



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 21, 2016 – 08:04 PM EDT

PDB ID : 2FKW  
Title : Structure of LH2 from Rps. acidophila crystallized in lipidic mesophases  
Authors : Papiz, M.Z.; Cherezov, V.; Clogston, J.; Caffrey, M.  
Deposited on : 2006-01-05  
Resolution : 2.45 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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

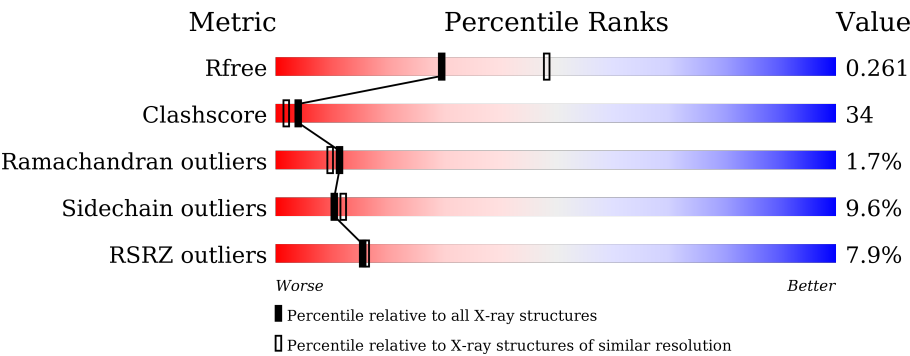
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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.

Mol	Chain	Length	Quality of chain
1	A	53	<div><div>11%</div><div><div></div><div>60%</div><div>30%</div><div>9%</div></div></div>
1	C	53	<div><div>13%</div><div><div></div><div>60%</div><div>30%</div><div>6%</div><div>.</div></div></div>
1	E	53	<div><div>11%</div><div><div></div><div>66%</div><div>23%</div><div>9%</div><div>.</div></div></div>
1	G	53	<div><div>11%</div><div><div></div><div>70%</div><div>23%</div><div>8%</div></div></div>
1	I	53	<div><div>11%</div><div><div></div><div>66%</div><div>28%</div><div>.</div><div>.</div></div></div>
1	K	53	<div><div>11%</div><div><div></div><div>68%</div><div>28%</div><div>.</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
1	M	53	
1	O	53	
1	R	53	
2	B	41	
2	D	41	
2	F	41	
2	H	41	
2	J	41	
2	L	41	
2	N	41	
2	P	41	
2	S	41	

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	A	1501	X	-	-	-
4	BCL	A	1701	X	-	-	-
4	BCL	B	1601	X	-	-	-
4	BCL	C	1502	X	-	-	-
4	BCL	C	1702	X	-	-	-
4	BCL	G	1704	X	-	X	-
4	BCL	H	1604	X	-	-	-
4	BCL	I	1705	-	-	X	-
4	BCL	J	1605	X	-	-	-
4	BCL	K	1506	X	-	-	-
4	BCL	K	1706	X	-	-	-
4	BCL	L	1606	X	-	X	-
4	BCL	M	1707	X	-	X	-
4	BCL	N	1607	X	-	-	-
4	BCL	O	1508	X	-	-	-
4	BCL	O	1708	X	-	-	-
4	BCL	P	1608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BCL	R	1509	X	-	-	-
4	BCL	R	1709	X	-	X	X
4	BCL	S	1609	X	-	-	-
5	LDA	A	1816	-	-	-	X
5	LDA	A	1817	-	-	-	X
5	LDA	B	1801	-	-	-	X
5	LDA	C	1815	-	-	-	X
5	LDA	C	1821	-	-	-	X
5	LDA	D	1802	-	-	-	X
5	LDA	E	1822	-	-	-	X
5	LDA	E	1823	-	-	-	X
5	LDA	F	1803	-	-	-	X
5	LDA	G	1814	-	-	-	X
5	LDA	G	1824	-	-	X	X
5	LDA	H	1804	-	-	-	X
5	LDA	I	1812	-	-	-	X
5	LDA	I	1825	-	-	-	X
5	LDA	K	1810	-	-	-	X
5	LDA	K	1826	-	-	-	X
5	LDA	L	1806	-	-	-	X
5	LDA	M	1811	-	-	-	X
5	LDA	M	1827	-	-	-	X
5	LDA	N	1807	-	-	-	X
5	LDA	O	1820	-	-	-	X
5	LDA	P	1808	-	-	-	X
5	LDA	R	1809	-	-	-	X
5	LDA	R	1818	-	-	X	X
5	LDA	R	1819	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9829 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 Light-harvesting protein B-800/850, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	C	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	E	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	G	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	I	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	K	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	M	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	O	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	R	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			

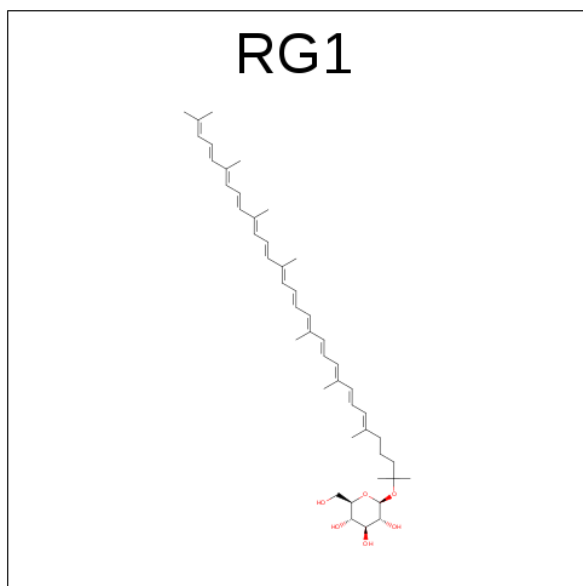
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
C	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
E	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
G	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
I	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
K	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
M	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
O	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
R	1	CXM	MET	MODIFIED RESIDUE	UNP P26789

- Molecule 2 is a protein called Light-harvesting protein B-800/850, beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	D	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	F	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	H	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	J	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	L	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	N	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	P	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	S	41	Total	C	N	O	0	0	0
			323	213	53	57			

- Molecule 3 is SUGAR (RHODOPIN B-D-GLUCOSIDE) (three-letter code: RG1) (formula:  $C_{46}H_{66}O_6$ ).



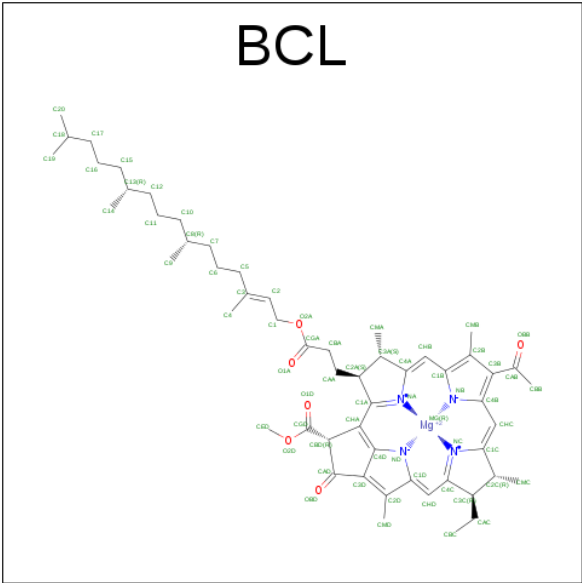
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	R	1	Total	C	O	0	0
			52	46	6		
3	D	1	Total	C	O	0	0
			52	46	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			52	46	6		
3	H	1	Total	C	O	0	0
			52	46	6		
3	J	1	Total	C	O	0	0
			52	46	6		
3	L	1	Total	C	O	0	0
			52	46	6		
3	N	1	Total	C	O	0	0
			52	46	6		
3	P	1	Total	C	O	0	0
			52	46	6		
3	S	1	Total	C	O	0	0
			52	46	6		

- 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	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	C	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	E	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	F	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	E	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	G	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	H	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	G	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	I	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	J	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	I	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	K	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	K	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	N	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	O	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	P	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	O	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	R	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

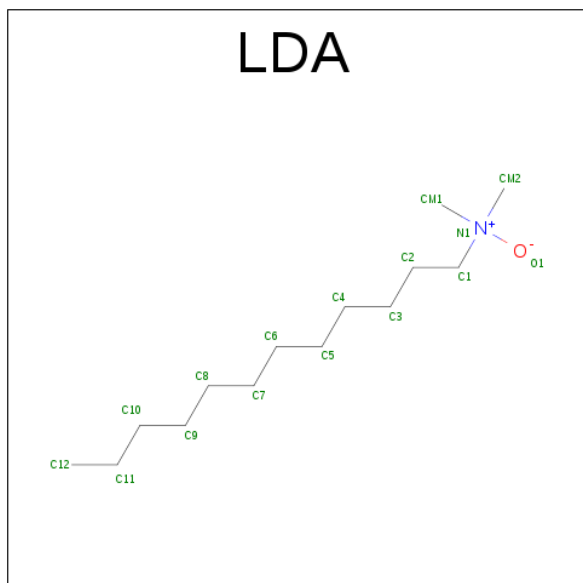
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	S	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			16	14	1	1		
5	D	1	Total	C	N	O	0	0
			16	14	1	1		
5	F	1	Total	C	N	O	0	0
			16	14	1	1		
5	H	1	Total	C	N	O	0	0
			16	14	1	1		
5	J	1	Total	C	N	O	0	0
			16	14	1	1		
5	L	1	Total	C	N	O	0	0
			16	14	1	1		
5	N	1	Total	C	N	O	0	0
			16	14	1	1		
5	P	1	Total	C	N	O	0	0
			16	14	1	1		
5	R	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	K	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		
5	I	1	Total	C	N	O	0	0
			16	14	1	1		
5	I	1	Total	C	N	O	0	0
			16	14	1	1		
5	G	1	Total	C	N	O	0	0
			16	14	1	1		
5	C	1	Total	C	N	O	0	0
			16	14	1	1		
5	A	1	Total	C	N	O	0	0
			16	14	1	1		
5	A	1	Total	C	N	O	0	0
			16	14	1	1		
5	R	1	Total	C	N	O	0	0
			16	14	1	1		
5	R	1	Total	C	N	O	0	0
			16	14	1	1		
5	O	1	Total	C	N	O	0	0
			16	14	1	1		
5	C	1	Total	C	N	O	0	0
			16	14	1	1		
5	E	1	Total	C	N	O	0	0
			16	14	1	1		
5	E	1	Total	C	N	O	0	0
			16	14	1	1		
5	G	1	Total	C	N	O	0	0
			16	14	1	1		
5	I	1	Total	C	N	O	0	0
			16	14	1	1		
5	K	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	33	Total	O	0	0
			33	33		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	26	Total 26	O 26	0	0
6	C	24	Total 24	O 24	0	0
6	D	27	Total 27	O 27	0	0
6	E	40	Total 40	O 40	0	0
6	F	28	Total 28	O 28	0	0
6	G	41	Total 41	O 41	0	0
6	H	37	Total 37	O 37	2	0
6	I	38	Total 38	O 38	0	0
6	J	39	Total 39	O 39	1	0
6	K	47	Total 47	O 47	0	0
6	L	29	Total 29	O 29	0	0
6	M	36	Total 36	O 36	0	0
6	N	30	Total 30	O 30	0	0
6	O	33	Total 33	O 33	1	0
6	P	32	Total 32	O 32	0	0
6	R	39	Total 39	O 39	0	0
6	S	34	Total 34	O 34	0	0

### 3 Residue-property plots [i](#)

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.

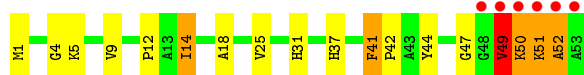
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



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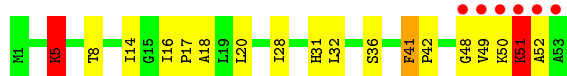
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



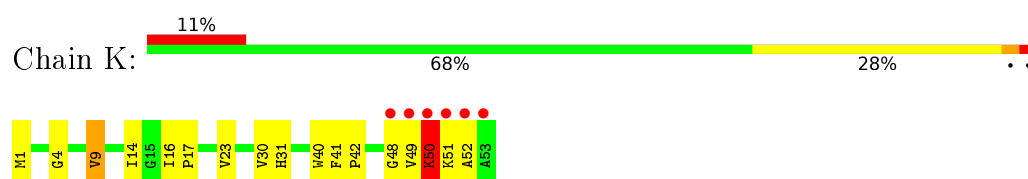
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



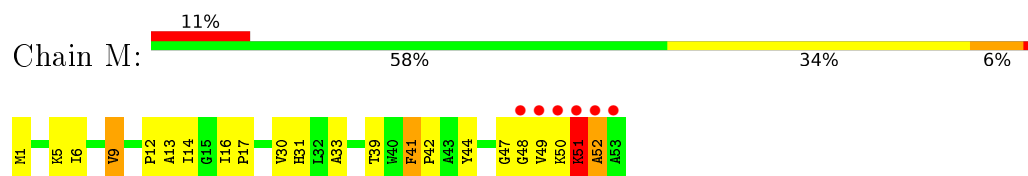
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



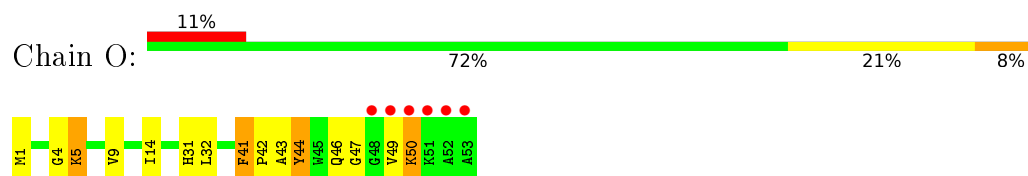
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



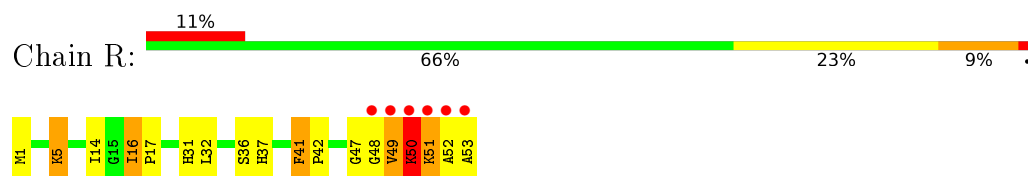
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



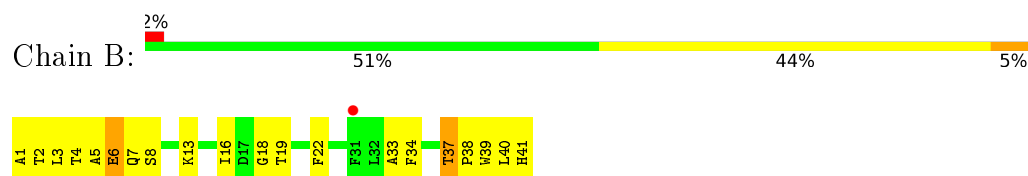
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



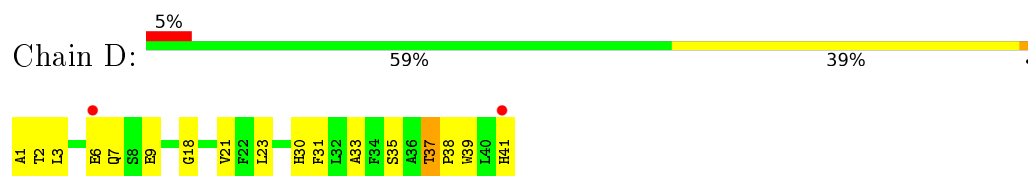
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



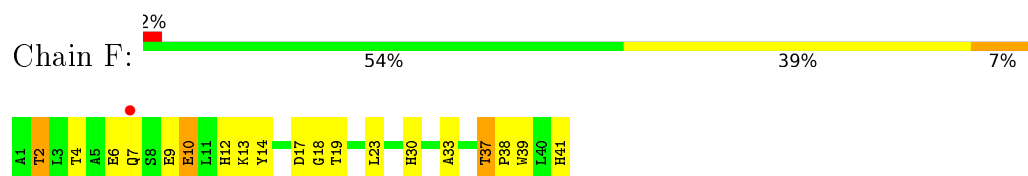
- Molecule 2: Light-harvesting protein B-800/850, beta chain



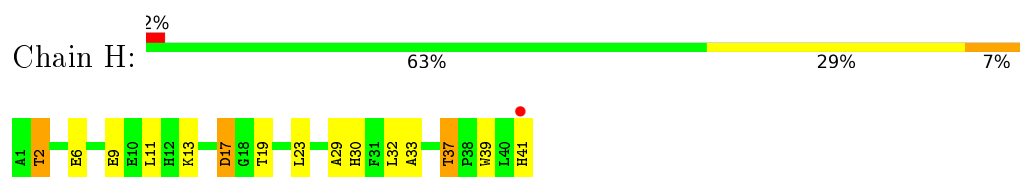
- Molecule 2: Light-harvesting protein B-800/850, beta chain



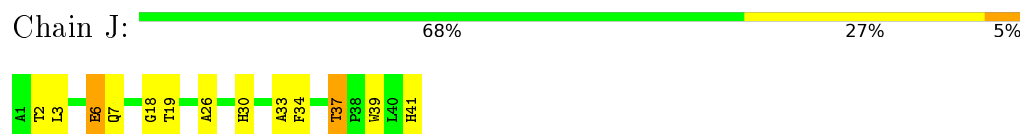
- Molecule 2: Light-harvesting protein B-800/850, beta chain



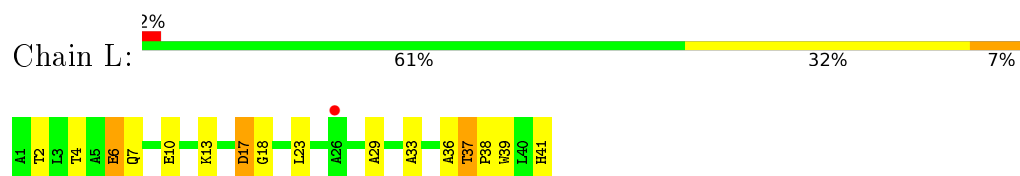
- Molecule 2: Light-harvesting protein B-800/850, beta chain



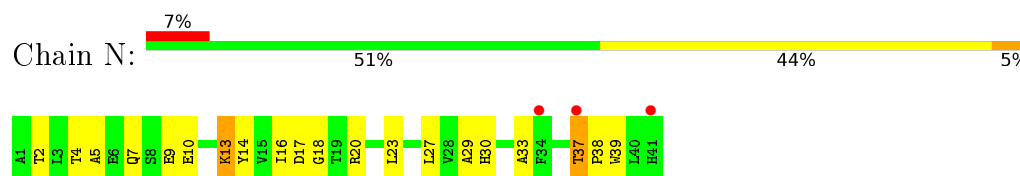
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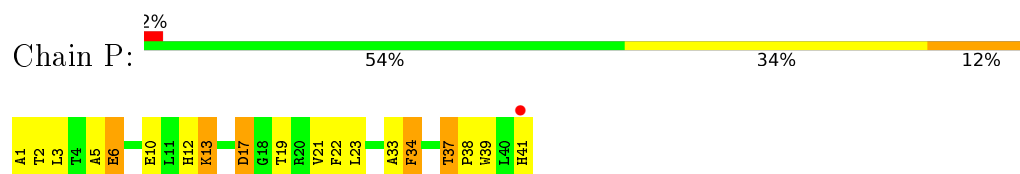
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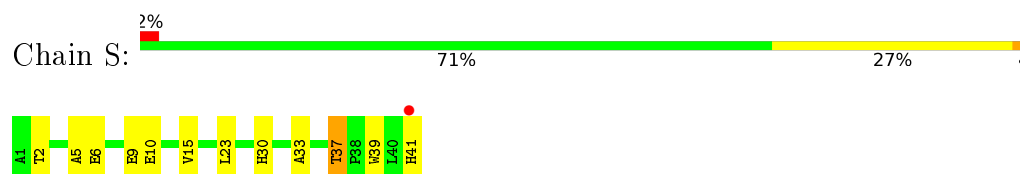
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- Molecule 2: Light-harvesting protein B-800/850, beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.44Å 126.38Å 129.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.45 38.85 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (10.00-2.45) 99.7 (38.85-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.183 , 0.254 0.203 , 0.261	Depositor DCC
$R_{free}$ test set	2531 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.0	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.7	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	10 of 49795 reflections (0.020%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9829	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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, RG1, LDA, CXM

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	A	1.27	1/404 (0.2%)	0.51	0/556
1	C	1.51	4/404 (1.0%)	0.51	0/556
1	E	1.35	1/404 (0.2%)	0.53	0/556
1	G	1.34	2/404 (0.5%)	0.50	0/556
1	I	1.38	1/404 (0.2%)	0.53	0/556
1	K	1.47	2/404 (0.5%)	0.55	0/556
1	M	1.35	1/404 (0.2%)	0.57	0/556
1	O	1.36	2/404 (0.5%)	0.51	0/556
1	R	1.35	3/404 (0.7%)	0.53	0/556
2	B	1.40	1/332 (0.3%)	0.49	0/453
2	D	1.25	1/332 (0.3%)	0.45	0/453
2	F	1.48	2/332 (0.6%)	0.42	0/453
2	H	1.40	2/332 (0.6%)	0.45	0/453
2	J	1.29	2/332 (0.6%)	0.44	0/453
2	L	1.62	5/332 (1.5%)	0.47	0/453
2	N	1.38	2/332 (0.6%)	0.44	0/453
2	P	1.60	3/332 (0.9%)	0.49	0/453
2	S	1.21	1/332 (0.3%)	0.45	0/453
All	All	1.39	36/6624 (0.5%)	0.50	0/9081

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	A	0	2
1	C	2	1
1	E	1	0
1	G	1	0
1	I	2	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	1	1
1	M	3	1
1	O	0	1
1	R	2	0
All	All	12	7

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	6	GLU	CG-CD	11.70	1.69	1.51
2	L	10	GLU	CG-CD	11.28	1.68	1.51
2	F	10	GLU	CG-CD	9.26	1.65	1.51
2	L	17	ASP	CB-CG	7.49	1.67	1.51
1	A	49	VAL	CA-CB	7.42	1.70	1.54
1	I	5	LYS	CD-CE	7.06	1.68	1.51
1	C	9	VAL	CB-CG1	-6.83	1.38	1.52
2	F	6	GLU	CG-CD	6.81	1.62	1.51
2	P	6	GLU	CB-CG	6.80	1.65	1.52
2	P	1	ALA	CA-CB	6.73	1.66	1.52
1	M	9	VAL	CB-CG2	-6.58	1.39	1.52
1	G	36	SER	C-O	-6.41	1.11	1.23
2	L	17	ASP	CG-OD1	6.39	1.40	1.25
2	H	17	ASP	CB-CG	-6.35	1.38	1.51
2	H	6	GLU	CG-CD	6.29	1.61	1.51
2	B	13	LYS	CD-CE	6.16	1.66	1.51
1	O	9	VAL	CB-CG2	-5.97	1.40	1.52
1	O	44	TYR	CD2-CE2	5.95	1.48	1.39
1	K	23	VAL	CB-CG2	-5.95	1.40	1.52
2	N	10	GLU	CG-CD	5.89	1.60	1.51
1	R	5	LYS	CD-CE	5.88	1.66	1.51
1	C	52	ALA	CA-CB	-5.75	1.40	1.52
1	C	53	ALA	CA-CB	-5.70	1.40	1.52
2	D	31	PHE	CE2-CZ	5.57	1.48	1.37
2	J	34	PHE	CE1-CZ	5.56	1.48	1.37
2	J	6	GLU	CD-OE2	5.42	1.31	1.25
2	N	14	TYR	CD1-CE1	-5.39	1.31	1.39
1	R	53	ALA	CA-CB	-5.34	1.41	1.52
1	K	9	VAL	CB-CG2	-5.31	1.41	1.52
1	E	49	VAL	N-CA	5.26	1.56	1.46
2	L	29	ALA	CA-CB	5.18	1.63	1.52
2	L	6	GLU	CG-CD	5.17	1.59	1.51
1	R	49	VAL	CA-CB	5.14	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	48	GLY	CA-C	5.07	1.59	1.51
1	C	36	SER	CB-OG	-5.06	1.35	1.42
2	S	15	VAL	CB-CG2	-5.04	1.42	1.52

There are no bond angle outliers.

