



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:25 PM GMT

PDB ID : 1K6N  
Title : E(L212)A,D(L213)A Double Mutant Structure of Photosynthetic Reaction Center from Rhodobacter Sphaeroides  
Authors : Pokkuluri, P.R.; Laible, P.D.; Deng, Y.-L.; Wong, T.N.; Hanson, D.K.; Schiffer, M.  
Deposited on : 2001-10-16  
Resolution : 3.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

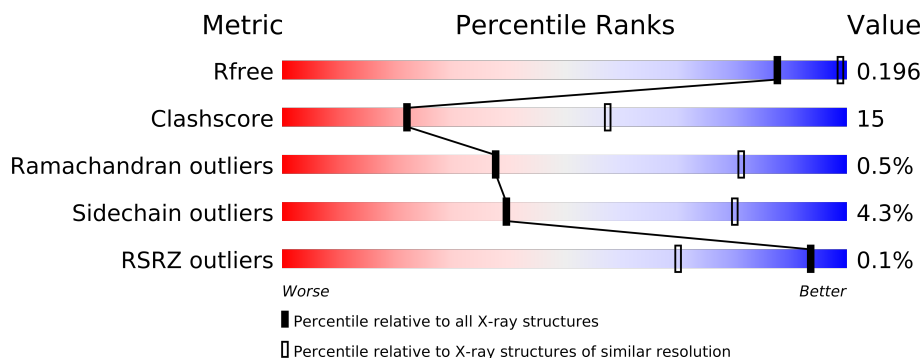
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	L	281	<div><div></div><div></div></div>
2	M	314	<div><div></div><div></div></div>
3	H	260	<div><div></div><div></div></div>

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	LDA	H	703	-	X
10	LDA	L	709	-	X
10	LDA	M	701	-	X
10	LDA	M	704	-	X
5	BCL	M	501	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
6	BPH	L	402	-	X
7	U10	L	502	-	X
8	SPN	M	600	-	X
9	CDL	M	800	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7270 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PHOTOSYNTHETIC REACTION CENTER L SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	0	0
			2225	1504	355	358	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	212	ALA	GLU	ENGINEERED	UNP P02954
L	213	ALA	ASP	ENGINEERED	UNP P02954

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

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	308	HIS	-	EXPRESSION TAG	UNP P02953
M	309	HIS	-	EXPRESSION TAG	UNP P02953
M	310	HIS	-	EXPRESSION TAG	UNP P02953
M	311	HIS	-	EXPRESSION TAG	UNP P02953
M	312	HIS	-	EXPRESSION TAG	UNP P02953
M	313	HIS	-	EXPRESSION TAG	UNP P02953
M	314	HIS	-	EXPRESSION TAG	UNP P02953

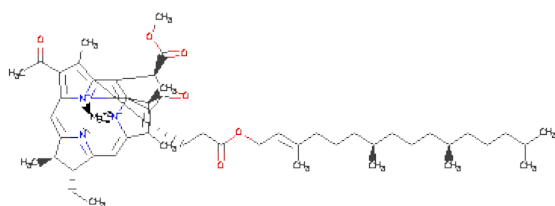
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER H SUBUNIT.

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

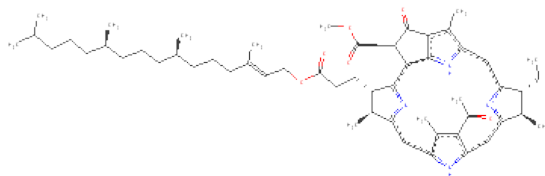
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



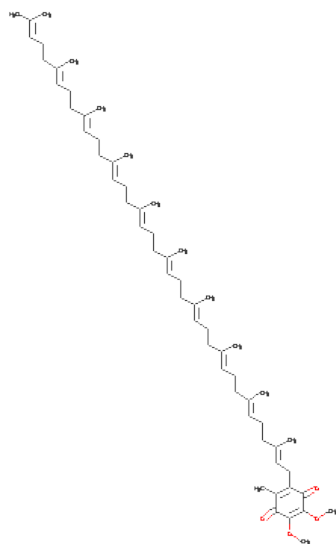
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 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
6	M	1	Total	C	N	O	10	0
			65	55	4	6		
6	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



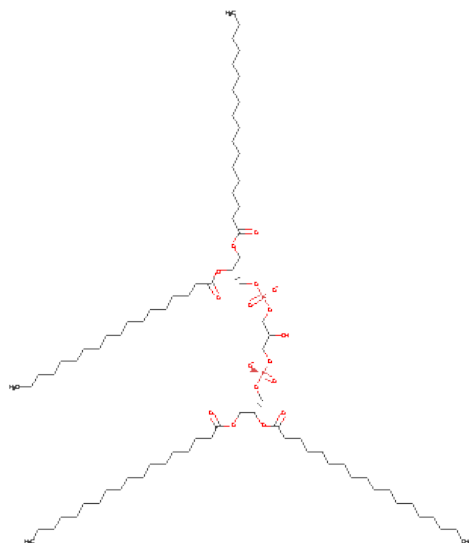
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			48	44	4		
7	L	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is SPEROIDENONE (three-letter code: SPN) (formula:  $C_{41}H_{70}O_2$ ).



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

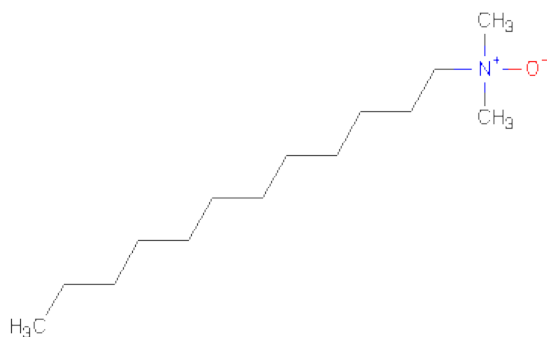
- Molecule 9 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

C<sub>14</sub>H<sub>31</sub>NO).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	51	Total	O	0	0
			51	51		
11	L	34	Total	O	0	0
			34	34		
11	M	44	Total	O	0	0
			44	44		

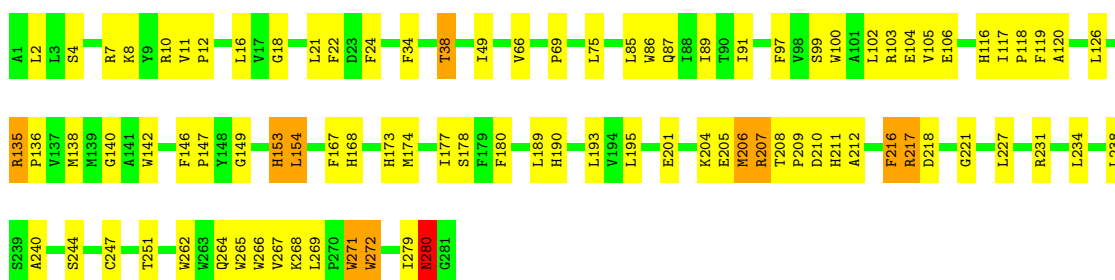


### 3 Residue-property plots

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.

