



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:01 AM UTC

PDB ID : 1PCR / pdb_00001pcr
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

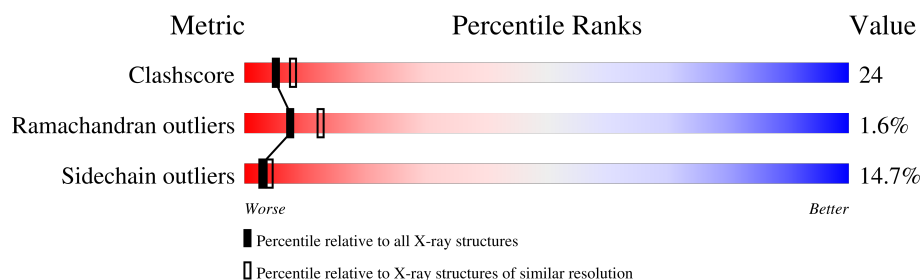
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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			

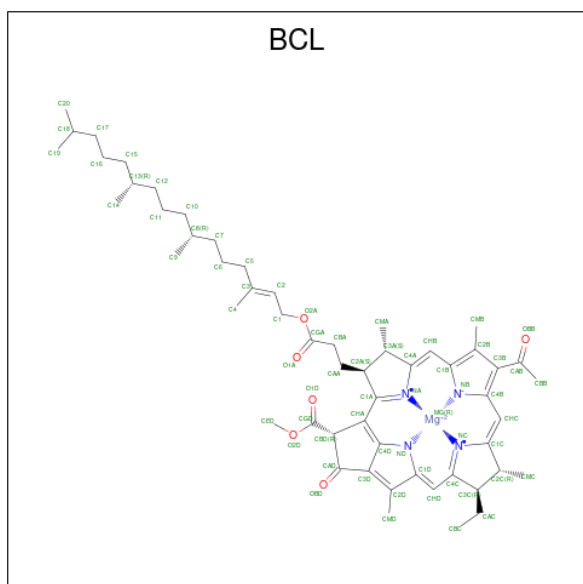
- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

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.

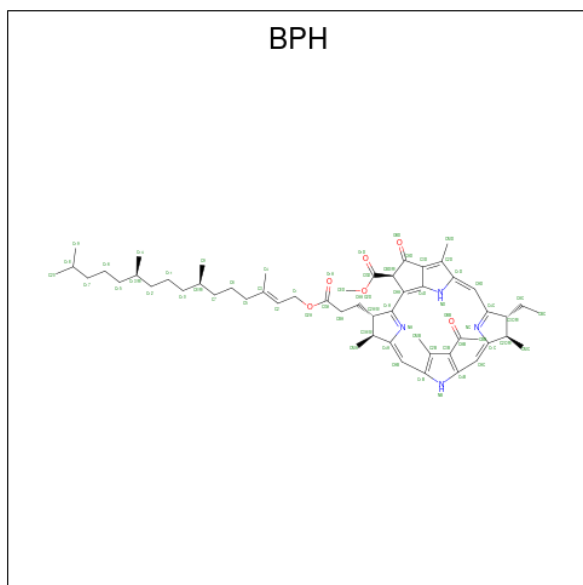
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



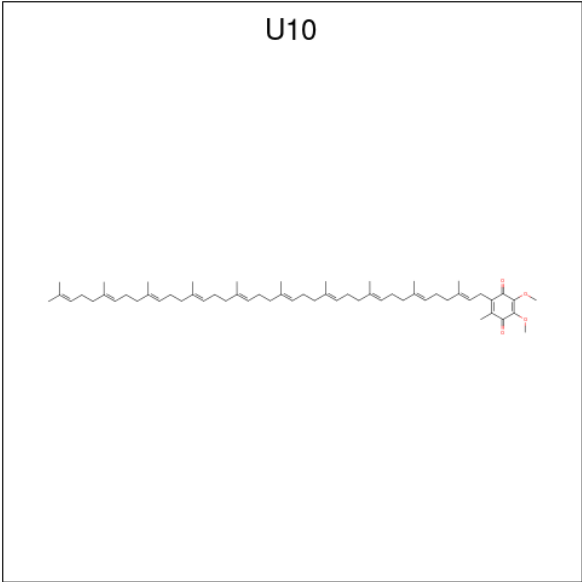
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



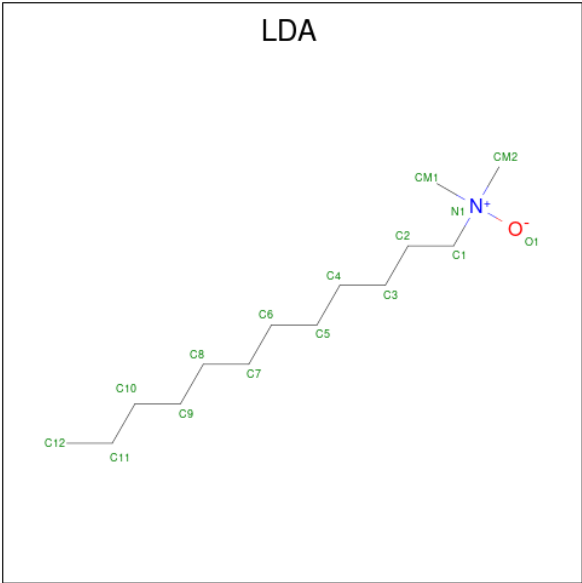
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



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

- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



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		

Continued on next page...

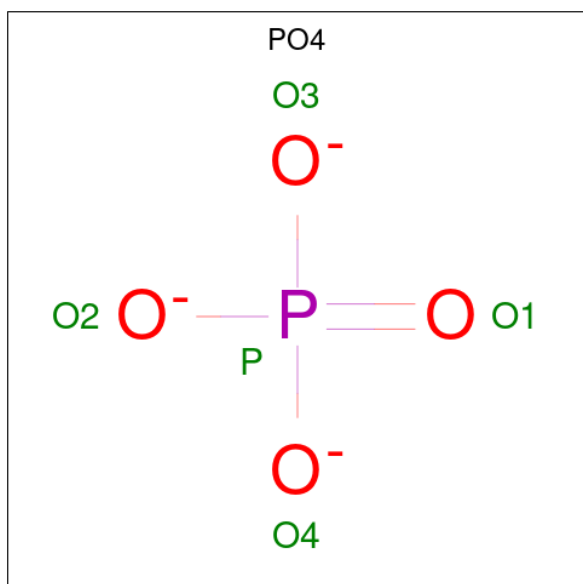
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	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 (CCD ID: FE) (formula: Fe).

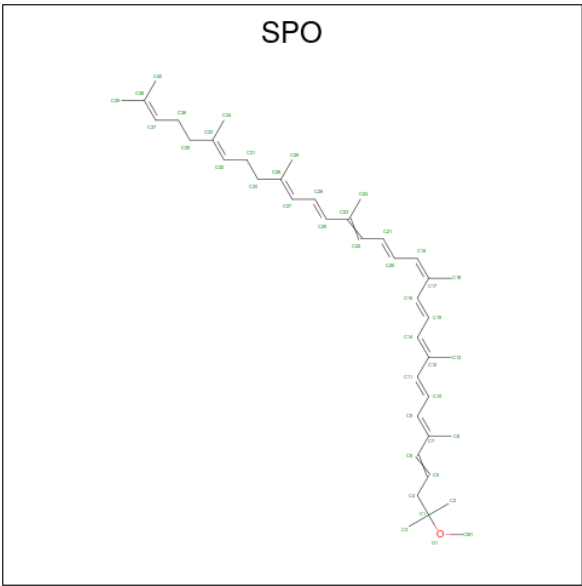
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 10 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).



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

- Molecule 11 is water.

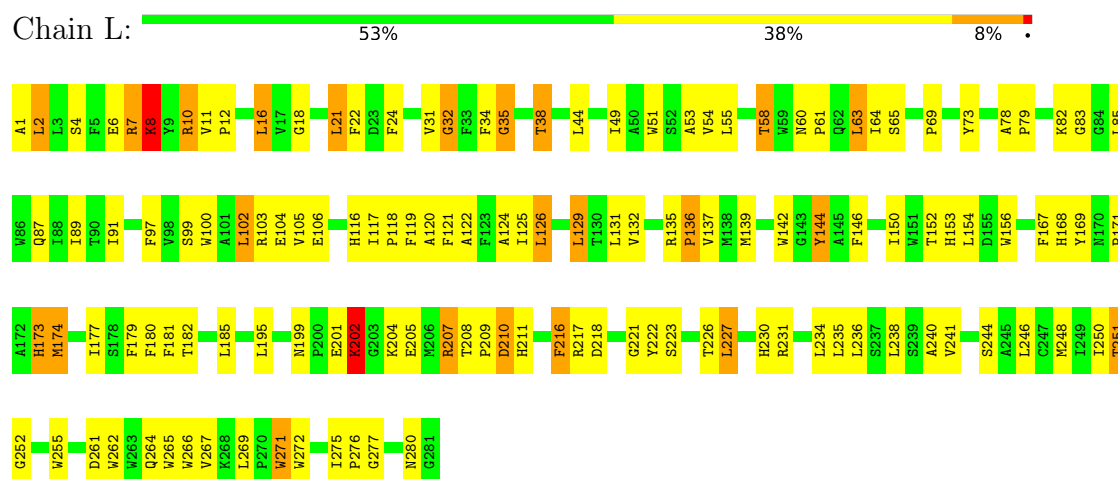
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	40	Total	O	0	0
			40	40		
11	M	50	Total	O	0	0
			50	50		
11	H	70	Total	O	0	0
			70	70		

