



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:51 PM GMT

PDB ID : 4TZ1
Title : Ensemble refinement of the E502A variant of sacteLam55A from Streptomyces sp. SirexAA-E in complex with laminaritriose
Authors : Bianchetti, C.M.; Takasuka, T.E.; Yik, E.J.; Bergeman, L.F.; Fox, B.G.
Deposited on : 2014-07-09
Resolution : 1.50 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : **FAILED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

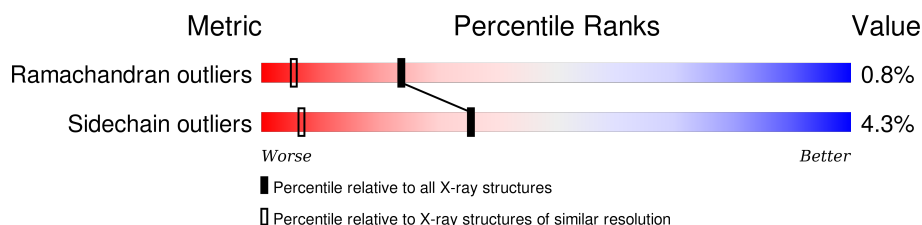
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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))
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)

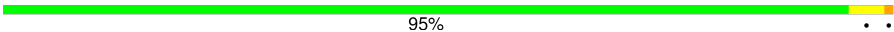
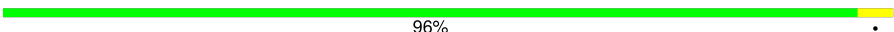
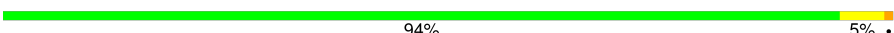









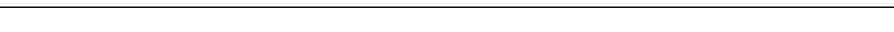

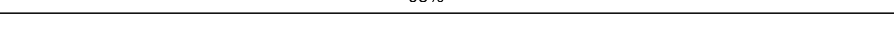
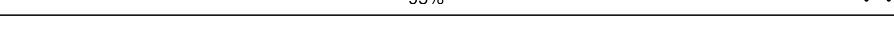
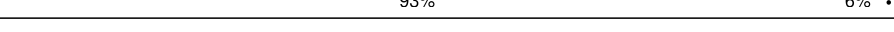
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	549	
1	10-A	549	
1	11-A	549	
1	12-A	549	
1	13-A	549	
1	14-A	549	
1	15-A	549	
1	16-A	549	

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Mol	Chain	Length	Quality of chain
1	17-A	549	 95% . .
1	18-A	549	 96% .
1	19-A	549	 94% 5% . .
1	2-A	549	 94% 6%
1	20-A	549	 93% 5% .
1	21-A	549	 94% 5% . .
1	22-A	549	 94% 6%
1	23-A	549	 95% 5%
1	24-A	549	 94% 6%
1	25-A	549	 93% 6% . .
1	3-A	549	 93% 6% . .
1	4-A	549	 94% 6%
1	5-A	549	 94% 5% .
1	6-A	549	 95% .
1	7-A	549	 95% . .
1	8-A	549	 93% 6% . .
1	9-A	549	 94% 5% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 211855 atoms, of which 97675 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 Putative secreted protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	2-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	3-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	4-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	5-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	6-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	7-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	8-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	9-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	10-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	11-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	12-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	13-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	14-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	15-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	16-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			

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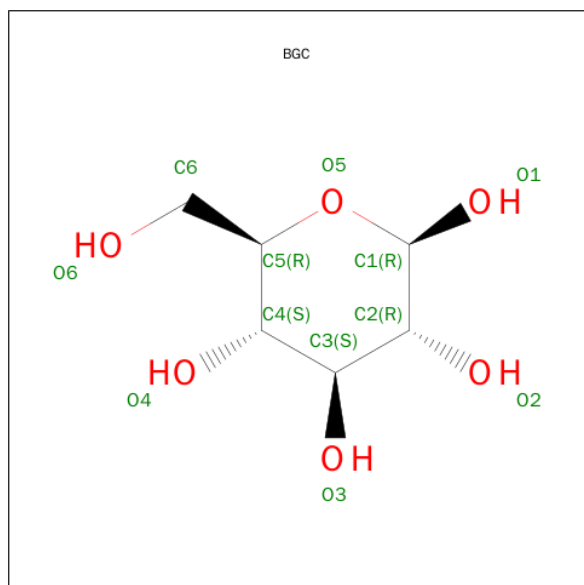
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	18-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	19-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	20-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	21-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	22-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	23-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	24-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	25-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	502	ALA	GLU	engineered mutation	UNP G2NFJ9

- Molecule 2 is BETA-D-GLUCOSE (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1-A	1	Total	C	O	0	0
			11	6	5		
2	2-A	1	Total	C	O	0	0
			11	6	5		
2	3-A	1	Total	C	O	0	0
			11	6	5		
2	4-A	1	Total	C	O	0	0
			11	6	5		
2	5-A	1	Total	C	O	0	0
			11	6	5		
2	6-A	1	Total	C	O	0	0
			11	6	5		
2	7-A	1	Total	C	O	0	0
			11	6	5		
2	8-A	1	Total	C	O	0	0
			11	6	5		
2	9-A	1	Total	C	O	0	0
			11	6	5		
2	10-A	1	Total	C	O	0	0
			11	6	5		
2	11-A	1	Total	C	O	0	0
			11	6	5		
2	12-A	1	Total	C	O	0	0
			11	6	5		
2	13-A	1	Total	C	O	0	0
			11	6	5		
2	14-A	1	Total	C	O	0	0
			11	6	5		
2	15-A	1	Total	C	O	0	0
			11	6	5		
2	16-A	1	Total	C	O	0	0
			11	6	5		
2	17-A	1	Total	C	O	0	0
			11	6	5		
2	18-A	1	Total	C	O	0	0
			11	6	5		
2	19-A	1	Total	C	O	0	0
			11	6	5		
2	20-A	1	Total	C	O	0	0
			11	6	5		
2	21-A	1	Total	C	O	0	0
			11	6	5		
2	22-A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	23-A	1	Total	C	O	0	0
			11	6	5		
2	24-A	1	Total	C	O	0	0
			11	6	5		
2	25-A	1	Total	C	O	0	0
			11	6	5		
2	1-A	1	Total	C	O	0	0
			11	6	5		
2	2-A	1	Total	C	O	0	0
			11	6	5		
2	3-A	1	Total	C	O	0	0
			11	6	5		
2	4-A	1	Total	C	O	0	0
			11	6	5		
2	5-A	1	Total	C	O	0	0
			11	6	5		
2	6-A	1	Total	C	O	0	0
			11	6	5		
2	7-A	1	Total	C	O	0	0
			11	6	5		
2	8-A	1	Total	C	O	0	0
			11	6	5		
2	9-A	1	Total	C	O	0	0
			11	6	5		
2	10-A	1	Total	C	O	0	0
			11	6	5		
2	11-A	1	Total	C	O	0	0
			11	6	5		
2	12-A	1	Total	C	O	0	0
			11	6	5		
2	13-A	1	Total	C	O	0	0
			11	6	5		
2	14-A	1	Total	C	O	0	0
			11	6	5		
2	15-A	1	Total	C	O	0	0
			11	6	5		
2	16-A	1	Total	C	O	0	0
			11	6	5		
2	17-A	1	Total	C	O	0	0
			11	6	5		
2	18-A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	19-A	1	Total	C	O	0	0
			11	6	5		
2	20-A	1	Total	C	O	0	0
			11	6	5		
2	21-A	1	Total	C	O	0	0
			11	6	5		
2	22-A	1	Total	C	O	0	0
			11	6	5		
2	23-A	1	Total	C	O	0	0
			11	6	5		
2	24-A	1	Total	C	O	0	0
			11	6	5		
2	25-A	1	Total	C	O	0	0
			11	6	5		
2	1-A	1	Total	C	O	0	0
			12	6	6		
2	2-A	1	Total	C	O	0	0
			12	6	6		
2	3-A	1	Total	C	O	0	0
			12	6	6		
2	4-A	1	Total	C	O	0	0
			12	6	6		
2	5-A	1	Total	C	O	0	0
			12	6	6		
2	6-A	1	Total	C	O	0	0
			12	6	6		
2	7-A	1	Total	C	O	0	0
			12	6	6		
2	8-A	1	Total	C	O	0	0
			12	6	6		
2	9-A	1	Total	C	O	0	0
			12	6	6		
2	10-A	1	Total	C	O	0	0
			12	6	6		
2	11-A	1	Total	C	O	0	0
			12	6	6		
2	12-A	1	Total	C	O	0	0
			12	6	6		
2	13-A	1	Total	C	O	0	0
			12	6	6		
2	14-A	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	15-A	1	Total	C	O	0	0
			12	6	6		
2	16-A	1	Total	C	O	0	0
			12	6	6		
2	17-A	1	Total	C	O	0	0
			12	6	6		
2	18-A	1	Total	C	O	0	0
			12	6	6		
2	19-A	1	Total	C	O	0	0
			12	6	6		
2	20-A	1	Total	C	O	0	0
			12	6	6		
2	21-A	1	Total	C	O	0	0
			12	6	6		
2	22-A	1	Total	C	O	0	0
			12	6	6		
2	23-A	1	Total	C	O	0	0
			12	6	6		
2	24-A	1	Total	C	O	0	0
			12	6	6		
2	25-A	1	Total	C	O	0	0
			12	6	6		
2	1-A	1	Total	C	O	0	0
			11	6	5		
2	2-A	1	Total	C	O	0	0
			11	6	5		
2	3-A	1	Total	C	O	0	0
			11	6	5		
2	4-A	1	Total	C	O	0	0
			11	6	5		
2	5-A	1	Total	C	O	0	0
			11	6	5		
2	6-A	1	Total	C	O	0	0
			11	6	5		
2	7-A	1	Total	C	O	0	0
			11	6	5		
2	8-A	1	Total	C	O	0	0
			11	6	5		
2	9-A	1	Total	C	O	0	0
			11	6	5		
2	10-A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	11-A	1	Total	C	O	0	0
			11	6	5		
2	12-A	1	Total	C	O	0	0
			11	6	5		
2	13-A	1	Total	C	O	0	0
			11	6	5		
2	14-A	1	Total	C	O	0	0
			11	6	5		
2	15-A	1	Total	C	O	0	0
			11	6	5		
2	16-A	1	Total	C	O	0	0
			11	6	5		
2	17-A	1	Total	C	O	0	0
			11	6	5		
2	18-A	1	Total	C	O	0	0
			11	6	5		
2	19-A	1	Total	C	O	0	0
			11	6	5		
2	20-A	1	Total	C	O	0	0
			11	6	5		
2	21-A	1	Total	C	O	0	0
			11	6	5		
2	22-A	1	Total	C	O	0	0
			11	6	5		
2	23-A	1	Total	C	O	0	0
			11	6	5		
2	24-A	1	Total	C	O	0	0
			11	6	5		
2	25-A	1	Total	C	O	0	0
			11	6	5		
2	1-A	1	Total	C	O	0	0
			11	6	5		
2	2-A	1	Total	C	O	0	0
			11	6	5		
2	3-A	1	Total	C	O	0	0
			11	6	5		
2	4-A	1	Total	C	O	0	0
			11	6	5		
2	5-A	1	Total	C	O	0	0
			11	6	5		
2	6-A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	7-A	1	Total	C	O	0	0
			11	6	5		
2	8-A	1	Total	C	O	0	0
			11	6	5		
2	9-A	1	Total	C	O	0	0
			11	6	5		
2	10-A	1	Total	C	O	0	0
			11	6	5		
2	11-A	1	Total	C	O	0	0
			11	6	5		
2	12-A	1	Total	C	O	0	0
			11	6	5		
2	13-A	1	Total	C	O	0	0
			11	6	5		
2	14-A	1	Total	C	O	0	0
			11	6	5		
2	15-A	1	Total	C	O	0	0
			11	6	5		
2	16-A	1	Total	C	O	0	0
			11	6	5		
2	17-A	1	Total	C	O	0	0
			11	6	5		
2	18-A	1	Total	C	O	0	0
			11	6	5		
2	19-A	1	Total	C	O	0	0
			11	6	5		
2	20-A	1	Total	C	O	0	0
			11	6	5		
2	21-A	1	Total	C	O	0	0
			11	6	5		
2	22-A	1	Total	C	O	0	0
			11	6	5		
2	23-A	1	Total	C	O	0	0
			11	6	5		
2	24-A	1	Total	C	O	0	0
			11	6	5		
2	25-A	1	Total	C	O	0	0
			11	6	5		
2	1-A	1	Total	C	O	0	0
			12	6	6		
2	2-A	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	3-A	1	Total	C	O	0	0
			12	6	6		
2	4-A	1	Total	C	O	0	0
			12	6	6		
2	5-A	1	Total	C	O	0	0
			12	6	6		
2	6-A	1	Total	C	O	0	0
			12	6	6		
2	7-A	1	Total	C	O	0	0
			12	6	6		
2	8-A	1	Total	C	O	0	0
			12	6	6		
2	9-A	1	Total	C	O	0	0
			12	6	6		
2	10-A	1	Total	C	O	0	0
			12	6	6		
2	11-A	1	Total	C	O	0	0
			12	6	6		
2	12-A	1	Total	C	O	0	0
			12	6	6		
2	13-A	1	Total	C	O	0	0
			12	6	6		
2	14-A	1	Total	C	O	0	0
			12	6	6		
2	15-A	1	Total	C	O	0	0
			12	6	6		
2	16-A	1	Total	C	O	0	0
			12	6	6		
2	17-A	1	Total	C	O	0	0
			12	6	6		
2	18-A	1	Total	C	O	0	0
			12	6	6		
2	19-A	1	Total	C	O	0	0
			12	6	6		
2	20-A	1	Total	C	O	0	0
			12	6	6		
2	21-A	1	Total	C	O	0	0
			12	6	6		
2	22-A	1	Total	C	O	0	0
			12	6	6		
2	23-A	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	24-A	1	Total	C	O	0	0
			12	6	6		
2	25-A	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1-A	339	Total	O		0	0
			339	339			
3	2-A	332	Total	O		0	0
			332	332			
3	3-A	343	Total	O		0	0
			343	343			
3	4-A	342	Total	O		0	0
			342	342			
3	5-A	340	Total	O		0	0
			340	340			
3	6-A	340	Total	O		0	0
			340	340			
3	7-A	327	Total	O		0	0
			327	327			
3	8-A	329	Total	O		0	0
			329	329			
3	9-A	329	Total	O		0	0
			329	329			
3	10-A	321	Total	O		0	0
			321	321			
3	11-A	342	Total	O		0	0
			342	342			
3	12-A	315	Total	O		0	0
			315	315			
3	13-A	340	Total	O		0	0
			340	340			
3	14-A	327	Total	O		0	0
			327	327			
3	15-A	354	Total	O		0	0
			354	354			
3	16-A	335	Total	O		0	0
			335	335			
3	17-A	333	Total	O		0	0
			333	333			

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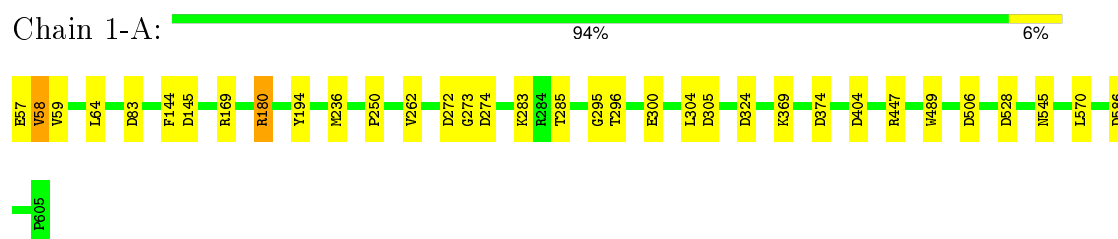
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	18-A	328	Total	O	0	0
			328	328		
3	19-A	320	Total	O	0	0
			320	320		
3	20-A	341	Total	O	0	0
			341	341		
3	21-A	321	Total	O	0	0
			321	321		
3	22-A	304	Total	O	0	0
			304	304		
3	23-A	341	Total	O	0	0
			341	341		
3	24-A	326	Total	O	0	0
			326	326		
3	25-A	336	Total	O	0	0
			336	336		

3 Residue-property plots

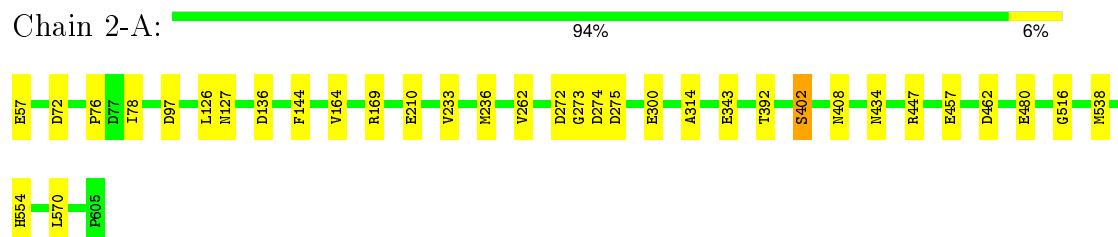
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS failed to run properly.

