



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:57 am GMT

PDB ID : 1PYH
Title : Crystal structure of RC-LH1 core complex from Rhodopseudomonas palustris
Authors : Roszak, A.W.; Howard, T.D.; Southall, J.; Gardiner, A.T.; Law, C.J.; Isaacs, N.W.; Cogdell, R.J.
Deposited on : 2003-07-08
Resolution : 4.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

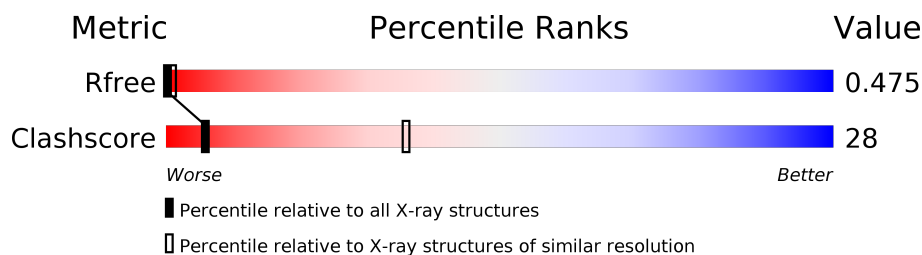
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

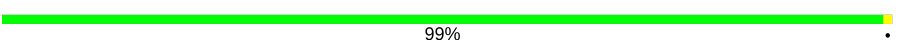


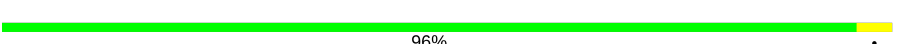

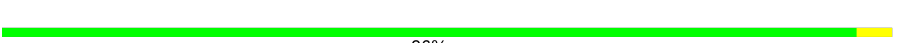

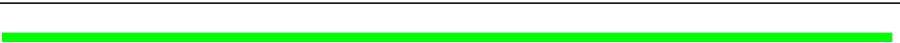

The reported resolution of this entry is 4.80 Å.

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.



















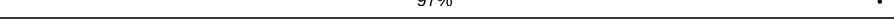
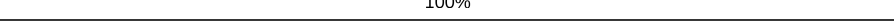
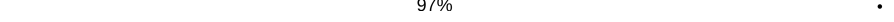
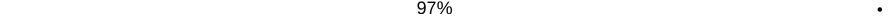
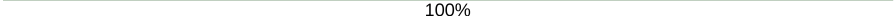

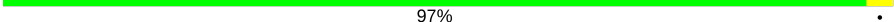
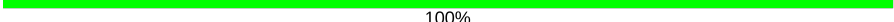

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	100719	1019 (5.94-3.66)
Clashscore	112137	1067 (5.90-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	281	 99% .
2	B	302	 99% .
3	C	241	 96% .
4	1	26	 96% .
4	3	26	 96% .
4	5	26	 96% .
4	7	26	 96% .
4	D	26	 100%
4	F	26	 92% 8%

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Mol	Chain	Length	Quality of chain
4	H	26	 100%
4	J	26	 88% 12%
4	L	26	 92% 8%
4	N	26	 100%
4	P	26	 100%
4	R	26	 96% .
4	T	26	 96% .
4	V	26	 85% 15%
4	X	26	 100%
4	Z	26	 92% 8%
5	2	30	 100%
5	4	30	 100%
5	6	30	 100%
5	8	30	 100%
5	E	30	 87% 13%
5	G	30	 97% .
5	I	30	 100%
5	K	30	 97% .
5	M	30	 97% .
5	O	30	 100%
5	Q	30	 97% .
5	S	30	 97% .
5	U	30	 100%
5	W	30	 97% .
5	Y	30	 93% 7%

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
7	BCL	J	8	-	-	X	-
7	BCL	L	10	-	-	X	-
7	BCL	N	38	-	-	X	-
7	BCL	P	38	-	-	X	-
7	BCL	P	39	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10100 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	0	0	0
			1373	811	281	281			

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	302	Total	C	N	O	0	0	0
			1474	870	302	302			

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	0	0	0
			1182	700	241	241			

- Molecule 4 is a protein called Light-harvesting protein B-800/850, alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	F	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	H	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	J	26	Total	C	N	O	0	0	0
			127	75	26	26			
4	L	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	N	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	P	26	Total	C	N	O	0	0	0
			128	76	26	26			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	R	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	T	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	V	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	X	26	Total	C	N	O	0	0	0
			127	75	26	26			
4	Z	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	1	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	3	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	5	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	7	26	Total	C	N	O	0	0	0
			128	76	26	26			

- Molecule 5 is a protein called Light-harvesting protein B-800/850, beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	G	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	I	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	K	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	M	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	O	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	Q	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	S	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	U	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	W	30	Total	C	N	O	0	0	0
			148	88	30	30			

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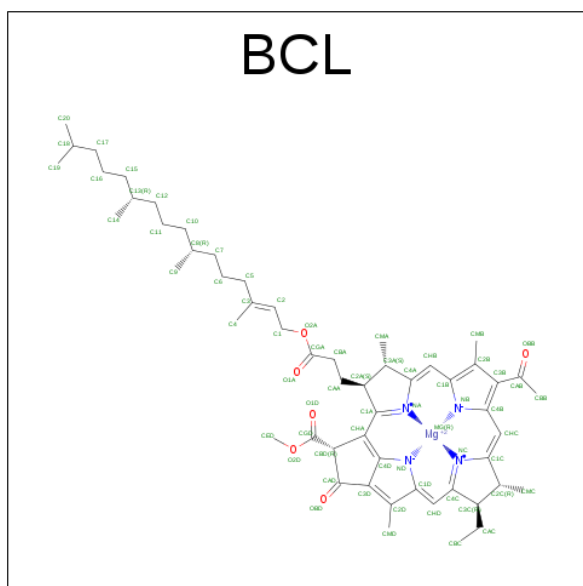
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Y	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	2	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	4	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	6	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	8	30	Total	C	N	O	0	0	0
			148	88	30	30			

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

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

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	0
7	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	0
7	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	0

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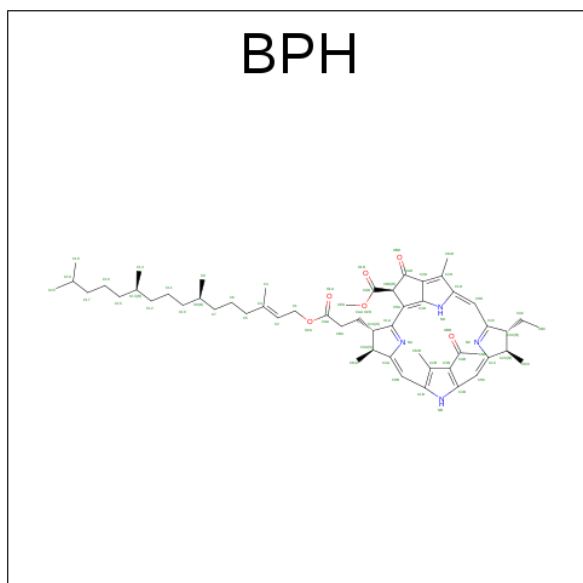
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	E	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	D	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	G	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	F	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	I	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	H	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	K	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	J	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	N	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	N	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	P	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	P	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	S	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	R	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	U	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	T	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	V	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	W	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	Y	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	Y	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	2	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	6	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	5	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	8	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	7	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			65	55	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			65	55	4	6		

3 Residue-property plots

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

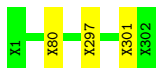
- Molecule 1: Reaction center protein L chain

Chain A:  99%



- Molecule 2: Reaction center protein M chain

Chain B:  99%



- Molecule 3: Reaction center protein H chain

Chain C:  96%



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain F:  92% 8%




- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain J:  88% 12%



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain L:  92% 8%



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain N:  100%

There are no outlier residues recorded for this chain.

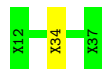
- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain R:  96% .



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain T:  96% .



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain V:  85% 15%



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain Z:  92% 8%



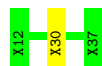
- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain 1:  96% .



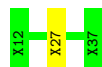
- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain 3:  96% .



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain 5:  96% .




- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain 7:  96% .



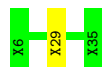
- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain E:  87% 13%



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain G:  97% .



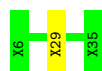
- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain K:  97%



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain M:  97%



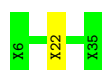
- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain O:  100%

There are no outlier residues recorded for this chain.

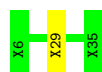
- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain Q:  97%



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain S:  97%



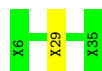
- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain W:  97%



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain Y:  93% 7%



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain 2:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain 4:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain 6:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain 8:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.04Å 119.02Å 130.43Å 69.32° 72.69° 66.52°	Depositor
Resolution (Å)	60.00 – 4.80 59.99 – 4.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (60.00-4.80) 88.6 (59.99-4.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 4.86Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, R_{free}	0.467 , 0.491 0.453 , 0.475	Depositor DCC
R_{free} test set	944 reflections (5.43%)	DCC
Wilson B-factor (Å ²)	202.7	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.03 , 289.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, BPH, FE

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1373	0	257	10	0
2	B	1474	0	274	2	0
3	C	1182	0	230	13	0
4	1	128	0	26	2	0
4	3	128	0	26	1	0
4	5	128	0	26	1	0
4	7	128	0	26	2	0
4	D	128	0	26	0	0
4	F	128	0	26	7	0
4	H	128	0	26	0	0
4	J	127	0	25	7	0
4	L	128	0	26	3	0
4	N	128	0	26	0	0
4	P	128	0	26	0	0
4	R	128	0	26	1	0
4	T	128	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	V	128	0	26	5	0
4	X	127	0	25	0	0
4	Z	128	0	26	4	0
5	2	148	0	30	0	0
5	4	148	0	30	0	0
5	6	148	0	30	0	0
5	8	148	0	30	0	0
5	E	148	0	30	11	0
5	G	148	0	30	3	0
5	I	148	0	30	0	0
5	K	148	0	30	4	0
5	M	148	0	30	1	0
5	O	148	0	30	0	0
5	Q	148	0	30	5	0
5	S	148	0	30	1	0
5	U	148	0	30	0	0
5	W	148	0	30	2	0
5	Y	148	0	30	4	0
6	B	1	0	0	0	0
7	1	47	0	34	18	0
7	2	47	0	34	10	0
7	3	94	0	68	15	0
7	5	47	0	33	12	0
7	6	47	0	34	3	0
7	7	47	0	34	8	0
7	8	47	0	34	5	0
7	A	132	0	148	9	0
7	B	132	0	148	6	0
7	D	47	0	34	14	0
7	E	47	0	34	14	0
7	F	47	0	34	7	0
7	G	47	0	34	11	0
7	H	47	0	33	11	0
7	I	47	0	34	6	0
7	J	47	0	33	32	0
7	K	47	0	34	18	0
7	L	47	0	34	25	0
7	M	47	0	34	13	0
7	N	94	0	68	39	0
7	P	94	0	68	51	0
7	R	47	0	34	16	0
7	S	47	0	34	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	T	47	0	34	10	0
7	U	47	0	34	8	0
7	V	47	0	34	8	0
7	W	47	0	34	6	0
7	Y	94	0	68	23	0
8	A	65	0	76	5	0
8	B	65	0	76	0	0
All	All	10100	0	3090	367	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 28.

