



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:06 PM GMT

PDB ID : 1E14  
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH PHE M197 REPLACED WITH ARG (CHAIN M, FM197R) AND GLY M203 REPLACED WITH ASP (CHAIN M, GM203D)  
Authors : Fyfe, P.K.; Ridge, J.P.; Mcauley, K.E.; Cogdell, R.J.; Isaacs, N.W.; Jones, M.R.  
Deposited on : 2000-04-18  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

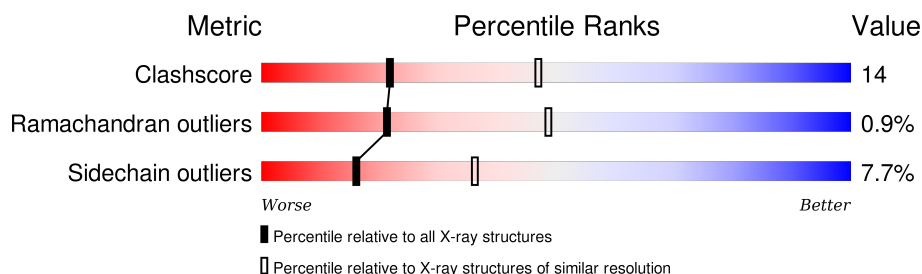
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	260	
2	L	281	
3	M	307	

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	M	1301	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BPH	L	401	X	-	-	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7250 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 H SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	0	0	1
			1830	1169	315	337	9			

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

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

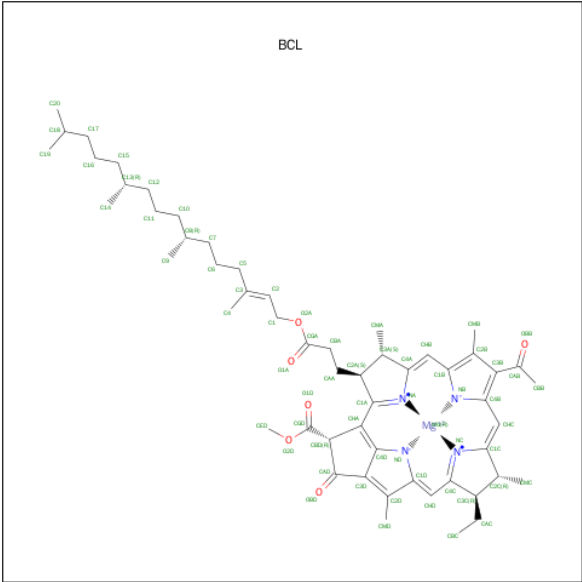
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER M SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2413	1606	398	399	10			

There are 2 discrepancies between the modelled and reference sequences:

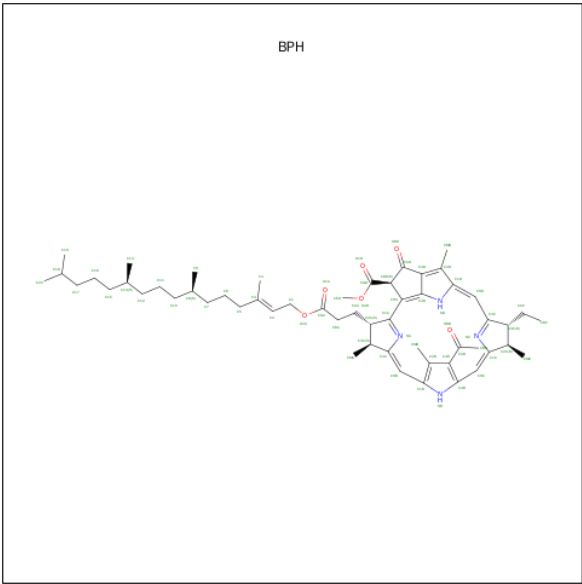
Chain	Residue	Modelled	Actual	Comment	Reference
M	197	ARG	PHE	ENGINEERED MUTATION	UNP P02953
M	203	ASP	GLY	ENGINEERED MUTATION	UNP P02953

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



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

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>).

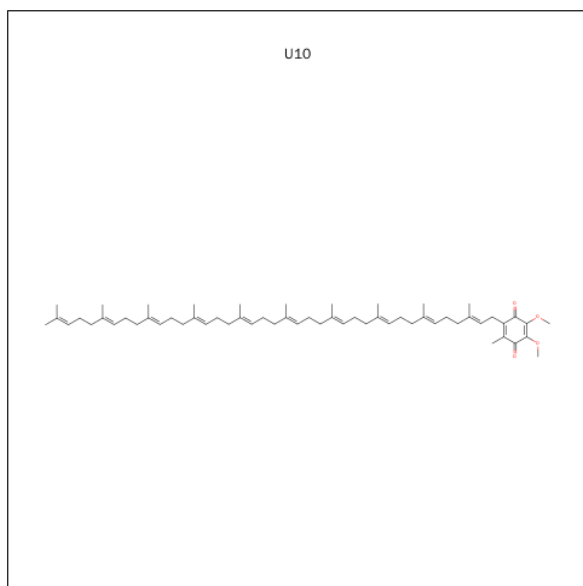


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

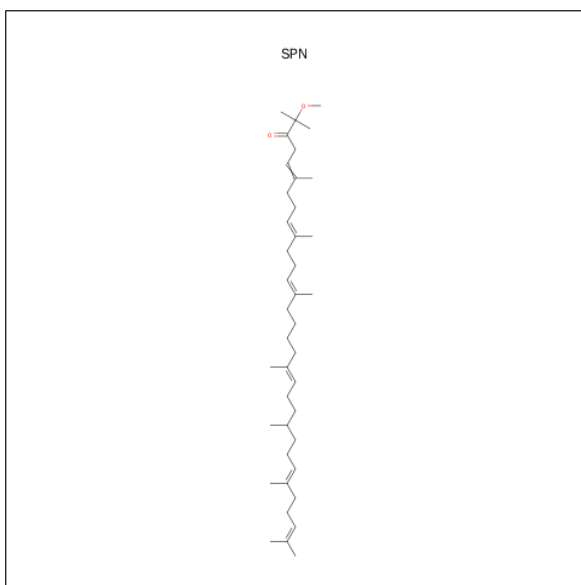
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total	Fe	0	0
			1	1		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).



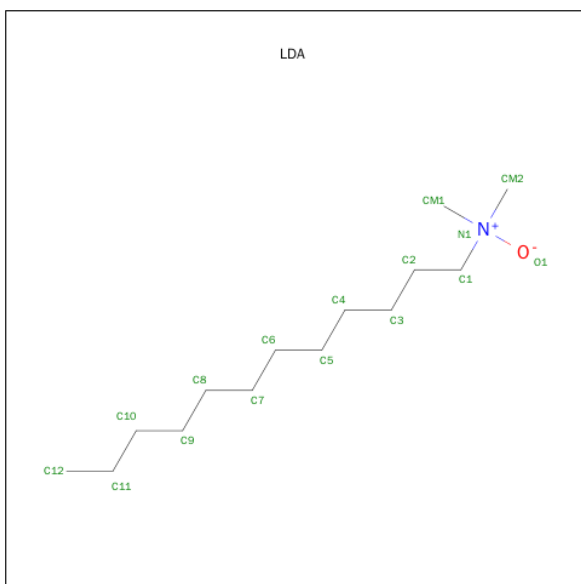
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	22	0
			48	44	4		
7	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is SPEROIDENONE (three-letter code: SPN) (formula: C<sub>41</sub>H<sub>70</sub>O<sub>2</sub>).