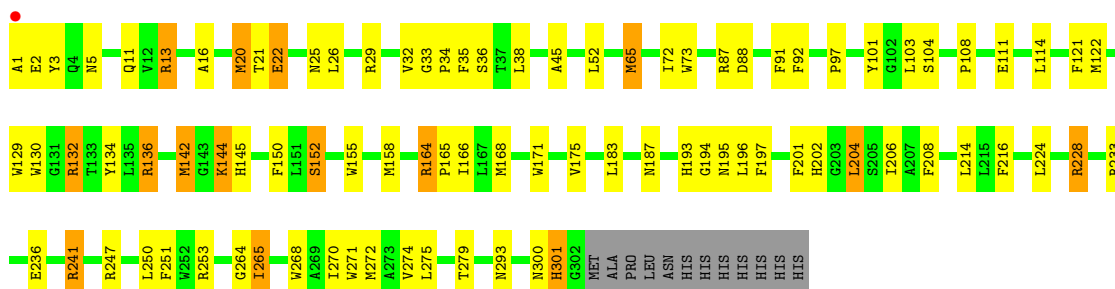
#### • Molecule 1: PHOTOSYNTHETIC REACTION CENTER L SUBUNIT

Chain L: 



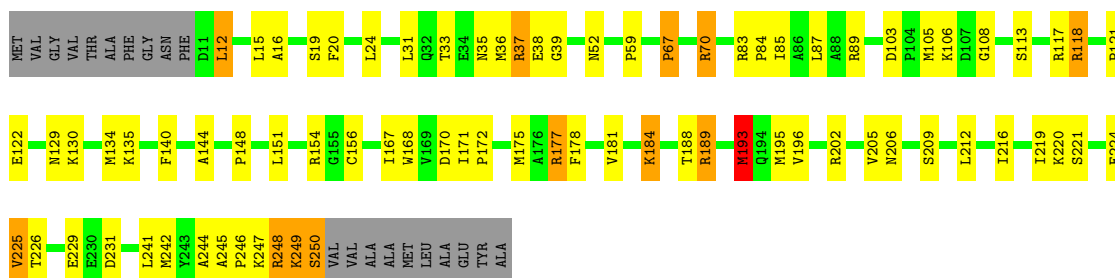
#### • Molecule 2: PHOTOSYNTHETIC REACTION CENTER M SUBUNIT

Chain M: 



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

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.50Å 141.50Å 187.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.10 14.99 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-3.10) 88.4 (14.99-3.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.13 (at 3.12Å)	Xtriage
Refinement program	?	Depositor
R, $R_{free}$	0.203 , 0.207 0.192 , 0.196	Depositor DCC
$R_{free}$ test set	2439 reflections (7.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.4	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.4	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 34959 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7270	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LDA, 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	L	0.95	0/2313	1.09	13/3166 (0.4%)
2	M	1.04	0/2500	1.10	16/3413 (0.5%)
3	H	0.94	1/1877 (0.1%)	1.21	20/2553 (0.8%)
All	All	0.98	1/6690 (0.0%)	1.13	49/9132 (0.5%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	250	SER	C-O	5.48	1.33	1.23