All (367) 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)
7:N:38:BCL:HMC3	7:P:38:BCL:CBB	1.44	1.47
7:H:6:BCL:C1	7:H:6:BCL:O2A	1.63	1.46
7:R:38:BCL:O2A	7:R:38:BCL:C1	1.63	1.42
7:P:38:BCL:CBC	7:P:39:BCL:HMD2	1.56	1.33
7:L:10:BCL:CMB	7:N:11:BCL:HMA1	1.64	1.26
7:N:38:BCL:CMC	7:P:38:BCL:HBB2	1.63	1.25
5:G:29:UNK:CB	7:G:3:BCL:HMD3	1.67	1.22
1:A:271:UNK:HA	4:V:37:UNK:CB	1.68	1.21
7:T:38:BCL:CBB	7:T:38:BCL:HHC	1.71	1.18
7:R:38:BCL:CBB	7:R:38:BCL:HHC	1.70	1.18
7:N:11:BCL:HBC1	7:N:38:BCL:HAC2	1.26	1.18
7:L:10:BCL:HMB3	7:N:11:BCL:CMA	1.74	1.17
7:3:39:BCL:CBB	7:3:39:BCL:HHC	1.70	1.17
7:P:39:BCL:CBB	7:P:39:BCL:HHC	1.70	1.17
7:5:38:BCL:CBB	7:5:38:BCL:HHC	1.70	1.16
7:D:2:BCL:HHC	7:D:2:BCL:CBB	1.71	1.16
7:J:8:BCL:HMA1	7:M:36:BCL:HMA1	1.27	1.14
7:P:38:BCL:HBC2	7:P:39:BCL:CMD	1.76	1.14
7:L:10:BCL:HED3	7:L:10:BCL:H2A	1.27	1.14
7:Y:37:BCL:HHC	7:Y:37:BCL:CBB	1.71	1.13
7:F:4:BCL:CBB	7:F:4:BCL:HHC	1.71	1.13
7:W:36:BCL:HHC	7:W:36:BCL:CBB	1.71	1.12
7:R:38:BCL:HBB2	7:R:38:BCL:HHC	1.13	1.12
7:D:2:BCL:HHC	7:D:2:BCL:HBB2	1.14	1.12
7:T:38:BCL:HBB2	7:T:38:BCL:HHC	1.14	1.12
7:L:10:BCL:HBB2	7:L:10:BCL:HHC	1.13	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:8:BCL:CBB	7:J:8:BCL:HHC	1.70	1.11
1:A:254:UNK:HA	4:Z:37:UNK:CB	1.79	1.11
7:P:38:BCL:CBC	7:P:39:BCL:CMD	2.28	1.11
7:7:38:BCL:HBB2	7:7:38:BCL:HHC	1.14	1.11
7:7:38:BCL:HHC	7:7:38:BCL:CBB	1.71	1.11
7:L:10:BCL:CBB	7:L:10:BCL:HHC	1.70	1.11
7:1:38:BCL:HHC	7:1:38:BCL:CBB	1.70	1.11
7:J:8:BCL:CED	7:J:8:BCL:C1	2.28	1.10
7:N:38:BCL:CBB	7:N:38:BCL:HHC	1.71	1.10
7:F:4:BCL:HBB2	7:F:4:BCL:HHC	1.14	1.10
7:N:38:BCL:HMA1	7:P:38:BCL:HMA1	1.32	1.09
7:W:36:BCL:HBB2	7:W:36:BCL:HHC	1.13	1.09
7:1:38:BCL:HBB2	7:1:38:BCL:HHC	1.12	1.09
7:P:39:BCL:HBB2	7:P:39:BCL:HHC	1.14	1.09
7:J:8:BCL:HBB2	7:J:8:BCL:HHC	1.13	1.09
7:H:6:BCL:HHC	7:H:6:BCL:HBB2	1.14	1.08
7:Y:36:BCL:CED	7:Y:36:BCL:HBA1	1.81	1.08
7:5:38:BCL:HHC	7:5:38:BCL:HBB2	1.13	1.08
7:3:39:BCL:HHC	7:3:39:BCL:HBB2	1.12	1.08
7:H:6:BCL:HHC	7:H:6:BCL:CBB	1.71	1.08
7:J:8:BCL:CBC	7:K:36:BCL:CBC	2.31	1.07
7:Y:37:BCL:HBB2	7:Y:37:BCL:HHC	1.14	1.07
7:N:38:BCL:HBB2	7:N:38:BCL:HHC	1.13	1.07
7:H:6:BCL:CHC	7:H:6:BCL:HBB2	1.86	1.06
7:T:38:BCL:HBB2	7:T:38:BCL:CHC	1.85	1.06
7:1:38:BCL:HBB2	7:1:38:BCL:CHC	1.84	1.05
7:5:38:BCL:CHC	7:5:38:BCL:HBB2	1.84	1.05
7:7:38:BCL:HBB2	7:7:38:BCL:CHC	1.85	1.05
7:W:36:BCL:CHC	7:W:36:BCL:HBB2	1.85	1.05
7:R:38:BCL:CHC	7:R:38:BCL:HBB2	1.85	1.05
7:L:10:BCL:CHC	7:L:10:BCL:HBB2	1.85	1.05
7:J:8:BCL:HBB2	7:J:8:BCL:CHC	1.85	1.05
7:D:2:BCL:CHC	7:D:2:BCL:HBB2	1.86	1.05
7:Y:37:BCL:CHC	7:Y:37:BCL:HBB2	1.85	1.05
7:3:39:BCL:CHC	7:3:39:BCL:HBB2	1.84	1.05
7:F:4:BCL:HBB2	7:F:4:BCL:CHC	1.86	1.05
7:J:8:BCL:HBC2	7:K:36:BCL:HBC2	1.36	1.04
7:P:39:BCL:CHC	7:P:39:BCL:HBB2	1.85	1.04
7:J:8:BCL:HMA1	7:M:36:BCL:CMA	1.87	1.04
7:P:38:BCL:HBC1	7:P:39:BCL:HHH	1.36	1.04
7:N:38:BCL:HMB3	7:P:38:BCL:HMA3	1.39	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:8:BCL:HBC1	7:K:36:BCL:CBC	1.84	1.04
7:N:38:BCL:HBB2	7:N:38:BCL:CHC	1.85	1.03
7:L:10:BCL:CMB	7:N:11:BCL:CMA	2.33	1.03
7:J:8:BCL:C1	7:J:8:BCL:HED1	1.87	1.03
7:Y:36:BCL:HED2	7:Y:36:BCL:HBA1	1.38	1.02
7:P:38:BCL:HBC2	7:P:39:BCL:HMD2	1.04	1.02
7:L:10:BCL:HMB3	7:N:11:BCL:HMA1	1.04	1.01
5:G:29:UNK:CB	7:G:3:BCL:CMD	2.39	1.00
8:A:401:BPH:H171	8:A:401:BPH:H141	1.44	0.99
7:R:38:BCL:O1A	7:R:38:BCL:H3A	1.62	0.98
7:R:38:BCL:C1	7:R:38:BCL:CGA	2.41	0.98
7:L:10:BCL:CHD	7:M:36:BCL:HMD2	1.94	0.98
7:H:6:BCL:C1	7:H:6:BCL:CGA	2.41	0.97
7:P:38:BCL:CBC	7:P:39:BCL:HHH	1.96	0.96
7:6:36:BCL:HBB3	7:6:36:BCL:HHC	1.47	0.96
7:3:38:BCL:HBB3	7:3:38:BCL:HHC	1.48	0.95
7:Y:36:BCL:HED2	7:Y:36:BCL:CBA	1.94	0.95
7:3:39:BCL:CBB	7:3:39:BCL:CHC	2.42	0.95
7:7:38:BCL:CHC	7:7:38:BCL:CBB	2.43	0.95
7:D:2:BCL:HMC3	7:G:3:BCL:HBB2	1.47	0.95
7:2:36:BCL:HHC	7:2:36:BCL:HBB3	1.49	0.94
7:V:38:BCL:HBB3	7:V:38:BCL:HHC	1.50	0.94
7:8:36:BCL:HBB3	7:8:36:BCL:HHC	1.48	0.94
7:K:36:BCL:HBB3	7:K:36:BCL:HHC	1.48	0.93
7:U:36:BCL:HHC	7:U:36:BCL:HBB3	1.49	0.93
7:N:11:BCL:HHC	7:N:11:BCL:HBB3	1.48	0.93
7:I:5:BCL:HHC	7:I:5:BCL:HBB3	1.49	0.92
7:E:1:BCL:HHC	7:E:1:BCL:HBB3	1.49	0.92
7:G:3:BCL:HBB3	7:G:3:BCL:HHC	1.50	0.92
7:J:8:BCL:CMA	7:M:36:BCL:HMA1	1.98	0.92
5:E:26:UNK:N	7:E:1:BCL:HED2	1.84	0.92
7:Y:37:BCL:CHC	7:Y:37:BCL:CBB	2.43	0.92
7:M:36:BCL:HBB3	7:M:36:BCL:HHC	1.48	0.92
7:P:38:BCL:HED2	5:Q:22:UNK:HA	1.51	0.92
7:R:38:BCL:CHC	7:R:38:BCL:CBB	2.43	0.91
3:C:52:UNK:HA	4:F:13:UNK:CB	2.00	0.91
7:U:36:BCL:CGD	7:U:36:BCL:HBA1	2.00	0.91
7:Y:36:BCL:HBB3	7:Y:36:BCL:HHC	1.50	0.91
7:N:38:BCL:HMA1	7:P:38:BCL:CMA	2.00	0.91
7:S:36:BCL:HHC	7:S:36:BCL:HBB3	1.49	0.91
7:P:38:BCL:HBC3	7:P:39:BCL:HMD2	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:2:BCL:CHC	7:D:2:BCL:CBB	2.44	0.89
7:P:38:BCL:HBB3	7:P:38:BCL:HHC	1.50	0.89
7:N:38:BCL:HMC3	7:P:38:BCL:HBB1	1.53	0.88
7:J:8:BCL:CBC	7:K:36:BCL:HBC2	1.99	0.88
7:T:38:BCL:CBB	7:T:38:BCL:CHC	2.43	0.88
5:E:22:UNK:O	7:E:1:BCL:HED1	1.73	0.87
7:Y:36:BCL:O2D	7:Y:36:BCL:HBA1	1.74	0.87
1:A:51:UNK:CB	4:7:36:UNK:CB	2.54	0.86
7:J:8:BCL:HBC1	7:K:36:BCL:CAC	2.05	0.85
7:N:38:BCL:CMA	7:P:38:BCL:HMA1	2.06	0.85
5:E:22:UNK:O	7:E:1:BCL:CED	2.25	0.85
3:C:51:UNK:O	4:F:13:UNK:CB	2.25	0.85
1:A:271:UNK:CA	4:V:37:UNK:CB	2.54	0.84
7:J:8:BCL:CBC	7:K:36:BCL:HBC1	2.07	0.84
7:P:38:BCL:HAC2	7:P:39:BCL:HBC2	1.59	0.83
7:1:38:BCL:CBB	7:1:38:BCL:CHC	2.42	0.83
3:C:10:UNK:O	4:J:36:UNK:CB	2.26	0.82
7:N:38:BCL:HMC3	7:P:38:BCL:HBB2	0.83	0.82
7:U:36:BCL:O2D	7:U:36:BCL:HBA1	1.78	0.82
7:J:8:BCL:HBC1	7:K:36:BCL:HAC2	1.59	0.81
7:N:38:BCL:CMC	7:P:38:BCL:CBB	2.40	0.81
7:N:38:BCL:CBB	7:N:38:BCL:CHC	2.43	0.81
7:J:8:BCL:HBC1	7:K:36:BCL:HBC1	1.60	0.81
7:Y:36:BCL:CGD	7:Y:36:BCL:HBA1	2.10	0.80
7:1:38:BCL:HMC3	7:3:38:BCL:HBB1	1.62	0.80
7:W:36:BCL:CHC	7:W:36:BCL:CBB	2.43	0.79
7:H:6:BCL:CBB	7:H:6:BCL:CHC	2.43	0.78
7:P:39:BCL:HBB3	7:P:39:BCL:HHC	1.66	0.77
7:P:38:BCL:HHC	7:P:38:BCL:CBB	2.11	0.77
7:1:38:BCL:HBB3	7:1:38:BCL:HHC	1.67	0.77
7:I:5:BCL:HBA2	7:I:5:BCL:CGD	2.15	0.76
7:W:36:BCL:HBB3	7:W:36:BCL:HHC	1.68	0.76
3:C:51:UNK:C	4:F:13:UNK:CB	2.63	0.76
7:L:10:BCL:CHC	7:L:10:BCL:CBB	2.43	0.76
7:5:38:BCL:CBB	7:5:38:BCL:CHC	2.42	0.76
7:L:10:BCL:HMB1	7:N:11:BCL:CMA	2.15	0.75
5:Y:29:UNK:CB	7:Y:36:BCL:CMD	2.64	0.75
7:3:39:BCL:HHC	7:3:39:BCL:HBB3	1.66	0.75
7:L:10:BCL:HHC	7:L:10:BCL:HBB3	1.67	0.75
4:J:27:UNK:CB	7:J:8:BCL:OBD	2.35	0.75
7:J:8:BCL:HBB3	7:J:8:BCL:HHC	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:10:BCL:HMB1	7:N:11:BCL:HMA1	1.68	0.75
7:Y:37:BCL:HBB3	7:Y:37:BCL:HHC	1.68	0.75
7:H:6:BCL:HHC	7:H:6:BCL:HBB3	1.67	0.74
7:T:38:BCL:HBB3	7:T:38:BCL:HHC	1.67	0.74
7:R:38:BCL:HHC	7:R:38:BCL:HBB3	1.67	0.74
7:D:2:BCL:HHC	7:D:2:BCL:HBB3	1.68	0.74
3:C:52:UNK:CA	4:F:13:UNK:CB	2.66	0.73
7:7:38:BCL:HBB3	7:7:38:BCL:HHC	1.67	0.73
7:Y:36:BCL:HED2	7:Y:36:BCL:CGA	2.18	0.73
4:L:23:UNK:CB	7:L:10:BCL:HED2	2.19	0.72
7:L:10:BCL:HED3	7:L:10:BCL:C2A	2.15	0.71
7:5:38:BCL:HHC	7:5:38:BCL:HBB3	1.66	0.71
5:Y:29:UNK:CB	7:Y:36:BCL:HMD3	2.20	0.71
7:F:4:BCL:HBB3	7:F:4:BCL:HHC	1.68	0.71
7:P:39:BCL:CHC	7:P:39:BCL:CBB	2.43	0.70
7:I:5:BCL:HBA2	7:I:5:BCL:O2D	1.91	0.70
7:J:8:BCL:CBB	7:J:8:BCL:CHC	2.43	0.70
7:N:38:BCL:HHC	7:N:38:BCL:HBB3	1.67	0.70
7:R:38:BCL:CGA	7:R:38:BCL:H3A	2.17	0.70
7:R:38:BCL:HBC2	7:S:36:BCL:HBC1	1.74	0.70
7:P:39:BCL:O2D	7:P:39:BCL:HBA2	1.92	0.70
7:R:38:BCL:O1A	7:R:38:BCL:C3A	2.37	0.70
7:N:38:BCL:CMB	7:P:38:BCL:HMA3	2.20	0.69
7:P:38:BCL:HED1	5:Q:22:UNK:CB	2.23	0.68
1:A:254:UNK:CB	4:Z:36:UNK:CB	2.71	0.68
7:U:36:BCL:CGD	7:U:36:BCL:CBA	2.71	0.68
7:5:38:BCL:C3A	7:5:38:BCL:O1A	2.42	0.68
7:P:38:BCL:HBC3	7:P:39:BCL:CMD	2.14	0.67
8:A:401:BPH:C17	8:A:401:BPH:H141	2.20	0.67
2:B:297:UNK:O	2:B:301:UNK:N	2.27	0.67
7:5:38:BCL:HMA2	7:5:38:BCL:O1A	1.95	0.67
3:C:54:UNK:O	4:F:14:UNK:CB	2.43	0.67
7:P:38:BCL:HAC2	7:P:39:BCL:CBC	2.25	0.67
7:M:36:BCL:HHC	7:M:36:BCL:CBB	2.24	0.66
7:T:38:BCL:C1	7:T:38:BCL:HMA2	2.25	0.66
3:C:54:UNK:C	4:F:14:UNK:CB	2.73	0.66
7:F:4:BCL:CBB	7:F:4:BCL:CHC	2.44	0.66
7:J:8:BCL:HBC2	7:K:36:BCL:CBC	2.04	0.66
7:E:1:BCL:CBB	7:E:1:BCL:HHC	2.24	0.66
7:U:36:BCL:CBD	7:U:36:BCL:HBA1	2.26	0.66
7:8:36:BCL:CBB	7:8:36:BCL:HHC	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:25:UNK:CB	7:E:1:BCL:HED2	2.25	0.65
7:N:11:BCL:HBC1	7:N:38:BCL:CAC	2.17	0.65
4:1:23:UNK:CB	7:1:38:BCL:CED	2.74	0.65
7:G:3:BCL:HHC	7:G:3:BCL:CBB	2.25	0.65
7:J:8:BCL:O2D	7:J:8:BCL:C1	2.44	0.65
7:1:38:BCL:CMD	7:2:36:BCL:HBC2	2.27	0.64
3:C:10:UNK:O	4:J:36:UNK:CA	2.46	0.64
7:P:38:BCL:HBC2	7:P:39:BCL:C2D	2.25	0.64
7:P:38:BCL:CBC	7:P:39:BCL:CHD	2.75	0.64
7:P:38:BCL:CAC	7:P:39:BCL:HBC2	2.26	0.64
7:2:36:BCL:CBB	7:2:36:BCL:HHC	2.24	0.63
3:C:10:UNK:O	4:J:36:UNK:HA	1.97	0.63
7:U:36:BCL:HBD	7:U:36:BCL:HBA1	1.79	0.63
7:Y:36:BCL:HHC	7:Y:36:BCL:CBB	2.25	0.63
7:D:2:BCL:HMA3	7:G:3:BCL:CMA	2.29	0.63
7:D:2:BCL:HBA2	7:D:2:BCL:O2D	2.00	0.62
7:N:38:BCL:HMB3	7:P:38:BCL:CMA	2.22	0.62
7:S:36:BCL:CBB	7:S:36:BCL:HHC	2.23	0.62
4:R:34:UNK:CB	7:R:38:BCL:HMD3	2.30	0.62
7:1:38:BCL:HMC3	7:3:38:BCL:CBB	2.30	0.62
5:Y:29:UNK:CB	7:Y:36:BCL:HMD1	2.29	0.61
7:V:38:BCL:CBB	7:V:38:BCL:HHC	2.25	0.61
7:5:38:BCL:H3A	7:5:38:BCL:O1A	1.99	0.61
7:Y:36:BCL:CED	7:Y:36:BCL:CBA	2.60	0.61
5:E:22:UNK:O	7:E:1:BCL:HED2	2.00	0.61
7:P:38:BCL:CED	5:Q:22:UNK:CB	2.79	0.61
7:3:38:BCL:HHC	7:3:38:BCL:CBB	2.23	0.60
5:E:25:UNK:CB	7:E:1:BCL:CED	2.78	0.60
7:R:38:BCL:O1A	7:R:38:BCL:C1	2.48	0.60
7:N:38:BCL:CHB	7:P:38:BCL:HMA1	2.31	0.60
7:1:38:BCL:HMD2	7:2:36:BCL:CHD	2.32	0.60
7:H:6:BCL:O1A	7:H:6:BCL:C1	2.49	0.60
5:K:29:UNK:CB	7:K:36:BCL:C2D	2.80	0.60
7:P:39:BCL:CGD	7:P:39:BCL:HBA2	2.32	0.59
7:Y:36:BCL:CGA	7:Y:36:BCL:CED	2.78	0.59
7:1:38:BCL:C1D	7:2:36:BCL:HMD2	2.32	0.59
7:K:36:BCL:HHC	7:K:36:BCL:CBB	2.23	0.59
7:B:303:BCL:HMB1	7:B:303:BCL:CBB	2.33	0.59
8:A:401:BPH:H142	8:A:401:BPH:H7C2	1.85	0.59
1:A:254:UNK:CA	4:Z:37:UNK:CB	2.69	0.59
5:E:29:UNK:CB	7:E:1:BCL:C3D	2.80	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:301:BCL:H102	7:B:303:BCL:H171	1.85	0.58
7:N:11:BCL:CBB	7:N:11:BCL:HHC	2.23	0.58
7:1:38:BCL:CHC	7:3:38:BCL:HBB2	2.34	0.58
7:B:304:BCL:HMB1	7:B:304:BCL:HBB2	1.85	0.58
7:I:5:BCL:CBB	7:I:5:BCL:HHC	2.24	0.58
7:U:36:BCL:O2D	7:U:36:BCL:CBA	2.50	0.58
7:1:38:BCL:HMB3	7:3:38:BCL:CHB	2.34	0.58
7:U:36:BCL:CBB	7:U:36:BCL:HHC	2.24	0.58
7:P:38:BCL:HED2	5:Q:22:UNK:CA	2.31	0.57
7:J:8:BCL:C1	7:J:8:BCL:HED3	2.31	0.57
7:5:38:BCL:CMA	7:5:38:BCL:O1A	2.53	0.57
8:A:401:BPH:HHH	8:A:401:BPH:HBC3	1.85	0.57
7:D:2:BCL:HMA3	7:G:3:BCL:HMA1	1.85	0.57
7:P:38:BCL:CBC	7:P:39:BCL:HMD3	2.31	0.57
7:L:10:BCL:HMD2	7:M:36:BCL:C1D	2.35	0.56
7:7:38:BCL:H2A	7:7:38:BCL:O1A	2.05	0.56
7:R:38:BCL:HBC2	7:S:36:BCL:CBC	2.35	0.56
7:Y:37:BCL:HMA2	7:Y:37:BCL:O1A	2.05	0.56
5:E:26:UNK:HA	7:E:1:BCL:OBD	2.06	0.56
4:L:23:UNK:CB	7:L:10:BCL:CED	2.84	0.56
7:N:11:BCL:O2D	7:N:11:BCL:HBA1	2.05	0.56
7:8:36:BCL:HAA2	7:8:36:BCL:HBD	1.88	0.55
7:N:38:BCL:HHB	7:P:38:BCL:HMA1	1.89	0.55
4:J:23:UNK:CB	7:J:8:BCL:HED1	2.36	0.55
7:P:39:BCL:CMA	7:S:36:BCL:HMA1	2.38	0.54
7:2:36:BCL:HBD	7:2:36:BCL:HAA2	1.90	0.54
7:5:38:BCL:H3A	7:5:38:BCL:CGA	2.38	0.54
4:J:23:UNK:CB	7:J:8:BCL:CED	2.85	0.54
7:6:36:BCL:CBB	7:6:36:BCL:HHC	2.23	0.54
5:E:25:UNK:C	7:E:1:BCL:HED2	2.37	0.54
7:P:39:BCL:HMA1	7:S:36:BCL:HMA1	1.89	0.53
3:C:249:UNK:O	3:C:250:UNK:C	2.55	0.53
7:Y:36:BCL:HBD	7:Y:37:BCL:OBD	2.08	0.53
7:T:38:BCL:HMA3	7:V:38:BCL:HMA3	1.91	0.53
7:A:301:BCL:C4	7:A:301:BCL:C7	2.84	0.53
2:B:80:UNK:O	4:T:36:UNK:O	2.27	0.53
4:1:23:UNK:O	7:1:38:BCL:HED2	2.09	0.52
5:E:26:UNK:HA	7:E:1:BCL:CGD	2.38	0.52
7:J:8:BCL:HMA1	7:M:36:BCL:HMA2	1.86	0.52
7:P:38:BCL:HBC2	7:P:39:BCL:HHH	1.89	0.52
7:A:302:BCL:HBB3	7:A:302:BCL:HMB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:10:BCL:C4C	7:M:36:BCL:HMD2	2.40	0.52
7:Y:36:BCL:HAA2	7:Y:37:BCL:OBD	2.10	0.51
7:J:8:BCL:HBB2	7:M:36:BCL:HBB2	1.92	0.51
7:P:38:BCL:HBC2	7:P:39:BCL:CHD	2.38	0.51
7:1:38:BCL:HMD2	7:2:36:BCL:HBC2	1.92	0.51
7:1:38:BCL:HMD3	7:2:36:BCL:HBC2	1.92	0.50
7:R:38:BCL:CBC	7:S:36:BCL:HBC1	2.41	0.50
7:B:303:BCL:HBB3	7:B:303:BCL:HMB1	1.94	0.50
7:S:36:BCL:HBD	7:S:36:BCL:HAA2	1.93	0.50
5:G:29:UNK:CB	7:G:3:BCL:HMD1	2.40	0.49
7:6:36:BCL:HAA2	7:6:36:BCL:HBD	1.94	0.49
7:J:8:BCL:HED3	7:J:8:BCL:O1A	2.13	0.49
7:A:302:BCL:CBB	7:A:302:BCL:HMB1	2.42	0.49
7:J:8:BCL:CMA	7:M:36:BCL:CMA	2.71	0.49
7:D:2:BCL:HMC3	7:G:3:BCL:CBB	2.32	0.49
7:N:11:BCL:HAC2	7:N:38:BCL:HBC2	1.94	0.49
7:T:38:BCL:CMA	7:V:38:BCL:HMA3	2.43	0.49
5:K:29:UNK:C	7:K:36:BCL:HMD3	2.42	0.48
4:3:30:UNK:CB	7:3:39:BCL:HMD3	2.43	0.48
7:D:2:BCL:CGD	7:D:2:BCL:HBA2	2.42	0.48
5:E:22:UNK:C	7:E:1:BCL:HED1	2.43	0.48
7:F:4:BCL:CAB	7:I:5:BCL:HBB2	2.44	0.48
3:C:75:UNK:HA	3:C:76:UNK:C	2.44	0.48
7:G:3:BCL:HAA2	7:G:3:BCL:HBD	1.96	0.48
7:H:6:BCL:HBA2	7:H:6:BCL:O2D	2.14	0.48
7:L:10:BCL:HMB1	7:N:11:BCL:HMA3	1.94	0.48
7:A:301:BCL:H8	7:B:303:BCL:H192	1.96	0.47
1:A:271:UNK:O	4:V:36:UNK:C	2.63	0.47
7:P:38:BCL:HBC2	7:P:39:BCL:C1D	2.45	0.47
7:T:38:BCL:HMA3	7:V:38:BCL:CMA	2.45	0.47
7:8:36:BCL:HAA2	7:8:36:BCL:CBD	2.44	0.47
7:L:10:BCL:HMB3	7:N:11:BCL:HMA2	1.85	0.46
7:L:10:BCL:HBC2	7:M:36:BCL:HHH	1.97	0.46
7:1:38:BCL:CMC	7:3:38:BCL:CBB	2.93	0.46
7:P:38:BCL:CED	5:Q:22:UNK:HA	2.34	0.46
7:7:38:BCL:C2A	7:7:38:BCL:O1A	2.64	0.45
7:F:4:BCL:H3A	7:F:4:BCL:HBA1	1.73	0.45
5:K:29:UNK:CB	7:K:36:BCL:CMD	2.94	0.45
7:A:301:BCL:HMB1	7:A:301:BCL:CBB	2.47	0.45
3:C:40:UNK:HA	3:C:41:UNK:C	2.46	0.45
7:2:36:BCL:HAA2	7:2:36:BCL:CBD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:8:BCL:CBC	7:K:36:BCL:CAC	2.85	0.45
8:A:401:BPH:C17	8:A:401:BPH:C14	2.93	0.45
7:E:1:BCL:HBA1	7:E:1:BCL:H3A	1.39	0.44
7:D:2:BCL:O1A	7:D:2:BCL:H2A	2.17	0.44
5:S:29:UNK:CB	7:S:36:BCL:HMD3	2.47	0.44
7:I:5:BCL:HBA2	7:I:5:BCL:CED	2.48	0.44
7:3:38:BCL:HAA2	7:3:38:BCL:HBD	1.99	0.43
4:5:27:UNK:CB	7:5:38:BCL:OBD	2.67	0.43
7:W:36:BCL:HBA1	7:W:36:BCL:H3A	1.71	0.43
7:T:38:BCL:CGA	7:T:38:BCL:C3A	2.96	0.43
7:N:11:BCL:CBC	7:N:38:BCL:HHH	2.48	0.43
7:1:38:BCL:C2D	7:2:36:BCL:HMD2	2.49	0.43
7:V:38:BCL:HMD3	5:W:29:UNK:CB	2.49	0.43
7:V:38:BCL:CMD	5:W:29:UNK:CB	2.97	0.42
7:J:8:BCL:CAC	7:K:36:BCL:HBC1	2.48	0.42
7:P:38:BCL:CHC	7:P:38:BCL:CBB	2.83	0.42
1:A:51:UNK:CA	4:7:36:UNK:CB	2.96	0.42
7:L:10:BCL:H2A	7:L:10:BCL:CED	2.20	0.42
7:N:38:BCL:HHB	7:P:38:BCL:CMA	2.49	0.42
7:3:39:BCL:CHC	7:3:39:BCL:HBB3	2.37	0.42
7:G:3:BCL:CBD	7:G:3:BCL:HAA2	2.49	0.42
7:H:6:BCL:O1A	7:H:6:BCL:H2A	2.19	0.42
7:L:10:BCL:C1D	7:M:36:BCL:HMD2	2.46	0.42
7:P:38:BCL:HBD	7:P:38:BCL:HAA2	2.01	0.42
7:P:39:BCL:CHC	7:P:39:BCL:HBB3	2.37	0.42
7:7:38:BCL:HBB3	7:7:38:BCL:CHC	2.37	0.42
7:A:301:BCL:C4	7:A:301:BCL:H71	2.49	0.42
4:V:34:UNK:O	4:V:35:UNK:C	2.68	0.42
7:V:38:BCL:HBA1	7:V:38:BCL:H3A	1.33	0.42
7:A:301:BCL:HMB1	7:A:301:BCL:HBB2	2.01	0.42
7:H:6:BCL:O1A	7:H:6:BCL:C2A	2.67	0.42
7:J:8:BCL:CBC	7:K:36:BCL:HAC2	2.40	0.42
7:B:304:BCL:HMB1	7:B:304:BCL:CBB	2.49	0.42
1:A:271:UNK:CB	4:V:37:UNK:CB	2.97	0.42
4:J:23:UNK:CB	7:J:8:BCL:HED2	2.50	0.42
7:N:38:BCL:HBB3	7:N:38:BCL:CHC	2.38	0.41
7:R:38:BCL:C3A	7:R:38:BCL:CGA	2.88	0.41
3:C:52:UNK:N	4:F:13:UNK:CB	2.83	0.41
7:N:11:BCL:HBC2	7:N:38:BCL:HHH	2.02	0.41
7:Y:36:BCL:C1D	7:Y:37:BCL:HMD2	2.50	0.41
7:N:38:BCL:HBA1	7:N:38:BCL:H3A	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:26:UNK:HA	7:Y:36:BCL:OBD	2.21	0.41
7:5:38:BCL:C2A	7:5:38:BCL:O1A	2.68	0.41
7:8:36:BCL:CED	7:8:36:BCL:HBA1	2.50	0.41
7:N:38:BCL:HMB3	7:P:38:BCL:C4A	2.51	0.41
7:D:2:BCL:CHC	7:D:2:BCL:HBB3	2.38	0.41
5:K:29:UNK:CB	7:K:36:BCL:HMD3	2.51	0.41
4:L:27:UNK:CB	7:L:10:BCL:OBD	2.69	0.41
7:N:11:BCL:HBD	7:N:11:BCL:HAA2	2.02	0.41
7:L:10:BCL:HBC1	5:M:33:UNK:CB	2.51	0.40
7:S:36:BCL:CBD	7:S:36:BCL:HAA2	2.50	0.40
7:A:301:BCL:H111	7:A:301:BCL:H91	1.75	0.40
7:D:2:BCL:C2A	7:D:2:BCL:O1A	2.69	0.40
1:A:254:UNK:O	4:Z:36:UNK:O	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
7	BCL	1	38	-	36,55,74	3.28	24 (66%)	43,92,115	2.96	16 (37%)
7	BCL	2	36	-	36,55,74	3.62	15 (41%)	43,92,115	2.54	17 (39%)
7	BCL	3	38	-	36,55,74	3.56	15 (41%)	43,92,115	2.52	16 (37%)
7	BCL	3	39	-	36,55,74	3.26	22 (61%)	43,92,115	2.94	17 (39%)
7	BCL	5	38	-	36,55,74	3.22	21 (58%)	43,92,115	2.97	16 (37%)
7	BCL	6	36	-	36,55,74	3.51	14 (38%)	43,92,115	2.52	18 (41%)
7	BCL	7	38	-	36,55,74	3.23	20 (55%)	43,92,115	2.91	16 (37%)
7	BCL	8	36	-	36,55,74	3.56	14 (38%)	43,92,115	2.60	19 (44%)
7	BCL	A	301	-	55,74,74	1.32	3 (5%)	65,115,115	1.84	17 (26%)
7	BCL	A	302	-	55,74,74	1.13	3 (5%)	65,115,115	1.53	14 (21%)
8	BPH	A	401	-	65,70,70	0.86	1 (1%)	75,101,101	1.52	14 (18%)
7	BCL	B	303	-	55,74,74	1.34	3 (5%)	65,115,115	1.38	8 (12%)
7	BCL	B	304	-	55,74,74	1.36	5 (9%)	65,115,115	1.47	13 (20%)
8	BPH	B	402	-	65,70,70	0.84	1 (1%)	75,101,101	1.44	9 (12%)
7	BCL	D	2	-	36,55,74	3.32	22 (61%)	43,92,115	2.90	15 (34%)
7	BCL	E	1	-	36,55,74	3.78	16 (44%)	43,92,115	2.54	19 (44%)
7	BCL	F	4	-	36,55,74	3.31	23 (63%)	43,92,115	2.89	14 (32%)
7	BCL	G	3	-	36,55,74	3.65	14 (38%)	43,92,115	2.57	18 (41%)
7	BCL	H	6	-	36,55,74	3.63	24 (66%)	43,92,115	2.93	16 (37%)
7	BCL	I	5	-	36,55,74	3.77	17 (47%)	43,92,115	2.68	20 (46%)
7	BCL	J	8	-	36,55,74	3.32	21 (58%)	43,92,115	2.94	15 (34%)
7	BCL	K	36	-	36,55,74	3.69	15 (41%)	43,92,115	2.55	16 (37%)
7	BCL	L	10	-	36,55,74	3.33	22 (61%)	43,92,115	2.95	16 (37%)
7	BCL	M	36	-	36,55,74	3.67	16 (44%)	43,92,115	2.65	19 (44%)
7	BCL	N	11	-	36,55,74	3.54	14 (38%)	43,92,115	2.91	20 (46%)
7	BCL	N	38	-	36,55,74	3.25	22 (61%)	43,92,115	2.95	16 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	P	38	-	36,55,74	3.65	16 (44%)	43,92,115	2.63	17 (39%)
7	BCL	P	39	-	36,55,74	3.44	23 (63%)	43,92,115	2.95	16 (37%)
7	BCL	R	38	-	36,55,74	3.49	22 (61%)	43,92,115	2.94	16 (37%)
7	BCL	S	36	-	36,55,74	3.75	17 (47%)	43,92,115	2.57	20 (46%)
7	BCL	T	38	-	36,55,74	3.51	23 (63%)	43,92,115	2.91	16 (37%)
7	BCL	U	36	-	36,55,74	3.70	16 (44%)	43,92,115	2.50	18 (41%)
7	BCL	V	38	-	36,55,74	3.66	15 (41%)	43,92,115	2.75	21 (48%)
7	BCL	W	36	-	36,55,74	3.26	22 (61%)	43,92,115	2.91	16 (37%)
7	BCL	Y	36	-	36,55,74	3.66	15 (41%)	43,92,115	2.48	16 (37%)
7	BCL	Y	37	-	36,55,74	3.28	23 (63%)	43,92,115	2.92	17 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	1	38	-	-	0/15/115/137	0/0/9/9
7	BCL	2	36	-	-	0/15/115/137	0/0/9/9
7	BCL	3	38	-	-	0/15/115/137	0/0/9/9
7	BCL	3	39	-	-	0/15/115/137	0/0/9/9
7	BCL	5	38	-	-	0/15/115/137	0/0/9/9
7	BCL	6	36	-	-	0/15/115/137	0/0/9/9
7	BCL	7	38	-	-	0/15/115/137	0/0/9/9
7	BCL	8	36	-	-	0/15/115/137	0/0/9/9
7	BCL	A	301	-	-	0/37/137/137	0/0/9/9
7	BCL	A	302	-	-	0/37/137/137	0/0/9/9
8	BPH	A	401	-	-	0/54/105/105	0/1/6/6
7	BCL	B	303	-	-	0/37/137/137	0/0/9/9
7	BCL	B	304	-	-	0/37/137/137	0/0/9/9
8	BPH	B	402	-	-	0/54/105/105	0/1/6/6
7	BCL	D	2	-	-	0/15/115/137	0/0/9/9
7	BCL	E	1	-	-	0/15/115/137	0/0/9/9
7	BCL	F	4	-	-	0/15/115/137	0/0/9/9
7	BCL	G	3	-	-	0/15/115/137	0/0/9/9
7	BCL	H	6	-	-	0/15/115/137	0/0/9/9
7	BCL	I	5	-	-	0/15/115/137	0/0/9/9
7	BCL	J	8	-	-	0/15/115/137	0/0/9/9
7	BCL	K	36	-	-	0/15/115/137	0/0/9/9
7	BCL	L	10	-	-	0/15/115/137	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	M	36	-	-	0/15/115/137	0/0/9/9
7	BCL	N	11	-	-	0/15/115/137	0/0/9/9
7	BCL	N	38	-	-	0/15/115/137	0/0/9/9
7	BCL	P	38	-	-	0/15/115/137	0/0/9/9
7	BCL	P	39	-	-	0/15/115/137	0/0/9/9
7	BCL	R	38	-	-	0/15/115/137	0/0/9/9
7	BCL	S	36	-	-	0/15/115/137	0/0/9/9
7	BCL	T	38	-	-	0/15/115/137	0/0/9/9
7	BCL	U	36	-	-	0/15/115/137	0/0/9/9
7	BCL	V	38	-	-	0/15/115/137	0/0/9/9
7	BCL	W	36	-	-	0/15/115/137	0/0/9/9
7	BCL	Y	36	-	-	1/15/115/137	0/0/9/9
7	BCL	Y	37	-	-	0/15/115/137	0/0/9/9