3 Residue-property plots

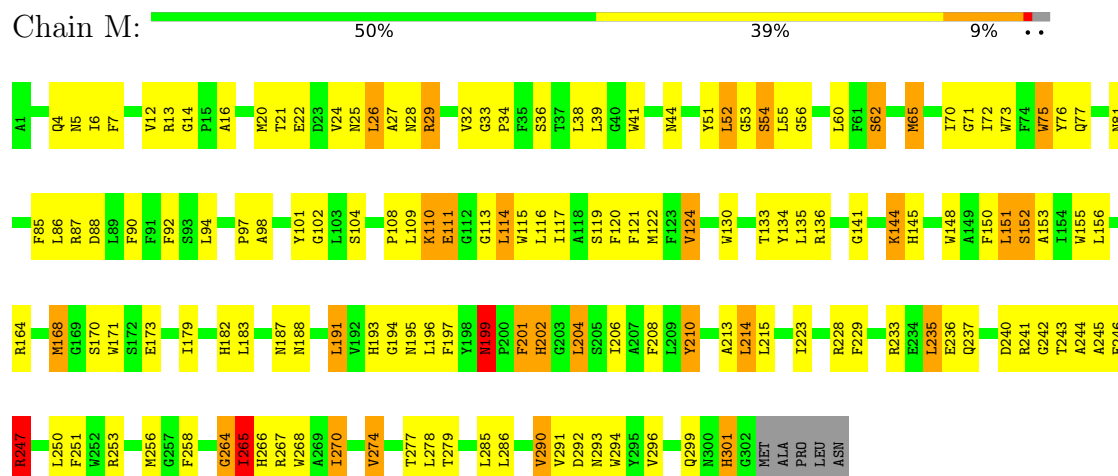
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: PHOTOSYNTHETIC REACTION CENTER



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER



ALA	L183	P94	MET
	GLU	I85	
TYR	D185	A86	VAL
ALA	T188	L87	THR
	R189	H98	ALA
	L190		PHE
	L191	D103	GLY
	P192		ASN
	P193		PHE
	P194	K106	D11
	H195		L12
	V196	P111	A13
	K197		S14
	V198	W114	L15
	Q199	V115	A16
	S200	A116	
	N201	R117	S19
	R202	D118	F20
	V203	L119	
	H204	L120	L24
	V205	P121	
	N206		L28
		D124	Y29
	S209		
	L212	N129	E34
		K130	N35
		I131	P36
	T219	K132	R37
	K220	P133	E38
	S221	M134	G39
	P222	K135	Y40
	T223		
	T224	F140	N44
	E225	H141	E45
	T226	V142	D46
			G47
	E229	N147	T48
	E230	P148	
	D231		Q53
	K232	L151	F56
	T233	P152	
			K60
	V237	C156	P61
			K62
	L241	I160	T63
	N242		
	A245	V165	
	P246	D166	L68
	K247	I167	R70
	R248	W168	G71
	K249	V169	L72
	S250	I171	L73
	VAL	A176	T74
	VAL	R177	V75
	ALA		P76
	ALA		G77
	MET	V181	
	TYR	E182	S20

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	141.30Å 141.30Å 187.20Å 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

5.1 Standard geometry

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

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	0.85	2/2320 (0.1%)	1.02	8/3175 (0.3%)
2	M	0.82	3/2500 (0.1%)	1.01	10/3413 (0.3%)
3	H	0.81	0/1877	1.04	8/2553 (0.3%)
All	All	0.82	5/6697 (0.1%)	1.02	26/9141 (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	6
2	M	0	4
3	H	0	4
All	All	0	14

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	173	HIS	ND1-CE1	5.90	1.38	1.32
2	M	202	HIS	ND1-CE1	5.49	1.38	1.32
2	M	182	HIS	ND1-CE1	5.45	1.38	1.32
2	M	266	HIS	ND1-CE1	5.14	1.37	1.32
1	L	174	MET	SD-CE	5.03	1.92	1.79

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	56	PHE	CA-C-N	6.68	126.65	120.03
3	H	56	PHE	C-N-CA	6.68	126.65	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	60	LYS	CA-C-N	6.62	126.60	119.78
3	H	60	LYS	C-N-CA	6.62	126.60	119.78
1	L	31	VAL	CA-C-N	-6.51	112.36	121.67
1	L	31	VAL	C-N-CA	-6.51	112.36	121.67
3	H	77	GLY	CA-C-N	6.21	127.61	119.84
3	H	77	GLY	C-N-CA	6.21	127.61	119.84
2	M	264	GLY	N-CA-C	6.03	119.94	112.64
1	L	210	ASP	N-CA-C	-5.56	105.30	111.36
1	L	227	LEU	N-CA-C	-5.51	105.29	112.23
2	M	199	ASN	CA-C-N	-5.47	114.03	119.56
2	M	199	ASN	C-N-CA	-5.47	114.03	119.56
2	M	14	GLY	CA-C-N	-5.41	114.22	119.90
2	M	14	GLY	C-N-CA	-5.41	114.22	119.90
1	L	199	ASN	CA-C-N	5.33	126.50	119.84
1	L	199	ASN	C-N-CA	5.33	126.50	119.84
1	L	8	LYS	N-CA-C	-5.23	106.85	113.18
3	H	114	TRP	CA-C-N	-5.07	115.65	122.91
3	H	114	TRP	C-N-CA	-5.07	115.65	122.91
2	M	210	TYR	N-CA-C	-5.07	105.76	111.28
2	M	81	ASN	CA-C-N	5.05	124.72	119.56
2	M	81	ASN	C-N-CA	5.05	124.72	119.56
1	L	35	GLY	N-CA-C	-5.03	106.69	112.73
2	M	286	LEU	N-CA-C	-5.02	107.10	113.18
2	M	168	MET	N-CA-C	-5.01	107.56	113.97

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	110	0
2	M	2408	0	2321	147	0
3	H	1829	0	1836	76	0
4	L	198	0	222	21	0
4	M	66	0	74	15	0
5	L	65	0	76	12	0
5	M	65	0	76	9	0
6	L	48	0	63	9	0
6	M	48	0	63	8	0
7	L	48	0	93	2	0
7	M	96	0	186	27	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	353	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 24.