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	52	ALA	CA
1	C	53	ALA	CA
1	E	51	LYS	CA
1	G	50	LYS	CA
1	I	49	VAL	CA
1	I	50	LYS	CA
1	K	51	LYS	CA
1	M	49	VAL	CA
1	M	51	LYS	CA
1	M	52	ALA	CA
1	R	50	LYS	CA
1	R	53	ALA	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	50	LYS	Peptide
1	A	51	LYS	Peptide
1	C	52	ALA	Peptide
1	I	51	LYS	Peptide
1	K	50	LYS	Peptide
1	M	51	LYS	Peptide
1	O	50	LYS	Peptide

## 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	A	403	0	422	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	403	0	422	27	0
1	E	403	0	422	27	0
1	G	403	0	422	21	0
1	I	403	0	422	21	0
1	K	403	0	422	27	0
1	M	403	0	422	32	0
1	O	403	0	422	17	0
1	R	403	0	422	22	0
2	B	323	0	321	25	0
2	D	323	0	321	22	0
2	F	323	0	321	24	0
2	H	323	0	321	19	0
2	J	323	0	321	23	0
2	L	323	0	321	22	0
2	N	323	0	321	29	0
2	P	323	0	321	30	0
2	S	323	0	321	11	0
3	D	52	0	66	5	0
3	F	52	0	66	5	0
3	H	52	0	66	5	0
3	J	52	0	66	1	0
3	L	52	0	66	4	0
3	N	52	0	66	4	0
3	P	52	0	66	4	0
3	R	52	0	66	4	0
3	S	52	0	66	5	0
4	A	132	0	146	25	0
4	B	66	0	74	11	0
4	C	132	0	148	15	0
4	D	66	0	74	8	0
4	E	132	0	147	12	0
4	F	66	0	74	12	0
4	G	132	0	147	27	0
4	H	66	0	73	12	0
4	I	132	0	148	33	0
4	J	66	0	73	17	0
4	K	132	0	146	14	0
4	L	66	0	74	25	0
4	M	132	0	147	28	0
4	N	66	0	74	16	0
4	O	132	0	147	21	0
4	P	66	0	73	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	132	0	147	28	0
4	S	66	0	74	13	0
5	A	32	0	62	11	0
5	B	16	0	31	2	0
5	C	32	0	62	6	0
5	D	16	0	31	3	0
5	E	32	0	62	14	0
5	F	16	0	31	7	0
5	G	32	0	62	17	0
5	H	16	0	31	3	0
5	I	48	0	93	15	0
5	J	16	0	31	1	0
5	K	32	0	62	12	0
5	L	16	0	31	5	0
5	M	32	0	62	6	0
5	N	16	0	31	2	0
5	O	16	0	31	7	0
5	P	16	0	31	3	0
5	R	48	0	93	12	0
6	A	33	0	0	9	0
6	B	26	0	0	6	0
6	C	24	0	0	3	0
6	D	27	0	0	8	0
6	E	40	0	0	20	0
6	F	28	0	0	7	0
6	G	41	0	0	22	0
6	H	37	0	0	5	0
6	I	38	0	0	11	0
6	J	39	0	0	14	0
6	K	47	0	0	28	0
6	L	29	0	0	2	0
6	M	36	0	0	10	0
6	N	30	0	0	8	0
6	O	33	0	0	11	0
6	P	32	0	0	8	0
6	R	39	0	0	24	0
6	S	34	0	0	4	0
All	All	9829	0	10104	659	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 34.