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	103	ARG	NE-CZ-NH1	11.02	125.81	120.30
3	H	154	ARG	NE-CZ-NH2	7.36	123.98	120.30
3	H	117	ARG	NE-CZ-NH2	7.36	123.98	120.30
2	M	13	ARG	NE-CZ-NH2	7.33	123.96	120.30
2	M	247	ARG	NE-CZ-NH2	7.33	123.96	120.30
1	L	217	ARG	NE-CZ-NH2	7.32	123.96	120.30
2	M	164	ARG	NE-CZ-NH2	7.31	123.96	120.30
3	H	202	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	L	231	ARG	NE-CZ-NH2	7.27	123.94	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	248	ARG	NE-CZ-NH2	7.25	123.92	120.30
3	H	70	ARG	NE-CZ-NH2	7.23	123.92	120.30
3	H	37	ARG	NE-CZ-NH2	7.19	123.90	120.30
3	H	189	ARG	NE-CZ-NH2	6.77	123.68	120.30
2	M	228	ARG	NE-CZ-NH2	6.75	123.68	120.30
1	L	207	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	L	135	ARG	NE-CZ-NH2	6.62	123.61	120.30
2	M	136	ARG	NE-CZ-NH2	6.58	123.59	120.30
2	M	253	ARG	NE-CZ-NH2	6.45	123.53	120.30
1	L	103	ARG	NH1-CZ-NH2	-6.40	112.36	119.40
2	M	132	ARG	NE-CZ-NH2	6.39	123.50	120.30
2	M	241	ARG	NE-CZ-NH2	6.29	123.45	120.30
1	L	280	ASN	O-C-N	-6.29	112.50	123.20
1	L	7	ARG	NE-CZ-NH2	6.27	123.44	120.30
3	H	177	ARG	NE-CZ-NH2	6.26	123.43	120.30
3	H	83	ARG	NE-CZ-NH2	6.25	123.43	120.30
1	L	10	ARG	NE-CZ-NH2	6.23	123.42	120.30
3	H	89	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	L	206	MET	CG-SD-CE	6.12	109.98	100.20
2	M	158	MET	CG-SD-CE	6.10	109.96	100.20
3	H	242	MET	CG-SD-CE	6.08	109.92	100.20
2	M	20	MET	CG-SD-CE	6.07	109.91	100.20
3	H	36	MET	CG-SD-CE	6.07	109.90	100.20
3	H	118	ARG	NE-CZ-NH2	6.05	123.32	120.30
3	H	175	MET	CG-SD-CE	6.01	109.81	100.20
1	L	174	MET	CG-SD-CE	5.90	109.64	100.20
3	H	134	MET	CG-SD-CE	5.89	109.63	100.20
2	M	1	ALA	CB-CA-C	5.87	118.91	110.10
2	M	142	MET	CG-SD-CE	5.81	109.50	100.20
2	M	272	MET	CG-SD-CE	5.74	109.38	100.20
3	H	193	MET	CG-SD-CE	5.74	109.38	100.20
3	H	178	PHE	CB-CA-C	-5.69	99.02	110.40
2	M	122	MET	CG-SD-CE	5.67	109.28	100.20
1	L	138	MET	CG-SD-CE	5.67	109.27	100.20
3	H	105	MET	CG-SD-CE	5.65	109.25	100.20
2	M	65	MET	CG-SD-CE	5.61	109.18	100.20
3	H	195	MET	CG-SD-CE	5.56	109.09	100.20
3	H	67	PRO	O-C-N	5.37	131.28	122.70
2	M	168	MET	CG-SD-CE	5.34	108.75	100.20
1	L	2	LEU	CB-CA-C	-5.08	100.56	110.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	280	ASN	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2225	0	2187	86	0
2	M	2408	0	2321	76	0
3	H	1829	0	1836	47	0
4	M	1	0	0	0	0
5	L	132	0	148	16	0
5	M	132	0	148	20	0
6	L	65	0	76	2	0
6	M	65	0	76	1	0
7	L	48	0	62	11	0
7	M	48	0	63	6	0
8	M	43	0	69	1	0
9	M	81	0	106	1	0
10	H	16	0	31	4	0
10	L	16	0	31	4	0
10	M	32	0	62	4	0
11	H	51	0	0	3	0
11	L	34	0	0	1	0
11	M	44	0	0	0	0
All	All	7270	0	7216	215	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (215) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:33:THR:O	3:H:59:PRO:HG3	1.69	0.91
1:L:34:PHE:O	1:L:38:THR:HG23	1.71	0.89
7:M:503:U10:H202	10:H:703:LDA:H112	1.54	0.88
1:L:204:LYS:HD3	1:L:207:ARG:HH22	1.36	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:204:LEU:HB3	2:M:279:THR:HG21	1.56	0.85
1:L:204:LYS:HD3	1:L:207:ARG:NH2	1.94	0.81
2:M:197:PHE:HZ	5:M:502:BCL:HBB2	1.47	0.80
5:L:302:BCL:HHC	5:L:302:BCL:OBB	1.81	0.79
1:L:227:LEU:HD21	2:M:5:ASN:ND2	1.98	0.78
7:L:502:U10:H151	5:M:501:BCL:C4	2.16	0.75
2:M:197:PHE:CZ	5:M:502:BCL:HBB2	2.22	0.75
5:M:502:BCL:HHC	5:M:502:BCL:CBB	2.19	0.73
2:M:270:ILE:HD13	9:M:800:CDL:H711	1.71	0.72
1:L:91:ILE:HG13	10:L:709:LDA:H91	1.71	0.72
1:L:193:LEU:HD23	7:L:502:U10:C3M	2.20	0.70
3:H:70:ARG:HB3	3:H:118:ARG:HH12	1.56	0.70
2:M:152:SER:O	2:M:155:TRP:HB3	1.91	0.70
2:M:208:PHE:HE1	10:M:701:LDA:H91	1.55	0.70
1:L:91:ILE:CG1	10:L:709:LDA:H91	2.22	0.70
5:M:502:BCL:HHC	5:M:502:BCL:HBB3	1.77	0.67
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.76	0.67
1:L:208:THR:HB	1:L:209:PRO:HD2	1.77	0.67
2:M:130:TRP:HD1	2:M:150:PHE:CD2	2.13	0.66
1:L:204:LYS:CD	1:L:207:ARG:NH2	2.58	0.66
5:M:501:BCL:C11	5:M:502:BCL:H203	2.26	0.66
1:L:227:LEU:HD21	2:M:5:ASN:HD21	1.58	0.66
5:L:304:BCL:HBB2	5:L:304:BCL:HMB1	1.79	0.65
1:L:217:ARG:O	1:L:221:GLY:HA2	1.97	0.65
1:L:189:LEU:HB3	7:L:502:U10:H1M3	1.78	0.64
7:M:503:U10:H202	10:H:703:LDA:C11	2.27	0.64
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.34	0.63
2:M:193:HIS:O	2:M:293:ASN:HA	1.98	0.62
1:L:38:THR:HG22	1:L:99:SER:HB3	1.80	0.62
5:M:501:BCL:H111	5:M:502:BCL:H203	1.80	0.62
3:H:241:LEU:O	3:H:248:ARG:NH2	2.32	0.62
2:M:134:TYR:CE2	2:M:144:LYS:HG2	2.36	0.61
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.83	0.61
5:L:304:BCL:H192	6:L:402:BPH:H7C2	1.83	0.61
3:H:37:ARG:HG2	3:H:37:ARG:HH11	1.66	0.60
2:M:13:ARG:O	3:H:140:PHE:HA	2.01	0.60
5:M:501:BCL:HMB1	5:M:501:BCL:CBB	2.32	0.60
1:L:16:LEU:N	1:L:106:GLU:OE2	2.31	0.60
1:L:227:LEU:CD2	2:M:5:ASN:HD21	2.13	0.60
2:M:130:TRP:HD1	2:M:150:PHE:HD2	1.49	0.59
3:H:249:LYS:O	3:H:250:SER:C	2.41	0.59
1:L:244:SER:OG	5:L:302:BCL:HMA2	2.02	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:148:PRO:HA	3:H:151:LEU:HD12	1.84	0.59
1:L:8:LYS:HA	3:H:87:LEU:CD1	2.33	0.58
1:L:178:SER:HB3	7:L:502:U10:H252	1.85	0.58
2:M:194:GLY:O	2:M:195:ASN:HB3	2.04	0.58
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.85	0.58
2:M:208:PHE:CE1	10:M:701:LDA:H91	2.37	0.58
2:M:11:GLN:HB2	3:H:144:ALA:HB3	1.85	0.58
1:L:116:HIS:O	1:L:119:PHE:HB3	2.04	0.58
2:M:21:THR:CG2	2:M:26:LEU:HD11	2.34	0.57
1:L:8:LYS:HA	3:H:87:LEU:HD11	1.86	0.57
1:L:227:LEU:HD21	2:M:5:ASN:CG	2.25	0.57
3:H:177:ARG:O	3:H:193:MET:HB2	2.03	0.57
5:M:501:BCL:HMB1	5:M:501:BCL:HBB2	1.85	0.57
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.40	0.57
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.86	0.56
1:L:85:LEU:O	1:L:89:ILE:HG13	2.06	0.56
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.88	0.55
1:L:38:THR:HG22	1:L:99:SER:CB	2.35	0.55
1:L:193:LEU:HD23	7:L:502:U10:H3M3	1.88	0.55
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.88	0.55
3:H:129:ASN:ND2	3:H:224:GLU:HG2	2.22	0.55
1:L:218:ASP:OD1	2:M:29:ARG:HD3	2.07	0.55
1:L:201:GLU:OE2	2:M:144:LYS:NZ	2.39	0.55
1:L:269:LEU:HB2	1:L:272:TRP:NE1	2.22	0.55
1:L:4:SER:OG	3:H:39:GLY:HA2	2.07	0.55
7:L:502:U10:C15	5:M:501:BCL:C4	2.84	0.54
1:L:206:MET:O	3:H:67:PRO:HG3	2.07	0.54
2:M:72:ILE:HG13	2:M:73:TRP:N	2.22	0.54
2:M:130:TRP:CD1	2:M:150:PHE:HD2	2.25	0.54
3:H:244:ALA:C	3:H:246:PRO:HD2	2.28	0.54
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.90	0.53
1:L:208:THR:O	1:L:211:HIS:HB2	2.08	0.53
1:L:267:VAL:HG21	1:L:280:ASN:ND2	2.24	0.53
5:L:302:BCL:H203	5:L:304:BCL:H102	1.91	0.52
5:L:304:BCL:HMD1	2:M:206:ILE:HD13	1.91	0.52
3:H:20:PHE:HE2	3:H:24:LEU:HD22	1.74	0.52
1:L:271:TRP:CD1	1:L:271:TRP:N	2.77	0.52
10:M:701:LDA:H101	10:H:703:LDA:C12	2.39	0.52
1:L:142:TRP:CZ2	10:L:709:LDA:H51	2.44	0.52
1:L:234:LEU:O	1:L:238:LEU:HG	2.09	0.52
2:M:32:VAL:HG12	2:M:33:GLY:O	2.10	0.52
2:M:187:ASN:HA	5:M:502:BCL:CBC	2.40	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:184:LYS:HG3	3:H:184:LYS:O	2.10	0.51
2:M:101:TYR:O	2:M:104:SER:HB2	2.10	0.51
2:M:300:ASN:O	2:M:301:HIS:HB2	2.10	0.51
1:L:168:HIS:CD2	5:L:302:BCL:HMC2	2.46	0.51
1:L:195:LEU:HB3	2:M:145:HIS:CD2	2.45	0.51
6:L:402:BPH:ND	2:M:214:LEU:HD13	2.26	0.51
3:H:168:TRP:CZ3	3:H:225:VAL:HG22	2.44	0.51
2:M:21:THR:HG23	2:M:26:LEU:HD21	1.92	0.51
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.10	0.51
2:M:20:MET:O	2:M:29:ARG:NH2	2.44	0.50
3:H:84:PRO:O	3:H:85:ILE:HD13	2.11	0.50
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.47	0.50
1:L:75:LEU:HD11	1:L:140:GLY:HA2	1.94	0.49
2:M:175:VAL:HG11	8:M:600:SPN:H161	1.93	0.49
2:M:241:ARG:NH1	3:H:38:GLU:OE1	2.40	0.49
5:L:302:BCL:HAA2	5:L:304:BCL:HAC1	1.93	0.49
1:L:11:VAL:HB	1:L:12:PRO:HD2	1.94	0.49
1:L:135:ARG:HB3	1:L:136:PRO:CD	2.42	0.49
1:L:262:TRP:O	1:L:265:TRP:HD1	1.95	0.49
3:H:12:LEU:O	3:H:15:LEU:HB3	2.12	0.49
1:L:207:ARG:HG3	1:L:211:HIS:CD2	2.48	0.49
1:L:190:HIS:HA	7:L:502:U10:O2	2.13	0.48
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.95	0.48
5:M:501:BCL:H112	5:M:501:BCL:H151	1.54	0.48
2:M:88:ASP:HB2	2:M:92:PHE:CZ	2.48	0.48
1:L:216:PHE:CE1	7:L:502:U10:H71	2.48	0.48
3:H:84:PRO:C	3:H:85:ILE:HD13	2.34	0.48
2:M:101:TYR:O	2:M:104:SER:CB	2.62	0.48
1:L:227:LEU:HD21	2:M:5:ASN:OD1	2.14	0.48
7:L:502:U10:H151	5:M:501:BCL:H41	1.93	0.48
1:L:104:GLU:HB3	1:L:118:PRO:HG3	1.96	0.48
3:H:20:PHE:CE2	3:H:24:LEU:HD22	2.48	0.47
5:L:302:BCL:CHC	5:L:302:BCL:OBB	2.55	0.47
3:H:219:ILE:HB	11:H:730:HOH:O	2.13	0.47
1:L:168:HIS:HB3	2:M:183:LEU:HD13	1.95	0.47
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.82	0.47
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.95	0.47
1:L:205:GLU:O	1:L:207:ARG:NH1	2.45	0.47
2:M:130:TRP:CD1	2:M:150:PHE:CD2	3.00	0.47
10:M:701:LDA:H101	10:H:703:LDA:H121	1.97	0.47
1:L:34:PHE:HB2	11:L:712:HOH:O	2.14	0.46
3:H:170:ASP:HB2	3:H:177:ARG:HG3	1.97	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:49:ILE:HG12	1:L:89:ILE:HD13	1.97	0.46
1:L:279:ILE:HG21	2:M:91:PHE:HB3	1.97	0.46
1:L:102:LEU:O	1:L:105:VAL:HB	2.15	0.46
1:L:189:LEU:HB3	7:L:502:U10:C1M	2.46	0.46
1:L:177:ILE:HG23	5:L:302:BCL:HMB3	1.97	0.45
1:L:22:PHE:HA	1:L:24:PHE:HE2	1.80	0.45
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.98	0.45
2:M:250:LEU:O	2:M:251:PHE:C	2.53	0.45
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.52	0.45
3:H:129:ASN:HD22	3:H:224:GLU:HG2	1.82	0.45
2:M:268:TRP:CD1	7:M:503:U10:H111	2.52	0.45
2:M:21:THR:O	2:M:22:GLU:C	2.55	0.45
3:H:148:PRO:HD2	3:H:167:ILE:HD11	1.98	0.44
2:M:201:PHE:HD1	2:M:279:THR:HG23	1.82	0.44
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.17	0.44
1:L:180:PHE:CE2	1:L:240:ALA:HB1	2.52	0.44
2:M:251:PHE:CD1	2:M:251:PHE:C	2.91	0.44
7:M:503:U10:H322	7:M:503:U10:H28	1.47	0.43
2:M:236:GLU:HB3	11:H:709:HOH:O	2.19	0.43
1:L:264:GLN:O	1:L:268:LYS:HB2	2.17	0.43
3:H:245:ALA:HB3	3:H:246:PRO:HD3	2.01	0.43
3:H:189:ARG:HD2	3:H:216:ILE:HB	1.99	0.43
5:M:502:BCL:HHC	5:M:502:BCL:HBB2	1.98	0.43
5:L:302:BCL:HMB1	5:L:302:BCL:HBB3	2.00	0.43
2:M:268:TRP:CE3	3:H:31:LEU:HD13	2.53	0.43
2:M:2:GLU:OE2	2:M:228:ARG:NH2	2.51	0.43
1:L:234:LEU:HD22	2:M:224:LEU:HD12	1.99	0.43
3:H:249:LYS:O	3:H:250:SER:O	2.37	0.43
1:L:117:ILE:HB	1:L:118:PRO:HD3	2.01	0.43
1:L:100:TRP:CH2	7:M:503:U10:H251	2.54	0.43
5:M:502:BCL:H121	5:M:502:BCL:H162	1.85	0.43
3:H:37:ARG:HG2	3:H:37:ARG:NH1	2.32	0.43
1:L:212:ALA:HA	2:M:142:MET:HE1	2.01	0.43
1:L:265:TRP:CG	1:L:266:TRP:N	2.87	0.43
1:L:180:PHE:CD2	1:L:240:ALA:HB1	2.54	0.43
1:L:153:HIS:CE1	1:L:154:LEU:HD23	2.54	0.43
2:M:114:LEU:HD12	2:M:114:LEU:HA	1.84	0.43
1:L:173:HIS:O	1:L:177:ILE:HG13	2.19	0.42
1:L:85:LEU:HD23	1:L:85:LEU:HA	1.89	0.42
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.49	0.42
3:H:16:ALA:O	3:H:19:SER:HB2	2.20	0.42
2:M:129:TRP:CH2	2:M:132:ARG:NH1	2.88	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:3:TYR:OH	2:M:5:ASN:HA	2.20	0.42
1:L:18:GLY:O	1:L:21:LEU:HB2	2.19	0.42
3:H:181:VAL:O	3:H:188:THR:HA	2.18	0.42
2:M:36:SER:OG	2:M:38:LEU:HB3	2.19	0.42
3:H:209:SER:OG	3:H:212:LEU:HD12	2.20	0.42
3:H:130:LYS:HD2	11:H:739:HOH:O	2.19	0.42
1:L:167:PHE:HB3	5:L:302:BCL:HMC3	2.02	0.42
3:H:156:CYS:HB3	3:H:206:ASN:O	2.19	0.42
2:M:197:PHE:HD1	2:M:197:PHE:HA	1.71	0.42
1:L:149:GLY:O	1:L:153:HIS:HB3	2.19	0.42
5:L:302:BCL:H162	5:L:302:BCL:H141	1.90	0.41
1:L:97:PHE:CE1	5:L:302:BCL:H121	2.55	0.41
2:M:2:GLU:HG2	2:M:3:TYR:N	2.35	0.41
1:L:120:ALA:HB1	1:L:238:LEU:HD21	2.01	0.41
2:M:65:MET:HB3	2:M:121:PHE:CD2	2.56	0.41
2:M:134:TYR:CD2	2:M:144:LYS:HG2	2.55	0.41
2:M:265:ILE:HG12	7:M:503:U10:C2	2.51	0.41
1:L:207:ARG:HD2	1:L:207:ARG:HA	1.62	0.41
3:H:247:LYS:O	3:H:249:LYS:NZ	2.53	0.41
1:L:267:VAL:HG21	1:L:280:ASN:HD22	1.85	0.41
2:M:271:TRP:O	2:M:275:LEU:HG	2.20	0.41
2:M:35:PHE:HA	2:M:45:ALA:O	2.20	0.41
2:M:25:ASN:OD1	2:M:25:ASN:C	2.59	0.41
3:H:103:ASP:HB3	3:H:106:LYS:HB2	2.02	0.41
5:L:304:BCL:H122	5:L:304:BCL:H161	1.80	0.41
5:M:501:BCL:C4A	5:M:501:BCL:HBA1	2.50	0.41
3:H:148:PRO:O	3:H:151:LEU:HG	2.21	0.41
1:L:206:MET:HB2	3:H:67:PRO:HD3	2.03	0.41
2:M:233:ARG:NH2	3:H:122:GLU:OE1	2.52	0.41
2:M:103:LEU:HD21	2:M:166:ILE:HA	2.03	0.41
1:L:267:VAL:HG23	2:M:87:ARG:HG2	2.03	0.41
1:L:146:PHE:HA	1:L:147:PRO:HD3	1.94	0.40
2:M:270:ILE:O	2:M:274:VAL:HB	2.20	0.40
2:M:187:ASN:HA	5:M:502:BCL:HBC3	2.03	0.40
5:M:502:BCL:H191	6:M:401:BPH:H8	2.04	0.40
5:M:501:BCL:OBB	5:M:501:BCL:HHC	2.21	0.40
5:M:502:BCL:CBB	5:M:502:BCL:CHC	2.92	0.40
1:L:97:PHE:CZ	5:L:302:BCL:H121	2.57	0.40
2:M:300:ASN:O	2:M:301:HIS:CB	2.70	0.40
1:L:66:VAL:HG12	1:L:86:TRP:HB2	2.03	0.40
1:L:193:LEU:HD23	7:L:502:U10:H3M2	2.02	0.40
1:L:91:ILE:HG12	10:L:709:LDA:H91	2.00	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:108:GLY:O	3:H:113:SER:HA	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/281 (99%)	264 (95%)	15 (5%)	0	100	100
2	M	300/314 (96%)	286 (95%)	10 (3%)	4 (1%)	18	60
3	H	238/260 (92%)	227 (95%)	11 (5%)	0	100	100
All	All	817/855 (96%)	777 (95%)	36 (4%)	4 (0%)	38	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	301	HIS
2	M	22	GLU
2	M	52	LEU
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	218/218 (100%)	208 (95%)	10 (5%)	37	78
2	M	236/247 (96%)	229 (97%)	7 (3%)	53	87
3	H	195/208 (94%)	184 (94%)	11 (6%)	30	70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	649/673 (96%)	621 (96%)	28 (4%)	40 80