All (579) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	8	36	BCL	CBB-CAB	-7.56	1.26	1.49
7	3	38	BCL	CBB-CAB	-7.48	1.26	1.49
7	Y	36	BCL	CBB-CAB	-7.47	1.26	1.49
7	G	3	BCL	CBB-CAB	-7.45	1.26	1.49
7	6	36	BCL	CBB-CAB	-7.45	1.26	1.49
7	2	36	BCL	CBB-CAB	-7.44	1.26	1.49
7	E	1	BCL	CBB-CAB	-7.44	1.26	1.49
7	I	5	BCL	CBB-CAB	-7.42	1.26	1.49
7	K	36	BCL	CBB-CAB	-7.40	1.26	1.49
7	M	36	BCL	CBB-CAB	-7.40	1.26	1.49
7	P	38	BCL	CBB-CAB	-7.40	1.26	1.49
7	N	11	BCL	CBB-CAB	-7.40	1.26	1.49
7	E	1	BCL	O2D-CED	-7.37	1.27	1.45
7	V	38	BCL	CBB-CAB	-7.35	1.27	1.49
7	S	36	BCL	CBB-CAB	-7.33	1.27	1.49
7	U	36	BCL	CBB-CAB	-7.31	1.27	1.49
7	5	38	BCL	C2C-C3C	-5.43	1.39	1.54
7	1	38	BCL	C2C-C3C	-5.32	1.39	1.54
7	R	38	BCL	C2C-C3C	-5.29	1.39	1.54
7	3	39	BCL	C2C-C3C	-5.25	1.39	1.54
7	J	8	BCL	CMB-C2B	-5.24	1.41	1.51
7	P	39	BCL	C2C-C3C	-5.24	1.39	1.54
7	L	10	BCL	C2C-C3C	-5.23	1.39	1.54
7	7	38	BCL	C2C-C3C	-5.22	1.39	1.54
7	L	10	BCL	CMB-C2B	-5.21	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	6	BCL	CMB-C2B	-5.20	1.41	1.51
7	D	2	BCL	C2C-C3C	-5.18	1.39	1.54
7	N	38	BCL	CMB-C2B	-5.17	1.41	1.51
7	5	38	BCL	CMB-C2B	-5.17	1.41	1.51
7	R	38	BCL	CMB-C2B	-5.16	1.41	1.51
7	N	38	BCL	C2C-C3C	-5.14	1.39	1.54
7	P	39	BCL	CMB-C2B	-5.13	1.41	1.51
7	W	36	BCL	C2C-C3C	-5.08	1.40	1.54
7	7	38	BCL	CMB-C2B	-5.08	1.41	1.51
7	Y	37	BCL	C2C-C3C	-5.07	1.40	1.54
7	J	8	BCL	C2C-C3C	-5.07	1.40	1.54
7	H	6	BCL	C2C-C3C	-5.05	1.40	1.54
7	T	38	BCL	C2C-C3C	-5.00	1.40	1.54
7	J	8	BCL	CMA-C3A	-5.00	1.41	1.53
7	H	6	BCL	CMA-C3A	-4.99	1.42	1.53
7	3	39	BCL	CMB-C2B	-4.97	1.41	1.51
7	F	4	BCL	CMA-C3A	-4.97	1.42	1.53
7	T	38	BCL	CMB-C2B	-4.96	1.41	1.51
7	D	2	BCL	CMB-C2B	-4.96	1.41	1.51
7	F	4	BCL	C2C-C3C	-4.95	1.40	1.54
7	H	6	BCL	CBB-CAB	-4.93	1.34	1.49
7	J	8	BCL	CBB-CAB	-4.93	1.34	1.49
7	L	10	BCL	C3B-C2B	-4.91	1.29	1.39
7	F	4	BCL	C3B-C2B	-4.89	1.29	1.39
7	F	4	BCL	CMB-C2B	-4.88	1.41	1.51
7	7	38	BCL	CBB-CAB	-4.87	1.34	1.49
7	J	8	BCL	C3B-C2B	-4.86	1.29	1.39
7	7	38	BCL	C3B-C2B	-4.85	1.29	1.39
7	Y	37	BCL	CMB-C2B	-4.84	1.41	1.51
7	5	38	BCL	CBB-CAB	-4.83	1.34	1.49
7	D	2	BCL	CBB-CAB	-4.82	1.34	1.49
7	1	38	BCL	CMB-C2B	-4.80	1.41	1.51
7	N	38	BCL	C3B-C2B	-4.80	1.29	1.39
7	3	39	BCL	C3B-C2B	-4.79	1.29	1.39
7	1	38	BCL	CMA-C3A	-4.79	1.42	1.53
7	Y	37	BCL	CMA-C3A	-4.78	1.42	1.53
7	H	6	BCL	C3B-C2B	-4.77	1.29	1.39
7	W	36	BCL	CMB-C2B	-4.76	1.42	1.51
7	W	36	BCL	C3B-C2B	-4.76	1.29	1.39
7	N	38	BCL	CBB-CAB	-4.76	1.35	1.49
7	L	10	BCL	CBB-CAB	-4.76	1.35	1.49
7	D	2	BCL	C3B-C2B	-4.75	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	6	BCL	O2D-CED	-4.75	1.33	1.45
7	Y	37	BCL	CBB-CAB	-4.73	1.35	1.49
7	W	36	BCL	CMA-C3A	-4.73	1.42	1.53
7	F	4	BCL	CBB-CAB	-4.73	1.35	1.49
7	P	39	BCL	CBB-CAB	-4.72	1.35	1.49
7	1	38	BCL	CBA-CGA	-4.72	1.37	1.50
7	F	4	BCL	CBA-CGA	-4.71	1.37	1.50
7	5	38	BCL	CMA-C3A	-4.71	1.42	1.53
7	1	38	BCL	C3B-C2B	-4.71	1.29	1.39
7	Y	37	BCL	C3B-C2B	-4.70	1.29	1.39
7	R	38	BCL	CBA-CGA	-4.70	1.37	1.50
7	1	38	BCL	CBB-CAB	-4.70	1.35	1.49
7	T	38	BCL	C3B-C2B	-4.69	1.29	1.39
7	R	38	BCL	C3B-C2B	-4.68	1.29	1.39
7	L	10	BCL	CMA-C3A	-4.68	1.42	1.53
7	7	38	BCL	CBA-CGA	-4.68	1.37	1.50
7	D	2	BCL	CMA-C3A	-4.67	1.42	1.53
7	L	10	BCL	CBA-CGA	-4.67	1.37	1.50
7	5	38	BCL	C3B-C2B	-4.65	1.29	1.39
7	J	8	BCL	CBA-CGA	-4.65	1.37	1.50
7	D	2	BCL	CBA-CGA	-4.65	1.37	1.50
7	3	39	BCL	CBB-CAB	-4.63	1.35	1.49
7	P	39	BCL	C3B-C2B	-4.62	1.29	1.39
7	3	39	BCL	CMA-C3A	-4.62	1.42	1.53
7	N	38	BCL	CMA-C3A	-4.62	1.42	1.53
7	K	36	BCL	O2D-CGD	-4.61	1.21	1.33
7	T	38	BCL	CBB-CAB	-4.60	1.35	1.49
7	H	6	BCL	CBA-CGA	-4.60	1.37	1.50
7	R	38	BCL	CBB-CAB	-4.59	1.35	1.49
7	7	38	BCL	CMA-C3A	-4.59	1.42	1.53
7	W	36	BCL	CBB-CAB	-4.58	1.35	1.49
7	T	38	BCL	CMA-C3A	-4.58	1.42	1.53
7	M	36	BCL	O2D-CGD	-4.56	1.21	1.33
7	J	8	BCL	CAC-C3C	-4.56	1.44	1.54
7	5	38	BCL	CBA-CGA	-4.55	1.37	1.50
7	S	36	BCL	O2D-CGD	-4.55	1.21	1.33
7	3	39	BCL	CBA-CGA	-4.54	1.37	1.50
7	8	36	BCL	O2D-CGD	-4.53	1.21	1.33
7	P	38	BCL	O2D-CGD	-4.52	1.21	1.33
7	I	5	BCL	O2D-CGD	-4.51	1.21	1.33
7	D	2	BCL	O2D-CED	-4.49	1.34	1.45
7	R	38	BCL	CMA-C3A	-4.49	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	38	BCL	CBA-CGA	-4.49	1.37	1.50
7	E	1	BCL	O2D-CGD	-4.47	1.21	1.33
7	U	36	BCL	O2D-CGD	-4.46	1.21	1.33
7	Y	37	BCL	CBA-CGA	-4.46	1.37	1.50
7	W	36	BCL	CBA-CGA	-4.46	1.37	1.50
7	P	39	BCL	CBA-CGA	-4.45	1.37	1.50
7	6	36	BCL	O2D-CGD	-4.45	1.21	1.33
7	G	3	BCL	O2D-CGD	-4.44	1.21	1.33
7	V	38	BCL	O2D-CGD	-4.43	1.21	1.33
7	P	39	BCL	CMA-C3A	-4.42	1.43	1.53
7	N	38	BCL	CBA-CGA	-4.42	1.37	1.50
7	K	36	BCL	CAC-C3C	-4.38	1.45	1.54
7	2	36	BCL	O2D-CGD	-4.35	1.22	1.33
7	N	11	BCL	O2D-CGD	-4.33	1.22	1.33
7	Y	36	BCL	O2D-CGD	-4.32	1.22	1.33
7	3	38	BCL	CAC-C3C	-4.31	1.45	1.54
7	H	6	BCL	CAC-C3C	-4.31	1.45	1.54
7	3	38	BCL	O2D-CGD	-4.27	1.22	1.33
7	N	11	BCL	CAC-C3C	-4.26	1.45	1.54
7	I	5	BCL	CAC-C3C	-4.23	1.45	1.54
7	F	4	BCL	CAC-C3C	-4.18	1.45	1.54
7	2	36	BCL	CAC-C3C	-4.17	1.45	1.54
7	L	10	BCL	CAC-C3C	-4.11	1.45	1.54
7	N	38	BCL	O2D-CGD	-4.11	1.22	1.33
7	N	38	BCL	CAC-C3C	-4.11	1.45	1.54
7	R	38	BCL	O2D-CGD	-4.10	1.22	1.33
7	P	38	BCL	CAC-C3C	-4.10	1.45	1.54
7	5	38	BCL	O2D-CGD	-4.10	1.22	1.33
7	W	36	BCL	O2D-CGD	-4.09	1.22	1.33
7	V	38	BCL	O2D-CED	-4.07	1.35	1.45
7	1	38	BCL	O2D-CGD	-4.06	1.22	1.33
7	U	36	BCL	CAC-C3C	-4.06	1.45	1.54
7	Y	37	BCL	O2D-CGD	-4.05	1.22	1.33
7	Y	36	BCL	CAC-C3C	-4.04	1.46	1.54
7	1	38	BCL	O2D-CED	-4.03	1.35	1.45
7	L	10	BCL	O2D-CGD	-4.03	1.22	1.33
7	1	38	BCL	CAC-C3C	-4.02	1.46	1.54
7	7	38	BCL	CAC-C3C	-4.02	1.46	1.54
7	J	8	BCL	O2D-CGD	-4.01	1.23	1.33
7	S	36	BCL	O2D-CED	-4.00	1.35	1.45
7	M	36	BCL	CAC-C3C	-4.00	1.46	1.54
7	P	39	BCL	O2D-CGD	-3.99	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	7	38	BCL	O2D-CGD	-3.98	1.23	1.33
7	F	4	BCL	O2D-CGD	-3.97	1.23	1.33
7	T	38	BCL	O2D-CGD	-3.96	1.23	1.33
7	5	38	BCL	CAC-C3C	-3.95	1.46	1.54
7	3	39	BCL	O2D-CGD	-3.95	1.23	1.33
7	V	38	BCL	CAC-C3C	-3.92	1.46	1.54
7	Y	37	BCL	CAC-C3C	-3.92	1.46	1.54
7	6	36	BCL	CAC-C3C	-3.92	1.46	1.54
7	3	39	BCL	CAC-C3C	-3.92	1.46	1.54
7	S	36	BCL	CAC-C3C	-3.90	1.46	1.54
7	H	6	BCL	O2D-CGD	-3.89	1.23	1.33
7	D	2	BCL	O2D-CGD	-3.87	1.23	1.33
7	T	38	BCL	CAC-C3C	-3.82	1.46	1.54
7	R	38	BCL	CAC-C3C	-3.80	1.46	1.54
7	P	39	BCL	CAC-C3C	-3.79	1.46	1.54
7	G	3	BCL	CAC-C3C	-3.75	1.46	1.54
7	P	38	BCL	O2D-CED	-3.70	1.36	1.45
7	D	2	BCL	CAC-C3C	-3.69	1.46	1.54
7	8	36	BCL	CAC-C3C	-3.67	1.46	1.54
7	W	36	BCL	CAC-C3C	-3.65	1.46	1.54
7	E	1	BCL	CAC-C3C	-3.63	1.46	1.54
7	K	36	BCL	O2A-CGA	-3.63	1.20	1.32
7	S	36	BCL	O2A-CGA	-3.52	1.21	1.32
7	U	36	BCL	O2A-CGA	-3.47	1.21	1.32
7	M	36	BCL	O2A-CGA	-3.46	1.21	1.32
7	T	38	BCL	O2D-CED	-3.41	1.37	1.45
7	3	38	BCL	O2A-CGA	-3.41	1.21	1.32
7	M	36	BCL	O2D-CED	-3.39	1.37	1.45
7	I	5	BCL	O2A-CGA	-3.39	1.21	1.32
7	Y	37	BCL	O2D-CED	-3.32	1.37	1.45
7	D	2	BCL	CBD-CGD	-3.29	1.42	1.52
7	7	38	BCL	CBD-CGD	-3.28	1.42	1.52
7	Y	36	BCL	O2A-C1	-3.26	1.37	1.45
7	H	6	BCL	CBD-CGD	-3.25	1.42	1.52
7	F	4	BCL	CBD-CGD	-3.24	1.42	1.52
7	1	38	BCL	CBD-CGD	-3.23	1.42	1.52
7	3	39	BCL	CBD-CGD	-3.22	1.42	1.52
7	G	3	BCL	O2A-C1	-3.22	1.37	1.45
7	Y	37	BCL	CBD-CGD	-3.19	1.42	1.52
7	5	38	BCL	CBD-CGD	-3.19	1.42	1.52
7	L	10	BCL	CBD-CGD	-3.15	1.42	1.52
7	J	8	BCL	CBD-CGD	-3.13	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	W	36	BCL	CBD-CGD	-3.09	1.42	1.52
7	T	38	BCL	CBD-CGD	-3.06	1.42	1.52
7	N	38	BCL	CBD-CGD	-3.06	1.43	1.52
7	J	8	BCL	O2D-CED	-3.03	1.38	1.45
7	P	39	BCL	CBD-CGD	-3.02	1.43	1.52
7	5	38	BCL	O2D-CED	-3.01	1.38	1.45
7	P	38	BCL	O2A-C1	-3.01	1.38	1.45
7	R	38	BCL	CBD-CGD	-3.00	1.43	1.52
7	5	38	BCL	C3A-C2A	-2.92	1.46	1.54
7	W	36	BCL	O2A-CGA	-2.90	1.23	1.32
7	8	36	BCL	O2A-C1	-2.89	1.38	1.45
7	J	8	BCL	O2A-CGA	-2.88	1.23	1.32
7	5	38	BCL	CMD-C2D	-2.87	1.45	1.51
7	V	38	BCL	O2A-C1	-2.85	1.38	1.45
7	L	10	BCL	CMD-C2D	-2.84	1.45	1.51
7	R	38	BCL	CMD-C2D	-2.82	1.45	1.51
7	J	8	BCL	CMD-C2D	-2.80	1.45	1.51
7	N	38	BCL	CMD-C2D	-2.79	1.45	1.51
7	P	39	BCL	O2D-CED	-2.74	1.38	1.45
7	P	39	BCL	O2A-CGA	-2.73	1.23	1.32
7	1	38	BCL	O2A-CGA	-2.71	1.23	1.32
7	D	2	BCL	CMD-C2D	-2.71	1.45	1.51
7	1	38	BCL	C3A-C2A	-2.67	1.46	1.54
7	P	39	BCL	CMD-C2D	-2.67	1.45	1.51
7	H	6	BCL	CMD-C2D	-2.67	1.45	1.51
7	7	38	BCL	CMD-C2D	-2.66	1.45	1.51
7	3	39	BCL	CMD-C2D	-2.66	1.45	1.51
7	N	38	BCL	O2A-CGA	-2.62	1.24	1.32
7	P	39	BCL	C3A-C2A	-2.61	1.47	1.54
7	3	39	BCL	C3A-C2A	-2.60	1.47	1.54
7	F	4	BCL	CMD-C2D	-2.60	1.46	1.51
7	T	38	BCL	O2A-CGA	-2.59	1.24	1.32
7	T	38	BCL	CMD-C2D	-2.59	1.46	1.51
7	Y	37	BCL	O2A-CGA	-2.59	1.24	1.32
7	H	6	BCL	O2A-CGA	-2.57	1.24	1.32
7	B	304	BCL	CHD-C4C	-2.56	1.33	1.41
7	R	38	BCL	C3A-C2A	-2.56	1.47	1.54
7	3	39	BCL	O2A-CGA	-2.55	1.24	1.32
7	P	38	BCL	C3B-CAB	-2.52	1.42	1.49
7	R	38	BCL	O2A-CGA	-2.52	1.24	1.32
7	N	38	BCL	C3A-C2A	-2.51	1.47	1.54
7	6	36	BCL	C3B-CAB	-2.51	1.42	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	7	38	BCL	C3A-C2A	-2.51	1.47	1.54
7	F	4	BCL	O2A-CGA	-2.50	1.24	1.32
7	D	2	BCL	C3A-C2A	-2.50	1.47	1.54
7	K	36	BCL	C3B-CAB	-2.48	1.42	1.49
7	L	10	BCL	C3A-C2A	-2.47	1.47	1.54
7	Y	37	BCL	CMD-C2D	-2.46	1.46	1.51
7	L	10	BCL	O2A-CGA	-2.46	1.24	1.32
7	J	8	BCL	C3A-C2A	-2.45	1.47	1.54
7	1	38	BCL	O2A-C1	-2.44	1.39	1.45
7	W	36	BCL	CMD-C2D	-2.43	1.46	1.51
7	H	6	BCL	C3A-C2A	-2.43	1.47	1.54
7	N	11	BCL	C3B-CAB	-2.43	1.42	1.49
7	8	36	BCL	C3B-CAB	-2.42	1.42	1.49
7	G	3	BCL	C3B-CAB	-2.40	1.42	1.49
7	Y	37	BCL	C3A-C2A	-2.40	1.47	1.54
8	B	402	BPH	C2A-C1A	-2.39	1.47	1.51
7	1	38	BCL	CMD-C2D	-2.39	1.46	1.51
7	T	38	BCL	C3A-C2A	-2.39	1.47	1.54
7	E	1	BCL	C3B-CAB	-2.38	1.42	1.49
7	W	36	BCL	O2D-CED	-2.36	1.39	1.45
7	M	36	BCL	C3B-CAB	-2.36	1.42	1.49
7	S	36	BCL	C3B-CAB	-2.35	1.42	1.49
7	D	2	BCL	O2A-CGA	-2.34	1.25	1.32
7	I	5	BCL	C3B-CAB	-2.34	1.42	1.49
7	V	38	BCL	C3B-CAB	-2.33	1.42	1.49
7	A	302	BCL	C1A-CHA	-2.33	1.33	1.43
7	N	11	BCL	C1A-CHA	-2.33	1.33	1.43
7	W	36	BCL	C3A-C2A	-2.33	1.47	1.54
7	U	36	BCL	C3B-CAB	-2.33	1.42	1.49
7	3	38	BCL	C3B-CAB	-2.31	1.42	1.49
7	6	36	BCL	C1A-CHA	-2.30	1.33	1.43
7	3	39	BCL	O2A-C1	-2.30	1.39	1.45
7	F	4	BCL	O2D-CED	-2.27	1.39	1.45
7	3	38	BCL	C1A-CHA	-2.24	1.33	1.43
7	Y	36	BCL	C3B-CAB	-2.21	1.43	1.49
7	2	36	BCL	C3B-CAB	-2.19	1.43	1.49
7	F	4	BCL	C3A-C2A	-2.18	1.48	1.54
7	B	304	BCL	C2C-C3C	-2.17	1.48	1.54
7	M	36	BCL	C1A-CHA	-2.14	1.34	1.43
7	8	36	BCL	C1A-CHA	-2.11	1.34	1.43
7	S	36	BCL	C1A-CHA	-2.10	1.34	1.43
7	Y	36	BCL	O2D-CED	-2.09	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	301	BCL	C1A-CHA	-2.09	1.34	1.43
7	2	36	BCL	C1A-CHA	-2.07	1.34	1.43
7	U	36	BCL	C1A-CHA	-2.06	1.34	1.43
7	B	304	BCL	O2D-CED	-2.06	1.40	1.45
7	E	1	BCL	C1A-CHA	-2.06	1.34	1.43
7	P	38	BCL	C1A-CHA	-2.06	1.34	1.43
7	N	38	BCL	O2D-CED	-2.06	1.40	1.45
7	6	36	BCL	C3A-C2A	-2.05	1.48	1.54