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

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



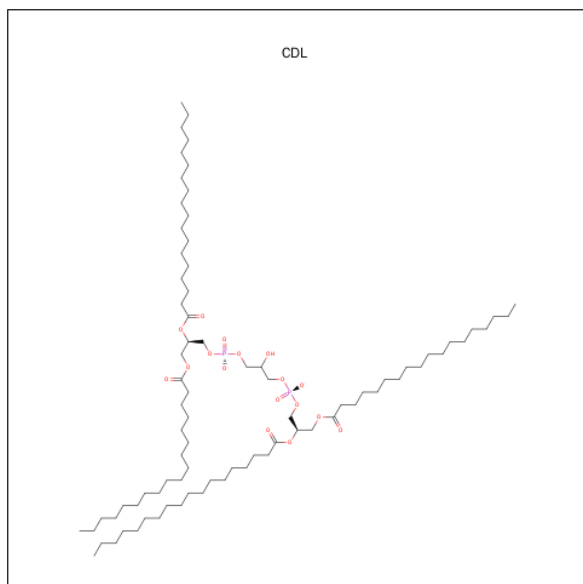
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	H	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		

*Continued on next page...*

*Continued from previous page...*

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

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



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	42	Total	O	0	0
			42	42		
11	L	28	Total	O	0	0
			28	28		
11	M	42	Total	O	0	0
			42	42		



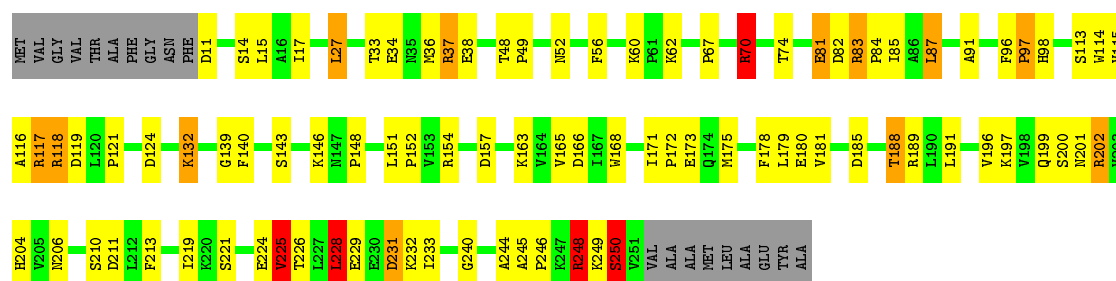
### 3 Residue-property plots

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

Note EDS was not executed.

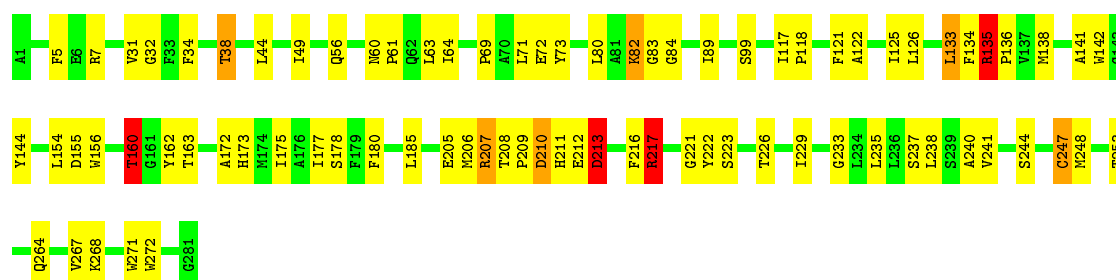
#### • Molecule 1: PHOTOSYNTHETIC REACTION CENTER H SUBUNIT

Chain H: 



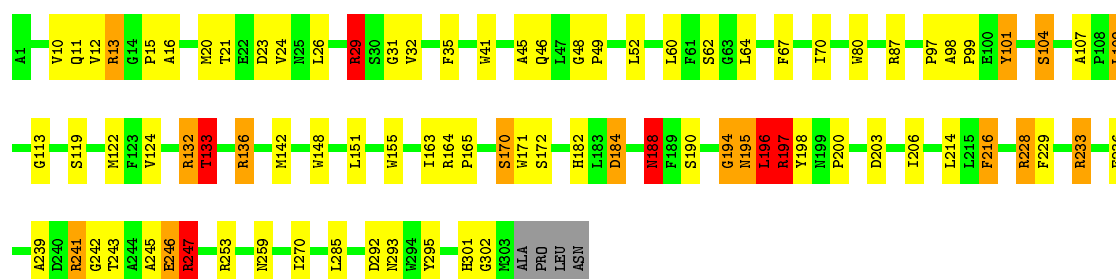
#### • Molecule 2: PHOTOSYNTHETIC REACTION CENTER L SUBUNIT

Chain L: 



#### • Molecule 3: PHOTOSYNTHETIC REACTION CENTER M SUBUNIT

Chain M: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.00 Å   140.00 Å   184.60 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	92.6 (30.00-2.70)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.226 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7250	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LDA, CDL, BPH, FE, SPN, 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	H	0.66	0/1878	1.75	30/2555 (1.2%)
2	L	0.63	0/2320	1.48	12/3175 (0.4%)
3	M	0.61	0/2504	1.56	36/3419 (1.1%)
All	All	0.63	0/6702	1.59	78/9149 (0.9%)

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	H	0	7
2	L	0	5
3	M	0	2
All	All	0	14

There are no bond length outliers.

