41
2:M:71:GLY:HA3	10:M:600:SPO:C6	2.50	0.41
1:L:97:PHE:CE1	4:L:302:BCL:H121	2.55	0.41
7:M:703:LDA:HM11	7:M:703:LDA:H22	1.80	0.41
3:H:98:HIS:HE1	11:H:276:HOH:O	2.03	0.41
1:L:1:ALA:C	1:L:2:LEU:HD23	2.41	0.41
4:L:301:BCL:CHC	4:L:301:BCL:CBB	2.92	0.41
2:M:25:ASN:OD1	2:M:25:ASN:C	2.58	0.41
2:M:36:SER:OG	2:M:38:LEU:HB3	2.20	0.41
2:M:7:PHE:CE1	7:M:702:LDA:HM22	2.55	0.41
3:H:148:PRO:HD2	3:H:167:ILE:HD11	2.02	0.41
1:L:120:ALA:HB1	1:L:238:LEU:HD21	2.01	0.41
2:M:77:GLN:NE2	2:M:92:PHE:HB3	2.35	0.41
2:M:101:TYR:HB3	2:M:104:SER:HB3	2.03	0.41
3:H:165:VAL:O	3:H:166:ASP:HB2	2.21	0.41
2:M:265:ILE:HG12	6:M:501:U10:C2	2.51	0.41
2:M:296:VAL:O	2:M:299:GLN:HB2	2.20	0.41
3:H:103:ASP:OD2	3:H:106:LYS:HD3	2.21	0.41
3:H:12:LEU:HD13	3:H:15:LEU:HD23	2.02	0.41
1:L:18:GLY:O	1:L:21:LEU:HB2	2.21	0.41
4:L:304:BCL:H122	4:L:304:BCL:H161	1.80	0.41
1:L:204:LYS:HE3	1:L:204:LYS:HB2	1.79	0.41
7:M:705:LDA:HM13	11:M:803:HOH:O	2.21	0.41
2:M:291:VAL:HG11	2:M:294:TRP:CD2	2.56	0.41
4:L:304:BCL:H202	4:L:304:BCL:H162	1.85	0.41
1:L:97:PHE:CZ	4:L:302:BCL:H121	2.56	0.41
1:L:139:MET:HB3	1:L:144:TYR:CD2	2.56	0.40
1:L:69:PRO:HD3	1:L:83:GLY:O	2.21	0.40
1:L:104:GLU:HB3	1:L:118:PRO:HG3	2.03	0.40
1:L:65:SER:HB2	1:L:152:THR:HG21	2.03	0.40
1:L:208:THR:O	1:L:211:HIS:HB2	2.21	0.40
1:L:21:LEU:HD13	1:L:22:PHE:CE1	2.56	0.40
2:M:98:ALA:HB3	2:M:101:TYR:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:208:PHE:CE1	7:M:701:LDA:H91	2.53	0.40
1:L:216:PHE:CE1	6:L:502:U10:H4M2	2.56	0.40
1:L:217:ARG:HD3	1:L:217:ARG:HH11	1.76	0.40
2:M:164:ARG:HH12	2:M:173:GLU:CG	2.34	0.40
2:M:36:SER:HB3	2:M:39:LEU:HB2	2.03	0.40
5:M:401:BPH:H6C2	5:M:401:BPH:H102	1.96	0.40
3:H:247:LYS:O	3:H:249:LYS:N	2.55	0.40
3:H:84:PRO:O	3:H:85:ILE:HD13	2.21	0.40
2:M:277:THR:CG2	5:M:401:BPH:HAC2	2.52	0.40
2:M:28:ASN:HB3	2:M:52:LEU:O	2.21	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%)	261 (94%)	15 (5%)	3 (1%)	14	21
2	M	300/307 (98%)	278 (93%)	18 (6%)	4 (1%)	12	18
3	H	238/260 (92%)	215 (90%)	17 (7%)	6 (2%)	5	7
All	All	817/848 (96%)	754 (92%)	50 (6%)	13 (2%)	9	14

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	202	LYS
2	M	54	SER
3	H	116	ALA
1	L	207	ARG
3	H	124	ASP
3	H	185	ASP
3	H	248	ARG

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Mol	Chain	Res	Type
2	M	22	GLU
3	H	201	ASN
2	M	290	VAL
1	L	276	PRO
3	H	222	PRO
2	M	34	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	220/220 (100%)	196 (89%)	24 (11%)	6	9
2	M	236/240 (98%)	206 (87%)	30 (13%)	4	6
3	H	195/208 (94%)	171 (88%)	24 (12%)	4	6
All	All	651/668 (98%)	573 (88%)	78 (12%)	5	7

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	ARG
1	L	8	LYS
1	L	16	LEU
1	L	21	LEU
1	L	38	THR
1	L	44	LEU
1	L	58	THR
1	L	63	LEU
1	L	102	LEU
1	L	126	LEU
1	L	129	LEU
1	L	136	PRO
1	L	153	HIS
1	L	185	LEU
1	L	202	LYS
1	L	205	GLU

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Mol	Chain	Res	Type
1	L	207	ARG
1	L	210	ASP
1	L	217	ARG
1	L	226	THR
1	L	246	LEU
1	L	251	THR
1	L	271	TRP
1	L	272	TRP
2	M	26	LEU
2	M	62	SER
2	M	65	MET
2	M	75	TRP
2	M	109	LEU
2	M	110	LYS
2	M	111	GLU
2	M	114	LEU
2	M	133	THR
2	M	136	ARG
2	M	144	LYS
2	M	151	LEU
2	M	152	SER
2	M	156	LEU
2	M	188	ASN
2	M	191	LEU
2	M	199	ASN
2	M	204	LEU
2	M	214	LEU
2	M	215	LEU
2	M	216	PHE
2	M	229	PHE
2	M	233	ARG
2	M	235	LEU
2	M	247	ARG
2	M	250	LEU
2	M	265	ILE
2	M	274	VAL
2	M	285	LEU
2	M	292	ASP
3	H	12	LEU
3	H	14	SER
3	H	28	ILE
3	H	53	GLN