All (659) 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)
1:M:1:CXM:CE	1:M:1:CXM:SD	2.21	1.28
1:G:48:GLY:HA2	6:G:1839:HOH:O	1.32	1.24
5:I:1825:LDA:HM22	6:I:1845:HOH:O	1.06	1.24
5:H:1804:LDA:H92	6:H:1825:HOH:O	1.38	1.22
1:E:49:VAL:HG11	6:E:1850:HOH:O	1.45	1.15
4:I:1705:BCL:H41	4:I:1705:BCL:H8	1.25	1.15
6:A:1831:HOH:O	2:D:21:VAL:HG11	1.53	1.08
4:R:1709:BCL:H2	6:R:1831:HOH:O	1.54	1.07
4:G:1504:BCL:H143	6:G:1853:HOH:O	1.54	1.05
4:O:1708:BCL:H2	6:O:1833:HOH:O	1.59	1.02
2:P:33:ALA:O	2:P:37:THR:HB	1.58	1.02
4:O:1708:BCL:C2	6:O:1833:HOH:O	2.08	1.01
5:I:1812:LDA:HM23	6:I:1829:HOH:O	1.59	1.01
2:D:6:GLU:HB3	6:D:1825:HOH:O	1.61	1.01
4:J:1605:BCL:O2D	6:J:1813:HOH:O	1.79	1.01
5:G:1824:LDA:CM1	6:G:1828:HOH:O	2.08	1.00
5:E:1822:LDA:CM2	6:E:1859:HOH:O	2.09	0.99
1:G:48:GLY:O	6:G:1832:HOH:O	1.79	0.98
1:I:48:GLY:HA2	6:I:1836:HOH:O	1.63	0.98
1:I:48:GLY:CA	6:I:1836:HOH:O	2.10	0.97
4:A:1501:BCL:H191	4:R:1709:BCL:HED1	1.41	0.97
4:A:1501:BCL:O1D	4:A:1501:BCL:CAA	2.14	0.96
1:E:14:ILE:HG22	6:E:1835:HOH:O	1.65	0.96
2:L:39:TRP:CE2	4:L:1606:BCL:CMC	2.49	0.95
4:J:1605:BCL:CBD	6:J:1813:HOH:O	2.12	0.95
2:P:23:LEU:HB2	4:P:1608:BCL:H2	1.46	0.95
5:G:1824:LDA:HM11	6:G:1828:HOH:O	1.66	0.94
4:M:1707:BCL:O2D	6:M:1859:HOH:O	1.86	0.94
1:E:44:TYR:CZ	6:E:1862:HOH:O	2.19	0.94
1:K:31:HIS:CE1	4:L:1606:BCL:HMD1	2.03	0.93
4:A:1501:BCL:HAA2	4:A:1501:BCL:O1D	1.68	0.93
1:C:13:ALA:HB2	6:D:1826:HOH:O	1.67	0.92
1:M:51:LYS:HG2	1:M:52:ALA:O	1.69	0.92
2:F:33:ALA:O	2:F:37:THR:HB	1.68	0.92
2:N:33:ALA:O	2:N:37:THR:HB	1.68	0.92
5:O:1820:LDA:HM12	6:O:1823:HOH:O	1.70	0.91
2:H:33:ALA:O	2:H:37:THR:HB	1.70	0.91
5:R:1818:LDA:H92	6:R:1852:HOH:O	1.70	0.90
1:C:14:ILE:HG21	5:C:1815:LDA:H21	1.53	0.90
4:M:1707:BCL:CBD	6:M:1859:HOH:O	2.20	0.89
1:M:51:LYS:HA	1:M:52:ALA:HB2	1.52	0.89
1:C:36:SER:OG	5:E:1822:LDA:HM21	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:ALA:O	2:D:37:THR:HB	1.74	0.87
2:S:33:ALA:O	2:S:37:THR:HG22	1.74	0.87
2:D:9:GLU:OE1	6:D:1809:HOH:O	1.91	0.87
6:K:1864:HOH:O	5:L:1806:LDA:H82	1.75	0.86
2:P:33:ALA:HB1	6:P:1837:HOH:O	1.76	0.86
1:A:31:HIS:CE1	4:B:1601:BCL:HMD1	2.10	0.86
1:R:5:LYS:HD3	6:R:1835:HOH:O	1.75	0.85
2:L:33:ALA:O	2:L:37:THR:HB	1.77	0.85
2:J:33:ALA:O	2:J:37:THR:HB	1.76	0.85
4:R:1709:BCL:H41	4:R:1709:BCL:H92	1.59	0.84
1:I:48:GLY:N	6:I:1836:HOH:O	2.10	0.84
2:J:41:HIS:NE2	1:K:49:VAL:HG12	1.92	0.84
1:I:5:LYS:HG3	6:J:1823:HOH:O	1.78	0.83
5:K:1810:LDA:HM22	1:M:14:ILE:HD11	1.58	0.83
5:O:1820:LDA:HM23	6:O:1823:HOH:O	1.76	0.83
4:I:1705:BCL:H41	4:I:1705:BCL:C8	2.06	0.82
6:K:1848:HOH:O	1:M:13:ALA:HB2	1.79	0.82
4:A:1501:BCL:C19	4:R:1709:BCL:HED1	2.08	0.82
5:O:1820:LDA:H122	6:O:1850:HOH:O	1.80	0.81
4:P:1608:BCL:HMB1	4:P:1608:BCL:HBB2	1.63	0.81
2:P:37:THR:HG22	2:P:39:TRP:H	1.45	0.81
4:A:1501:BCL:H62	4:R:1709:BCL:HED2	1.59	0.81
4:J:1605:BCL:CBB	6:K:1864:HOH:O	2.28	0.81
6:R:1835:HOH:O	2:S:5:ALA:HB1	1.81	0.81
4:N:1607:BCL:HBB2	4:N:1607:BCL:HMB1	1.62	0.81
2:L:39:TRP:CE2	4:L:1606:BCL:HMC3	2.14	0.80
4:R:1709:BCL:CAD	4:S:1609:BCL:H203	2.10	0.80
5:I:1825:LDA:H92	6:K:1842:HOH:O	1.80	0.80
5:A:1816:LDA:H31	1:C:14:ILE:HD13	1.64	0.80
1:A:14:ILE:HG21	5:A:1816:LDA:H42	1.62	0.80
2:B:4:THR:OG1	2:B:7:GLN:HG3	1.81	0.80
1:C:31:HIS:CE1	4:D:1602:BCL:HMD1	2.17	0.80
6:A:1850:HOH:O	2:B:8:SER:HB2	1.82	0.80
2:P:41:HIS:NE2	1:R:49:VAL:CG1	2.46	0.79
4:M:1707:BCL:H8	4:M:1707:BCL:H41	1.65	0.78
2:B:37:THR:HG23	2:B:39:TRP:H	1.47	0.78
4:G:1704:BCL:CED	4:I:1505:BCL:H191	2.14	0.78
1:M:31:HIS:CE1	4:N:1607:BCL:HMD1	2.19	0.77
4:R:1709:BCL:H102	6:S:419:HOH:O	1.85	0.77
5:K:1810:LDA:H21	1:M:14:ILE:HD13	1.68	0.76
4:R:1709:BCL:C9	4:R:1709:BCL:H41	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:5:LYS:CG	6:J:1823:HOH:O	2.32	0.75
5:O:1820:LDA:HM22	1:R:32:LEU:HD22	1.67	0.75
2:S:37:THR:HG23	2:S:39:TRP:H	1.49	0.75
2:P:33:ALA:CB	6:P:1837:HOH:O	2.31	0.75
1:M:48:GLY:HA2	6:M:1829:HOH:O	1.86	0.75
5:I:1812:LDA:H121	6:K:1856:HOH:O	1.85	0.75
5:G:1824:LDA:CM2	6:G:1828:HOH:O	2.35	0.75
2:S:23:LEU:HB2	4:S:1609:BCL:H2	1.67	0.74
2:F:10:GLU:OE1	3:F:1403:RG1:O2'	2.03	0.74
5:R:1818:LDA:C11	6:R:1856:HOH:O	2.35	0.74
1:A:14:ILE:HD13	5:A:1816:LDA:H22	1.68	0.74
5:A:1816:LDA:C3	1:C:14:ILE:HD13	2.18	0.74
2:L:39:TRP:CD2	4:L:1606:BCL:CMC	2.71	0.74
5:R:1818:LDA:H122	6:R:1856:HOH:O	1.88	0.74
1:E:18:ALA:O	6:E:1860:HOH:O	2.05	0.74
2:H:32:LEU:HD12	5:H:1804:LDA:H122	1.70	0.73
1:M:41:PHE:HB3	1:M:42:PRO:HD3	1.69	0.73
4:I:1705:BCL:C4	4:I:1705:BCL:H8	2.15	0.73
2:N:39:TRP:CE2	4:N:1607:BCL:CMC	2.72	0.73
2:P:39:TRP:CE2	4:P:1608:BCL:HMC2	2.24	0.73
5:G:1824:LDA:HM21	6:G:1843:HOH:O	1.89	0.72
1:O:31:HIS:CE1	4:P:1608:BCL:HMD1	2.24	0.72
5:G:1824:LDA:H31	6:G:1844:HOH:O	1.86	0.72
4:P:1608:BCL:CBB	4:P:1608:BCL:HMB1	2.19	0.72
5:R:1818:LDA:C9	6:R:1852:HOH:O	2.30	0.72
5:A:1817:LDA:H11	6:A:1820:HOH:O	1.90	0.72
2:D:37:THR:HG22	2:D:39:TRP:H	1.54	0.71
1:M:33:ALA:HA	5:M:1827:LDA:HM11	1.70	0.71
4:P:1608:BCL:HBC1	6:P:1837:HOH:O	1.90	0.71
5:G:1824:LDA:HM23	6:I:1859:HOH:O	1.89	0.71
5:E:1822:LDA:HM22	6:E:1859:HOH:O	1.83	0.71
2:H:23:LEU:HB2	4:H:1604:BCL:H2	1.72	0.71
1:E:14:ILE:CG2	6:E:1835:HOH:O	2.30	0.70
1:A:20:LEU:HD13	4:R:1709:BCL:HED3	1.73	0.70
2:N:39:TRP:CD2	4:N:1607:BCL:HMC2	2.26	0.70
4:O:1508:BCL:HHC	4:O:1508:BCL:OBB	1.89	0.70
5:R:1818:LDA:C9	6:R:1856:HOH:O	2.39	0.70
2:B:1:ALA:N	6:B:278:HOH:O	2.23	0.70
2:H:39:TRP:CE3	4:H:1604:BCL:CBC	2.75	0.70
1:M:49:VAL:HG12	6:M:1843:HOH:O	1.91	0.70
5:N:1807:LDA:HM12	6:N:1810:HOH:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:1824:LDA:C6	6:G:1865:HOH:O	2.38	0.70
1:K:48:GLY:HA2	6:K:1829:HOH:O	1.90	0.70
5:R:1818:LDA:C10	6:R:1856:HOH:O	2.40	0.70
5:K:1810:LDA:H101	6:K:1856:HOH:O	1.92	0.70
4:K:1506:BCL:HMC3	5:L:1806:LDA:H51	1.71	0.70
2:P:41:HIS:NE2	1:R:49:VAL:HG13	2.06	0.70
4:F:1603:BCL:HMB1	4:F:1603:BCL:HBB2	1.72	0.69
4:R:1509:BCL:O1D	4:R:1509:BCL:H2A	1.92	0.69
4:M:1707:BCL:C7	4:M:1707:BCL:H41	2.22	0.69
1:E:44:TYR:CE1	6:E:1862:HOH:O	2.44	0.69
1:E:49:VAL:CG1	6:E:1850:HOH:O	2.16	0.69
2:J:26:ALA:HB1	6:J:1825:HOH:O	1.92	0.69
2:F:2:THR:HG22	6:F:1823:HOH:O	1.92	0.69
4:K:1706:BCL:HBB2	4:K:1706:BCL:HHC	1.73	0.69
2:P:41:HIS:NE2	1:R:49:VAL:HG12	2.07	0.69
1:G:41:PHE:HB3	1:G:42:PRO:HD3	1.75	0.68
2:N:39:TRP:CE2	4:N:1607:BCL:HMC2	2.27	0.68
5:R:1818:LDA:H71	6:R:1852:HOH:O	1.93	0.68
4:I:1705:BCL:HHB	2:J:19:THR:HG21	1.76	0.68
1:R:48:GLY:HA2	6:R:1823:HOH:O	1.92	0.68
6:A:1850:HOH:O	2:B:3:LEU:HB2	1.94	0.68
1:K:30:VAL:CG2	3:L:1406:RG1:HM03	2.24	0.68
1:R:37:HIS:ND1	6:R:1845:HOH:O	2.27	0.68
4:J:1605:BCL:CGD	6:J:1813:HOH:O	2.27	0.68
4:G:1704:BCL:C10	6:H:1808:HOH:O	2.40	0.67
4:A:1501:BCL:O1D	4:A:1501:BCL:C2A	2.42	0.67
4:O:1508:BCL:O1D	4:O:1508:BCL:HAA2	1.95	0.67
6:E:1862:HOH:O	5:F:1803:LDA:C3	2.42	0.67
2:F:41:HIS:CE1	1:G:49:VAL:H	2.12	0.67
4:L:1606:BCL:CHB	4:M:1507:BCL:HMB3	2.24	0.67
1:A:35:LEU:HD21	1:R:37:HIS:CD2	2.30	0.67
1:I:31:HIS:CE1	4:J:1605:BCL:HMD1	2.30	0.66
4:R:1709:BCL:C10	6:S:419:HOH:O	2.41	0.66
5:I:1825:LDA:HM11	6:I:1859:HOH:O	1.95	0.66
1:I:41:PHE:HB3	1:I:42:PRO:HD3	1.78	0.66
2:J:41:HIS:NE2	1:K:49:VAL:CG1	2.58	0.66
4:F:1603:BCL:H62	4:F:1603:BCL:H112	1.76	0.66
5:K:1810:LDA:H21	1:M:14:ILE:CD1	2.25	0.66
4:G:1704:BCL:H101	6:H:1808:HOH:O	1.96	0.65
1:A:14:ILE:HG21	5:A:1816:LDA:C4	2.26	0.65
2:B:41:HIS:O	6:B:186:HOH:O	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1403:RG1:O1'	6:F:1827:HOH:O	2.13	0.65
1:I:51:LYS:HB2	1:I:52:ALA:HA	1.77	0.65
4:F:1603:BCL:H142	4:F:1603:BCL:C10	2.26	0.65
5:E:1823:LDA:H11	6:E:1854:HOH:O	1.97	0.65
1:R:1:CXM:HE2	6:R:1842:HOH:O	1.96	0.65
4:G:1704:BCL:CB D	6:G:1854:HOH:O	2.44	0.64
1:O:41:PHE:HB3	1:O:42:PRO:HD3	1.77	0.64
5:E:1823:LDA:HM21	6:E:1853:HOH:O	1.96	0.64
1:G:50:LYS:NZ	6:G:1840:HOH:O	2.29	0.64
5:I:1825:LDA:C9	6:K:1842:HOH:O	2.41	0.64
1:R:5:LYS:CD	6:R:1835:HOH:O	2.37	0.64
1:C:36:SER:OG	5:E:1822:LDA:CM2	2.43	0.64
1:K:14:ILE:HG21	5:K:1810:LDA:H31	1.79	0.64
1:K:30:VAL:HG22	3:L:1406:RG1:HM03	1.80	0.64
2:B:41:HIS:NE2	1:C:49:VAL:HG12	2.13	0.64
1:E:49:VAL:HG21	6:E:1849:HOH:O	1.96	0.63
2:D:37:THR:CG2	2:D:39:TRP:H	2.11	0.63
5:F:1803:LDA:C8	6:F:1809:HOH:O	2.44	0.63
2:B:19:THR:CG2	4:B:1601:BCL:H42	2.27	0.63
4:M:1707:BCL:H141	2:N:30:HIS:ND1	2.12	0.63
4:M:1707:BCL:C8	4:M:1707:BCL:H41	2.27	0.63
5:G:1824:LDA:H52	6:G:1865:HOH:O	1.98	0.63
2:N:23:LEU:HD22	4:N:1607:BCL:H61	1.79	0.63
4:H:1604:BCL:HMB1	4:H:1604:BCL:HBB2	1.79	0.63
1:A:48:GLY:HA2	6:A:1843:HOH:O	1.98	0.63
4:G:1704:BCL:HAA1	4:G:1704:BCL:O1D	1.98	0.63
2:H:39:TRP:CE2	4:H:1604:BCL:HMC2	2.34	0.63
2:J:30:HIS:CE1	6:J:1825:HOH:O	2.50	0.63
2:N:17:ASP:CG	6:N:1829:HOH:O	2.35	0.63
2:P:37:THR:CG2	2:P:39:TRP:H	2.12	0.63
2:D:41:HIS:NE2	1:E:49:VAL:HG23	2.14	0.62
4:J:1605:BCL:HBB2	4:J:1605:BCL:HMB1	1.81	0.62
5:O:1820:LDA:C12	6:O:1850:HOH:O	2.42	0.62
2:D:38:PRO:O	1:E:47:GLY:HA3	1.99	0.62
5:G:1824:LDA:C5	6:G:1865:HOH:O	2.46	0.62
4:I:1705:BCL:H2	4:J:1605:BCL:H192	1.82	0.62
4:S:1609:BCL:HBB2	4:S:1609:BCL:HMB1	1.80	0.62
2:B:4:THR:H	2:B:7:GLN:HE21	1.47	0.62
4:A:1701:BCL:HBB2	4:A:1701:BCL:HHC	1.82	0.62
5:G:1824:LDA:H61	6:G:1865:HOH:O	1.99	0.62
1:R:16:ILE:HB	1:R:17:PRO:HD3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:1709:BCL:C2	6:R:1831:HOH:O	2.28	0.62
5:E:1822:LDA:HM23	6:E:1859:HOH:O	1.82	0.62
2:H:37:THR:HG22	2:H:39:TRP:H	1.65	0.62
2:J:7:GLN:NE2	6:J:1812:HOH:O	2.31	0.62
5:I:1812:LDA:C2	6:K:1860:HOH:O	2.47	0.61
4:G:1704:BCL:HED2	4:I:1505:BCL:H191	1.81	0.61
4:R:1709:BCL:H41	4:R:1709:BCL:C8	2.31	0.61
4:B:1601:BCL:CHB	4:C:1502:BCL:HMB3	2.31	0.61
2:P:41:HIS:CD2	1:R:49:VAL:N	2.69	0.61
2:F:37:THR:CG2	2:F:39:TRP:H	2.14	0.60
1:E:31:HIS:CE1	4:F:1603:BCL:HMD1	2.37	0.60
4:G:1704:BCL:O1D	4:I:1505:BCL:C5	2.49	0.60
4:G:1704:BCL:HBB	2:H:19:THR:HG21	1.83	0.60
4:N:1607:BCL:CBB	4:N:1607:BCL:HMB1	2.30	0.60
4:A:1501:BCL:HMB1	4:A:1501:BCL:CBB	2.32	0.60
2:F:9:GLU:OE1	6:F:1804:HOH:O	2.15	0.60
2:J:37:THR:HG23	2:J:39:TRP:H	1.67	0.60
4:C:1702:BCL:HBB2	4:C:1702:BCL:HHC	1.84	0.60
4:M:1707:BCL:O1D	4:O:1508:BCL:C5	2.50	0.60
2:P:34:PHE:CG	6:P:1817:HOH:O	2.51	0.60
4:F:1603:BCL:C6	4:F:1603:BCL:H112	2.31	0.60
4:A:1501:BCL:O1D	4:A:1501:BCL:CBA	2.49	0.60
5:G:1824:LDA:HM21	6:G:1828:HOH:O	1.99	0.60
2:H:33:ALA:N	6:H:1825:HOH:O	2.35	0.60
4:K:1506:BCL:HBB1	6:K:1851:HOH:O	2.02	0.59
2:L:39:TRP:HA	6:M:1862:HOH:O	2.01	0.59
4:O:1708:BCL:H91	4:P:1608:BCL:HBB	1.84	0.59
1:A:41:PHE:HB3	1:A:42:PRO:HD3	1.84	0.59
1:R:31:HIS:CE1	4:S:1609:BCL:HMD1	2.37	0.59
4:A:1701:BCL:C1D	6:A:1831:HOH:O	2.49	0.59
2:J:37:THR:CG2	2:J:39:TRP:H	2.15	0.59
1:R:48:GLY:CA	6:R:1823:HOH:O	2.49	0.59
4:M:1707:BCL:H143	2:N:27:LEU:HD23	1.83	0.59
4:M:1707:BCL:CED	4:O:1508:BCL:H191	2.33	0.59
2:D:33:ALA:HB2	6:D:1806:HOH:O	2.00	0.59
1:M:5:LYS:HE3	6:M:1856:HOH:O	2.01	0.59
6:E:1862:HOH:O	5:F:1803:LDA:H42	2.02	0.59
1:A:14:ILE:CD1	5:A:1816:LDA:H22	2.33	0.58
1:G:14:ILE:HD13	5:G:1814:LDA:C4	2.33	0.58
3:N:1407:RG1:HM82	4:O:1508:BCL:HAA1	1.84	0.58
2:J:41:HIS:HB3	1:K:50:LYS:NZ	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:34:PHE:CD2	2:P:34:PHE:C	2.77	0.58
2:B:41:HIS:NE2	1:C:49:VAL:CG1	2.66	0.58
4:A:1701:BCL:CHD	6:A:1831:HOH:O	2.51	0.58
2:P:34:PHE:CD1	6:P:1817:HOH:O	2.55	0.58
4:G:1704:BCL:C7	6:G:1863:HOH:O	2.52	0.58
4:M:1707:BCL:O1D	4:M:1707:BCL:HAA1	2.04	0.58
5:R:1818:LDA:H92	6:R:1856:HOH:O	2.02	0.58
6:E:1862:HOH:O	5:F:1803:LDA:C4	2.51	0.57
4:P:1608:BCL:CAC	6:P:1837:HOH:O	2.51	0.57
4:K:1706:BCL:H191	6:M:1849:HOH:O	2.04	0.57
4:R:1509:BCL:HBB3	4:R:1509:BCL:HMB1	1.86	0.57
1:G:31:HIS:CE1	4:H:1604:BCL:HMD1	2.40	0.57
6:K:1861:HOH:O	1:M:12:PRO:C	2.43	0.57
4:M:1707:BCL:H71	6:N:1831:HOH:O	2.04	0.57
3:P:1408:RG1:HM82	4:R:1509:BCL:HAA1	1.87	0.57
2:S:33:ALA:O	2:S:37:THR:CG2	2.50	0.57
5:M:1827:LDA:HM22	1:O:32:LEU:HD22	1.85	0.57
3:P:1408:RG1:HM82	4:R:1509:BCL:CAA	2.35	0.57
1:C:8:THR:HG22	2:D:3:LEU:O	2.05	0.57
2:H:37:THR:CG2	2:H:39:TRP:H	2.18	0.57
4:C:1702:BCL:H42	4:E:1503:BCL:CMA	2.35	0.57
2:L:39:TRP:CZ2	4:L:1606:BCL:CMC	2.88	0.57
2:L:37:THR:CG2	2:L:39:TRP:H	2.18	0.57
5:R:1818:LDA:C12	6:R:1856:HOH:O	2.48	0.56
1:C:5:LYS:NZ	2:D:9:GLU:OE2	2.34	0.56
2:J:6:GLU:CD	6:J:1821:HOH:O	2.42	0.56
2:L:39:TRP:CD2	4:L:1606:BCL:HMC1	2.40	0.56
2:J:41:HIS:CD2	1:K:49:VAL:N	2.74	0.56
2:D:41:HIS:NE2	1:E:49:VAL:CG2	2.69	0.56
1:C:9:VAL:CG2	1:E:12:PRO:HB2	2.36	0.56
4:C:1502:BCL:CBB	4:C:1502:BCL:HMB1	2.36	0.55
1:E:37:HIS:CD2	1:G:35:LEU:HD21	2.41	0.55
5:K:1810:LDA:HM22	1:M:14:ILE:CD1	2.31	0.55
1:R:5:LYS:CE	6:R:1835:HOH:O	2.54	0.55
1:A:44:TYR:HB2	5:B:1801:LDA:HM22	1.88	0.55
2:D:23:LEU:HD13	4:D:1602:BCL:H2	1.87	0.55
4:G:1504:BCL:HMB1	4:G:1504:BCL:CBB	2.37	0.55
4:I:1705:BCL:C9	4:I:1705:BCL:C4	2.84	0.55
1:K:14:ILE:HG21	5:K:1810:LDA:C5	2.36	0.55
2:B:33:ALA:O	2:B:37:THR:HB	2.07	0.55
4:R:1709:BCL:C4	4:R:1709:BCL:H92	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1501:BCL:H191	4:R:1709:BCL:CED	2.26	0.55
2:L:41:HIS:NE2	1:M:49:VAL:N	2.54	0.55
4:C:1702:BCL:CAD	4:D:1602:BCL:H192	2.36	0.55
2:F:37:THR:HG22	2:F:39:TRP:H	1.71	0.55
5:I:1812:LDA:H21	6:K:1860:HOH:O	2.05	0.55
2:P:39:TRP:HB2	6:R:1857:HOH:O	2.07	0.55
2:D:41:HIS:CD2	1:E:49:VAL:N	2.75	0.55
5:F:1803:LDA:C7	6:F:1809:HOH:O	2.54	0.55
4:A:1501:BCL:C1D	4:B:1601:BCL:HMD2	2.37	0.54
1:C:41:PHE:HB3	1:C:42:PRO:HD3	1.88	0.54
1:A:5:LYS:HG2	3:D:1402:RG1:HM12	1.90	0.54
1:K:41:PHE:HB3	1:K:42:PRO:HD3	1.88	0.54
2:L:39:TRP:CE2	4:L:1606:BCL:HMC2	2.37	0.54
4:B:1601:BCL:HMB1	4:B:1601:BCL:HBB2	1.87	0.54
1:M:14:ILE:HG13	5:M:1811:LDA:H12	1.90	0.54
4:R:1709:BCL:H122	4:R:1709:BCL:H91	1.88	0.54
2:H:2:THR:CG2	6:H:1822:HOH:O	2.55	0.54
4:M:1707:BCL:HED3	4:O:1508:BCL:H62	1.90	0.54
2:N:38:PRO:O	1:O:47:GLY:HA3	2.07	0.54
4:C:1702:BCL:H42	4:E:1503:BCL:HMA2	1.90	0.54
4:L:1606:BCL:HMA3	4:L:1606:BCL:HBA2	1.89	0.54
3:H:1404:RG1:HM01	1:I:32:LEU:HD21	1.89	0.54
2:B:18:GLY:HA2	4:R:1709:BCL:CMD	2.38	0.53
1:G:48:GLY:CA	6:G:1839:HOH:O	2.15	0.53
4:L:1606:BCL:HBC2	4:L:1606:BCL:HMC1	1.89	0.53
4:N:1607:BCL:HBC3	4:N:1607:BCL:HMC2	1.90	0.53
1:A:28:ILE:HG22	1:A:32:LEU:HD12	1.88	0.53
4:G:1704:BCL:HHC	4:G:1704:BCL:HBB2	1.90	0.53
4:K:1506:BCL:CBB	4:K:1506:BCL:HMB1	2.39	0.53
4:M:1707:BCL:HBB2	4:M:1707:BCL:HHC	1.89	0.53
1:A:39:THR:OG1	1:C:46:GLN:NE2	2.33	0.53
1:C:16:ILE:HB	1:C:17:PRO:HD3	1.89	0.53
4:E:1703:BCL:H11	4:F:1603:BCL:H192	1.90	0.53
2:J:7:GLN:NE2	6:J:1818:HOH:O	2.41	0.53
4:I:1705:BCL:H92	4:I:1705:BCL:H43	1.90	0.53
1:E:41:PHE:HB3	1:E:42:PRO:HD3	1.91	0.53
2:N:37:THR:CG2	2:N:39:TRP:H	2.22	0.53
4:R:1709:BCL:H41	4:R:1709:BCL:H8	1.91	0.53
1:A:16:ILE:HB	1:A:17:PRO:HD3	1.91	0.52
4:G:1704:BCL:O1D	4:I:1505:BCL:H62	2.09	0.52
5:G:1824:LDA:H11	6:G:1843:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:LYS:N	6:G:1832:HOH:O	2.29	0.52
1:K:4:GLY:N	6:K:1840:HOH:O	2.41	0.52
4:C:1502:BCL:HMB1	4:C:1502:BCL:HBB3	1.91	0.52
5:C:1815:LDA:HM21	1:E:14:ILE:HD13	1.91	0.52
2:N:39:TRP:CD2	4:N:1607:BCL:CMC	2.90	0.52
4:E:1503:BCL:OBB	4:E:1503:BCL:HHC	2.10	0.52
4:M:1707:BCL:CGD	6:M:1859:HOH:O	2.35	0.52
2:S:33:ALA:HB2	6:S:296:HOH:O	2.08	0.52
4:I:1705:BCL:C2	4:J:1605:BCL:H192	2.39	0.52
6:C:1838:HOH:O	4:D:1602:BCL:H121	2.10	0.52
4:E:1703:BCL:H2	4:F:1603:BCL:H162	1.92	0.52
4:A:1701:BCL:CMD	2:D:18:GLY:HA2	2.40	0.52