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	70	ARG	NE-CZ-NH2	-21.92	109.34	120.30
3	M	247	ARG	NE-CZ-NH1	17.87	129.24	120.30
2	L	135	ARG	NE-CZ-NH1	16.24	128.42	120.30
2	L	135	ARG	CD-NE-CZ	15.24	144.93	123.60
2	L	135	ARG	NE-CZ-NH2	-14.98	112.81	120.30
1	H	117	ARG	NE-CZ-NH2	-14.97	112.82	120.30
1	H	37	ARG	NE-CZ-NH1	-14.23	113.18	120.30
3	M	132	ARG	NE-CZ-NH1	-14.16	113.22	120.30
2	L	217	ARG	NE-CZ-NH1	14.12	127.36	120.30
3	M	241	ARG	NE-CZ-NH2	-13.14	113.73	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	202	ARG	NE-CZ-NH1	11.98	126.29	120.30
1	H	118	ARG	NE-CZ-NH2	-11.66	114.47	120.30
1	H	70	ARG	NE-CZ-NH1	11.11	125.85	120.30
1	H	83	ARG	CD-NE-CZ	11.06	139.08	123.60
2	L	217	ARG	CD-NE-CZ	10.66	138.53	123.60
3	M	241	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	H	70	ARG	CD-NE-CZ	10.20	137.88	123.60
3	M	29	ARG	NE-CZ-NH2	-10.11	115.25	120.30
3	M	13	ARG	NE-CZ-NH2	-9.97	115.32	120.30
2	L	155	ASP	CB-CG-OD2	-9.91	109.38	118.30
3	M	198	TYR	CB-CG-CD2	9.38	126.63	121.00
1	H	117	ARG	CD-NE-CZ	8.52	135.52	123.60
3	M	253	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	H	189	ARG	CD-NE-CZ	8.27	135.18	123.60
1	H	224	GLU	OE1-CD-OE2	8.22	133.17	123.30
3	M	247	ARG	CD-NE-CZ	8.17	135.03	123.60
1	H	211	ASP	CB-CG-OD2	-8.06	111.04	118.30
3	M	241	ARG	CD-NE-CZ	8.02	134.83	123.60
3	M	136	ARG	NE-CZ-NH1	7.80	124.20	120.30
2	L	213	ASP	CB-CG-OD2	7.72	125.25	118.30
3	M	247	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	H	37	ARG	NE-CZ-NH2	7.54	124.07	120.30
3	M	188	ASN	OD1-CG-ND2	7.39	138.89	121.90
2	L	31	VAL	CA-C-N	7.36	130.93	116.20
3	M	136	ARG	NE-CZ-NH2	7.27	123.93	120.30
3	M	132	ARG	NE-CZ-NH2	7.21	123.91	120.30
3	M	198	TYR	CG-CD1-CE1	7.09	126.97	121.30
3	M	228	ARG	NE-CZ-NH1	-6.97	116.82	120.30
3	M	136	ARG	NH1-CZ-NH2	-6.86	111.86	119.40
2	L	217	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	H	231	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	H	225	VAL	CB-CA-C	-6.44	99.16	111.40
1	H	228	LEU	CA-CB-CG	6.42	130.08	115.30
1	H	211	ASP	CB-CG-OD1	6.34	124.01	118.30
3	M	29	ARG	NE-CZ-NH1	6.33	123.46	120.30
3	M	23	ASP	CB-CG-OD2	-6.28	112.64	118.30
1	H	81	GLU	OE1-CD-OE2	6.19	130.73	123.30
3	M	253	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	L	31	VAL	C-N-CA	-6.11	109.47	122.30
1	H	163	LYS	CA-CB-CG	6.03	126.66	113.40
3	M	29	ARG	CD-NE-CZ	6.03	132.04	123.60
3	M	233	ARG	NE-CZ-NH2	-6.01	117.30	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	101	TYR	CB-CG-CD1	5.95	124.57	121.00
1	H	119	ASP	C-N-CA	5.92	136.50	121.70
3	M	246	GLU	CG-CD-OE2	-5.88	106.53	118.30
3	M	101	TYR	CB-CG-CD2	-5.71	117.57	121.00
3	M	133	THR	CA-CB-CG2	5.68	120.35	112.40
1	H	175	MET	CA-CB-CG	5.62	122.86	113.30
3	M	12	VAL	N-CA-CB	-5.61	99.15	111.50
3	M	236	GLU	OE1-CD-OE2	-5.61	116.57	123.30
3	M	87	ARG	NE-CZ-NH1	-5.58	117.51	120.30
3	M	188	ASN	CA-CB-CG	-5.54	101.21	113.40
3	M	182	HIS	CA-CB-CG	5.53	123.00	113.60
1	H	117	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	H	67	PRO	N-CA-C	5.49	126.37	112.10
3	M	184	ASP	CB-CG-OD1	5.41	123.17	118.30
2	L	31	VAL	O-C-N	-5.33	114.14	123.20
1	H	132	LYS	CB-CA-C	-5.29	99.81	110.40
1	H	202	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	H	11	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	H	152	PRO	N-CA-CB	5.26	109.62	103.30
1	H	248	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	L	222	TYR	CB-CG-CD2	5.23	124.14	121.00
3	M	292	ASP	CB-CG-OD2	-5.15	113.67	118.30
3	M	197	ARG	NE-CZ-NH1	5.13	122.87	120.30
3	M	188	ASN	CB-CG-OD1	-5.11	111.38	121.60
1	H	118	ARG	CD-NE-CZ	-5.08	116.48	123.60
1	H	97	PRO	N-CA-CB	5.02	109.33	103.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	113	SER	Mainchain
1	H	114	TRP	Mainchain
1	H	115	VAL	Mainchain
1	H	185	ASP	Mainchain
1	H	250	SER	Mainchain
1	H	87	LEU	Mainchain
1	H	91	ALA	Mainchain
2	L	141	ALA	Mainchain
2	L	160	THR	Mainchain
2	L	162	TYR	Mainchain
2	L	213	ASP	Mainchain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	L	253	THR	Mainchain
3	M	196	LEU	Mainchain
3	M	29	ARG	Mainchain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1830	0	1836	61	0
2	L	2232	0	2187	59	0
3	M	2413	0	2326	58	0
4	L	132	0	148	15	0
4	M	132	0	148	10	0
5	L	65	0	76	10	0
5	M	65	0	76	3	0
6	M	1	0	0	0	0
7	L	48	0	58	1	0
7	M	48	0	63	0	0
8	M	43	0	69	5	0
9	H	16	0	31	0	0
9	M	32	0	62	5	0
10	M	81	0	106	16	0
11	H	42	0	0	3	0
11	L	28	0	0	1	0
11	M	42	0	0	1	0
All	All	7250	0	7186	200	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 14.

All (200) 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)
10:M:800:CDL:CA6	10:M:800:CDL:HB4	1.62	1.28
10:M:800:CDL:HA61	10:M:800:CDL:HB4	1.10	1.10
10:M:800:CDL:CB4	10:M:800:CDL:HA61	1.83	1.08