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Mol	Chain	Res	Type
3	H	66	LEU
3	H	70	ARG
3	H	72	THR
3	H	80	SER
3	H	115	VAL
3	H	117	ARG
3	H	120	LEU
3	H	135	LYS
3	H	151	LEU
3	H	177	ARG
3	H	184	LYS
3	H	191	LEU
3	H	202	ARG
3	H	220	LYS
3	H	221	SER
3	H	223	THR
3	H	225	VAL
3	H	231	ASP
3	H	237	VAL
3	H	250	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	159	ASN
1	L	183	ASN
1	L	280	ASN
2	M	44	ASN
2	M	77	GLN
2	M	193	HIS
2	M	199	ASN
2	M	301	HIS
3	H	44	ASN
3	H	68	HIS
3	H	98	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\# Z > 2$
5	BPH	L	402	-	64,70,70	1.18	4 (6%)	76,101,101	1.61	15 (19%)
7	LDA	M	704	-	12,15,15	2.06	1 (8%)	14,17,17	0.52	0
4	BCL	L	302	1,4	58,74,74	1.61	10 (17%)	69,115,115	2.49	14 (20%)
6	U10	M	501	-	48,48,63	2.45	21 (43%)	58,61,79	1.30	7 (12%)
7	LDA	M	701	-	12,15,15	2.57	1 (8%)	14,17,17	0.40	0
4	BCL	L	301	2	58,74,74	1.49	8 (13%)	69,115,115	2.12	12 (17%)
7	LDA	M	705	-	12,15,15	2.23	1 (8%)	14,17,17	0.57	0
7	LDA	L	709	-	12,15,15	2.43	1 (8%)	14,17,17	0.49	0
4	BCL	L	304	1	58,74,74	1.38	8 (13%)	69,115,115	2.75	15 (21%)
7	LDA	L	707	-	12,15,15	2.33	1 (8%)	14,17,17	0.44	0
9	PO4	M	800	-	4,4,4	1.93	1 (25%)	6,6,6	0.90	0
7	LDA	M	702	-	12,15,15	2.54	1 (8%)	14,17,17	0.52	0
4	BCL	M	801	2,4	58,74,74	1.30	7 (12%)	69,115,115	1.94	14 (20%)
7	LDA	M	703	-	12,15,15	2.41	1 (8%)	14,17,17	0.65	0
7	LDA	M	706	-	12,15,15	2.37	1 (8%)	14,17,17	0.48	0
7	LDA	L	708	-	12,15,15	2.20	1 (8%)	14,17,17	0.45	0
5	BPH	M	401	-	64,70,70	1.24	8 (12%)	76,101,101	1.67	12 (15%)
10	SPO	M	600	-	40,41,41	3.46	23 (57%)	47,50,50	2.08	15 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	U10	L	502	-	48,48,63	2.15	20 (41%)	58,61,79	1.01	3 (5%)

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
5	BPH	L	402	-	-	12/54/105/105	0/5/6/6
7	LDA	M	704	-	-	2/13/13/13	-
4	BCL	L	302	1,4	-	6/37/137/137	-
6	U10	M	501	-	-	10/45/69/87	0/1/1/1
7	LDA	M	701	-	-	8/13/13/13	-
4	BCL	L	301	2	2/2/21/25	12/37/137/137	-
7	LDA	M	705	-	-	7/13/13/13	-
7	LDA	L	709	-	-	4/13/13/13	-
4	BCL	L	304	1	1/1/21/25	10/37/137/137	-
7	LDA	L	707	-	-	7/13/13/13	-
7	LDA	M	702	-	-	4/13/13/13	-
4	BCL	M	801	2,4	-	8/37/137/137	-
7	LDA	M	703	-	-	5/13/13/13	-
7	LDA	M	706	-	-	7/13/13/13	-
7	LDA	L	708	-	-	5/13/13/13	-
5	BPH	M	401	-	-	19/54/105/105	0/5/6/6
10	SPO	M	600	-	-	15/47/47/47	-
6	U10	L	502	-	-	9/45/69/87	0/1/1/1

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	600	SPO	C15-C16	9.49	1.59	1.34
7	M	701	LDA	O1-N1	-8.77	1.21	1.42
7	M	702	LDA	O1-N1	-8.70	1.21	1.42
7	M	703	LDA	O1-N1	-8.33	1.22	1.42
7	L	709	LDA	O1-N1	-8.32	1.22	1.42
7	M	706	LDA	O1-N1	-8.14	1.23	1.42
7	L	707	LDA	O1-N1	-7.97	1.23	1.42
7	M	705	LDA	O1-N1	-7.65	1.24	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	708	LDA	O1-N1	-7.54	1.24	1.42
10	M	600	SPO	C6-C5	7.39	1.51	1.32
6	M	501	U10	C27-C28	-7.28	1.26	1.50
6	M	501	U10	O3-C3	7.24	1.54	1.36
10	M	600	SPO	C10-C11	7.18	1.53	1.34
7	M	704	LDA	O1-N1	-6.98	1.25	1.42
10	M	600	SPO	C21-C20	6.03	1.51	1.36
10	M	600	SPO	C26-C25	5.31	1.48	1.34
4	L	302	BCL	O2D-CED	-5.17	1.33	1.45
4	L	301	BCL	O2A-CGA	5.04	1.48	1.33
4	L	304	BCL	O2D-CGD	4.63	1.44	1.33
10	M	600	SPO	C15-C14	4.59	1.57	1.43
6	L	502	U10	O3-C3	4.53	1.47	1.36
10	M	600	SPO	C14-C12	4.45	1.41	1.35
10	M	600	SPO	C27-C28	4.43	1.38	1.34
4	L	302	BCL	C1-C2	-4.30	1.36	1.49
4	L	302	BCL	O2A-CGA	4.18	1.45	1.33
4	L	302	BCL	MG-NA	4.14	2.16	2.06
5	M	401	BPH	O2D-CED	-4.10	1.35	1.45