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	38	THR
1	L	126	LEU
1	L	153	HIS
1	L	154	LEU
1	L	210	ASP
1	L	216	PHE
1	L	247	CYS
1	L	251	THR
1	L	271	TRP
1	L	272	TRP
2	M	136	ARG
2	M	144	LYS
2	M	152	SER
2	M	196	LEU
2	M	204	LEU
2	M	216	PHE
2	M	265	ILE
3	H	12	LEU
3	H	52	ASN
3	H	121	PRO
3	H	135	LYS
3	H	184	LYS
3	H	193	MET
3	H	220	LYS
3	H	221	SER
3	H	225	VAL
3	H	231	ASP
3	H	249	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	280	ASN
2	M	4	GLN
2	M	188	ASN
3	H	206	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
10	LDA	H	703	-	15,15,15	4.76	4 (26%)	17,17,17	1.25	2 (11%)
5	BCL	L	302	1	74,74,74	1.61	13 (17%)	97,115,115	1.90	17 (17%)
5	BCL	L	304	1	74,74,74	1.57	14 (18%)	97,115,115	1.71	15 (15%)
6	BPH	L	402	-	70,70,70	1.47	13 (18%)	94,101,101	1.79	22 (23%)
7	U10	L	502	-	48,48,63	1.91	14 (29%)	59,61,79	2.99	17 (28%)
10	LDA	L	709	-	15,15,15	4.58	2 (13%)	17,17,17	3.73	1 (5%)
6	BPH	M	401	-	70,70,70	1.56	13 (18%)	94,101,101	2.13	34 (36%)
5	BCL	M	501	2	74,74,74	1.56	15 (20%)	97,115,115	2.14	24 (24%)
5	BCL	M	502	2	74,74,74	1.43	11 (14%)	97,115,115	1.46	14 (14%)
7	U10	M	503	-	48,48,63	2.60	23 (47%)	59,61,79	1.39	10 (16%)
8	SPN	M	600	-	42,42,42	4.15	17 (40%)	52,52,52	2.73	18 (34%)
10	LDA	M	701	-	15,15,15	4.88	2 (13%)	17,17,17	5.44	1 (5%)
10	LDA	M	704	-	15,15,15	3.74	1 (6%)	17,17,17	4.37	1 (5%)
9	CDL	M	800	-	80,80,99	1.36	4 (5%)	92,92,111	0.99	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
10	LDA	H	703	-	-	0/13/13/13	0/0/0/0
5	BCL	L	302	1	-	0/41/137/137	0/0/9/9
5	BCL	L	304	1	1/1/21/25	0/41/137/137	0/0/9/9
6	BPH	L	402	-	2/2/18/22	0/49/105/105	0/0/6/6
7	U10	L	502	-	-	0/45/69/87	0/1/1/1
10	LDA	L	709	-	-	0/13/13/13	0/0/0/0
6	BPH	M	401	-	1/1/18/22	0/49/105/105	0/0/6/6
5	BCL	M	501	2	2/2/21/25	1/41/137/137	0/0/9/9
5	BCL	M	502	2	-	0/41/137/137	0/0/9/9
7	U10	M	503	-	-	0/45/69/87	0/1/1/1
8	SPN	M	600	-	-	0/51/51/51	0/0/0/0
10	LDA	M	701	-	-	0/13/13/13	0/0/0/0
10	LDA	M	704	-	-	0/13/13/13	0/0/0/0
9	CDL	M	800	-	1/1/9/9	0/91/91/110	0/0/0/0