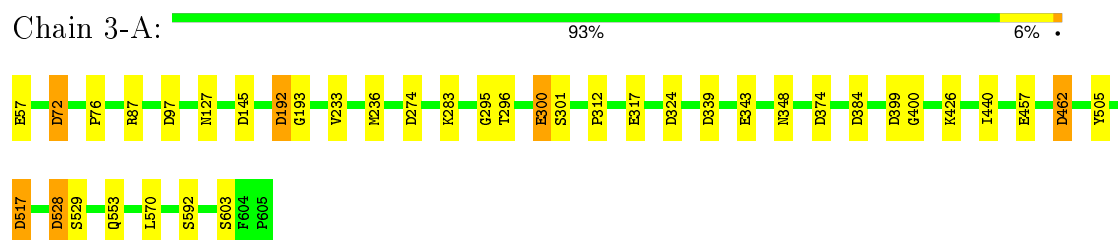
- Molecule 1: Putative secreted protein



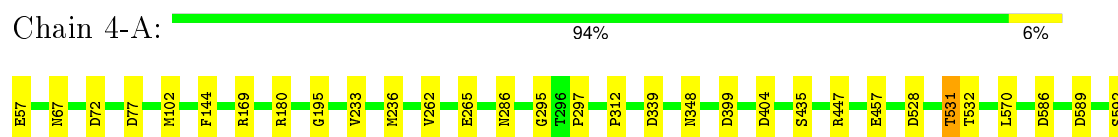
- Molecule 1: Putative secreted protein

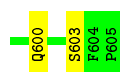


- Molecule 1: Putative secreted protein



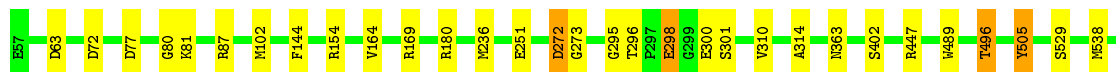
- Molecule 1: Putative secreted protein





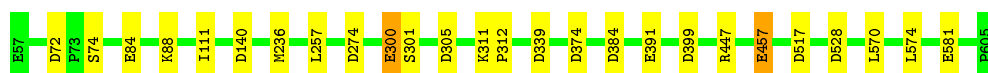
- Molecule 1: Putative secreted protein

Chain 5-A: 94% 5% •



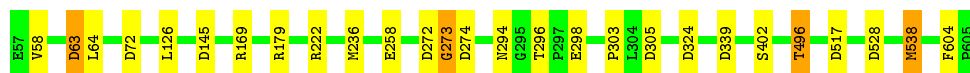
- Molecule 1: Putative secreted protein

Chain 6-A: 95% •



- Molecule 1: Putative secreted protein

Chain 7-A: 95% • •



- Molecule 1: Putative secreted protein

Chain 8-A: 93% 6% •



- Molecule 1: Putative secreted protein

Chain 9-A: 94% 5% •



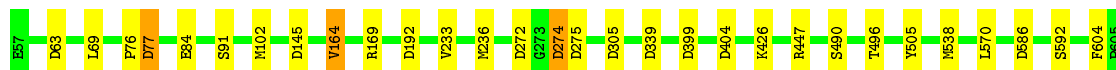
- Molecule 1: Putative secreted protein

Chain 10-A: 96% • •



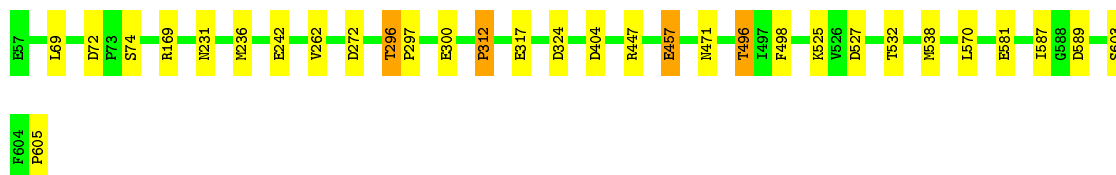
- Molecule 1: Putative secreted protein

Chain 11-A: 95% 5%



- Molecule 1: Putative secreted protein

Chain 12-A: 94% 5%



- Molecule 1: Putative secreted protein

Chain 13-A: 95% 5%



- Molecule 1: Putative secreted protein

Chain 14-A: 95% 5%



- Molecule 1: Putative secreted protein

Chain 15-A: 95% 5%



- Molecule 1: Putative secreted protein

Chain 16-A: 94% 5%



- Molecule 1: Putative secreted protein

Chain 17-A: 95% . .



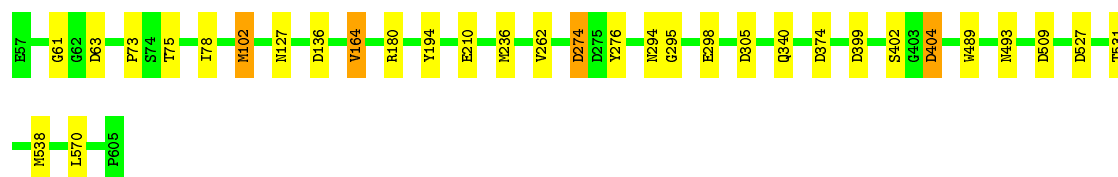
- Molecule 1: Putative secreted protein

Chain 18-A: 96%



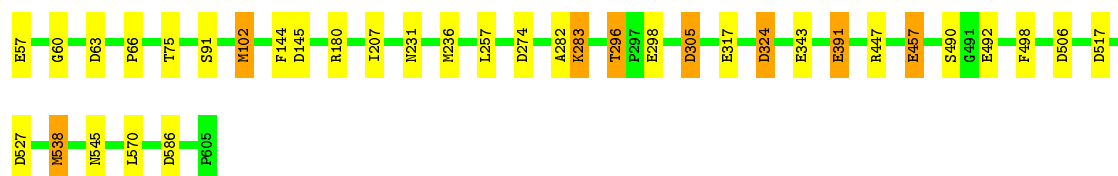
- Molecule 1: Putative secreted protein

Chain 19-A: 94% 5%



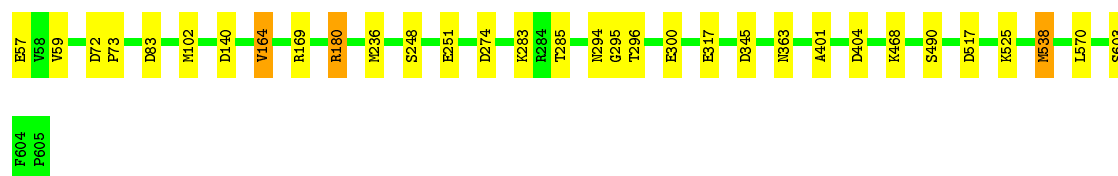
- Molecule 1: Putative secreted protein

Chain 20-A: 93% 5%



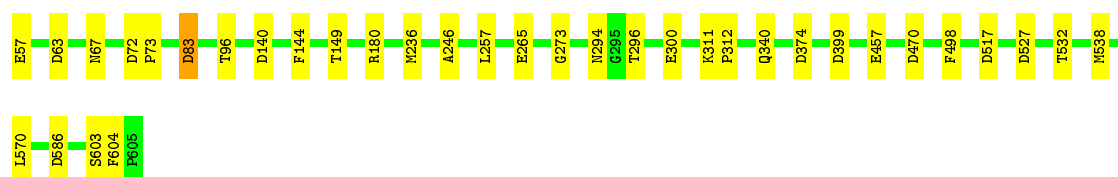
- Molecule 1: Putative secreted protein

Chain 21-A: 94% 5%



- Molecule 1: Putative secreted protein

Chain 22-A: 94% 6%



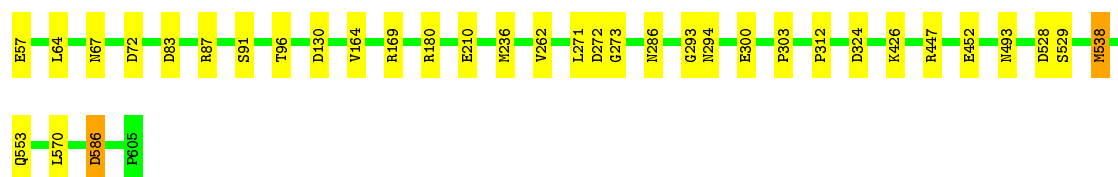
- Molecule 1: Putative secreted protein

Chain 23-A:  95% 5%



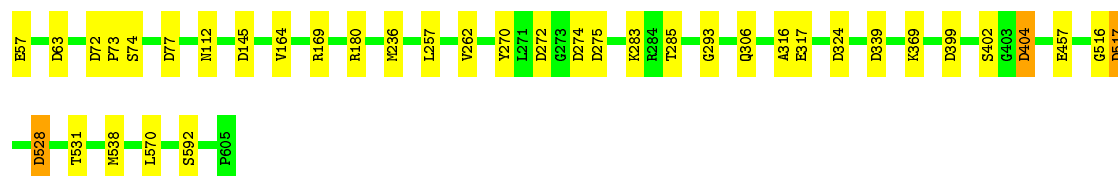
- Molecule 1: Putative secreted protein

Chain 24-A:  94% 6%



- Molecule 1: Putative secreted protein

Chain 25-A:  93% 6%



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.77Å 100.19Å 53.86Å 90.00° 103.49° 90.00°	Depositor
Resolution (Å)	24.23 – 1.50	Depositor
% Data completeness (in resolution range)	99.4 (24.23-1.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.37 (at 1.50Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement: 1.9_1692)	Depositor
R, R_{free}	0.100 , 0.124	Depositor
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.107	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 81428 reflections	Xtriage
Total number of atoms	211855	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BGC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1-A	0.78	5/4280 (0.1%)	0.94	11/5848 (0.2%)
1	2-A	0.74	3/4280 (0.1%)	0.92	6/5848 (0.1%)
1	3-A	0.79	5/4280 (0.1%)	0.94	8/5848 (0.1%)
1	4-A	0.72	2/4280 (0.0%)	0.92	6/5848 (0.1%)
1	5-A	0.77	1/4280 (0.0%)	0.99	14/5848 (0.2%)
1	6-A	0.77	5/4280 (0.1%)	0.95	6/5848 (0.1%)
1	7-A	0.75	1/4280 (0.0%)	0.94	10/5848 (0.2%)
1	8-A	0.77	3/4280 (0.1%)	0.95	14/5848 (0.2%)
1	9-A	0.78	4/4280 (0.1%)	0.97	12/5848 (0.2%)
1	10-A	0.76	3/4280 (0.1%)	0.98	11/5848 (0.2%)
1	11-A	0.75	3/4280 (0.1%)	0.95	12/5848 (0.2%)
1	12-A	0.78	8/4280 (0.2%)	0.94	11/5848 (0.2%)
1	13-A	0.77	4/4280 (0.1%)	0.99	15/5848 (0.3%)
1	14-A	0.75	1/4280 (0.0%)	0.93	7/5848 (0.1%)
1	15-A	0.76	5/4280 (0.1%)	0.97	9/5848 (0.2%)
1	16-A	0.74	3/4280 (0.1%)	0.98	16/5848 (0.3%)
1	17-A	0.75	3/4280 (0.1%)	0.92	8/5848 (0.1%)
1	18-A	0.77	6/4280 (0.1%)	0.94	8/5848 (0.1%)
1	19-A	0.75	3/4280 (0.1%)	0.95	12/5848 (0.2%)
1	20-A	0.78	7/4280 (0.2%)	0.95	12/5848 (0.2%)
1	21-A	0.74	4/4280 (0.1%)	0.98	10/5848 (0.2%)
1	22-A	0.77	4/4280 (0.1%)	0.98	10/5848 (0.2%)
1	23-A	0.74	2/4280 (0.0%)	0.97	10/5848 (0.2%)
1	24-A	0.76	5/4280 (0.1%)	0.93	9/5848 (0.2%)
1	25-A	0.75	4/4280 (0.1%)	0.95	10/5848 (0.2%)
All	All	0.76	94/107000 (0.1%)	0.95	257/146200 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	1
1	2-A	0	1
1	3-A	0	1
1	4-A	0	2
1	7-A	0	2
1	9-A	0	1
1	10-A	0	1
1	11-A	0	2
1	13-A	0	2
1	14-A	0	2
1	15-A	0	1
1	18-A	0	1
1	20-A	0	2
1	21-A	0	1
1	23-A	0	2
1	25-A	0	2
All	All	0	24