4	L	304	BCL	MG-NA	4.09	2.16	2.06
4	M	801	BCL	MG-NA	4.01	2.15	2.06
6	L	502	U10	O4-C4	3.96	1.46	1.36
6	L	502	U10	C7-C6	3.89	1.57	1.51
4	L	301	BCL	MG-NA	3.88	2.15	2.06
4	M	801	BCL	C1B-NB	3.84	1.38	1.35
6	M	501	U10	C17-C18	-3.83	1.38	1.50
4	M	801	BCL	C4B-NB	3.74	1.38	1.35
4	L	301	BCL	C1B-NB	3.70	1.38	1.35
10	M	600	SPO	C10-C9	3.65	1.54	1.43
6	M	501	U10	O4-C4	3.61	1.45	1.36
6	M	501	U10	C36-C34	3.48	1.58	1.51
4	L	301	BCL	O2D-CED	-3.43	1.37	1.45
5	M	401	BPH	O2D-CGD	3.40	1.41	1.33
6	L	502	U10	C33-C34	3.40	1.41	1.33
6	L	502	U10	C28-C29	3.37	1.41	1.33
10	M	600	SPO	C11-C12	-3.32	1.38	1.45
4	L	304	BCL	C4B-NB	3.29	1.38	1.35
10	M	600	SPO	C4-C5	-3.26	1.45	1.50
10	M	600	SPO	C6-C7	-3.25	1.39	1.45
6	M	501	U10	C37-C38	-3.24	1.39	1.50
6	M	501	U10	C22-C23	-3.24	1.39	1.50
10	M	600	SPO	C13-C12	3.24	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	502	U10	C36-C34	3.23	1.58	1.51
6	M	501	U10	C35-C34	3.21	1.58	1.50
6	L	502	U10	C23-C24	3.16	1.40	1.33
5	L	402	BPH	O2D-CED	-3.14	1.37	1.45
4	L	302	BCL	C4B-NB	3.13	1.38	1.35
5	L	402	BPH	O2D-CGD	3.12	1.40	1.33
6	L	502	U10	C17-C18	-3.11	1.40	1.50
4	L	301	BCL	C4B-NB	3.10	1.38	1.35
4	L	302	BCL	MG-NC	3.09	2.13	2.06
6	M	501	U10	C33-C34	3.09	1.40	1.33
10	M	600	SPO	O1-CM1	3.05	1.52	1.43
10	M	600	SPO	C31-C32	-3.04	1.40	1.50
6	L	502	U10	C8-C9	3.01	1.40	1.33
6	L	502	U10	C13-C14	2.97	1.40	1.33
6	L	502	U10	C31-C29	2.96	1.57	1.51
6	L	502	U10	C38-C39	2.93	1.40	1.32
6	L	502	U10	O4-C4M	-2.93	1.38	1.45
5	M	401	BPH	O2A-CGA	2.92	1.41	1.33
6	M	501	U10	C8-C9	2.84	1.39	1.33
10	M	600	SPO	C25-C23	-2.80	1.39	1.45
4	L	301	BCL	C2-C3	2.80	1.39	1.33
10	M	600	SPO	C37-C38	2.80	1.40	1.32
6	L	502	U10	C21-C19	2.77	1.57	1.51
10	M	600	SPO	C32-C33	2.76	1.39	1.33
5	L	402	BPH	C2-C3	2.75	1.39	1.33
6	M	501	U10	C23-C24	2.73	1.39	1.33
4	M	801	BCL	C2-C3	2.73	1.39	1.33
10	M	600	SPO	C9-C7	2.66	1.39	1.35
5	M	401	BPH	C2-C3	2.65	1.39	1.33
6	M	501	U10	C38-C39	2.64	1.40	1.32
4	L	304	BCL	C2-C3	2.63	1.39	1.33
10	M	600	SPO	C19-C17	2.63	1.39	1.35
5	L	402	BPH	O2A-CGA	2.62	1.41	1.33
10	M	600	SPO	C35-C33	2.60	1.56	1.51
4	L	304	BCL	C1B-NB	2.57	1.37	1.35
4	L	304	BCL	O2A-CGA	2.51	1.40	1.33
6	M	501	U10	C13-C14	2.50	1.39	1.33
4	L	304	BCL	CMB-C2B	-2.50	1.46	1.51
6	M	501	U10	O4-C4M	-2.49	1.39	1.45
4	L	301	BCL	C3D-C2D	-2.43	1.35	1.39
6	M	501	U10	C18-C19	2.42	1.38	1.33
6	M	501	U10	C30-C29	2.41	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	502	U10	C18-C19	2.41	1.38	1.33
6	L	502	U10	C7-C8	-2.39	1.47	1.50
6	M	501	U10	C15-C14	2.37	1.56	1.50
4	M	801	BCL	O2D-CED	-2.32	1.39	1.45
6	M	501	U10	O2-C2	2.32	1.28	1.23
4	L	304	BCL	C3D-C2D	-2.32	1.35	1.39
6	M	501	U10	C7-C8	-2.30	1.47	1.50
6	M	501	U10	O3-C3M	-2.29	1.39	1.45
6	L	502	U10	C10-C9	2.28	1.56	1.50
6	L	502	U10	C15-C14	2.28	1.56	1.50
6	L	502	U10	C16-C14	2.27	1.56	1.51
5	M	401	BPH	C3D-C2D	-2.23	1.35	1.39
5	M	401	BPH	C5-C3	2.22	1.55	1.51
9	M	800	PO4	P-O3	-2.22	1.47	1.54
10	M	600	SPO	C16-C17	-2.22	1.41	1.45
10	M	600	SPO	O1-C1	2.19	1.53	1.41
4	L	302	BCL	C4-C3	2.19	1.56	1.50
4	L	302	BCL	CMC-C2C	-2.18	1.48	1.53
6	L	502	U10	C35-C34	2.16	1.56	1.50
5	M	401	BPH	C3A-C2A	-2.13	1.48	1.54
4	M	801	BCL	OBD-CAD	2.13	1.25	1.22
4	M	801	BCL	O2A-CGA	2.11	1.39	1.33
4	L	302	BCL	O2D-CGD	2.11	1.38	1.33
6	M	501	U10	C40-C39	2.06	1.55	1.50
5	M	401	BPH	CHA-C1A	2.03	1.42	1.38
4	L	301	BCL	C1-C2	2.02	1.55	1.49
4	L	302	BCL	C3D-C2D	-2.01	1.35	1.39