All (353) 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:HHC	4:M:801:BCL:HBB3	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:32:GLY:HA3	11:L:712:HOH:O	1.74	0.87
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
3:H:148:PRO:HA	3:H:151:LEU:HD22	1.56	0.86
4:L:301:BCL:HBB2	4:L:301:BCL:HHC	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
1:L:7:ARG:HH11	3:H:98:HIS:CD2	2.06	0.74
3:H:61:PRO:HA	3:H:76:PRO:HD2	1.69	0.74
2:M:256:MET:HE3	2:M:258:PHE:CE1	2.22	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:HM21	7:M:706:LDA:H71	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
2:M:256:MET:HE3	2:M:258:PHE:CZ	2.28	0.68
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.75	0.67
2:M:130:TRP:HD1	2:M:150:PHE:CD2	2.12	0.67
3:H:156:CYS:SG	3:H:248:ARG:HA	2.34	0.67
2:M:197:PHE:HZ	4:M:801:BCL:CBB	2.07	0.66
2:M:62:SER:HA	2:M:65:MET:HB2	1.77	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:202:LYS:C	1:L:204:LYS:H	2.05	0.63
1:L:208:THR:HB	1:L:209:PRO:HD2	1.80	0.63
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.81	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
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
3:H:233:ILE:O	3:H:237:VAL:HG13	1.99	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:181:PHE:CD2	5:M:401:BPH:HBB1	2.35	0.61
1:L:269:LEU:HB2	1:L:272:TRP:NE1	2.15	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
4:L:301:BCL:HMD2	4:L:302:BCL:OBB	2.02	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:H51	7:L:708:LDA:H92	1.85	0.59
3:H:156:CYS:HB3	3:H:206:ASN:O	2.02	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
2:M:242:GLY:CA	3:H:117:ARG:HD2	2.31	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
2:M:270:ILE:O	2:M:274:VAL:HB	2.04	0.57
3:H:132:LYS:HB2	3:H:171:ILE:HD11	1.86	0.57
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:CD2	2:M:301:HIS:N	2.73	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:L:201:GLU:HG3	2:M:141:GLY:C	2.30	0.56
3:H:66:LEU:HD12	3:H:118:ARG:NH2	2.20	0.56
1:L:180:PHE:CE2	1:L:240:ALA:HB1	2.40	0.56
2:M:90:PHE:CD1	2:M:179:ILE:HD13	2.40	0.56
5:M:401:BPH:HBB3	5:M:401:BPH:HH1	1.85	0.56
1:L:241:VAL:HG21	5:L:402:BPH:HAC2	1.87	0.56
7:M:706:LDA:HM11	7:M:706:LDA:H72	1.87	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
3:H:202:ARG:HG2	3:H:203:VAL:N	2.19	0.56
2:M:130:TRP:CD1	2:M:150:PHE:HD2	2.23	0.55
3:H:66:LEU:N	3:H:66:LEU:HD23	2.21	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
1:L:87:GLN:HE21	1:L:142:TRP:CD1	2.25	0.55
2:M:199:ASN:C	2:M:199:ASN:HD22	2.15	0.54
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
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:118:ARG:HD2	11:H:311:HOH:O	2.07	0.54
1:L:202:LYS:C	1:L:204:LYS:N	2.63	0.53
7:M:706:LDA:H52	7:M:706:LDA:H12	1.90	0.53
3:H:148:PRO:HA	3:H:151:LEU:CD2	2.34	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
1:L:280:ASN:HD22	2:M:88:ASP:CG	2.16	0.53
4:L:302:BCL:H203	4:L:304:BCL:H102	1.91	0.53
5:L:402:BPH:HBB3	5:L:402:BPH:CHC	2.36	0.53
2:M:85:PHE:HD2	2:M:86:LEU:HD12	1.74	0.53
1:L:4:SER:OG	3:H:39:GLY:HA2	2.09	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
3:H:20:PHE:HE2	3:H:24:LEU:HD22	1.74	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:195:LEU:HB3	2:M:145:HIS:CD2	2.45	0.52
2:M:32:VAL:HG12	2:M:33:GLY:O	2.10	0.52
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
3:H:245:ALA:N	3:H:246:PRO:HD2	2.25	0.52
4:L:301:BCL:H51	5:M:401:BPH:HMB3	1.92	0.52
6:L:502:U10:H122	7:M:702:LDA:H92	1.92	0.52
1:L:267:VAL:HG23	2:M:87:ARG:HG2	1.92	0.51
4:L:301:BCL:HBB3	4:M:801:BCL:C4	2.38	0.51
2:M:77:GLN:NE2	2:M:92:PHE:CD1	2.77	0.51
2:M:152:SER:HB2	2:M:274:VAL:HG22	1.91	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
1:L:271:TRP:CD1	1:L:271:TRP:H	2.30	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:CD2	2:M:301:HIS:H	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:102:LEU:O	1:L:105:VAL:HB	2.13	0.48
2:M:88:ASP:HB2	2:M:92:PHE:CZ	2.48	0.48
3:H:44:ASN:HB2	3:H:46:ASP:OD1	2.12	0.48
1:L:135:ARG:HB3	1:L:136:PRO:CD	2.41	0.48
1:L:227:LEU:O	1:L:231:ARG:HG3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:234:LEU:O	1:L:238:LEU:HG	2.13	0.48
3:H:170:ASP:OD2	3:H:177:ARG:NH1	2.46	0.48
1:L:201:GLU:O	1:L:202:LYS:CB	2.62	0.48
2:M:134:TYR:CD1	2:M:134:TYR:C	2.91	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
6:L:502:U10:H122	7:M:702:LDA:C9	2.44	0.48
3:H:206:ASN:O	3:H:248:ARG:NH1	2.47	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
1:L:171:PRO:HA	1:L:174:MET:HG3	1.96	0.47
4:L:302:BCL:HBB2	4:M:801:BCL:C1B	2.43	0.47
5:L:402:BPH:H6C2	5:L:402:BPH:H2	1.66	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: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
1:L:139:MET:HE3	1:L:252:GLY:HA3	1.96	0.47
3:H:84:PRO:C	3:H:85:ILE:HD13	2.39	0.47
1:L:6:GLU:OE2	1:L:10:ARG:NH1	2.44	0.47
2:M:75:TRP:CZ3	10:M:600:SPO:O1	2.67	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
3:H:117:ARG:HA	11:H:290:HOH:O	2.13	0.47
2:M:20:MET:O	2:M:29:ARG:NH2	2.48	0.47
6:L:502:U10:H1M1	7:M:702:LDA:H112	1.97	0.46
2:M:265:ILE:HG21	6:M:501:U10:H3M3	1.97	0.46
1:L:12:PRO:O	3:H:242:MET:HE1	2.15	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
3:H:70:ARG:NH2	3:H:120:LEU:CB	2.79	0.46
1:L:58:THR:HG21	1:L:63:LEU:HD23	1.97	0.46
2:M:25:ASN:OD1	2:M:25:ASN:C	2.58	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:70:ILE:O	2:M:73:TRP:HB3	2.15	0.46
1:L:169:TYR:HA	1:L:174:MET:HE3	1.97	0.46
2:M:242:GLY:HA2	3:H:117:ARG:CD	2.38	0.46
2:M:267:ARG:HD2	3:H:34:GLU:HG2	1.98	0.46
1:L:53:ALA:HB2	1:L:64:ILE:HD13	1.97	0.46
1:L:60:ASN:HA	1:L:61:PRO:HD3	1.75	0.46
1:L:22:PHE:HA	1:L:24:PHE:HE2	1.80	0.46
1:L:124:ALA:HB2	5:L:402:BPH:HAC1	1.97	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
3:H:16:ALA:O	3:H:19:SER:HB2	2.16	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:241:LEU:O	3:H:248:ARG:NH2	2.49	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
1:L:1:ALA:C	1:L:2:LEU:HD23	2.41	0.45
2:M:114:LEU:HD23	2:M:117:ILE:HD12	1.97	0.45
2:M:29:ARG:HA	2:M:51:TYR:HA	1.98	0.45
2:M:65:MET:HE3	7:M:706:LDA:H42	1.98	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
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: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
3:H:193:MET:HE3	3:H:193:MET:HA	1.97	0.45
1:L:135:ARG:HH12	1:L:251:THR:HG22	1.80	0.45
2:M:24:VAL:HG13	2:M:51:TYR:CD2	2.51	0.45
5:M:401:BPH:HBB3	5:M:401:BPH:CHC	2.47	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
1:L:218:ASP:OD1	2:M:29:ARG:HD3	2.17	0.44
3:H:241:LEU:HA	3:H:248:ARG:NH2	2.33	0.44
1:L:2:LEU:HD23	1:L:2:LEU:N	2.32	0.44
3:H:62:LYS:O	3:H:74:THR:HA	2.17	0.44
1:L:54:VAL:HG23	1:L:55:LEU:N	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:24:VAL:HG11	2:M:29:ARG:CZ	2.47	0.44
2:M:151:LEU:HD13	2:M:151:LEU:HA	1.65	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
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.48	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:228:ARG:HG3	2:M:229:PHE:CE1	2.53	0.44
3:H:181:VAL:O	3:H:188:THR:HA	2.17	0.44
2:M:53:GLY:O	2:M:56:GLY:N	2.51	0.44
2:M:148:TRP:HB3	7:M:705:LDA:H61	2.00	0.44
2:M:41:TRP:HA	2:M:41:TRP:CE3	2.53	0.43
2:M:135:LEU:HD23	2:M:135:LEU:HA	1.83	0.43
3:H:209:SER:OG	3:H:212:LEU:HD12	2.17	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
3:H:176:ALA:O	3:H:193:MET:HG2	2.18	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:H61	7:M:705:LDA:H31	1.83	0.43
3:H:148:PRO:CG	3:H:167:ILE:HD11	2.48	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:HA	2:M:235:LEU:HD12	1.62	0.43
2:M:245:ALA:HB1	11:M:807:HOH:O	2.18	0.43
3:H:130:LYS:HD2	11:H:284:HOH:O	2.18	0.43
1:L:261:ASP:O	1:L:264:GLN:HB2	2.19	0.43
1:L:264:GLN:HA	1:L:267:VAL:HG12	2.00	0.43
2:M:94:LEU:HD21	2:M:115:TRP:HA	2.00	0.43
3:H:60:LYS:HA	3:H:61:PRO:HD3	1.78	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:85:LEU:HD23	1:L:85:LEU:HA	1.89	0.42
1:L:223:SER:OG	6:L:502:U10:H3M1	2.19	0.42
2:M:265:ILE:HG21	6:M:501:U10:C3M	2.49	0.42
7:L:707:LDA:H71	7:L:707:LDA:H42	1.88	0.42
2:M:110:LYS:HB2	2:M:110:LYS:HE3	1.69	0.42
2:M:130:TRP:HE1	2:M:151:LEU:HD22	1.84	0.42
2:M:191:LEU:HD13	2:M:191:LEU:HA	1.59	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:152:PRO:HB2	3:H:160:ILE:HD13	2.00	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
3:H:37:ARG:HH21	3:H:61:PRO:HA	1.84	0.42
4:L:302:BCL:H141	4:L:302:BCL:H162	1.90	0.42
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
2:M:251:PHE:CD1	2:M:251:PHE:C	2.97	0.42
1:L:49:ILE:HG12	1:L:89:ILE:HD13	2.02	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
3:H:248:ARG:CZ	3:H:248:ARG:HB2	2.49	0.42
2:M:71:GLY:HA3	10:M:600:SPO:C6	2.50	0.41
3:H:134:MET:HB2	3:H:167:ILE:O	2.19	0.41
1:L:97:PHE:CE1	4:L:302:BCL:H121	2.55	0.41
7:M:703:LDA:H22	7:M:703:LDA:HM11	1.80	0.41
4:L:301:BCL:CBB	4:L:301:BCL:CHC	2.92	0.41
2:M:7:PHE:CE1	7:M:702:LDA:HM22	2.55	0.41
2:M:36:SER:OG	2:M:38:LEU:HB3	2.20	0.41
3:H:98:HIS:HE1	11:H:276:HOH:O	2.03	0.41
1:L:120:ALA:HB1	1:L:238:LEU:HD21	2.01	0.41
4:L:301:BCL:H51	5:M:401:BPH:CMB	2.50	0.41
2:M:77:GLN:NE2	2:M:92:PHE:HB3	2.35	0.41
3:H:148:PRO:HD2	3:H:167:ILE:HD11	2.02	0.41
2:M:122:MET:HE2	4:M:801:BCL:H13	2.02	0.41
2:M:101:TYR:HB3	2:M:104:SER:HB3	2.03	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:165:VAL:O	3:H:166:ASP:HB2	2.21	0.41
1:L:18:GLY:O	1:L:21:LEU:HB2	2.21	0.41
4:L:304:BCL:H161	4:L:304:BCL:H122	1.80	0.41
3:H:12:LEU:HD13	3:H:15:LEU:HD23	2.02	0.41
3:H:103:ASP:OD2	3:H:106:LYS:HD3	2.21	0.41
1:L:204:LYS:HB2	1:L:204:LYS:HE3	1.79	0.41
2:M:291:VAL:HG11	2:M:294:TRP:CD2	2.56	0.41
2:M:293:ASN:OD1	2:M:293:ASN:C	2.63	0.41
7:M:705:LDA:HM13	11:M:803:HOH:O	2.21	0.41
3:H:75:VAL:HA	3:H:76:PRO:C	2.46	0.41
1:L:97:PHE:CZ	4:L:302:BCL:H121	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:304:BCL:H162	4:L:304:BCL:H202	1.85	0.41
1:L:69:PRO:HD3	1:L:83:GLY:O	2.21	0.40
1:L:139:MET:HB3	1:L:144:TYR:CD2	2.56	0.40
1:L:21:LEU:HD13	1:L:22:PHE:CE1	2.56	0.40
1:L:32:GLY:C	1:L:35:GLY:H	2.30	0.40
1:L:65:SER:HB2	1:L:152:THR:HG21	2.03	0.40
1:L:104:GLU:HB3	1:L:118:PRO:HG3	2.03	0.40
1:L:208:THR:O	1:L:211:HIS:HB2	2.21	0.40
2:M:98:ALA:HB3	2:M:101:TYR:HE1	1.86	0.40
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:HH11	1:L:217:ARG:HD3	1.76	0.40
2:M:36:SER:HB3	2:M:39:LEU:HB2	2.03	0.40
2:M:164:ARG:HH12	2:M:173:GLU:CG	2.34	0.40
5:M:401:BPH:H6C2	5:M:401:BPH:H102	1.96	0.40
3:H:195:MET:HE3	3:H:195:MET:HB3	1.91	0.40
2:M:28:ASN:HB3	2:M:52:LEU:O	2.21	0.40
2:M:277:THR:CG2	5:M:401:BPH:HAC2	2.52	0.40
3:H:84:PRO:O	3:H:85:ILE:HD13	2.21	0.40
3:H:247:LYS:O	3:H:249:LYS: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	279/281 (99%)	261 (94%)	15 (5%)	3 (1%)	11	19
2	M	300/307 (98%)	278 (93%)	18 (6%)	4 (1%)	9	16
3	H	238/260 (92%)	215 (90%)	17 (7%)	6 (2%)	4	7
All	All	817/848 (96%)	754 (92%)	50 (6%)	13 (2%)	7	12