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	18-A	180	ARG	CB-CG	-10.28	1.24	1.52
1	20-A	538	MET	CB-CG	-10.08	1.19	1.51
1	3-A	462	ASP	CB-CG	-9.78	1.31	1.51
1	22-A	538	MET	CG-SD	9.54	2.06	1.81
1	1-A	300	GLU	CB-CG	9.27	1.69	1.52
1	13-A	457	GLU	CG-CD	8.99	1.65	1.51
1	6-A	391	GLU	CB-CG	-8.98	1.35	1.52
1	16-A	538	MET	CG-SD	8.77	2.04	1.81
1	18-A	265	GLU	CB-CG	-8.36	1.36	1.52
1	1-A	262	VAL	CB-CG1	-8.19	1.35	1.52
1	12-A	300	GLU	CB-CG	7.95	1.67	1.52
1	21-A	300	GLU	CB-CG	-7.93	1.37	1.52
1	13-A	496	THR	CB-CG2	-7.83	1.26	1.52
1	16-A	242	GLU	CG-CD	-7.58	1.40	1.51
1	9-A	102	MET	CB-CG	7.30	1.74	1.51
1	17-A	102	MET	CB-CG	7.17	1.74	1.51
1	18-A	457	GLU	CB-CG	7.15	1.65	1.52
1	15-A	538	MET	CB-CG	-7.05	1.28	1.51
1	20-A	538	MET	CG-SD	-7.03	1.62	1.81
1	1-A	300	GLU	CG-CD	7.00	1.62	1.51
1	6-A	581	GLU	CD-OE2	6.94	1.33	1.25
1	12-A	300	GLU	CG-CD	6.93	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	13-A	457	GLU	CB-CG	6.79	1.65	1.52
1	19-A	102	MET	CB-CG	6.78	1.73	1.51
1	15-A	538	MET	CG-SD	-6.67	1.63	1.81
1	15-A	457	GLU	CG-CD	6.65	1.61	1.51
1	24-A	300	GLU	CG-CD	6.63	1.61	1.51
1	9-A	343	GLU	CG-CD	-6.63	1.42	1.51
1	11-A	84	GLU	CG-CD	6.58	1.61	1.51
1	20-A	457	GLU	CB-CG	6.48	1.64	1.52
1	22-A	265	GLU	CD-OE2	-6.26	1.18	1.25
1	17-A	180	ARG	CZ-NH1	-6.25	1.25	1.33
1	20-A	317	GLU	CB-CG	6.22	1.64	1.52
1	4-A	265	GLU	CB-CG	-6.21	1.40	1.52
1	24-A	300	GLU	CB-CG	6.20	1.64	1.52
1	25-A	457	GLU	CG-CD	6.13	1.61	1.51
1	17-A	82	VAL	CB-CG1	-6.10	1.40	1.52
1	3-A	300	GLU	CB-CG	6.09	1.63	1.52
1	15-A	99	TYR	CD2-CE2	-6.09	1.30	1.39
1	20-A	391	GLU	CB-CG	6.08	1.63	1.52
1	12-A	457	GLU	CG-CD	6.07	1.61	1.51
1	20-A	492	GLU	CG-CD	-6.06	1.42	1.51
1	3-A	300	GLU	CG-CD	6.04	1.61	1.51
1	19-A	102	MET	CG-SD	6.03	1.96	1.81
1	21-A	317	GLU	CG-CD	-6.01	1.43	1.51
1	18-A	298	GLU	CB-CG	5.97	1.63	1.52
1	22-A	457	GLU	CG-CD	5.91	1.60	1.51
1	8-A	265	GLU	CD-OE1	5.86	1.32	1.25
1	23-A	242	GLU	CB-CG	5.85	1.63	1.52
1	8-A	164	VAL	CB-CG1	-5.80	1.40	1.52
1	24-A	180	ARG	CB-CG	-5.80	1.36	1.52
1	11-A	102	MET	CG-SD	-5.75	1.66	1.81
1	4-A	457	GLU	CG-CD	5.67	1.60	1.51
1	12-A	242	GLU	CB-CG	5.64	1.62	1.52
1	1-A	369	LYS	CD-CE	5.59	1.65	1.51
1	2-A	457	GLU	CG-CD	5.57	1.60	1.51
1	6-A	391	GLU	CG-CD	-5.56	1.43	1.51
1	24-A	262	VAL	CB-CG2	5.55	1.64	1.52
1	3-A	505	TYR	CB-CG	5.54	1.59	1.51
1	3-A	317	GLU	CD-OE2	5.51	1.31	1.25
1	15-A	102	MET	CG-SD	-5.50	1.66	1.81
1	14-A	87	ARG	CB-CG	5.48	1.67	1.52
1	6-A	300	GLU	CD-OE1	5.47	1.31	1.25
1	6-A	457	GLU	CB-CG	-5.46	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	18-A	457	GLU	CG-CD	5.44	1.60	1.51
1	12-A	457	GLU	CB-CG	5.43	1.62	1.52
1	21-A	180	ARG	CD-NE	-5.42	1.37	1.46
1	18-A	298	GLU	CG-CD	5.42	1.60	1.51
1	21-A	140	ASP	CB-CG	5.42	1.63	1.51
1	22-A	180	ARG	CB-CG	-5.38	1.38	1.52
1	25-A	164	VAL	CB-CG1	-5.37	1.41	1.52
1	12-A	242	GLU	CG-CD	5.37	1.59	1.51
1	2-A	262	VAL	CB-CG1	-5.34	1.41	1.52
1	9-A	265	GLU	CD-OE2	-5.34	1.19	1.25
1	12-A	300	GLU	CD-OE1	5.32	1.31	1.25
1	12-A	581	GLU	CD-OE2	-5.30	1.19	1.25
1	25-A	517	ASP	CB-CG	-5.27	1.40	1.51
1	10-A	471	ASN	CB-CG	5.27	1.63	1.51
1	24-A	452	GLU	CG-CD	5.24	1.59	1.51
1	13-A	180	ARG	CD-NE	-5.19	1.37	1.46
1	25-A	528	ASP	CB-CG	-5.16	1.41	1.51
1	19-A	402	SER	CB-OG	5.15	1.49	1.42
1	16-A	493	ASN	CB-CG	5.13	1.62	1.51
1	2-A	300	GLU	CG-CD	5.12	1.59	1.51
1	11-A	505	TYR	CD1-CE1	-5.11	1.31	1.39
1	20-A	305	ASP	CB-CG	5.10	1.62	1.51
1	5-A	505	TYR	CD2-CE2	-5.10	1.31	1.39
1	9-A	538	MET	CB-CG	-5.10	1.35	1.51
1	10-A	496	THR	CB-CG2	-5.08	1.35	1.52
1	10-A	306	GLN	CB-CG	-5.06	1.38	1.52
1	23-A	242	GLU	CG-CD	5.06	1.59	1.51
1	1-A	545	ASN	CB-CG	5.04	1.62	1.51
1	7-A	258	GLU	CD-OE2	5.04	1.31	1.25
1	8-A	493	ASN	CB-CG	-5.02	1.39	1.51