7	K	36	BCL	C1A-CHA	-2.05	1.34	1.43
7	I	5	BCL	O2D-CED	-2.04	1.40	1.45
8	A	401	BPH	O2D-CED	-2.04	1.40	1.45
7	B	303	BCL	CBA-CGA	-2.03	1.44	1.50
7	L	10	BCL	O2A-C1	-2.03	1.40	1.45
7	2	36	BCL	O2D-CED	-2.03	1.40	1.45
7	K	36	BCL	O2A-C1	-2.02	1.40	1.45
7	I	5	BCL	C1A-CHA	-2.01	1.34	1.43
7	N	11	BCL	CHD-C4C	2.01	1.47	1.41
7	Y	37	BCL	CHD-C4C	2.01	1.47	1.41
7	H	6	BCL	O1D-CGD	2.01	1.26	1.21
7	S	36	BCL	CHD-C4C	2.01	1.47	1.41
7	1	38	BCL	C2A-C1A	2.01	1.56	1.52
7	1	38	BCL	CAA-C2A	2.04	1.58	1.54
7	I	5	BCL	CHD-C4C	2.07	1.47	1.41
7	H	6	BCL	CAA-C2A	2.09	1.58	1.54
7	J	8	BCL	O1D-CGD	2.09	1.26	1.21
7	M	36	BCL	CHD-C4C	2.10	1.47	1.41
7	P	38	BCL	CHD-C4C	2.11	1.47	1.41
7	6	36	BCL	C2C-C1C	2.11	1.58	1.51
7	E	1	BCL	CHD-C4C	2.11	1.47	1.41
7	U	36	BCL	CHD-C4C	2.11	1.47	1.41
7	H	6	BCL	CHD-C4C	2.12	1.47	1.41
7	3	38	BCL	C2C-C1C	2.13	1.58	1.51
7	F	4	BCL	CHD-C4C	2.14	1.47	1.41
7	Y	37	BCL	O1D-CGD	2.18	1.26	1.21
7	2	36	BCL	C2C-C1C	2.20	1.59	1.51
7	1	38	BCL	O1D-CGD	2.21	1.26	1.21
7	N	11	BCL	C2C-C1C	2.21	1.59	1.51
7	3	38	BCL	CHD-C4C	2.21	1.47	1.41
7	3	39	BCL	CAA-C2A	2.22	1.58	1.54
7	W	36	BCL	CAA-C2A	2.22	1.58	1.54
7	Y	36	BCL	C2C-C1C	2.22	1.59	1.51
7	3	39	BCL	O1D-CGD	2.23	1.26	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2	36	BCL	CHD-C4C	2.23	1.47	1.41
7	E	1	BCL	C2C-C1C	2.24	1.59	1.51
7	Y	36	BCL	CHD-C4C	2.24	1.47	1.41
7	P	38	BCL	C2C-C1C	2.26	1.59	1.51
7	T	38	BCL	O1D-CGD	2.27	1.26	1.21
7	V	38	BCL	CHD-C4C	2.27	1.47	1.41
7	G	3	BCL	CHD-C4C	2.27	1.47	1.41
7	S	36	BCL	C2C-C1C	2.27	1.59	1.51
7	W	36	BCL	O1D-CGD	2.29	1.27	1.21
7	L	10	BCL	CAA-C2A	2.29	1.58	1.54
7	K	36	BCL	C2C-C1C	2.29	1.59	1.51
7	I	5	BCL	C2C-C1C	2.30	1.59	1.51
7	8	36	BCL	C2C-C1C	2.30	1.59	1.51
7	V	38	BCL	C2C-C1C	2.31	1.59	1.51
7	P	39	BCL	O1D-CGD	2.32	1.27	1.21
7	U	36	BCL	C2C-C1C	2.32	1.59	1.51
7	T	38	BCL	CAA-C2A	2.32	1.58	1.54
7	Y	37	BCL	CAA-C2A	2.33	1.58	1.54
7	F	4	BCL	O1D-CGD	2.33	1.27	1.21
7	F	4	BCL	CAA-C2A	2.33	1.58	1.54
7	R	38	BCL	CAA-C2A	2.35	1.58	1.54
7	N	38	BCL	O1D-CGD	2.37	1.27	1.21
7	M	36	BCL	C2C-C1C	2.37	1.59	1.51
7	L	10	BCL	O1D-CGD	2.37	1.27	1.21
7	G	3	BCL	C2C-C1C	2.37	1.59	1.51
7	D	2	BCL	O1D-CGD	2.39	1.27	1.21
7	N	38	BCL	CAA-C2A	2.42	1.58	1.54
7	P	39	BCL	CAA-C2A	2.42	1.58	1.54
7	5	38	BCL	C3D-CAD	2.42	1.53	1.46
7	R	38	BCL	O1D-CGD	2.43	1.27	1.21
7	T	38	BCL	C3D-CAD	2.49	1.53	1.46
7	D	2	BCL	CAA-C2A	2.50	1.58	1.54
7	D	2	BCL	C3D-CAD	2.50	1.53	1.46
7	1	38	BCL	C3D-CAD	2.51	1.53	1.46
7	5	38	BCL	O1D-CGD	2.53	1.27	1.21
7	7	38	BCL	O1D-CGD	2.53	1.27	1.21
7	J	8	BCL	C3D-CAD	2.56	1.53	1.46
7	F	4	BCL	C3D-CAD	2.57	1.53	1.46
7	W	36	BCL	C3D-CAD	2.57	1.53	1.46
7	P	39	BCL	C3D-CAD	2.60	1.53	1.46
7	N	38	BCL	C3D-CAD	2.60	1.53	1.46
7	Y	36	BCL	CMA-C3A	2.60	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	7	38	BCL	C3D-CAD	2.61	1.53	1.46
7	3	39	BCL	C3D-CAD	2.61	1.53	1.46
7	K	36	BCL	CMA-C3A	2.62	1.59	1.53
7	R	38	BCL	C3D-CAD	2.64	1.53	1.46
7	Y	37	BCL	C3D-CAD	2.65	1.53	1.46
7	J	8	BCL	C2C-C1C	2.66	1.60	1.51
7	7	38	BCL	CAA-C2A	2.66	1.59	1.54
7	L	10	BCL	C3D-CAD	2.67	1.53	1.46
7	7	38	BCL	C2C-C1C	2.67	1.60	1.51
7	F	4	BCL	C2C-C1C	2.68	1.60	1.51
7	I	5	BCL	CMA-C3A	2.70	1.59	1.53
7	N	38	BCL	C2C-C1C	2.70	1.60	1.51
7	E	1	BCL	O2A-CGA	2.72	1.41	1.32
7	V	38	BCL	CMA-C3A	2.73	1.59	1.53
7	5	38	BCL	CAA-C2A	2.75	1.59	1.54
7	D	2	BCL	C2C-C1C	2.75	1.60	1.51
7	3	38	BCL	CMA-C3A	2.75	1.59	1.53
7	H	6	BCL	C3D-CAD	2.76	1.54	1.46
7	L	10	BCL	C2C-C1C	2.77	1.61	1.51
7	H	6	BCL	C2C-C1C	2.77	1.61	1.51
7	3	39	BCL	C2C-C1C	2.78	1.61	1.51
7	2	36	BCL	CMA-C3A	2.78	1.59	1.53
7	P	39	BCL	C2C-C1C	2.79	1.61	1.51
7	T	38	BCL	C2C-C1C	2.80	1.61	1.51
7	N	11	BCL	CMA-C3A	2.80	1.59	1.53
7	R	38	BCL	C2C-C1C	2.81	1.61	1.51
7	5	38	BCL	C2C-C1C	2.82	1.61	1.51
7	U	36	BCL	CMA-C3A	2.83	1.59	1.53
7	M	36	BCL	CMA-C3A	2.83	1.59	1.53
7	W	36	BCL	C2C-C1C	2.86	1.61	1.51
7	Y	37	BCL	C2C-C1C	2.87	1.61	1.51
7	1	38	BCL	C2C-C1C	2.89	1.61	1.51
7	G	3	BCL	CMA-C3A	2.90	1.59	1.53
7	P	38	BCL	CMA-C3A	2.91	1.59	1.53
7	E	1	BCL	CMA-C3A	2.92	1.59	1.53
7	8	36	BCL	CMA-C3A	2.96	1.59	1.53
7	S	36	BCL	CMA-C3A	2.97	1.59	1.53
7	6	36	BCL	CMA-C3A	3.14	1.60	1.53
7	7	38	BCL	C3C-C4C	3.18	1.55	1.51
7	5	38	BCL	C3C-C4C	3.31	1.55	1.51
7	D	2	BCL	C3C-C4C	3.31	1.55	1.51
7	W	36	BCL	C3C-C4C	3.34	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Y	37	BCL	C3C-C4C	3.36	1.55	1.51
7	1	38	BCL	C3C-C4C	3.39	1.56	1.51
7	3	39	BCL	C3C-C4C	3.46	1.56	1.51
7	T	38	BCL	C3C-C4C	3.51	1.56	1.51
7	F	4	BCL	C3C-C4C	3.52	1.56	1.51
7	R	38	BCL	C3C-C4C	3.52	1.56	1.51
7	N	38	BCL	C3C-C4C	3.54	1.56	1.51
7	1	38	BCL	C3B-CAB	3.57	1.58	1.49
7	P	39	BCL	C3C-C4C	3.58	1.56	1.51
7	J	8	BCL	C3C-C4C	3.63	1.56	1.51
7	6	36	BCL	C3B-C2B	3.64	1.47	1.39
7	Y	36	BCL	C3B-C2B	3.65	1.47	1.39
7	I	5	BCL	C3B-C2B	3.71	1.47	1.39
7	2	36	BCL	C3B-C2B	3.75	1.48	1.39
7	U	36	BCL	C3B-C2B	3.76	1.48	1.39
7	M	36	BCL	C3B-C2B	3.78	1.48	1.39
7	3	38	BCL	C3B-C2B	3.78	1.48	1.39
7	K	36	BCL	C3B-C2B	3.79	1.48	1.39
7	8	36	BCL	C3B-C2B	3.80	1.48	1.39
7	5	38	BCL	C3B-CAB	3.81	1.59	1.49
7	H	6	BCL	C3C-C4C	3.81	1.56	1.51
7	V	38	BCL	C3B-C2B	3.82	1.48	1.39
7	S	36	BCL	C3B-C2B	3.85	1.48	1.39
7	E	1	BCL	C3B-C2B	3.86	1.48	1.39
7	N	11	BCL	C3B-C2B	3.86	1.48	1.39
7	Y	37	BCL	C3B-CAB	3.87	1.59	1.49
7	3	39	BCL	C3B-CAB	3.87	1.59	1.49
7	R	38	BCL	C3B-CAB	3.89	1.59	1.49
7	P	38	BCL	C3B-C2B	3.91	1.48	1.39
7	T	38	BCL	C3B-CAB	3.92	1.59	1.49
7	G	3	BCL	C3B-C2B	3.93	1.48	1.39
7	P	39	BCL	C3B-CAB	3.94	1.59	1.49
7	J	8	BCL	C3B-CAB	3.96	1.59	1.49
7	L	10	BCL	C3C-C4C	3.96	1.56	1.51
7	W	36	BCL	C3B-CAB	3.97	1.59	1.49
7	A	302	BCL	CHC-C1C	3.97	1.38	1.33
7	1	38	BCL	CHB-C4A	4.00	1.38	1.33
7	N	38	BCL	C3B-CAB	4.00	1.59	1.49
7	5	38	BCL	CHB-C4A	4.04	1.38	1.33
7	D	2	BCL	C3B-CAB	4.07	1.60	1.49
7	L	10	BCL	C3B-CAB	4.07	1.60	1.49
7	F	4	BCL	C3B-CAB	4.15	1.60	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	6	BCL	C3B-CAB	4.17	1.60	1.49
7	K	36	BCL	O1D-CGD	4.19	1.31	1.21
7	7	38	BCL	C3B-CAB	4.22	1.60	1.49
7	E	1	BCL	O1D-CGD	4.33	1.32	1.21
7	G	3	BCL	O1D-CGD	4.33	1.32	1.21
7	2	36	BCL	O1D-CGD	4.38	1.32	1.21
7	7	38	BCL	CHB-C4A	4.40	1.39	1.33
7	Y	36	BCL	O1D-CGD	4.41	1.32	1.21
7	A	302	BCL	CHB-C4A	4.42	1.39	1.33
7	I	5	BCL	O1D-CGD	4.44	1.32	1.21
7	6	36	BCL	O1D-CGD	4.46	1.32	1.21
7	3	38	BCL	O1D-CGD	4.47	1.32	1.21
7	M	36	BCL	O1D-CGD	4.50	1.32	1.21
7	U	36	BCL	O2A-C1	4.55	1.56	1.45
7	P	39	BCL	CHB-C4A	4.56	1.39	1.33
7	8	36	BCL	O1D-CGD	4.58	1.32	1.21
7	V	38	BCL	O1D-CGD	4.59	1.32	1.21
7	3	39	BCL	CHB-C4A	4.61	1.39	1.33
7	U	36	BCL	O1D-CGD	4.61	1.32	1.21
7	N	11	BCL	O1D-CGD	4.63	1.32	1.21
7	P	38	BCL	O1D-CGD	4.63	1.32	1.21
7	J	8	BCL	CHB-C4A	4.66	1.39	1.33
7	N	38	BCL	CHB-C4A	4.67	1.39	1.33
7	D	2	BCL	CHB-C4A	4.68	1.39	1.33
7	S	36	BCL	O2A-C1	4.68	1.56	1.45
7	I	5	BCL	O2A-C1	4.68	1.56	1.45
7	S	36	BCL	O1D-CGD	4.75	1.33	1.21
7	W	36	BCL	CHB-C4A	4.76	1.39	1.33
7	R	38	BCL	CHB-C4A	4.76	1.39	1.33
7	Y	37	BCL	CHB-C4A	4.83	1.39	1.33
7	L	10	BCL	CHB-C4A	4.85	1.39	1.33
7	J	8	BCL	C4B-CHC	4.85	1.53	1.40
7	T	38	BCL	CHB-C4A	4.94	1.39	1.33
7	R	38	BCL	C4B-CHC	4.96	1.53	1.40
7	5	38	BCL	C4B-CHC	4.99	1.53	1.40
7	L	10	BCL	C4B-CHC	4.99	1.53	1.40
7	F	4	BCL	C4B-CHC	5.00	1.53	1.40
7	7	38	BCL	C4B-CHC	5.01	1.53	1.40
7	D	2	BCL	C4B-CHC	5.03	1.53	1.40
7	H	6	BCL	C4B-CHC	5.03	1.53	1.40
7	3	39	BCL	C4B-CHC	5.05	1.53	1.40
7	P	39	BCL	C4B-CHC	5.05	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	38	BCL	C4B-CHC	5.05	1.53	1.40
7	H	6	BCL	CHB-C4A	5.06	1.40	1.33
7	W	36	BCL	C4B-CHC	5.06	1.53	1.40
7	B	304	BCL	CHB-C4A	5.07	1.40	1.33
7	T	38	BCL	C4B-CHC	5.10	1.53	1.40
7	1	38	BCL	C4B-CHC	5.14	1.53	1.40
7	Y	37	BCL	C4B-CHC	5.17	1.53	1.40
7	A	301	BCL	CHC-C1C	5.19	1.40	1.33
7	F	4	BCL	CHB-C4A	5.21	1.40	1.33
7	B	303	BCL	CHB-C4A	5.42	1.40	1.33
7	B	303	BCL	CHC-C1C	5.62	1.40	1.33
7	B	304	BCL	CHC-C1C	5.69	1.40	1.33
7	A	301	BCL	CHB-C4A	5.89	1.41	1.33
7	8	36	BCL	CMB-C2B	6.30	1.64	1.51
7	6	36	BCL	CMB-C2B	6.36	1.64	1.51
7	3	38	BCL	CMB-C2B	6.38	1.64	1.51
7	N	11	BCL	CMB-C2B	6.55	1.65	1.51
7	V	38	BCL	CMB-C2B	6.63	1.65	1.51
7	S	36	BCL	CMB-C2B	6.66	1.65	1.51
7	P	38	BCL	CMB-C2B	6.68	1.65	1.51
7	E	1	BCL	CMB-C2B	6.68	1.65	1.51
7	U	36	BCL	CMB-C2B	6.75	1.65	1.51
7	5	38	BCL	CHC-C1C	6.79	1.42	1.33
7	2	36	BCL	CMB-C2B	6.80	1.65	1.51
7	Y	36	BCL	CMB-C2B	6.85	1.65	1.51
7	G	3	BCL	CMB-C2B	6.95	1.65	1.51
7	M	36	BCL	CMB-C2B	6.97	1.65	1.51
7	K	36	BCL	CMB-C2B	7.04	1.65	1.51
7	N	38	BCL	CHC-C1C	7.08	1.42	1.33
7	I	5	BCL	CMB-C2B	7.13	1.66	1.51
7	P	39	BCL	CHC-C1C	7.14	1.42	1.33
7	1	38	BCL	CHC-C1C	7.16	1.42	1.33
7	P	39	BCL	O2A-C1	7.23	1.62	1.45
7	J	8	BCL	CHC-C1C	7.24	1.42	1.33
7	7	38	BCL	CHC-C1C	7.29	1.42	1.33
7	H	6	BCL	CHC-C1C	7.35	1.42	1.33
7	R	38	BCL	CHC-C1C	7.41	1.42	1.33
7	Y	37	BCL	CHC-C1C	7.43	1.43	1.33
7	D	2	BCL	CHC-C1C	7.44	1.43	1.33
7	T	38	BCL	O2A-C1	7.49	1.63	1.45
7	6	36	BCL	CHC-C1C	7.61	1.43	1.33
7	R	38	BCL	O2A-C1	7.63	1.63	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	3	39	BCL	CHC-C1C	7.63	1.43	1.33
7	L	10	BCL	CHC-C1C	7.64	1.43	1.33
7	T	38	BCL	CHC-C1C	7.71	1.43	1.33
7	H	6	BCL	O2A-C1	7.72	1.63	1.45
7	W	36	BCL	CHC-C1C	7.73	1.43	1.33
7	F	4	BCL	CHC-C1C	7.75	1.43	1.33
7	8	36	BCL	OBB-CAB	7.81	1.48	1.22
7	6	36	BCL	OBB-CAB	7.88	1.48	1.22
7	N	11	BCL	CHC-C1C	7.89	1.43	1.33
7	3	38	BCL	CHC-C1C	7.94	1.43	1.33
7	E	1	BCL	OBB-CAB	8.02	1.49	1.22
7	3	38	BCL	OBB-CAB	8.02	1.49	1.22
7	N	11	BCL	OBB-CAB	8.03	1.49	1.22
7	S	36	BCL	OBB-CAB	8.07	1.49	1.22
7	P	38	BCL	OBB-CAB	8.12	1.49	1.22
7	U	36	BCL	OBB-CAB	8.12	1.49	1.22
7	8	36	BCL	CHC-C1C	8.15	1.43	1.33
7	V	38	BCL	OBB-CAB	8.18	1.49	1.22
7	2	36	BCL	OBB-CAB	8.19	1.49	1.22
7	G	3	BCL	OBB-CAB	8.21	1.49	1.22
7	M	36	BCL	OBB-CAB	8.21	1.49	1.22
7	K	36	BCL	OBB-CAB	8.27	1.50	1.22
7	I	5	BCL	OBB-CAB	8.33	1.50	1.22
7	Y	36	BCL	OBB-CAB	8.35	1.50	1.22
7	P	38	BCL	CHC-C1C	8.36	1.44	1.33
7	V	38	BCL	CHC-C1C	8.38	1.44	1.33
7	M	36	BCL	CHC-C1C	8.39	1.44	1.33
7	S	36	BCL	CHC-C1C	8.42	1.44	1.33
7	U	36	BCL	CHC-C1C	8.44	1.44	1.33
7	E	1	BCL	CHC-C1C	8.50	1.44	1.33
7	2	36	BCL	CHC-C1C	8.57	1.44	1.33
7	Y	36	BCL	CHC-C1C	8.65	1.44	1.33
7	G	3	BCL	CHC-C1C	8.71	1.44	1.33
7	K	36	BCL	CHC-C1C	8.81	1.44	1.33
7	I	5	BCL	CHC-C1C	8.88	1.44	1.33
7	N	11	BCL	CHB-C4A	9.28	1.45	1.33
7	P	38	BCL	CHB-C4A	9.43	1.45	1.33
7	6	36	BCL	CHB-C4A	9.52	1.45	1.33
7	3	38	BCL	CHB-C4A	9.60	1.45	1.33
7	S	36	BCL	CHB-C4A	9.64	1.45	1.33
7	8	36	BCL	CHB-C4A	9.66	1.45	1.33
7	E	1	BCL	CHB-C4A	9.78	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	36	BCL	CHB-C4A	9.81	1.46	1.33
7	K	36	BCL	CHB-C4A	9.81	1.46	1.33
7	V	38	BCL	CHB-C4A	9.87	1.46	1.33
7	2	36	BCL	CHB-C4A	9.90	1.46	1.33
7	U	36	BCL	CHB-C4A	9.90	1.46	1.33
7	G	3	BCL	CHB-C4A	9.91	1.46	1.33
7	I	5	BCL	CHB-C4A	9.94	1.46	1.33
7	Y	36	BCL	CHB-C4A	9.95	1.46	1.33