All (146) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	701	LDA	O1-N1	-18.69	1.21	1.39
10	H	703	LDA	O1-N1	-17.65	1.22	1.39
10	L	709	LDA	O1-N1	-17.50	1.22	1.39
10	M	704	LDA	O1-N1	-14.40	1.25	1.39
8	M	600	SPN	C4-C5	10.60	1.54	1.32
8	M	600	SPN	C19-C18	10.47	1.54	1.32
8	M	600	SPN	C8-C9	10.04	1.53	1.32
8	M	600	SPN	C12-C13	9.75	1.52	1.32
7	M	503	U10	C27-C28	-8.23	1.26	1.50
8	M	600	SPN	C3-C2	7.86	1.61	1.51
7	M	503	U10	O3-C3	7.01	1.54	1.36
9	M	800	CDL	C43-C42	-6.72	1.52	1.55
9	M	800	CDL	C58-C57	-6.34	1.52	1.55
8	M	600	SPN	C3-C4	-6.02	1.41	1.50
6	M	401	BPH	C1D-CHD	5.26	1.41	1.35
8	M	600	SPN	C17-C18	-5.18	1.39	1.51
8	M	600	SPN	C10-C9	-5.09	1.39	1.51
9	M	800	CDL	C84-C83	-5.08	1.53	1.55
9	M	800	CDL	C24-C23	-4.83	1.53	1.55
5	L	302	BCL	O2D-CED	-4.79	1.33	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	600	SPN	C14-C13	-4.73	1.40	1.51
5	M	502	BCL	C3B-C4B	4.65	1.47	1.40
8	M	600	SPN	C6-C5	-4.55	1.40	1.51
5	L	302	BCL	C3B-C4B	4.48	1.47	1.40
5	M	501	BCL	O2D-CGD	4.45	1.44	1.33
7	L	502	U10	O4-C4	4.32	1.47	1.36
7	M	503	U10	C17-C18	-4.31	1.38	1.50
6	L	402	BPH	C1D-CHD	4.29	1.40	1.35
5	L	304	BCL	O2D-CGD	4.22	1.44	1.33
5	L	304	BCL	C3B-C4B	4.17	1.46	1.40
5	M	502	BCL	C4C-NC	4.10	1.41	1.32
7	L	502	U10	C13-C14	4.04	1.41	1.32
8	M	600	SPN	C20-C19	-3.99	1.39	1.50
5	L	304	BCL	MG-ND	-3.99	1.96	2.05
5	L	302	BCL	C1A-NA	3.99	1.41	1.32
5	L	302	BCL	C4C-NC	3.98	1.41	1.32
8	M	600	SPN	C25-C26	3.94	1.40	1.32
5	L	304	BCL	C1A-NA	3.93	1.40	1.32
5	M	501	BCL	C4C-NC	3.92	1.40	1.32
5	L	302	BCL	O2A-CGA	3.92	1.45	1.33
5	M	502	BCL	C1B-C2B	3.88	1.45	1.40
6	L	402	BPH	C1B-NB	3.86	1.40	1.36
6	M	401	BPH	C4B-NB	3.85	1.40	1.36
5	L	304	BCL	C1B-C2B	3.83	1.44	1.40
5	L	304	BCL	C4C-NC	3.82	1.40	1.32
7	M	503	U10	C33-C34	3.79	1.40	1.32
5	M	501	BCL	C3B-C4B	3.78	1.46	1.40
5	L	302	BCL	C1-C2	-3.72	1.36	1.49
7	M	503	U10	C37-C38	-3.71	1.39	1.50
7	M	503	U10	C22-C23	-3.70	1.39	1.50
7	L	502	U10	C23-C24	3.70	1.40	1.32
6	M	401	BPH	O2A-CGA	3.62	1.44	1.33
10	H	703	LDA	CM1-N1	-3.58	1.43	1.49
6	L	402	BPH	O2D-CGD	3.58	1.42	1.33
6	M	401	BPH	O2D-CGD	3.58	1.42	1.33
5	M	501	BCL	O2A-CGA	3.53	1.44	1.33
7	M	503	U10	O4-C4	3.52	1.45	1.36
7	L	502	U10	C7-C8	-3.51	1.45	1.50
8	M	600	SPN	C7-C8	-3.51	1.40	1.50
8	M	600	SPN	C11-C12	-3.47	1.40	1.50
5	M	502	BCL	C1B-NB	3.47	1.38	1.34
7	M	503	U10	C8-C9	3.40	1.39	1.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	503	U10	C23-C24	3.38	1.39	1.32
5	M	502	BCL	C2-C3	3.30	1.39	1.32
7	L	502	U10	C8-C9	3.30	1.39	1.32
5	M	501	BCL	MG-NA	3.28	2.16	2.07
7	M	503	U10	C35-C34	3.25	1.59	1.50
5	M	501	BCL	C1B-C2B	3.24	1.44	1.40
5	M	501	BCL	C1B-NB	3.22	1.38	1.34
6	L	402	BPH	O2A-CGA	3.22	1.43	1.33
5	L	304	BCL	C2-C3	3.15	1.39	1.32
7	L	502	U10	C18-C19	3.14	1.39	1.32
7	L	502	U10	O3-C3	3.12	1.44	1.36
10	H	703	LDA	C1-N1	-3.10	1.45	1.51
7	L	502	U10	C32-C33	-3.09	1.41	1.50
5	L	302	BCL	MG-NA	3.08	2.16	2.07
5	M	502	BCL	C4B-NB	3.08	1.38	1.34
6	L	402	BPH	C2-C3	3.02	1.39	1.32
7	M	503	U10	C36-C34	3.02	1.58	1.51
6	L	402	BPH	C3B-C4B	2.96	1.44	1.40
5	L	304	BCL	MG-NA	2.94	2.15	2.07
7	M	503	U10	C13-C14	2.94	1.38	1.32
5	M	501	BCL	C1A-NA	2.92	1.38	1.32
5	M	502	BCL	MG-NA	2.90	2.15	2.07
5	M	502	BCL	C1A-NA	2.90	1.38	1.32
8	M	600	SPN	O1-CMA	2.88	1.52	1.43
7	L	502	U10	O3-C3M	-2.84	1.38	1.45
7	M	503	U10	C18-C19	2.84	1.38	1.32
5	L	302	BCL	C1B-C2B	2.83	1.43	1.40
6	M	401	BPH	C2-C3	2.82	1.38	1.32
5	L	302	BCL	C4B-NB	2.81	1.38	1.34
5	M	501	BCL	C2-C3	2.80	1.38	1.32
5	M	501	BCL	C4B-NB	2.79	1.38	1.34
7	M	503	U10	C38-C39	2.79	1.40	1.34
6	M	401	BPH	C1B-NB	2.78	1.39	1.36
6	L	402	BPH	C4C-NC	2.73	1.41	1.34
7	L	502	U10	C38-C39	2.71	1.40	1.34
8	M	600	SPN	C29-C30	2.71	1.41	1.32
5	M	501	BCL	CAA-C2A	2.70	1.58	1.54
6	M	401	BPH	O2D-CED	-2.69	1.38	1.45
5	L	304	BCL	C4B-NB	2.67	1.38	1.34
6	M	401	BPH	C3B-C4B	2.62	1.44	1.40
7	M	503	U10	C41-C39	2.60	1.54	1.40
6	L	402	BPH	CAA-C2A	2.55	1.58	1.54