All (257) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16-A	538	MET	CG-SD-CE	-20.07	68.09	100.20
1	10-A	538	MET	CG-SD-CE	-19.51	68.99	100.20
1	21-A	538	MET	CG-SD-CE	-19.04	69.73	100.20
1	22-A	538	MET	CG-SD-CE	-18.99	69.81	100.20
1	23-A	538	MET	CG-SD-CE	-18.91	69.94	100.20
1	13-A	538	MET	CG-SD-CE	-18.14	71.18	100.20
1	24-A	538	MET	CG-SD-CE	-15.77	74.96	100.20
1	8-A	538	MET	CG-SD-CE	-15.36	75.63	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-A	384	ASP	CB-CG-OD2	13.41	130.37	118.30
1	14-A	538	MET	CG-SD-CE	-13.37	78.81	100.20
1	11-A	538	MET	CG-SD-CE	-13.36	78.83	100.20
1	11-A	102	MET	CB-CG-SD	-12.55	74.75	112.40
1	12-A	538	MET	CG-SD-CE	-12.41	80.34	100.20
1	25-A	538	MET	CG-SD-CE	-12.15	80.76	100.20
1	19-A	180	ARG	NE-CZ-NH2	11.67	126.14	120.30
1	5-A	169	ARG	NE-CZ-NH2	-11.67	114.46	120.30
1	19-A	180	ARG	NE-CZ-NH1	-11.46	114.57	120.30
1	17-A	102	MET	CG-SD-CE	-11.22	82.25	100.20
1	22-A	180	ARG	NE-CZ-NH1	-11.05	114.77	120.30
1	3-A	462	ASP	CB-CG-OD1	-9.90	109.39	118.30
1	9-A	538	MET	CG-SD-CE	-9.77	84.57	100.20
1	19-A	538	MET	CB-CG-SD	-9.71	83.26	112.40
1	2-A	169	ARG	NE-CZ-NH2	-9.65	115.47	120.30
1	10-A	296	THR	N-CA-C	-9.65	84.94	111.00
1	1-A	180	ARG	NE-CZ-NH1	-9.58	115.51	120.30
1	23-A	538	MET	CB-CG-SD	9.46	140.78	112.40
1	15-A	102	MET	CB-CG-SD	-9.45	84.06	112.40
1	18-A	169	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	22-A	180	ARG	NE-CZ-NH2	9.15	124.87	120.30
1	7-A	538	MET	CG-SD-CE	-8.97	85.84	100.20
1	20-A	102	MET	CA-CB-CG	8.96	128.53	113.30
1	5-A	538	MET	CG-SD-CE	8.78	114.25	100.20
1	16-A	272	ASP	CB-CG-OD2	8.76	126.18	118.30
1	9-A	72	ASP	CB-CG-OD1	-8.57	110.59	118.30
1	2-A	169	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	1-A	180	ARG	NE-CZ-NH2	8.39	124.50	120.30
1	5-A	496	THR	N-CA-CB	-8.32	94.48	110.30
1	21-A	180	ARG	NE-CZ-NH2	8.32	124.46	120.30
1	13-A	180	ARG	NE-CZ-NH2	8.24	124.42	120.30
1	10-A	180	ARG	NE-CZ-NH1	-8.20	116.20	120.30
1	25-A	180	ARG	NE-CZ-NH2	8.20	124.40	120.30
1	20-A	538	MET	CG-SD-CE	-8.20	87.08	100.20
1	12-A	169	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	9-A	102	MET	CG-SD-CE	-8.09	87.26	100.20
1	10-A	140	ASP	CB-CG-OD1	7.86	125.38	118.30
1	25-A	402	SER	N-CA-CB	-7.86	98.72	110.50
1	15-A	538	MET	CG-SD-CE	-7.79	87.74	100.20
1	8-A	77	ASP	CB-CG-OD1	7.74	125.27	118.30
1	5-A	102	MET	CG-SD-CE	-7.74	87.82	100.20
1	10-A	180	ARG	NE-CZ-NH2	7.69	124.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	13-A	192	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	24-A	169	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	13-A	538	MET	CB-CG-SD	-7.57	89.70	112.40
1	17-A	324	ASP	CB-CG-OD1	7.57	125.11	118.30
1	2-A	97	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	25-A	169	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	5-A	169	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	10-A	496	THR	CA-CB-OG1	7.46	124.66	109.00
1	20-A	102	MET	CG-SD-CE	-7.44	88.30	100.20
1	3-A	72	ASP	CB-CG-OD1	7.38	124.94	118.30
1	16-A	527	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	16-A	460	ARG	NE-CZ-NH1	-7.35	116.63	120.30
1	22-A	140	ASP	CB-CG-OD2	7.34	124.91	118.30
1	18-A	180	ARG	NE-CZ-NH1	-7.33	116.64	120.30
1	12-A	300	GLU	N-CA-C	-7.28	91.35	111.00
1	13-A	192	ASP	CB-CG-OD1	7.27	124.84	118.30
1	13-A	140	ASP	CB-CG-OD1	7.25	124.82	118.30
1	23-A	528	ASP	CB-CG-OD1	7.23	124.81	118.30
1	21-A	102	MET	CG-SD-CE	-7.21	88.66	100.20
1	22-A	83	ASP	CB-CG-OD2	7.18	124.76	118.30
1	9-A	266	LYS	CD-CE-NZ	7.16	128.16	111.70
1	15-A	538	MET	CB-CG-SD	-7.09	91.12	112.40
1	17-A	140	ASP	CB-CG-OD1	7.01	124.61	118.30
1	13-A	63	ASP	CB-CG-OD1	7.00	124.60	118.30
1	19-A	404	ASP	CB-CG-OD1	-6.93	112.07	118.30
1	21-A	180	ARG	CG-CD-NE	-6.87	97.37	111.80
1	24-A	528	ASP	CB-CG-OD1	6.85	124.46	118.30
1	1-A	145	ASP	CB-CG-OD1	6.84	124.45	118.30
1	19-A	102	MET	CB-CG-SD	6.82	132.87	112.40
1	7-A	179	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	4-A	180	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	8-A	272	ASP	CB-CG-OD2	6.78	124.40	118.30
1	21-A	164	VAL	CB-CA-C	-6.76	98.56	111.40
1	5-A	154	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	23-A	517	ASP	CB-CG-OD1	6.72	124.35	118.30
1	1-A	369	LYS	CD-CE-NZ	6.69	127.08	111.70
1	23-A	180	ARG	NE-CZ-NH1	-6.67	116.96	120.30
1	14-A	531	THR	CB-CA-C	-6.66	93.61	111.60
1	5-A	447	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	5-A	295	GLY	N-CA-C	6.65	129.73	113.10
1	14-A	169	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	14-A	180	ARG	NE-CZ-NH2	-6.64	116.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	20-A	538	MET	CB-CG-SD	-6.59	92.62	112.40
1	9-A	447	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	19-A	399	ASP	CB-CG-OD1	6.58	124.22	118.30
1	15-A	538	MET	CB-CA-C	-6.57	97.26	110.40
1	5-A	447	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	21-A	140	ASP	CB-CG-OD1	6.56	124.20	118.30
1	10-A	496	THR	CA-CB-CG2	-6.54	103.25	112.40
1	23-A	271	LEU	CA-CB-CG	6.51	130.28	115.30
1	15-A	180	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	24-A	586	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	20-A	527	ASP	CB-CG-OD1	6.37	124.03	118.30
1	18-A	169	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	21-A	83	ASP	CB-CG-OD1	6.33	124.00	118.30
1	20-A	102	MET	CB-CG-SD	6.32	131.37	112.40
1	20-A	506	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	5-A	63	ASP	CB-CG-OD1	-6.28	112.65	118.30
1	8-A	273	GLY	N-CA-C	6.28	128.79	113.10
1	17-A	426	LYS	CD-CE-NZ	-6.27	97.28	111.70
1	16-A	180	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	19-A	538	MET	CG-SD-CE	6.26	110.21	100.20
1	19-A	298	GLU	N-CA-C	6.23	127.83	111.00
1	25-A	180	ARG	NE-CZ-NH1	-6.23	117.18	120.30
1	19-A	102	MET	CG-SD-CE	-6.23	90.23	100.20
1	17-A	447	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	10-A	58	VAL	CB-CA-C	-6.22	99.59	111.40
1	21-A	300	GLU	CB-CA-C	-6.20	97.99	110.40
1	9-A	72	ASP	CB-CG-OD2	6.20	123.88	118.30
1	18-A	179	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	16-A	447	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	4-A	169	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	9-A	140	ASP	CB-CG-OD1	6.15	123.83	118.30
1	14-A	538	MET	CB-CG-SD	6.14	130.83	112.40
1	1-A	528	ASP	CB-CG-OD1	6.12	123.81	118.30
1	20-A	180	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	15-A	102	MET	CG-SD-CE	6.08	109.93	100.20
1	6-A	447	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	9-A	72	ASP	CB-CA-C	6.07	122.54	110.40
1	6-A	447	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	4-A	447	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	3-A	462	ASP	CB-CG-OD2	6.03	123.73	118.30
1	12-A	538	MET	CB-CG-SD	6.02	130.47	112.40
1	16-A	180	ARG	NE-CZ-NH2	6.00	123.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16-A	447	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	18-A	180	ARG	CB-CA-C	5.99	122.38	110.40
1	7-A	273	GLY	N-CA-C	-5.98	98.16	113.10
1	21-A	169	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	10-A	527	ASP	CB-CG-OD1	5.97	123.67	118.30
1	4-A	399	ASP	CB-CG-OD1	5.97	123.67	118.30
1	7-A	145	ASP	CB-CG-OD1	5.94	123.64	118.30
1	16-A	102	MET	CG-SD-CE	-5.93	90.70	100.20
1	11-A	275	ASP	CB-CG-OD1	5.88	123.59	118.30
1	24-A	447	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	11-A	102	MET	CG-SD-CE	-5.86	90.82	100.20
1	7-A	305	ASP	CB-CG-OD2	5.84	123.56	118.30
1	5-A	505	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	22-A	374	ASP	CB-CG-OD1	5.80	123.52	118.30
1	17-A	374	ASP	CB-CG-OD1	5.80	123.52	118.30
1	5-A	298	GLU	CB-CA-C	-5.77	98.86	110.40
1	13-A	97	ASP	CB-CG-OD2	5.76	123.48	118.30
1	7-A	63	ASP	CB-CG-OD2	5.76	123.48	118.30
1	17-A	528	ASP	CB-CG-OD1	5.76	123.48	118.30
1	14-A	169	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	4-A	180	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	16-A	460	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	18-A	180	ARG	CG-CD-NE	-5.70	99.83	111.80
1	14-A	315	THR	CB-CA-C	-5.69	96.23	111.60
1	1-A	447	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	11-A	447	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	12-A	404	ASP	CB-CG-OD1	5.67	123.40	118.30
1	3-A	517	ASP	N-CA-CB	5.64	120.75	110.60
1	18-A	180	ARG	N-CA-CB	-5.64	100.44	110.60
1	16-A	77	ASP	CB-CG-OD1	5.60	123.34	118.30
1	24-A	426	LYS	CD-CE-NZ	-5.59	98.84	111.70
1	16-A	75	THR	CB-CA-C	-5.59	96.51	111.60
1	11-A	496	THR	OG1-CB-CG2	5.58	122.83	110.00
1	23-A	288	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	25-A	72	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	22-A	257	LEU	CB-CG-CD1	-5.57	101.54	111.00
1	9-A	536	TRP	CA-CB-CG	5.56	124.26	113.70
1	20-A	274	ASP	CB-CG-OD1	5.55	123.30	118.30
1	8-A	449	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	9-A	79	GLN	CA-CB-CG	5.54	125.59	113.40
1	23-A	242	GLU	OE1-CD-OE2	-5.54	116.65	123.30
1	13-A	77	ASP	CB-CG-OD2	-5.53	113.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	22-A	517	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	13-A	374	ASP	CB-CG-OD1	5.53	123.28	118.30
1	11-A	272	ASP	CB-CG-OD1	-5.53	113.33	118.30
1	19-A	374	ASP	CB-CG-OD1	5.53	123.27	118.30
1	1-A	374	ASP	CB-CG-OD1	5.52	123.27	118.30
1	12-A	496	THR	N-CA-CB	-5.51	99.84	110.30
1	12-A	447	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	25-A	538	MET	CA-CB-CG	-5.49	103.96	113.30
1	11-A	426	LYS	CD-CE-NZ	-5.48	99.09	111.70
1	8-A	468	LYS	CD-CE-NZ	5.48	124.30	111.70
1	9-A	460	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	23-A	505	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	1-A	64	LEU	CA-CB-CG	5.47	127.88	115.30
1	15-A	457	GLU	CA-CB-CG	5.47	125.42	113.40
1	12-A	242	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	9-A	283	LYS	CD-CE-NZ	5.44	124.22	111.70
1	6-A	384	ASP	CB-CG-OD1	-5.42	113.43	118.30
1	19-A	298	GLU	CB-CA-C	-5.41	99.58	110.40
1	16-A	426	LYS	CD-CE-NZ	5.41	124.14	111.70
1	8-A	447	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	22-A	374	ASP	CB-CG-OD2	-5.39	113.44	118.30
1	20-A	586	ASP	CB-CG-OD2	5.38	123.15	118.30
1	12-A	447	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	2-A	447	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	7-A	222	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	3-A	528	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	25-A	275	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	1-A	169	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	13-A	222	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	1-A	145	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	20-A	447	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	8-A	525	LYS	CD-CE-NZ	5.29	123.88	111.70
1	8-A	528	ASP	CB-CG-OD1	5.29	123.06	118.30
1	25-A	404	ASP	CB-CG-OD1	5.28	123.05	118.30
1	3-A	374	ASP	CB-CG-OD1	5.25	123.03	118.30
1	21-A	83	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	20-A	180	ARG	CD-NE-CZ	-5.24	116.27	123.60
1	12-A	589	ASP	CB-CG-OD1	5.21	122.99	118.30
1	3-A	426	LYS	CD-CE-NZ	5.21	123.67	111.70
1	3-A	87	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	11-A	169	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	7-A	63	ASP	CB-CG-OD1	-5.18	113.63	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	374	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	25-A	145	ASP	CB-CG-OD1	5.18	122.96	118.30
1	11-A	164	VAL	CB-CA-C	-5.16	101.59	111.40
1	10-A	462	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	23-A	140	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	16-A	374	ASP	CB-CG-OD1	5.15	122.93	118.30
1	4-A	531	THR	CB-CA-C	-5.15	97.70	111.60
1	15-A	462	ASP	CB-CG-OD2	5.14	122.93	118.30
1	13-A	496	THR	OG1-CB-CG2	-5.12	98.21	110.00
1	12-A	169	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	13-A	145	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	11-A	69	LEU	CA-CB-CG	5.11	127.04	115.30
1	5-A	180	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	8-A	179	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	16-A	77	ASP	CB-CG-OD2	-5.09	113.71	118.30
1	10-A	74	SER	CB-CA-C	5.09	119.77	110.10
1	22-A	311	LYS	C-N-CD	-5.09	109.40	120.60
1	24-A	169	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	11-A	77	ASP	CB-CG-OD1	5.09	122.88	118.30
1	5-A	272	ASP	CB-CG-OD1	5.08	122.88	118.30
1	8-A	447	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	24-A	130	ASP	CB-CG-OD1	5.08	122.87	118.30
1	8-A	528	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	13-A	527	ASP	CB-CG-OD1	5.07	122.86	118.30
1	6-A	528	ASP	CB-CG-OD1	5.06	122.85	118.30
1	7-A	496	THR	N-CA-CB	-5.06	100.69	110.30
1	15-A	549	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	8-A	496	THR	CA-CB-CG2	-5.05	105.33	112.40
1	2-A	402	SER	N-CA-CB	-5.05	102.93	110.50
1	6-A	374	ASP	CB-CG-OD1	5.04	122.84	118.30
1	7-A	528	ASP	CB-CG-OD2	5.04	122.84	118.30
1	24-A	300	GLU	OE1-CD-OE2	-5.04	117.26	123.30
1	17-A	589	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	18-A	87	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	19-A	164	VAL	CB-CA-C	-5.02	101.87	111.40
1	2-A	538	MET	CG-SD-CE	5.01	108.22	100.20
1	8-A	104	LYS	CD-CE-NZ	-5.01	100.18	111.70
1	16-A	528	ASP	CB-CG-OD2	5.00	122.81	118.30
1	13-A	589	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	57	GLU	Peptide
1	10-A	295	GLY	Peptide
1	11-A	274	ASP	Peptide
1	11-A	76	PRO	Peptide
1	13-A	272	ASP	Peptide
1	13-A	293	GLY	Peptide
1	14-A	193	GLY	Peptide
1	14-A	293	GLY	Peptide
1	15-A	314	ALA	Peptide
1	18-A	401	ALA	Peptide
1	2-A	126	LEU	Peptide
1	20-A	57	GLU	Peptide
1	20-A	66	PRO	Peptide
1	21-A	294	ASN	Peptide
1	23-A	312	PRO	Peptide
1	23-A	57	GLU	Peptide
1	25-A	272	ASP	Peptide
1	25-A	316	ALA	Peptide
1	3-A	295	GLY	Peptide
1	4-A	295	GLY	Peptide
1	4-A	57	GLU	Peptide
1	7-A	272	ASP	Peptide
1	7-A	273	GLY	Peptide
1	9-A	296	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	4167	3907	3919	0	0
1	2-A	4167	3907	3919	0	0
1	3-A	4167	3907	3919	0	0
1	4-A	4167	3907	3919	0	0
1	5-A	4167	3907	3919	0	0
1	6-A	4167	3907	3919	0	0
1	7-A	4167	3907	3919	0	0
1	8-A	4167	3907	3919	0	0
1	9-A	4167	3907	3919	0	0
1	10-A	4167	3907	3919	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	11-A	4167	3907	3919	0	0
1	12-A	4167	3907	3919	0	0
1	13-A	4167	3907	3919	0	0
1	14-A	4167	3907	3919	0	0
1	15-A	4167	3907	3919	0	0
1	16-A	4167	3907	3919	0	0
1	17-A	4167	3907	3919	0	0
1	18-A	4167	3907	3919	0	0
1	19-A	4167	3907	3919	0	0
1	20-A	4167	3907	3919	0	0
1	21-A	4167	3907	3919	0	0
1	22-A	4167	3907	3919	0	0
1	23-A	4167	3907	3919	0	0
1	24-A	4167	3907	3919	0	0
1	25-A	4167	3907	3919	0	0
2	1-A	68	0	60	0	0
2	2-A	68	0	60	0	0
2	3-A	68	0	60	0	0
2	4-A	68	0	60	0	0
2	5-A	68	0	59	0	0
2	6-A	68	0	60	0	0
2	7-A	68	0	60	0	0
2	8-A	68	0	60	0	0
2	9-A	68	0	60	0	0
2	10-A	68	0	60	0	0
2	11-A	68	0	60	0	0
2	12-A	68	0	60	0	0
2	13-A	68	0	60	0	0
2	14-A	68	0	60	0	0
2	15-A	68	0	60	0	0
2	16-A	68	0	60	0	0
2	17-A	68	0	60	0	0
2	18-A	68	0	59	0	0
2	19-A	68	0	60	0	0
2	20-A	68	0	60	0	0
2	21-A	68	0	59	0	0
2	22-A	68	0	60	0	0
2	23-A	68	0	60	0	0
2	24-A	68	0	60	0	0
2	25-A	68	0	60	0	0
3	1-A	339	0	0	0	0
3	2-A	332	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3-A	343	0	0	0	0
3	4-A	342	0	0	0	0
3	5-A	340	0	0	0	0
3	6-A	340	0	0	0	0
3	7-A	327	0	0	0	0
3	8-A	329	0	0	0	0
3	9-A	329	0	0	0	0
3	10-A	321	0	0	0	0
3	11-A	342	0	0	0	0
3	12-A	315	0	0	0	0
3	13-A	340	0	0	0	0
3	14-A	327	0	0	0	0
3	15-A	354	0	0	0	0
3	16-A	335	0	0	0	0
3	17-A	333	0	0	0	0
3	18-A	328	0	0	0	0
3	19-A	320	0	0	0	0
3	20-A	341	0	0	0	0
3	21-A	321	0	0	0	0
3	22-A	304	0	0	0	0
3	23-A	341	0	0	0	0
3	24-A	326	0	0	0	0
3	25-A	336	0	0	0	0
All	All	114180	97675	99472	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	547/549 (100%)	510 (93%)	31 (6%)	6 (1%)	17	3
1	2-A	547/549 (100%)	515 (94%)	28 (5%)	4 (1%)	26	6
1	3-A	547/549 (100%)	513 (94%)	27 (5%)	7 (1%)	15	2
1	4-A	547/549 (100%)	510 (93%)	31 (6%)	6 (1%)	17	3
1	5-A	547/549 (100%)	516 (94%)	26 (5%)	5 (1%)	21	4
1	6-A	547/549 (100%)	509 (93%)	37 (7%)	1 (0%)	52	25
1	7-A	547/549 (100%)	517 (94%)	28 (5%)	2 (0%)	39	14
1	8-A	547/549 (100%)	513 (94%)	31 (6%)	3 (0%)	34	10
1	9-A	547/549 (100%)	514 (94%)	28 (5%)	5 (1%)	21	4
1	10-A	547/549 (100%)	512 (94%)	30 (6%)	5 (1%)	21	4
1	11-A	547/549 (100%)	512 (94%)	32 (6%)	3 (0%)	34	10
1	12-A	547/549 (100%)	517 (94%)	25 (5%)	5 (1%)	21	4
1	13-A	547/549 (100%)	513 (94%)	32 (6%)	2 (0%)	39	14
1	14-A	547/549 (100%)	509 (93%)	31 (6%)	7 (1%)	15	2
1	15-A	547/549 (100%)	513 (94%)	31 (6%)	3 (0%)	34	10
1	16-A	547/549 (100%)	510 (93%)	33 (6%)	4 (1%)	26	6
1	17-A	547/549 (100%)	513 (94%)	32 (6%)	2 (0%)	39	14
1	18-A	547/549 (100%)	507 (93%)	36 (7%)	4 (1%)	26	6
1	19-A	547/549 (100%)	511 (93%)	29 (5%)	7 (1%)	15	2
1	20-A	547/549 (100%)	508 (93%)	32 (6%)	7 (1%)	15	2
1	21-A	547/549 (100%)	509 (93%)	33 (6%)	5 (1%)	21	4
1	22-A	547/549 (100%)	514 (94%)	27 (5%)	6 (1%)	17	3
1	23-A	547/549 (100%)	510 (93%)	31 (6%)	6 (1%)	17	3
1	24-A	547/549 (100%)	512 (94%)	30 (6%)	5 (1%)	21	4
1	25-A	547/549 (100%)	510 (93%)	31 (6%)	6 (1%)	17	3
All	All	13675/13725 (100%)	12797 (94%)	762 (6%)	116 (1%)	24	5

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	58	VAL
1	1-A	194	TYR
1	3-A	400	GLY
1	4-A	77	ASP

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Mol	Chain	Res	Type
1	5-A	80	GLY
1	5-A	81	LYS
1	7-A	58	VAL
1	9-A	63	ASP
1	9-A	296	THR
1	10-A	77	ASP
1	11-A	77	ASP
1	14-A	316	ALA
1	15-A	77	ASP
1	16-A	293	GLY
1	18-A	77	ASP
1	20-A	60	GLY
1	20-A	282	ALA
1	21-A	295	GLY
1	21-A	296	THR
1	22-A	312	PRO
1	23-A	296	THR
1	25-A	274	ASP
1	1-A	83	ASP
1	1-A	273	GLY
1	1-A	295	GLY
1	2-A	314	ALA
1	2-A	516	GLY
1	3-A	193	GLY
1	3-A	233	VAL
1	3-A	324	ASP
1	5-A	273	GLY
1	8-A	74	SER
1	9-A	61	GLY
1	18-A	399	ASP
1	19-A	194	TYR
1	19-A	274	ASP
1	19-A	295	GLY
1	20-A	283	LYS
1	22-A	246	ALA
1	22-A	273	GLY
1	24-A	64	LEU
1	24-A	293	GLY
1	25-A	77	ASP
1	25-A	317	GLU
1	25-A	516	GLY
1	4-A	195	GLY

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Mol	Chain	Res	Type
1	4-A	312	PRO
1	5-A	77	ASP
1	9-A	74	SER
1	10-A	272	ASP
1	10-A	297	PRO
1	10-A	401	ALA
1	14-A	63	ASP
1	14-A	66	PRO
1	14-A	145	ASP
1	14-A	399	ASP
1	15-A	312	PRO
1	15-A	402	SER
1	16-A	297	PRO
1	19-A	61	GLY
1	21-A	59	VAL
1	21-A	401	ALA
1	23-A	77	ASP
1	23-A	272	ASP
1	24-A	273	GLY
1	24-A	294	ASN
1	24-A	312	PRO
1	25-A	73	PRO
1	3-A	312	PRO
1	4-A	286	ASN
1	12-A	296	THR
1	16-A	73	PRO
1	17-A	399	ASP
1	18-A	449	ASP
1	23-A	76	PRO
1	23-A	297	PRO
1	3-A	192	ASP
1	5-A	314	ALA
1	6-A	312	PRO
1	7-A	296	THR
1	8-A	297	PRO
1	13-A	61	GLY
1	16-A	76	PRO
1	19-A	73	PRO
1	20-A	296	THR
1	22-A	296	THR
1	8-A	251	GLU
1	9-A	312	PRO