1:C:9:VAL:HG21	1:E:12:PRO:HB2	1.92	0.52
4:J:1605:BCL:C19	6:K:1854:HOH:O	2.57	0.52
4:L:1606:BCL:CMA	6:L:1835:HOH:O	2.58	0.52
1:K:9:VAL:HB	6:K:1861:HOH:O	2.09	0.52
6:K:1864:HOH:O	5:L:1806:LDA:C8	2.47	0.52
1:K:31:HIS:ND1	4:L:1606:BCL:HMD1	2.26	0.51
1:M:47:GLY:N	6:M:1862:HOH:O	2.43	0.51
4:A:1501:BCL:O1D	4:A:1501:BCL:H2A	2.10	0.51
1:G:14:ILE:HD13	5:G:1814:LDA:H42	1.91	0.51
1:E:1:CXM:HG2	4:E:1703:BCL:CHC	2.41	0.51
1:O:44:TYR:CE1	5:P:1808:LDA:H11	2.45	0.51
2:L:39:TRP:CD2	4:L:1606:BCL:HMC2	2.44	0.51
4:D:1602:BCL:HMB1	4:D:1602:BCL:HBB2	1.92	0.51
4:I:1705:BCL:H92	4:I:1705:BCL:C4	2.40	0.51
1:M:6:ILE:N	3:P:1408:RG1:HM32	2.25	0.51
1:O:1:CXM:HG2	4:O:1708:BCL:CHC	2.40	0.51
5:A:1816:LDA:C3	1:C:14:ILE:CD1	2.88	0.51
4:E:1703:BCL:HBB2	4:E:1703:BCL:HHC	1.93	0.51
4:I:1505:BCL:HMC3	5:J:1805:LDA:H51	1.93	0.51
1:K:1:CXM:C	6:K:1840:HOH:O	2.59	0.51
4:L:1606:BCL:HBB2	4:L:1606:BCL:HMB1	1.93	0.51
5:O:1820:LDA:CM1	6:O:1823:HOH:O	2.45	0.51
1:I:18:ALA:HA	5:I:1813:LDA:H91	1.93	0.51
2:L:37:THR:HG22	2:L:39:TRP:H	1.75	0.51
2:P:38:PRO:O	1:R:47:GLY:HA3	2.11	0.51
2:F:41:HIS:CE1	1:G:49:VAL:N	2.79	0.51
1:M:30:VAL:HG22	3:N:1407:RG1:HM03	1.93	0.51
1:R:49:VAL:O	1:R:49:VAL:HG22	2.10	0.51
5:C:1815:LDA:HM11	1:E:14:ILE:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1705:BCL:C4	4:I:1705:BCL:C8	2.83	0.50
2:J:41:HIS:NE2	1:K:49:VAL:N	2.59	0.50
4:K:1706:BCL:CMD	2:N:18:GLY:HA2	2.40	0.50
4:A:1501:BCL:O1D	4:A:1501:BCL:HBA1	2.11	0.50
4:I:1705:BCL:H141	6:J:1825:HOH:O	2.11	0.50
4:F:1603:BCL:CHB	4:G:1504:BCL:HMB3	2.42	0.50
4:L:1606:BCL:HMA2	6:L:1835:HOH:O	2.11	0.50
2:F:41:HIS:HB3	1:G:50:LYS:HE2	1.92	0.50
2:N:39:TRP:CE2	4:N:1607:BCL:HMC3	2.45	0.50
1:A:20:LEU:HD13	4:R:1709:BCL:CED	2.41	0.50
1:K:30:VAL:HG23	3:L:1406:RG1:HM03	1.93	0.50
1:G:19:LEU:O	1:G:23:VAL:HG23	2.11	0.50
2:D:7:GLN:HB3	6:D:1829:HOH:O	2.10	0.50
2:N:20:ARG:NH1	6:N:1812:HOH:O	2.45	0.49
4:O:1708:BCL:HED3	3:S:1409:RG1:HM42	1.92	0.49
1:E:25:VAL:HG11	5:E:1823:LDA:C12	2.43	0.49
5:I:1812:LDA:H111	6:K:1863:HOH:O	2.11	0.49
1:C:14:ILE:HG21	5:C:1815:LDA:C2	2.36	0.49
4:G:1504:BCL:HMD1	2:H:30:HIS:CE1	2.47	0.49
4:J:1605:BCL:HMC3	6:K:1851:HOH:O	2.12	0.49
4:M:1707:BCL:H101	6:N:1831:HOH:O	2.13	0.49
5:R:1818:LDA:C7	6:R:1852:HOH:O	2.57	0.49
4:H:1604:BCL:CHB	4:I:1505:BCL:HMB3	2.43	0.49
1:M:51:LYS:HA	1:M:52:ALA:CB	2.29	0.49
2:N:17:ASP:CB	6:N:1829:HOH:O	2.60	0.49
4:R:1509:BCL:HMB1	4:R:1509:BCL:CBB	2.42	0.49
5:E:1823:LDA:CM2	6:E:1853:HOH:O	2.57	0.49
2:H:37:THR:HG22	2:H:39:TRP:HB3	1.94	0.49
1:K:51:LYS:HD3	1:K:52:ALA:O	2.12	0.49
4:G:1704:BCL:H91	4:G:1704:BCL:H122	1.94	0.49
4:R:1509:BCL:HMD1	2:S:30:HIS:CE1	2.48	0.49
2:B:34:PHE:CD1	2:B:40:LEU:HD12	2.48	0.48
2:L:39:TRP:CZ2	4:L:1606:BCL:HMC3	2.46	0.48
2:J:41:HIS:HB3	1:K:50:LYS:HZ1	1.77	0.48
4:M:1707:BCL:HED1	4:O:1508:BCL:H191	1.94	0.48
4:M:1707:BCL:HBC3	4:N:1607:BCL:H143	1.95	0.48
1:A:49:VAL:HG12	2:S:41:HIS:NE2	2.28	0.48
4:B:1601:BCL:CBB	4:B:1601:BCL:HMB1	2.43	0.48
4:K:1706:BCL:CBB	4:K:1706:BCL:HHC	2.42	0.48
2:B:6:GLU:CG	6:B:597:HOH:O	2.62	0.48
4:F:1603:BCL:H142	4:F:1603:BCL:H101	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:5:LYS:NZ	2:S:9:GLU:OE2	2.46	0.48
4:E:1503:BCL:HMB1	4:E:1503:BCL:CBB	2.44	0.48
4:O:1508:BCL:HAA2	4:O:1508:BCL:CGD	2.44	0.48
4:O:1708:BCL:H3C	6:O:1822:HOH:O	2.14	0.48
1:C:14:ILE:HG13	5:C:1815:LDA:O1	2.13	0.48
1:I:5:LYS:HG2	6:J:1823:HOH:O	2.09	0.47
4:J:1605:BCL:CHB	4:K:1506:BCL:HMB3	2.44	0.47
6:C:1843:HOH:O	5:E:1822:LDA:C3	2.62	0.47
4:G:1704:BCL:C6	6:G:1863:HOH:O	2.62	0.47
4:I:1705:BCL:H2	4:J:1605:BCL:H161	1.95	0.47
1:O:5:LYS:CE	2:P:5:ALA:HB1	2.44	0.47
2:P:39:TRP:CD2	4:P:1608:BCL:HMC2	2.49	0.47
4:R:1709:BCL:C3D	4:S:1609:BCL:H203	2.44	0.47
4:S:1609:BCL:HHC	4:S:1609:BCL:OBB	2.14	0.47
2:H:39:TRP:CE3	4:H:1604:BCL:HBC2	2.47	0.47
4:G:1704:BCL:HED1	4:I:1505:BCL:H191	1.92	0.47
1:O:4:GLY:HA2	2:P:12:HIS:CD2	2.49	0.47
4:D:1602:BCL:HMB1	4:D:1602:BCL:CBB	2.44	0.47
1:M:14:ILE:HG13	5:M:1811:LDA:C1	2.44	0.47
5:M:1811:LDA:H41	1:O:14:ILE:HD12	1.95	0.47
4:M:1707:BCL:C4D	4:N:1607:BCL:H172	2.45	0.47
4:L:1606:BCL:C4A	4:M:1507:BCL:HMB3	2.45	0.47
5:O:1820:LDA:CM2	6:O:1823:HOH:O	2.49	0.47
2:F:37:THR:HG22	2:F:39:TRP:HB3	1.96	0.47
1:I:8:THR:HG22	2:J:3:LEU:O	2.15	0.47
2:L:39:TRP:CZ2	4:L:1606:BCL:HMC2	2.50	0.47
1:M:1:CXM:CN	2:N:16:ILE:HD11	2.44	0.47
1:R:50:LYS:O	1:R:51:LYS:HB2	2.14	0.47
5:A:1816:LDA:H32	1:C:14:ILE:CD1	2.44	0.47
4:F:1603:BCL:HMB1	4:F:1603:BCL:CBB	2.40	0.47
6:C:1843:HOH:O	5:E:1822:LDA:C2	2.63	0.47
2:N:37:THR:HG22	2:N:39:TRP:HB3	1.96	0.47
6:E:1862:HOH:O	5:F:1803:LDA:H31	2.08	0.47
4:B:1601:BCL:OBB	4:B:1601:BCL:HHC	2.14	0.47
1:I:31:HIS:ND1	4:J:1605:BCL:HMD1	2.30	0.47
1:M:1:CXM:HG2	4:M:1707:BCL:CHC	2.45	0.47
2:D:37:THR:HG22	2:D:39:TRP:HB3	1.97	0.46
5:G:1824:LDA:HM12	6:G:1828:HOH:O	1.94	0.46
1:O:5:LYS:HE2	2:P:5:ALA:HB1	1.96	0.46
4:B:1601:BCL:H62	4:B:1601:BCL:H112	1.97	0.46
1:R:14:ILE:HD11	5:R:1818:LDA:H11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1502:BCL:CHD	6:D:1806:HOH:O	2.62	0.46
5:E:1823:LDA:HM11	6:E:1853:HOH:O	2.14	0.46
4:I:1705:BCL:C9	4:I:1705:BCL:H41	2.46	0.46
1:K:14:ILE:HG21	5:K:1810:LDA:H52	1.95	0.46
4:L:1606:BCL:CGD	4:L:1606:BCL:H2A	2.45	0.46
2:L:4:THR:OG1	2:L:7:GLN:HG3	2.14	0.46
4:S:1609:BCL:H43	6:S:515:HOH:O	2.14	0.46
6:R:1831:HOH:O	4:S:1609:BCL:C19	2.62	0.46
4:J:1605:BCL:HAA1	6:J:1825:HOH:O	2.14	0.46
1:M:30:VAL:CG2	3:N:1407:RG1:HM03	2.46	0.46
2:H:39:TRP:CD2	4:H:1604:BCL:HBC3	2.51	0.46
4:I:1705:BCL:HMB1	4:I:1705:BCL:OBB	2.16	0.46
1:M:1:CXM:SD	2:N:20:ARG:NH2	2.88	0.46
4:J:1605:BCL:HBB3	6:K:1864:HOH:O	2.03	0.46
4:C:1702:BCL:CMD	2:F:18:GLY:HA2	2.45	0.46
2:J:37:THR:HG22	2:J:39:TRP:HB3	1.97	0.46
4:A:1501:BCL:HMB1	4:A:1501:BCL:HBB3	1.98	0.46
4:O:1708:BCL:HBC3	6:O:1822:HOH:O	2.16	0.46
2:F:38:PRO:O	1:G:47:GLY:HA3	2.16	0.45
2:H:11:LEU:CD1	3:H:1404:RG1:H41	2.47	0.45
5:K:1826:LDA:C12	6:K:1863:HOH:O	2.64	0.45
4:K:1506:BCL:CMC	5:L:1806:LDA:H51	2.45	0.45
5:I:1825:LDA:HM12	6:I:1840:HOH:O	2.16	0.45
5:K:1826:LDA:H121	6:K:1847:HOH:O	2.17	0.45
2:P:37:THR:HG22	2:P:39:TRP:N	2.23	0.45
1:I:51:LYS:HB2	1:I:52:ALA:CA	2.45	0.45
1:I:14:ILE:HD11	6:I:1862:HOH:O	2.15	0.45
2:J:37:THR:CG2	2:J:39:TRP:HB3	2.47	0.45
4:M:1507:BCL:HMD2	4:N:1607:BCL:CHD	2.46	0.45
2:P:3:LEU:HD21	6:P:1824:HOH:O	2.16	0.45
2:B:4:THR:HG23	2:B:7:GLN:NE2	2.32	0.45
2:D:1:ALA:N	6:D:1826:HOH:O	2.49	0.45
4:G:1704:BCL:CED	1:I:20:LEU:HD13	2.47	0.45
3:H:1404:RG1:H7	3:H:1404:RG1:HM31	1.83	0.45
4:G:1704:BCL:HMB2	4:H:1604:BCL:H61	1.98	0.45
2:N:17:ASP:HB3	6:N:1829:HOH:O	2.15	0.45
1:O:4:GLY:HA2	2:P:12:HIS:CG	2.52	0.45
2:B:19:THR:HG21	4:B:1601:BCL:H42	1.99	0.45
2:B:37:THR:CG2	2:B:39:TRP:H	2.25	0.45
2:F:2:THR:HG21	6:F:1825:HOH:O	2.17	0.45
4:G:1704:BCL:C4D	4:H:1604:BCL:H172	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:1708:BCL:HMB1	4:O:1708:BCL:OBB	2.16	0.45
3:H:1404:RG1:HM41	3:H:1404:RG1:H11	1.87	0.45
4:I:1705:BCL:C9	4:I:1705:BCL:H43	2.47	0.45
4:G:1704:BCL:CMD	2:J:18:GLY:HA2	2.46	0.45
1:A:21:GLY:HA3	5:A:1817:LDA:H101	1.99	0.45
1:A:49:VAL:CG1	2:S:41:HIS:NE2	2.80	0.45
4:B:1601:BCL:H2	6:B:282:HOH:O	2.15	0.45
2:H:29:ALA:HA	5:H:1804:LDA:H112	1.99	0.45
4:A:1701:BCL:H92	4:B:1601:BCL:H92	1.99	0.44
4:I:1705:BCL:HBB2	4:I:1705:BCL:HHC	1.99	0.44
1:C:5:LYS:HZ1	2:D:9:GLU:HG3	1.81	0.44
1:E:51:LYS:O	1:E:52:ALA:HB2	2.18	0.44
4:I:1505:BCL:HMD1	2:J:30:HIS:CE1	2.53	0.44
4:I:1705:BCL:C14	6:J:1825:HOH:O	2.65	0.44
2:L:36:ALA:HB1	5:L:1806:LDA:H32	1.99	0.44
4:M:1507:BCL:HMD1	2:N:30:HIS:CE1	2.52	0.44
4:E:1703:BCL:HHB	2:F:19:THR:HG21	1.98	0.44
4:G:1504:BCL:HBB3	4:G:1504:BCL:HMB1	1.98	0.44
2:P:19:THR:CG2	4:P:1608:BCL:H42	2.47	0.44
4:J:1605:BCL:HBB1	6:K:1864:HOH:O	2.06	0.44
1:K:9:VAL:HG12	6:K:1853:HOH:O	2.17	0.44
1:C:23:VAL:HG13	4:D:1602:BCL:HED1	1.98	0.44
2:J:39:TRP:CD2	4:J:1605:BCL:HBC2	2.53	0.44
3:L:1406:RG1:H11	3:L:1406:RG1:HM41	1.86	0.44
2:F:4:THR:HG1	2:F:7:GLN:CD	2.21	0.44
5:M:1811:LDA:H21	1:O:14:ILE:CD1	2.47	0.44
2:B:38:PRO:O	1:C:47:GLY:HA3	2.18	0.44
3:D:1402:RG1:HM31	3:D:1402:RG1:H7	1.82	0.44
1:E:25:VAL:HG11	5:E:1823:LDA:H111	1.99	0.44
4:I:1505:BCL:HMB1	4:I:1505:BCL:CBB	2.48	0.44
1:M:39:THR:OG1	1:O:46:GLN:NE2	2.37	0.44
4:A:1701:BCL:HMB1	4:A:1701:BCL:OBB	2.18	0.44
4:E:1503:BCL:HMD1	2:F:30:HIS:CE1	2.52	0.44
1:A:43:ALA:HA	6:A:1825:HOH:O	2.17	0.43
2:B:37:THR:CG2	2:B:39:TRP:HB3	2.48	0.43
1:R:41:PHE:HB3	1:R:42:PRO:CD	2.48	0.43
2:D:6:GLU:CB	6:D:1825:HOH:O	2.41	0.43
2:L:39:TRP:CE3	4:L:1606:BCL:HMC2	2.53	0.43
4:O:1708:BCL:HHC	4:O:1708:BCL:HBB2	2.00	0.43
5:K:1826:LDA:H121	6:K:1863:HOH:O	2.17	0.43
2:N:37:THR:HG23	2:N:39:TRP:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1822:LDA:O1	6:E:1859:HOH:O	2.20	0.43
1:K:16:ILE:HB	1:K:17:PRO:HD3	1.99	0.43
3:R:1401:RG1:H20	3:R:1401:RG1:HM61	1.85	0.43
2:B:6:GLU:HG2	6:B:597:HOH:O	2.18	0.43
3:J:1405:RG1:H7	3:J:1405:RG1:HM31	1.84	0.43
4:L:1606:BCL:CMA	4:L:1606:BCL:HBA2	2.49	0.43
4:M:1507:BCL:HBD	4:M:1507:BCL:HAA2	2.00	0.43
4:M:1707:BCL:H91	4:M:1707:BCL:H112	1.77	0.43
2:N:33:ALA:CB	4:N:1607:BCL:HBC1	2.48	0.43
4:A:1501:BCL:H3C	5:B:1801:LDA:H71	2.01	0.43
1:A:8:THR:HG22	2:B:3:LEU:O	2.19	0.43
4:G:1704:BCL:CGD	6:G:1854:HOH:O	2.64	0.43
1:E:14:ILE:HG13	5:G:1814:LDA:H12	2.00	0.43
2:F:41:HIS:HB3	1:G:50:LYS:CG	2.49	0.43
4:I:1705:BCL:C4	4:K:1506:BCL:HMA2	2.47	0.43
4:C:1502:BCL:C1D	4:D:1602:BCL:HMD2	2.49	0.43
1:E:4:GLY:HA2	2:F:12:HIS:CD2	2.54	0.43
2:F:41:HIS:HE1	1:G:49:VAL:H	1.60	0.43
4:I:1705:BCL:O1A	4:K:1506:BCL:H2	2.19	0.43
2:F:14:TYR:CE1	3:F:1403:RG1:HM11	2.53	0.43
4:F:1603:BCL:C14	4:F:1603:BCL:C10	2.97	0.43
3:H:1404:RG1:HM22	3:H:1404:RG1:H1'	1.73	0.43
1:A:49:VAL:N	2:S:41:HIS:CD2	2.87	0.42
1:A:50:LYS:HG3	6:A:1833:HOH:O	2.18	0.42
4:I:1705:BCL:C2	6:K:1854:HOH:O	2.67	0.42
3:S:1409:RG1:H7	3:S:1409:RG1:HM31	1.77	0.42
2:N:29:ALA:HB1	5:N:1807:LDA:H112	2.01	0.42
5:R:1818:LDA:C8	6:R:1852:HOH:O	2.64	0.42
5:K:1826:LDA:H22	5:K:1826:LDA:HM22	1.87	0.42
1:M:14:ILE:HG22	6:M:1852:HOH:O	2.19	0.42
1:G:26:ILE:HG12	1:I:28:ILE:HD11	2.01	0.42
1:K:40:TRP:HH2	4:K:1506:BCL:CBC	2.32	0.42
2:J:41:HIS:CE1	1:K:49:VAL:HG12	2.53	0.42
3:N:1407:RG1:H7	3:N:1407:RG1:HM31	1.85	0.42
2:F:4:THR:OG1	2:F:7:GLN:CD	2.58	0.42
2:P:13:LYS:NZ	6:P:1835:HOH:O	2.52	0.42
3:R:1401:RG1:HM31	3:R:1401:RG1:H7	1.80	0.42
4:C:1702:BCL:OBD	3:F:1403:RG1:H11	2.19	0.42
2:F:23:LEU:HB2	4:F:1603:BCL:H2	2.01	0.42
4:R:1509:BCL:HMD2	4:S:1609:BCL:CHD	2.50	0.42
4:A:1701:BCL:OBD	3:D:1402:RG1:H11	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:1847:HOH:O	2:J:6:GLU:HA	2.20	0.42
4:M:1507:BCL:CBB	4:M:1507:BCL:HMB1	2.50	0.42
2:N:4:THR:H	2:N:7:GLN:HE21	1.67	0.42
1:O:44:TYR:HB2	5:P:1808:LDA:HM11	2.02	0.42
4:A:1501:BCL:HED3	2:B:22:PHE:CE1	2.55	0.42
2:L:39:TRP:CG	4:L:1606:BCL:HMC1	2.54	0.42
2:N:37:THR:HG22	2:N:39:TRP:H	1.85	0.42
2:P:17:ASP:O	2:P:21:VAL:HG23	2.20	0.42
4:S:1609:BCL:CBB	4:S:1609:BCL:HMB1	2.48	0.42
4:A:1501:BCL:OBB	4:A:1501:BCL:HHC	2.20	0.42
3:P:1408:RG1:H7	3:P:1408:RG1:HM31	1.91	0.42
1:A:13:ALA:HB1	5:A:1817:LDA:HM11	2.02	0.42
4:A:1701:BCL:HMB3	2:B:16:ILE:HG23	2.01	0.42
3:D:1402:RG1:HM51	3:D:1402:RG1:H15	1.92	0.42
3:S:1409:RG1:C17	4:S:1609:BCL:H12	2.50	0.42
1:C:44:TYR:CD1	5:D:1802:LDA:HM21	2.55	0.41
2:F:37:THR:HG23	2:F:39:TRP:H	1.84	0.41
1:I:14:ILE:HD13	5:I:1812:LDA:HM12	2.02	0.41
2:N:9:GLU:O	2:N:13:LYS:HD2	2.19	0.41
4:O:1508:BCL:H12	2:P:22:PHE:HE1	1.85	0.41
3:S:1409:RG1:H15	3:S:1409:RG1:HM51	1.91	0.41
3:F:1403:RG1:HM13	3:F:1403:RG1:H1'	1.79	0.41
1:G:5:LYS:HE2	2:H:9:GLU:OE2	2.20	0.41
4:M:1507:BCL:H102	4:M:1507:BCL:H61	1.93	0.41
1:O:43:ALA:HB2	6:O:1830:HOH:O	2.20	0.41
4:C:1702:BCL:H41	4:C:1702:BCL:C8	2.49	0.41
4:I:1705:BCL:CMD	2:L:18:GLY:HA2	2.50	0.41
5:I:1812:LDA:H22	6:K:1860:HOH:O	2.13	0.41
5:I:1825:LDA:CM1	6:I:1859:HOH:O	2.60	0.41
4:M:1707:BCL:OBB	4:M:1707:BCL:HMB1	2.19	0.41
1:M:41:PHE:O	1:M:44:TYR:HB3	2.19	0.41
1:O:49:VAL:O	1:O:49:VAL:HG13	2.21	0.41
4:C:1702:BCL:H192	2:D:39:TRP:HZ2	1.85	0.41
4:G:1504:BCL:HHC	4:G:1504:BCL:OBB	2.20	0.41
1:I:18:ALA:HA	5:I:1813:LDA:C9	2.50	0.41
1:M:16:ILE:HB	1:M:17:PRO:HD3	2.02	0.41
3:R:1401:RG1:CM1	3:R:1401:RG1:O5'	2.68	0.41
1:I:16:ILE:HB	1:I:17:PRO:HD3	2.02	0.41
4:K:1706:BCL:H2C	4:K:1706:BCL:HBC3	1.87	0.41
4:O:1508:BCL:H3C	5:P:1808:LDA:H51	2.02	0.41
1:O:32:LEU:HD23	1:O:32:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:O	1:A:8:THR:OG1	2.31	0.41
1:C:44:TYR:CD1	5:D:1802:LDA:H11	2.55	0.41
1:K:48:GLY:CA	6:K:1829:HOH:O	2.60	0.41
1:C:16:ILE:O	1:C:20:LEU:HG	2.21	0.41
4:E:1703:BCL:H161	4:E:1703:BCL:H202	1.74	0.41
4:I:1505:BCL:HMB1	4:I:1505:BCL:HBB3	2.03	0.41
1:K:1:CXM:C	1:K:1:CXM:ON1	2.69	0.41
4:L:1606:BCL:HMA1	4:L:1606:BCL:HHB	1.93	0.41
5:C:1815:LDA:HM11	1:E:14:ILE:HD13	2.03	0.41
1:E:1:CXM:HG2	4:E:1703:BCL:HHC	2.03	0.41
5:F:1803:LDA:H82	6:F:1809:HOH:O	2.17	0.41
1:K:50:LYS:O	1:K:51:LYS:CB	2.69	0.41
2:L:38:PRO:O	1:M:47:GLY:HA3	2.21	0.41
4:O:1708:BCL:HHC	4:O:1708:BCL:CBB	2.51	0.41
2:P:6:GLU:HG2	2:P:10:GLU:OE2	2.21	0.41
1:A:5:LYS:HE3	2:B:5:ALA:HB1	2.01	0.41
4:C:1502:BCL:HMD1	2:D:30:HIS:CE1	2.56	0.41
2:L:37:THR:HG22	2:L:39:TRP:HB3	2.02	0.41
1:M:31:HIS:ND1	4:N:1607:BCL:HMD1	2.35	0.41
2:N:4:THR:H	2:N:7:GLN:NE2	2.19	0.41
3:D:1402:RG1:H11	3:D:1402:RG1:HM41	1.98	0.40
2:F:41:HIS:HB3	1:G:50:LYS:CE	2.51	0.40
5:G:1824:LDA:HM22	5:G:1824:LDA:H22	1.78	0.40
1:G:30:VAL:HG12	4:H:1604:BCL:HMD3	2.03	0.40
4:O:1508:BCL:CHD	4:O:1508:BCL:HBC2	2.50	0.40
6:B:517:HOH:O	1:R:5:LYS:HE2	2.21	0.40
1:C:44:TYR:CE1	5:D:1802:LDA:H11	2.56	0.40
4:G:1704:BCL:O1D	4:I:1505:BCL:C6	2.69	0.40
2:N:5:ALA:HB3	6:N:1826:HOH:O	2.20	0.40
4:R:1709:BCL:H92	4:S:1609:BCL:H51	2.03	0.40
4:C:1502:BCL:HHC	4:C:1502:BCL:OBB	2.21	0.40
2:H:39:TRP:NE1	4:H:1604:BCL:HMC2	2.35	0.40
4:R:1709:BCL:C4D	4:S:1609:BCL:H172	2.52	0.40
4:A:1501:BCL:HED3	2:B:22:PHE:CZ	2.56	0.40
2:L:23:LEU:HB2	4:L:1606:BCL:H2	2.04	0.40
2:N:39:TRP:CZ3	4:N:1607:BCL:HBC3	2.57	0.40
2:P:41:HIS:HA	6:R:1823:HOH:O	2.22	0.40
4:G:1704:BCL:O1D	4:I:1505:BCL:H52	2.22	0.40
2:H:41:HIS:CD2	1:I:49:VAL:C	2.95	0.40
4:K:1506:BCL:HBC1	4:L:1606:BCL:CBC	2.51	0.40
2:P:37:THR:HG23	2:P:38:PRO:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:1401:RG1:HM41	3:R:1401:RG1:H11	1.87	0.40
3:S:1409:RG1:HM61	3:S:1409:RG1:H20	1.79	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	A	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
1	C	51/53 (96%)	47 (92%)	1 (2%)	3 (6%)	2	0
1	E	51/53 (96%)	46 (90%)	2 (4%)	3 (6%)	2	0
1	G	51/53 (96%)	51 (100%)	0	0	100	100
1	I	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
1	K	51/53 (96%)	47 (92%)	3 (6%)	1 (2%)	9	7
1	M	51/53 (96%)	47 (92%)	1 (2%)	3 (6%)	2	0
1	O	51/53 (96%)	47 (92%)	3 (6%)	1 (2%)	9	7
1	R	51/53 (96%)	46 (90%)	2 (4%)	3 (6%)	2	0
2	B	39/41 (95%)	39 (100%)	0	0	100	100
2	D	39/41 (95%)	39 (100%)	0	0	100	100
2	F	39/41 (95%)	39 (100%)	0	0	100	100
2	H	39/41 (95%)	39 (100%)	0	0	100	100
2	J	39/41 (95%)	39 (100%)	0	0	100	100
2	L	39/41 (95%)	39 (100%)	0	0	100	100
2	N	39/41 (95%)	39 (100%)	0	0	100	100
2	P	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
2	S	39/41 (95%)	39 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	810/846 (96%)	775 (96%)	21 (3%)	14 (2%)	11	10