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	401	BPH	C4D-ND	-2.52	1.34	1.38
8	M	600	SPN	C21-C22	-2.52	1.39	1.52
5	L	304	BCL	CMB-C2B	-2.51	1.46	1.51
7	L	502	U10	C28-C29	2.51	1.38	1.32
6	M	401	BPH	C4C-NC	2.46	1.41	1.34
7	M	503	U10	C30-C29	2.43	1.56	1.50
7	L	502	U10	C41-C39	2.43	1.53	1.40
5	M	501	BCL	CHC-C1C	2.42	1.42	1.36
7	M	503	U10	C15-C14	2.41	1.56	1.50
6	L	402	BPH	O1D-CGD	2.40	1.27	1.21
6	L	402	BPH	C4B-NB	2.36	1.39	1.36
5	L	304	BCL	O2A-CGA	2.34	1.40	1.33
10	H	703	LDA	CM2-N1	-2.34	1.45	1.49
7	M	503	U10	O4-C4M	-2.34	1.39	1.45
6	L	402	BPH	O2D-CED	-2.34	1.39	1.45
6	M	401	BPH	C15-C13	2.34	1.65	1.52
7	L	502	U10	C27-C28	-2.28	1.44	1.50
5	M	501	BCL	C2C-C3C	-2.27	1.47	1.54
5	L	302	BCL	C4-C3	2.26	1.56	1.50
5	M	501	BCL	CMA-C3A	2.26	1.58	1.53
6	M	401	BPH	C2C-C3C	-2.26	1.47	1.54
5	L	304	BCL	C1B-NB	2.23	1.37	1.34
6	M	401	BPH	CAA-C2A	2.23	1.58	1.54
5	L	302	BCL	C2-C3	2.23	1.37	1.32
5	L	304	BCL	C4D-C3D	2.18	1.44	1.41
5	M	502	BCL	O2D-CED	-2.18	1.39	1.45
7	M	503	U10	C28-C29	2.17	1.37	1.32
7	M	503	U10	C40-C39	2.17	1.55	1.48
10	M	701	LDA	CM2-N1	-2.17	1.46	1.49
7	M	503	U10	O3-C3M	-2.15	1.39	1.45
5	L	302	BCL	MG-NC	2.12	2.13	2.07
6	L	402	BPH	C3B-C2B	-2.09	1.34	1.40
10	L	709	LDA	CM2-N1	-2.09	1.46	1.49
5	L	304	BCL	C3D-CAD	-2.08	1.43	1.47
7	M	503	U10	O2-C2	2.07	1.28	1.23
7	M	503	U10	C7-C8	-2.07	1.47	1.50
5	M	501	BCL	C4D-C3D	2.05	1.44	1.41
5	M	502	BCL	C4D-C3D	2.04	1.44	1.41
6	L	402	BPH	C4D-C3D	2.04	1.44	1.41
5	L	302	BCL	CMC-C2C	-2.03	1.48	1.53
7	L	502	U10	C15-C14	2.01	1.55	1.50
5	M	502	BCL	O2A-CGA	2.01	1.39	1.33