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	302	BCL	C4B-C3B-CAB	-11.03	105.83	127.13
4	L	304	BCL	C4B-C3B-CAB	-9.82	108.18	127.13
4	L	304	BCL	C4A-NA-C1A	8.51	110.53	106.71
4	L	302	BCL	C4A-NA-C1A	8.29	110.43	106.71
4	L	304	BCL	CBB-CAB-C3B	-8.17	96.08	120.34
4	L	304	BCL	O2D-CGD-CBD	7.89	125.28	111.27
4	M	801	BCL	C4A-NA-C1A	7.67	110.16	106.71
4	L	301	BCL	C1-C2-C3	7.14	138.39	126.04
4	L	304	BCL	OBB-CAB-C3B	7.06	132.52	119.99
4	L	301	BCL	C4A-NA-C1A	7.02	109.86	106.71
5	M	401	BPH	O2D-CGD-CBD	6.88	123.50	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	302	BCL	CBB-CAB-C3B	-6.50	101.04	120.34
4	L	302	BCL	C1C-NC-C4C	6.42	109.59	106.71
5	L	402	BPH	O2D-CGD-CBD	6.36	122.58	111.27
4	L	301	BCL	O2D-CGD-CBD	6.32	122.51	111.27
4	L	301	BCL	C1C-NC-C4C	5.68	109.26	106.71
4	M	801	BCL	C1C-NC-C4C	5.65	109.25	106.71
4	M	801	BCL	O2D-CGD-CBD	5.64	121.29	111.27
4	L	304	BCL	O1D-CGD-CBD	-5.51	113.22	124.48
4	L	304	BCL	C1C-NC-C4C	5.46	109.16	106.71
4	L	302	BCL	O2D-CGD-CBD	4.96	120.09	111.27
5	M	401	BPH	O1D-CGD-CBD	-4.96	114.34	124.48
10	M	600	SPO	C25-C23-C22	-4.86	111.48	118.94
4	L	301	BCL	CMB-C2B-C1B	-4.76	121.15	128.46
4	L	301	BCL	O1D-CGD-CBD	-4.66	114.96	124.48
5	L	402	BPH	O1D-CGD-CBD	-4.63	115.00	124.48
10	M	600	SPO	C20-C21-C22	-4.49	114.28	123.47
4	L	304	BCL	OBB-CAB-CBB	-4.43	110.20	120.17
10	M	600	SPO	C15-C14-C12	-4.20	121.32	127.31
4	L	302	BCL	OBB-CAB-CBB	-4.05	111.06	120.17
10	M	600	SPO	C15-C16-C17	-4.01	115.15	126.42
10	M	600	SPO	C20-C19-C17	-3.99	121.61	127.31
10	M	600	SPO	C18-C17-C19	-3.94	117.40	122.92
10	M	600	SPO	C10-C9-C7	-3.94	121.69	127.31
5	L	402	BPH	OBD-CAD-CBD	-3.89	120.34	125.89
10	M	600	SPO	C5-C6-C7	-3.79	120.16	125.89
5	M	401	BPH	OBD-CAD-CBD	-3.79	120.48	125.89
4	M	801	BCL	O1D-CGD-CBD	-3.72	116.86	124.48
5	M	401	BPH	O2A-CGA-CBA	3.49	122.87	111.91
6	M	501	U10	C27-C28-C29	3.45	135.96	127.66
4	M	801	BCL	O2A-CGA-CBA	3.42	122.64	111.91
5	L	402	BPH	C1-C2-C3	3.33	131.81	126.04
6	M	501	U10	C26-C27-C28	-3.25	101.20	111.88
4	M	801	BCL	C4D-C3D-CAD	-3.23	106.67	108.47
4	L	302	BCL	O2A-CGA-CBA	3.17	121.85	111.91
5	L	402	BPH	O2A-CGA-CBA	3.17	121.85	111.91
4	L	302	BCL	OBD-CAD-CBD	-3.16	121.38	125.89
4	L	301	BCL	CMB-C2B-C3B	3.16	130.59	124.68
4	M	801	BCL	OBB-CAB-C3B	3.12	125.53	119.99
4	L	301	BCL	O2A-CGA-CBA	3.05	121.47	111.91
4	L	304	BCL	CMB-C2B-C1B	-3.03	123.81	128.46
4	L	302	BCL	OBB-CAB-C3B	2.95	125.23	119.99
4	M	801	BCL	CED-O2D-CGD	2.91	122.51	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	302	BCL	O1D-CGD-CBD	-2.88	118.59	124.48
5	L	402	BPH	C4D-CHA-C1A	-2.87	123.43	130.51
4	L	304	BCL	CMD-C2D-C3D	2.86	130.02	124.68
4	M	801	BCL	OBD-CAD-CBD	-2.83	121.85	125.89
5	M	401	BPH	C4A-NA-C1A	2.81	110.41	108.14
4	L	304	BCL	O2A-CGA-CBA	2.79	120.67	111.91
6	L	502	U10	C7-C8-C9	2.77	131.40	126.79
5	M	401	BPH	C3A-C4A-CHB	2.75	126.58	121.83
5	M	401	BPH	C3A-C4A-NA	-2.72	108.42	113.05
4	L	302	BCL	CMB-C2B-C1B	-2.72	124.29	128.46
4	L	301	BCL	OBD-CAD-CBD	-2.69	122.05	125.89
5	M	401	BPH	C4D-CHA-C1A	-2.68	123.90	130.51
4	L	304	BCL	C4D-C3D-CAD	-2.68	106.98	108.47
5	M	401	BPH	OBB-CAB-C3B	2.65	125.31	120.41
4	L	302	BCL	C4D-C3D-CAD	-2.57	107.04	108.47
4	L	304	BCL	O2A-CGA-O1A	-2.51	117.26	123.59
4	M	801	BCL	C4B-C3B-CAB	-2.48	122.33	127.13
4	M	801	BCL	C1-C2-C3	2.45	130.27	126.04
6	M	501	U10	C25-C24-C26	-2.44	111.16	115.27
6	M	501	U10	C7-C8-C9	2.44	130.85	126.79
10	M	600	SPO	C21-C22-C23	-2.42	123.86	127.31
4	L	302	BCL	C1-C2-C3	2.40	130.19	126.04
4	L	304	BCL	CAC-C3C-C4C	-2.38	107.31	112.58
5	L	402	BPH	CBB-CAB-C3B	-2.36	115.38	120.43
4	L	302	BCL	CED-O2D-CGD	2.33	121.22	115.94
5	M	401	BPH	C2A-C1A-NA	-2.33	109.19	111.86
5	M	401	BPH	CBB-CAB-C3B	-2.32	115.48	120.43
5	M	401	BPH	O2A-CGA-O1A	-2.31	117.76	123.59
10	M	600	SPO	C10-C11-C12	-2.26	120.07	126.42
5	L	402	BPH	CMD-C2D-C3D	2.26	128.90	124.68
4	M	801	BCL	CMB-C2B-C1B	-2.24	125.02	128.46
6	L	502	U10	C3M-O3-C3	2.24	124.41	116.47
10	M	600	SPO	C6-C7-C9	-2.24	115.51	118.94
5	L	402	BPH	C4A-NA-C1A	2.23	109.94	108.14
10	M	600	SPO	C8-C7-C6	2.23	121.59	118.08
6	M	501	U10	C3M-O3-C3	2.20	124.25	116.47
4	M	801	BCL	C3A-C2A-C1A	2.19	104.62	101.34
5	L	402	BPH	O2A-CGA-O1A	-2.19	118.07	123.59
6	L	502	U10	C4M-O4-C4	2.17	124.14	116.47
5	L	402	BPH	C3A-C4A-CHB	2.14	125.52	121.83
5	L	402	BPH	C3A-C4A-NA	-2.13	109.42	113.05
10	M	600	SPO	C11-C12-C14	-2.12	115.68	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	304	BCL	OBD-CAD-CBD	-2.12	122.87	125.89
4	L	301	BCL	C4B-C3B-CAB	-2.11	123.06	127.13
10	M	600	SPO	C24-C23-C22	-2.11	119.97	122.92
4	L	301	BCL	C4D-C3D-CAD	-2.08	107.31	108.47
6	M	501	U10	C31-C29-C28	-2.08	116.91	121.12
4	M	801	BCL	O2A-CGA-O1A	-2.07	118.38	123.59
5	L	402	BPH	C4D-C3D-CAD	-2.06	106.56	107.87
4	L	301	BCL	C1B-CHB-C4A	-2.06	126.04	130.12
5	L	402	BPH	C3A-C2A-C1A	2.05	104.09	101.64
6	M	501	U10	C4M-O4-C4	2.03	123.66	116.47
5	L	402	BPH	C2A-C1A-NA	-2.01	109.55	111.86
10	M	600	SPO	C24-C23-C25	2.01	121.24	118.08