All (587) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	8	BCL	CMB-C2B-C1B	-6.85	117.93	128.46
7	N	38	BCL	CMB-C2B-C1B	-6.77	118.06	128.46
7	1	38	BCL	CMB-C2B-C1B	-6.77	118.06	128.46
7	3	39	BCL	CMB-C2B-C1B	-6.76	118.07	128.46
7	L	10	BCL	CMB-C2B-C1B	-6.73	118.12	128.46
7	H	6	BCL	CMB-C2B-C1B	-6.72	118.14	128.46
7	5	38	BCL	CMB-C2B-C1B	-6.71	118.16	128.46
7	7	38	BCL	CMB-C2B-C1B	-6.67	118.22	128.46
7	P	39	BCL	CMB-C2B-C1B	-6.66	118.22	128.46
7	F	4	BCL	CMB-C2B-C1B	-6.63	118.27	128.46
7	R	38	BCL	CMB-C2B-C1B	-6.63	118.27	128.46
7	Y	37	BCL	CMB-C2B-C1B	-6.61	118.31	128.46
7	T	38	BCL	CMB-C2B-C1B	-6.59	118.33	128.46
7	D	2	BCL	CMB-C2B-C1B	-6.53	118.43	128.46
7	W	36	BCL	CMB-C2B-C1B	-6.49	118.50	128.46
7	N	11	BCL	O2A-CGA-O1A	-5.35	105.40	123.12
7	A	301	BCL	CED-O2D-CGD	-5.26	103.63	115.97
7	A	301	BCL	CMB-C2B-C1B	-4.92	120.90	128.46
7	5	38	BCL	OBD-CAD-CBD	-4.75	118.77	125.94
7	I	5	BCL	O2A-CGA-O1A	-4.69	107.58	123.12
7	K	36	BCL	OBD-CAD-C3D	-4.67	119.42	128.03
7	P	39	BCL	OBD-CAD-CBD	-4.63	118.95	125.94
7	N	38	BCL	OBD-CAD-CBD	-4.56	119.06	125.94
7	M	36	BCL	OBD-CAD-C3D	-4.55	119.65	128.03
7	L	10	BCL	OBD-CAD-CBD	-4.54	119.08	125.94
7	H	6	BCL	OBD-CAD-CBD	-4.53	119.11	125.94
7	P	38	BCL	OBD-CAD-C3D	-4.52	119.69	128.03
7	U	36	BCL	OBD-CAD-C3D	-4.52	119.69	128.03
7	J	8	BCL	OBD-CAD-CBD	-4.51	119.13	125.94
7	S	36	BCL	OBD-CAD-C3D	-4.50	119.73	128.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	38	BCL	OBD-CAD-CBD	-4.50	119.15	125.94
7	V	38	BCL	OBD-CAD-C3D	-4.50	119.74	128.03
7	G	3	BCL	OBD-CAD-C3D	-4.48	119.78	128.03
7	T	38	BCL	OBD-CAD-CBD	-4.46	119.21	125.94
7	I	5	BCL	OBD-CAD-C3D	-4.42	119.89	128.03
7	F	4	BCL	OBD-CAD-CBD	-4.42	119.27	125.94
7	B	304	BCL	CAC-C3C-C2C	-4.41	103.15	114.24
7	Y	37	BCL	OBD-CAD-CBD	-4.41	119.29	125.94
7	7	38	BCL	OBD-CAD-CBD	-4.40	119.30	125.94
7	E	1	BCL	OBD-CAD-C3D	-4.40	119.93	128.03
7	N	11	BCL	OBD-CAD-C3D	-4.39	119.93	128.03
7	D	2	BCL	OBD-CAD-CBD	-4.39	119.31	125.94
7	3	39	BCL	OBD-CAD-CBD	-4.37	119.35	125.94
7	Y	36	BCL	OBD-CAD-C3D	-4.36	119.98	128.03
7	1	38	BCL	OBD-CAD-CBD	-4.36	119.35	125.94
7	W	36	BCL	OBD-CAD-CBD	-4.36	119.36	125.94
7	2	36	BCL	OBD-CAD-C3D	-4.32	120.07	128.03
7	3	38	BCL	OBD-CAD-C3D	-4.29	120.12	128.03
7	M	36	BCL	O2A-CGA-O1A	-4.29	108.91	123.12
7	8	36	BCL	OBD-CAD-C3D	-4.27	120.15	128.03
7	6	36	BCL	OBD-CAD-C3D	-4.23	120.24	128.03
7	1	38	BCL	O2D-CGD-O1D	-4.22	115.32	123.82
7	V	38	BCL	O1D-CGD-CBD	-4.20	117.06	124.60
7	K	36	BCL	O1D-CGD-CBD	-4.20	117.06	124.60
7	3	39	BCL	O2D-CGD-O1D	-4.17	115.42	123.82
7	B	303	BCL	CMB-C2B-C1B	-4.16	122.07	128.46
7	W	36	BCL	O2D-CGD-O1D	-4.16	115.46	123.82
7	L	10	BCL	O2D-CGD-O1D	-4.14	115.49	123.82
7	6	36	BCL	CMB-C2B-C1B	-4.14	122.10	128.46
7	R	38	BCL	O2D-CGD-O1D	-4.12	115.52	123.82
7	S	36	BCL	O1D-CGD-CBD	-4.12	117.19	124.60
7	8	36	BCL	O1D-CGD-CBD	-4.12	117.20	124.60
7	M	36	BCL	O1D-CGD-CBD	-4.12	117.21	124.60
7	G	3	BCL	O1D-CGD-CBD	-4.10	117.23	124.60
7	I	5	BCL	O1D-CGD-CBD	-4.08	117.28	124.60
7	3	38	BCL	CMB-C2B-C1B	-4.07	122.21	128.46
7	P	39	BCL	O2D-CGD-O1D	-4.06	115.64	123.82
7	E	1	BCL	O1D-CGD-CBD	-4.06	117.32	124.60
7	N	11	BCL	CMB-C2B-C1B	-4.05	122.23	128.46
7	P	38	BCL	O1D-CGD-CBD	-4.05	117.33	124.60
7	N	38	BCL	O2D-CGD-O1D	-4.05	115.67	123.82
7	J	8	BCL	O2D-CGD-O1D	-4.05	115.68	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	2	36	BCL	O1D-CGD-CBD	-4.04	117.34	124.60
7	T	38	BCL	O2D-CGD-O1D	-4.04	115.69	123.82
7	U	36	BCL	O1D-CGD-CBD	-4.04	117.35	124.60
7	N	11	BCL	O1D-CGD-CBD	-4.04	117.35	124.60
7	Y	37	BCL	O2D-CGD-O1D	-4.04	115.70	123.82
7	Y	36	BCL	O1D-CGD-CBD	-4.03	117.36	124.60
7	6	36	BCL	O1D-CGD-CBD	-4.02	117.39	124.60
7	2	36	BCL	CMB-C2B-C1B	-4.01	122.30	128.46
7	Y	36	BCL	CMB-C2B-C1B	-4.01	122.30	128.46
7	M	36	BCL	CMB-C2B-C1B	-4.00	122.32	128.46
7	S	36	BCL	CMB-C2B-C1B	-3.99	122.33	128.46
7	H	6	BCL	O2D-CGD-O1D	-3.98	115.81	123.82
7	I	5	BCL	CMB-C2B-C1B	-3.98	122.34	128.46
7	U	36	BCL	CMB-C2B-C1B	-3.98	122.35	128.46
7	K	36	BCL	CMB-C2B-C1B	-3.98	122.35	128.46
7	7	38	BCL	O2D-CGD-O1D	-3.98	115.82	123.82
7	V	38	BCL	O2A-CGA-O1A	-3.96	110.00	123.12
7	P	38	BCL	CMB-C2B-C1B	-3.95	122.40	128.46
8	A	401	BPH	C3D-CAD-CBD	-3.94	102.02	107.60
7	3	38	BCL	O1D-CGD-CBD	-3.94	117.53	124.60
7	5	38	BCL	O2D-CGD-O1D	-3.92	115.94	123.82
7	D	2	BCL	O2D-CGD-O1D	-3.91	115.94	123.82
7	8	36	BCL	CMB-C2B-C1B	-3.91	122.45	128.46
7	E	1	BCL	CMB-C2B-C1B	-3.91	122.45	128.46
7	G	3	BCL	CMB-C2B-C1B	-3.91	122.46	128.46
7	F	4	BCL	O2D-CGD-O1D	-3.90	115.98	123.82
7	V	38	BCL	CMB-C2B-C1B	-3.90	122.47	128.46
8	B	402	BPH	C1C-NC-C4C	-3.89	107.04	110.54
7	L	10	BCL	C4B-CHC-C1C	-3.70	122.79	130.12
7	J	8	BCL	C4B-CHC-C1C	-3.66	122.86	130.12
7	H	6	BCL	C4B-CHC-C1C	-3.65	122.89	130.12
7	P	39	BCL	C4B-CHC-C1C	-3.59	123.02	130.12
7	R	38	BCL	C4B-CHC-C1C	-3.55	123.08	130.12
7	T	38	BCL	C4B-CHC-C1C	-3.55	123.08	130.12
7	N	38	BCL	C4B-CHC-C1C	-3.52	123.14	130.12
7	5	38	BCL	C4B-CHC-C1C	-3.50	123.19	130.12
7	3	39	BCL	C4B-CHC-C1C	-3.48	123.23	130.12
7	D	2	BCL	C4B-CHC-C1C	-3.47	123.25	130.12
7	F	4	BCL	C4B-CHC-C1C	-3.44	123.30	130.12
7	W	36	BCL	C4B-CHC-C1C	-3.39	123.40	130.12
7	7	38	BCL	C4B-CHC-C1C	-3.38	123.42	130.12
7	1	38	BCL	C4B-CHC-C1C	-3.38	123.43	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	301	BCL	C3D-CAD-CBD	-3.37	102.83	107.60
7	Y	37	BCL	C4B-CHC-C1C	-3.36	123.45	130.12
7	B	304	BCL	CMB-C2B-C1B	-3.36	123.30	128.46
7	J	8	BCL	C2A-C1A-CHA	-3.32	118.03	123.92
8	A	401	BPH	C1-C2-C3	-3.27	119.93	125.96
7	L	10	BCL	C2A-C1A-CHA	-3.26	118.14	123.92
7	N	38	BCL	C2A-C1A-CHA	-3.26	118.14	123.92
7	P	39	BCL	C2A-C1A-CHA	-3.25	118.16	123.92
7	H	6	BCL	C2A-C1A-CHA	-3.25	118.16	123.92
7	S	36	BCL	O2A-CGA-O1A	-3.24	112.39	123.12
7	7	38	BCL	C2A-C1A-CHA	-3.20	118.24	123.92
7	B	304	BCL	CAA-C2A-C3A	-3.20	104.05	112.81
7	H	6	BCL	O1D-CGD-CBD	-3.18	118.89	124.60
7	8	36	BCL	O2A-CGA-O1A	-3.16	112.64	123.12
7	3	39	BCL	C2A-C1A-CHA	-3.15	118.33	123.92
7	R	38	BCL	C2A-C1A-CHA	-3.14	118.35	123.92
7	F	4	BCL	O1D-CGD-CBD	-3.14	118.97	124.60
7	Y	37	BCL	C2A-C1A-CHA	-3.13	118.38	123.92
7	D	2	BCL	C2A-C1A-CHA	-3.12	118.38	123.92
7	F	4	BCL	C2A-C1A-CHA	-3.12	118.38	123.92
7	T	38	BCL	C2A-C1A-CHA	-3.12	118.39	123.92
7	D	2	BCL	O1D-CGD-CBD	-3.10	119.03	124.60
7	J	8	BCL	O1D-CGD-CBD	-3.10	119.03	124.60
7	5	38	BCL	C1-O2A-CGA	-3.08	105.51	116.14
7	5	38	BCL	C2A-C1A-CHA	-3.07	118.48	123.92
7	N	38	BCL	O1D-CGD-CBD	-3.05	119.12	124.60
7	W	36	BCL	C2A-C1A-CHA	-3.05	118.51	123.92
7	1	38	BCL	C2A-C1A-CHA	-3.05	118.51	123.92
7	7	38	BCL	O1D-CGD-CBD	-3.05	119.13	124.60
7	A	302	BCL	CMB-C2B-C1B	-3.04	123.79	128.46
7	A	302	BCL	CHA-C1A-NA	-3.04	119.12	126.18
8	B	402	BPH	O2A-CGA-O1A	-3.02	116.05	123.55
7	A	301	BCL	OBG-CAB-CBB	-3.01	113.29	120.16
7	V	38	BCL	CMA-C3A-C4A	-3.01	103.69	111.77
7	A	302	BCL	O1D-CGD-CBD	-2.99	119.23	124.60
7	S	36	BCL	CMA-C3A-C4A	-2.99	103.74	111.77
7	Y	37	BCL	O1D-CGD-CBD	-2.98	119.24	124.60
7	5	38	BCL	O1D-CGD-CBD	-2.97	119.28	124.60
7	W	36	BCL	O1D-CGD-CBD	-2.97	119.28	124.60
7	A	301	BCL	CAA-C2A-C3A	-2.96	104.69	112.81
7	U	36	BCL	CMA-C3A-C4A	-2.96	103.83	111.77
7	A	302	BCL	C15-C13-C12	-2.95	97.92	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	303	BCL	CAC-C3C-C2C	-2.95	106.83	114.24
7	P	38	BCL	CMA-C3A-C4A	-2.93	103.90	111.77
7	N	11	BCL	CMA-C3A-C4A	-2.92	103.91	111.77
7	R	38	BCL	O1D-CGD-CBD	-2.92	119.35	124.60
7	L	10	BCL	O1D-CGD-CBD	-2.92	119.36	124.60
7	2	36	BCL	CMA-C3A-C4A	-2.92	103.93	111.77
7	1	38	BCL	O1D-CGD-CBD	-2.91	119.37	124.60
7	Y	36	BCL	CMA-C3A-C4A	-2.90	103.98	111.77
7	G	3	BCL	CMA-C3A-C4A	-2.88	104.05	111.77
7	T	38	BCL	O1D-CGD-CBD	-2.88	119.44	124.60
7	P	39	BCL	O1D-CGD-CBD	-2.87	119.44	124.60
8	A	401	BPH	C1C-NC-C4C	-2.87	107.96	110.54
7	3	39	BCL	O1D-CGD-CBD	-2.86	119.46	124.60
7	E	1	BCL	CMA-C3A-C4A	-2.86	104.08	111.77
7	M	36	BCL	CMA-C3A-C4A	-2.85	104.11	111.77
7	6	36	BCL	CMA-C3A-C4A	-2.84	104.13	111.77
7	K	36	BCL	CMA-C3A-C4A	-2.82	104.18	111.77
7	8	36	BCL	CMA-C3A-C4A	-2.81	104.23	111.77
7	3	38	BCL	CMA-C3A-C4A	-2.80	104.25	111.77
7	I	5	BCL	CMA-C3A-C4A	-2.79	104.27	111.77
7	5	38	BCL	CHB-C4A-NA	-2.79	120.66	124.51
7	B	304	BCL	OBD-CAD-CBD	-2.78	121.74	125.94
7	B	304	BCL	CHA-C1A-NA	-2.78	119.72	126.18
7	L	10	BCL	CHB-C4A-NA	-2.76	120.69	124.51
7	A	302	BCL	CAA-C2A-C3A	-2.75	105.28	112.81
7	R	38	BCL	CHB-C4A-NA	-2.74	120.72	124.51
7	P	39	BCL	CHB-C4A-NA	-2.71	120.76	124.51
7	Y	37	BCL	CHB-C4A-NA	-2.71	120.76	124.51
7	A	302	BCL	OBB-CAB-CBB	-2.71	113.98	120.16
7	3	39	BCL	CHB-C4A-NA	-2.70	120.78	124.51
7	A	301	BCL	CHA-C1A-NA	-2.68	119.94	126.18
7	A	302	BCL	CAC-C3C-C2C	-2.67	107.52	114.24
7	1	38	BCL	CHB-C4A-NA	-2.67	120.82	124.51
7	T	38	BCL	CHB-C4A-NA	-2.67	120.82	124.51
8	B	402	BPH	CAA-C2A-C3A	-2.66	105.53	112.81
7	A	302	BCL	CMA-C3A-C2A	-2.64	103.04	113.77
7	6	36	BCL	CHC-C1C-NC	-2.64	120.86	124.51
7	N	38	BCL	CHB-C4A-NA	-2.64	120.87	124.51
8	A	401	BPH	C7-C6-C5	-2.61	105.86	113.11
7	B	303	BCL	O2D-CGD-O1D	-2.60	118.59	123.82
7	B	303	BCL	CHA-C1A-NA	-2.56	120.22	126.18
8	B	402	BPH	C2B-C1B-NB	-2.56	106.03	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	6	BCL	CHB-C4A-NA	-2.55	120.99	124.51
7	A	301	BCL	C4-C3-C2	-2.54	116.90	123.69
7	J	8	BCL	CHB-C4A-NA	-2.53	121.01	124.51
7	A	301	BCL	O2A-CGA-O1A	-2.53	117.28	123.55
7	7	38	BCL	CHB-C4A-NA	-2.52	121.02	124.51
7	N	11	BCL	CHC-C1C-NC	-2.52	121.02	124.51
7	W	36	BCL	CHB-C4A-NA	-2.52	121.03	124.51
7	D	2	BCL	CHB-C4A-NA	-2.50	121.05	124.51
7	F	4	BCL	CHB-C4A-NA	-2.50	121.05	124.51
7	P	38	BCL	CHC-C1C-NC	-2.49	121.07	124.51
7	B	303	BCL	CAC-C3C-C4C	-2.47	107.09	112.58
7	W	36	BCL	CAA-C2A-C1A	-2.47	103.89	111.97
7	K	36	BCL	CHC-C1C-NC	-2.44	121.14	124.51
7	T	38	BCL	CAA-C2A-C1A	-2.44	103.98	111.97
7	R	38	BCL	CAA-C2A-C1A	-2.42	104.05	111.97
7	8	36	BCL	CHC-C1C-NC	-2.42	121.17	124.51
7	Y	37	BCL	CAA-C2A-C1A	-2.40	104.10	111.97
7	S	36	BCL	CHC-C1C-NC	-2.40	121.19	124.51
7	P	39	BCL	CAA-C2A-C1A	-2.38	104.16	111.97
7	5	38	BCL	CAA-C2A-C1A	-2.38	104.16	111.97
8	A	401	BPH	CAA-C2A-C3A	-2.38	106.28	112.81
7	1	38	BCL	CAA-C2A-C1A	-2.38	104.17	111.97
7	D	2	BCL	CAA-C2A-C1A	-2.36	104.23	111.97
8	A	401	BPH	C2B-C1B-NB	-2.35	106.34	109.82
7	3	38	BCL	O2A-CGA-O1A	-2.35	115.35	123.12
7	A	302	BCL	C17-C16-C15	-2.35	101.91	113.25
7	B	304	BCL	CMA-C3A-C4A	-2.34	105.47	111.77
7	3	38	BCL	CHC-C1C-NC	-2.34	121.28	124.51
7	I	5	BCL	CHC-C1C-NC	-2.34	121.28	124.51
7	N	38	BCL	CAA-C2A-C1A	-2.33	104.33	111.97
7	M	36	BCL	CHC-C1C-NC	-2.33	121.29	124.51
7	L	10	BCL	CAA-C2A-C1A	-2.33	104.35	111.97
7	3	39	BCL	CAA-C2A-C1A	-2.33	104.35	111.97
7	A	301	BCL	C6-C5-C3	-2.31	107.42	112.66
7	F	4	BCL	CAA-C2A-C1A	-2.31	104.41	111.97
8	B	402	BPH	CAA-C2A-C1A	-2.31	106.32	112.28
7	5	38	BCL	C4A-NA-C1A	-2.30	103.59	106.45
7	7	38	BCL	CAA-C2A-C1A	-2.30	104.44	111.97
7	2	36	BCL	CHC-C1C-NC	-2.30	121.33	124.51
7	A	301	BCL	CMA-C3A-C2A	-2.29	104.46	113.77
7	V	38	BCL	CHC-C1C-NC	-2.29	121.34	124.51
7	Y	36	BCL	CHC-C1C-NC	-2.29	121.35	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	6	BCL	CAA-C2A-C1A	-2.29	104.48	111.97
7	G	3	BCL	CHC-C1C-NC	-2.28	121.36	124.51
7	E	1	BCL	CHC-C1C-NC	-2.28	121.36	124.51
7	B	304	BCL	C5-C3-C2	-2.28	116.44	121.10
7	U	36	BCL	CHC-C1C-NC	-2.28	121.36	124.51
7	P	39	BCL	C4A-NA-C1A	-2.26	103.64	106.45
7	K	36	BCL	CMA-C3A-C2A	-2.23	104.72	113.77
7	J	8	BCL	CAA-C2A-C1A	-2.22	104.71	111.97
8	A	401	BPH	C4B-C3B-CAB	-2.21	121.92	130.09
7	1	38	BCL	OBD-CAD-C3D	-2.21	123.95	128.03
7	I	5	BCL	C1B-CHB-C4A	-2.21	125.74	130.12
7	L	10	BCL	C4A-NA-C1A	-2.21	103.72	106.45
7	R	38	BCL	C4A-NA-C1A	-2.20	103.72	106.45
7	A	302	BCL	O2A-CGA-O1A	-2.19	118.11	123.55
7	2	36	BCL	CMA-C3A-C2A	-2.19	104.89	113.77
7	3	39	BCL	C4A-NA-C1A	-2.19	103.73	106.45
7	3	38	BCL	CMA-C3A-C2A	-2.19	104.90	113.77
7	1	38	BCL	C4A-NA-C1A	-2.18	103.74	106.45
7	N	11	BCL	CMA-C3A-C2A	-2.16	105.02	113.77
7	B	304	BCL	OBB-CAB-CBB	-2.16	115.24	120.16
7	M	36	BCL	C1B-CHB-C4A	-2.15	125.85	130.12
7	Y	36	BCL	CMA-C3A-C2A	-2.15	105.04	113.77
7	I	5	BCL	CMA-C3A-C2A	-2.14	105.08	113.77
8	A	401	BPH	CAA-C2A-C1A	-2.13	106.78	112.28
7	6	36	BCL	CMA-C3A-C2A	-2.12	105.16	113.77
7	N	38	BCL	C4A-NA-C1A	-2.12	103.82	106.45
7	A	302	BCL	C3D-CAD-CBD	-2.12	104.60	107.60
7	M	36	BCL	CMA-C3A-C2A	-2.11	105.20	113.77
7	U	36	BCL	C1B-CHB-C4A	-2.10	125.95	130.12
7	K	36	BCL	C1B-CHB-C4A	-2.10	125.96	130.12
7	8	36	BCL	C1B-CHB-C4A	-2.10	125.97	130.12
7	G	3	BCL	C1B-CHB-C4A	-2.09	125.97	130.12
7	3	39	BCL	OBD-CAD-C3D	-2.09	124.18	128.03
7	P	38	BCL	CMA-C3A-C2A	-2.09	105.30	113.77
7	E	1	BCL	C1B-CHB-C4A	-2.09	125.98	130.12
7	8	36	BCL	CBA-CAA-C2A	-2.09	107.56	113.80
7	Y	37	BCL	C4A-NA-C1A	-2.08	103.87	106.45
7	G	3	BCL	CMA-C3A-C2A	-2.07	105.35	113.77
7	N	11	BCL	C1B-CHB-C4A	-2.07	126.02	130.12
7	T	38	BCL	C4A-NA-C1A	-2.07	103.89	106.45
7	P	38	BCL	C1B-CHB-C4A	-2.07	126.03	130.12
7	S	36	BCL	C1B-CHB-C4A	-2.06	126.04	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	36	BCL	CMA-C3A-C2A	-2.05	105.46	113.77
7	B	303	BCL	OBD-CAD-CBD	-2.05	122.84	125.94
7	I	5	BCL	CBA-CAA-C2A	-2.05	107.67	113.80
7	S	36	BCL	CBA-CAA-C2A	-2.05	107.67	113.80
7	B	303	BCL	C1-C2-C3	-2.05	122.18	125.96
7	V	38	BCL	CMA-C3A-C2A	-2.04	105.48	113.77
7	Y	37	BCL	OBD-CAD-C3D	-2.04	124.28	128.03
7	E	1	BCL	CBA-CAA-C2A	-2.03	107.72	113.80