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:27:LEU:HD23	10:M:800:CDL:H132	1.51	0.92
2:L:206:MET:HE1	3:M:239:ALA:HB2	1.51	0.89
10:M:800:CDL:HA62	10:M:800:CDL:HB4	1.55	0.86
1:H:81:GLU:HG3	1:H:85:ILE:HD11	1.57	0.86
10:M:800:CDL:CA7	10:M:800:CDL:OB7	2.25	0.84
3:M:31:GLY:H	9:M:702:LDA:H92	1.40	0.84
3:M:197:ARG:HH11	3:M:197:ARG:HG3	1.44	0.81
1:H:154:ARG:HE	1:H:204:HIS:HD2	1.29	0.80
10:M:800:CDL:HA61	10:M:800:CDL:CB6	2.13	0.78
3:M:197:ARG:HG3	3:M:197:ARG:NH1	1.97	0.77
1:H:154:ARG:HE	1:H:204:HIS:CD2	2.03	0.76
2:L:154:LEU:HB3	3:M:197:ARG:HG2	1.67	0.76
10:M:800:CDL:C31	10:M:800:CDL:OB7	2.34	0.75
1:H:132:LYS:HG3	1:H:171:ILE:HD13	1.72	0.72
1:H:70:ARG:O	1:H:118:ARG:NH2	2.24	0.71
1:H:96:PHE:HB3	1:H:97:PRO:CD	2.20	0.70
3:M:203:ASP:HB2	9:M:703:LDA:HM11	1.73	0.68
4:M:1303:BCL:HBB3	4:M:1303:BCL:HMB1	1.76	0.68
2:L:221:GLY:HA3	9:M:702:LDA:HM21	1.75	0.67
2:L:267:VAL:HG13	2:L:268:LYS:HD3	1.76	0.66
4:L:1302:BCL:OBB	4:L:1302:BCL:HHC	1.93	0.66
2:L:208:THR:HB	2:L:209:PRO:HD2	1.77	0.66
3:M:190:SER:HA	3:M:196:LEU:HD13	1.78	0.65
1:H:171:ILE:N	1:H:172:PRO:HD2	2.11	0.65
2:L:135:ARG:HB2	2:L:136:PRO:HD3	1.78	0.65
2:L:221:GLY:HA3	9:M:702:LDA:CM2	2.26	0.65
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.44	0.64
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.16	0.63
4:L:1304:BCL:C1C	4:L:1304:BCL:CBC	2.77	0.63
1:H:96:PHE:HB3	1:H:97:PRO:HD2	1.79	0.63
2:L:34:PHE:O	2:L:38:THR:HG23	1.99	0.62
2:L:49:ILE:HG12	2:L:89:ILE:HD13	1.79	0.62
2:L:71:LEU:H	2:L:71:LEU:HD12	1.64	0.62
4:L:1302:BCL:HBD	4:L:1304:BCL:HAC1	1.81	0.62
4:M:1303:BCL:CBB	4:M:1303:BCL:HMB1	2.29	0.62
1:H:197:LYS:NZ	1:H:199:GLN:HE21	1.98	0.62
2:L:264:GLN:HA	2:L:267:VAL:HG12	1.83	0.60
1:H:14:SER:HA	1:H:17:ILE:HG22	1.82	0.60
3:M:197:ARG:HH11	3:M:197:ARG:CG	2.13	0.60
4:M:1301:BCL:H61	4:M:1303:BCL:H18	1.83	0.60
1:H:132:LYS:HG3	1:H:171:ILE:CD1	2.32	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:101:TYR:O	3:M:104:SER:HB3	2.02	0.59
2:L:156:TRP:O	2:L:160:THR:HG23	2.02	0.59
2:L:5:PHE:CD1	3:M:246:GLU:HG2	2.37	0.59
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.84	0.59
10:M:800:CDL:OB7	10:M:800:CDL:H312	2.03	0.58
3:M:70:ILE:HD13	8:M:600:SPN:H102	1.86	0.58
4:M:1301:BCL:HHC	4:M:1301:BCL:OBB	2.04	0.57
2:L:5:PHE:CE1	3:M:246:GLU:HG2	2.40	0.57
1:H:219:ILE:HG21	1:H:225:VAL:HG13	1.86	0.56
10:M:800:CDL:HA61	10:M:800:CDL:HB61	1.86	0.56
3:M:233:ARG:HA	11:M:2031:HOH:O	2.06	0.56
1:H:117:ARG:HD3	3:M:242:GLY:CA	2.36	0.56
4:L:1304:BCL:HBB2	4:L:1304:BCL:HMB1	1.88	0.56
3:M:16:ALA:HB1	3:M:32:VAL:HG21	1.89	0.55
2:L:229:ILE:HG13	2:L:229:ILE:O	2.06	0.55
1:H:121:PRO:HB3	1:H:225:VAL:O	2.06	0.55
3:M:170:SER:HG	3:M:172:SER:HG	1.53	0.55
2:L:49:ILE:CG1	2:L:89:ILE:HD13	2.37	0.55
2:L:156:TRP:CE2	2:L:160:THR:HG21	2.42	0.55
1:H:34:GLU:OE1	1:H:37:ARG:NH1	2.40	0.55
3:M:21:THR:HG23	3:M:26:LEU:HD11	1.87	0.54
2:L:121:PHE:CE2	2:L:125:ILE:HD11	2.43	0.54
4:L:1302:BCL:HBB3	4:L:1302:BCL:HMB1	1.89	0.54
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.89	0.54
5:L:401:BPH:OBB	5:L:401:BPH:HHC	2.08	0.54
1:H:249:LYS:O	1:H:250:SER:HB2	2.08	0.54
3:M:97:PRO:HG2	3:M:171:TRP:HB2	1.90	0.54
5:M:402:BPH:HHH	5:M:402:BPH:HBC3	1.90	0.53
1:H:146:LYS:HE2	1:H:200:SER:O	2.09	0.52
1:H:139:GLY:HA3	3:M:15:PRO:HD3	1.91	0.52
1:H:226:THR:OG1	1:H:229:GLU:HG3	2.09	0.52
1:H:181:VAL:HG21	1:H:191:LEU:HD12	1.90	0.52
2:L:241:VAL:HG21	5:L:401:BPH:HAC2	1.92	0.52
1:H:228:LEU:O	1:H:232:LYS:HG3	2.09	0.52
3:M:119:SER:HB3	8:M:600:SPN:H232	1.91	0.52
1:H:62:LYS:HE3	11:H:2006:HOH:O	2.09	0.52
1:H:245:ALA:HB3	1:H:246:PRO:HD3	1.92	0.52
3:M:98:ALA:HB1	3:M:99:PRO:HD2	1.92	0.51
2:L:60:ASN:O	2:L:64:ILE:HG13	2.10	0.51
3:M:293:ASN:OD1	3:M:295:TYR:HB3	2.09	0.51
3:M:109:LEU:HA	3:M:113:GLY:HA3	1.93	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:80:LEU:HA	2:L:84:GLY:HA3	1.91	0.51
2:L:135:ARG:HD3	2:L:248:MET:O	2.11	0.51
1:H:83:ARG:HB2	1:H:84:PRO:HD2	1.92	0.51
2:L:135:ARG:CB	2:L:136:PRO:HD3	2.39	0.51
3:M:148:TRP:CD1	10:M:800:CDL:H511	2.46	0.50
3:M:67:PHE:CE1	8:M:600:SPN:H61	2.46	0.50
2:L:154:LEU:HD13	3:M:197:ARG:HG2	1.94	0.50
1:H:132:LYS:NZ	11:H:2028:HOH:O	2.45	0.50
1:H:197:LYS:HZ3	1:H:199:GLN:HE21	1.59	0.50
3:M:101:TYR:CG	3:M:107:ALA:HB2	2.47	0.50
2:L:69:PRO:HG2	2:L:142:TRP:CB	2.42	0.49
5:L:401:BPH:CMB	5:L:401:BPH:HBB3	2.42	0.49
2:L:122:ALA:O	2:L:126:LEU:HG	2.12	0.49
2:L:233:GLY:HA3	3:M:216:PHE:CE1	2.47	0.49
4:L:1304:BCL:C1C	4:L:1304:BCL:HBC2	2.43	0.48
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.47	0.48
2:L:73:TYR:OH	2:L:82:LYS:HD2	2.12	0.48