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	701	LDA	C2-C1-N1	22.33	152.29	113.80
10	M	704	LDA	C2-C1-N1	17.84	144.55	113.80
7	L	502	U10	C32-C33-C34	16.29	162.93	127.80
10	L	709	LDA	C2-C1-N1	15.21	140.02	113.80
5	L	302	BCL	OBB-CAB-C3B	10.98	136.55	120.07
8	M	600	SPN	CM6-C18-C17	7.67	127.05	115.39
5	M	501	BCL	C1-C2-C3	7.54	139.59	126.19
6	M	401	BPH	O2D-CGD-CBD	7.20	126.00	111.33
7	L	502	U10	C27-C28-C29	7.09	143.10	127.80
8	M	600	SPN	CM5-C13-C14	7.05	126.10	115.39
5	L	304	BCL	O2D-CGD-CBD	6.87	125.33	111.33
5	M	501	BCL	OBB-CAB-C3B	6.87	130.38	120.07
6	L	402	BPH	O2D-CGD-CBD	6.87	125.32	111.33
7	L	502	U10	C3M-O3-C3	6.65	139.08	116.48
5	M	501	BCL	C4-C3-C5	-6.64	105.30	115.39
5	L	304	BCL	OBB-CAB-C3B	6.14	129.28	120.07
6	M	401	BPH	C1-C2-C3	5.68	136.28	126.19
5	L	304	BCL	O1D-CGD-CBD	-5.50	113.14	124.42
8	M	600	SPN	C6-C5-C4	-5.40	110.70	121.08
6	M	401	BPH	C16-C15-C13	5.15	129.98	115.14
8	M	600	SPN	C17-C18-C19	-5.12	111.22	121.08
5	M	502	BCL	O2D-CGD-CBD	4.91	121.34	111.33
5	L	302	BCL	C4B-C3B-CAB	-4.86	105.78	127.09
5	M	501	BCL	CAA-C2A-C3A	-4.68	101.97	113.04
6	L	402	BPH	O2A-CGA-O1A	-4.66	110.69	123.43
5	M	501	BCL	O2A-CGA-CBA	4.62	126.47	111.94
8	M	600	SPN	C3-C4-C5	-4.53	119.10	126.76
8	M	600	SPN	C20-C19-C18	-4.49	118.11	127.80
5	M	501	BCL	OBD-CAD-CBD	-4.47	119.19	125.94
6	L	402	BPH	O2D-CGD-O1D	-4.38	114.89	123.79
7	L	502	U10	O5-C5-C6	-4.33	113.71	121.67
8	M	600	SPN	C7-C8-C9	-4.29	118.55	127.80
5	L	302	BCL	O2D-CGD-CBD	4.29	120.06	111.33
8	M	600	SPN	CM7-C22-C21	4.27	126.67	111.02
5	M	501	BCL	O2A-CGA-O1A	-4.27	111.78	123.43
8	M	600	SPN	C11-C12-C13	-4.25	118.63	127.80
8	M	600	SPN	CM4-C9-C10	4.23	121.81	115.39
5	M	502	BCL	OBB-CAB-C3B	4.14	126.29	120.07
5	M	501	BCL	C5-C3-C2	4.11	129.00	121.08
8	M	600	SPN	C10-C9-C8	-4.03	113.33	121.08
7	L	502	U10	C30-C29-C31	-4.01	109.30	115.39
5	M	501	BCL	O2D-CGD-CBD	3.98	119.44	111.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	304	BCL	OBB-CAB-CBB	-3.93	110.36	120.13
10	H	703	LDA	C2-C1-N1	3.87	120.48	113.80
8	M	600	SPN	C14-C13-C12	-3.87	113.63	121.08
6	M	401	BPH	O2D-CGD-O1D	-3.87	115.94	123.79
6	M	401	BPH	CAA-C2A-C3A	-3.86	103.92	113.04
7	M	503	U10	C27-C28-C29	3.79	135.97	127.80
6	M	401	BPH	C6-C5-C3	3.77	121.73	112.78
5	M	501	BCL	CMB-C2B-C1B	-3.72	122.90	128.62
5	L	302	BCL	OBB-CAB-CBB	-3.71	110.91	120.13
5	M	502	BCL	O1D-CGD-CBD	-3.70	116.83	124.42
8	M	600	SPN	C16-C17-C18	3.67	121.49	112.78
7	M	503	U10	C26-C27-C28	-3.63	101.24	111.62
6	L	402	BPH	CAA-C2A-C3A	-3.63	104.45	113.04
6	M	401	BPH	CED-O2D-CGD	3.54	124.44	116.02
6	L	402	BPH	OBD-CAD-CBD	-3.50	120.66	125.94
6	L	402	BPH	C2C-C1C-NC	-3.48	108.21	112.90
7	L	502	U10	C16-C14-C13	3.47	127.76	121.08
6	M	401	BPH	C3C-C4C-CHD	3.45	129.01	121.83
5	M	501	BCL	C2C-C3C-C4C	3.44	105.82	101.05
6	L	402	BPH	O2A-CGA-CBA	3.41	122.66	111.94
6	M	401	BPH	C2C-C1C-NC	-3.40	108.32	112.90
5	M	502	BCL	O2A-CGA-CBA	3.38	122.59	111.94
6	M	401	BPH	CBC-CAC-C3C	3.31	121.75	113.61
7	L	502	U10	O2-C2-C3	-3.23	113.80	120.96
7	L	502	U10	C20-C19-C21	-3.19	110.54	115.39
6	M	401	BPH	C11-C12-C13	-3.18	105.97	115.14
5	L	304	BCL	CMD-C2D-C3D	3.15	129.94	124.97
5	L	302	BCL	O2A-CGA-CBA	3.15	121.85	111.94
6	M	401	BPH	O1D-CGD-CBD	-3.12	118.03	124.42
6	L	402	BPH	CAC-C3C-C2C	3.11	121.03	113.89
5	L	302	BCL	C3A-C4A-NA	-3.11	107.16	110.95
5	M	501	BCL	O2D-CGD-O1D	-3.10	117.49	123.79
5	L	304	BCL	CMB-C2B-C1B	-3.10	123.85	128.62
5	L	302	BCL	CBB-CAB-C3B	-3.05	111.39	120.30
6	M	401	BPH	CMB-C2B-C1B	-3.04	124.03	128.65
9	M	800	CDL	OB8-CB6-CB4	3.04	116.78	108.83
5	L	302	BCL	C2B-C3B-CAB	3.00	137.68	127.43
5	L	302	BCL	OBD-CAD-CBD	-2.99	121.42	125.94
5	L	304	BCL	C4A-NA-C1A	2.92	110.54	106.52
5	M	501	BCL	OBB-CAB-CBB	-2.90	112.92	120.13
5	M	501	BCL	C4B-CHC-C1C	-2.89	124.04	130.06
6	L	402	BPH	C3A-C4A-NA	-2.89	109.01	112.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	402	BPH	C3C-C4C-CHD	2.88	127.82	121.83
5	M	501	BCL	CMD-C2D-C3D	2.87	129.49	124.97
5	L	302	BCL	C4A-NA-C1A	2.86	110.47	106.52
6	M	401	BPH	CMB-C2B-C3B	2.84	129.45	124.97
6	L	402	BPH	C4-C3-C5	-2.85	111.06	115.39
5	L	302	BCL	O1D-CGD-CBD	-2.84	118.59	124.42
5	L	304	BCL	C3C-C4C-NC	-2.83	107.96	111.60
6	L	402	BPH	CMA-C3A-C4A	-2.83	103.94	112.94
5	L	302	BCL	CMB-C2B-C1B	-2.79	124.33	128.62
5	L	304	BCL	O2A-CGA-CBA	2.78	120.70	111.94
6	M	401	BPH	C17-C16-C15	2.77	127.20	113.02
5	M	502	BCL	CED-O2D-CGD	2.74	122.54	116.02
7	M	503	U10	C25-C24-C26	-2.74	111.22	115.39
5	M	502	BCL	C2C-C1C-NC	-2.74	107.61	110.95
6	M	401	BPH	C3C-C4C-NC	-2.73	108.73	113.49
9	M	800	CDL	CB6-CB4-CB3	-2.73	105.64	111.86
5	M	501	BCL	CMA-C3A-C2A	-2.70	102.54	114.14
5	M	502	BCL	C4A-NA-C1A	2.70	110.24	106.52
6	M	401	BPH	C11-C10-C8	2.69	122.89	115.14
5	M	502	BCL	OBD-CAD-CBD	-2.68	121.90	125.94
6	M	401	BPH	CMD-C2D-C3D	2.66	129.16	124.97
5	M	502	BCL	C3C-C4C-NC	-2.66	108.17	111.60
5	M	501	BCL	CGD-CBD-CHA	-2.66	101.93	110.96
5	L	302	BCL	C4B-C3B-C2B	-2.66	103.75	106.97
8	M	600	SPN	CM3-C5-C6	2.65	119.42	115.39
6	L	402	BPH	C3C-C4C-NC	-2.64	108.89	113.49
7	L	502	U10	C7-C6-C5	-2.62	115.91	118.75
6	M	401	BPH	O2A-CGA-O1A	-2.62	116.28	123.43
6	M	401	BPH	C2C-C3C-C4C	2.60	105.61	102.06
6	M	401	BPH	C5-C3-C2	-2.56	116.16	121.08
6	L	402	BPH	CED-O2D-CGD	2.50	121.97	116.02
5	M	501	BCL	C3C-C2C-C1C	2.49	105.23	101.40
6	L	402	BPH	CAA-C2A-C1A	-2.49	106.18	112.72
5	M	502	BCL	C3A-C2A-C1A	2.46	104.56	101.08
6	M	401	BPH	CAA-C2A-C1A	-2.46	106.26	112.72
7	L	502	U10	C31-C29-C28	2.45	125.80	121.08
7	L	502	U10	C17-C18-C19	2.42	133.01	127.80
5	L	304	BCL	C4B-C3B-C2B	-2.42	104.05	106.97
6	M	401	BPH	C3B-C4B-NB	2.40	109.81	107.10
7	M	503	U10	C7-C8-C9	2.40	130.81	126.76
5	M	502	BCL	CMB-C2B-C1B	-2.40	124.94	128.62
6	M	401	BPH	C1D-C2D-C3D	-2.39	104.84	106.89