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Mol	Chain	Res	Type
1	11-A	145	ASP
1	12-A	297	PRO
1	12-A	317	GLU
1	12-A	498	PHE
1	17-A	296	THR
1	18-A	314	ALA
1	20-A	324	ASP
1	20-A	498	PHE
1	21-A	73	PRO
1	22-A	498	PHE
1	10-A	295	GLY
1	25-A	293	GLY
1	2-A	233	VAL
1	3-A	76	PRO
1	13-A	76	PRO
1	14-A	312	PRO
1	2-A	273	GLY
1	4-A	297	PRO
1	14-A	251	GLU
1	19-A	78	ILE
1	20-A	75	THR
1	23-A	233	VAL
1	11-A	233	VAL
1	19-A	75	THR
1	22-A	73	PRO
1	4-A	233	VAL
1	12-A	312	PRO
1	1-A	250	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	436/436 (100%)	418 (96%)	18 (4%)	37	7
1	2-A	436/436 (100%)	414 (95%)	22 (5%)	30	5
1	3-A	436/436 (100%)	409 (94%)	27 (6%)	23	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4-A	436/436 (100%)	417 (96%)	19 (4%)	35	6
1	5-A	436/436 (100%)	417 (96%)	19 (4%)	35	6
1	6-A	436/436 (100%)	417 (96%)	19 (4%)	35	6
1	7-A	436/436 (100%)	419 (96%)	17 (4%)	39	8
1	8-A	436/436 (100%)	413 (95%)	23 (5%)	28	4
1	9-A	436/436 (100%)	417 (96%)	19 (4%)	35	6
1	10-A	436/436 (100%)	424 (97%)	12 (3%)	51	17
1	11-A	436/436 (100%)	421 (97%)	15 (3%)	44	11
1	12-A	436/436 (100%)	416 (95%)	20 (5%)	33	6
1	13-A	436/436 (100%)	421 (97%)	15 (3%)	44	11
1	14-A	436/436 (100%)	420 (96%)	16 (4%)	41	10
1	15-A	436/436 (100%)	416 (95%)	20 (5%)	33	6
1	16-A	436/436 (100%)	418 (96%)	18 (4%)	37	7
1	17-A	436/436 (100%)	419 (96%)	17 (4%)	39	8
1	18-A	436/436 (100%)	422 (97%)	14 (3%)	46	13
1	19-A	436/436 (100%)	416 (95%)	20 (5%)	33	6
1	20-A	436/436 (100%)	414 (95%)	22 (5%)	30	5
1	21-A	436/436 (100%)	416 (95%)	20 (5%)	33	6
1	22-A	436/436 (100%)	416 (95%)	20 (5%)	33	6
1	23-A	436/436 (100%)	422 (97%)	14 (3%)	46	13
1	24-A	436/436 (100%)	415 (95%)	21 (5%)	31	5
1	25-A	436/436 (100%)	415 (95%)	21 (5%)	31	5
All	All	10900/10900 (100%)	10432 (96%)	468 (4%)	35	7

All (468) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	58	VAL
1	1-A	59	VAL
1	1-A	144	PHE
1	1-A	180	ARG
1	1-A	236	MET
1	1-A	272	ASP
1	1-A	274	ASP

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Mol	Chain	Res	Type
1	1-A	283	LYS
1	1-A	285	THR
1	1-A	296	THR
1	1-A	304	LEU
1	1-A	305	ASP
1	1-A	324	ASP
1	1-A	404	ASP
1	1-A	489	TRP
1	1-A	506	ASP
1	1-A	570	LEU
1	1-A	586	ASP
1	2-A	57	GLU
1	2-A	72	ASP
1	2-A	76	PRO
1	2-A	78	ILE
1	2-A	127	ASN
1	2-A	136	ASP
1	2-A	144	PHE
1	2-A	164	VAL
1	2-A	210	GLU
1	2-A	236	MET
1	2-A	272	ASP
1	2-A	274	ASP
1	2-A	275	ASP
1	2-A	343	GLU
1	2-A	392	THR
1	2-A	402	SER
1	2-A	408	ASN
1	2-A	434	ASN
1	2-A	462	ASP
1	2-A	480	GLU
1	2-A	554	HIS
1	2-A	570	LEU
1	3-A	57	GLU
1	3-A	72	ASP
1	3-A	97	ASP
1	3-A	127	ASN
1	3-A	145	ASP
1	3-A	192	ASP
1	3-A	236	MET
1	3-A	274	ASP
1	3-A	283	LYS

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Mol	Chain	Res	Type
1	3-A	296	THR
1	3-A	300	GLU
1	3-A	301	SER
1	3-A	339	ASP
1	3-A	343	GLU
1	3-A	348	ASN
1	3-A	384	ASP
1	3-A	399	ASP
1	3-A	440	ILE
1	3-A	457	GLU
1	3-A	462	ASP
1	3-A	517	ASP
1	3-A	528	ASP
1	3-A	529	SER
1	3-A	553	GLN
1	3-A	570	LEU
1	3-A	592	SER
1	3-A	603	SER
1	4-A	67	ASN
1	4-A	72	ASP
1	4-A	102	MET
1	4-A	144	PHE
1	4-A	236	MET
1	4-A	262	VAL
1	4-A	339	ASP
1	4-A	348	ASN
1	4-A	404	ASP
1	4-A	435	SER
1	4-A	528	ASP
1	4-A	531	THR
1	4-A	532	THR
1	4-A	570	LEU
1	4-A	586	ASP
1	4-A	589	ASP
1	4-A	592	SER
1	4-A	600	GLN
1	4-A	603	SER
1	5-A	72	ASP
1	5-A	87	ARG
1	5-A	144	PHE
1	5-A	164	VAL
1	5-A	236	MET

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Mol	Chain	Res	Type
1	5-A	251	GLU
1	5-A	272	ASP
1	5-A	296	THR
1	5-A	298	GLU
1	5-A	300	GLU
1	5-A	301	SER
1	5-A	310	VAL
1	5-A	363	ASN
1	5-A	402	SER
1	5-A	489	TRP
1	5-A	496	THR
1	5-A	505	TYR
1	5-A	529	SER
1	5-A	570	LEU
1	6-A	72	ASP
1	6-A	74	SER
1	6-A	84	GLU
1	6-A	88	LYS
1	6-A	111	ILE
1	6-A	140	ASP
1	6-A	236	MET
1	6-A	257	LEU
1	6-A	274	ASP
1	6-A	300	GLU
1	6-A	301	SER
1	6-A	305	ASP
1	6-A	311	LYS
1	6-A	339	ASP
1	6-A	399	ASP
1	6-A	457	GLU
1	6-A	517	ASP
1	6-A	570	LEU
1	6-A	574	LEU
1	7-A	63	ASP
1	7-A	64	LEU
1	7-A	72	ASP
1	7-A	126	LEU
1	7-A	169	ARG
1	7-A	236	MET
1	7-A	274	ASP
1	7-A	294	ASN
1	7-A	298	GLU

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Mol	Chain	Res	Type
1	7-A	303	PRO
1	7-A	324	ASP
1	7-A	339	ASP
1	7-A	402	SER
1	7-A	496	THR
1	7-A	517	ASP
1	7-A	538	MET
1	7-A	604	PHE
1	8-A	57	GLU
1	8-A	59	VAL
1	8-A	63	ASP
1	8-A	77	ASP
1	8-A	136	ASP
1	8-A	144	PHE
1	8-A	236	MET
1	8-A	251	GLU
1	8-A	265	GLU
1	8-A	274	ASP
1	8-A	294	ASN
1	8-A	296	THR
1	8-A	305	ASP
1	8-A	306	GLN
1	8-A	310	VAL
1	8-A	312	PRO
1	8-A	340	GLN
1	8-A	363	ASN
1	8-A	391	GLU
1	8-A	517	ASP
1	8-A	527	ASP
1	8-A	570	LEU
1	8-A	586	ASP
1	9-A	74	SER
1	9-A	79	GLN
1	9-A	102	MET
1	9-A	127	ASN
1	9-A	128	PRO
1	9-A	144	PHE
1	9-A	145	ASP
1	9-A	207	ILE
1	9-A	236	MET
1	9-A	275	ASP
1	9-A	300	GLU

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Mol	Chain	Res	Type
1	9-A	301	SER
1	9-A	340	GLN
1	9-A	343	GLU
1	9-A	528	ASP
1	9-A	536	TRP
1	9-A	545	ASN
1	9-A	570	LEU
1	9-A	587	ILE
1	10-A	72	ASP
1	10-A	91	SER
1	10-A	236	MET
1	10-A	262	VAL
1	10-A	296	THR
1	10-A	298	GLU
1	10-A	306	GLN
1	10-A	339	ASP
1	10-A	402	SER
1	10-A	527	ASP
1	10-A	538	MET
1	10-A	570	LEU
1	11-A	63	ASP
1	11-A	91	SER
1	11-A	164	VAL
1	11-A	192	ASP
1	11-A	236	MET
1	11-A	274	ASP
1	11-A	305	ASP
1	11-A	339	ASP
1	11-A	399	ASP
1	11-A	404	ASP
1	11-A	490	SER
1	11-A	570	LEU
1	11-A	586	ASP
1	11-A	592	SER
1	11-A	604	PHE
1	12-A	69	LEU
1	12-A	72	ASP
1	12-A	74	SER
1	12-A	231	ASN
1	12-A	236	MET
1	12-A	262	VAL
1	12-A	272	ASP

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Mol	Chain	Res	Type
1	12-A	296	THR
1	12-A	312	PRO
1	12-A	324	ASP
1	12-A	457	GLU
1	12-A	471	ASN
1	12-A	496	THR
1	12-A	525	LYS
1	12-A	527	ASP
1	12-A	532	THR
1	12-A	570	LEU
1	12-A	587	ILE
1	12-A	603	SER
1	12-A	605	PRO
1	13-A	57	GLU
1	13-A	72	ASP
1	13-A	77	ASP
1	13-A	91	SER
1	13-A	236	MET
1	13-A	274	ASP
1	13-A	285	THR
1	13-A	300	GLU
1	13-A	343	GLU
1	13-A	346	ARG
1	13-A	496	THR
1	13-A	529	SER
1	13-A	538	MET
1	13-A	570	LEU
1	13-A	592	SER
1	14-A	57	GLU
1	14-A	67	ASN
1	14-A	69	LEU
1	14-A	97	ASP
1	14-A	102	MET
1	14-A	145	ASP
1	14-A	180	ARG
1	14-A	236	MET
1	14-A	275	ASP
1	14-A	301	SER
1	14-A	324	ASP
1	14-A	339	ASP
1	14-A	489	TRP
1	14-A	529	SER

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Mol	Chain	Res	Type
1	14-A	538	MET
1	14-A	570	LEU
1	15-A	57	GLU
1	15-A	72	ASP
1	15-A	97	ASP
1	15-A	102	MET
1	15-A	144	PHE
1	15-A	207	ILE
1	15-A	231	ASN
1	15-A	236	MET
1	15-A	248	SER
1	15-A	262	VAL
1	15-A	265	GLU
1	15-A	296	THR
1	15-A	304	LEU
1	15-A	311	LYS
1	15-A	462	ASP
1	15-A	506	ASP
1	15-A	517	ASP
1	15-A	538	MET
1	15-A	562	PRO
1	15-A	570	LEU
1	16-A	59	VAL
1	16-A	63	ASP
1	16-A	74	SER
1	16-A	75	THR
1	16-A	102	MET
1	16-A	222	ARG
1	16-A	236	MET
1	16-A	272	ASP
1	16-A	274	ASP
1	16-A	275	ASP
1	16-A	296	THR
1	16-A	297	PRO
1	16-A	489	TRP
1	16-A	492	GLU
1	16-A	528	ASP
1	16-A	529	SER
1	16-A	570	LEU
1	16-A	586	ASP
1	17-A	57	GLU
1	17-A	63	ASP

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Mol	Chain	Res	Type
1	17-A	72	ASP
1	17-A	84	GLU
1	17-A	91	SER
1	17-A	102	MET
1	17-A	194	TYR
1	17-A	236	MET
1	17-A	262	VAL
1	17-A	285	THR
1	17-A	296	THR
1	17-A	391	GLU
1	17-A	528	ASP
1	17-A	570	LEU
1	17-A	589	ASP
1	17-A	603	SER
1	17-A	604	PHE
1	18-A	72	ASP
1	18-A	111	ILE
1	18-A	129	ASP
1	18-A	180	ARG
1	18-A	236	MET
1	18-A	270	TYR
1	18-A	310	VAL
1	18-A	315	THR
1	18-A	348	ASN
1	18-A	399	ASP
1	18-A	440	ILE
1	18-A	517	ASP
1	18-A	528	ASP
1	18-A	532	THR
1	19-A	63	ASP
1	19-A	102	MET
1	19-A	127	ASN
1	19-A	136	ASP
1	19-A	164	VAL
1	19-A	210	GLU
1	19-A	236	MET
1	19-A	262	VAL
1	19-A	274	ASP
1	19-A	276	TYR
1	19-A	294	ASN
1	19-A	305	ASP
1	19-A	340	GLN

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Mol	Chain	Res	Type
1	19-A	404	ASP
1	19-A	489	TRP
1	19-A	493	ASN
1	19-A	509	ASP
1	19-A	527	ASP
1	19-A	531	THR
1	19-A	570	LEU
1	20-A	63	ASP
1	20-A	91	SER
1	20-A	102	MET
1	20-A	144	PHE
1	20-A	145	ASP
1	20-A	207	ILE
1	20-A	231	ASN
1	20-A	236	MET
1	20-A	257	LEU
1	20-A	283	LYS
1	20-A	296	THR
1	20-A	298	GLU
1	20-A	305	ASP
1	20-A	324	ASP
1	20-A	343	GLU
1	20-A	391	GLU
1	20-A	457	GLU
1	20-A	490	SER
1	20-A	517	ASP
1	20-A	538	MET
1	20-A	545	ASN
1	20-A	570	LEU
1	21-A	57	GLU
1	21-A	72	ASP
1	21-A	164	VAL
1	21-A	180	ARG
1	21-A	236	MET
1	21-A	248	SER
1	21-A	251	GLU
1	21-A	274	ASP
1	21-A	283	LYS
1	21-A	285	THR
1	21-A	345	ASP
1	21-A	363	ASN
1	21-A	404	ASP

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Mol	Chain	Res	Type
1	21-A	468	LYS
1	21-A	490	SER
1	21-A	517	ASP
1	21-A	525	LYS
1	21-A	538	MET
1	21-A	570	LEU
1	21-A	603	SER
1	22-A	57	GLU
1	22-A	63	ASP
1	22-A	67	ASN
1	22-A	72	ASP
1	22-A	83	ASP
1	22-A	96	THR
1	22-A	144	PHE
1	22-A	149	THR
1	22-A	236	MET
1	22-A	294	ASN
1	22-A	300	GLU
1	22-A	340	GLN
1	22-A	399	ASP
1	22-A	470	ASP
1	22-A	527	ASP
1	22-A	532	THR
1	22-A	570	LEU
1	22-A	586	ASP
1	22-A	603	SER
1	22-A	604	PHE
1	23-A	59	VAL
1	23-A	69	LEU
1	23-A	147	ASN
1	23-A	180	ARG
1	23-A	236	MET
1	23-A	258	GLU
1	23-A	285	THR
1	23-A	296	THR
1	23-A	310	VAL
1	23-A	317	GLU
1	23-A	340	GLN
1	23-A	346	ARG
1	23-A	490	SER
1	23-A	595	THR
1	24-A	57	GLU

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Mol	Chain	Res	Type
1	24-A	67	ASN
1	24-A	72	ASP
1	24-A	83	ASP
1	24-A	87	ARG
1	24-A	91	SER
1	24-A	96	THR
1	24-A	164	VAL
1	24-A	210	GLU
1	24-A	236	MET
1	24-A	271	LEU
1	24-A	272	ASP
1	24-A	286	ASN
1	24-A	303	PRO
1	24-A	324	ASP
1	24-A	493	ASN
1	24-A	529	SER
1	24-A	538	MET
1	24-A	553	GLN
1	24-A	570	LEU
1	24-A	586	ASP
1	25-A	57	GLU
1	25-A	63	ASP
1	25-A	74	SER
1	25-A	112	ASN
1	25-A	236	MET
1	25-A	257	LEU
1	25-A	262	VAL
1	25-A	270	TYR
1	25-A	283	LYS
1	25-A	285	THR
1	25-A	306	GLN
1	25-A	324	ASP
1	25-A	339	ASP
1	25-A	369	LYS
1	25-A	399	ASP
1	25-A	404	ASP
1	25-A	517	ASP
1	25-A	528	ASP
1	25-A	531	THR
1	25-A	570	LEU
1	25-A	592	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such

sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	93	GLN
1	1-A	127	ASN
1	1-A	408	ASN
1	2-A	79	GLN
1	2-A	127	ASN
1	2-A	325	GLN
1	2-A	408	ASN
1	2-A	434	ASN
1	3-A	127	ASN
1	3-A	217	GLN
1	3-A	493	ASN
1	4-A	93	GLN
1	4-A	127	ASN
1	4-A	340	GLN
1	4-A	348	ASN
1	4-A	434	ASN
1	5-A	217	GLN
1	6-A	217	GLN
1	6-A	306	GLN
1	6-A	466	HIS
1	7-A	217	GLN
1	7-A	340	GLN
1	7-A	600	GLN
1	8-A	165	ASN
1	8-A	217	GLN
1	8-A	306	GLN
1	9-A	79	GLN
1	9-A	217	GLN
1	9-A	471	ASN
1	9-A	514	GLN
1	10-A	93	GLN
1	11-A	217	GLN
1	11-A	471	ASN
1	11-A	514	GLN
1	12-A	127	ASN
1	12-A	348	ASN
1	12-A	557	GLN
1	13-A	114	GLN
1	13-A	231	ASN
1	14-A	127	ASN
1	14-A	231	ASN
1	14-A	515	ASN