4:L:1302:BCL:H42	4:L:1304:BCL:HBC3	1.95	0.48
3:M:197:ARG:NH2	4:M:1303:BCL:OBB	2.46	0.48
3:M:24:VAL:HG11	3:M:29:ARG:NH2	2.28	0.48
3:M:194:GLY:O	3:M:195:ASN:CB	2.61	0.48
4:L:1302:BCL:OBB	4:L:1302:BCL:CHC	2.62	0.48
1:H:191:LEU:HD11	1:H:213:PHE:CE2	2.49	0.48
2:L:32:GLY:HA3	11:L:2016:HOH:O	2.13	0.48
1:H:201:ASN:O	1:H:202:ARG:HB3	2.13	0.47
1:H:33:THR:O	1:H:36:MET:HB2	2.14	0.47
3:M:155:TRP:CD2	10:M:800:CDL:H812	2.50	0.47
2:L:154:LEU:HD13	3:M:197:ARG:CG	2.45	0.47
1:H:171:ILE:N	1:H:172:PRO:CD	2.78	0.47
1:H:140:PHE:HA	3:M:13:ARG:O	2.15	0.47
3:M:148:TRP:CE2	10:M:800:CDL:H511	2.50	0.47
2:L:172:ALA:HB3	2:L:247:CYS:HA	1.95	0.47
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.96	0.47
1:H:37:ARG:HD2	1:H:37:ARG:HH11	1.46	0.46
1:H:191:LEU:HD11	1:H:213:PHE:HE2	1.80	0.46
2:L:233:GLY:HA3	3:M:216:PHE:CD1	2.50	0.46
2:L:210:ASP:HB2	3:M:20:MET:HE3	1.97	0.46
2:L:117:ILE:HB	2:L:118:PRO:HD3	1.97	0.46
2:L:134:PHE:O	2:L:138:MET:HG3	2.15	0.46
2:L:208:THR:O	2:L:211:HIS:HB2	2.15	0.46
1:H:206:ASN:HD21	1:H:248:ARG:HD3	1.81	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.51	0.46
4:L:1304:BCL:CBB	4:L:1304:BCL:HMB1	2.46	0.45
1:H:121:PRO:HA	1:H:226:THR:HA	1.98	0.45
3:M:35:PHE:CE1	3:M:46:GLN:HB2	2.51	0.45
4:L:1304:BCL:HMD1	3:M:206:ILE:HD13	1.98	0.45
4:M:1301:BCL:H141	4:M:1301:BCL:H162	1.65	0.45
1:H:197:LYS:HD3	1:H:199:GLN:NE2	2.30	0.45
2:L:117:ILE:HB	2:L:118:PRO:CD	2.46	0.45
1:H:206:ASN:O	1:H:248:ARG:NH1	2.49	0.45
2:L:175:ILE:O	2:L:178:SER:HB2	2.16	0.45
1:H:180:GLU:OE2	1:H:188:THR:HG21	2.16	0.45
1:H:199:GLN:HB2	1:H:202:ARG:O	2.17	0.45
3:M:132:ARG:O	3:M:133:THR:C	2.52	0.45
1:H:165:VAL:O	1:H:166:ASP:HB2	2.17	0.45
1:H:87:LEU:HD13	1:H:98:HIS:HB2	1.99	0.44
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.98	0.44
1:H:38:GLU:OE1	3:M:241:ARG:NH1	2.47	0.44
3:M:270:ILE:HD13	10:M:800:CDL:H711	1.98	0.44
5:M:402:BPH:H9C2	5:M:402:BPH:H6C1	1.73	0.44
1:H:240:GLY:O	1:H:244:ALA:HB3	2.18	0.44
1:H:34:GLU:CD	1:H:37:ARG:HH12	2.22	0.43
2:L:241:VAL:HG21	5:L:401:BPH:H2C	2.00	0.43
5:L:401:BPH:ND	3:M:214:LEU:HD13	2.34	0.43
1:H:229:GLU:O	1:H:233:ILE:HD12	2.18	0.43
1:H:62:LYS:O	1:H:74:THR:HA	2.17	0.43
2:L:209:PRO:O	2:L:212:GLU:HB2	2.19	0.43
5:L:401:BPH:H141	5:L:401:BPH:H162	1.72	0.43
3:M:200:PRO:HA	9:M:703:LDA:HM12	2.00	0.43
5:M:402:BPH:H4C1	5:M:402:BPH:H6C1	1.34	0.43
3:M:228:ARG:HG3	3:M:229:PHE:CE2	2.54	0.43
4:L:1302:BCL:H2C	4:M:1303:BCL:H2C	2.00	0.43
2:L:38:THR:HG22	2:L:99:SER:CB	2.49	0.43
1:H:82:ASP:O	1:H:83:ARG:HB3	2.18	0.43
10:M:800:CDL:H522	10:M:800:CDL:H311	2.00	0.43
4:M:1301:BCL:CBB	4:M:1301:BCL:HMB1	2.48	0.43
4:M:1303:BCL:HHC	4:M:1303:BCL:OBB	2.19	0.43
1:H:168:TRP:CZ3	1:H:225:VAL:HG22	2.53	0.42
4:L:1304:BCL:H203	5:L:401:BPH:H112	2.00	0.42
2:L:238:LEU:HD23	5:L:401:BPH:CBC	2.50	0.42
1:H:124:ASP:HB2	2:L:210:ASP:OD2	2.19	0.42
3:M:184:ASP:O	3:M:188:ASN:HB2	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:226:THR:HG22	7:L:501:U10:H3M2	2.02	0.42
4:L:1302:BCL:H122	5:L:401:BPH:H3A	2.01	0.42
2:L:247:CYS:SG	2:L:248:MET:HG2	2.59	0.42
1:H:225:VAL:HG12	1:H:229:GLU:HB2	2.01	0.42
1:H:228:LEU:HD22	1:H:232:LYS:HE3	2.01	0.42
5:L:401:BPH:CMB	5:L:401:BPH:CBB	2.98	0.41
3:M:163:ILE:HG22	3:M:285:LEU:HD11	2.03	0.41
1:H:179:LEU:HD11	1:H:196:VAL:HG21	2.01	0.41
1:H:98:HIS:HE1	11:H:2019:HOH:O	2.02	0.41
1:H:36:MET:CE	1:H:56:PHE:HB2	2.50	0.41
10:M:800:CDL:C52	10:M:800:CDL:H312	2.50	0.41
2:L:69:PRO:HD3	2:L:83:GLY:O	2.21	0.41
3:M:243:THR:O	3:M:247:ARG:HG2	2.20	0.41
3:M:11:GLN:NE2	3:M:41:TRP:CD2	2.88	0.41
4:L:1302:BCL:H2C	4:L:1302:BCL:HBC2	1.89	0.41
2:L:207:ARG:HG2	3:M:142:MET:HG2	2.02	0.41
2:L:133:LEU:HD12	2:L:133:LEU:O	2.20	0.41
4:L:1302:BCL:CBB	4:L:1302:BCL:HMB1	2.49	0.41
3:M:241:ARG:HG3	3:M:245:ALA:HB3	2.03	0.41
2:L:213:ASP:O	2:L:217:ARG:HG3	2.20	0.41
2:L:163:THR:O	2:L:163:THR:HG22	2.21	0.41
3:M:122:MET:SD	8:M:600:SPN:H19	2.60	0.41
2:L:60:ASN:HA	2:L:61:PRO:HD3	1.82	0.41
4:M:1301:BCL:H193	4:M:1301:BCL:H161	1.86	0.40
2:L:241:VAL:O	2:L:244:SER:HB2	2.20	0.40
3:M:48:GLY:HA2	3:M:49:PRO:C	2.42	0.40
2:L:71:LEU:HD23	2:L:144:TYR:CZ	2.56	0.40
2:L:210:ASP:CB	3:M:20:MET:HE3	2.52	0.40
3:M:60:LEU:HD23	3:M:64:LEU:HD11	2.04	0.40
1:H:48:THR:HB	1:H:49:PRO:HD2	2.02	0.40
3:M:67:PHE:CZ	8:M:600:SPN:H61	2.57	0.40
3:M:35:PHE:HA	3:M:45:ALA:O	2.21	0.40
1:H:157:ASP:OD2	1:H:210:SER:OG	2.33	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	H	239/260 (92%)	224 (94%)	13 (5%)	2 (1%)	24	51
2	L	279/281 (99%)	262 (94%)	17 (6%)	0	100	100
3	M	301/307 (98%)	275 (91%)	21 (7%)	5 (2%)	11	29
All	All	819/848 (97%)	761 (93%)	51 (6%)	7 (1%)	21	49