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	501	BCL	CMB-C2B-C3B	2.38	128.72	124.97
5	L	304	BCL	CAC-C3C-C4C	-2.37	107.31	112.58
6	M	401	BPH	C14-C13-C12	2.35	119.66	111.02
5	M	501	BCL	CHA-C1A-NA	-2.35	121.39	126.22
5	M	502	BCL	C2D-C1D-ND	2.35	111.18	109.41
7	L	502	U10	C1-C6-C5	-2.33	117.33	120.26
7	L	502	U10	C21-C19-C18	2.33	125.56	121.08
6	L	402	BPH	C3B-C4B-NB	2.32	109.72	107.10
5	M	501	BCL	C2D-C1D-ND	2.31	111.16	109.41
7	L	502	U10	C12-C13-C14	-2.30	122.84	127.80
6	M	401	BPH	C3A-C4A-NA	-2.29	109.81	112.90
5	M	502	BCL	C1-C2-C3	2.29	130.26	126.19
7	M	503	U10	C3M-O3-C3	2.29	124.25	116.48
6	L	402	BPH	O1D-CGD-CBD	-2.28	119.74	124.42
5	L	302	BCL	C1-C2-C3	2.27	130.22	126.19
6	M	401	BPH	C3C-C2C-C1C	2.25	106.19	101.11
8	M	600	SPN	C7-C6-C5	2.25	120.19	112.74
5	L	304	BCL	O2A-CGA-O1A	-2.25	117.29	123.43
7	L	502	U10	C31-C32-C33	2.24	118.02	111.62
7	M	503	U10	C20-C19-C21	-2.24	111.98	115.39
5	L	304	BCL	C2D-C1D-ND	2.23	111.09	109.41
5	M	501	BCL	C2A-C3A-C4A	2.22	104.82	101.40
6	M	401	BPH	C2A-C1A-NA	-2.21	109.31	112.61
7	L	502	U10	C15-C14-C13	-2.20	119.17	123.52
5	L	302	BCL	C2A-C1A-NA	-2.18	108.83	111.24
7	M	503	U10	C31-C29-C28	-2.19	116.88	121.08
8	M	600	SPN	O1-C1-C2	-2.18	104.97	109.32
6	M	401	BPH	C4-C3-C5	2.18	118.71	115.39
9	M	800	CDL	CA6-CA4-CA3	-2.18	106.89	111.86
6	M	401	BPH	C4A-NA-C1A	2.18	111.93	107.76
5	M	502	BCL	C2A-C3A-C4A	2.18	104.75	101.40
5	L	302	BCL	CED-O2D-CGD	2.17	121.19	116.02
5	L	304	BCL	C2C-C1C-NC	-2.16	108.31	110.95
6	M	401	BPH	OBD-CAD-CBD	-2.15	122.69	125.94
6	M	401	BPH	CMA-C3A-C4A	-2.15	106.11	112.94
8	M	600	SPN	C15-C16-C17	2.13	121.30	113.28
5	L	302	BCL	C2C-C3C-C4C	2.12	103.99	101.05
5	M	501	BCL	C1B-CHB-C4A	-2.11	125.66	130.06
6	L	402	BPH	O2A-C1-C2	-2.11	103.98	108.55
7	M	503	U10	C4M-O4-C4	2.09	123.59	116.48
6	L	402	BPH	C2A-C3A-C4A	2.08	105.81	101.11
6	L	402	BPH	CMB-C2B-C1B	-2.08	125.48	128.65

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	503	U10	C22-C23-C24	2.08	132.28	127.80
7	L	502	U10	O5-C5-C4	2.06	125.55	120.96
6	L	402	BPH	C2C-C3C-C4C	2.05	104.86	102.06
6	M	401	BPH	CBD-CHA-C1A	2.05	128.96	123.62
5	M	501	BCL	O1D-CGD-CBD	-2.05	120.23	124.42
5	L	304	BCL	OBD-CAD-CBD	-2.05	122.85	125.94
6	L	402	BPH	C3C-C2C-C1C	2.04	105.71	101.11
7	M	503	U10	C10-C9-C11	-2.04	112.28	115.39
8	M	600	SPN	C11-C10-C9	2.02	119.43	112.74
10	H	703	LDA	O1-N1-CM2	2.01	111.71	109.01
6	M	401	BPH	C6-C7-C8	-2.01	109.36	115.14

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	304	BCL	C13
9	M	800	CDL	CA4
5	M	501	BCL	C8
5	M	501	BCL	C13
6	M	401	BPH	C13
6	L	402	BPH	C8
6	L	402	BPH	C13

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	501	BCL	C1-C2-C3-C4

There are no ring outliers.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	L	281/281 (100%)	-0.55	0 100 100	10, 27, 66, 94	0
2	M	302/314 (96%)	-0.54	1 (0%) 91 53	11, 32, 68, 97	0
3	H	240/260 (92%)	-0.49	0 100 100	13, 29, 58, 95	0
All	All	823/855 (96%)	-0.53	1 (0%) 93 70	10, 29, 66, 97	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	2.3

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	U10	L	502	48/63	0.45	13.90	43,72,101,102	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
10	LDA	L	709	16/16	0.47	8.03	67,85,95,97	0
10	LDA	M	704	16/16	0.33	7.85	48,75,109,109	0
10	LDA	H	703	16/16	0.26	4.11	34,50,64,67	0
9	CDL	M	800	81/100	0.38	3.51	41,62,76,77	81
6	BPH	L	402	65/65	0.17	2.56	23,27,38,40	0
10	LDA	M	701	16/16	0.18	2.53	29,44,52,58	0
5	BCL	M	501	66/66	0.17	2.26	27,32,92,94	0
8	SPN	M	600	43/43	0.21	2.12	36,47,64,67	0
7	U10	M	503	48/63	0.15	1.59	15,29,60,62	0
5	BCL	M	502	66/66	0.12	0.44	10,19,52,68	0
5	BCL	L	304	66/66	0.12	0.08	2,14,40,49	0
6	BPH	M	401	65/65	0.13	-0.02	29,33,63,67	10
5	BCL	L	302	66/66	0.10	-0.50	5,17,40,54	0
4	FE	M	500	1/1	0.02	-2.98	18,18,18,18	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.