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
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%)	191 (87%)	29 (13%)	4	6
2	M	236/240 (98%)	197 (84%)	39 (16%)	2	3
3	H	195/208 (94%)	167 (86%)	28 (14%)	3	4
All	All	651/668 (98%)	555 (85%)	96 (15%)	3	4

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	LEU
1	L	7	ARG
1	L	8	LYS
1	L	10	ARG
1	L	16	LEU
1	L	21	LEU
1	L	38	THR
1	L	44	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	58	THR
1	L	63	LEU
1	L	91	ILE
1	L	102	LEU
1	L	126	LEU
1	L	129	LEU
1	L	136	PRO
1	L	137	VAL
1	L	150	ILE
1	L	153	HIS
1	L	154	LEU
1	L	185	LEU
1	L	202	LYS
1	L	205	GLU
1	L	207	ARG
1	L	210	ASP
1	L	226	THR
1	L	235	LEU
1	L	246	LEU
1	L	251	THR
1	L	271	TRP
2	M	12	VAL
2	M	26	LEU
2	M	29	ARG
2	M	52	LEU
2	M	54	SER
2	M	55	LEU
2	M	60	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	124	VAL
2	M	133	THR
2	M	136	ARG
2	M	144	LYS
2	M	151	LEU
2	M	152	SER
2	M	156	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	188	ASN
2	M	191	LEU
2	M	196	LEU
2	M	199	ASN
2	M	204	LEU
2	M	214	LEU
2	M	215	LEU
2	M	233	ARG
2	M	235	LEU
2	M	247	ARG
2	M	250	LEU
2	M	265	ILE
2	M	270	ILE
2	M	274	VAL
2	M	285	LEU
2	M	290	VAL
2	M	292	ASP
2	M	301	HIS
3	H	12	LEU
3	H	14	SER
3	H	28	ILE
3	H	53	GLN
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	160	ILE
3	H	177	ARG
3	H	184	LYS
3	H	191	LEU
3	H	200	SER
3	H	202	ARG
3	H	203	VAL
3	H	220	LYS
3	H	221	SER
3	H	223	THR
3	H	225	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	231	ASP
3	H	237	VAL
3	H	249	LYS
3	H	250	SER

Sometimes 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	199	ASN
2	M	301	HIS
3	H	44	ASN
3	H	68	HIS
3	H	98	HIS
3	H	201	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
4	BCL	M	801	4,2	69,74,74	1.07	5 (7%)	79,115,115	1.80	12 (15%)
7	LDA	L	708	-	13,15,15	2.11	2 (15%)	14,17,17	0.45	0
4	BCL	L	302	4,1	69,74,74	1.52	10 (14%)	79,115,115	2.14	12 (15%)
9	PO4	M	800	-	4,4,4	1.99	2 (50%)	6,6,6	0.95	0
7	LDA	L	707	-	13,15,15	2.42	2 (15%)	14,17,17	0.43	0
6	U10	L	502	-	48,48,63	2.18	21 (43%)	60,61,79	1.03	4 (6%)
7	LDA	M	703	-	13,15,15	2.74	2 (15%)	14,17,17	0.65	0
7	LDA	L	709	-	13,15,15	2.29	1 (7%)	14,17,17	0.49	0
7	LDA	M	701	-	13,15,15	2.43	2 (15%)	14,17,17	0.40	0
7	LDA	M	706	-	13,15,15	2.25	1 (7%)	14,17,17	0.47	0
6	U10	M	501	-	48,48,63	2.54	21 (43%)	60,61,79	1.28	7 (11%)
5	BPH	L	402	-	59,70,70	1.77	12 (20%)	59,101,101	2.21	14 (23%)
7	LDA	M	702	-	13,15,15	2.34	1 (7%)	14,17,17	0.52	0
5	BPH	M	401	-	59,70,70	1.92	13 (22%)	59,101,101	2.31	12 (20%)
10	SPO	M	600	-	41,41,41	3.21	20 (48%)	47,50,50	2.31	16 (34%)
7	LDA	M	704	-	13,15,15	1.90	1 (7%)	14,17,17	0.51	0
4	BCL	L	304	1	69,74,74	1.32	8 (11%)	79,115,115	2.56	12 (15%)
4	BCL	L	301	2	69,74,74	1.39	8 (11%)	79,115,115	1.96	9 (11%)
7	LDA	M	705	-	13,15,15	2.35	2 (15%)	14,17,17	0.57	0

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
7	LDA	L	707	-	-	7/13/13/13	-
6	U10	L	502	-	-	9/45/69/87	0/1/1/1
7	LDA	M	702	-	-	4/13/13/13	-
7	LDA	M	703	-	-	5/13/13/13	-
7	LDA	L	709	-	-	4/13/13/13	-
7	LDA	M	701	-	-	8/13/13/13	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BPH	M	401	-	-	12/37/105/105	0/5/6/6
4	BCL	L	304	1	1/1/21/25	13/41/137/137	-
4	BCL	M	801	4,2	-	9/41/137/137	-
4	BCL	L	301	2	2/2/21/25	14/41/137/137	-
7	LDA	M	706	-	-	7/13/13/13	-
7	LDA	L	708	-	-	5/13/13/13	-
10	SPO	M	600	-	-	15/47/47/47	-
4	BCL	L	302	4,1	-	8/41/137/137	-
6	U10	M	501	-	-	10/45/69/87	0/1/1/1
5	BPH	L	402	-	-	9/37/105/105	0/5/6/6
7	LDA	M	704	-	-	2/13/13/13	-
7	LDA	M	705	-	-	7/13/13/13	-