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Mol	Chain	Res	Type
1	14-A	600	GLN
1	15-A	109	ASN
1	15-A	217	GLN
1	15-A	231	ASN
1	15-A	325	GLN
1	16-A	127	ASN
1	16-A	217	GLN
1	16-A	481	HIS
1	17-A	217	GLN
1	17-A	554	HIS
1	18-A	127	ASN
1	18-A	217	GLN
1	19-A	165	ASN
1	19-A	217	GLN
1	20-A	67	ASN
1	20-A	114	GLN
1	20-A	217	GLN
1	20-A	408	ASN
1	20-A	481	HIS
1	21-A	127	ASN
1	21-A	363	ASN
1	22-A	127	ASN
1	22-A	306	GLN
1	23-A	217	GLN
1	23-A	340	GLN
1	23-A	493	ASN
1	24-A	286	ASN
1	24-A	340	GLN
1	24-A	471	ASN
1	25-A	217	GLN
1	25-A	600	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

150 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	BGC	1-A	701	2	11,11,12	2.47	5 (45%)	14,15,17	1.30	1 (7%)
2	BGC	1-A	702	2	11,11,12	2.56	5 (45%)	14,15,17	1.61	2 (14%)
2	BGC	1-A	703	2	12,12,12	2.07	4 (33%)	17,17,17	1.25	2 (11%)
2	BGC	1-A	704	2	11,11,12	3.02	4 (36%)	14,15,17	1.16	1 (7%)
2	BGC	1-A	705	2	11,11,12	3.04	5 (45%)	14,15,17	2.22	3 (21%)
2	BGC	1-A	706	2	12,12,12	2.62	7 (58%)	17,17,17	2.31	6 (35%)
2	BGC	10-A	701	2	11,11,12	2.66	5 (45%)	14,15,17	1.27	2 (14%)
2	BGC	10-A	702	2	11,11,12	2.53	5 (45%)	14,15,17	1.57	2 (14%)
2	BGC	10-A	703	2	12,12,12	2.08	4 (33%)	17,17,17	1.18	2 (11%)
2	BGC	10-A	704	2	11,11,12	2.97	5 (45%)	14,15,17	1.42	1 (7%)
2	BGC	10-A	705	2	11,11,12	3.07	6 (54%)	14,15,17	1.98	3 (21%)
2	BGC	10-A	706	2	12,12,12	2.40	5 (41%)	17,17,17	1.47	5 (29%)
2	BGC	11-A	701	2	11,11,12	2.54	5 (45%)	14,15,17	1.26	1 (7%)
2	BGC	11-A	702	2	11,11,12	2.52	4 (36%)	14,15,17	1.47	2 (14%)
2	BGC	11-A	703	2	12,12,12	2.04	5 (41%)	17,17,17	1.57	2 (11%)
2	BGC	11-A	704	2	11,11,12	3.06	6 (54%)	14,15,17	1.53	3 (21%)
2	BGC	11-A	705	2	11,11,12	3.09	6 (54%)	14,15,17	1.91	7 (50%)
2	BGC	11-A	706	2	12,12,12	2.43	6 (50%)	17,17,17	1.51	3 (17%)
2	BGC	12-A	701	2	11,11,12	2.66	5 (45%)	14,15,17	1.52	1 (7%)
2	BGC	12-A	702	2	11,11,12	2.47	4 (36%)	14,15,17	1.84	4 (28%)
2	BGC	12-A	703	2	12,12,12	2.05	4 (33%)	17,17,17	1.21	2 (11%)
2	BGC	12-A	704	2	11,11,12	2.96	5 (45%)	14,15,17	1.46	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	12-A	705	2	11,11,12	2.94	5 (45%)	14,15,17	1.52	2 (14%)
2	BGC	12-A	706	2	12,12,12	2.50	6 (50%)	17,17,17	1.41	3 (17%)
2	BGC	13-A	701	2	11,11,12	2.54	5 (45%)	14,15,17	1.30	1 (7%)
2	BGC	13-A	702	2	11,11,12	2.42	4 (36%)	14,15,17	1.89	3 (21%)
2	BGC	13-A	703	2	12,12,12	2.18	4 (33%)	17,17,17	1.25	2 (11%)
2	BGC	13-A	704	2	11,11,12	3.09	4 (36%)	14,15,17	1.11	1 (7%)
2	BGC	13-A	705	2	11,11,12	3.00	5 (45%)	14,15,17	1.41	2 (14%)
2	BGC	13-A	706	2	12,12,12	2.14	5 (41%)	17,17,17	2.06	6 (35%)
2	BGC	14-A	701	2	11,11,12	2.63	4 (36%)	14,15,17	1.32	1 (7%)
2	BGC	14-A	702	2	11,11,12	2.45	4 (36%)	14,15,17	1.65	1 (7%)
2	BGC	14-A	703	2	12,12,12	2.05	5 (41%)	17,17,17	1.37	1 (5%)
2	BGC	14-A	704	2	11,11,12	3.05	4 (36%)	14,15,17	1.19	1 (7%)
2	BGC	14-A	705	2	11,11,12	3.07	7 (63%)	14,15,17	1.13	0
2	BGC	14-A	706	2	12,12,12	2.37	6 (50%)	17,17,17	2.65	10 (58%)
2	BGC	15-A	701	2	11,11,12	2.59	5 (45%)	14,15,17	1.39	1 (7%)
2	BGC	15-A	702	2	11,11,12	2.62	5 (45%)	14,15,17	1.62	2 (14%)
2	BGC	15-A	703	2	12,12,12	2.07	4 (33%)	17,17,17	1.32	2 (11%)
2	BGC	15-A	704	2	11,11,12	3.10	5 (45%)	14,15,17	1.92	5 (35%)
2	BGC	15-A	705	2	11,11,12	3.03	5 (45%)	14,15,17	1.87	3 (21%)
2	BGC	15-A	706	2	12,12,12	2.52	6 (50%)	17,17,17	3.04	11 (64%)
2	BGC	16-A	701	2	11,11,12	2.58	6 (54%)	14,15,17	1.23	1 (7%)
2	BGC	16-A	702	2	11,11,12	2.46	4 (36%)	14,15,17	1.45	2 (14%)
2	BGC	16-A	703	2	12,12,12	2.03	4 (33%)	17,17,17	1.33	2 (11%)
2	BGC	16-A	704	2	11,11,12	3.05	4 (36%)	14,15,17	1.26	1 (7%)
2	BGC	16-A	705	2	11,11,12	3.30	6 (54%)	14,15,17	1.85	5 (35%)
2	BGC	16-A	706	2	12,12,12	2.59	6 (50%)	17,17,17	1.93	6 (35%)
2	BGC	17-A	701	2	11,11,12	2.66	4 (36%)	14,15,17	1.52	2 (14%)
2	BGC	17-A	702	2	11,11,12	2.52	5 (45%)	14,15,17	1.60	2 (14%)
2	BGC	17-A	703	2	12,12,12	2.07	4 (33%)	17,17,17	1.32	2 (11%)
2	BGC	17-A	704	2	11,11,12	3.02	4 (36%)	14,15,17	1.34	2 (14%)
2	BGC	17-A	705	2	11,11,12	2.95	5 (45%)	14,15,17	1.37	2 (14%)
2	BGC	17-A	706	2	12,12,12	2.56	5 (41%)	17,17,17	2.60	7 (41%)
2	BGC	18-A	701	2	11,11,12	2.51	5 (45%)	14,15,17	1.36	1 (7%)
2	BGC	18-A	702	2	11,11,12	2.65	5 (45%)	14,15,17	1.59	2 (14%)
2	BGC	18-A	703	2	12,12,12	2.18	4 (33%)	17,17,17	1.37	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	18-A	704	2	11,11,12	3.06	4 (36%)	14,15,17	1.24	1 (7%)
2	BGC	18-A	705	2	11,11,12	2.84	6 (54%)	14,15,17	2.10	3 (21%)
2	BGC	18-A	706	2	12,12,12	2.72	6 (50%)	17,17,17	2.48	8 (47%)
2	BGC	19-A	701	2	11,11,12	2.57	4 (36%)	14,15,17	1.30	1 (7%)
2	BGC	19-A	702	2	11,11,12	2.55	4 (36%)	14,15,17	1.66	1 (7%)
2	BGC	19-A	703	2	12,12,12	2.14	5 (41%)	17,17,17	1.34	2 (11%)
2	BGC	19-A	704	2	11,11,12	3.04	4 (36%)	14,15,17	1.20	1 (7%)
2	BGC	19-A	705	2	11,11,12	3.05	5 (45%)	14,15,17	1.22	3 (21%)
2	BGC	19-A	706	2	12,12,12	2.34	5 (41%)	17,17,17	1.39	3 (17%)
2	BGC	2-A	701	2	11,11,12	2.60	4 (36%)	14,15,17	1.16	1 (7%)
2	BGC	2-A	702	2	11,11,12	2.56	5 (45%)	14,15,17	1.68	2 (14%)
2	BGC	2-A	703	2	12,12,12	2.15	4 (33%)	17,17,17	1.19	1 (5%)
2	BGC	2-A	704	2	11,11,12	3.00	4 (36%)	14,15,17	1.20	2 (14%)
2	BGC	2-A	705	2	11,11,12	3.19	6 (54%)	14,15,17	1.07	0
2	BGC	2-A	706	2	12,12,12	2.64	6 (50%)	17,17,17	3.32	7 (41%)
2	BGC	20-A	701	2	11,11,12	2.63	5 (45%)	14,15,17	1.58	2 (14%)
2	BGC	20-A	702	2	11,11,12	2.53	5 (45%)	14,15,17	1.48	1 (7%)
2	BGC	20-A	703	2	12,12,12	2.10	4 (33%)	17,17,17	1.17	1 (5%)
2	BGC	20-A	704	2	11,11,12	3.05	5 (45%)	14,15,17	1.74	3 (21%)
2	BGC	20-A	705	2	11,11,12	3.03	5 (45%)	14,15,17	2.14	2 (14%)
2	BGC	20-A	706	2	12,12,12	2.34	5 (41%)	17,17,17	1.46	4 (23%)
2	BGC	21-A	701	2	11,11,12	2.52	5 (45%)	14,15,17	1.24	1 (7%)
2	BGC	21-A	702	2	11,11,12	2.65	5 (45%)	14,15,17	1.42	1 (7%)
2	BGC	21-A	703	2	12,12,12	2.10	5 (41%)	17,17,17	1.35	1 (5%)
2	BGC	21-A	704	2	11,11,12	3.05	5 (45%)	14,15,17	1.80	3 (21%)
2	BGC	21-A	705	2	11,11,12	3.09	5 (45%)	14,15,17	2.88	8 (57%)
2	BGC	21-A	706	2	12,12,12	2.44	6 (50%)	17,17,17	2.76	11 (64%)
2	BGC	22-A	701	2	11,11,12	2.66	5 (45%)	14,15,17	1.34	1 (7%)
2	BGC	22-A	702	2	11,11,12	2.50	5 (45%)	14,15,17	1.48	2 (14%)
2	BGC	22-A	703	2	12,12,12	2.11	4 (33%)	17,17,17	1.21	1 (5%)
2	BGC	22-A	704	2	11,11,12	3.02	4 (36%)	14,15,17	1.25	1 (7%)
2	BGC	22-A	705	2	11,11,12	3.07	6 (54%)	14,15,17	1.25	2 (14%)
2	BGC	22-A	706	2	12,12,12	2.70	6 (50%)	17,17,17	2.70	6 (35%)
2	BGC	23-A	701	2	11,11,12	2.57	5 (45%)	14,15,17	1.24	1 (7%)
2	BGC	23-A	702	2	11,11,12	2.50	5 (45%)	14,15,17	1.55	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	23-A	703	2	12,12,12	2.10	5 (41%)	17,17,17	1.50	1 (5%)
2	BGC	23-A	704	2	11,11,12	3.23	5 (45%)	14,15,17	1.73	6 (42%)
2	BGC	23-A	705	2	11,11,12	2.99	6 (54%)	14,15,17	1.42	3 (21%)
2	BGC	23-A	706	2	12,12,12	2.69	6 (50%)	17,17,17	2.18	5 (29%)
2	BGC	24-A	701	2	11,11,12	2.58	5 (45%)	14,15,17	1.51	1 (7%)
2	BGC	24-A	702	2	11,11,12	2.42	4 (36%)	14,15,17	1.73	2 (14%)
2	BGC	24-A	703	2	12,12,12	2.11	5 (41%)	17,17,17	1.32	2 (11%)
2	BGC	24-A	704	2	11,11,12	3.02	4 (36%)	14,15,17	1.24	1 (7%)
2	BGC	24-A	705	2	11,11,12	3.19	6 (54%)	14,15,17	1.22	2 (14%)
2	BGC	24-A	706	2	12,12,12	2.43	5 (41%)	17,17,17	1.45	4 (23%)
2	BGC	25-A	701	2	11,11,12	2.54	5 (45%)	14,15,17	1.33	1 (7%)
2	BGC	25-A	702	2	11,11,12	2.41	4 (36%)	14,15,17	1.77	2 (14%)
2	BGC	25-A	703	2	12,12,12	2.22	5 (41%)	17,17,17	1.25	1 (5%)
2	BGC	25-A	704	2	11,11,12	2.86	4 (36%)	14,15,17	1.47	3 (21%)
2	BGC	25-A	705	2	11,11,12	3.07	5 (45%)	14,15,17	1.23	2 (14%)
2	BGC	25-A	706	2	12,12,12	2.56	6 (50%)	17,17,17	2.07	8 (47%)
2	BGC	3-A	701	2	11,11,12	2.57	4 (36%)	14,15,17	1.12	1 (7%)
2	BGC	3-A	702	2	11,11,12	2.46	6 (54%)	14,15,17	1.77	3 (21%)
2	BGC	3-A	703	2	12,12,12	2.02	5 (41%)	17,17,17	1.15	1 (5%)
2	BGC	3-A	704	2	11,11,12	2.91	4 (36%)	14,15,17	1.39	2 (14%)
2	BGC	3-A	705	2	11,11,12	2.88	5 (45%)	14,15,17	1.58	2 (14%)
2	BGC	3-A	706	2	12,12,12	2.57	5 (41%)	17,17,17	2.14	7 (41%)
2	BGC	4-A	701	2	11,11,12	2.51	4 (36%)	14,15,17	1.27	1 (7%)
2	BGC	4-A	702	2	11,11,12	2.58	5 (45%)	14,15,17	1.64	2 (14%)
2	BGC	4-A	703	2	12,12,12	2.11	4 (33%)	17,17,17	1.37	3 (17%)
2	BGC	4-A	704	2	11,11,12	3.09	4 (36%)	14,15,17	1.44	3 (21%)
2	BGC	4-A	705	2	11,11,12	3.19	6 (54%)	14,15,17	2.88	5 (35%)
2	BGC	4-A	706	2	12,12,12	2.59	6 (50%)	17,17,17	2.54	8 (47%)
2	BGC	5-A	701	2	11,11,12	2.61	5 (45%)	14,15,17	1.26	1 (7%)
2	BGC	5-A	702	2	11,11,12	2.58	5 (45%)	14,15,17	1.66	2 (14%)
2	BGC	5-A	703	2	12,12,12	2.01	4 (33%)	17,17,17	1.27	1 (5%)
2	BGC	5-A	704	2	11,11,12	2.99	4 (36%)	14,15,17	1.34	2 (14%)
2	BGC	5-A	705	2	11,11,12	3.23	6 (54%)	14,15,17	1.32	2 (14%)
2	BGC	5-A	706	2	12,12,12	2.56	5 (41%)	17,17,17	2.17	8 (47%)
2	BGC	6-A	701	2	11,11,12	2.50	5 (45%)	14,15,17	1.61	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	6-A	702	2	11,11,12	2.62	4 (36%)	14,15,17	1.76	2 (14%)
2	BGC	6-A	703	2	12,12,12	2.04	4 (33%)	17,17,17	1.21	2 (11%)
2	BGC	6-A	704	2	11,11,12	2.97	4 (36%)	14,15,17	1.29	2 (14%)
2	BGC	6-A	705	2	11,11,12	2.81	6 (54%)	14,15,17	1.23	2 (14%)
2	BGC	6-A	706	2	12,12,12	2.77	7 (58%)	17,17,17	2.43	6 (35%)
2	BGC	7-A	701	2	11,11,12	2.44	5 (45%)	14,15,17	1.43	1 (7%)
2	BGC	7-A	702	2	11,11,12	2.57	4 (36%)	14,15,17	1.85	4 (28%)
2	BGC	7-A	703	2	12,12,12	2.09	4 (33%)	17,17,17	1.18	2 (11%)
2	BGC	7-A	704	2	11,11,12	2.90	5 (45%)	14,15,17	1.23	2 (14%)
2	BGC	7-A	705	2	11,11,12	2.98	4 (36%)	14,15,17	0.81	1 (7%)
2	BGC	7-A	706	2	12,12,12	2.60	6 (50%)	17,17,17	2.08	6 (35%)
2	BGC	8-A	701	2	11,11,12	2.54	5 (45%)	14,15,17	1.40	1 (7%)
2	BGC	8-A	702	2	11,11,12	2.49	4 (36%)	14,15,17	1.52	2 (14%)
2	BGC	8-A	703	2	12,12,12	2.07	5 (41%)	17,17,17	1.68	4 (23%)
2	BGC	8-A	704	2	11,11,12	3.00	5 (45%)	14,15,17	1.43	2 (14%)
2	BGC	8-A	705	2	11,11,12	3.28	6 (54%)	14,15,17	1.82	5 (35%)
2	BGC	8-A	706	2	12,12,12	2.71	7 (58%)	17,17,17	2.42	7 (41%)
2	BGC	9-A	701	2	11,11,12	2.59	4 (36%)	14,15,17	1.43	3 (21%)
2	BGC	9-A	702	2	11,11,12	2.48	5 (45%)	14,15,17	1.69	3 (21%)
2	BGC	9-A	703	2	12,12,12	2.10	4 (33%)	17,17,17	1.41	4 (23%)
2	BGC	9-A	704	2	11,11,12	2.97	4 (36%)	14,15,17	1.16	2 (14%)
2	BGC	9-A	705	2	11,11,12	2.97	5 (45%)	14,15,17	1.32	3 (21%)
2	BGC	9-A	706	2	12,12,12	2.29	6 (50%)	17,17,17	2.38	4 (23%)