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	50	LYS
1	E	51	LYS
1	E	52	ALA
1	K	50	LYS
1	M	50	LYS
1	M	51	LYS
1	M	52	ALA
1	R	51	LYS
1	C	51	LYS
1	R	50	LYS
1	R	52	ALA
1	C	52	ALA
1	E	50	LYS
1	O	50	LYS

### 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	A	40/40 (100%)	37 (92%)	3 (8%)	17	22
1	C	40/40 (100%)	37 (92%)	3 (8%)	17	22
1	E	40/40 (100%)	34 (85%)	6 (15%)	3	2
1	G	40/40 (100%)	36 (90%)	4 (10%)	9	10
1	I	40/40 (100%)	35 (88%)	5 (12%)	6	5
1	K	40/40 (100%)	39 (98%)	1 (2%)	55	72
1	M	40/40 (100%)	38 (95%)	2 (5%)	30	42
1	O	40/40 (100%)	38 (95%)	2 (5%)	30	42
1	R	40/40 (100%)	36 (90%)	4 (10%)	9	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	33/33 (100%)	30 (91%)	3 (9%)	12	13
2	D	33/33 (100%)	30 (91%)	3 (9%)	12	13
2	F	33/33 (100%)	29 (88%)	4 (12%)	6	6
2	H	33/33 (100%)	29 (88%)	4 (12%)	6	6
2	J	33/33 (100%)	31 (94%)	2 (6%)	23	32
2	L	33/33 (100%)	28 (85%)	5 (15%)	3	2
2	N	33/33 (100%)	30 (91%)	3 (9%)	12	13
2	P	33/33 (100%)	28 (85%)	5 (15%)	3	2
2	S	33/33 (100%)	29 (88%)	4 (12%)	6	6
All	All	657/657 (100%)	594 (90%)	63 (10%)	10	12

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	41	PHE
1	A	51	LYS
2	B	2	THR
2	B	6	GLU
2	B	37	THR
1	C	9	VAL
1	C	41	PHE
1	C	50	LYS
2	D	2	THR
2	D	35	SER
2	D	37	THR
1	E	5	LYS
1	E	9	VAL
1	E	14	ILE
1	E	41	PHE
1	E	49	VAL
1	E	50	LYS
2	F	2	THR
2	F	13	LYS
2	F	17	ASP
2	F	37	THR
1	G	36	SER
1	G	41	PHE
1	G	50	LYS

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Mol	Chain	Res	Type
1	G	51	LYS
2	H	2	THR
2	H	13	LYS
2	H	17	ASP
2	H	37	THR
1	I	5	LYS
1	I	36	SER
1	I	41	PHE
1	I	50	LYS
1	I	51	LYS
2	J	2	THR
2	J	37	THR
1	K	50	LYS
2	L	2	THR
2	L	6	GLU
2	L	13	LYS
2	L	17	ASP
2	L	37	THR
1	M	9	VAL
1	M	41	PHE
2	N	2	THR
2	N	13	LYS
2	N	37	THR
1	O	5	LYS
1	O	41	PHE
2	P	2	THR
2	P	13	LYS
2	P	17	ASP
2	P	34	PHE
2	P	37	THR
1	R	16	ILE
1	R	36	SER
1	R	41	PHE
1	R	50	LYS
2	S	2	THR
2	S	6	GLU
2	S	10	GLU
2	S	37	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:



Mol	Chain	Res	Type
2	B	7	GLN
2	D	7	GLN
1	E	37	HIS
2	H	7	GLN
1	I	37	HIS
1	K	37	HIS
2	L	7	GLN
2	N	7	GLN
1	R	37	HIS
2	S	7	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	CXM	A	1	1,4	6,10,11	1.64	1 (16%)	5,11,13	1.00	1 (20%)
1	CXM	C	1	1,4	6,10,11	1.66	1 (16%)	5,11,13	0.74	0
1	CXM	E	1	1,4	6,10,11	1.31	1 (16%)	5,11,13	1.08	1 (20%)
1	CXM	G	1	1,4	6,10,11	1.64	1 (16%)	5,11,13	1.10	1 (20%)
1	CXM	I	1	1,4	6,10,11	1.25	1 (16%)	5,11,13	0.77	0
1	CXM	K	1	1,4	6,10,11	1.60	2 (33%)	5,11,13	1.03	0
1	CXM	M	1	1,4	6,10,11	3.00	1 (16%)	5,11,13	0.83	0
1	CXM	O	1	1,4	6,10,11	1.24	1 (16%)	5,11,13	0.71	0
1	CXM	R	1	1,4	6,10,11	1.14	0	5,11,13	0.78	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
1	CXM	A	1	1,4	-	0/6/10/12	0/0/0/0
1	CXM	C	1	1,4	-	0/6/10/12	0/0/0/0
1	CXM	E	1	1,4	-	0/6/10/12	0/0/0/0
1	CXM	G	1	1,4	-	0/6/10/12	0/0/0/0
1	CXM	I	1	1,4	-	0/6/10/12	0/0/0/0
1	CXM	K	1	1,4	-	0/6/10/12	0/0/0/0
1	CXM	M	1	1,4	-	0/6/10/12	0/0/0/0
1	CXM	O	1	1,4	-	0/6/10/12	0/0/0/0
1	CXM	R	1	1,4	-	0/6/10/12	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	1	CXM	CB-CA	-2.52	1.48	1.53
1	K	1	CXM	CB-CA	-2.16	1.49	1.53
1	I	1	CXM	CA-N	2.32	1.49	1.46
1	K	1	CXM	CA-N	2.36	1.49	1.46
1	E	1	CXM	CE-SD	2.38	1.93	1.78
1	A	1	CXM	CA-N	2.89	1.50	1.46
1	C	1	CXM	CE-SD	3.07	1.97	1.78
1	G	1	CXM	CE-SD	3.60	2.00	1.78
1	M	1	CXM	CE-SD	7.14	2.21	1.78

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1	CXM	O-C-CA	-2.35	119.26	125.69
1	E	1	CXM	O-C-CA	-2.21	119.65	125.69
1	A	1	CXM	O-C-CA	-2.17	119.76	125.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	1	CXM	2	0
1	K	1	CXM	2	0
1	M	1	CXM	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	O	1	CXM	1	0
1	R	1	CXM	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

63 ligands are modelled in this entry.

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	A	1501	1	55,74,74	2.66	16 (29%)	55,115,115	1.89	15 (27%)
4	BCL	A	1701	1	55,74,74	2.87	19 (34%)	55,115,115	1.84	19 (34%)
5	LDA	A	1816	-	15,15,15	3.52	2 (13%)	16,17,17	0.53	0
5	LDA	A	1817	-	15,15,15	3.66	1 (6%)	16,17,17	0.53	0
4	BCL	B	1601	2	55,74,74	2.26	14 (25%)	55,115,115	1.91	15 (27%)
5	LDA	B	1801	-	15,15,15	3.58	1 (6%)	16,17,17	0.74	0
4	BCL	C	1502	1	55,74,74	2.66	15 (27%)	55,115,115	1.99	16 (29%)
4	BCL	C	1702	1	55,74,74	2.70	12 (21%)	55,115,115	1.68	15 (27%)
5	LDA	C	1815	-	15,15,15	3.71	1 (6%)	16,17,17	0.32	0
5	LDA	C	1821	-	15,15,15	3.40	1 (6%)	16,17,17	0.43	0
3	RG1	D	1402	-	52,52,52	1.31	7 (13%)	63,67,67	1.67	16 (25%)
4	BCL	D	1602	2	55,74,74	2.61	16 (29%)	55,115,115	1.83	15 (27%)
5	LDA	D	1802	-	15,15,15	3.86	2 (13%)	16,17,17	0.85	1 (6%)
4	BCL	E	1503	1	55,74,74	2.27	10 (18%)	55,115,115	1.83	14 (25%)
4	BCL	E	1703	1	55,74,74	2.24	9 (16%)	55,115,115	1.63	14 (25%)
5	LDA	E	1822	-	15,15,15	3.41	1 (6%)	16,17,17	0.45	0
5	LDA	E	1823	-	15,15,15	3.31	1 (6%)	16,17,17	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	RG1	F	1403	-	52,52,52	1.35	5 (9%)	63,67,67	1.61	14 (22%)
4	BCL	F	1603	2	55,74,74	2.40	14 (25%)	55,115,115	1.78	15 (27%)
5	LDA	F	1803	-	15,15,15	3.92	1 (6%)	16,17,17	1.09	1 (6%)
4	BCL	G	1504	1	55,74,74	2.56	11 (20%)	55,115,115	1.77	18 (32%)
4	BCL	G	1704	1	55,74,74	2.47	13 (23%)	55,115,115	1.84	17 (30%)
5	LDA	G	1814	-	15,15,15	3.59	1 (6%)	16,17,17	0.43	0
5	LDA	G	1824	-	15,15,15	3.77	1 (6%)	16,17,17	0.47	0
3	RG1	H	1404	-	52,52,52	1.39	6 (11%)	63,67,67	1.68	12 (19%)
4	BCL	H	1604	2	55,74,74	2.56	17 (30%)	55,115,115	2.14	20 (36%)
5	LDA	H	1804	-	15,15,15	3.56	2 (13%)	16,17,17	0.91	1 (6%)
4	BCL	I	1505	1	55,74,74	2.38	14 (25%)	55,115,115	1.65	12 (21%)
4	BCL	I	1705	1	55,74,74	2.26	15 (27%)	55,115,115	1.74	11 (20%)
5	LDA	I	1812	-	15,15,15	4.32	1 (6%)	16,17,17	0.34	0
5	LDA	I	1813	-	15,15,15	3.71	1 (6%)	16,17,17	0.40	0
5	LDA	I	1825	-	15,15,15	3.72	1 (6%)	16,17,17	0.52	0
3	RG1	J	1405	-	52,52,52	1.30	7 (13%)	63,67,67	1.62	14 (22%)
4	BCL	J	1605	2	55,74,74	2.53	17 (30%)	55,115,115	1.87	18 (32%)
5	LDA	J	1805	-	15,15,15	3.11	1 (6%)	16,17,17	0.80	1 (6%)
4	BCL	K	1506	1	55,74,74	2.86	17 (30%)	55,115,115	1.93	15 (27%)
4	BCL	K	1706	1	55,74,74	2.39	12 (21%)	55,115,115	1.74	13 (23%)
5	LDA	K	1810	-	15,15,15	3.85	1 (6%)	16,17,17	0.41	0
5	LDA	K	1826	-	15,15,15	3.44	1 (6%)	16,17,17	0.50	0
3	RG1	L	1406	-	52,52,52	1.38	7 (13%)	63,67,67	1.56	13 (20%)
4	BCL	L	1606	2	55,74,74	2.77	18 (32%)	55,115,115	2.27	17 (30%)
5	LDA	L	1806	-	15,15,15	3.68	1 (6%)	16,17,17	0.89	1 (6%)
4	BCL	M	1507	1	55,74,74	2.49	13 (23%)	55,115,115	1.81	15 (27%)
4	BCL	M	1707	1	55,74,74	2.62	13 (23%)	55,115,115	1.65	12 (21%)
5	LDA	M	1811	-	15,15,15	3.31	1 (6%)	16,17,17	0.49	0
5	LDA	M	1827	-	15,15,15	3.62	1 (6%)	16,17,17	0.42	0
3	RG1	N	1407	-	52,52,52	1.23	4 (7%)	63,67,67	1.63	14 (22%)
4	BCL	N	1607	2	55,74,74	2.37	13 (23%)	55,115,115	1.91	14 (25%)
5	LDA	N	1807	-	15,15,15	3.16	1 (6%)	16,17,17	0.66	0
4	BCL	O	1508	1	55,74,74	2.36	12 (21%)	55,115,115	1.96	20 (36%)
4	BCL	O	1708	1	55,74,74	2.67	13 (23%)	55,115,115	1.74	13 (23%)
5	LDA	O	1820	-	15,15,15	3.85	1 (6%)	16,17,17	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	RG1	P	1408	-	52,52,52	1.41	10 (19%)	63,67,67	1.66	11 (17%)
4	BCL	P	1608	2	55,74,74	2.73	17 (30%)	55,115,115	1.74	15 (27%)
5	LDA	P	1808	-	15,15,15	3.40	1 (6%)	16,17,17	0.67	0
3	RG1	R	1401	-	52,52,52	1.25	6 (11%)	63,67,67	1.68	12 (19%)
4	BCL	R	1509	1	55,74,74	2.78	14 (25%)	55,115,115	1.93	16 (29%)
4	BCL	R	1709	1	55,74,74	2.65	20 (36%)	55,115,115	1.88	14 (25%)
5	LDA	R	1809	-	15,15,15	3.40	1 (6%)	16,17,17	0.78	0
5	LDA	R	1818	-	15,15,15	3.48	1 (6%)	16,17,17	0.46	0
5	LDA	R	1819	-	15,15,15	3.48	2 (13%)	16,17,17	0.53	0
3	RG1	S	1409	-	52,52,52	1.43	9 (17%)	63,67,67	1.64	17 (26%)
4	BCL	S	1609	2	55,74,74	2.28	12 (21%)	55,115,115	1.94	18 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	A	1501	1	1/1/21/25	0/37/137/137	0/0/9/9
4	BCL	A	1701	1	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	A	1816	-	-	0/13/13/13	0/0/0/0
5	LDA	A	1817	-	-	0/13/13/13	0/0/0/0
4	BCL	B	1601	2	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	B	1801	-	-	0/13/13/13	0/0/0/0
4	BCL	C	1502	1	1/1/21/25	0/37/137/137	0/0/9/9
4	BCL	C	1702	1	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	C	1815	-	-	0/13/13/13	0/0/0/0
5	LDA	C	1821	-	-	0/13/13/13	0/0/0/0
3	RG1	D	1402	-	-	0/51/71/71	0/1/1/1
4	BCL	D	1602	2	-	0/37/137/137	0/0/9/9
5	LDA	D	1802	-	-	0/13/13/13	0/0/0/0
4	BCL	E	1503	1	-	0/37/137/137	0/0/9/9
4	BCL	E	1703	1	-	0/37/137/137	0/0/9/9
5	LDA	E	1822	-	-	0/13/13/13	0/0/0/0
5	LDA	E	1823	-	-	0/13/13/13	0/0/0/0
3	RG1	F	1403	-	-	0/51/71/71	0/1/1/1
4	BCL	F	1603	2	-	0/37/137/137	0/0/9/9
5	LDA	F	1803	-	-	0/13/13/13	0/0/0/0
4	BCL	G	1504	1	-	0/37/137/137	0/0/9/9
4	BCL	G	1704	1	1/1/21/25	0/37/137/137	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LDA	G	1814	-	-	0/13/13/13	0/0/0/0
5	LDA	G	1824	-	-	0/13/13/13	0/0/0/0
3	RG1	H	1404	-	-	0/51/71/71	0/1/1/1
4	BCL	H	1604	2	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	H	1804	-	-	0/13/13/13	0/0/0/0
4	BCL	I	1505	1	-	0/37/137/137	0/0/9/9
4	BCL	I	1705	1	-	0/37/137/137	0/0/9/9
5	LDA	I	1812	-	-	0/13/13/13	0/0/0/0
5	LDA	I	1813	-	-	0/13/13/13	0/0/0/0
5	LDA	I	1825	-	-	0/13/13/13	0/0/0/0
3	RG1	J	1405	-	-	0/51/71/71	0/1/1/1
4	BCL	J	1605	2	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	J	1805	-	-	0/13/13/13	0/0/0/0
4	BCL	K	1506	1	1/1/21/25	0/37/137/137	0/0/9/9
4	BCL	K	1706	1	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	K	1810	-	-	0/13/13/13	0/0/0/0
5	LDA	K	1826	-	-	0/13/13/13	0/0/0/0
3	RG1	L	1406	-	-	0/51/71/71	0/1/1/1
4	BCL	L	1606	2	3/3/21/25	0/37/137/137	0/0/9/9
5	LDA	L	1806	-	-	0/13/13/13	0/0/0/0
4	BCL	M	1507	1	-	0/37/137/137	0/0/9/9
4	BCL	M	1707	1	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	M	1811	-	-	0/13/13/13	0/0/0/0
5	LDA	M	1827	-	-	0/13/13/13	0/0/0/0
3	RG1	N	1407	-	-	0/51/71/71	0/1/1/1
4	BCL	N	1607	2	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	N	1807	-	-	0/13/13/13	0/0/0/0
4	BCL	O	1508	1	2/2/21/25	0/37/137/137	0/0/9/9
4	BCL	O	1708	1	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	O	1820	-	-	0/13/13/13	0/0/0/0
3	RG1	P	1408	-	-	0/51/71/71	0/1/1/1
4	BCL	P	1608	2	2/2/21/25	0/37/137/137	0/0/9/9
5	LDA	P	1808	-	-	0/13/13/13	0/0/0/0
3	RG1	R	1401	-	-	0/51/71/71	0/1/1/1
4	BCL	R	1509	1	1/1/21/25	0/37/137/137	0/0/9/9
4	BCL	R	1709	1	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	R	1809	-	-	0/13/13/13	0/0/0/0
5	LDA	R	1818	-	-	0/13/13/13	0/0/0/0
5	LDA	R	1819	-	-	0/13/13/13	0/0/0/0
3	RG1	S	1409	-	-	0/51/71/71	0/1/1/1
4	BCL	S	1609	2	1/1/21/25	0/37/137/137	0/0/9/9