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	600	SPO	C15-C16	9.33	1.59	1.34
7	M	701	LDA	O1-N1	-8.37	1.21	1.42
7	M	702	LDA	O1-N1	-8.30	1.21	1.42
7	M	703	LDA	O1-N1	-7.95	1.22	1.42
7	L	709	LDA	O1-N1	-7.94	1.22	1.42
6	M	501	U10	C27-C28	-7.86	1.26	1.50
7	M	706	LDA	O1-N1	-7.77	1.23	1.42
7	L	707	LDA	O1-N1	-7.61	1.23	1.42
6	M	501	U10	O3-C3	7.38	1.54	1.36
7	M	705	LDA	O1-N1	-7.30	1.24	1.42
7	L	708	LDA	O1-N1	-7.20	1.24	1.42
5	M	401	BPH	C3A-C2A	-7.18	1.48	1.54
10	M	600	SPO	C10-C11	7.05	1.53	1.34
10	M	600	SPO	C6-C5	6.94	1.51	1.32
7	M	704	LDA	O1-N1	-6.66	1.25	1.42
5	L	402	BPH	C1D-C2D	6.59	1.46	1.39
7	M	703	LDA	C1-N1	-5.82	1.45	1.51
10	M	600	SPO	C21-C20	5.65	1.51	1.36
4	L	302	BCL	O2D-CED	-5.45	1.33	1.45
10	M	600	SPO	C26-C25	5.21	1.48	1.34
5	M	401	BPH	C1D-C2D	5.10	1.45	1.39
4	L	301	BCL	O2A-CGA	5.05	1.48	1.33
4	L	304	BCL	MG-ND	-4.86	1.96	2.05
5	L	402	BPH	C3A-C2A	-4.71	1.50	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	600	SPO	C15-C14	4.67	1.57	1.43
6	L	502	U10	O3-C3	4.63	1.47	1.36
4	L	304	BCL	O2D-CGD	4.59	1.44	1.33
4	L	302	BCL	C1-C2	-4.57	1.36	1.49
5	M	401	BPH	C2C-C3C	-4.47	1.50	1.54
5	M	401	BPH	O2D-CED	-4.32	1.35	1.45
4	L	301	BCL	MG-ND	-4.27	1.97	2.05
4	L	302	BCL	O2A-CGA	4.19	1.45	1.33
4	L	302	BCL	MG-NA	4.14	2.16	2.06
6	M	501	U10	C17-C18	-4.14	1.38	1.50
7	M	705	LDA	C1-N1	-4.13	1.47	1.51
4	L	304	BCL	MG-NA	4.09	2.16	2.06
6	L	502	U10	O4-C4	4.06	1.46	1.36
7	L	707	LDA	C1-N1	-4.02	1.47	1.51
4	M	801	BCL	MG-NA	4.01	2.15	2.06
4	L	301	BCL	MG-NA	3.88	2.15	2.06
10	M	600	SPO	C10-C9	3.73	1.54	1.43
6	M	501	U10	O4-C4	3.70	1.45	1.36
5	L	402	BPH	C1B-C2B	3.66	1.43	1.39
4	L	301	BCL	O2D-CED	-3.61	1.37	1.45
6	M	501	U10	C37-C38	-3.51	1.39	1.50
6	M	501	U10	C22-C23	-3.51	1.39	1.50
6	M	501	U10	C36-C34	3.51	1.58	1.51
6	L	502	U10	C33-C34	3.51	1.41	1.33
6	L	502	U10	C28-C29	3.47	1.41	1.33
10	M	600	SPO	C4-C5	-3.45	1.45	1.50
6	L	502	U10	C7-C6	3.44	1.57	1.51
5	M	401	BPH	C1B-C2B	3.44	1.43	1.39
5	M	401	BPH	O2D-CGD	3.36	1.41	1.33
6	M	501	U10	C35-C34	3.36	1.58	1.50
6	L	502	U10	C17-C18	-3.36	1.40	1.50
10	M	600	SPO	C11-C12	-3.34	1.38	1.46
10	M	600	SPO	C13-C12	3.33	1.57	1.50
5	L	402	BPH	O2D-CED	-3.30	1.37	1.45
10	M	600	SPO	C31-C32	-3.28	1.40	1.50
10	M	600	SPO	C6-C7	-3.27	1.39	1.46
6	L	502	U10	C23-C24	3.26	1.40	1.33
6	L	502	U10	C36-C34	3.25	1.58	1.51
6	M	501	U10	C33-C34	3.18	1.40	1.33
4	M	801	BCL	C3B-C4B	3.17	1.47	1.41
6	L	502	U10	C8-C9	3.10	1.40	1.33
4	L	302	BCL	C3B-C4B	3.09	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	302	BCL	MG-NC	3.09	2.13	2.06
5	L	402	BPH	O2D-CGD	3.09	1.40	1.33
6	L	502	U10	O4-C4M	-3.08	1.38	1.45
6	L	502	U10	C13-C14	3.06	1.40	1.33
10	M	600	SPO	O1-CM1	3.05	1.52	1.43
5	L	402	BPH	C3B-C2B	-3.01	1.34	1.39
6	L	502	U10	C31-C29	2.98	1.57	1.51
4	L	301	BCL	C3B-C4B	2.95	1.46	1.41
6	M	501	U10	C8-C9	2.92	1.39	1.33
5	M	401	BPH	O2A-CGA	2.92	1.41	1.33
4	L	301	BCL	C2-C3	2.88	1.39	1.33
5	M	401	BPH	CHA-CBD	2.85	1.55	1.51
10	M	600	SPO	C32-C33	2.84	1.39	1.33
5	L	402	BPH	C2-C3	2.83	1.39	1.33
4	L	304	BCL	C3B-C4B	2.83	1.46	1.41
10	M	600	SPO	C25-C23	-2.81	1.39	1.46
6	M	501	U10	C23-C24	2.81	1.39	1.33
4	M	801	BCL	C2-C3	2.80	1.39	1.33
6	L	502	U10	C21-C19	2.79	1.57	1.51
6	L	502	U10	C38-C39	2.78	1.40	1.32
5	L	402	BPH	C2C-C3C	-2.77	1.52	1.54
5	M	401	BPH	C2-C3	2.73	1.39	1.33
4	L	304	BCL	C2-C3	2.70	1.39	1.33
10	M	600	SPO	C37-C38	2.65	1.40	1.32
10	M	600	SPO	C35-C33	2.62	1.56	1.51
5	L	402	BPH	O2A-CGA	2.62	1.41	1.33
6	M	501	U10	O4-C4M	-2.61	1.39	1.45
5	L	402	BPH	CHA-CBD	2.59	1.54	1.51
6	M	501	U10	C13-C14	2.57	1.39	1.33
10	M	600	SPO	C14-C12	2.54	1.41	1.35
6	M	501	U10	C30-C29	2.53	1.56	1.50
4	L	304	BCL	O2A-CGA	2.51	1.40	1.33
6	M	501	U10	C38-C39	2.50	1.40	1.32
6	M	501	U10	C18-C19	2.48	1.38	1.33
6	M	501	U10	C15-C14	2.48	1.56	1.50
6	L	502	U10	C18-C19	2.47	1.38	1.33
5	M	401	BPH	C3D-C2D	-2.47	1.35	1.39
4	M	801	BCL	O2D-CED	-2.44	1.39	1.45
6	M	501	U10	O3-C3M	-2.41	1.39	1.45
6	L	502	U10	C10-C9	2.39	1.56	1.50
6	L	502	U10	C15-C14	2.38	1.56	1.50
9	M	800	PO4	P-O3	-2.31	1.47	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	302	BCL	C4-C3	2.29	1.56	1.50
6	L	502	U10	C16-C14	2.29	1.56	1.51
6	L	502	U10	C35-C34	2.27	1.56	1.50
6	M	501	U10	O2-C2	2.25	1.28	1.23
5	M	401	BPH	C5-C3	2.24	1.55	1.51
10	M	600	SPO	C16-C17	-2.24	1.41	1.46
4	L	302	BCL	CMC-C2C	-2.22	1.48	1.53
4	L	302	BCL	MG-ND	-2.22	2.01	2.05
10	M	600	SPO	O1-C1	2.19	1.53	1.41
5	M	401	BPH	C4D-ND	-2.18	1.35	1.38
4	L	301	BCL	MG-NB	-2.16	2.01	2.05
7	L	708	LDA	C1-N1	-2.16	1.49	1.51
5	L	402	BPH	CMA-C3A	-2.15	1.49	1.53
6	L	502	U10	C7-C8	-2.14	1.47	1.50
5	M	401	BPH	C3B-C4B	2.14	1.44	1.41
4	L	304	BCL	CMB-C2B	-2.11	1.46	1.50
4	M	801	BCL	O2A-CGA	2.11	1.39	1.33
4	L	301	BCL	C1-C2	2.10	1.55	1.49
4	L	304	BCL	O2D-CED	-2.09	1.40	1.45
4	L	302	BCL	O2D-CGD	2.08	1.38	1.33
6	L	502	U10	C25-C24	2.08	1.55	1.50
6	M	501	U10	C40-C39	2.06	1.55	1.50
6	M	501	U10	C7-C8	-2.06	1.47	1.50
5	L	402	BPH	C4-C3	2.04	1.55	1.50
9	M	800	PO4	P-O4	-2.02	1.48	1.54
7	M	701	LDA	C1-N1	-2.01	1.49	1.51

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	304	BCL	CBB-CAB-C3B	-11.54	96.08	120.40
5	M	401	BPH	O2D-CGD-CBD	11.43	123.50	110.95
5	L	402	BPH	O2D-CGD-CBD	10.58	122.58	110.95
4	L	302	BCL	CBB-CAB-C3B	-9.18	101.04	120.40
4	L	304	BCL	C4A-NA-C1A	8.44	110.53	106.68
4	L	302	BCL	C4A-NA-C1A	8.22	110.43	106.68
4	L	304	BCL	O2D-CGD-CBD	8.04	125.28	111.23
4	M	801	BCL	C4A-NA-C1A	7.62	110.16	106.68
4	L	301	BCL	C1-C2-C3	7.44	138.39	126.20
4	L	301	BCL	C4A-NA-C1A	6.98	109.86	106.68
5	M	401	BPH	O1D-CGD-CBD	-6.85	114.34	124.72
4	L	304	BCL	OBB-CAB-C3B	6.84	132.52	120.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	301	BCL	O2D-CGD-CBD	6.45	122.51	111.23
5	L	402	BPH	O1D-CGD-CBD	-6.41	115.00	124.72
4	L	302	BCL	C1C-NC-C4C	6.39	109.59	106.68
10	M	600	SPO	C26-C27-C28	-6.26	118.89	127.69
4	M	801	BCL	O2D-CGD-CBD	5.75	121.29	111.23
4	L	304	BCL	O1D-CGD-CBD	-5.73	113.22	124.52
5	M	401	BPH	C4D-CHA-CBD	-5.72	105.71	108.45
4	L	301	BCL	C1C-NC-C4C	5.66	109.26	106.68
4	L	304	BCL	CAB-C3B-C2B	5.64	139.46	127.74
4	M	801	BCL	C1C-NC-C4C	5.63	109.25	106.68
4	L	304	BCL	C1C-NC-C4C	5.44	109.16	106.68
4	L	302	BCL	O2D-CGD-CBD	5.07	120.09	111.23
4	L	301	BCL	O1D-CGD-CBD	-4.85	114.96	124.52
4	L	302	BCL	CAB-C3B-C2B	4.78	137.68	127.74
10	M	600	SPO	C25-C23-C22	-4.78	111.48	119.01
5	L	402	BPH	C4D-CHA-CBD	-4.71	106.20	108.45
10	M	600	SPO	C20-C21-C22	-4.52	114.28	123.52
4	L	304	BCL	OBB-CAB-CBB	-4.27	110.20	119.77
10	M	600	SPO	C15-C14-C12	-4.25	121.32	127.28
10	M	600	SPO	C15-C16-C17	-4.09	115.15	126.36
10	M	600	SPO	C20-C19-C17	-4.04	121.61	127.28
10	M	600	SPO	C10-C9-C7	-3.99	121.69	127.28
4	L	302	BCL	OBB-CAB-CBB	-3.89	111.06	119.77
4	M	801	BCL	O1D-CGD-CBD	-3.88	116.86	124.52
10	M	600	SPO	C4-C5-C6	-3.83	119.54	124.91
10	M	600	SPO	C5-C6-C7	-3.79	120.16	125.89
5	L	402	BPH	OBD-CAD-CBD	-3.74	120.34	125.82
5	M	401	BPH	OBD-CAD-CBD	-3.64	120.48	125.82
6	M	501	U10	C27-C28-C29	3.64	135.96	127.62
5	M	401	BPH	O2A-CGA-CBA	3.62	122.87	111.83
4	M	801	BCL	O2A-CGA-CBA	3.54	122.64	111.83
5	L	402	BPH	C1-C2-C3	3.42	131.81	126.20
10	M	600	SPO	C18-C17-C19	-3.34	117.40	122.82
4	L	302	BCL	O2A-CGA-CBA	3.28	121.85	111.83
5	L	402	BPH	O2A-CGA-CBA	3.28	121.85	111.83
5	M	401	BPH	OBB-CAB-C3B	3.19	125.31	119.99
4	L	301	BCL	O2A-CGA-CBA	3.16	121.47	111.83
4	L	302	BCL	O1D-CGD-CBD	-3.00	118.59	124.52
4	M	801	BCL	CED-O2D-CGD	2.91	122.51	115.92
5	M	401	BPH	C4D-ND-C1D	-2.90	105.39	108.87
4	L	304	BCL	O2A-CGA-CBA	2.90	120.67	111.83
5	L	402	BPH	C1B-NB-C4B	-2.88	104.61	108.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	801	BCL	OBB-CAB-C3B	2.88	125.53	120.43
4	L	301	BCL	CMB-C2B-C1B	-2.80	121.15	125.42
5	L	402	BPH	C3D-C4D-ND	2.79	111.29	107.71
4	L	302	BCL	OBB-CAB-C3B	2.72	125.23	120.43
6	L	502	U10	C7-C8-C9	2.65	131.40	126.83
6	M	501	U10	C7-C6-C1	-2.65	120.35	124.89
5	L	402	BPH	C4D-ND-C1D	-2.64	105.71	108.87
4	L	304	BCL	C1D-ND-C4D	-2.63	104.47	106.31
4	L	304	BCL	O2A-CGA-O1A	-2.55	117.26	123.63
4	M	801	BCL	C1-C2-C3	2.49	130.27	126.20
4	L	301	BCL	CHB-C1B-NB	2.48	127.77	124.05
5	M	401	BPH	C1B-NB-C4B	-2.46	105.23	108.82
10	M	600	SPO	C21-C22-C23	-2.44	123.86	127.28
4	L	302	BCL	C1-C2-C3	2.44	130.19	126.20
5	M	401	BPH	C3D-C4D-ND	2.38	110.75	107.71
4	L	304	BCL	CAC-C3C-C4C	-2.38	107.31	112.58
5	M	401	BPH	O2A-CGA-O1A	-2.35	117.76	123.63
6	M	501	U10	C25-C24-C26	-2.34	111.16	115.23
4	L	302	BCL	CED-O2D-CGD	2.34	121.22	115.92
6	M	501	U10	C7-C8-C9	2.33	130.85	126.83
10	M	600	SPO	C10-C11-C12	-2.30	120.07	126.36
10	M	600	SPO	C8-C7-C6	2.29	121.59	118.09
6	L	502	U10	C7-C6-C1	-2.29	120.97	124.89
6	L	502	U10	C3M-O3-C3	2.26	124.41	116.47
4	M	801	BCL	CBB-CAB-C3B	-2.25	115.66	120.40
5	L	402	BPH	CMA-C3A-C4A	-2.24	109.78	114.61
4	M	801	BCL	C1D-ND-C4D	-2.24	104.74	106.31
10	M	600	SPO	C6-C7-C9	-2.22	115.51	119.01
5	L	402	BPH	O2A-CGA-O1A	-2.22	118.07	123.63
6	M	501	U10	C3M-O3-C3	2.22	124.25	116.47
4	M	801	BCL	C3A-C2A-C1A	2.19	104.62	101.34
6	M	501	U10	C26-C27-C28	-2.19	101.20	112.02
6	L	502	U10	C4M-O4-C4	2.18	124.14	116.47
4	L	301	BCL	C1D-ND-C4D	-2.18	104.78	106.31
10	M	600	SPO	C11-C12-C14	-2.12	115.68	119.01
5	L	402	BPH	CMD-C2D-C3D	2.11	128.90	124.68
4	M	801	BCL	O2A-CGA-O1A	-2.10	118.38	123.63
4	L	302	BCL	C2B-C1B-NB	-2.08	108.17	110.33
5	L	402	BPH	OBD-CAD-C3D	2.07	131.12	127.89
10	M	600	SPO	C24-C23-C25	2.06	121.24	118.09
6	M	501	U10	C4M-O4-C4	2.05	123.66	116.47
5	M	401	BPH	C2D-C1D-ND	2.03	110.90	109.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	402	BPH	OBB-CAB-C3B	2.02	123.38	119.99
5	M	401	BPH	C4A-C3A-C2A	2.02	104.76	102.84