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	L	301	BCL	C8
4	L	301	BCL	C13
4	L	304	BCL	C13

All (150) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	402	BPH	C4C-C3C-CAC-CBC
5	L	402	BPH	C2C-C3C-CAC-CBC
5	L	402	BPH	C4B-C3B-CAB-CBB
5	L	402	BPH	C4B-C3B-CAB-OB
5	L	402	BPH	O2A-C1-C2-C3
7	M	701	LDA	C2-C1-N1-O1
7	M	701	LDA	C2-C1-N1-CM1
4	L	301	BCL	C1A-C2A-CAA-CBA
4	L	301	BCL	C4C-C3C-CAC-CBC
4	L	301	BCL	O2A-C1-C2-C3
7	M	705	LDA	C2-C1-N1-CM1
7	M	705	LDA	C2-C1-N1-CM2
7	L	709	LDA	N1-C1-C2-C3
4	L	304	BCL	C2C-C3C-CAC-CBC
4	L	304	BCL	C4C-C3C-CAC-CBC
7	L	707	LDA	C2-C1-N1-O1
7	L	707	LDA	C2-C1-N1-CM1
7	L	707	LDA	N1-C1-C2-C3
7	M	702	LDA	N1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	M	703	LDA	C2-C1-N1-O1
7	M	703	LDA	C2-C1-N1-CM1
7	M	706	LDA	C2-C1-N1-O1
7	M	706	LDA	C2-C1-N1-CM1
7	M	706	LDA	N1-C1-C2-C3
5	M	401	BPH	C4C-C3C-CAC-CBC
5	M	401	BPH	C2C-C3C-CAC-CBC
5	M	401	BPH	C2C-C1C-CHC-C4B
5	M	401	BPH	C4B-C3B-CAB-CBB
5	M	401	BPH	C4B-C3B-CAB-OB
10	M	600	SPO	C4-C5-C6-C7
10	M	600	SPO	C21-C22-C23-C24
10	M	600	SPO	C24-C23-C25-C26
10	M	600	SPO	C36-C37-C38-C39
6	L	502	U10	C23-C24-C26-C27
6	L	502	U10	C25-C24-C26-C27
6	L	502	U10	C35-C34-C36-C37
4	L	304	BCL	CBD-CGD-O2D-CED
4	L	304	BCL	O1D-CGD-O2D-CED
10	M	600	SPO	C36-C37-C38-C40
5	L	402	BPH	C3-C5-C6-C7
6	L	502	U10	C33-C34-C36-C37
10	M	600	SPO	C20-C21-C22-C23
5	M	401	BPH	C4-C3-C5-C6
5	M	401	BPH	C2-C3-C5-C6
6	M	501	U10	C24-C26-C27-C28
4	M	801	BCL	C3-C5-C6-C7
5	M	401	BPH	CBA-CGA-O2A-C1
5	M	401	BPH	O1A-CGA-O2A-C1
5	M	401	BPH	C11-C10-C8-C7
6	L	502	U10	C29-C31-C32-C33
4	M	801	BCL	C13-C15-C16-C17
4	M	801	BCL	C15-C16-C17-C18
4	L	302	BCL	C15-C16-C17-C18
5	M	401	BPH	C2B-C3B-CAB-CBB
7	M	703	LDA	C7-C8-C9-C10
7	L	708	LDA	C4-C5-C6-C7
6	M	501	U10	C35-C34-C36-C37
7	M	702	LDA	C7-C8-C9-C10
5	L	402	BPH	C6-C7-C8-C9
7	M	703	LDA	C6-C7-C8-C9
5	M	401	BPH	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
7	M	705	LDA	C2-C3-C4-C5
4	L	301	BCL	C16-C17-C18-C20
7	L	708	LDA	C6-C7-C8-C9
5	M	401	BPH	O2A-C1-C2-C3
6	M	501	U10	C33-C34-C36-C37
7	M	701	LDA	C7-C8-C9-C10
5	L	402	BPH	C6-C7-C8-C10
4	M	801	BCL	C6-C7-C8-C10
7	L	707	LDA	C2-C3-C4-C5
6	M	501	U10	C14-C16-C17-C18
7	M	701	LDA	C1-C2-C3-C4
7	L	709	LDA	C2-C3-C4-C5
10	M	600	SPO	C19-C20-C21-C22
7	M	706	LDA	C2-C3-C4-C5
5	L	402	BPH	C11-C10-C8-C9
4	M	801	BCL	C6-C7-C8-C9
5	M	401	BPH	C11-C10-C8-C9
5	M	401	BPH	O1D-CGD-O2D-CED
4	L	304	BCL	C15-C16-C17-C18
7	M	706	LDA	C4-C5-C6-C7
7	M	703	LDA	C11-C10-C9-C8
7	L	709	LDA	C3-C4-C5-C6
5	M	401	BPH	C2B-C3B-CAB-OBB
7	M	705	LDA	C1-C2-C3-C4
4	L	301	BCL	C10-C11-C12-C13
6	M	501	U10	C30-C29-C31-C32
5	L	402	BPH	C11-C10-C8-C7
4	L	302	BCL	C11-C12-C13-C15
6	M	501	U10	C28-C29-C31-C32
4	L	301	BCL	C6-C7-C8-C10
4	L	301	BCL	C6-C7-C8-C9
7	M	701	LDA	C9-C10-C11-C12
6	M	501	U10	C25-C24-C26-C27
6	M	501	U10	C23-C24-C26-C27
4	L	301	BCL	C3A-C2A-CAA-CBA
4	L	301	BCL	C8-C10-C11-C12
7	M	701	LDA	C4-C5-C6-C7
4	L	301	BCL	C16-C17-C18-C19
6	M	501	U10	C29-C31-C32-C33
6	L	502	U10	C14-C16-C17-C18
7	M	705	LDA	C6-C7-C8-C9
5	L	402	BPH	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
7	L	708	LDA	C11-C10-C9-C8
7	M	701	LDA	C2-C1-N1-CM2
4	L	304	BCL	CHA-CBD-CGD-O1D
4	L	304	BCL	CHA-CBD-CGD-O2D
7	L	707	LDA	C2-C1-N1-CM2
7	M	706	LDA	C2-C1-N1-CM2
4	L	302	BCL	C16-C17-C18-C20
7	M	705	LDA	C5-C6-C7-C8
10	M	600	SPO	C35-C36-C37-C38
4	L	304	BCL	C6-C7-C8-C10
7	M	704	LDA	C3-C4-C5-C6
7	M	704	LDA	C5-C6-C7-C8
4	L	304	BCL	C6-C7-C8-C9
10	M	600	SPO	C4-C1-O1-CM1
7	M	701	LDA	C5-C6-C7-C8
7	L	708	LDA	C2-C3-C4-C5
4	L	301	BCL	C2-C1-O2A-CGA
10	M	600	SPO	C2-C1-O1-CM1
7	L	707	LDA	C4-C5-C6-C7
4	L	302	BCL	C11-C12-C13-C14
4	M	801	BCL	C10-C11-C12-C13
7	L	709	LDA	C5-C6-C7-C8
7	L	707	LDA	C3-C4-C5-C6
10	M	600	SPO	C28-C30-C31-C32
7	M	702	LDA	C5-C6-C7-C8
4	L	304	BCL	C11-C10-C8-C9
10	M	600	SPO	C18-C17-C19-C20
7	M	702	LDA	C6-C7-C8-C9
6	L	502	U10	C2-C3-O3-C3M
10	M	600	SPO	C16-C17-C19-C20
6	L	502	U10	C26-C27-C28-C29
10	M	600	SPO	C29-C28-C30-C31
6	L	502	U10	C12-C11-C9-C10
4	L	302	BCL	CAD-CBD-CGD-O2D
4	L	301	BCL	CBA-CGA-O2A-C1
7	L	708	LDA	C3-C4-C5-C6
6	M	501	U10	C5-C4-O4-C4M
5	L	402	BPH	C2-C3-C5-C6
10	M	600	SPO	C3-C1-O1-CM1
7	M	706	LDA	C6-C7-C8-C9
4	M	801	BCL	C2-C1-O2A-CGA
7	M	705	LDA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
5	M	401	BPH	CAD-CBD-CGD-O1D
4	L	302	BCL	O1A-CGA-O2A-C1
5	M	401	BPH	C11-C12-C13-C14
5	M	401	BPH	C10-C11-C12-C13
4	M	801	BCL	CAA-CBA-CGA-O2A