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	250	SER
1	H	116	ALA
3	M	195	ASN
3	M	301	HIS
3	M	80	TRP
3	M	194	GLY
3	M	302	GLY

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/208 (94%)	182 (93%)	13 (7%)	20	44
2	L	220/220 (100%)	199 (90%)	21 (10%)	11	24
3	M	237/241 (98%)	221 (93%)	16 (7%)	20	43
All	All	652/669 (98%)	602 (92%)	50 (8%)	16	36

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	15	LEU
1	H	27	LEU
1	H	52	ASN
1	H	60	LYS
1	H	70	ARG
1	H	143	SER
1	H	173	GLU
1	H	188	THR
1	H	221	SER
1	H	225	VAL
1	H	228	LEU
1	H	231	ASP
1	H	248	ARG
2	L	38	THR
2	L	44	LEU
2	L	56	GLN
2	L	63	LEU
2	L	72	GLU
2	L	82	LYS
2	L	133	LEU
2	L	135	ARG
2	L	160	THR
2	L	185	LEU
2	L	205	GLU
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	217	ARG
2	L	223	SER
2	L	235	LEU
2	L	237	SER
2	L	247	CYS
2	L	271	TRP
2	L	272	TRP
3	M	10	VAL
3	M	52	LEU
3	M	62	SER
3	M	104	SER
3	M	109	LEU
3	M	124	VAL
3	M	133	THR
3	M	136	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	M	151	LEU
3	M	170	SER
3	M	188	ASN
3	M	196	LEU
3	M	197	ARG
3	M	216	PHE
3	M	247	ARG
3	M	259	ASN