7	7	38	BCL	CHD-C4C-NC	-2.03	122.83	125.08
7	6	36	BCL	CBA-CAA-C2A	-2.02	107.76	113.80
7	V	38	BCL	C1B-CHB-C4A	-2.02	126.12	130.12
7	S	36	BCL	CMA-C3A-C2A	-2.01	105.61	113.77
7	Y	36	BCL	CBA-CAA-C2A	-2.01	107.78	113.80
7	H	6	BCL	C4A-NA-C1A	-2.01	103.96	106.45
7	A	301	BCL	CMA-C3A-C4A	-2.00	106.39	111.77
7	W	36	BCL	OBD-CAD-C3D	-2.00	124.34	128.03
7	B	304	BCL	CMA-C3A-C2A	-2.00	105.66	113.77
7	U	36	BCL	CBA-CAA-C2A	-2.00	107.81	113.80
7	B	304	BCL	OBD-CAD-C3D	2.00	131.71	128.03
7	D	2	BCL	C1D-CHD-C4C	2.01	128.91	125.92
7	6	36	BCL	CAA-C2A-C3A	2.01	118.32	112.81
7	V	38	BCL	CAA-C2A-C3A	2.01	118.32	112.81
7	Y	37	BCL	C1D-CHD-C4C	2.03	128.95	125.92
7	U	36	BCL	CAA-C2A-C3A	2.04	118.39	112.81
7	6	36	BCL	O2A-CGA-CBA	2.04	120.75	112.33
8	A	401	BPH	CMC-C2C-C1C	2.04	117.81	112.09
7	T	38	BCL	C1D-CHD-C4C	2.05	128.97	125.92
7	W	36	BCL	C1D-CHD-C4C	2.05	128.97	125.92
7	A	301	BCL	C2C-C3C-C4C	2.06	104.42	101.34
7	E	1	BCL	CAA-C2A-C3A	2.07	118.48	112.81
7	3	39	BCL	C1D-CHD-C4C	2.09	129.03	125.92
7	S	36	BCL	CAA-C2A-C3A	2.09	118.55	112.81
7	E	1	BCL	C2A-C3A-C4A	2.10	105.26	101.87
8	B	402	BPH	CAC-C3C-C4C	2.11	118.09	112.67
7	P	38	BCL	C2A-C3A-C4A	2.11	105.28	101.87
7	J	8	BCL	C1D-CHD-C4C	2.12	129.08	125.92
7	L	10	BCL	C1D-CHD-C4C	2.12	129.08	125.92
7	G	3	BCL	C2A-C3A-C4A	2.13	105.31	101.87
7	7	38	BCL	C1D-CHD-C4C	2.13	129.09	125.92
7	I	5	BCL	C2A-C3A-C4A	2.13	105.31	101.87
7	B	304	BCL	CMB-C2B-C3B	2.14	128.86	124.89
7	M	36	BCL	C2A-C3A-C4A	2.15	105.35	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	38	BCL	C1D-CHD-C4C	2.15	129.13	125.92
7	8	36	BCL	C2A-C3A-C4A	2.16	105.35	101.87
7	H	6	BCL	C1D-CHD-C4C	2.17	129.16	125.92
7	8	36	BCL	CAA-C2A-C3A	2.18	118.78	112.81
7	U	36	BCL	C2A-C3A-C4A	2.19	105.41	101.87
7	P	39	BCL	C1D-CHD-C4C	2.20	129.20	125.92
7	V	38	BCL	C2A-C3A-C4A	2.22	105.45	101.87
7	A	302	BCL	C14-C13-C15	2.23	119.50	111.36
8	A	401	BPH	C1-O2A-CGA	2.26	122.19	116.77
7	N	38	BCL	C1D-CHD-C4C	2.28	129.31	125.92
7	S	36	BCL	C2A-C3A-C4A	2.28	105.55	101.87
7	S	36	BCL	O1A-CGA-CBA	2.28	132.70	123.68
7	6	36	BCL	C2A-C3A-C4A	2.30	105.59	101.87
7	B	304	BCL	O2D-CGD-CBD	2.31	115.42	111.30
7	N	11	BCL	C2A-C3A-C4A	2.32	105.62	101.87
7	3	38	BCL	C2A-C3A-C4A	2.32	105.62	101.87
7	2	36	BCL	C2A-C3A-C4A	2.32	105.62	101.87
7	2	36	BCL	O2A-CGA-CBA	2.34	121.98	112.33
7	Y	36	BCL	C2A-C3A-C4A	2.39	105.73	101.87
8	B	402	BPH	C1B-NB-C4B	2.41	111.28	106.52
7	8	36	BCL	CAA-CBA-CGA	2.47	120.79	113.35
7	3	38	BCL	CAA-CBA-CGA	2.48	120.81	113.35
7	I	5	BCL	CAA-CBA-CGA	2.48	120.82	113.35
7	8	36	BCL	CHB-C4A-NA	2.48	127.95	124.51
7	6	36	BCL	CAA-CBA-CGA	2.49	120.83	113.35
7	V	38	BCL	CAA-CBA-CGA	2.49	120.85	113.35
7	E	1	BCL	O2A-CGA-CBA	2.49	122.61	112.33
7	S	36	BCL	CAA-CBA-CGA	2.50	120.87	113.35
7	U	36	BCL	CAA-CBA-CGA	2.51	120.91	113.35
7	B	303	BCL	CMB-C2B-C3B	2.52	129.56	124.89
7	G	3	BCL	CED-O2D-CGD	2.54	121.92	115.97
7	2	36	BCL	CAA-CBA-CGA	2.54	121.00	113.35
7	6	36	BCL	CHB-C4A-NA	2.55	128.03	124.51
7	P	38	BCL	CAA-CBA-CGA	2.55	121.02	113.35
7	E	1	BCL	CAA-CBA-CGA	2.55	121.03	113.35
7	G	3	BCL	CAA-CBA-CGA	2.56	121.06	113.35
7	M	36	BCL	CAA-CBA-CGA	2.56	121.06	113.35
7	K	36	BCL	CHB-C4A-NA	2.56	128.06	124.51
7	I	5	BCL	CED-O2D-CGD	2.56	121.98	115.97
7	Y	36	BCL	CAA-CBA-CGA	2.57	121.10	113.35
7	N	11	BCL	CED-O2D-CGD	2.57	122.00	115.97
8	A	401	BPH	C1B-NB-C4B	2.58	111.63	106.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	302	BCL	C2C-C3C-C4C	2.59	105.21	101.34
7	K	36	BCL	CAA-CBA-CGA	2.61	121.21	113.35
7	E	1	BCL	CED-O2D-CGD	2.62	122.11	115.97
7	N	11	BCL	CHB-C4A-NA	2.62	128.13	124.51
7	N	11	BCL	CAA-CBA-CGA	2.63	121.26	113.35
8	B	402	BPH	CAC-C3C-C2C	2.64	120.87	114.24
7	E	1	BCL	CHB-C4A-NA	2.64	128.16	124.51
7	A	302	BCL	O2D-CGD-CBD	2.64	116.02	111.30
7	3	38	BCL	CHB-C4A-NA	2.65	128.18	124.51
7	B	304	BCL	C4-C3-C5	2.67	119.92	115.29
7	A	301	BCL	OBB-CAB-C3B	2.69	125.07	119.95
7	2	36	BCL	CMB-C2B-C3B	2.69	129.88	124.89
7	S	36	BCL	CHB-C4A-NA	2.71	128.27	124.51
7	M	36	BCL	CED-O2D-CGD	2.74	122.39	115.97
7	P	38	BCL	CHB-C4A-NA	2.74	128.30	124.51
7	6	36	BCL	CMB-C2B-C3B	2.74	129.98	124.89
7	3	38	BCL	CMB-C2B-C3B	2.76	130.01	124.89
7	2	36	BCL	CHB-C4A-NA	2.77	128.34	124.51
7	U	36	BCL	CHB-C4A-NA	2.78	128.35	124.51
7	Y	36	BCL	CMB-C2B-C3B	2.78	130.05	124.89
7	8	36	BCL	CMB-C2B-C3B	2.79	130.06	124.89
7	V	38	BCL	CHB-C4A-NA	2.79	128.38	124.51
7	M	36	BCL	CHB-C4A-NA	2.80	128.38	124.51
7	G	3	BCL	CHB-C4A-NA	2.80	128.39	124.51
7	G	3	BCL	CMB-C2B-C3B	2.80	130.09	124.89
7	V	38	BCL	CMB-C2B-C3B	2.81	130.10	124.89
7	M	36	BCL	CMB-C2B-C3B	2.83	130.14	124.89
7	P	38	BCL	CMB-C2B-C3B	2.84	130.16	124.89
7	E	1	BCL	CMB-C2B-C3B	2.84	130.17	124.89
7	N	11	BCL	CMB-C2B-C3B	2.85	130.19	124.89
7	K	36	BCL	CMB-C2B-C3B	2.86	130.20	124.89
7	Y	36	BCL	CHB-C4A-NA	2.86	128.47	124.51
8	A	401	BPH	O1D-CGD-CBD	2.90	129.81	124.60
7	I	5	BCL	CMB-C2B-C3B	2.90	130.28	124.89
7	U	36	BCL	CMB-C2B-C3B	2.91	130.29	124.89
7	I	5	BCL	CHB-C4A-NA	2.93	128.56	124.51
7	S	36	BCL	CMB-C2B-C3B	2.95	130.36	124.89
7	A	301	BCL	OBD-CAD-C3D	2.97	133.49	128.03
7	K	36	BCL	CED-O2D-CGD	3.03	123.07	115.97
7	2	36	BCL	CED-O2D-CGD	3.13	123.30	115.97
7	A	301	BCL	C5-C3-C2	3.15	127.54	121.10
7	A	301	BCL	CMB-C2B-C3B	3.18	130.79	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	401	BPH	C4D-C3D-CAD	3.21	109.61	107.78
7	M	36	BCL	O1A-CGA-CBA	3.25	136.52	123.68
7	G	3	BCL	C1-O2A-CGA	3.30	127.54	116.14
7	V	38	BCL	CED-O2D-CGD	3.37	123.88	115.97
7	I	5	BCL	O1A-CGA-CBA	3.42	137.20	123.68
7	Y	36	BCL	CBC-CAC-C3C	3.51	121.46	113.51
7	M	36	BCL	CBC-CAC-C3C	3.52	121.49	113.51
7	I	5	BCL	CBC-CAC-C3C	3.55	121.56	113.51
7	K	36	BCL	CBC-CAC-C3C	3.56	121.57	113.51
7	J	8	BCL	CGD-CBD-CAD	3.58	122.69	110.71
7	V	38	BCL	CBC-CAC-C3C	3.62	121.72	113.51
7	2	36	BCL	CBC-CAC-C3C	3.64	121.76	113.51
7	S	36	BCL	CBC-CAC-C3C	3.65	121.79	113.51
7	3	38	BCL	CBC-CAC-C3C	3.66	121.79	113.51
7	N	11	BCL	CBC-CAC-C3C	3.66	121.80	113.51
7	E	1	BCL	CBC-CAC-C3C	3.66	121.80	113.51
7	L	10	BCL	CGD-CBD-CAD	3.67	123.00	110.71
7	U	36	BCL	CBC-CAC-C3C	3.67	121.83	113.51
7	G	3	BCL	CBC-CAC-C3C	3.70	121.89	113.51
7	8	36	BCL	O2A-CGA-CBA	3.73	127.72	112.33
7	P	38	BCL	CBC-CAC-C3C	3.75	122.00	113.51
7	H	6	BCL	CGD-CBD-CAD	3.75	123.27	110.71
7	N	38	BCL	CGD-CBD-CAD	3.75	123.28	110.71
7	1	38	BCL	CGD-CBD-CAD	3.76	123.30	110.71
7	3	39	BCL	CGD-CBD-CAD	3.76	123.30	110.71
7	Y	37	BCL	CGD-CBD-CAD	3.77	123.33	110.71
7	V	38	BCL	C1-O2A-CGA	3.77	129.15	116.14
7	F	4	BCL	CGD-CBD-CAD	3.78	123.39	110.71
7	R	38	BCL	CGD-CBD-CAD	3.79	123.42	110.71
7	6	36	BCL	CBC-CAC-C3C	3.80	122.12	113.51
7	D	2	BCL	CGD-CBD-CAD	3.81	123.49	110.71
7	V	38	BCL	CAC-C3C-C4C	3.81	121.05	112.58
7	P	39	BCL	CGD-CBD-CAD	3.82	123.50	110.71
7	8	36	BCL	CAC-C3C-C4C	3.82	121.06	112.58
7	T	38	BCL	CGD-CBD-CAD	3.82	123.52	110.71
7	2	36	BCL	CAC-C3C-C4C	3.82	121.07	112.58
7	U	36	BCL	CAC-C3C-C4C	3.84	121.10	112.58
7	W	36	BCL	CGD-CBD-CAD	3.84	123.60	110.71
7	7	38	BCL	CGD-CBD-CAD	3.85	123.62	110.71
7	S	36	BCL	CAC-C3C-C4C	3.86	121.14	112.58
7	G	3	BCL	CAC-C3C-C4C	3.86	121.15	112.58
7	Y	36	BCL	CAC-C3C-C4C	3.88	121.20	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	8	36	BCL	CBC-CAC-C3C	3.89	122.32	113.51
7	5	38	BCL	CGD-CBD-CAD	3.89	123.74	110.71
7	P	38	BCL	CAC-C3C-C4C	3.91	121.27	112.58
7	6	36	BCL	CAC-C3C-C4C	3.93	121.31	112.58
7	N	11	BCL	CAC-C3C-C4C	3.93	121.31	112.58
7	M	36	BCL	CAC-C3C-C4C	3.97	121.39	112.58
7	I	5	BCL	CAC-C3C-C4C	3.97	121.39	112.58
7	E	1	BCL	CAC-C3C-C4C	3.97	121.40	112.58
7	K	36	BCL	CAC-C3C-C4C	3.98	121.42	112.58
7	3	38	BCL	CAC-C3C-C4C	3.98	121.42	112.58
7	V	38	BCL	O2A-CGA-CBA	4.32	130.16	112.33
7	A	301	BCL	C1-O2A-CGA	4.37	127.25	116.77
8	A	401	BPH	C3C-C4C-NC	4.59	112.29	107.97
7	1	38	BCL	C2C-C3C-C4C	4.75	108.46	101.34
7	5	38	BCL	C2C-C3C-C4C	4.87	108.63	101.34
7	3	39	BCL	C2C-C3C-C4C	4.90	108.68	101.34
7	Y	37	BCL	C2C-C3C-C4C	4.94	108.74	101.34
7	T	38	BCL	C2C-C3C-C4C	4.94	108.74	101.34
7	F	4	BCL	C2C-C3C-C4C	4.95	108.76	101.34
7	7	38	BCL	C2C-C3C-C4C	4.99	108.82	101.34
7	W	36	BCL	C2C-C3C-C4C	5.03	108.88	101.34
7	R	38	BCL	C2C-C3C-C4C	5.05	108.90	101.34
7	P	39	BCL	C2C-C3C-C4C	5.05	108.90	101.34
7	D	2	BCL	CAC-C3C-C4C	5.05	123.79	112.58
7	N	38	BCL	C2C-C3C-C4C	5.08	108.95	101.34
8	B	402	BPH	C3C-C4C-NC	5.10	112.78	107.97
7	D	2	BCL	C2C-C3C-C4C	5.12	109.01	101.34
7	7	38	BCL	CAC-C3C-C4C	5.15	124.01	112.58
7	R	38	BCL	CAC-C3C-C4C	5.15	124.02	112.58
7	F	4	BCL	CAC-C3C-C4C	5.16	124.04	112.58
7	W	36	BCL	CAC-C3C-C4C	5.17	124.06	112.58
7	L	10	BCL	CAC-C3C-C4C	5.17	124.06	112.58
7	H	6	BCL	C2C-C3C-C4C	5.17	109.09	101.34
7	P	38	BCL	CED-O2D-CGD	5.23	128.22	115.97
7	N	38	BCL	CAC-C3C-C4C	5.23	124.18	112.58
7	H	6	BCL	CAC-C3C-C4C	5.23	124.19	112.58
7	J	8	BCL	C2C-C3C-C4C	5.23	109.17	101.34
7	P	39	BCL	CAC-C3C-C4C	5.23	124.19	112.58
7	5	38	BCL	CAC-C3C-C4C	5.23	124.20	112.58
7	J	8	BCL	CAC-C3C-C4C	5.23	124.20	112.58
7	T	38	BCL	CAC-C3C-C4C	5.25	124.23	112.58
7	1	38	BCL	CAC-C3C-C4C	5.27	124.27	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	10	BCL	C2C-C3C-C4C	5.27	109.24	101.34
7	Y	37	BCL	CAC-C3C-C4C	5.28	124.31	112.58
7	3	39	BCL	CAC-C3C-C4C	5.29	124.32	112.58
7	Y	36	BCL	CMD-C2D-C3D	5.38	134.87	124.89
7	2	36	BCL	CMD-C2D-C3D	5.38	134.88	124.89
7	V	38	BCL	CMD-C2D-C3D	5.44	134.98	124.89
7	6	36	BCL	CMD-C2D-C3D	5.46	135.02	124.89
7	N	11	BCL	O2A-CGA-CBA	5.49	134.96	112.33
7	U	36	BCL	CMD-C2D-C3D	5.51	135.11	124.89
7	N	11	BCL	CMD-C2D-C3D	5.52	135.13	124.89
7	E	1	BCL	CMD-C2D-C3D	5.52	135.14	124.89
7	M	36	BCL	CMD-C2D-C3D	5.54	135.17	124.89
7	S	36	BCL	CMD-C2D-C3D	5.54	135.18	124.89
7	8	36	BCL	CMD-C2D-C3D	5.55	135.19	124.89
7	3	38	BCL	CMD-C2D-C3D	5.60	135.28	124.89
7	I	5	BCL	CMD-C2D-C3D	5.60	135.29	124.89
7	P	38	BCL	CMD-C2D-C3D	5.61	135.30	124.89
7	G	3	BCL	CMD-C2D-C3D	5.69	135.44	124.89
7	K	36	BCL	CMD-C2D-C3D	5.70	135.46	124.89
7	N	11	BCL	O2D-CGD-CBD	5.76	121.59	111.30
7	N	11	BCL	C1-O2A-CGA	5.81	136.21	116.14
7	U	36	BCL	O2D-CGD-CBD	5.86	121.77	111.30
7	P	38	BCL	O2D-CGD-CBD	5.86	121.78	111.30
7	E	1	BCL	O2D-CGD-CBD	5.89	121.83	111.30
7	S	36	BCL	O2D-CGD-CBD	5.90	121.85	111.30
7	6	36	BCL	O2D-CGD-CBD	5.93	121.91	111.30
7	J	8	BCL	C3D-CAD-CBD	5.94	115.99	107.60
7	M	36	BCL	O2D-CGD-CBD	5.95	121.93	111.30
7	2	36	BCL	O2D-CGD-CBD	5.96	121.95	111.30
7	D	2	BCL	CMB-C2B-C3B	5.98	135.98	124.89
7	H	6	BCL	C3D-CAD-CBD	5.98	116.05	107.60
7	T	38	BCL	CMB-C2B-C3B	5.98	136.00	124.89
7	V	38	BCL	O2D-CGD-CBD	5.99	122.01	111.30
7	P	39	BCL	CMB-C2B-C3B	6.00	136.02	124.89
7	H	6	BCL	CMB-C2B-C3B	6.01	136.05	124.89
7	3	38	BCL	O2D-CGD-CBD	6.02	122.05	111.30
7	G	3	BCL	C3D-CAD-CBD	6.02	116.10	107.60
7	W	36	BCL	CMB-C2B-C3B	6.03	136.08	124.89
7	8	36	BCL	O2D-CGD-CBD	6.03	122.08	111.30
7	I	5	BCL	O2D-CGD-CBD	6.04	122.09	111.30
7	5	38	BCL	CMB-C2B-C3B	6.05	136.11	124.89
7	F	4	BCL	CMB-C2B-C3B	6.05	136.12	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	3	BCL	O2D-CGD-CBD	6.06	122.13	111.30
7	K	36	BCL	O2D-CGD-CBD	6.06	122.13	111.30
7	8	36	BCL	C3D-CAD-CBD	6.07	116.18	107.60
7	Y	36	BCL	C3D-CAD-CBD	6.07	116.18	107.60
7	J	8	BCL	CMB-C2B-C3B	6.07	136.16	124.89
7	Y	36	BCL	O2D-CGD-CBD	6.08	122.17	111.30
7	2	36	BCL	C3D-CAD-CBD	6.09	116.20	107.60
7	L	10	BCL	CMB-C2B-C3B	6.09	136.19	124.89
7	F	4	BCL	C3D-CAD-CBD	6.09	116.20	107.60
7	7	38	BCL	C3D-CAD-CBD	6.09	116.20	107.60
7	N	38	BCL	CMB-C2B-C3B	6.09	136.20	124.89
7	3	38	BCL	C3D-CAD-CBD	6.11	116.23	107.60
7	I	5	BCL	C3D-CAD-CBD	6.11	116.23	107.60
7	L	10	BCL	C3D-CAD-CBD	6.11	116.24	107.60
7	7	38	BCL	CMB-C2B-C3B	6.11	136.23	124.89
7	R	38	BCL	CMB-C2B-C3B	6.12	136.24	124.89
7	E	1	BCL	C3D-CAD-CBD	6.12	116.25	107.60
7	Y	37	BCL	CMB-C2B-C3B	6.14	136.28	124.89
7	D	2	BCL	C3D-CAD-CBD	6.14	116.28	107.60
7	W	36	BCL	C3D-CAD-CBD	6.14	116.28	107.60
7	R	38	BCL	C3D-CAD-CBD	6.16	116.31	107.60
7	U	36	BCL	C3D-CAD-CBD	6.21	116.38	107.60
7	T	38	BCL	C3D-CAD-CBD	6.21	116.38	107.60
7	3	39	BCL	CMB-C2B-C3B	6.22	136.43	124.89
7	S	36	BCL	C3D-CAD-CBD	6.23	116.40	107.60
7	1	38	BCL	CMB-C2B-C3B	6.24	136.47	124.89
7	Y	37	BCL	C3D-CAD-CBD	6.24	116.42	107.60
7	K	36	BCL	C3D-CAD-CBD	6.25	116.43	107.60
7	N	38	BCL	C3D-CAD-CBD	6.25	116.43	107.60
7	V	38	BCL	C3D-CAD-CBD	6.26	116.44	107.60
7	6	36	BCL	C3D-CAD-CBD	6.27	116.46	107.60
7	3	39	BCL	C3D-CAD-CBD	6.27	116.46	107.60
7	P	39	BCL	C3D-CAD-CBD	6.29	116.49	107.60
7	M	36	BCL	C3D-CAD-CBD	6.30	116.51	107.60
7	N	11	BCL	C3D-CAD-CBD	6.33	116.55	107.60
7	P	38	BCL	C3D-CAD-CBD	6.39	116.62	107.60
7	5	38	BCL	C3D-CAD-CBD	6.42	116.67	107.60
7	1	38	BCL	C3D-CAD-CBD	6.43	116.68	107.60
7	5	38	BCL	O2D-CGD-CBD	7.55	124.79	111.30
7	T	38	BCL	O2D-CGD-CBD	7.59	124.87	111.30
7	P	39	BCL	O2D-CGD-CBD	7.62	124.91	111.30
7	D	2	BCL	O2D-CGD-CBD	7.68	125.02	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	7	38	BCL	O2D-CGD-CBD	7.69	125.05	111.30
7	F	4	BCL	O2D-CGD-CBD	7.70	125.05	111.30
7	Y	37	BCL	O2D-CGD-CBD	7.70	125.05	111.30
7	3	39	BCL	O2D-CGD-CBD	7.73	125.12	111.30
7	R	38	BCL	O2D-CGD-CBD	7.73	125.12	111.30
7	L	10	BCL	O2D-CGD-CBD	7.75	125.16	111.30
7	N	38	BCL	O2D-CGD-CBD	7.78	125.21	111.30
7	W	36	BCL	O2D-CGD-CBD	7.82	125.27	111.30
7	J	8	BCL	O2D-CGD-CBD	7.83	125.28	111.30
7	H	6	BCL	O2D-CGD-CBD	7.83	125.30	111.30
7	1	38	BCL	O2D-CGD-CBD	7.84	125.31	111.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	Y	36	BCL	CED-O2D-CGD-CBD