All (478) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1812	LDA	O1-N1	-16.38	1.23	1.39
5	F	1803	LDA	O1-N1	-14.82	1.25	1.39
5	K	1810	LDA	O1-N1	-14.69	1.25	1.39
5	O	1820	LDA	O1-N1	-14.69	1.25	1.39
5	D	1802	LDA	O1-N1	-14.66	1.25	1.39
5	G	1824	LDA	O1-N1	-14.46	1.25	1.39
5	I	1813	LDA	O1-N1	-14.23	1.26	1.39
5	I	1825	LDA	O1-N1	-14.22	1.26	1.39
5	A	1817	LDA	O1-N1	-13.99	1.26	1.39
5	L	1806	LDA	O1-N1	-13.96	1.26	1.39
5	C	1815	LDA	O1-N1	-13.95	1.26	1.39
5	M	1827	LDA	O1-N1	-13.70	1.26	1.39
5	G	1814	LDA	O1-N1	-13.48	1.26	1.39
5	B	1801	LDA	O1-N1	-13.38	1.26	1.39
5	H	1804	LDA	O1-N1	-13.24	1.27	1.39
5	A	1816	LDA	O1-N1	-13.17	1.27	1.39
5	R	1819	LDA	O1-N1	-13.16	1.27	1.39
5	R	1818	LDA	O1-N1	-13.16	1.27	1.39
5	K	1826	LDA	O1-N1	-13.15	1.27	1.39
5	C	1821	LDA	O1-N1	-12.97	1.27	1.39
5	E	1822	LDA	O1-N1	-12.96	1.27	1.39
5	P	1808	LDA	O1-N1	-12.96	1.27	1.39
5	R	1809	LDA	O1-N1	-12.77	1.27	1.39
5	E	1823	LDA	O1-N1	-12.72	1.27	1.39
5	M	1811	LDA	O1-N1	-12.54	1.27	1.39
5	N	1807	LDA	O1-N1	-11.68	1.28	1.39
5	J	1805	LDA	O1-N1	-11.52	1.28	1.39
4	K	1506	BCL	CAC-C3C	-8.04	1.38	1.54
4	A	1701	BCL	C3C-C4C	-7.08	1.42	1.51
4	M	1707	BCL	CBD-CGD	-6.29	1.30	1.52
4	L	1606	BCL	C2C-C3C	-5.24	1.39	1.54
4	N	1607	BCL	CMC-C2C	-5.11	1.41	1.53
4	H	1604	BCL	C3C-C4C	-5.04	1.45	1.51
4	R	1509	BCL	C3A-C2A	-4.98	1.40	1.54
4	A	1701	BCL	CAC-C3C	-4.67	1.44	1.54
4	J	1605	BCL	CBD-CGD	-4.39	1.37	1.52
3	N	1407	RG1	O1'-C1	-4.27	1.40	1.46
4	N	1607	BCL	C2C-C3C	-4.25	1.42	1.54
4	G	1704	BCL	CBD-CGD	-4.11	1.38	1.52
4	K	1506	BCL	C4D-ND	-4.03	1.28	1.37
4	C	1502	BCL	C4D-ND	-4.01	1.28	1.37
4	O	1508	BCL	C14-C13	-3.84	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1606	BCL	CMC-C2C	-3.81	1.44	1.53
4	L	1606	BCL	C4D-ND	-3.77	1.28	1.37
4	O	1508	BCL	C4D-ND	-3.77	1.28	1.37
4	G	1704	BCL	C4D-ND	-3.68	1.29	1.37
4	P	1608	BCL	C2C-C3C	-3.55	1.44	1.54
4	D	1602	BCL	C2A-C1A	-3.50	1.43	1.52
4	O	1508	BCL	CBD-CGD	-3.48	1.40	1.52
5	H	1804	LDA	C1-N1	-3.48	1.45	1.51
4	M	1707	BCL	C4D-ND	-3.40	1.29	1.37
4	E	1503	BCL	C4D-ND	-3.29	1.29	1.37
3	J	1405	RG1	C6-C5	-3.25	1.30	1.34
4	F	1603	BCL	C4D-ND	-3.24	1.30	1.37
4	G	1704	BCL	C3C-C4C	-3.23	1.47	1.51
4	K	1506	BCL	C2C-C3C	-3.22	1.45	1.54
4	M	1707	BCL	C3C-C4C	-3.22	1.47	1.51
3	S	1409	RG1	O1'-C1	-3.19	1.42	1.46
4	R	1509	BCL	C3C-C4C	-3.12	1.47	1.51
4	P	1608	BCL	CMC-C2C	-3.08	1.46	1.53
4	L	1606	BCL	C3A-C2A	-3.05	1.45	1.54
3	J	1405	RG1	O1'-C1	-3.03	1.42	1.46
4	L	1606	BCL	CMA-C3A	-3.03	1.46	1.53
4	M	1507	BCL	C4D-ND	-2.96	1.30	1.37
3	S	1409	RG1	C14-C13	-2.95	1.31	1.35
4	J	1605	BCL	CBA-CGA	-2.91	1.42	1.50
4	A	1701	BCL	C2C-C3C	-2.88	1.46	1.54
4	A	1501	BCL	CBD-CGD	-2.81	1.42	1.52
3	H	1404	RG1	CM5-C13	-2.75	1.45	1.50
3	P	1408	RG1	CM7-C22	-2.74	1.45	1.50
4	R	1709	BCL	C2A-C1A	-2.68	1.45	1.52
3	D	1402	RG1	C28-C27	-2.68	1.28	1.34
4	N	1607	BCL	CBD-CGD	-2.62	1.43	1.52
4	S	1609	BCL	C4D-ND	-2.61	1.31	1.37
4	D	1602	BCL	C4D-ND	-2.61	1.31	1.37
4	D	1602	BCL	CMD-C2D	-2.61	1.45	1.51
4	I	1705	BCL	CMB-C2B	-2.61	1.46	1.51
3	P	1408	RG1	CM5-C13	-2.59	1.46	1.50
4	P	1608	BCL	C4D-ND	-2.59	1.31	1.37
4	A	1501	BCL	C4D-ND	-2.59	1.31	1.37
4	I	1505	BCL	C4D-ND	-2.58	1.31	1.37
3	R	1401	RG1	C25-C26	-2.58	1.32	1.35
4	B	1601	BCL	C4D-ND	-2.58	1.31	1.37
4	M	1507	BCL	C2A-C1A	-2.58	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1704	BCL	CBD-CHA	-2.58	1.38	1.52
4	J	1605	BCL	C4D-ND	-2.57	1.31	1.37
4	O	1708	BCL	CMD-C2D	-2.55	1.46	1.51
4	P	1608	BCL	CBA-CGA	-2.54	1.43	1.50
4	R	1709	BCL	C3C-C4C	-2.53	1.48	1.51
5	D	1802	LDA	C1-N1	-2.53	1.46	1.51
4	C	1502	BCL	C2A-C1A	-2.51	1.46	1.52
4	I	1505	BCL	C2A-C1A	-2.50	1.46	1.52
4	G	1504	BCL	CMD-C2D	-2.50	1.46	1.51
4	N	1607	BCL	C4D-ND	-2.49	1.31	1.37
4	H	1604	BCL	C2A-C1A	-2.48	1.46	1.52
4	R	1709	BCL	C4D-ND	-2.48	1.31	1.37
4	H	1604	BCL	C4D-ND	-2.47	1.31	1.37
4	D	1602	BCL	C3C-C4C	-2.45	1.48	1.51
4	G	1504	BCL	CBD-CGD	-2.45	1.43	1.52
4	F	1603	BCL	CMC-C2C	-2.44	1.47	1.53
3	J	1405	RG1	C2-C1	-2.44	1.50	1.53
3	S	1409	RG1	CM6-C18	-2.42	1.46	1.50
5	A	1816	LDA	C1-N1	-2.41	1.47	1.51
4	N	1607	BCL	C3C-C4C	-2.41	1.48	1.51
4	R	1709	BCL	CMD-C2D	-2.40	1.46	1.51
4	J	1605	BCL	C3A-C2A	-2.39	1.47	1.54
4	M	1507	BCL	C2C-C3C	-2.39	1.47	1.54
5	R	1819	LDA	C1-N1	-2.38	1.47	1.51
4	D	1602	BCL	CBD-CGD	-2.38	1.44	1.52
3	F	1403	RG1	C25-C26	-2.38	1.32	1.35
4	R	1709	BCL	CBD-CGD	-2.36	1.44	1.52
4	J	1605	BCL	CAA-C2A	-2.36	1.49	1.54
4	A	1701	BCL	CBD-CGD	-2.33	1.44	1.52
4	H	1604	BCL	CMD-C2D	-2.30	1.46	1.51
4	F	1603	BCL	C3C-C4C	-2.29	1.48	1.51
4	C	1502	BCL	CAC-C3C	-2.29	1.49	1.54
4	J	1605	BCL	O2D-CED	-2.29	1.39	1.45
4	G	1704	BCL	CMB-C2B	-2.28	1.47	1.51
4	I	1705	BCL	CBD-CGD	-2.27	1.44	1.52
4	F	1603	BCL	O2D-CED	-2.25	1.39	1.45
4	I	1505	BCL	CBD-CGD	-2.25	1.44	1.52
4	S	1609	BCL	C2A-C1A	-2.24	1.46	1.52
4	K	1506	BCL	CBD-CGD	-2.19	1.44	1.52
4	B	1601	BCL	C3A-C2A	-2.18	1.48	1.54
4	C	1702	BCL	C3C-C4C	-2.14	1.48	1.51
4	M	1707	BCL	CBD-CHA	-2.13	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	1409	RG1	CM5-C13	-2.11	1.47	1.50
4	K	1506	BCL	CMD-C2D	-2.06	1.47	1.51
4	C	1702	BCL	C2A-C1A	-2.04	1.47	1.52
4	P	1608	BCL	C3C-C4C	-2.03	1.49	1.51
4	L	1606	BCL	CAC-C3C	-2.02	1.50	1.54
4	G	1504	BCL	C4D-ND	-2.02	1.33	1.37
4	L	1606	BCL	O2D-CED	-2.01	1.40	1.45
4	R	1709	BCL	CHD-C4C	2.00	1.47	1.41
4	G	1704	BCL	C1A-CHA	2.00	1.51	1.43
4	O	1708	BCL	C1D-ND	2.01	1.42	1.37
4	J	1605	BCL	C1A-CHA	2.03	1.51	1.43
3	H	1404	RG1	C7-C6	2.04	1.49	1.43
4	E	1703	BCL	C1D-ND	2.05	1.42	1.37
4	M	1707	BCL	O1D-CGD	2.06	1.26	1.21
4	P	1608	BCL	OBB-CAB	2.07	1.29	1.22
3	R	1401	RG1	C2-C1	2.08	1.55	1.53
4	K	1506	BCL	C3D-CAD	2.09	1.51	1.45
3	J	1405	RG1	C12-C13	2.10	1.50	1.45
3	P	1408	RG1	C11-C10	2.10	1.49	1.43
4	A	1501	BCL	C4B-CHC	2.11	1.45	1.40
3	H	1404	RG1	C11-C10	2.11	1.49	1.43
3	L	1406	RG1	C20-C21	2.11	1.49	1.43
4	M	1507	BCL	OBD-CAD	2.12	1.25	1.22
4	R	1509	BCL	C1B-CHB	2.12	1.45	1.40
3	P	1408	RG1	O5'-C1'	2.12	1.47	1.41
4	R	1709	BCL	OBB-CAB	2.12	1.29	1.22
4	M	1507	BCL	C1B-CHB	2.13	1.45	1.40
3	J	1405	RG1	C15-C14	2.15	1.49	1.43
3	J	1405	RG1	C11-C10	2.15	1.49	1.43
4	O	1708	BCL	OBB-CAB	2.17	1.30	1.22
4	I	1505	BCL	OBD-CAD	2.17	1.25	1.22
4	C	1502	BCL	O2D-CGD	2.18	1.38	1.33
4	I	1505	BCL	OBB-CAB	2.18	1.30	1.22
4	O	1708	BCL	C4B-CHC	2.19	1.46	1.40
4	M	1707	BCL	C5-C3	2.20	1.56	1.51
4	A	1501	BCL	C3D-CAD	2.20	1.52	1.45
4	C	1702	BCL	O2A-CGA	2.20	1.39	1.33
3	L	1406	RG1	O2'-C2'	2.22	1.48	1.43
4	K	1706	BCL	O2D-CGD	2.23	1.38	1.33
4	E	1703	BCL	O1A-CGA	2.23	1.29	1.22
4	M	1507	BCL	OBB-CAB	2.24	1.30	1.22
4	J	1605	BCL	C4B-CHC	2.25	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1403	RG1	C6-C5	2.26	1.36	1.34
4	I	1705	BCL	C1B-CHB	2.26	1.46	1.40
3	S	1409	RG1	O5'-C1'	2.28	1.47	1.41
4	R	1509	BCL	C3B-CAB	2.28	1.55	1.49
4	R	1709	BCL	O2A-CGA	2.29	1.40	1.33
3	P	1408	RG1	C19-C18	2.29	1.51	1.45
4	A	1701	BCL	C5-C3	2.30	1.56	1.51
3	S	1409	RG1	C12-C13	2.30	1.51	1.45
4	F	1603	BCL	O1D-CGD	2.31	1.27	1.21
3	S	1409	RG1	C25-C26	2.31	1.38	1.35
3	P	1408	RG1	C6-C5	2.34	1.36	1.34
3	D	1402	RG1	C8-C9	2.35	1.51	1.45
4	C	1702	BCL	C1B-CHB	2.35	1.46	1.40
4	O	1508	BCL	C3D-C2D	2.36	1.45	1.40
3	D	1402	RG1	O5'-C1'	2.37	1.47	1.41
4	A	1701	BCL	CHD-C4C	2.37	1.48	1.41
4	O	1708	BCL	O1A-CGA	2.39	1.29	1.22
4	E	1703	BCL	C3B-CAB	2.40	1.55	1.49
4	H	1604	BCL	O2A-CGA	2.41	1.40	1.33
4	S	1609	BCL	O2D-CGD	2.42	1.39	1.33
4	B	1601	BCL	O1A-CGA	2.43	1.29	1.22
3	P	1408	RG1	C28-C29	2.43	1.50	1.43
4	K	1706	BCL	C9-C8	2.45	1.61	1.52
3	R	1401	RG1	C11-C10	2.45	1.50	1.43
4	R	1709	BCL	C1D-ND	2.49	1.43	1.37
3	J	1405	RG1	C8-C9	2.49	1.51	1.45
4	R	1709	BCL	C4B-CHC	2.51	1.46	1.40
4	A	1701	BCL	C4B-CHC	2.52	1.46	1.40
4	I	1705	BCL	O1D-CGD	2.52	1.27	1.21
4	M	1707	BCL	C3B-C2B	2.52	1.45	1.40
4	A	1501	BCL	O2A-CGA	2.53	1.40	1.33
4	F	1603	BCL	O1A-CGA	2.53	1.30	1.22
3	N	1407	RG1	C27-C26	2.55	1.51	1.45
4	H	1604	BCL	OBB-CAB	2.56	1.31	1.22
4	R	1709	BCL	OBD-CAD	2.57	1.26	1.22
4	R	1509	BCL	OBB-CAB	2.57	1.31	1.22
4	O	1708	BCL	OBD-CAD	2.57	1.26	1.22
3	N	1407	RG1	C15-C14	2.58	1.51	1.43
3	R	1401	RG1	C8-C9	2.58	1.51	1.45
4	H	1604	BCL	O2D-CGD	2.58	1.39	1.33
4	A	1701	BCL	OBB-CAB	2.58	1.31	1.22
3	L	1406	RG1	C19-C18	2.60	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1702	BCL	OBD-CAD	2.62	1.26	1.22
4	D	1602	BCL	O2D-CGD	2.62	1.39	1.33
4	C	1502	BCL	O1D-CGD	2.63	1.27	1.21
4	P	1608	BCL	O1A-CGA	2.63	1.30	1.22
4	N	1607	BCL	C3B-C2B	2.63	1.45	1.40
4	P	1608	BCL	C3B-C2B	2.63	1.45	1.40
4	B	1601	BCL	O2A-CGA	2.65	1.41	1.33
4	O	1508	BCL	O1D-CGD	2.65	1.28	1.21
4	E	1503	BCL	O2A-CGA	2.66	1.41	1.33
4	O	1708	BCL	C1B-CHB	2.67	1.47	1.40
4	G	1704	BCL	O1A-CGA	2.67	1.30	1.22
4	C	1502	BCL	O1A-CGA	2.67	1.30	1.22
4	K	1506	BCL	O1A-CGA	2.69	1.30	1.22
4	C	1502	BCL	C1D-ND	2.69	1.44	1.37
4	B	1601	BCL	C1B-CHB	2.70	1.47	1.40
4	P	1608	BCL	O2D-CGD	2.70	1.40	1.33
4	I	1705	BCL	C3B-CAB	2.71	1.56	1.49
4	I	1505	BCL	O1D-CGD	2.72	1.28	1.21
4	H	1604	BCL	OBD-CAD	2.72	1.26	1.22
3	P	1408	RG1	C24-C25	2.73	1.51	1.43
4	R	1709	BCL	C5-C3	2.73	1.57	1.51
4	L	1606	BCL	O2A-CGA	2.74	1.41	1.33
4	I	1705	BCL	C3B-C2B	2.74	1.46	1.40
4	O	1508	BCL	OB B-CAB	2.77	1.32	1.22
3	D	1402	RG1	C7-C6	2.77	1.51	1.43
4	B	1601	BCL	O2D-CGD	2.79	1.40	1.33
4	M	1707	BCL	O1A-CGA	2.81	1.30	1.22
3	H	1404	RG1	C27-C26	2.81	1.52	1.45
4	J	1605	BCL	O1D-CGD	2.82	1.28	1.21
4	L	1606	BCL	O1A-CGA	2.83	1.31	1.22
4	F	1603	BCL	O2D-CGD	2.83	1.40	1.33
3	D	1402	RG1	C11-C10	2.83	1.51	1.43
3	R	1401	RG1	CM1-C1	2.84	1.58	1.52
4	A	1701	BCL	O2A-CGA	2.85	1.41	1.33
4	C	1502	BCL	C4B-CHC	2.86	1.47	1.40
4	K	1506	BCL	C3B-CAB	2.86	1.56	1.49
3	P	1408	RG1	C23-C22	2.86	1.52	1.45
4	I	1705	BCL	C3D-CAD	2.87	1.53	1.45
4	N	1607	BCL	O1A-CGA	2.87	1.31	1.22
4	F	1603	BCL	C5-C3	2.87	1.57	1.51
3	L	1406	RG1	C11-C10	2.88	1.51	1.43
4	D	1602	BCL	O1D-CGD	2.88	1.28	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1601	BCL	C4B-CHC	2.89	1.47	1.40
4	L	1606	BCL	C3D-C2D	2.91	1.46	1.40
3	P	1408	RG1	C17-C18	2.91	1.39	1.35
4	C	1702	BCL	O1A-CGA	2.91	1.31	1.22
4	R	1709	BCL	O1A-CGA	2.93	1.31	1.22
4	J	1605	BCL	O2A-CGA	2.93	1.42	1.33
4	E	1503	BCL	O1D-CGD	2.94	1.28	1.21
4	A	1501	BCL	O2D-CGD	2.95	1.40	1.33
4	S	1609	BCL	O2A-CGA	2.95	1.42	1.33
3	H	1404	RG1	C23-C22	2.95	1.52	1.45
4	L	1606	BCL	C1B-CHB	2.97	1.48	1.40
3	F	1403	RG1	C11-C10	2.97	1.52	1.43
4	J	1605	BCL	C3D-C2D	2.98	1.46	1.40
3	D	1402	RG1	C6-C5	3.00	1.37	1.34
3	F	1403	RG1	C24-C25	3.01	1.52	1.43
3	N	1407	RG1	C21-C22	3.01	1.39	1.35
3	S	1409	RG1	C24-C25	3.03	1.52	1.43
4	K	1506	BCL	O2A-CGA	3.05	1.42	1.33
4	R	1709	BCL	O1D-CGD	3.06	1.29	1.21
4	E	1503	BCL	O1A-CGA	3.06	1.31	1.22
4	K	1706	BCL	O1A-CGA	3.08	1.31	1.22
4	C	1502	BCL	C3D-C2D	3.08	1.46	1.40
4	R	1509	BCL	C4B-CHC	3.09	1.48	1.40
4	A	1501	BCL	C1B-CHB	3.09	1.48	1.40
4	G	1504	BCL	C3D-C2D	3.14	1.46	1.40
4	K	1706	BCL	OBB-CAB	3.14	1.33	1.22
3	L	1406	RG1	C15-C16	3.15	1.44	1.35
3	L	1406	RG1	C17-C18	3.15	1.40	1.35
4	S	1609	BCL	O1D-CGD	3.15	1.29	1.21
3	L	1406	RG1	C16-C17	3.16	1.52	1.43
4	K	1706	BCL	C3B-C2B	3.16	1.47	1.40
4	N	1607	BCL	C1B-CHB	3.17	1.48	1.40
4	I	1705	BCL	CAA-C2A	3.18	1.60	1.54
4	K	1706	BCL	C1B-CHB	3.19	1.48	1.40
4	J	1605	BCL	C1B-CHB	3.21	1.48	1.40
4	G	1504	BCL	C1B-CHB	3.21	1.48	1.40
4	P	1608	BCL	C4B-CHC	3.21	1.48	1.40
4	A	1501	BCL	C3C-C4C	3.23	1.55	1.51
3	D	1402	RG1	C2-C1	3.25	1.57	1.53
4	J	1605	BCL	O1A-CGA	3.25	1.32	1.22
4	P	1608	BCL	C1B-CHB	3.26	1.48	1.40
4	S	1609	BCL	C1B-CHB	3.26	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1704	BCL	C1B-CHB	3.27	1.48	1.40
4	C	1502	BCL	C1B-CHB	3.31	1.49	1.40
4	M	1507	BCL	O2D-CGD	3.32	1.41	1.33
4	K	1706	BCL	OBD-CAD	3.34	1.27	1.22
4	I	1505	BCL	O1A-CGA	3.38	1.32	1.22
4	D	1602	BCL	O2A-CGA	3.38	1.43	1.33
4	B	1601	BCL	O1D-CGD	3.38	1.29	1.21
4	D	1602	BCL	OBD-CAD	3.39	1.27	1.22
4	A	1501	BCL	C3B-C2B	3.39	1.47	1.40
4	H	1604	BCL	O1A-CGA	3.40	1.32	1.22
4	B	1601	BCL	C3D-C2D	3.43	1.47	1.40
4	A	1701	BCL	O2D-CGD	3.43	1.42	1.33
4	R	1509	BCL	O1A-CGA	3.43	1.32	1.22
3	R	1401	RG1	C6-C5	3.45	1.38	1.34
4	I	1705	BCL	O2D-CGD	3.46	1.42	1.33
4	C	1502	BCL	C3B-C2B	3.47	1.47	1.40
4	L	1606	BCL	OBD-CAD	3.49	1.27	1.22
4	H	1604	BCL	C4B-CHC	3.49	1.49	1.40
4	D	1602	BCL	O1A-CGA	3.50	1.33	1.22
4	N	1607	BCL	OBD-CAD	3.51	1.27	1.22
4	F	1603	BCL	OBD-CAD	3.51	1.27	1.22
4	I	1505	BCL	O2D-CGD	3.52	1.42	1.33
4	A	1701	BCL	C1B-CHB	3.52	1.49	1.40
4	H	1604	BCL	C1B-CHB	3.52	1.49	1.40
4	K	1506	BCL	C3D-C2D	3.53	1.47	1.40
4	E	1503	BCL	OBD-CAD	3.55	1.27	1.22
4	L	1606	BCL	C4B-CHC	3.62	1.49	1.40
4	A	1501	BCL	C3D-C2D	3.65	1.48	1.40
4	A	1501	BCL	O1D-CGD	3.66	1.30	1.21
4	I	1505	BCL	C1B-CHB	3.66	1.50	1.40
4	I	1705	BCL	OBD-CAD	3.66	1.27	1.22
4	M	1707	BCL	C1B-CHB	3.67	1.50	1.40
4	I	1705	BCL	O1A-CGA	3.69	1.33	1.22
4	O	1508	BCL	O1A-CGA	3.69	1.33	1.22
4	H	1604	BCL	C3D-C2D	3.69	1.48	1.40
4	C	1502	BCL	OBD-CAD	3.71	1.27	1.22
4	D	1602	BCL	C1B-CHB	3.72	1.50	1.40
4	A	1701	BCL	C3B-C2B	3.73	1.48	1.40
4	M	1507	BCL	O1D-CGD	3.74	1.30	1.21
4	S	1609	BCL	OBD-CAD	3.74	1.28	1.22
4	P	1608	BCL	C3D-C2D	3.75	1.48	1.40
4	G	1704	BCL	C3D-C2D	3.75	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	1509	BCL	C3D-C2D	3.87	1.48	1.40
4	R	1509	BCL	C3B-C2B	3.87	1.48	1.40
4	I	1505	BCL	C4B-CHC	3.90	1.50	1.40
4	R	1709	BCL	C1B-CHB	3.92	1.50	1.40
4	H	1604	BCL	C3B-C2B	3.92	1.48	1.40
4	A	1701	BCL	O1A-CGA	3.92	1.34	1.22
4	I	1705	BCL	C3D-C2D	3.92	1.48	1.40
4	A	1501	BCL	O1A-CGA	3.94	1.34	1.22
4	A	1701	BCL	O1D-CGD	3.95	1.31	1.21
4	I	1505	BCL	C3B-C2B	3.96	1.48	1.40
4	G	1704	BCL	C3B-C2B	3.96	1.48	1.40
4	B	1601	BCL	OBD-CAD	3.99	1.28	1.22
4	I	1505	BCL	C2-C3	4.00	1.43	1.32
4	L	1606	BCL	O1D-CGD	4.04	1.31	1.21
4	R	1509	BCL	O1D-CGD	4.04	1.31	1.21
3	H	1404	RG1	C2-C1	4.07	1.58	1.53
4	H	1604	BCL	O1D-CGD	4.09	1.31	1.21
4	S	1609	BCL	C3B-C2B	4.11	1.49	1.40
4	G	1504	BCL	OBD-CAD	4.12	1.28	1.22
4	A	1701	BCL	C3D-C2D	4.14	1.49	1.40
4	K	1506	BCL	O2D-CGD	4.18	1.44	1.33
3	S	1409	RG1	C2-C1	4.20	1.58	1.53
4	K	1706	BCL	C3D-C2D	4.20	1.49	1.40
4	K	1706	BCL	O1D-CGD	4.20	1.31	1.21
4	N	1607	BCL	C3D-C2D	4.26	1.49	1.40
4	R	1709	BCL	C3D-C2D	4.32	1.49	1.40
4	S	1609	BCL	C3D-C2D	4.33	1.49	1.40
4	O	1708	BCL	C3B-C2B	4.35	1.49	1.40
4	D	1602	BCL	C3D-C2D	4.37	1.49	1.40
4	B	1601	BCL	C3B-C2B	4.39	1.49	1.40
4	F	1603	BCL	C3B-C2B	4.42	1.49	1.40
4	O	1708	BCL	C3D-C2D	4.43	1.49	1.40
4	O	1708	BCL	O1D-CGD	4.44	1.32	1.21
4	J	1605	BCL	C3B-C2B	4.45	1.49	1.40
4	E	1503	BCL	C3D-C2D	4.59	1.50	1.40
3	F	1403	RG1	C19-C18	4.65	1.56	1.45
4	E	1703	BCL	C3D-C2D	4.66	1.50	1.40
4	K	1506	BCL	O1D-CGD	4.77	1.33	1.21
4	K	1506	BCL	CAA-C2A	4.79	1.63	1.54
4	G	1504	BCL	O1D-CGD	4.81	1.33	1.21
4	I	1705	BCL	C2-C3	4.82	1.45	1.32
4	E	1703	BCL	C3B-C2B	4.82	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1702	BCL	C3D-C2D	4.82	1.50	1.40
4	M	1707	BCL	OBD-CAD	4.87	1.29	1.22
4	C	1702	BCL	C3B-C2B	4.90	1.50	1.40
4	R	1709	BCL	C3B-C2B	4.91	1.50	1.40
4	C	1702	BCL	O1D-CGD	4.93	1.33	1.21
4	D	1602	BCL	C3B-C2B	4.96	1.50	1.40
4	A	1701	BCL	OBD-CAD	4.97	1.29	1.22
4	L	1606	BCL	C2-C3	5.02	1.45	1.32
4	F	1603	BCL	C3D-C2D	5.10	1.51	1.40
4	E	1503	BCL	C3B-C2B	5.13	1.51	1.40
4	O	1508	BCL	OBD-CAD	5.15	1.30	1.22
4	O	1508	BCL	C2-C3	5.16	1.46	1.32
4	L	1606	BCL	C3B-C2B	5.24	1.51	1.40
4	K	1506	BCL	C3B-C2B	5.24	1.51	1.40
4	P	1608	BCL	OBD-CAD	5.27	1.30	1.22
4	G	1504	BCL	C3B-C2B	5.31	1.51	1.40
4	M	1507	BCL	C3D-C2D	5.32	1.51	1.40
4	M	1507	BCL	C3B-C2B	5.34	1.51	1.40
4	O	1508	BCL	C3B-C2B	5.35	1.51	1.40
4	P	1608	BCL	O1D-CGD	5.39	1.34	1.21
4	A	1501	BCL	OBD-CAD	5.43	1.30	1.22
4	E	1503	BCL	CHC-C1C	5.52	1.40	1.33
4	R	1509	BCL	C2-C3	5.53	1.47	1.32
4	S	1609	BCL	CHC-C1C	5.58	1.41	1.33
4	K	1706	BCL	C2-C3	5.58	1.47	1.32
4	G	1504	BCL	C2-C3	5.61	1.47	1.32
4	C	1502	BCL	C2-C3	5.69	1.47	1.32
4	R	1509	BCL	OBD-CAD	5.74	1.31	1.22
4	E	1703	BCL	C2-C3	5.74	1.47	1.32
4	E	1703	BCL	O1D-CGD	5.78	1.35	1.21
4	H	1604	BCL	C2-C3	5.83	1.47	1.32
4	F	1603	BCL	C2-C3	5.84	1.47	1.32
4	P	1608	BCL	C2-C3	5.87	1.47	1.32
4	D	1602	BCL	C2-C3	6.05	1.48	1.32
4	B	1601	BCL	C2-C3	6.06	1.48	1.32
4	E	1703	BCL	CHC-C1C	6.06	1.41	1.33
4	K	1506	BCL	C2-C3	6.08	1.48	1.32
4	M	1507	BCL	C2-C3	6.11	1.48	1.32
4	M	1707	BCL	C2-C3	6.17	1.48	1.32
4	A	1501	BCL	C2-C3	6.25	1.48	1.32
4	N	1607	BCL	C2-C3	6.30	1.49	1.32
4	G	1704	BCL	CHC-C1C	6.30	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	1709	BCL	C2-C3	6.30	1.49	1.32
4	O	1508	BCL	CHC-C1C	6.40	1.42	1.33
4	E	1503	BCL	C2-C3	6.45	1.49	1.32
4	G	1704	BCL	C2-C3	6.65	1.49	1.32
4	O	1708	BCL	C2-C3	6.74	1.50	1.32
4	J	1605	BCL	C2-C3	6.81	1.50	1.32
4	J	1605	BCL	CHC-C1C	6.88	1.42	1.33
4	S	1609	BCL	C2-C3	6.95	1.50	1.32
4	A	1701	BCL	C2-C3	6.96	1.50	1.32
4	B	1601	BCL	CHB-C4A	7.09	1.43	1.33
4	F	1603	BCL	CHC-C1C	7.10	1.43	1.33
4	I	1705	BCL	CHC-C1C	7.25	1.43	1.33
4	N	1607	BCL	CHC-C1C	7.30	1.43	1.33
4	K	1506	BCL	CHC-C1C	7.67	1.43	1.33
4	I	1705	BCL	CHB-C4A	7.74	1.43	1.33
4	A	1701	BCL	CHC-C1C	7.74	1.43	1.33
4	P	1608	BCL	CHC-C1C	7.76	1.43	1.33
4	B	1601	BCL	CHC-C1C	7.77	1.43	1.33
4	M	1707	BCL	CHC-C1C	7.77	1.43	1.33
4	C	1702	BCL	C2-C3	7.81	1.52	1.32
4	H	1604	BCL	CHC-C1C	7.93	1.44	1.33
4	K	1706	BCL	CHB-C4A	8.04	1.44	1.33
4	L	1606	BCL	CHB-C4A	8.06	1.44	1.33
4	D	1602	BCL	CHC-C1C	8.09	1.44	1.33
4	E	1703	BCL	CHB-C4A	8.20	1.44	1.33
4	C	1702	BCL	CHC-C1C	8.20	1.44	1.33
4	N	1607	BCL	CHB-C4A	8.38	1.44	1.33
4	M	1507	BCL	CHB-C4A	8.47	1.44	1.33
4	I	1505	BCL	CHB-C4A	8.48	1.44	1.33
4	E	1503	BCL	CHB-C4A	8.66	1.45	1.33
4	S	1609	BCL	CHB-C4A	8.79	1.45	1.33
4	G	1504	BCL	CHC-C1C	8.94	1.45	1.33
4	O	1508	BCL	CHB-C4A	8.97	1.45	1.33
4	C	1502	BCL	CHC-C1C	8.97	1.45	1.33
4	A	1501	BCL	CHC-C1C	9.02	1.45	1.33
4	O	1708	BCL	CHC-C1C	9.04	1.45	1.33
4	M	1507	BCL	CHC-C1C	9.09	1.45	1.33
4	R	1709	BCL	CHC-C1C	9.15	1.45	1.33
4	H	1604	BCL	CHB-C4A	9.31	1.46	1.33
4	R	1709	BCL	CHB-C4A	9.37	1.46	1.33
4	R	1509	BCL	CHB-C4A	9.41	1.46	1.33
4	K	1706	BCL	CHC-C1C	9.45	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1701	BCL	CHB-C4A	9.55	1.46	1.33
4	I	1505	BCL	CHC-C1C	9.63	1.46	1.33
4	K	1506	BCL	CHB-C4A	9.68	1.46	1.33
4	F	1603	BCL	CHB-C4A	9.72	1.46	1.33
4	D	1602	BCL	CHB-C4A	9.98	1.46	1.33
4	A	1501	BCL	CHB-C4A	10.09	1.47	1.33
4	G	1504	BCL	CHB-C4A	10.35	1.47	1.33
4	J	1605	BCL	CHB-C4A	10.37	1.47	1.33
4	G	1704	BCL	CHB-C4A	10.68	1.47	1.33
4	R	1509	BCL	CHC-C1C	10.89	1.48	1.33
4	M	1707	BCL	CHB-C4A	10.93	1.48	1.33
4	L	1606	BCL	CHC-C1C	11.10	1.48	1.33
4	C	1702	BCL	CHB-C4A	11.17	1.48	1.33
4	O	1708	BCL	CHB-C4A	11.28	1.48	1.33
4	P	1608	BCL	CHB-C4A	11.55	1.49	1.33
4	C	1502	BCL	CHB-C4A	11.87	1.49	1.33