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

Mol	Chain	Res	Type
1	H	98	HIS
1	H	126	HIS
1	H	199	GLN
1	H	204	HIS
1	H	206	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
9	LDA	H	701	-	15,15,15	4.80	4 (26%)	16,17,17	1.22	1 (6%)
4	BCL	L	1302	2	53,74,74	1.35	6 (11%)	57,115,115	1.97	13 (22%)
4	BCL	L	1304	2	53,74,74	1.30	3 (5%)	57,115,115	2.97	18 (31%)
5	BPH	L	401	-	64,70,70	1.41	6 (9%)	73,101,101	2.79	17 (23%)
7	U10	L	501	-	47,47,63	2.09	14 (29%)	55,58,79	2.78	21 (38%)
4	BCL	M	1301	3	53,74,74	1.33	4 (7%)	57,115,115	2.12	18 (31%)
4	BCL	M	1303	3	53,74,74	1.23	6 (11%)	57,115,115	1.71	14 (24%)
5	BPH	M	402	-	64,70,70	1.25	8 (12%)	73,101,101	2.66	18 (24%)
7	U10	M	502	-	48,48,63	1.91	17 (35%)	58,61,79	1.66	13 (22%)
8	SPN	M	600	-	41,42,42	4.29	20 (48%)	41,52,52	3.42	21 (51%)
9	LDA	M	702	-	15,15,15	4.83	4 (26%)	16,17,17	1.15	2 (12%)
9	LDA	M	703	-	15,15,15	4.77	4 (26%)	16,17,17	0.86	1 (6%)
10	CDL	M	800	-	80,80,99	0.51	0	82,92,111	0.89	3 (3%)

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
9	LDA	H	701	-	-	0/13/13/13	0/0/0/0
4	BCL	L	1302	2	-	0/37/137/137	0/0/9/9
4	BCL	L	1304	2	-	0/37/137/137	0/0/9/9
5	BPH	L	401	-	2/2/18/22	0/54/105/105	0/1/6/6
7	U10	L	501	-	-	1/41/65/87	0/1/1/1
4	BCL	M	1301	3	1/1/21/25	0/37/137/137	0/0/9/9
4	BCL	M	1303	3	-	0/37/137/137	0/0/9/9
5	BPH	M	402	-	-	0/54/105/105	0/1/6/6
7	U10	M	502	-	-	0/45/69/87	0/1/1/1
8	SPN	M	600	-	-	0/50/51/51	0/0/0/0
9	LDA	M	702	-	-	0/13/13/13	0/0/0/0
9	LDA	M	703	-	-	0/13/13/13	0/0/0/0
10	CDL	M	800	-	-	0/91/91/110	0/0/0/0

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	701	LDA	O1-N1	-18.04	1.22	1.39
9	M	702	LDA	O1-N1	-18.01	1.22	1.39
9	M	703	LDA	O1-N1	-17.78	1.22	1.39
8	M	600	SPN	C3-C4	-6.44	1.40	1.50
8	M	600	SPN	C10-C9	-6.16	1.37	1.51
8	M	600	SPN	C6-C5	-5.72	1.38	1.51
7	L	501	U10	C20-C19	-5.48	1.25	1.49
8	M	600	SPN	C17-C18	-4.91	1.40	1.51
8	M	600	SPN	C14-C13	-4.84	1.40	1.51
7	L	501	U10	C7-C8	-4.75	1.43	1.50
8	M	600	SPN	C20-C19	-4.06	1.39	1.50
8	M	600	SPN	C11-C12	-4.03	1.39	1.50
5	L	401	BPH	O2D-CED	-3.39	1.37	1.45
9	M	703	LDA	C1-N1	-3.39	1.45	1.51
7	L	501	U10	C37-C38	-3.25	1.41	1.50
8	M	600	SPN	C7-C8	-3.08	1.41	1.50
9	M	702	LDA	C1-N1	-3.06	1.45	1.51
9	M	702	LDA	CM1-N1	-3.04	1.44	1.49
7	M	502	U10	C7-C8	-2.96	1.46	1.50
9	H	701	LDA	C1-N1	-2.88	1.46	1.51
9	M	703	LDA	CM2-N1	-2.77	1.45	1.49
9	M	702	LDA	CM2-N1	-2.71	1.45	1.49
8	M	600	SPN	C21-C22	-2.62	1.39	1.52
4	L	1302	BCL	C2C-C3C	-2.56	1.46	1.54
9	H	701	LDA	CM2-N1	-2.53	1.45	1.49
5	M	402	BPH	O2D-CED	-2.52	1.39	1.45
7	L	501	U10	C42-C43	-2.45	1.43	1.50
9	M	703	LDA	CM1-N1	-2.44	1.45	1.49
7	L	501	U10	O3-C3M	-2.41	1.39	1.45
7	L	501	U10	C32-C33	-2.39	1.43	1.50
4	M	1303	BCL	C2C-C3C	-2.35	1.47	1.54
9	H	701	LDA	CM1-N1	-2.33	1.45	1.49
4	L	1302	BCL	O2D-CED	-2.31	1.39	1.45
7	M	502	U10	C17-C18	-2.27	1.44	1.50
7	M	502	U10	O4-C4M	-2.22	1.39	1.45
7	M	502	U10	C22-C23	-2.20	1.44	1.50
7	M	502	U10	C12-C13	-2.19	1.44	1.50
4	M	1303	BCL	O2D-CED	-2.18	1.40	1.45
4	M	1301	BCL	C3B-C2B	-2.16	1.34	1.40
8	M	600	SPN	C16-C15	-2.05	1.39	1.51
7	M	502	U10	O3-C3M	-2.03	1.40	1.45
4	M	1303	BCL	O1D-CGD	2.02	1.26	1.21
5	M	402	BPH	O1D-CGD	2.03	1.26	1.21

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	502	U10	C40-C39	2.05	1.56	1.50
7	L	501	U10	C43-C44	2.05	1.38	1.32
7	L	501	U10	C38-C39	2.10	1.37	1.33
7	M	502	U10	C35-C34	2.23	1.56	1.50
4	L	1302	BCL	O1D-CGD	2.24	1.26	1.21
5	M	402	BPH	C4A-NA	2.28	1.40	1.34
8	M	600	SPN	O1-C1	2.32	1.53	1.41
8	M	600	SPN	CM4-C9	2.40	1.56	1.50
7	M	502	U10	C38-C39	2.46	1.39	1.32
7	L	501	U10	C33-C34	2.52	1.37	1.33
5	M	402	BPH	C3D-C4D	2.54	1.44	1.41
5	M	402	BPH	C4-C3	2.59	1.57	1.50
5	L	401	BPH	O1D-CGD	2.64	1.27	1.21
8	M	600	SPN	C29-C30	2.68	1.40	1.32
5	L	401	BPH	C3D-C4D	2.82	1.45	1.41
5	M	402	BPH	C2-C3	2.97	1.38	1.33
7	L	501	U10	C8-C9	3.05	1.38	1.33
5	L	401	BPH	C2-C3	3.05	1.39	1.33
7	M	502	U10	C18-C19	3.14	1.39	1.33
7	M	502	U10	O3-C3	3.17	1.45	1.37
7	M	502	U10	C28-C29	3.26	1.39	1.33
7	L	501	U10	O3-C3	3.34	1.45	1.37
7	M	502	U10	C23-C24	3.41	1.39	1.33
4	L	1302	BCL	O2A-CGA	3.41	1.43	1.33
4	L	1304	BCL	C2-C3	3.46	1.39	1.33
4	M	1301	BCL	C2-C3	3.49	1.39	1.33
4	M	1303	BCL	O2A-CGA	3.51	1.43	1.33
7	L	501	U10	C28-C29	3.65	1.40	1.33
7	M	502	U10	C8-C9	3.66	1.40	1.33
4	M	1303	BCL	C2-C3	3.66	1.40	1.33
7	L	501	U10	O4-C4	3.66	1.46	1.37
7	M	502	U10	C13-C14	3.66	1.40	1.33
7	M	502	U10	O4-C4	3.69	1.46	1.37
5	M	402	BPH	O2A-CGA	3.71	1.44	1.33
7	M	502	U10	C33-C34	3.76	1.40	1.33
8	M	600	SPN	C25-C26	3.77	1.40	1.33
4	L	1302	BCL	C2-C3	3.94	1.40	1.33
8	M	600	SPN	O1-CMA	3.96	1.55	1.43
5	M	402	BPH	O2D-CGD	3.99	1.43	1.33
4	M	1301	BCL	O2A-CGA	4.12	1.45	1.33
4	L	1304	BCL	O2A-CGA	4.17	1.45	1.33
7	L	501	U10	C13-C14	4.38	1.41	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1303	BCL	O2D-CGD	4.49	1.44	1.33
5	L	401	BPH	O2A-CGA	4.75	1.47	1.33
5	L	401	BPH	O2D-CGD	4.93	1.45	1.33
4	M	1301	BCL	O2D-CGD	5.43	1.47	1.33
4	L	1302	BCL	O2D-CGD	5.59	1.47	1.33
4	L	1304	BCL	O2D-CGD	5.61	1.47	1.33
8	M	600	SPN	C3-C2	6.64	1.60	1.52
8	M	600	SPN	C12-C13	9.88	1.52	1.33
8	M	600	SPN	C19-C18	10.15	1.52	1.33
8	M	600	SPN	C8-C9	10.39	1.53	1.33
8	M	600	SPN	C4-C5	10.86	1.54	1.33