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
2	BGC	1-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	1-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	1-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	1-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	1-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	1-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	10-A	701	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	10-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	10-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	10-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	10-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	10-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	11-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	11-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	11-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	11-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	11-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	11-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	12-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	12-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	12-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	12-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	12-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	12-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	13-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	13-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	13-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	13-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	13-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	13-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	14-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	14-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	14-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	14-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	14-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	14-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	15-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	15-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	15-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	15-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	15-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	15-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	16-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	16-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	16-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	16-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	16-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	16-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	17-A	701	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	17-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	17-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	17-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	17-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	17-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	18-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	18-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	18-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	18-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	18-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	18-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	19-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	19-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	19-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	19-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	19-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	19-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	2-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	2-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	2-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	2-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	2-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	2-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	20-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	20-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	20-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	20-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	20-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	20-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	21-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	21-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	21-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	21-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	21-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	21-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	22-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	22-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	22-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	22-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	22-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	22-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	23-A	701	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	23-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	23-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	23-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	23-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	23-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	24-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	24-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	24-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	24-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	24-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	24-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	25-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	25-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	25-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	25-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	25-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	25-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	3-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	3-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	3-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	3-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	3-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	3-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	4-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	4-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	4-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	4-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	4-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	4-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	5-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	5-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	5-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	5-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	5-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	5-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	6-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	6-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	6-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	6-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	6-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	6-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	7-A	701	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	7-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	7-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	7-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	7-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	7-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	8-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	8-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	8-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	8-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	8-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	8-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	9-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	9-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	9-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	9-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	9-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	9-A	706	2	-	0/2/22/22	0/1/1/1