All (3) chirality outliers are listed below:

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

All (148) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	301	BCL	C1A-C2A-CAA-CBA
4	L	301	BCL	C4C-C3C-CAC-CBC
4	L	301	BCL	O2A-C1-C2-C3
4	L	302	BCL	C2B-C3B-CAB-OBB
4	L	302	BCL	C2B-C3B-CAB-CBB
4	L	302	BCL	C4B-C3B-CAB-OBB
4	L	304	BCL	C2B-C3B-CAB-OBB
4	L	304	BCL	C2B-C3B-CAB-CBB
4	L	304	BCL	C2C-C3C-CAC-CBC
4	L	304	BCL	C4C-C3C-CAC-CBC
4	L	304	BCL	CHA-CBD-CGD-O1D
4	L	304	BCL	CHA-CBD-CGD-O2D
5	L	402	BPH	C4C-C3C-CAC-CBC
5	L	402	BPH	C2C-C3C-CAC-CBC
5	M	401	BPH	C4C-C3C-CAC-CBC
5	M	401	BPH	C2C-C3C-CAC-CBC
6	L	502	U10	C23-C24-C26-C27
6	L	502	U10	C25-C24-C26-C27
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	L	709	LDA	N1-C1-C2-C3
7	M	701	LDA	C2-C1-N1-O1
7	M	701	LDA	C2-C1-N1-CM1
7	M	702	LDA	N1-C1-C2-C3
7	M	703	LDA	C2-C1-N1-O1
7	M	703	LDA	C2-C1-N1-CM1
7	M	705	LDA	C2-C1-N1-CM1
7	M	705	LDA	C2-C1-N1-CM2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	M	706	LDA	C2-C1-N1-O1
7	M	706	LDA	C2-C1-N1-CM1
7	M	706	LDA	N1-C1-C2-C3
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
4	L	304	BCL	CBD-CGD-O2D-CED
10	M	600	SPO	C36-C37-C38-C40
4	L	304	BCL	O1D-CGD-O2D-CED
5	L	402	BPH	C3-C5-C6-C7
6	L	502	U10	C35-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	L	502	U10	C33-C34-C36-C37
6	M	501	U10	C24-C26-C27-C28
5	M	401	BPH	CBA-CGA-O2A-C1
4	M	801	BCL	C3-C5-C6-C7
5	M	401	BPH	O1A-CGA-O2A-C1
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
7	M	703	LDA	C7-C8-C9-C10
4	L	301	BCL	C16-C17-C18-C20
7	M	702	LDA	C7-C8-C9-C10
5	M	401	BPH	CBD-CGD-O2D-CED
7	L	708	LDA	C4-C5-C6-C7
7	M	705	LDA	C2-C3-C4-C5
7	L	708	LDA	C6-C7-C8-C9
7	M	703	LDA	C6-C7-C8-C9
10	M	600	SPO	C19-C20-C21-C22
6	M	501	U10	C35-C34-C36-C37
7	M	701	LDA	C7-C8-C9-C10
6	M	501	U10	C33-C34-C36-C37
7	M	701	LDA	C1-C2-C3-C4
7	L	709	LDA	C2-C3-C4-C5
7	M	706	LDA	C2-C3-C4-C5
4	L	301	BCL	C6-C7-C8-C10
5	L	402	BPH	C11-C10-C8-C7
4	L	304	BCL	C4B-C3B-CAB-OB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	M	401	BPH	O1D-CGD-O2D-CED
4	L	301	BCL	C6-C7-C8-C9
7	L	707	LDA	C2-C3-C4-C5
4	L	304	BCL	C15-C16-C17-C18
7	M	706	LDA	C4-C5-C6-C7
5	L	402	BPH	O2A-C1-C2-C3
5	M	401	BPH	O2A-C1-C2-C3
6	M	501	U10	C14-C16-C17-C18
7	L	709	LDA	C3-C4-C5-C6
7	M	703	LDA	C11-C10-C9-C8
7	M	705	LDA	C1-C2-C3-C4
4	L	301	BCL	C10-C11-C12-C13
4	L	302	BCL	C11-C12-C13-C15
4	L	301	BCL	C3A-C2A-CAA-CBA
6	M	501	U10	C25-C24-C26-C27
7	M	701	LDA	C9-C10-C11-C12
6	M	501	U10	C30-C29-C31-C32
6	M	501	U10	C23-C24-C26-C27
4	L	301	BCL	C8-C10-C11-C12
7	M	701	LDA	C4-C5-C6-C7
6	M	501	U10	C28-C29-C31-C32
4	M	801	BCL	C4B-C3B-CAB-CBB
6	L	502	U10	C14-C16-C17-C18
6	M	501	U10	C29-C31-C32-C33
4	L	301	BCL	C16-C17-C18-C19
7	M	705	LDA	C6-C7-C8-C9
5	L	402	BPH	C11-C10-C8-C9
7	L	708	LDA	C11-C10-C9-C8
10	M	600	SPO	C35-C36-C37-C38
7	L	707	LDA	C2-C1-N1-CM2
7	M	701	LDA	C2-C1-N1-CM2
7	M	706	LDA	C2-C1-N1-CM2
4	L	304	BCL	C6-C7-C8-C10
4	L	302	BCL	C16-C17-C18-C20
7	M	705	LDA	C5-C6-C7-C8
4	L	304	BCL	C6-C7-C8-C9
10	M	600	SPO	C4-C1-O1-CM1
7	M	704	LDA	C3-C4-C5-C6
4	L	301	BCL	CHA-CBD-CGD-O1D
4	L	301	BCL	CHA-CBD-CGD-O2D
7	M	704	LDA	C5-C6-C7-C8
7	M	701	LDA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	L	302	BCL	C11-C12-C13-C14
5	M	401	BPH	C11-C10-C8-C9
7	L	708	LDA	C2-C3-C4-C5
10	M	600	SPO	C2-C1-O1-CM1
7	L	707	LDA	C4-C5-C6-C7
4	M	801	BCL	C10-C11-C12-C13
5	M	401	BPH	C11-C10-C8-C7
7	L	709	LDA	C5-C6-C7-C8
7	L	707	LDA	C3-C4-C5-C6
10	M	600	SPO	C18-C17-C19-C20
10	M	600	SPO	C29-C28-C30-C31
10	M	600	SPO	C28-C30-C31-C32
4	L	304	BCL	C11-C10-C8-C9
4	M	801	BCL	C6-C7-C8-C9
10	M	600	SPO	C16-C17-C19-C20
7	M	702	LDA	C5-C6-C7-C8
6	L	502	U10	C2-C3-O3-C3M
7	M	702	LDA	C6-C7-C8-C9
6	L	502	U10	C26-C27-C28-C29
6	L	502	U10	C12-C11-C9-C10
5	L	402	BPH	CHA-CBD-CGD-O1D
5	L	402	BPH	C6-C7-C8-C9
6	M	501	U10	C5-C4-O4-C4M
7	L	708	LDA	C3-C4-C5-C6
4	L	301	BCL	CBA-CGA-O2A-C1
4	M	801	BCL	C6-C7-C8-C10
5	L	402	BPH	C6-C7-C8-C10
4	L	301	BCL	C2-C1-O2A-CGA
10	M	600	SPO	C3-C1-O1-CM1
7	M	706	LDA	C6-C7-C8-C9
7	M	705	LDA	C3-C4-C5-C6
4	M	801	BCL	C2B-C3B-CAB-CBB
5	M	401	BPH	C10-C11-C12-C13
4	L	302	BCL	O1A-CGA-O2A-C1
4	M	801	BCL	CAA-CBA-CGA-O2A

There are no ring outliers.