There are no ring outliers.

35 monomers are involved in 341 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	1	38	BCL	18	0
7	2	36	BCL	10	0
7	3	38	BCL	8	0
7	3	39	BCL	7	0
7	5	38	BCL	12	0
7	6	36	BCL	3	0
7	7	38	BCL	8	0
7	8	36	BCL	5	0
7	A	301	BCL	7	0
7	A	302	BCL	2	0
8	A	401	BPH	5	0
7	B	303	BCL	4	0
7	B	304	BCL	2	0
7	D	2	BCL	14	0
7	E	1	BCL	14	0
7	F	4	BCL	7	0
7	G	3	BCL	11	0
7	H	6	BCL	11	0
7	I	5	BCL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	8	BCL	32	0
7	K	36	BCL	18	0
7	L	10	BCL	25	0
7	M	36	BCL	13	0
7	N	11	BCL	17	0
7	N	38	BCL	27	0
7	P	38	BCL	41	0
7	P	39	BCL	27	0
7	R	38	BCL	16	0
7	S	36	BCL	10	0
7	T	38	BCL	10	0
7	U	36	BCL	8	0
7	V	38	BCL	8	0
7	W	36	BCL	6	0
7	Y	36	BCL	17	0
7	Y	37	BCL	9	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, 95th 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 ²)	Q<0.9
1	A	0/281	-	-	-	-
2	B	0/302	-	-	-	-
3	C	0/241	-	-	-	-
4	1	0/26	-	-	-	-
4	3	0/26	-	-	-	-
4	5	0/26	-	-	-	-
4	7	0/26	-	-	-	-
4	D	0/26	-	-	-	-
4	F	0/26	-	-	-	-
4	H	0/26	-	-	-	-
4	J	0/26	-	-	-	-
4	L	0/26	-	-	-	-
4	N	0/26	-	-	-	-
4	P	0/26	-	-	-	-
4	R	0/26	-	-	-	-
4	T	0/26	-	-	-	-
4	V	0/26	-	-	-	-
4	X	0/26	-	-	-	-
4	Z	0/26	-	-	-	-
5	2	0/30	-	-	-	-
5	4	0/30	-	-	-	-
5	6	0/30	-	-	-	-
5	8	0/30	-	-	-	-
5	E	0/30	-	-	-	-
5	G	0/30	-	-	-	-
5	I	0/30	-	-	-	-
5	K	0/30	-	-	-	-
5	M	0/30	-	-	-	-
5	O	0/30	-	-	-	-
5	Q	0/30	-	-	-	-
5	S	0/30	-	-	-	-
5	U	0/30	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	W	0/30	-	-	-	-
5	Y	0/30	-	-	-	-
All	All	0/1690	-	-	-	-