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	401	BPH	O1D-CGD-CBD	-9.16	111.50	124.62
8	M	600	SPN	C7-C8-C9	-7.80	110.81	127.76
4	L	1304	BCL	O1D-CGD-CBD	-6.89	114.75	124.62
5	M	402	BPH	OBD-CAD-CBD	-6.30	116.44	125.94
5	M	402	BPH	O2D-CGD-O1D	-6.22	110.94	123.79
5	M	402	BPH	O1D-CGD-CBD	-5.82	116.29	124.62
8	M	600	SPN	C14-C13-C12	-5.69	110.26	121.05
8	M	600	SPN	C6-C5-C4	-5.55	110.53	121.05
4	M	1301	BCL	CMB-C2B-C1B	-5.33	119.54	128.36
4	L	1304	BCL	O2D-CGD-O1D	-5.14	113.18	123.79
7	M	502	U10	C27-C28-C29	-5.07	116.74	127.76
5	L	401	BPH	O2D-CGD-O1D	-5.05	113.36	123.79
8	M	600	SPN	C3-C4-C5	-4.97	118.28	126.70
4	M	1301	BCL	C4-C3-C5	-4.93	107.88	115.41
4	L	1304	BCL	CAC-C3C-C4C	-4.81	101.91	112.58
4	L	1302	BCL	O2A-CGA-O1A	-4.78	111.15	123.49
5	L	401	BPH	O2A-CGA-O1A	-4.56	111.73	123.49
4	L	1304	BCL	O2A-CGA-O1A	-4.50	111.88	123.49
7	M	502	U10	C20-C19-C21	-4.49	108.55	115.41
8	M	600	SPN	C17-C18-C19	-4.20	113.09	121.05
4	L	1304	BCL	CMB-C2B-C1B	-4.14	121.52	128.36
8	M	600	SPN	C20-C19-C18	-3.99	119.08	127.76
4	M	1301	BCL	CAA-C2A-C3A	-3.97	101.79	113.22
7	L	501	U10	C35-C34-C36	-3.97	109.34	115.41
5	M	402	BPH	C4-C3-C2	-3.96	115.73	123.50
4	M	1301	BCL	CAC-C3C-C4C	-3.84	104.07	112.58
7	L	501	U10	C40-C39-C38	-3.78	116.07	123.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	402	BPH	C4-C3-C5	-3.78	109.63	115.41
4	L	1304	BCL	CAC-C3C-C2C	-3.67	104.90	114.13
4	M	1301	BCL	CBC-CAC-C3C	-3.65	104.64	113.57
4	M	1303	BCL	O1D-CGD-CBD	-3.49	119.63	124.62
4	L	1302	BCL	O1D-CGD-CBD	-3.42	119.73	124.62
4	L	1302	BCL	OBD-CAD-CBD	-3.33	120.91	125.94
7	L	501	U10	C30-C29-C28	-3.30	117.02	123.50
4	L	1302	BCL	O2D-CGD-O1D	-3.19	117.20	123.79
4	L	1302	BCL	CAC-C3C-C4C	-3.13	105.64	112.58
5	L	401	BPH	CMA-C3A-C4A	-3.10	102.91	113.01
4	M	1303	BCL	OBD-CAD-CBD	-2.99	121.43	125.94
10	M	800	CDL	CA4-OA6-CA5	-2.97	110.77	117.89
4	M	1303	BCL	OBB-CAB-CBB	-2.94	113.09	120.13
4	L	1304	BCL	CAA-C2A-C3A	-2.93	104.79	113.22
7	L	501	U10	O2-C2-C3	-2.82	114.68	120.79
5	M	402	BPH	CAA-C2A-C3A	-2.80	105.16	113.22
7	L	501	U10	C15-C14-C13	-2.80	118.01	123.50
4	M	1303	BCL	CAC-C3C-C4C	-2.79	106.39	112.58
7	L	501	U10	C12-C13-C14	-2.76	121.76	127.76
8	M	600	SPN	C10-C9-C8	-2.74	115.85	121.05
4	L	1304	BCL	C6-C5-C3	-2.72	106.52	112.48
8	M	600	SPN	CM6-C18-C19	-2.69	118.21	123.50
4	M	1301	BCL	O2A-CGA-O1A	-2.69	116.54	123.49
5	M	402	BPH	C3A-C4A-NA	-2.68	108.88	113.57
5	L	401	BPH	C3A-C4A-NA	-2.67	108.90	113.57
7	M	502	U10	C25-C24-C26	-2.66	111.34	115.41
4	M	1303	BCL	CAC-C3C-C2C	-2.62	107.55	114.13
7	L	501	U10	O5-C5-C6	-2.57	116.85	121.68
5	L	401	BPH	C1C-NC-C4C	-2.54	107.84	110.44
5	M	402	BPH	CBB-CAB-C3B	-2.52	114.92	120.52
7	M	502	U10	C26-C27-C28	-2.48	105.19	111.69
4	M	1301	BCL	OBD-CAD-CBD	-2.46	122.22	125.94
5	M	402	BPH	C6-C5-C3	-2.46	107.10	112.48
4	L	1302	BCL	CMA-C3A-C2A	-2.44	103.53	114.35
5	L	401	BPH	CMA-C3A-C2A	-2.44	103.57	114.35
5	M	402	BPH	CMA-C3A-C2A	-2.41	103.69	114.35
4	M	1303	BCL	C4-C3-C2	-2.38	118.83	123.50
4	M	1301	BCL	CAC-C3C-C2C	-2.37	108.17	114.13
4	L	1304	BCL	OBB-CAB-CBB	-2.37	114.45	120.13
4	M	1301	BCL	C1D-CHD-C4C	-2.36	122.47	126.07
4	M	1301	BCL	O1D-CGD-CBD	-2.35	121.26	124.62
5	L	401	BPH	CHB-C1B-C2B	-2.35	120.30	125.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1303	BCL	O2A-CGA-O1A	-2.29	117.57	123.49
7	M	502	U10	C35-C34-C36	-2.27	111.94	115.41
10	M	800	CDL	OB8-CB7-OB9	-2.23	117.73	123.49
5	L	401	BPH	CBB-CAB-C3B	-2.22	115.59	120.52
7	L	501	U10	C1M-C1-C6	-2.16	119.49	124.10
4	M	1303	BCL	CAA-C2A-C3A	-2.14	107.08	113.22
7	M	502	U10	C15-C14-C16	-2.12	112.17	115.41
9	M	702	LDA	O1-N1-CM2	-2.10	106.25	109.05
5	M	402	BPH	CHB-C4A-NA	-2.08	120.92	124.40
7	M	502	U10	C27-C26-C24	-2.07	105.95	112.71
8	M	600	SPN	C11-C12-C13	-2.07	123.27	127.76
7	M	502	U10	C22-C21-C19	-2.02	106.15	112.71
8	M	600	SPN	CM5-C13-C12	-2.01	119.55	123.50
5	L	401	BPH	C4-C3-C2	2.03	127.49	123.50
7	L	501	U10	C4M-O4-C4	2.03	123.84	116.61
8	M	600	SPN	C6-C7-C8	2.04	117.03	111.69
5	L	401	BPH	OBB-CAB-C3B	2.05	124.26	120.31
4	M	1301	BCL	C4A-NA-C1A	2.05	109.01	106.36
5	L	401	BPH	CMB-C2B-C1B	2.06	128.41	125.06
4	L	1304	BCL	C2C-C3C-C4C	2.11	105.08	101.50
7	M	502	U10	C30-C29-C31	2.16	118.70	115.41
10	M	800	CDL	OA6-CA5-C11	2.17	116.25	111.53
9	M	703	LDA	O1-N1-C1	2.22	112.77	110.27
4	M	1301	BCL	CAA-CBA-CGA	2.22	119.81	113.32
5	L	401	BPH	C2A-C3A-C4A	2.25	106.25	101.10
4	M	1303	BCL	C6-C7-C8	2.31	123.15	115.49
7	L	501	U10	C16-C14-C13	2.40	125.60	121.05
7	M	502	U10	C36-C34-C33	2.42	125.64	121.05
4	L	1304	BCL	O2A-CGA-CBA	2.48	119.45	111.90
4	M	1303	BCL	C4A-NA-C1A	2.49	109.58	106.36
4	L	1304	BCL	CAA-CBA-CGA	2.51	120.66	113.32
7	L	501	U10	C10-C9-C8	2.52	128.45	123.50
9	M	702	LDA	CM2-N1-CM1	2.64	111.81	108.83
4	L	1302	BCL	CHC-C1C-NC	2.67	128.20	124.51
4	L	1302	BCL	C2C-C3C-C4C	2.77	106.20	101.50
4	L	1302	BCL	C4A-NA-C1A	2.79	109.97	106.36
7	L	501	U10	C36-C37-C38	2.82	119.07	111.69
4	M	1301	BCL	C2C-C3C-C4C	2.82	106.29	101.50
7	L	501	U10	C41-C39-C38	2.84	126.44	121.05
8	M	600	SPN	C15-C16-C17	2.86	123.80	113.29
4	M	1303	BCL	O2A-CGA-CBA	2.89	120.71	111.90
7	L	501	U10	C36-C34-C33	3.01	126.76	121.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	600	SPN	C16-C15-C14	3.02	124.37	113.29
4	L	1304	BCL	CMD-C2D-C3D	3.02	131.00	125.09
4	L	1304	BCL	CHD-C4C-NC	3.05	128.59	125.06
7	M	502	U10	C12-C13-C14	3.11	134.52	127.76
4	L	1302	BCL	CBA-CAA-C2A	3.13	122.56	113.73
4	L	1304	BCL	CMB-C2B-C3B	3.13	131.22	125.09
5	M	402	BPH	OBD-CAD-C3D	3.14	134.76	128.35
4	L	1304	BCL	C4A-NA-C1A	3.17	110.45	106.36
4	M	1303	BCL	C5-C3-C2	3.20	127.12	121.05
4	M	1301	BCL	OBB-CAB-C3B	3.23	125.11	120.00
5	M	402	BPH	C2C-C3C-C4C	3.30	107.09	101.50
5	L	401	BPH	C4A-NA-C1A	3.39	111.24	108.21
5	L	401	BPH	O2A-CGA-CBA	3.39	122.24	111.90
5	L	401	BPH	C3C-C4C-NC	3.42	111.36	107.93
8	M	600	SPN	CM7-C22-C21	3.43	124.27	111.08
4	M	1301	BCL	C4-C3-C2	3.53	130.42	123.50
7	M	502	U10	C20-C19-C18	3.56	130.50	123.50
4	M	1303	BCL	O2D-CGD-CBD	3.69	116.36	111.30
7	L	501	U10	C3M-O3-C3	3.69	129.72	116.61
7	L	501	U10	C7-C8-C9	3.72	133.00	126.70
5	M	402	BPH	OBB-CAB-C3B	3.74	127.53	120.31
7	M	502	U10	C25-C24-C23	3.75	130.86	123.50
4	L	1302	BCL	CMD-C2D-C3D	3.79	132.50	125.09
7	L	501	U10	C20-C19-C18	3.83	163.06	127.19
7	L	501	U10	C31-C29-C28	3.89	128.44	121.05
9	H	701	LDA	O1-N1-CM1	3.98	114.38	109.05
4	M	1301	BCL	O2D-CGD-CBD	4.09	116.91	111.30
4	M	1301	BCL	O2A-CGA-CBA	4.10	124.39	111.90
8	M	600	SPN	C15-C14-C13	4.11	121.50	112.48
5	M	402	BPH	O2A-CGA-CBA	4.12	124.45	111.90
4	M	1303	BCL	OBB-CAB-C3B	4.16	126.58	120.00
8	M	600	SPN	CM4-C9-C10	4.22	121.85	115.41
4	M	1301	BCL	CMB-C2B-C3B	4.30	133.50	125.09
5	M	402	BPH	C3A-C4A-CHB	4.41	130.04	121.84
8	M	600	SPN	C7-C6-C5	4.42	127.11	112.71
8	M	600	SPN	C16-C17-C18	4.53	122.43	112.48
7	L	501	U10	C42-C43-C44	4.61	145.47	127.73
4	L	1304	BCL	OBB-CAB-C3B	4.76	127.54	120.00
4	L	1302	BCL	O2A-CGA-CBA	5.70	129.28	111.90
8	M	600	SPN	CM3-C5-C6	6.02	124.60	115.41
4	L	1302	BCL	O2D-CGD-CBD	6.29	119.93	111.30
5	M	402	BPH	C5-C3-C2	7.16	134.63	121.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	600	SPN	CM5-C13-C14	7.17	126.36	115.41
8	M	600	SPN	CM6-C18-C17	7.86	127.41	115.41
7	L	501	U10	C32-C33-C34	7.90	144.94	127.76
7	L	501	U10	C37-C38-C39	11.35	152.45	127.76
5	M	402	BPH	O2D-CGD-CBD	12.85	128.94	111.30
4	L	1304	BCL	O2D-CGD-CBD	14.47	131.15	111.30
5	L	401	BPH	O2D-CGD-CBD	17.21	134.91	111.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	1301	BCL	C13
5	L	401	BPH	C8
5	L	401	BPH	C13

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	501	U10	C17-C18-C19-C20

There are no ring outliers.

11 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1302	BCL	9	0
4	L	1304	BCL	8	0
5	L	401	BPH	10	0
7	L	501	U10	1	0
4	M	1301	BCL	5	0
4	M	1303	BCL	6	0
5	M	402	BPH	3	0
8	M	600	SPN	5	0
9	M	702	LDA	3	0
9	M	703	LDA	2	0
10	M	800	CDL	16	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.