16 monomers are involved in 97 short contacts:

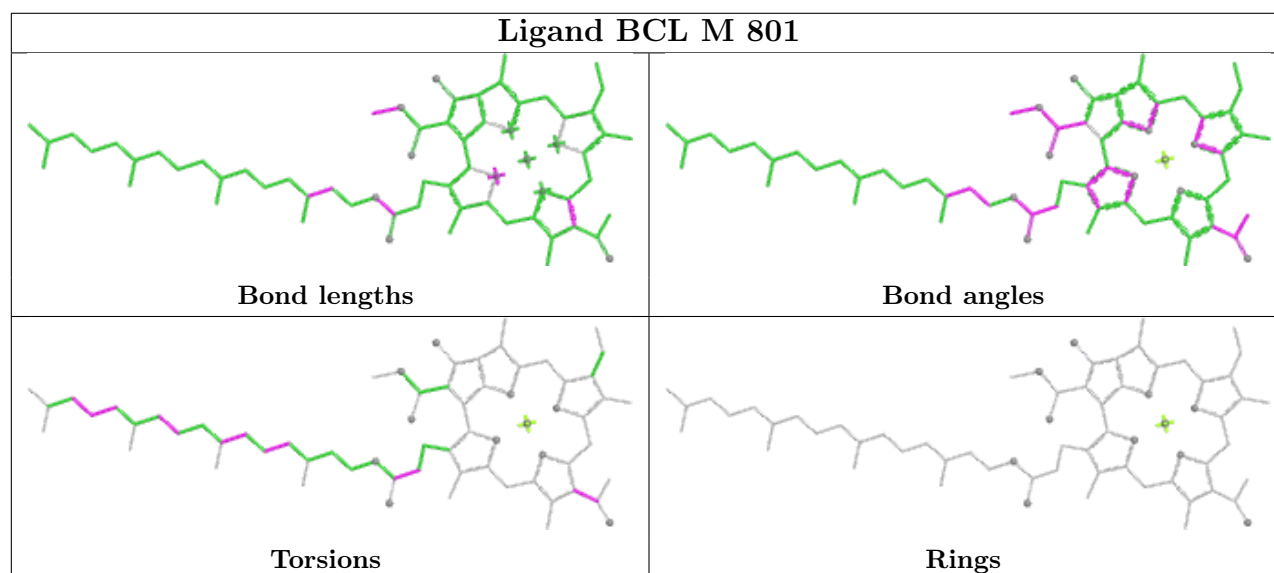
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	801	BCL	15	0
7	L	708	LDA	1	0

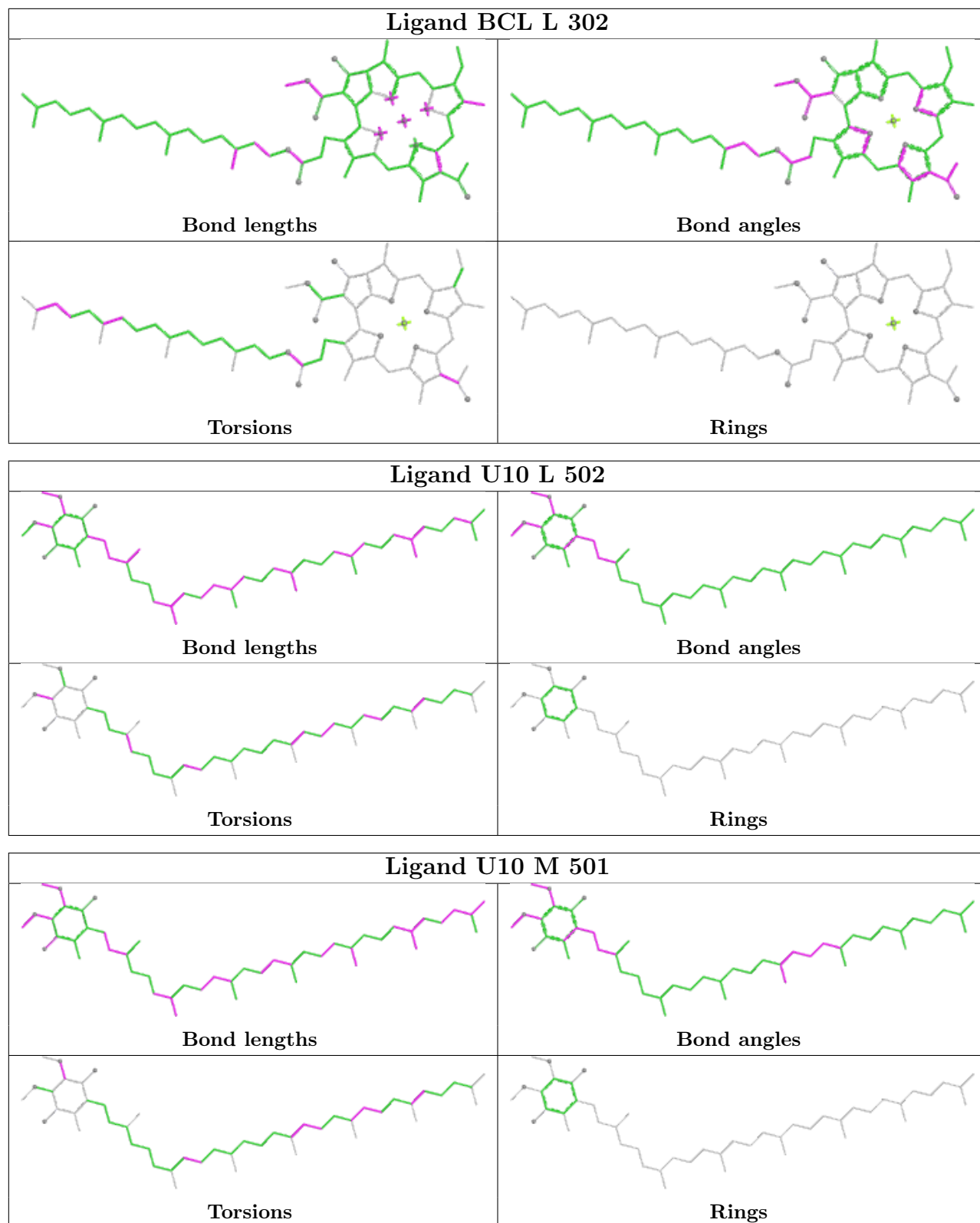
Continued on next page...

Continued from previous page...

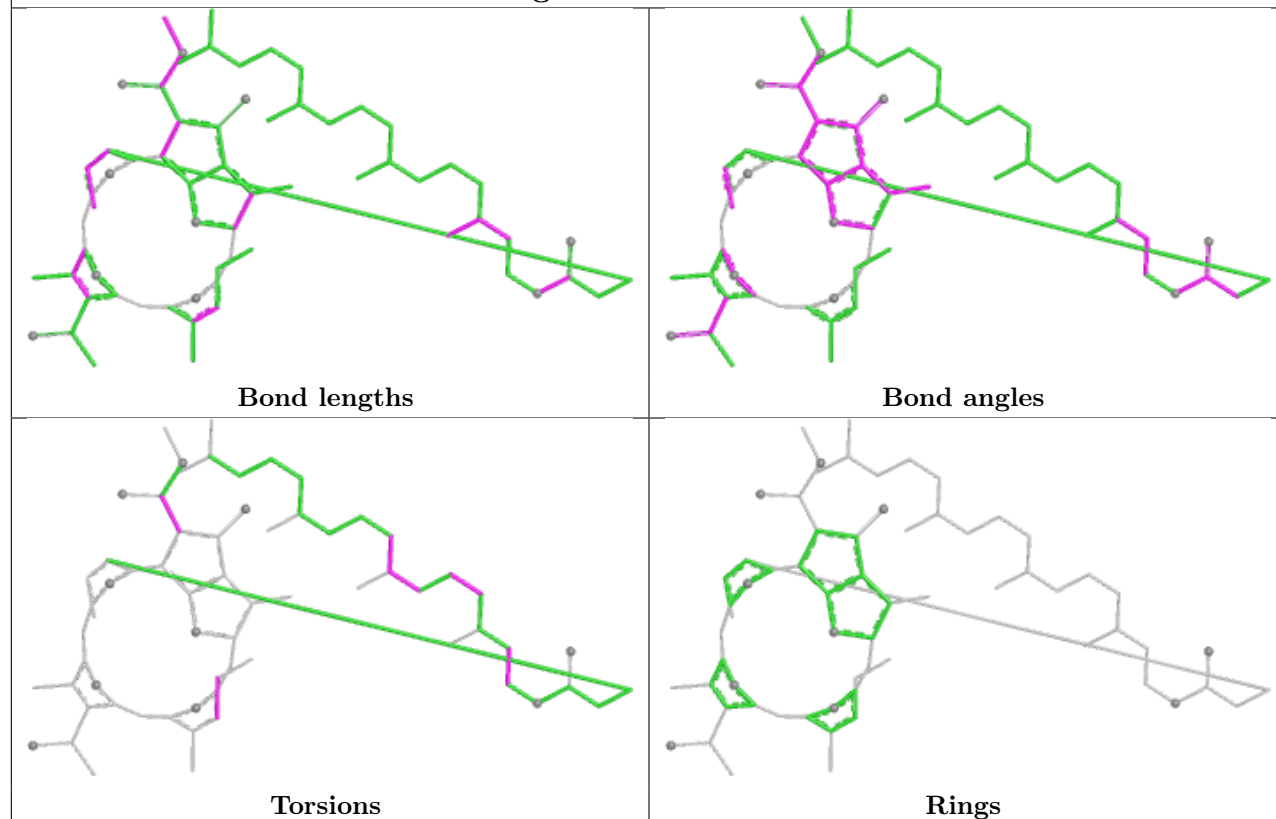
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	302	BCL	10	0
7	L	707	LDA	1	0
6	L	502	U10	9	0
7	M	703	LDA	8	0
7	M	701	LDA	4	0
7	M	706	LDA	6	0
6	M	501	U10	8	0
5	L	402	BPH	12	0
7	M	702	LDA	7	0
5	M	401	BPH	9	0
10	M	600	SPO	7	0
4	L	304	BCL	4	0
4	L	301	BCL	10	0
7	M	705	LDA	4	0

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.