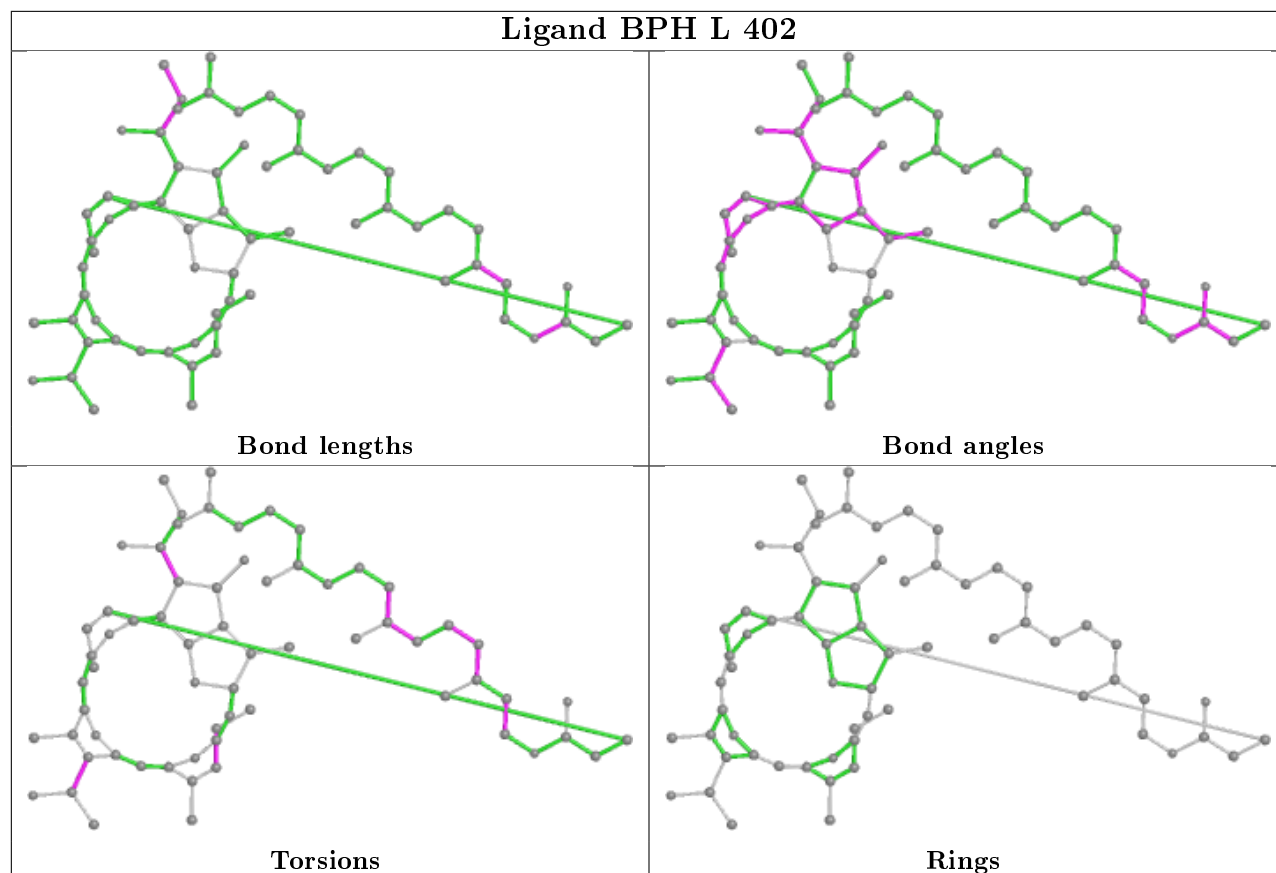
There are no ring outliers.

16 monomers are involved in 94 short contacts:

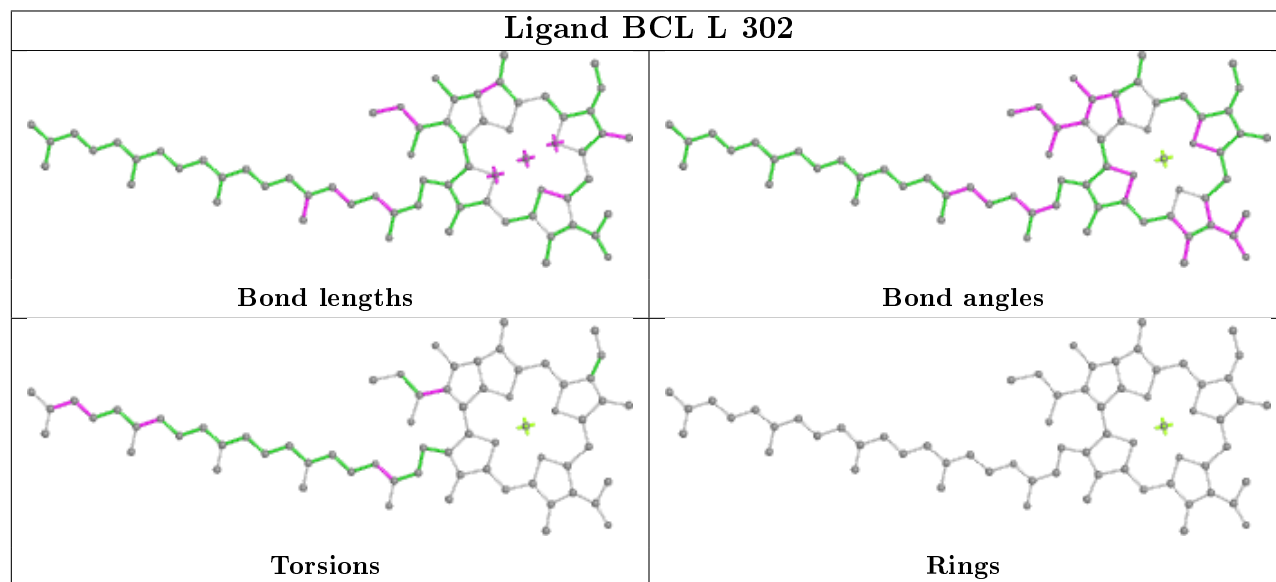
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	402	BPH	12	0
4	L	302	BCL	10	0
6	M	501	U10	8	0
7	M	701	LDA	4	0
4	L	301	BCL	9	0
7	M	705	LDA	4	0
4	L	304	BCL	5	0
7	L	707	LDA	1	0
7	M	702	LDA	6	0
4	M	801	BCL	14	0
7	M	703	LDA	8	0
7	M	706	LDA	5	0
7	L	708	LDA	1	0
5	M	401	BPH	8	0
10	M	600	SPO	7	0
6	L	502	U10	8	0