All (544) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1502	BCL	C6-C5-C3	-5.94	102.09	112.76
3	H	1404	RG1	C16-C17-C18	-5.56	119.14	127.22
3	J	1405	RG1	C16-C17-C18	-5.48	119.25	127.22
3	R	1401	RG1	C16-C17-C18	-5.40	119.38	127.22
3	R	1401	RG1	C7-C6-C5	-5.37	121.10	127.69
3	D	1402	RG1	C16-C17-C18	-5.30	119.52	127.22
3	D	1402	RG1	C7-C6-C5	-5.27	121.23	127.69
4	L	1606	BCL	C4A-NA-C1A	-4.95	100.09	106.38
3	N	1407	RG1	C7-C6-C5	-4.90	121.67	127.69
3	N	1407	RG1	C16-C17-C18	-4.87	120.14	127.22
3	S	1409	RG1	C7-C6-C5	-4.84	121.75	127.69
4	K	1506	BCL	C1D-CHD-C4C	-4.72	118.70	126.06
4	F	1603	BCL	C6-C5-C3	-4.63	104.46	112.76
4	G	1704	BCL	C6-C5-C3	-4.61	104.48	112.76
3	L	1406	RG1	C7-C6-C5	-4.60	122.04	127.69
3	P	1408	RG1	C16-C17-C18	-4.60	120.54	127.22
4	B	1601	BCL	C4A-NA-C1A	-4.59	100.55	106.38
4	A	1701	BCL	C1D-CHD-C4C	-4.57	118.93	126.06
4	J	1605	BCL	CBA-CAA-C2A	-4.57	102.19	113.96
3	P	1408	RG1	C7-C6-C5	-4.52	122.14	127.69
3	S	1409	RG1	C16-C17-C18	-4.51	120.67	127.22
4	G	1504	BCL	C6-C5-C3	-4.49	104.71	112.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	1506	BCL	C6-C5-C3	-4.34	104.98	112.76
3	H	1404	RG1	C7-C6-C5	-4.29	122.43	127.69
3	F	1403	RG1	C11-C10-C9	-4.29	120.99	127.22
4	L	1606	BCL	O2D-CGD-O1D	-4.27	114.78	123.77
4	O	1708	BCL	O2A-CGA-O1A	-4.22	112.44	123.51
4	H	1604	BCL	CBA-CAA-C2A	-4.16	103.24	113.96
4	I	1705	BCL	OB- CAB-C3B	-4.16	111.90	119.97
4	O	1508	BCL	OB- CAB-C3B	-4.15	111.91	119.97
4	R	1509	BCL	C4A-NA-C1A	-4.15	101.11	106.38
4	P	1608	BCL	CBA-CAA-C2A	-4.13	103.31	113.96
4	S	1609	BCL	CBA-CAA-C2A	-4.02	103.59	113.96
4	S	1609	BCL	OB- CAD-C3D	-4.01	120.99	128.09
4	N	1607	BCL	C1D-CHD-C4C	-4.01	119.80	126.06
4	M	1507	BCL	C4A-NA-C1A	-4.00	101.30	106.38
4	C	1502	BCL	OB- CAB-C3B	-3.98	112.24	119.97
4	E	1503	BCL	C6-C5-C3	-3.97	105.64	112.76
4	L	1606	BCL	OB- CAB-C3B	-3.97	112.26	119.97
4	H	1604	BCL	C6-C5-C3	-3.95	105.67	112.76
4	D	1602	BCL	C6-C5-C3	-3.95	105.68	112.76
4	D	1602	BCL	C4A-NA-C1A	-3.94	101.37	106.38
3	F	1403	RG1	C16-C17-C18	-3.94	121.49	127.22
4	G	1504	BCL	O2A-CGA-O1A	-3.93	113.20	123.51
4	A	1701	BCL	OB- CAB-C3B	-3.92	112.35	119.97
4	J	1605	BCL	OB- CAB-C3B	-3.89	112.42	119.97
4	J	1605	BCL	C6-C5-C3	-3.88	105.80	112.76
4	O	1708	BCL	OB- CAB-C3B	-3.86	112.47	119.97
4	B	1601	BCL	C6-C5-C3	-3.81	105.92	112.76
4	M	1707	BCL	O2A-CGA-O1A	-3.81	113.53	123.51
4	K	1706	BCL	O2A-CGA-O1A	-3.80	113.55	123.51
4	K	1506	BCL	CBA-CAA-C2A	-3.80	104.17	113.96
3	L	1406	RG1	C11-C10-C9	-3.79	121.70	127.22
4	C	1702	BCL	OB- CAB-C3B	-3.79	112.60	119.97
4	O	1708	BCL	C6-C5-C3	-3.78	105.98	112.76
4	E	1703	BCL	OB- CAD-C3D	-3.77	121.43	128.09
4	O	1508	BCL	C6-C5-C3	-3.77	106.00	112.76
4	A	1501	BCL	CBA-CAA-C2A	-3.76	104.26	113.96
4	R	1509	BCL	C6-C5-C3	-3.75	106.04	112.76
4	I	1705	BCL	C6-C5-C3	-3.74	106.05	112.76
4	I	1705	BCL	O2A-CGA-O1A	-3.71	113.79	123.51
4	N	1607	BCL	O2A-CGA-O1A	-3.70	113.82	123.51
4	B	1601	BCL	OB- CAB-C3B	-3.68	112.82	119.97
4	G	1704	BCL	O2A-CGA-O1A	-3.67	113.90	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1703	BCL	O2A-CGA-O1A	-3.66	113.91	123.51
4	C	1502	BCL	O2A-CGA-O1A	-3.66	113.91	123.51
4	O	1708	BCL	C1D-CHD-C4C	-3.66	120.35	126.06
4	R	1709	BCL	C1D-CHD-C4C	-3.65	120.36	126.06
4	H	1604	BCL	C3C-C4C-CHD	-3.64	117.03	123.17
4	E	1503	BCL	CBA-CAA-C2A	-3.62	104.63	113.96
3	R	1401	RG1	C16-C15-C14	-3.61	115.45	123.23
4	M	1507	BCL	O2A-CGA-O1A	-3.61	114.05	123.51
4	S	1609	BCL	C6-C5-C3	-3.60	106.30	112.76
4	R	1509	BCL	O2A-CGA-O1A	-3.60	114.08	123.51
4	L	1606	BCL	OBD-CAD-C3D	-3.59	121.74	128.09
4	A	1501	BCL	OBB-CAB-C3B	-3.59	113.00	119.97
4	M	1707	BCL	OBB-CAB-C3B	-3.59	113.00	119.97
4	N	1607	BCL	C6-C5-C3	-3.58	106.33	112.76
3	P	1408	RG1	C24-C25-C26	-3.58	122.02	127.22
4	R	1709	BCL	O2A-CGA-O1A	-3.57	114.16	123.51
4	N	1607	BCL	OBB-CAB-C3B	-3.56	113.05	119.97
4	A	1701	BCL	O2A-CGA-O1A	-3.56	114.19	123.51
4	O	1508	BCL	O2A-CGA-O1A	-3.56	114.19	123.51
4	R	1709	BCL	OBD-CAD-C3D	-3.55	121.81	128.09
4	J	1605	BCL	C4A-NA-C1A	-3.54	101.89	106.38
3	J	1405	RG1	C7-C6-C5	-3.53	123.35	127.69
4	I	1505	BCL	CBA-CAA-C2A	-3.53	104.86	113.96
4	E	1503	BCL	C4A-NA-C1A	-3.52	101.90	106.38
4	E	1503	BCL	O2A-CGA-O1A	-3.51	114.32	123.51
4	K	1706	BCL	C1D-CHD-C4C	-3.50	120.60	126.06
4	L	1606	BCL	C1D-CHD-C4C	-3.48	120.63	126.06
4	B	1601	BCL	O2A-CGA-O1A	-3.46	114.44	123.51
4	D	1602	BCL	OBB-CAB-C3B	-3.45	113.27	119.97
4	N	1607	BCL	CBA-CAA-C2A	-3.45	105.08	113.96
4	S	1609	BCL	OBB-CAB-C3B	-3.44	113.29	119.97
4	M	1507	BCL	C6-C5-C3	-3.43	106.61	112.76
4	D	1602	BCL	CBA-CAA-C2A	-3.42	105.14	113.96
4	B	1601	BCL	CBA-CAA-C2A	-3.42	105.15	113.96
3	L	1406	RG1	C16-C15-C14	-3.40	115.90	123.23
4	N	1607	BCL	OBD-CAD-C3D	-3.40	122.09	128.09
4	F	1603	BCL	O2A-CGA-O1A	-3.39	114.61	123.51
4	D	1602	BCL	C1D-CHD-C4C	-3.39	120.77	126.06
4	N	1607	BCL	C4A-NA-C1A	-3.39	102.08	106.38
4	I	1505	BCL	O2A-CGA-O1A	-3.38	114.64	123.51
4	C	1702	BCL	O2A-CGA-O1A	-3.37	114.67	123.51
4	I	1505	BCL	C1D-CHD-C4C	-3.37	120.81	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1502	BCL	OBD-CAD-C3D	-3.36	122.15	128.09
4	K	1706	BCL	C6-C5-C3	-3.36	106.73	112.76
3	P	1408	RG1	C16-C15-C14	-3.34	116.03	123.23
4	R	1509	BCL	C1D-CHD-C4C	-3.34	120.85	126.06
3	P	1408	RG1	C11-C10-C9	-3.33	122.38	127.22
3	J	1405	RG1	C20-C21-C22	-3.33	122.38	127.22
4	I	1505	BCL	OBB-CAB-C3B	-3.33	113.50	119.97
4	G	1704	BCL	OBB-CAB-C3B	-3.33	113.51	119.97
4	K	1706	BCL	OBB-CAB-C3B	-3.31	113.55	119.97
4	O	1508	BCL	O2D-CGD-O1D	-3.29	116.84	123.77
4	F	1603	BCL	C4A-NA-C1A	-3.29	102.20	106.38
4	M	1707	BCL	C6-C5-C3	-3.27	106.89	112.76
4	L	1606	BCL	O2A-CGA-O1A	-3.24	115.03	123.51
4	M	1507	BCL	OBB-CAB-C3B	-3.23	113.69	119.97
3	N	1407	RG1	C11-C10-C9	-3.23	122.53	127.22
4	R	1709	BCL	OBB-CAB-C3B	-3.22	113.72	119.97
4	C	1502	BCL	O2D-CGD-O1D	-3.20	117.03	123.77
4	K	1506	BCL	C3C-C2C-C1C	-3.20	98.55	101.84
4	H	1604	BCL	OBD-CAD-C3D	-3.19	122.46	128.09
4	M	1507	BCL	C1D-CHD-C4C	-3.18	121.10	126.06
4	A	1501	BCL	C1D-CHD-C4C	-3.18	121.10	126.06
4	O	1708	BCL	OBD-CAD-C3D	-3.16	122.50	128.09
4	C	1502	BCL	C4A-NA-C1A	-3.16	102.37	106.38
4	G	1704	BCL	C1D-CHD-C4C	-3.15	121.14	126.06
3	R	1401	RG1	C11-C10-C9	-3.15	122.65	127.22
4	S	1609	BCL	O2D-CGD-O1D	-3.14	117.15	123.77
4	P	1608	BCL	OBB-CAB-C3B	-3.14	113.88	119.97
4	D	1602	BCL	O2A-CGA-O1A	-3.13	115.30	123.51
4	F	1603	BCL	CBA-CAA-C2A	-3.13	105.89	113.96
4	E	1703	BCL	C6-C5-C3	-3.12	107.16	112.76
4	F	1603	BCL	OBB-CAB-C3B	-3.11	113.92	119.97
4	A	1501	BCL	O2D-CGD-O1D	-3.11	117.22	123.77
4	E	1503	BCL	OBD-CAD-C3D	-3.10	122.61	128.09
4	B	1601	BCL	OBD-CAD-C3D	-3.09	122.63	128.09
4	G	1504	BCL	C1D-CHD-C4C	-3.09	121.24	126.06
4	A	1701	BCL	C4A-NA-C1A	-3.07	102.47	106.38
4	A	1701	BCL	C3C-C2C-C1C	-3.07	98.69	101.84
3	N	1407	RG1	C16-C15-C14	-3.06	116.63	123.23
4	I	1705	BCL	C1D-CHD-C4C	-3.06	121.28	126.06
4	K	1506	BCL	C4A-NA-C1A	-3.06	102.50	106.38
4	G	1704	BCL	CHA-C1A-NA	-3.05	118.58	126.21
4	A	1501	BCL	O2A-CGA-O1A	-3.05	115.52	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1604	BCL	OBB-CAB-C3B	-3.04	114.06	119.97
4	E	1503	BCL	OBB-CAB-C3B	-3.04	114.06	119.97
4	C	1502	BCL	C1D-CHD-C4C	-3.03	121.33	126.06
4	H	1604	BCL	C1D-CHD-C4C	-3.03	121.33	126.06
4	K	1506	BCL	O2A-CGA-O1A	-3.03	115.57	123.51
4	D	1602	BCL	OBD-CAD-C3D	-3.03	122.74	128.09
4	C	1502	BCL	CBA-CAA-C2A	-3.02	106.16	113.96
3	J	1405	RG1	C2-C3-C4	-3.01	105.82	112.54
3	S	1409	RG1	C16-C15-C14	-3.00	116.76	123.23
4	K	1706	BCL	O2D-CGD-O1D	-2.99	117.48	123.77
3	J	1405	RG1	C25-C24-C23	-2.98	113.91	123.11
5	F	1803	LDA	O1-N1-CM1	-2.98	105.08	109.05
3	R	1401	RG1	C20-C21-C22	-2.97	122.90	127.22
4	K	1506	BCL	CBC-CAC-C3C	-2.97	106.07	113.43
4	A	1501	BCL	C4A-NA-C1A	-2.97	102.61	106.38
3	F	1403	RG1	C12-C13-C14	-2.97	114.17	118.95
3	S	1409	RG1	C20-C21-C22	-2.96	122.91	127.22
3	D	1402	RG1	C15-C14-C13	-2.96	122.92	127.22
4	A	1501	BCL	C6-C5-C3	-2.94	107.48	112.76
4	S	1609	BCL	C4A-NA-C1A	-2.94	102.64	106.38
4	E	1703	BCL	C1D-CHD-C4C	-2.94	121.48	126.06
4	R	1509	BCL	O2D-CGD-O1D	-2.91	117.64	123.77
4	M	1507	BCL	CBA-CAA-C2A	-2.90	106.47	113.96
4	K	1706	BCL	C4A-NA-C1A	-2.90	102.69	106.38
4	I	1505	BCL	C6-C5-C3	-2.89	107.57	112.76
4	I	1505	BCL	C4A-NA-C1A	-2.89	102.70	106.38
4	S	1609	BCL	C1D-CHD-C4C	-2.89	121.55	126.06
4	R	1509	BCL	OBD-CAD-C3D	-2.87	123.02	128.09
3	F	1403	RG1	C24-C25-C26	-2.86	123.06	127.22
4	L	1606	BCL	C6-C5-C3	-2.86	107.63	112.76
4	B	1601	BCL	O2D-CGD-O1D	-2.86	117.75	123.77
3	L	1406	RG1	C16-C17-C18	-2.85	123.08	127.22
4	S	1609	BCL	O2A-CGA-O1A	-2.83	116.08	123.51
4	P	1608	BCL	O2A-CGA-O1A	-2.83	116.09	123.51
3	H	1404	RG1	C16-C15-C14	-2.83	117.13	123.23
4	H	1604	BCL	O2A-CGA-O1A	-2.83	116.10	123.51
4	L	1606	BCL	CBA-CAA-C2A	-2.82	106.69	113.96
4	O	1708	BCL	CBA-CAA-C2A	-2.81	106.71	113.96
4	E	1503	BCL	C1D-CHD-C4C	-2.81	121.67	126.06
4	N	1607	BCL	O2D-CGD-O1D	-2.80	117.87	123.77
4	P	1608	BCL	OBD-CAD-C3D	-2.80	123.14	128.09
4	G	1504	BCL	CBA-CAA-C2A	-2.80	106.75	113.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1505	BCL	OBD-CAD-C3D	-2.79	123.17	128.09
4	B	1601	BCL	C1D-CHD-C4C	-2.77	121.74	126.06
4	O	1508	BCL	C4A-NA-C1A	-2.77	102.86	106.38
4	A	1701	BCL	C6-C5-C3	-2.76	107.81	112.76
4	C	1702	BCL	C4A-NA-C1A	-2.76	102.87	106.38
3	L	1406	RG1	C20-C21-C22	-2.75	123.23	127.22
4	G	1504	BCL	OBB-CAB-C3B	-2.72	114.68	119.97
3	D	1402	RG1	C16-C15-C14	-2.72	117.37	123.23
4	J	1605	BCL	C1D-CHD-C4C	-2.71	121.83	126.06
4	K	1706	BCL	CBA-CAA-C2A	-2.71	106.98	113.96
4	F	1603	BCL	O2D-CGD-O1D	-2.70	118.08	123.77
4	E	1703	BCL	OBB-CAB-C3B	-2.70	114.72	119.97
4	S	1609	BCL	C5-C3-C2	-2.70	115.95	120.98
4	G	1704	BCL	CBA-CAA-C2A	-2.70	107.00	113.96
3	L	1406	RG1	C12-C13-C14	-2.70	114.61	118.95
3	H	1404	RG1	C25-C24-C23	-2.69	114.79	123.11
4	O	1508	BCL	C1D-CHD-C4C	-2.69	121.86	126.06
4	G	1504	BCL	C4A-NA-C1A	-2.69	102.96	106.38
4	R	1709	BCL	O2D-CGD-O1D	-2.69	118.11	123.77
4	P	1608	BCL	C4A-NA-C1A	-2.67	102.98	106.38
4	E	1503	BCL	O2D-CGD-O1D	-2.67	118.15	123.77
4	M	1507	BCL	O2D-CGD-O1D	-2.67	118.15	123.77
3	J	1405	RG1	C16-C15-C14	-2.67	117.48	123.23
3	R	1401	RG1	C25-C24-C23	-2.65	114.91	123.11
4	O	1508	BCL	OBD-CAD-C3D	-2.65	123.40	128.09
4	O	1508	BCL	C5-C3-C2	-2.65	116.04	120.98
3	J	1405	RG1	CM6-C18-C17	-2.64	119.05	122.89
4	P	1608	BCL	C6-C5-C3	-2.64	108.03	112.76
4	O	1708	BCL	C4A-NA-C1A	-2.63	103.04	106.38
4	C	1702	BCL	OBD-CAD-C3D	-2.63	123.45	128.09
4	M	1707	BCL	CHA-C1A-NA	-2.63	119.64	126.21
4	R	1509	BCL	OBB-CAB-C3B	-2.63	114.87	119.97
4	H	1604	BCL	CAC-C3C-C4C	-2.62	106.78	112.58
3	N	1407	RG1	C29-C28-C27	-2.61	115.04	123.11
3	H	1404	RG1	C11-C10-C9	-2.61	123.43	127.22
4	C	1502	BCL	C5-C3-C2	-2.60	116.14	120.98
4	G	1504	BCL	O2D-CGD-O1D	-2.59	118.31	123.77
4	R	1709	BCL	C6-C5-C3	-2.59	108.11	112.76
4	R	1709	BCL	C4A-NA-C1A	-2.58	103.10	106.38
4	C	1702	BCL	C1D-CHD-C4C	-2.58	122.04	126.06
4	C	1702	BCL	C6-C5-C3	-2.56	108.17	112.76
3	D	1402	RG1	C20-C21-C22	-2.56	123.50	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	1708	BCL	O2D-CGD-O1D	-2.56	118.39	123.77
3	F	1403	RG1	C16-C15-C14	-2.55	117.73	123.23
4	G	1704	BCL	O2D-CGD-O1D	-2.54	118.42	123.77
3	J	1405	RG1	C28-C27-C26	-2.51	118.97	126.34
3	H	1404	RG1	C28-C27-C26	-2.51	118.97	126.34
4	P	1608	BCL	C1D-CHD-C4C	-2.51	122.14	126.06
4	A	1501	BCL	CHA-C1A-NA	-2.51	119.93	126.21
3	H	1404	RG1	C20-C21-C22	-2.51	123.58	127.22
4	H	1604	BCL	C4A-NA-C1A	-2.50	103.20	106.38
4	K	1706	BCL	OBD-CAD-C3D	-2.50	123.68	128.09
4	R	1709	BCL	CGD-CBD-CAD	-2.49	102.27	110.70
4	M	1707	BCL	C1D-CHD-C4C	-2.48	122.18	126.06
4	I	1705	BCL	C4A-NA-C1A	-2.48	103.22	106.38
3	N	1407	RG1	C24-C25-C26	-2.48	123.62	127.22
3	N	1407	RG1	CM6-C18-C17	-2.46	119.31	122.89
3	S	1409	RG1	C28-C27-C26	-2.46	119.13	126.34
3	S	1409	RG1	C24-C25-C26	-2.46	123.65	127.22
4	F	1603	BCL	C1D-CHD-C4C	-2.45	122.23	126.06
3	P	1408	RG1	C2-C3-C4	-2.45	107.07	112.54
4	E	1703	BCL	CBA-CAA-C2A	-2.44	107.67	113.96
3	J	1405	RG1	C11-C10-C9	-2.43	123.69	127.22
4	J	1605	BCL	O2A-CGA-O1A	-2.43	117.14	123.51
5	D	1802	LDA	O1-N1-C1	-2.42	107.55	110.27
4	K	1506	BCL	OBD-CAD-C3D	-2.42	123.81	128.09
4	J	1605	BCL	C3C-C4C-CHD	-2.42	119.09	123.17
3	F	1403	RG1	C7-C6-C5	-2.40	124.75	127.69
4	C	1702	BCL	O2D-CGD-O1D	-2.40	118.72	123.77
4	A	1501	BCL	OBD-CAD-C3D	-2.39	123.86	128.09
3	D	1402	RG1	C10-C11-C12	-2.39	115.74	123.11
4	G	1504	BCL	OBD-CAD-C3D	-2.38	123.89	128.09
4	S	1609	BCL	C3C-C4C-CHD	-2.38	119.16	123.17
3	N	1407	RG1	C20-C21-C22	-2.37	123.77	127.22
4	A	1701	BCL	OBD-CAD-C3D	-2.36	123.91	128.09
4	M	1507	BCL	C2A-C1A-CHA	-2.34	120.02	123.80
3	D	1402	RG1	C24-C25-C26	-2.34	123.81	127.22
4	G	1704	BCL	CBC-CAC-C3C	-2.34	107.64	113.43
4	E	1503	BCL	C5-C3-C2	-2.33	116.63	120.98
3	D	1402	RG1	C28-C27-C26	-2.33	119.50	126.34
3	F	1403	RG1	CM8-C26-C25	-2.33	119.50	122.89
4	C	1502	BCL	C2A-C1A-CHA	-2.32	120.06	123.80
4	A	1701	BCL	CBA-CAA-C2A	-2.32	107.98	113.96
4	F	1603	BCL	OBD-CAD-C3D	-2.30	124.02	128.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1504	BCL	C5-C3-C2	-2.29	116.71	120.98
3	S	1409	RG1	C25-C24-C23	-2.29	116.03	123.11
3	P	1408	RG1	CM8-C26-C25	-2.29	119.56	122.89
3	J	1405	RG1	C24-C25-C26	-2.29	123.90	127.22
4	A	1701	BCL	CBC-CAC-C3C	-2.28	107.78	113.43
3	F	1403	RG1	C29-C28-C27	-2.27	116.08	123.11
3	R	1401	RG1	C23-C22-C21	-2.27	115.30	118.95
4	K	1506	BCL	OBB-CAB-C3B	-2.27	115.57	119.97
4	G	1704	BCL	C3C-C4C-CHD	-2.26	119.36	123.17
3	N	1407	RG1	C15-C14-C13	-2.26	123.94	127.22
3	N	1407	RG1	C12-C13-C14	-2.26	115.32	118.95
4	M	1707	BCL	C3D-CAD-CBD	-2.25	104.42	107.60
3	L	1406	RG1	C2-C3-C4	-2.25	107.53	112.54
3	H	1404	RG1	CM2-C1-C2	-2.25	106.37	111.15
3	D	1402	RG1	C29-C28-C27	-2.25	116.17	123.11
4	G	1504	BCL	CHA-C1A-NA	-2.24	120.60	126.21
4	O	1508	BCL	CBA-CAA-C2A	-2.24	108.19	113.96
3	S	1409	RG1	C23-C22-C21	-2.23	115.36	118.95
3	D	1402	RG1	C25-C24-C23	-2.23	116.23	123.11
3	L	1406	RG1	C29-C28-C27	-2.22	116.25	123.11
4	R	1509	BCL	CBA-CAA-C2A	-2.22	108.23	113.96
3	F	1403	RG1	C28-C27-C26	-2.22	119.84	126.34
3	P	1408	RG1	C10-C11-C12	-2.22	116.26	123.11
3	L	1406	RG1	CM4-C9-C10	-2.21	119.67	122.89
4	I	1505	BCL	C11-C10-C8	-2.21	108.63	115.46
3	S	1409	RG1	C29-C28-C27	-2.20	116.30	123.11
3	F	1403	RG1	C25-C24-C23	-2.20	116.32	123.11
3	F	1403	RG1	C6-C7-C8	-2.19	116.34	123.11
4	M	1507	BCL	C5-C3-C2	-2.18	116.92	120.98
4	R	1509	BCL	C5-C3-C2	-2.17	116.95	120.98
4	H	1604	BCL	O2D-CGD-O1D	-2.15	119.24	123.77
4	M	1707	BCL	C3C-C4C-CHD	-2.14	119.56	123.17
3	R	1401	RG1	C28-C27-C26	-2.14	120.07	126.34
5	L	1806	LDA	O1-N1-CM1	-2.14	106.20	109.05
4	P	1608	BCL	C5-C3-C2	-2.13	117.02	120.98
4	D	1602	BCL	O2D-CGD-O1D	-2.12	119.31	123.77
3	S	1409	RG1	C20-C19-C18	-2.11	120.14	126.34
3	J	1405	RG1	C6-C7-C8	-2.11	116.59	123.11
3	N	1407	RG1	C25-C24-C23	-2.09	116.64	123.11
3	R	1401	RG1	C15-C14-C13	-2.09	124.18	127.22
3	S	1409	RG1	C7-C8-C9	-2.08	120.25	126.34
3	H	1404	RG1	CM6-C18-C17	-2.08	119.87	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1605	BCL	C5-C3-C2	-2.07	117.12	120.98
4	G	1504	BCL	C14-C13-C15	-2.07	103.36	111.10
4	J	1605	BCL	CHA-C1A-NA	-2.07	121.03	126.21
4	G	1704	BCL	C4A-NA-C1A	-2.07	103.75	106.38
3	J	1405	RG1	C29-C28-C27	-2.07	116.71	123.11
4	O	1508	BCL	CHA-C1A-NA	-2.06	121.05	126.21
4	C	1702	BCL	CBC-CAC-C3C	-2.06	108.33	113.43
4	E	1703	BCL	C4A-NA-C1A	-2.06	103.76	106.38
4	G	1504	BCL	CBC-CAC-C3C	-2.06	108.34	113.43
4	F	1603	BCL	C5-C3-C2	-2.05	117.16	120.98
4	E	1703	BCL	CHA-C1A-NA	-2.05	121.09	126.21
3	S	1409	RG1	C11-C10-C9	-2.04	124.25	127.22
4	I	1705	BCL	CBA-CAA-C2A	-2.04	108.70	113.96
4	H	1604	BCL	C5-C3-C2	-2.04	117.18	120.98
4	D	1602	BCL	C5-C3-C2	-2.03	117.19	120.98
4	I	1705	BCL	O2D-CGD-O1D	-2.03	119.49	123.77
4	J	1605	BCL	C16-C15-C13	-2.03	109.19	115.46
4	M	1507	BCL	CHA-C1A-NA	-2.02	121.16	126.21
3	S	1409	RG1	C10-C11-C12	-2.02	116.88	123.11
4	J	1605	BCL	O2D-CGD-O1D	-2.01	119.53	123.77
4	B	1601	BCL	C2A-C1A-CHA	-2.01	120.55	123.80
4	L	1606	BCL	CMB-C2B-C1B	-2.01	124.89	128.31
4	A	1701	BCL	CHA-C1A-NA	-2.00	121.20	126.21
4	P	1608	BCL	CHA-C1A-NA	-2.00	121.20	126.21
4	R	1709	BCL	CMD-C2D-C3D	2.00	129.01	125.09
4	C	1702	BCL	OBB-CAB-CBB	2.01	124.94	120.14
4	D	1602	BCL	OBB-CAB-CBB	2.01	124.95	120.14
4	I	1505	BCL	O2A-CGA-CBA	2.02	118.06	111.85
4	R	1509	BCL	CMA-C3A-C2A	2.02	122.86	113.99
3	J	1405	RG1	CM0-C30-CM9	2.03	119.53	114.61
3	L	1406	RG1	C1'-O5'-C5'	2.03	117.73	113.74
4	G	1704	BCL	CGD-CBD-CAD	2.03	117.58	110.70
3	D	1402	RG1	CM7-C22-C23	2.04	121.41	118.08
4	J	1605	BCL	OBB-CAB-CBB	2.04	125.02	120.14
3	H	1404	RG1	CM4-C9-C8	2.05	121.43	118.08
4	O	1508	BCL	OBB-CAB-CBB	2.05	125.05	120.14
4	O	1708	BCL	CMD-C2D-C3D	2.05	129.10	125.09
5	J	1805	LDA	CM2-N1-CM1	2.06	111.16	108.83
3	N	1407	RG1	CM5-C13-C12	2.07	121.46	118.08
3	R	1401	RG1	CM3-C5-C4	2.07	118.53	115.37
4	E	1703	BCL	CMD-C2D-C3D	2.08	129.15	125.09
4	A	1701	BCL	CMD-C2D-C3D	2.09	129.18	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1501	BCL	OBB-CAB-CBB	2.10	125.16	120.14
4	E	1703	BCL	C3D-CAD-CBD	2.11	110.57	107.60
4	O	1508	BCL	CGD-CBD-CAD	2.11	117.83	110.70
3	N	1407	RG1	CM4-C9-C8	2.12	121.54	118.08
4	O	1708	BCL	CMB-C2B-C3B	2.12	129.23	125.09
4	M	1507	BCL	C4-C3-C5	2.13	118.62	115.37
4	S	1609	BCL	OBD-CAD-CBD	2.13	129.15	125.94
4	F	1603	BCL	OBB-CAB-CBB	2.15	125.27	120.14
4	R	1509	BCL	O2A-CGA-CBA	2.17	118.52	111.85
3	R	1401	RG1	CM5-C13-C12	2.17	121.63	118.08
4	O	1508	BCL	O2A-CGA-CBA	2.18	118.56	111.85
4	G	1704	BCL	OBD-CAD-CBD	2.18	129.23	125.94
4	D	1602	BCL	O2A-CGA-CBA	2.19	118.60	111.85
4	J	1605	BCL	CGD-CBD-CAD	2.20	118.14	110.70
4	J	1605	BCL	C4-C3-C5	2.20	118.72	115.37
4	H	1604	BCL	OBB-CAB-CBB	2.22	125.45	120.14
3	L	1406	RG1	CM5-C13-C12	2.22	121.71	118.08
3	S	1409	RG1	CM0-C30-CM9	2.23	120.02	114.61
4	N	1607	BCL	C4-C3-C5	2.23	118.76	115.37
4	H	1604	BCL	O2A-CGA-CBA	2.23	118.72	111.85
4	R	1709	BCL	OBB-CAB-CBB	2.23	125.48	120.14
4	S	1609	BCL	CMB-C2B-C3B	2.24	129.46	125.09
4	A	1701	BCL	C2A-C3A-C4A	2.24	104.14	101.84
4	M	1507	BCL	O2A-CGA-CBA	2.25	118.78	111.85
4	P	1608	BCL	OBB-CAB-CBB	2.26	125.54	120.14
3	F	1403	RG1	CM0-C30-CM9	2.27	120.13	114.61
3	D	1402	RG1	CM3-C5-C4	2.27	118.83	115.37
4	P	1608	BCL	O2A-CGA-CBA	2.28	118.88	111.85
4	A	1701	BCL	CMB-C2B-C3B	2.29	129.56	125.09
4	B	1601	BCL	OBB-CAB-CBB	2.29	125.62	120.14
5	H	1804	LDA	CM2-N1-CM1	2.29	111.42	108.83
4	N	1607	BCL	OBB-CAB-CBB	2.30	125.63	120.14
4	M	1707	BCL	CMD-C2D-C3D	2.30	129.59	125.09
3	D	1402	RG1	CM5-C13-C12	2.33	121.90	118.08
4	F	1603	BCL	O2A-CGA-CBA	2.34	119.06	111.85
4	L	1606	BCL	C4-C3-C5	2.34	118.94	115.37
4	O	1508	BCL	C14-C13-C12	2.36	119.92	111.10
4	S	1609	BCL	C4-C3-C5	2.36	118.97	115.37
4	C	1502	BCL	O2A-CGA-CBA	2.36	119.12	111.85
4	R	1509	BCL	CMB-C2B-C3B	2.37	129.72	125.09
4	S	1609	BCL	C2A-C3A-C4A	2.37	104.26	101.84
4	H	1604	BCL	C4-C3-C5	2.39	119.02	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1606	BCL	OBB-CAB-CBB	2.40	125.87	120.14
4	A	1501	BCL	CMB-C2B-C3B	2.40	129.79	125.09
4	K	1506	BCL	CMB-C2B-C3B	2.42	129.83	125.09
4	L	1606	BCL	O2A-CGA-CBA	2.43	119.32	111.85
4	B	1601	BCL	C4-C3-C5	2.43	119.08	115.37
4	R	1509	BCL	CMD-C2D-C3D	2.44	129.85	125.09
3	D	1402	RG1	C1'-C2'-C3'	2.44	114.83	109.98
4	P	1608	BCL	C4-C3-C5	2.45	119.10	115.37
4	K	1706	BCL	CMD-C2D-C3D	2.45	129.88	125.09
4	E	1503	BCL	C4-C3-C5	2.45	119.10	115.37
4	G	1504	BCL	CMD-C2D-C3D	2.46	129.89	125.09
4	C	1702	BCL	C4-C3-C5	2.46	119.12	115.37
4	S	1609	BCL	O2A-CGA-CBA	2.47	119.44	111.85
4	K	1706	BCL	OBB-CAB-CBB	2.47	126.05	120.14
4	G	1704	BCL	C4-C3-C5	2.49	119.16	115.37
4	C	1502	BCL	C14-C13-C12	2.51	120.49	111.10
4	G	1504	BCL	O2A-CGA-CBA	2.51	119.58	111.85
4	A	1701	BCL	OBB-CAB-CBB	2.51	126.15	120.14
4	G	1704	BCL	CGD-CBD-CHA	2.53	119.56	110.88
4	O	1708	BCL	C4-C3-C5	2.54	119.24	115.37
3	L	1406	RG1	O5'-C1'-C2'	2.54	115.56	110.28
4	J	1605	BCL	CMB-C2B-C3B	2.55	130.07	125.09
4	K	1706	BCL	O2A-CGA-CBA	2.55	119.70	111.85
3	P	1408	RG1	C1'-O5'-C5'	2.55	118.75	113.74
4	E	1503	BCL	O2A-CGA-CBA	2.56	119.73	111.85
4	E	1703	BCL	O2A-CGA-CBA	2.56	119.73	111.85
4	G	1504	BCL	C2A-C3A-C4A	2.56	104.47	101.84
4	C	1502	BCL	CMD-C2D-C3D	2.58	130.13	125.09
4	J	1605	BCL	O2A-CGA-CBA	2.58	119.80	111.85
3	D	1402	RG1	CM4-C9-C8	2.59	122.31	118.08
4	O	1508	BCL	CMB-C2B-C3B	2.60	130.17	125.09
3	P	1408	RG1	CM7-C22-C23	2.60	122.34	118.08
4	I	1505	BCL	CMB-C2B-C3B	2.60	130.18	125.09
4	C	1702	BCL	O2A-CGA-CBA	2.62	119.92	111.85
3	D	1402	RG1	CM0-C30-CM9	2.62	120.98	114.61
4	O	1508	BCL	CMD-C2D-C3D	2.64	130.25	125.09
4	A	1701	BCL	CAC-C3C-C4C	2.65	118.46	112.58
4	F	1603	BCL	CMB-C2B-C3B	2.65	130.27	125.09
4	G	1504	BCL	C4-C3-C5	2.67	119.43	115.37
4	I	1705	BCL	CMD-C2D-C3D	2.67	130.31	125.09
4	G	1504	BCL	CMB-C2B-C3B	2.68	130.32	125.09
3	S	1409	RG1	CM5-C13-C12	2.68	122.46	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1404	RG1	CM7-C22-C23	2.68	122.46	118.08
4	O	1508	BCL	C4-C3-C5	2.68	119.45	115.37
4	N	1607	BCL	O2A-CGA-CBA	2.68	120.11	111.85
3	R	1401	RG1	CM7-C22-C23	2.70	122.50	118.08
4	I	1505	BCL	O2D-CGD-CBD	2.71	115.13	111.22
4	E	1703	BCL	O2D-CGD-CBD	2.73	115.16	111.22
4	A	1701	BCL	O2A-CGA-CBA	2.74	120.27	111.85
4	I	1505	BCL	C4-C3-C5	2.78	119.60	115.37
4	R	1709	BCL	CMB-C2B-C3B	2.78	130.53	125.09
3	F	1403	RG1	CM5-C13-C12	2.80	122.66	118.08
4	C	1502	BCL	C2A-C3A-C4A	2.82	104.73	101.84
4	R	1509	BCL	C4-C3-C5	2.83	119.68	115.37
4	M	1707	BCL	CGD-CBD-CHA	2.84	120.62	110.88
4	B	1601	BCL	CMB-C2B-C3B	2.85	130.67	125.09
3	J	1405	RG1	CM3-C5-C4	2.86	119.72	115.37
4	A	1501	BCL	CGD-CBD-CAD	2.86	120.38	110.70
4	E	1503	BCL	CMB-C2B-C3B	2.89	130.74	125.09
4	B	1601	BCL	O2A-CGA-CBA	2.89	120.75	111.85
4	A	1501	BCL	CMD-C2D-C3D	2.92	130.80	125.09
4	G	1704	BCL	O2A-CGA-CBA	2.93	120.87	111.85
3	N	1407	RG1	CM3-C5-C4	2.94	119.85	115.37
4	D	1602	BCL	C4-C3-C5	2.94	119.85	115.37
3	L	1406	RG1	CM3-C5-C4	2.94	119.85	115.37
4	C	1702	BCL	CMB-C2B-C3B	2.94	130.84	125.09
4	M	1507	BCL	CMB-C2B-C3B	2.94	130.84	125.09
4	D	1602	BCL	CMB-C2B-C3B	2.94	130.84	125.09
4	C	1502	BCL	C4-C3-C5	2.95	119.87	115.37
4	H	1604	BCL	CMC-C2C-C3C	2.95	126.95	113.99
4	A	1501	BCL	C4-C3-C5	2.96	119.88	115.37
4	I	1705	BCL	O2A-CGA-CBA	2.96	120.97	111.85
4	O	1708	BCL	O2D-CGD-CBD	2.98	115.52	111.22
4	K	1706	BCL	C4-C3-C5	2.98	119.92	115.37
4	A	1701	BCL	CAC-C3C-C2C	2.98	121.62	114.17
4	C	1702	BCL	C2A-C3A-C4A	2.99	104.90	101.84
4	R	1709	BCL	C4-C3-C5	2.99	119.93	115.37
4	K	1506	BCL	CAC-C3C-C2C	3.02	121.70	114.17
4	K	1506	BCL	C4-C3-C5	3.05	120.01	115.37
4	M	1707	BCL	O2A-CGA-CBA	3.06	121.27	111.85
4	K	1506	BCL	CAC-C3C-C4C	3.08	119.43	112.58
4	F	1603	BCL	C4-C3-C5	3.10	120.09	115.37
4	A	1701	BCL	C4-C3-C5	3.11	120.10	115.37
3	P	1408	RG1	CM3-C5-C4	3.12	120.12	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	1506	BCL	O2D-CGD-CBD	3.12	115.73	111.22
4	N	1607	BCL	C3C-C2C-C1C	3.14	105.06	101.84
4	E	1703	BCL	CMB-C2B-C3B	3.16	131.26	125.09
4	D	1602	BCL	CMD-C2D-C3D	3.21	131.36	125.09
4	O	1508	BCL	CGD-CBD-CHA	3.22	121.92	110.88
4	H	1604	BCL	CMD-C2D-C3D	3.22	131.39	125.09
4	J	1605	BCL	CMD-C2D-C3D	3.23	131.40	125.09
4	C	1702	BCL	CMD-C2D-C3D	3.23	131.40	125.09
4	G	1704	BCL	CMD-C2D-C3D	3.23	131.41	125.09
4	O	1508	BCL	OBD-CAD-CBD	3.26	130.86	125.94
4	M	1707	BCL	O2D-CGD-CBD	3.27	115.94	111.22
4	K	1506	BCL	CMD-C2D-C3D	3.28	131.50	125.09
4	M	1707	BCL	C4-C3-C5	3.29	120.38	115.37
3	S	1409	RG1	CM3-C5-C4	3.29	120.39	115.37
4	N	1607	BCL	CMD-C2D-C3D	3.33	131.59	125.09
4	O	1708	BCL	O2A-CGA-CBA	3.34	122.12	111.85
4	B	1601	BCL	CMD-C2D-C3D	3.37	131.68	125.09
4	H	1604	BCL	CMB-C2B-C3B	3.37	131.68	125.09
4	R	1709	BCL	O2A-CGA-CBA	3.39	122.27	111.85
4	L	1606	BCL	CMB-C2B-C3B	3.39	131.71	125.09
4	P	1608	BCL	CMD-C2D-C3D	3.40	131.73	125.09
4	S	1609	BCL	C14-C13-C12	3.40	123.79	111.10
4	E	1503	BCL	CMD-C2D-C3D	3.40	131.74	125.09
3	F	1403	RG1	CM3-C5-C4	3.40	120.56	115.37
4	F	1603	BCL	CMD-C2D-C3D	3.43	131.80	125.09
4	M	1507	BCL	CMD-C2D-C3D	3.48	131.90	125.09
3	S	1409	RG1	CM7-C22-C23	3.52	123.84	118.08
4	P	1608	BCL	C3C-C2C-C1C	3.54	105.47	101.84
4	A	1701	BCL	O2D-CGD-CBD	3.60	116.41	111.22
4	G	1504	BCL	O2D-CGD-CBD	3.60	116.41	111.22
4	S	1609	BCL	CMD-C2D-C3D	3.61	132.14	125.09
4	C	1702	BCL	O2D-CGD-CBD	3.62	116.44	111.22
4	E	1703	BCL	C4-C3-C5	3.69	121.00	115.37
4	P	1608	BCL	O2D-CGD-CBD	3.76	116.64	111.22
4	L	1606	BCL	CMD-C2D-C3D	3.78	132.49	125.09
3	H	1404	RG1	CM3-C5-C4	3.96	121.40	115.37
4	I	1705	BCL	C4-C3-C5	4.01	121.47	115.37
4	H	1604	BCL	CAC-C3C-C2C	4.19	124.63	114.17
4	R	1509	BCL	C2A-C3A-C4A	4.19	106.14	101.84
4	D	1602	BCL	O2D-CGD-CBD	4.21	117.30	111.22
4	G	1704	BCL	O2D-CGD-CBD	4.36	117.51	111.22
4	M	1507	BCL	O2D-CGD-CBD	4.39	117.56	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1503	BCL	O2D-CGD-CBD	4.56	117.79	111.22
4	I	1705	BCL	O2D-CGD-CBD	4.58	117.82	111.22
4	J	1605	BCL	O2D-CGD-CBD	4.59	117.84	111.22
4	F	1603	BCL	O2D-CGD-CBD	4.61	117.87	111.22
4	C	1502	BCL	O2D-CGD-CBD	4.78	118.12	111.22
4	H	1604	BCL	O2D-CGD-CBD	4.87	118.25	111.22
4	K	1706	BCL	O2D-CGD-CBD	4.88	118.26	111.22
4	O	1508	BCL	O2D-CGD-CBD	4.94	118.35	111.22
4	L	1606	BCL	O2D-CGD-CBD	4.96	118.37	111.22
4	B	1601	BCL	O2D-CGD-CBD	5.06	118.52	111.22
4	S	1609	BCL	O2D-CGD-CBD	5.19	118.70	111.22
4	N	1607	BCL	O2D-CGD-CBD	5.23	118.76	111.22
4	A	1501	BCL	O2D-CGD-CBD	5.49	119.14	111.22
4	L	1606	BCL	C3C-C2C-C1C	5.57	107.55	101.84
4	L	1606	BCL	C2A-C3A-C4A	5.62	107.60	101.84
4	H	1604	BCL	C3C-C2C-C1C	5.72	107.70	101.84
4	R	1709	BCL	O2D-CGD-CBD	6.14	120.08	111.22
4	R	1509	BCL	O2D-CGD-CBD	6.17	120.12	111.22