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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, 95th 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 ²)	Q<0.9
7	BCL	L	10	47/66	0.73	0.27	-	198,198,198,198	0
6	FE	B	500	1/1	0.94	0.53	-	198,198,198,198	0
7	BCL	B	303	66/66	0.70	0.50	-	198,198,198,198	0
7	BCL	P	39	47/66	0.65	0.30	-	198,198,198,198	0
7	BCL	H	6	47/66	0.77	0.24	-	198,198,198,198	0
7	BCL	S	36	47/66	0.60	0.44	-	198,198,198,198	0
7	BCL	U	36	47/66	0.60	0.37	-	198,198,198,198	0
7	BCL	F	4	47/66	0.67	0.51	-	198,198,198,198	0
7	BCL	V	38	47/66	0.65	0.41	-	198,198,198,198	0
7	BCL	5	38	47/66	0.58	0.57	-	198,198,198,198	0
7	BCL	D	2	47/66	0.68	0.31	-	198,198,198,198	0
7	BCL	Y	37	47/66	0.67	0.47	-	198,198,198,198	0
7	BCL	A	301	66/66	0.71	0.50	-	198,198,198,198	0
7	BCL	N	11	47/66	0.79	0.20	-	198,198,198,198	0
8	BPH	B	402	65/65	0.63	0.55	-	198,198,198,198	0
7	BCL	A	302	66/66	0.69	0.56	-	198,198,198,198	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	BCL	N	38	47/66	0.81	0.19	-	198,198,198,198	0
7	BCL	3	39	47/66	0.73	0.30	-	198,198,198,198	0
7	BCL	7	38	47/66	0.68	0.35	-	198,198,198,198	0
7	BCL	3	38	47/66	0.82	0.19	-	198,198,198,198	0
7	BCL	R	38	47/66	0.67	0.33	-	198,198,198,198	0
7	BCL	E	1	47/66	0.70	0.34	-	198,198,198,198	0
7	BCL	2	36	47/66	0.82	0.32	-	198,198,198,198	0
7	BCL	Y	36	47/66	0.83	0.30	-	198,198,198,198	0
7	BCL	I	5	47/66	0.79	0.31	-	198,198,198,198	0
7	BCL	G	3	47/66	0.79	0.28	-	198,198,198,198	0
7	BCL	W	36	47/66	0.79	0.81	-	198,198,198,198	0
7	BCL	K	36	47/66	0.72	0.29	-	198,198,198,198	0
7	BCL	T	38	47/66	0.67	0.28	-	198,198,198,198	0
7	BCL	M	36	47/66	0.72	0.27	-	198,198,198,198	0
7	BCL	J	8	47/66	0.67	0.27	-	198,198,198,198	0
8	BPH	A	401	65/65	0.52	0.71	-	198,198,198,198	0
7	BCL	6	36	47/66	0.74	0.40	-	198,198,198,198	0
7	BCL	8	36	47/66	0.65	0.59	-	198,198,198,198	0
7	BCL	B	304	66/66	0.70	0.57	-	198,198,198,198	0
7	BCL	1	38	47/66	0.74	0.26	-	198,198,198,198	0
7	BCL	P	38	47/66	0.73	0.24	-	198,198,198,198	0

6.5 Other polymers [i](#)

There are no such residues in this entry.