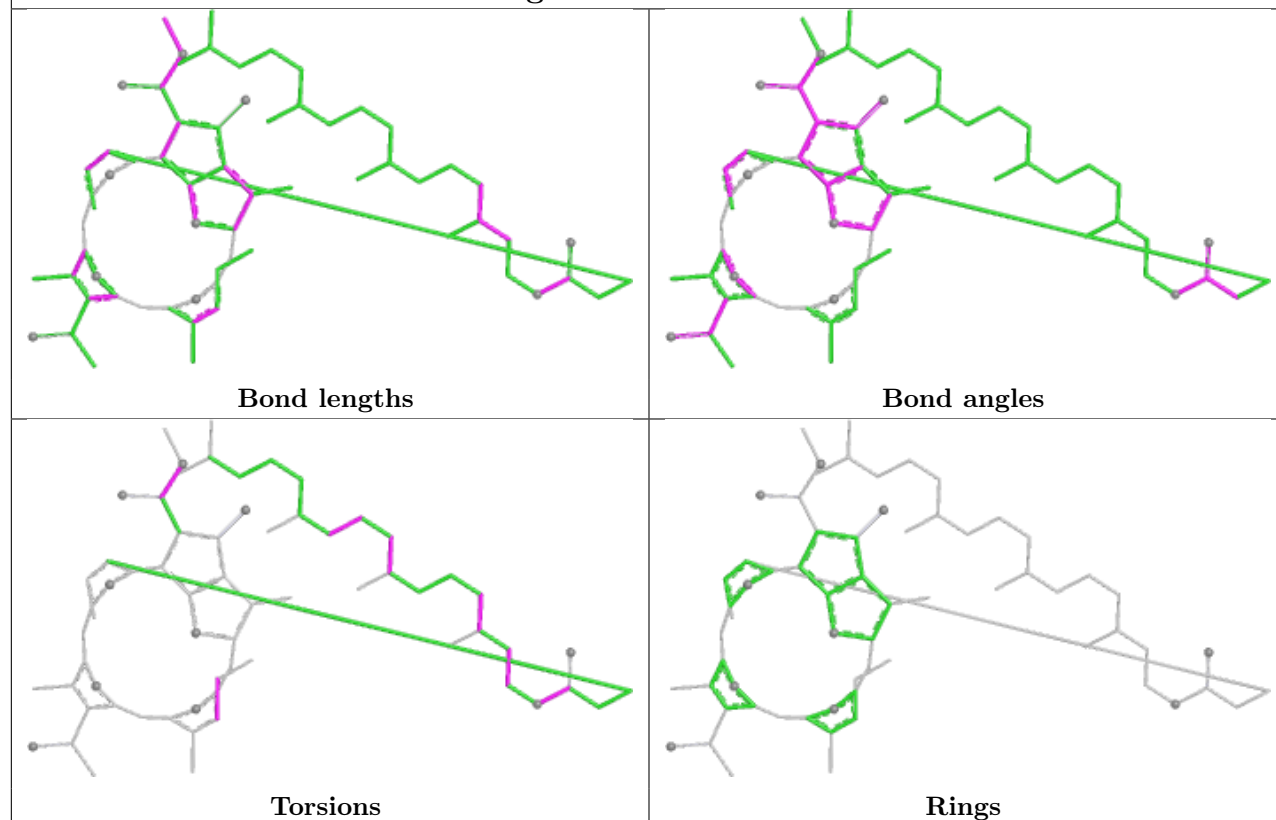


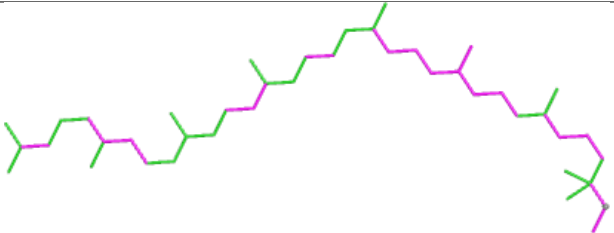
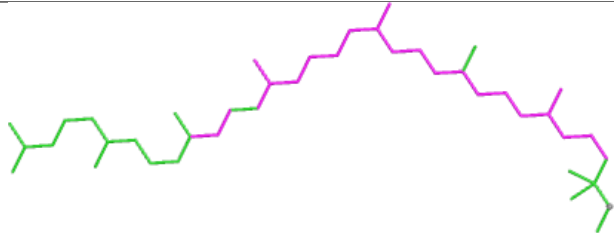
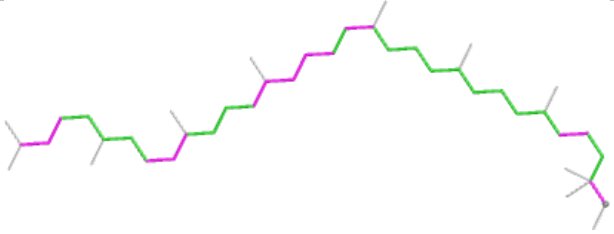
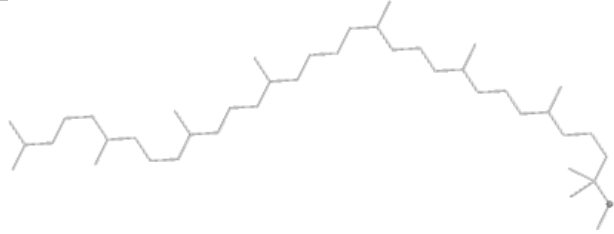


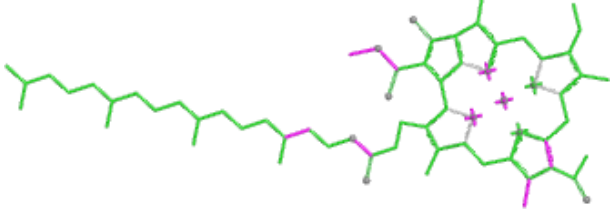
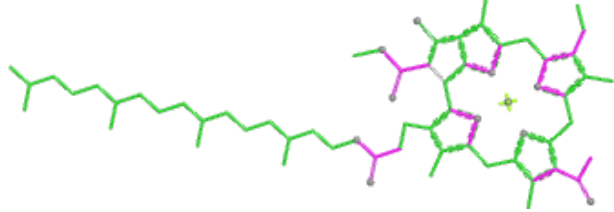
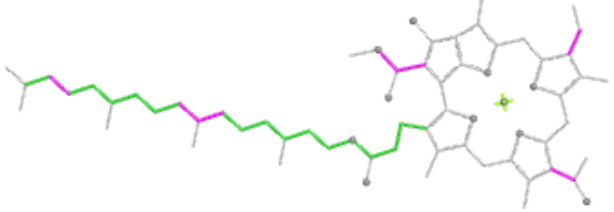
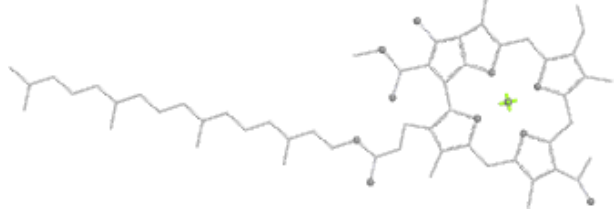
Ligand BPH L 402

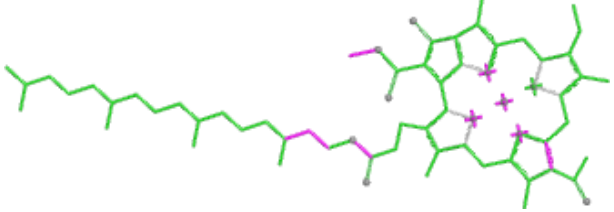
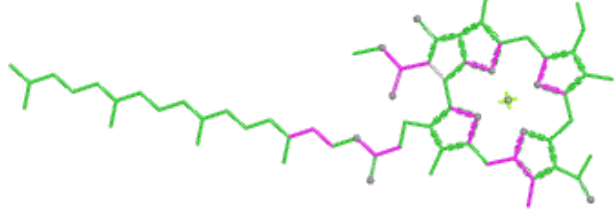
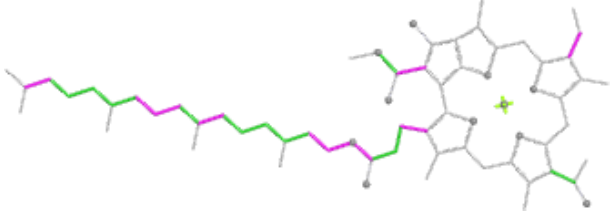
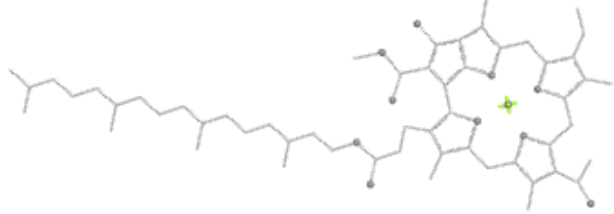


Ligand BPH M 401



Ligand SPO M 600	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL L 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL L 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

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.