All (23) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1501	BCL	CBD
4	R	1709	BCL	C13
4	C	1502	BCL	C13
4	N	1607	BCL	C2C
4	R	1509	BCL	C3A
4	P	1608	BCL	C2C
4	P	1608	BCL	C8
4	K	1706	BCL	C8
4	M	1707	BCL	CBD
4	G	1704	BCL	CBD
4	O	1708	BCL	C8
4	L	1606	BCL	C2C
4	L	1606	BCL	C8
4	L	1606	BCL	C3A
4	A	1701	BCL	C3C
4	J	1605	BCL	CBD
4	O	1508	BCL	CBD
4	O	1508	BCL	C13
4	S	1609	BCL	C13
4	C	1702	BCL	C13

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Mol	Chain	Res	Type	Atom
4	B	1601	BCL	C8
4	K	1506	BCL	C3C
4	H	1604	BCL	C2C

There are no torsion outliers.

There are no ring outliers.

60 monomers are involved in 432 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1501	BCL	17	0
4	A	1701	BCL	8	0
5	A	1816	LDA	8	0
5	A	1817	LDA	3	0
4	B	1601	BCL	11	0
5	B	1801	LDA	2	0
4	C	1502	BCL	7	0
4	C	1702	BCL	8	0
5	C	1815	LDA	6	0
3	D	1402	RG1	5	0
4	D	1602	BCL	8	0
5	D	1802	LDA	3	0
4	E	1503	BCL	5	0
4	E	1703	BCL	7	0
5	E	1822	LDA	8	0
5	E	1823	LDA	6	0
3	F	1403	RG1	5	0
4	F	1603	BCL	12	0
5	F	1803	LDA	7	0
4	G	1504	BCL	6	0
4	G	1704	BCL	21	0
5	G	1814	LDA	3	0
5	G	1824	LDA	14	0
3	H	1404	RG1	5	0
4	H	1604	BCL	12	0
5	H	1804	LDA	3	0
4	I	1505	BCL	12	0
4	I	1705	BCL	21	0
5	I	1812	LDA	7	0
5	I	1813	LDA	2	0
5	I	1825	LDA	6	0
3	J	1405	RG1	1	0
4	J	1605	BCL	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	1805	LDA	1	0
4	K	1506	BCL	9	0
4	K	1706	BCL	5	0
5	K	1810	LDA	8	0
5	K	1826	LDA	4	0
3	L	1406	RG1	4	0
4	L	1606	BCL	25	0
5	L	1806	LDA	5	0
4	M	1507	BCL	7	0
4	M	1707	BCL	21	0
5	M	1811	LDA	4	0
5	M	1827	LDA	2	0
3	N	1407	RG1	4	0
4	N	1607	BCL	16	0
5	N	1807	LDA	2	0
4	O	1508	BCL	11	0
4	O	1708	BCL	10	0
5	O	1820	LDA	7	0
3	P	1408	RG1	4	0
4	P	1608	BCL	10	0
5	P	1808	LDA	3	0
3	R	1401	RG1	4	0
4	R	1509	BCL	7	0
4	R	1709	BCL	21	0
5	R	1818	LDA	12	0
3	S	1409	RG1	5	0
4	S	1609	BCL	13	0

## 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

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	A	52/53 (98%)	0.40	6 (11%) 6 6	35, 41, 88, 98	0
1	C	52/53 (98%)	0.95	7 (13%) 4 4	34, 41, 88, 102	0
1	E	52/53 (98%)	1.40	6 (11%) 6 6	35, 40, 88, 101	0
1	G	52/53 (98%)	0.74	6 (11%) 6 6	33, 40, 87, 99	0
1	I	52/53 (98%)	0.93	6 (11%) 6 6	34, 39, 88, 100	0
1	K	52/53 (98%)	0.65	6 (11%) 6 6	33, 40, 88, 100	0
1	M	52/53 (98%)	0.58	6 (11%) 6 6	35, 40, 88, 101	0
1	O	52/53 (98%)	0.88	6 (11%) 6 6	34, 41, 87, 100	0
1	R	52/53 (98%)	0.71	6 (11%) 6 6	35, 41, 87, 97	0
2	B	41/41 (100%)	-0.24	1 (2%) 62 65	42, 46, 54, 67	0
2	D	41/41 (100%)	-0.01	2 (4%) 33 36	41, 46, 55, 64	0
2	F	41/41 (100%)	-0.01	1 (2%) 62 65	38, 45, 52, 65	0
2	H	41/41 (100%)	-0.23	1 (2%) 62 65	37, 45, 52, 64	0
2	J	41/41 (100%)	-0.26	0 100 100	40, 45, 53, 65	0
2	L	41/41 (100%)	0.41	1 (2%) 62 65	39, 43, 52, 65	0
2	N	41/41 (100%)	0.19	3 (7%) 18 19	41, 45, 52, 69	0
2	P	41/41 (100%)	-0.04	1 (2%) 62 65	40, 46, 53, 68	0
2	S	41/41 (100%)	-0.36	1 (2%) 62 65	41, 46, 54, 67	0
All	All	837/846 (98%)	0.42	66 (7%) 15 16	33, 43, 79, 102	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	53	ALA	23.6
1	E	52	ALA	20.3
1	E	49	VAL	17.0

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Mol	Chain	Res	Type	RSRZ
1	M	49	VAL	16.6
1	C	52	ALA	16.1
1	I	52	ALA	14.5
1	R	52	ALA	14.3
1	C	49	VAL	13.2
1	I	49	VAL	12.3
1	G	49	VAL	11.9
1	E	51	LYS	11.8
1	A	49	VAL	11.7
1	K	53	ALA	11.4
1	K	49	VAL	11.3
1	R	49	VAL	11.3
1	G	53	ALA	10.5
1	K	52	ALA	9.8
1	O	53	ALA	9.8
1	O	49	VAL	9.6
1	I	53	ALA	9.6
1	E	50	LYS	9.5
1	M	52	ALA	9.5
1	O	52	ALA	9.5
1	G	52	ALA	9.4
1	I	51	LYS	9.1
1	A	52	ALA	9.0
1	M	51	LYS	9.0
1	E	53	ALA	9.0
1	R	53	ALA	8.7
1	A	51	LYS	8.6
1	I	50	LYS	8.5
1	A	53	ALA	8.3
1	O	51	LYS	8.0
1	R	51	LYS	6.8
1	K	51	LYS	6.7
1	M	50	LYS	6.6
1	M	53	ALA	6.6
1	E	48	GLY	6.4
1	A	50	LYS	5.8
1	R	50	LYS	5.5
1	K	50	LYS	5.3
1	O	50	LYS	5.1
1	G	51	LYS	5.0
1	C	51	LYS	5.0
1	C	50	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	R	48	GLY	4.0
1	O	48	GLY	3.7
1	I	48	GLY	3.7
1	G	50	LYS	3.3
2	L	26	ALA	3.2
2	N	41	HIS	3.2
2	D	41	HIS	3.1
2	D	6	GLU	3.1
1	G	48	GLY	3.0
2	H	41	HIS	3.0
1	K	48	GLY	2.9
2	B	31	PHE	2.7
2	P	41	HIS	2.6
1	C	39	THR	2.6
1	M	48	GLY	2.5
1	A	48	GLY	2.4
2	N	37	THR	2.3
2	F	7	GLN	2.3
2	S	41	HIS	2.2
2	N	34	PHE	2.2
1	C	48	GLY	2.1

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

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CXM	M	1	11/12	0.95	0.13	-	40,45,51,52	0
1	CXM	I	1	11/12	0.95	0.15	-	38,45,51,52	0
1	CXM	O	1	11/12	0.96	0.14	-	45,47,54,58	0
1	CXM	E	1	11/12	0.96	0.14	-	41,46,48,50	0
1	CXM	K	1	11/12	0.94	0.12	-	40,46,54,54	0
1	CXM	A	1	11/12	0.95	0.12	-	45,48,60,62	0
1	CXM	G	1	11/12	0.95	0.16	-	45,46,52,58	0
1	CXM	R	1	11/12	0.95	0.21	-	45,48,54,59	0
1	CXM	C	1	11/12	0.95	0.28	-	45,47,55,58	0

### 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	LDA	K	1810	16/16	0.57	0.55	26.23	107,110,116,116	0
5	LDA	I	1812	16/16	0.57	0.46	19.30	87,106,111,111	0
5	LDA	R	1818	16/16	0.58	0.41	18.90	85,90,95,96	0
5	LDA	E	1823	16/16	0.19	0.64	17.77	89,99,122,123	0
5	LDA	C	1821	16/16	0.62	0.34	16.34	82,90,101,103	0
5	LDA	R	1819	16/16	0.76	0.32	14.55	80,83,85,87	0
5	LDA	M	1811	16/16	0.60	0.36	13.14	75,77,84,84	0
5	LDA	C	1815	16/16	0.47	0.53	11.16	79,96,103,103	0
5	LDA	M	1827	16/16	0.48	0.40	9.76	96,101,105,107	0
5	LDA	A	1816	16/16	0.61	0.42	9.08	86,87,91,93	0
5	LDA	I	1825	16/16	0.65	0.39	8.98	95,101,108,108	0
5	LDA	G	1824	16/16	0.62	0.36	8.38	89,105,120,121	0
5	LDA	H	1804	16/16	0.85	0.26	7.85	49,57,66,67	0
5	LDA	P	1808	16/16	0.65	0.38	7.45	53,61,84,86	0
5	LDA	A	1817	16/16	0.82	0.21	5.81	67,69,87,87	0
5	LDA	O	1820	16/16	0.71	0.29	5.78	71,80,92,95	0
5	LDA	E	1822	16/16	0.58	0.33	5.43	69,91,107,108	0
5	LDA	G	1814	16/16	0.63	0.29	5.36	70,74,83,84	0
5	LDA	D	1802	16/16	0.71	0.33	4.83	53,57,75,77	0
5	LDA	B	1801	16/16	0.70	0.29	4.24	49,62,76,78	0
5	LDA	R	1809	16/16	0.71	0.26	4.11	57,63,71,73	0
5	LDA	F	1803	16/16	0.74	0.24	3.97	50,56,67,67	0
5	LDA	L	1806	16/16	0.71	0.29	3.25	44,52,74,75	0
4	BCL	R	1709	66/66	0.89	0.19	3.22	43,53,78,82	0
5	LDA	K	1826	16/16	0.80	0.24	2.93	83,88,103,104	0
5	LDA	N	1807	16/16	0.53	0.32	2.45	61,66,76,78	0
3	RG1	J	1405	52/52	0.82	0.24	1.85	28,37,76,80	0
3	RG1	F	1403	52/52	0.78	0.25	1.84	28,38,77,82	0
3	RG1	R	1401	52/52	0.88	0.22	1.82	30,40,74,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BCL	A	1701	66/66	0.91	0.17	1.80	42,49,80,83	0
3	RG1	P	1408	52/52	0.88	0.22	1.77	32,42,75,78	0
4	BCL	G	1704	66/66	0.90	0.20	1.55	32,45,73,76	0
4	BCL	C	1702	66/66	0.88	0.19	1.47	41,48,78,80	0
3	RG1	H	1404	52/52	0.89	0.21	1.46	27,37,78,80	0
5	LDA	J	1805	16/16	0.76	0.21	1.42	44,54,67,68	0
3	RG1	S	1409	52/52	0.85	0.20	1.40	29,40,77,78	0
3	RG1	N	1407	52/52	0.85	0.20	1.32	29,37,69,73	0
4	BCL	A	1501	66/66	0.92	0.17	1.30	33,42,51,65	0
5	LDA	I	1813	16/16	0.76	0.19	1.23	50,54,76,76	0
3	RG1	D	1402	52/52	0.84	0.18	1.01	30,44,77,81	0
4	BCL	B	1601	66/66	0.95	0.15	0.97	33,42,67,68	0
4	BCL	O	1708	66/66	0.92	0.16	0.76	42,50,79,81	0
4	BCL	P	1608	66/66	0.94	0.16	0.75	34,42,66,68	0
4	BCL	R	1509	66/66	0.94	0.17	0.74	31,38,49,57	0
4	BCL	M	1707	66/66	0.92	0.17	0.61	29,44,74,76	0
4	BCL	S	1609	66/66	0.93	0.15	0.56	31,41,69,72	0
4	BCL	F	1603	66/66	0.94	0.17	0.55	26,35,62,64	0
4	BCL	I	1705	66/66	0.93	0.17	0.47	34,41,73,75	0
4	BCL	H	1604	66/66	0.94	0.14	0.43	29,39,63,64	0
4	BCL	J	1605	66/66	0.90	0.16	0.35	31,39,64,66	0
3	RG1	L	1406	52/52	0.91	0.17	0.33	26,35,74,77	0
4	BCL	I	1505	66/66	0.94	0.15	0.12	28,36,42,48	0
4	BCL	N	1607	66/66	0.90	0.15	0.09	31,41,63,65	0
4	BCL	K	1506	66/66	0.94	0.17	0.08	28,35,47,51	0
4	BCL	D	1602	66/66	0.95	0.13	0.06	30,37,64,67	0
4	BCL	E	1703	66/66	0.93	0.16	0.01	29,37,69,72	0
4	BCL	G	1504	66/66	0.95	0.15	-0.03	26,34,44,49	0
4	BCL	L	1606	66/66	0.94	0.15	-0.15	27,36,66,69	0
4	BCL	O	1508	66/66	0.93	0.14	-0.20	30,37,46,54	0
4	BCL	C	1502	66/66	0.96	0.12	-0.22	33,38,50,57	0
4	BCL	K	1706	66/66	0.94	0.15	-0.45	27,36,78,82	0
4	BCL	M	1507	66/66	0.96	0.12	-0.49	27,35,41,48	0
4	BCL	E	1503	66/66	0.97	0.11	-0.68	28,35,46,49	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.