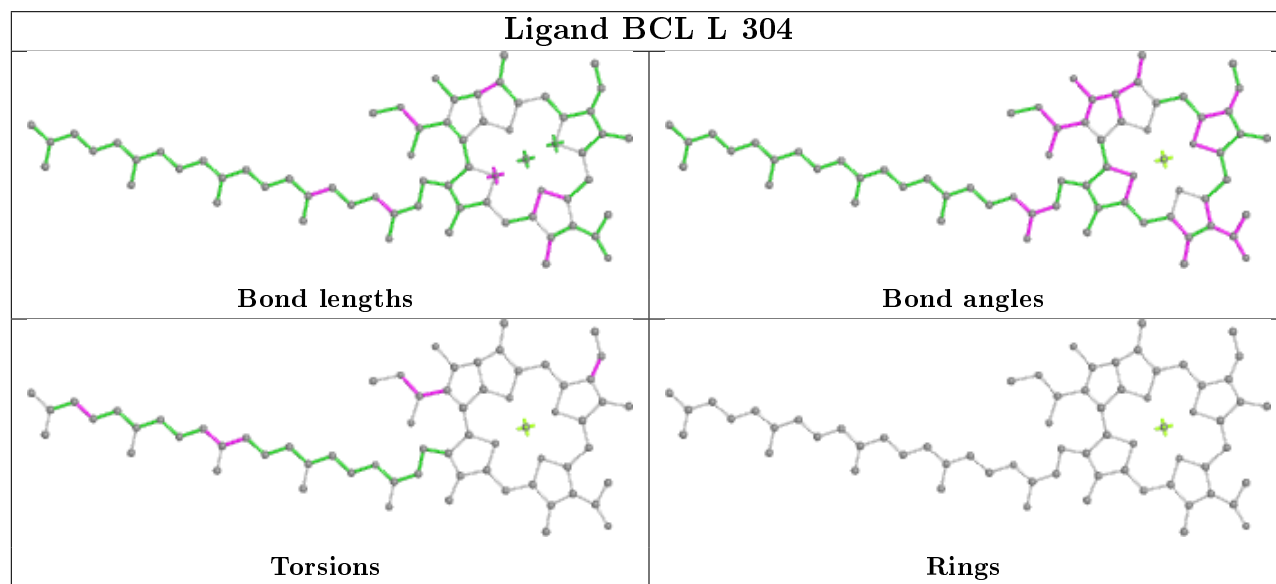
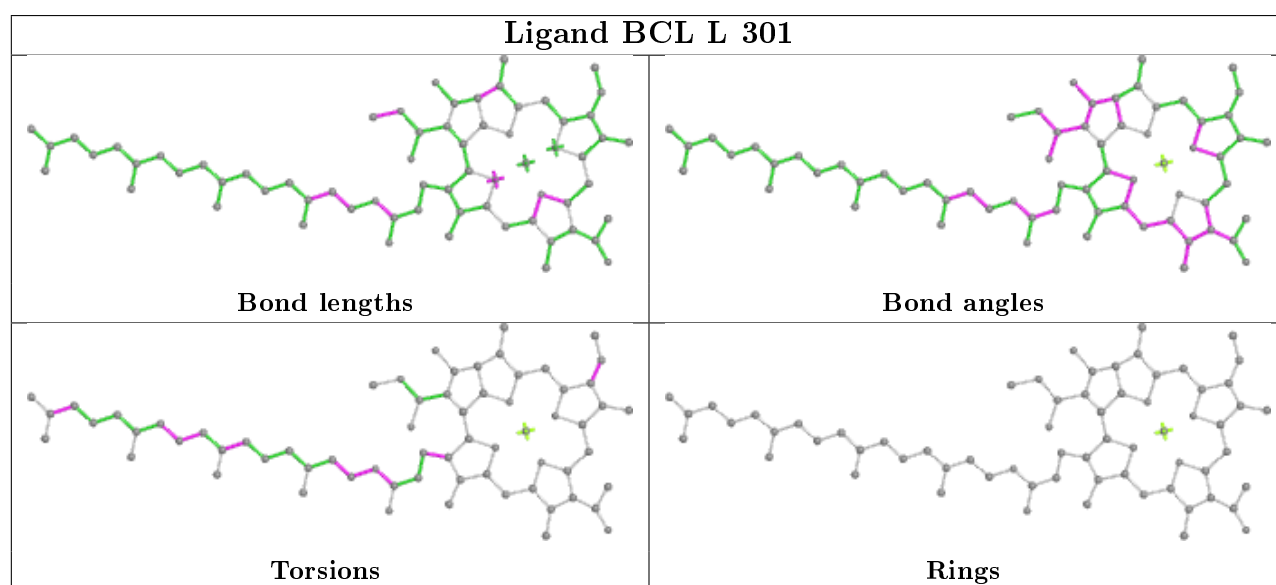
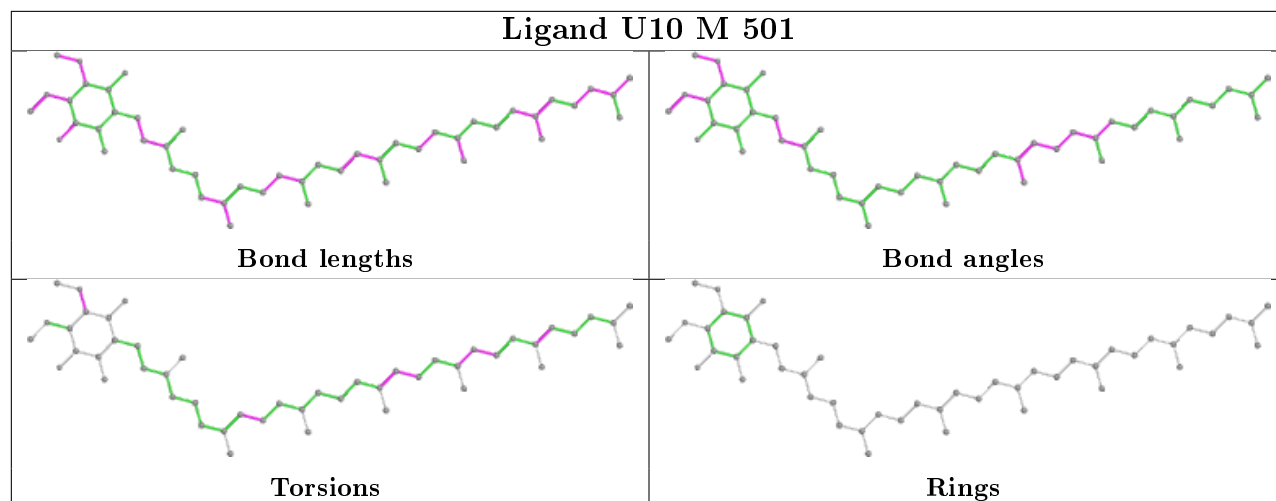
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

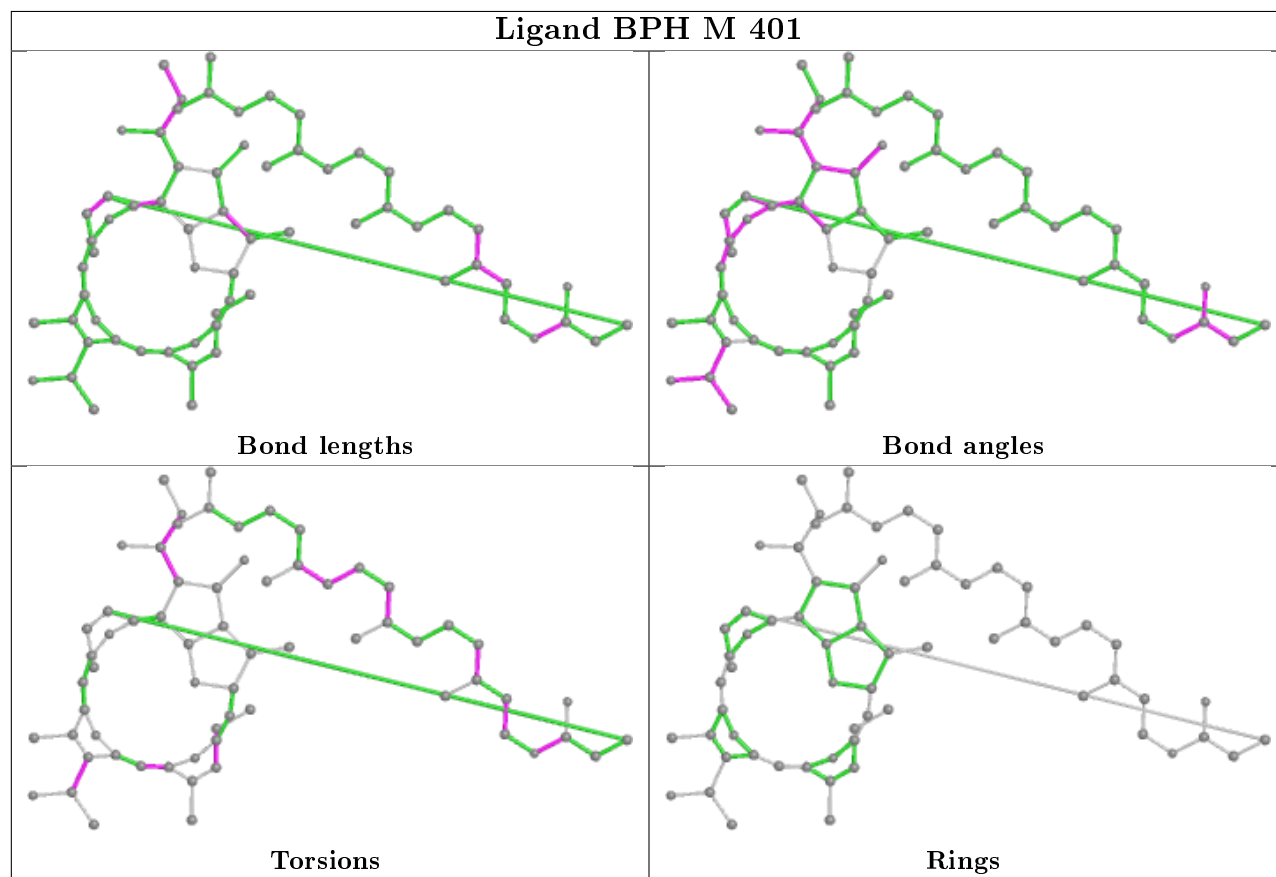
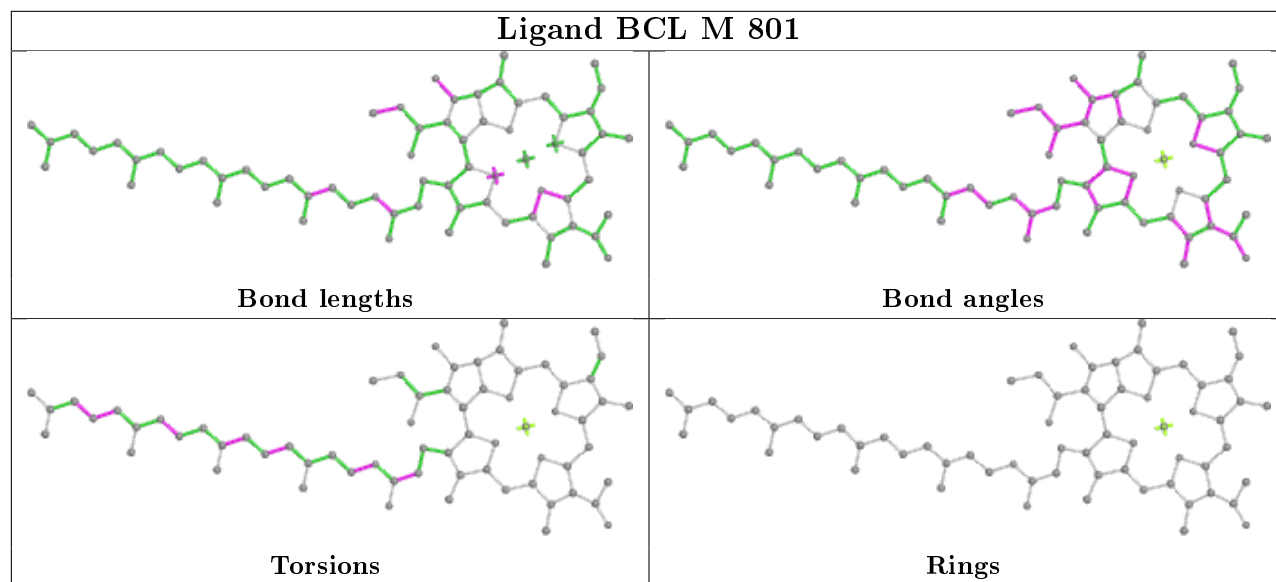
Ligand BPH L 402

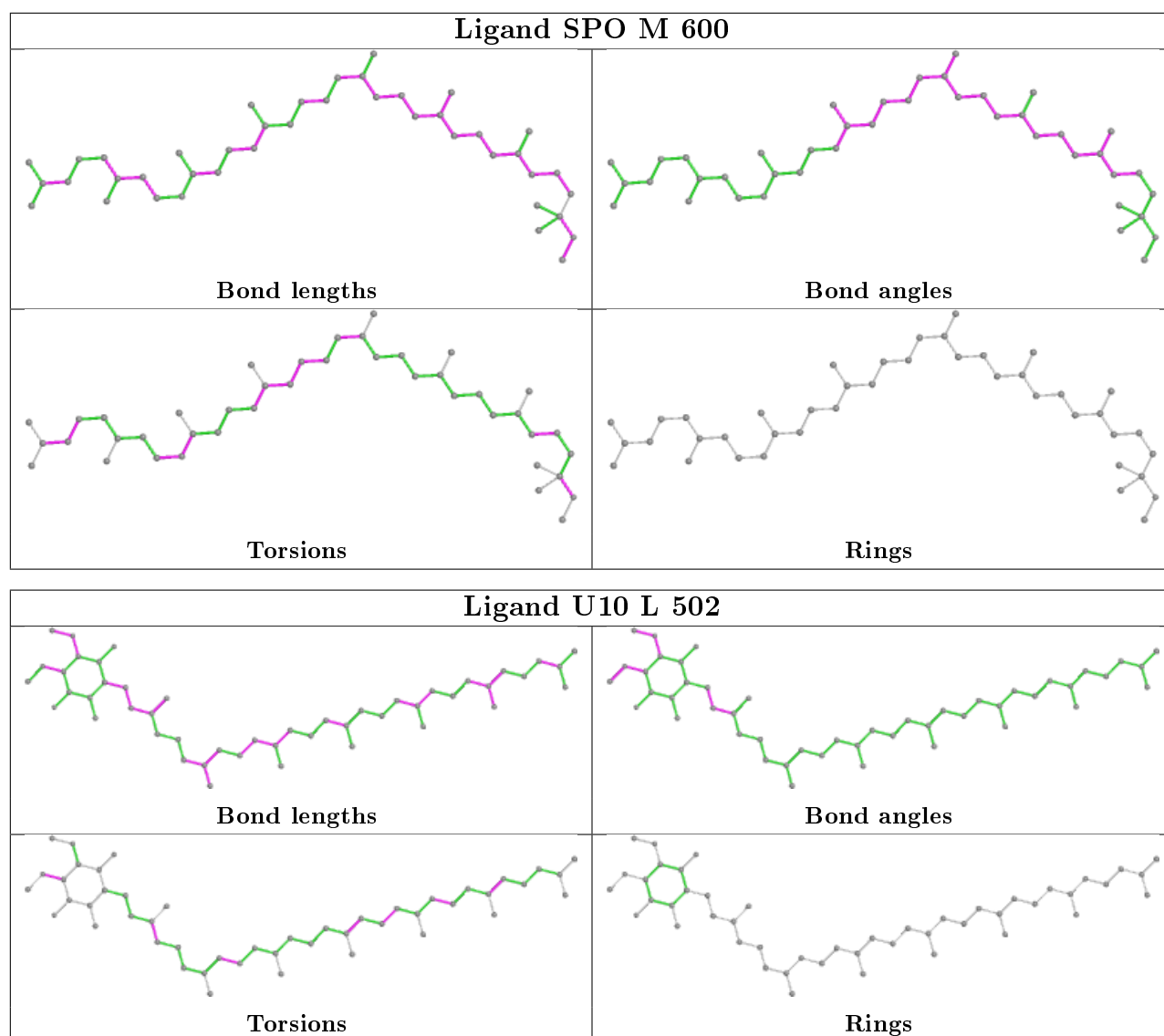


Ligand BCL L 302









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 ⓘ

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.