All (736) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	23-A	704	BGC	C2-C3	-8.07	1.41	1.52
2	13-A	704	BGC	C2-C3	-7.91	1.41	1.52
2	14-A	704	BGC	C2-C3	-7.61	1.42	1.52
2	15-A	704	BGC	C2-C3	-7.58	1.42	1.52
2	18-A	704	BGC	C2-C3	-7.57	1.42	1.52
2	24-A	704	BGC	C2-C3	-7.54	1.42	1.52
2	19-A	704	BGC	C2-C3	-7.53	1.42	1.52
2	22-A	704	BGC	C2-C3	-7.52	1.42	1.52
2	21-A	704	BGC	C2-C3	-7.51	1.42	1.52
2	16-A	704	BGC	C2-C3	-7.51	1.42	1.52
2	4-A	704	BGC	C2-C3	-7.49	1.42	1.52
2	2-A	704	BGC	C2-C3	-7.48	1.42	1.52
2	20-A	704	BGC	C2-C3	-7.40	1.42	1.52
2	1-A	704	BGC	C2-C3	-7.38	1.42	1.52
2	8-A	704	BGC	C2-C3	-7.38	1.42	1.52
2	17-A	704	BGC	C2-C3	-7.35	1.42	1.52
2	10-A	704	BGC	C2-C3	-7.33	1.42	1.52
2	5-A	704	BGC	C2-C3	-7.32	1.42	1.52
2	9-A	704	BGC	C2-C3	-7.29	1.42	1.52
2	11-A	704	BGC	C2-C3	-7.27	1.42	1.52
2	6-A	704	BGC	C2-C3	-7.23	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	12-A	704	BGC	C2-C3	-7.07	1.42	1.52
2	3-A	704	BGC	C2-C3	-7.07	1.42	1.52
2	16-A	705	BGC	C2-C3	-6.94	1.43	1.52
2	24-A	705	BGC	C2-C3	-6.90	1.43	1.52
2	25-A	704	BGC	C2-C3	-6.88	1.43	1.52
2	8-A	705	BGC	C2-C3	-6.85	1.43	1.52
2	5-A	705	BGC	C2-C3	-6.85	1.43	1.52
2	7-A	704	BGC	C2-C3	-6.75	1.43	1.52
2	2-A	705	BGC	C2-C3	-6.69	1.43	1.52
2	25-A	705	BGC	C2-C3	-6.46	1.43	1.52
2	4-A	705	BGC	C2-C3	-6.45	1.43	1.52
2	14-A	705	BGC	C2-C3	-6.43	1.43	1.52
2	19-A	705	BGC	C2-C3	-6.41	1.43	1.52
2	10-A	705	BGC	C2-C3	-6.35	1.43	1.52
2	15-A	705	BGC	C2-C3	-6.33	1.43	1.52
2	1-A	705	BGC	C2-C3	-6.33	1.43	1.52
2	22-A	705	BGC	C2-C3	-6.31	1.43	1.52
2	17-A	701	BGC	C2-C3	-6.30	1.43	1.52
2	11-A	705	BGC	C2-C3	-6.22	1.44	1.52
2	22-A	701	BGC	C2-C3	-6.21	1.44	1.52
2	12-A	701	BGC	C2-C3	-6.17	1.44	1.52
2	13-A	705	BGC	C2-C3	-6.13	1.44	1.52
2	20-A	701	BGC	C2-C3	-6.06	1.44	1.52
2	9-A	705	BGC	C2-C3	-6.01	1.44	1.52
2	15-A	701	BGC	C2-C3	-6.01	1.44	1.52
2	9-A	701	BGC	C2-C3	-5.99	1.44	1.52
2	20-A	705	BGC	C2-C3	-5.98	1.44	1.52
2	14-A	701	BGC	C2-C3	-5.97	1.44	1.52
2	12-A	705	BGC	C2-C3	-5.95	1.44	1.52
2	17-A	705	BGC	C2-C3	-5.91	1.44	1.52
2	3-A	701	BGC	C2-C3	-5.88	1.44	1.52
2	7-A	705	BGC	C2-C3	-5.85	1.44	1.52
2	2-A	701	BGC	C2-C3	-5.85	1.44	1.52
2	5-A	701	BGC	C2-C3	-5.84	1.44	1.52
2	10-A	701	BGC	C2-C3	-5.77	1.44	1.52
2	19-A	701	BGC	C2-C3	-5.75	1.44	1.52
2	21-A	705	BGC	C2-C3	-5.74	1.44	1.52
2	23-A	705	BGC	C2-C3	-5.73	1.44	1.52
2	23-A	701	BGC	C2-C3	-5.66	1.44	1.52
2	24-A	701	BGC	C2-C3	-5.65	1.44	1.52
2	18-A	701	BGC	C2-C3	-5.65	1.44	1.52
2	6-A	701	BGC	C2-C3	-5.62	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	16-A	701	BGC	C2-C3	-5.61	1.44	1.52
2	11-A	701	BGC	C2-C3	-5.56	1.44	1.52
2	13-A	701	BGC	C2-C3	-5.55	1.44	1.52
2	4-A	701	BGC	C2-C3	-5.53	1.44	1.52
2	21-A	701	BGC	C2-C3	-5.46	1.45	1.52
2	21-A	702	BGC	C2-C3	-5.43	1.45	1.52
2	25-A	701	BGC	C2-C3	-5.43	1.45	1.52
2	8-A	701	BGC	C2-C3	-5.42	1.45	1.52
2	18-A	702	BGC	C2-C3	-5.27	1.45	1.52
2	18-A	705	BGC	C2-C3	-5.20	1.45	1.52
2	1-A	701	BGC	C2-C3	-5.17	1.45	1.52
2	3-A	705	BGC	C2-C3	-5.15	1.45	1.52
2	17-A	702	BGC	C2-C3	-5.13	1.45	1.52
2	6-A	705	BGC	C2-C3	-5.12	1.45	1.52
2	4-A	702	BGC	C2-C3	-5.12	1.45	1.52
2	1-A	702	BGC	C2-C3	-5.12	1.45	1.52
2	5-A	702	BGC	C2-C3	-5.11	1.45	1.52
2	2-A	702	BGC	C2-C3	-5.09	1.45	1.52
2	7-A	701	BGC	C2-C3	-5.07	1.45	1.52
2	23-A	702	BGC	C2-C3	-5.05	1.45	1.52
2	11-A	702	BGC	C2-C3	-5.00	1.45	1.52
2	10-A	702	BGC	C2-C3	-4.99	1.45	1.52
2	19-A	702	BGC	C2-C3	-4.98	1.45	1.52
2	22-A	702	BGC	C2-C3	-4.94	1.45	1.52
2	6-A	706	BGC	C3-C2	-4.94	1.39	1.52
2	15-A	702	BGC	C2-C3	-4.94	1.45	1.52
2	8-A	702	BGC	C2-C3	-4.91	1.45	1.52
2	6-A	702	BGC	C2-C3	-4.89	1.45	1.52
2	3-A	702	BGC	C2-C3	-4.88	1.45	1.52
2	20-A	702	BGC	C2-C3	-4.83	1.45	1.52
2	16-A	702	BGC	C2-C3	-4.80	1.45	1.52
2	12-A	702	BGC	C2-C3	-4.79	1.46	1.52
2	17-A	705	BGC	C6-C5	-4.77	1.35	1.51
2	16-A	705	BGC	C6-C5	-4.77	1.35	1.51
2	16-A	706	BGC	C3-C2	-4.77	1.39	1.52
2	25-A	702	BGC	C2-C3	-4.74	1.46	1.52
2	7-A	702	BGC	C2-C3	-4.74	1.46	1.52
2	14-A	702	BGC	C2-C3	-4.72	1.46	1.52
2	24-A	702	BGC	C2-C3	-4.71	1.46	1.52
2	15-A	705	BGC	C6-C5	-4.63	1.35	1.51
2	1-A	705	BGC	C6-C5	-4.62	1.35	1.51
2	12-A	705	BGC	C6-C5	-4.61	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	10-A	705	BGC	C6-C5	-4.59	1.35	1.51
2	2-A	706	BGC	C3-C2	-4.58	1.40	1.52
2	13-A	705	BGC	C6-C5	-4.58	1.35	1.51
2	21-A	705	BGC	C6-C5	-4.57	1.35	1.51
2	14-A	705	BGC	C6-C5	-4.55	1.35	1.51
2	9-A	702	BGC	C2-C3	-4.55	1.46	1.52
2	7-A	705	BGC	C6-C5	-4.55	1.35	1.51
2	25-A	705	BGC	C6-C5	-4.54	1.35	1.51
2	22-A	705	BGC	C6-C5	-4.53	1.35	1.51
2	25-A	706	BGC	C1-C2	-4.52	1.44	1.52
2	4-A	705	BGC	C6-C5	-4.50	1.35	1.51
2	19-A	705	BGC	C6-C5	-4.49	1.36	1.51
2	4-A	706	BGC	C6-C5	-4.49	1.36	1.51
2	13-A	702	BGC	C2-C3	-4.49	1.46	1.52
2	2-A	705	BGC	C6-C5	-4.48	1.36	1.51
2	22-A	706	BGC	C3-C2	-4.45	1.40	1.52
2	8-A	706	BGC	C3-C2	-4.44	1.40	1.52
2	6-A	705	BGC	C6-C5	-4.43	1.36	1.51
2	20-A	705	BGC	C6-C5	-4.42	1.36	1.51
2	9-A	705	BGC	C6-C5	-4.42	1.36	1.51
2	23-A	706	BGC	C3-C2	-4.41	1.40	1.52
2	24-A	705	BGC	C6-C5	-4.40	1.36	1.51
2	18-A	705	BGC	C6-C5	-4.39	1.36	1.51
2	5-A	706	BGC	C3-C2	-4.37	1.40	1.52
2	10-A	706	BGC	C3-C2	-4.35	1.41	1.52
2	5-A	705	BGC	C6-C5	-4.34	1.36	1.51
2	23-A	705	BGC	C6-C5	-4.30	1.36	1.51
2	16-A	706	BGC	C1-C2	-4.30	1.44	1.52
2	8-A	705	BGC	C6-C5	-4.29	1.36	1.51
2	1-A	706	BGC	C3-C2	-4.28	1.41	1.52
2	3-A	705	BGC	C6-C5	-4.27	1.36	1.51
2	25-A	706	BGC	C3-C2	-4.26	1.41	1.52
2	11-A	705	BGC	C6-C5	-4.22	1.36	1.51
2	14-A	706	BGC	C6-C5	-4.19	1.37	1.51
2	12-A	702	BGC	C6-C5	-4.19	1.37	1.51
2	4-A	704	BGC	C6-C5	-4.18	1.37	1.51
2	22-A	706	BGC	C1-C2	-4.17	1.44	1.52
2	17-A	702	BGC	C6-C5	-4.17	1.37	1.51
2	6-A	702	BGC	C6-C5	-4.16	1.37	1.51
2	19-A	706	BGC	C1-C2	-4.16	1.44	1.52
2	2-A	704	BGC	C6-C5	-4.15	1.37	1.51
2	7-A	706	BGC	C6-C5	-4.14	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	8-A	702	BGC	C6-C5	-4.12	1.37	1.51
2	9-A	702	BGC	C6-C5	-4.12	1.37	1.51
2	20-A	704	BGC	C6-C5	-4.12	1.37	1.51
2	9-A	706	BGC	C3-C2	-4.11	1.41	1.52
2	7-A	702	BGC	C6-C5	-4.10	1.37	1.51
2	19-A	702	BGC	C6-C5	-4.10	1.37	1.51
2	2-A	702	BGC	C6-C5	-4.10	1.37	1.51
2	5-A	704	BGC	C6-C5	-4.09	1.37	1.51
2	11-A	704	BGC	C6-C5	-4.09	1.37	1.51
2	23-A	706	BGC	C6-C5	-4.08	1.37	1.51
2	18-A	706	BGC	C3-C2	-4.08	1.41	1.52
2	21-A	702	BGC	C6-C5	-4.08	1.37	1.51
2	8-A	704	BGC	C6-C5	-4.07	1.37	1.51
2	16-A	704	BGC	C6-C5	-4.06	1.37	1.51
2	17-A	706	BGC	C3-C2	-4.06	1.41	1.52
2	16-A	702	BGC	C6-C5	-4.06	1.37	1.51
2	5-A	706	BGC	C1-C2	-4.05	1.45	1.52
2	22-A	704	BGC	C6-C5	-4.05	1.37	1.51
2	24-A	704	BGC	C6-C5	-4.05	1.37	1.51
2	4-A	702	BGC	C6-C5	-4.05	1.37	1.51
2	1-A	704	BGC	C6-C5	-4.03	1.37	1.51
2	19-A	704	BGC	C6-C5	-4.03	1.37	1.51
2	1-A	702	BGC	C6-C5	-4.03	1.37	1.51
2	3-A	704	BGC	C6-C5	-4.03	1.37	1.51
2	14-A	704	BGC	C6-C5	-4.02	1.37	1.51
2	15-A	704	BGC	C6-C5	-4.02	1.37	1.51
2	11-A	702	BGC	C6-C5	-4.02	1.37	1.51
2	23-A	702	BGC	C6-C5	-4.02	1.37	1.51
2	13-A	704	BGC	C6-C5	-4.01	1.37	1.51
2	7-A	704	BGC	C6-C5	-4.00	1.37	1.51
2	10-A	702	BGC	C6-C5	-3.99	1.37	1.51
2	24-A	706	BGC	C6-C5	-3.99	1.37	1.51
2	18-A	702	BGC	C6-C5	-3.99	1.37	1.51
2	18-A	704	BGC	C6-C5	-3.99	1.37	1.51
2	9-A	704	BGC	C6-C5	-3.99	1.37	1.51
2	5-A	702	BGC	C6-C5	-3.98	1.37	1.51
2	14-A	702	BGC	C6-C5	-3.98	1.37	1.51
2	24-A	706	BGC	C3-C2	-3.98	1.42	1.52
2	25-A	702	BGC	C6-C5	-3.97	1.37	1.51
2	13-A	702	BGC	C6-C5	-3.97	1.37	1.51
2	20-A	702	BGC	C6-C5	-3.97	1.37	1.51
2	24-A	702	BGC	C6-C5	-3.96	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3-A	706	BGC	C3-C2	-3.95	1.42	1.52
2	6-A	704	BGC	C6-C5	-3.95	1.37	1.51
2	16-A	706	BGC	C6-C5	-3.95	1.37	1.51
2	12-A	706	BGC	C3-C2	-3.94	1.42	1.52
2	15-A	706	BGC	C3-C2	-3.94	1.42	1.52
2	10-A	704	BGC	C6-C5	-3.94	1.37	1.51
2	22-A	702	BGC	C6-C5	-3.94	1.37	1.51
2	15-A	702	BGC	C6-C5	-3.94	1.37	1.51
2	25-A	701	BGC	C6-C5	-3.93	1.38	1.51
2	25-A	704	BGC	C6-C5	-3.93	1.38	1.51
2	3-A	702	BGC	C6-C5	-3.92	1.38	1.51
2	21-A	704	BGC	C6-C5	-3.92	1.38	1.51
2	12-A	704	BGC	C6-C5	-3.92	1.38	1.51
2	9-A	706	BGC	C6-C5	-3.91	1.38	1.51
2	23-A	704	BGC	C6-C5	-3.90	1.38	1.51
2	24-A	701	BGC	C6-C5	-3.89	1.38	1.51
2	17-A	704	BGC	C6-C5	-3.89	1.38	1.51
2	15-A	701	BGC	C6-C5	-3.88	1.38	1.51
2	25-A	706	BGC	C6-C5	-3.88	1.38	1.51
2	14-A	701	BGC	C6-C5	-3.88	1.38	1.51
2	19-A	706	BGC	C3-C2	-3.87	1.42	1.52
2	8-A	701	BGC	C6-C5	-3.86	1.38	1.51
2	25-A	703	BGC	C6-C5	-3.86	1.38	1.51
2	4-A	703	BGC	C6-C5	-3.86	1.38	1.51
2	22-A	701	BGC	C6-C5	-3.85	1.38	1.51
2	13-A	701	BGC	C6-C5	-3.83	1.38	1.51
2	10-A	701	BGC	C6-C5	-3.82	1.38	1.51
2	5-A	701	BGC	C6-C5	-3.81	1.38	1.51
2	2-A	703	BGC	C6-C5	-3.80	1.38	1.51
2	9-A	701	BGC	C6-C5	-3.80	1.38	1.51
2	13-A	703	BGC	C6-C5	-3.80	1.38	1.51
2	17-A	701	BGC	C6-C5	-3.79	1.38	1.51
2	9-A	703	BGC	C6-C5	-3.79	1.38	1.51
2	11-A	706	BGC	C6-C5	-3.79	1.38	1.51
2	21-A	706	BGC	C6-C5	-3.77	1.38	1.51
2	19-A	701	BGC	C6-C5	-3.77	1.38	1.51
2	18-A	703	BGC	C6-C5	-3.77	1.38	1.51
2	21-A	701	BGC	C6-C5	-3.77	1.38	1.51
2	3-A	701	BGC	C6-C5	-3.76	1.38	1.51
2	23-A	701	BGC	C6-C5	-3.75	1.38	1.51
2	4-A	701	BGC	C6-C5	-3.73	1.38	1.51
2	12-A	701	BGC	C6-C5	-3.71	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7-A	701	BGC	C6-C5	-3.71	1.38	1.51
2	7-A	706	BGC	C3-C2	-3.70	1.42	1.52
2	20-A	706	BGC	C6-C5	-3.70	1.38	1.51
2	22-A	703	BGC	C6-C5	-3.69	1.38	1.51
2	11-A	701	BGC	C6-C5	-3.69	1.38	1.51
2	1-A	703	BGC	C6-C5	-3.69	1.38	1.51
2	22-A	706	BGC	C6-C5	-3.68	1.38	1.51
2	20-A	703	BGC	C6-C5	-3.68	1.38	1.51
2	7-A	703	BGC	C6-C5	-3.68	1.38	1.51
2	1-A	701	BGC	C6-C5	-3.67	1.38	1.51
2	2-A	701	BGC	C6-C5	-3.66	1.38	1.51
2	15-A	703	BGC	C6-C5	-3.66	1.38	1.51
2	17-A	706	BGC	C6-C5	-3.66	1.38	1.51
2	13-A	706	BGC	C3-C2	-3.62	1.42	1.52
2	14-A	706	BGC	C3-C2	-3.62	1.42	1.52
2	12-A	706	BGC	C6-C5	-3.61	1.39	1.51
2	3-A	706	BGC	C6-C5	-3.61	1.39	1.51
2	8-A	706	BGC	C6-C5	-3.61	1.39	1.51
2	18-A	701	BGC	C6-C5	-3.60	1.39	1.51
2	16-A	701	BGC	C6-C5	-3.59	1.39	1.51
2	2-A	706	BGC	C6-C5	-3.58	1.39	1.51
2	6-A	706	BGC	C6-C5	-3.58	1.39	1.51
2	21-A	703	BGC	C6-C5	-3.56	1.39	1.51
2	17-A	703	BGC	C6-C5	-3.56	1.39	1.51
2	6-A	703	BGC	C6-C5	-3.54	1.39	1.51
2	19-A	706	BGC	C6-C5	-3.54	1.39	1.51
2	12-A	703	BGC	C6-C5	-3.53	1.39	1.51
2	10-A	703	BGC	C6-C5	-3.53	1.39	1.51
2	1-A	706	BGC	C1-C2	-3.52	1.46	1.52
2	6-A	701	BGC	C6-C5	-3.52	1.39	1.51
2	24-A	703	BGC	C6-C5	-3.51	1.39	1.51
2	1-A	706	BGC	C6-C5	-3.51	1.39	1.51
2	16-A	703	BGC	C6-C5	-3.51	1.39	1.51
2	14-A	703	BGC	C6-C5	-3.50	1.39	1.51
2	20-A	706	BGC	C3-C2	-3.48	1.43	1.52
2	10-A	706	BGC	C6-C5	-3.48	1.39	1.51
2	19-A	703	BGC	C6-C5	-3.47	1.39	1.51
2	5-A	703	BGC	C6-C5	-3.44	1.39	1.51
2	13-A	706	BGC	C6-C5	-3.43	1.39	1.51
2	8-A	703	BGC	C6-C5	-3.43	1.39	1.51
2	3-A	703	BGC	C6-C5	-3.43	1.39	1.51
2	19-A	703	BGC	C3-C2	-3.42	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	12-A	706	BGC	C1-C2	-3.41	1.46	1.52
2	23-A	703	BGC	C6-C5	-3.41	1.39	1.51
2	15-A	706	BGC	C6-C5	-3.40	1.39	1.51
2	4-A	706	BGC	C3-C2	-3.36	1.43	1.52
2	11-A	703	BGC	C6-C5	-3.35	1.40	1.51
2	5-A	706	BGC	C6-C5	-3.33	1.40	1.51
2	6-A	706	BGC	C1-C2	-3.33	1.46	1.52
2	20-A	701	BGC	C6-C5	-3.32	1.40	1.51
2	21-A	703	BGC	C3-C2	-3.27	1.43	1.52
2	11-A	706	BGC	C3-C2	-3.22	1.43	1.52
2	7-A	706	BGC	C1-C2	-3.15	1.46	1.52
2	23-A	703	BGC	C3-C2	-3.15	1.44	1.52
2	11-A	703	BGC	C3-C2	-3.13	1.44	1.52
2	8-A	706	BGC	C1-C2	-3.13	1.46	1.52
2	20-A	706	BGC	C1-C2	-3.11	1.46	1.52
2	3-A	703	BGC	C3-C2	-3.11	1.44	1.52
2	8-A	703	BGC	C3-C2	-3.10	1.44	1.52
2	14-A	703	BGC	C3-C2	-3.08	1.44	1.52
2	10-A	706	BGC	C1-C2	-3.08	1.47	1.52
2	23-A	706	BGC	C1-C2	-3.05	1.47	1.52
2	10-A	703	BGC	C3-C2	-3.03	1.44	1.52
2	24-A	706	BGC	C1-C2	-3.02	1.47	1.52
2	24-A	703	BGC	C3-C2	-3.02	1.44	1.52
2	5-A	703	BGC	C3-C2	-3.01	1.44	1.52
2	15-A	703	BGC	C3-C2	-2.99	1.44	1.52
2	2-A	703	BGC	C3-C2	-2.98	1.44	1.52
2	15-A	706	BGC	C4-C3	-2.96	1.44	1.52
2	17-A	706	BGC	C1-C2	-2.95	1.47	1.52
2	16-A	703	BGC	C3-C2	-2.94	1.44	1.52
2	4-A	703	BGC	C3-C2	-2.94	1.44	1.52
2	6-A	703	BGC	C3-C2	-2.93	1.44	1.52
2	17-A	703	BGC	C3-C2	-2.93	1.44	1.52
2	16-A	705	BGC	C4-C3	-2.92	1.44	1.52
2	12-A	703	BGC	C3-C2	-2.92	1.44	1.52
2	7-A	703	BGC	C3-C2	-2.90	1.44	1.52
2	9-A	703	BGC	C3-C2	-2.90	1.44	1.52
2	25-A	703	BGC	C3-C2	-2.89	1.44	1.52
2	18-A	703	BGC	C3-C2	-2.89	1.44	1.52
2	22-A	703	BGC	C3-C2	-2.89	1.44	1.52
2	20-A	703	BGC	C3-C2	-2.88	1.44	1.52
2	13-A	703	BGC	C3-C2	-2.87	1.44	1.52
2	1-A	703	BGC	C3-C2	-2.87	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	25-A	703	BGC	C1-C2	-2.85	1.47	1.52
2	18-A	706	BGC	C6-C5	-2.83	1.41	1.51
2	22-A	706	BGC	C4-C3	-2.81	1.45	1.52
2	3-A	706	BGC	C1-C2	-2.79	1.47	1.52
2	1-A	705	BGC	C4-C3	-2.77	1.45	1.52
2	4-A	706	BGC	C1-C2	-2.75	1.47	1.52
2	14-A	706	BGC	C1-C2	-2.72	1.47	1.52
2	13-A	705	BGC	C4-C3	-2.72	1.45	1.52
2	15-A	706	BGC	C1-C2	-2.66	1.47	1.52
2	11-A	705	BGC	C4-C3	-2.63	1.45	1.52
2	17-A	705	BGC	C4-C3	-2.63	1.45	1.52
2	21-A	705	BGC	C4-C3	-2.59	1.45	1.52
2	21-A	706	BGC	C3-C2	-2.53	1.45	1.52
2	2-A	703	BGC	C1-C2	-2.53	1.48	1.52
2	18-A	706	BGC	C1-C2	-2.49	1.48	1.52
2	21-A	706	BGC	C4-C3	-2.48	1.45	1.52
2	6-A	706	BGC	C4-C3	-2.47	1.45	1.52
2	9-A	703	BGC	C1-C2	-2.46	1.48	1.52
2	20-A	703	BGC	C1-C2	-2.46	1.48	1.52
2	19-A	703	BGC	C1-C2	-2.45	1.48	1.52
2	11-A	703	BGC	C1-C2	-2.44	1.48	1.52
2	15-A	703	BGC	C1-C2	-2.43	1.48	1.52
2	10-A	702	BGC	C4-C3	-2.43	1.46	1.52
2	1-A	706	BGC	C4-C3	-2.42	1.46	1.52
2	21-A	702	BGC	C4-C3	-2.42	1.46	1.52
2	15-A	702	BGC	C4-C3	-2.42	1.46	1.52
2	12-A	706	BGC	C4-C3	-2.42	1.46	1.52
2	15-A	705	BGC	C4-C3	-2.42	1.46	1.52
2	24-A	703	BGC	C1-C2	-2.39	1.48	1.52
2	4-A	705	BGC	C4-C3	-2.39	1.46	1.52
2	18-A	703	BGC	C1-C2	-2.39	1.48	1.52
2	17-A	703	BGC	C1-C2	-2.38	1.48	1.52
2	8-A	705	BGC	C1-C2	-2.38	1.46	1.52
2	22-A	705	BGC	C4-C3	-2.38	1.46	1.52
2	21-A	703	BGC	C1-C2	-2.36	1.48	1.52
2	18-A	705	BGC	C4-C3	-2.36	1.46	1.52
2	24-A	705	BGC	C4-C3	-2.36	1.46	1.52
2	19-A	705	BGC	C4-C3	-2.35	1.46	1.52
2	23-A	703	BGC	C1-C2	-2.34	1.48	1.52
2	23-A	705	BGC	C4-C3	-2.34	1.46	1.52
2	14-A	703	BGC	C1-C2	-2.33	1.48	1.52
2	14-A	705	BGC	C4-C3	-2.33	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	22-A	702	BGC	C4-C3	-2.32	1.46	1.52
2	11-A	706	BGC	C1-C2	-2.31	1.48	1.52
2	12-A	705	BGC	C4-C3	-2.31	1.46	1.52
2	5-A	705	BGC	C1-C2	-2.31	1.46	1.52
2	7-A	703	BGC	C1-C2	-2.29	1.48	1.52
2	16-A	705	BGC	C1-C2	-2.29	1.46	1.52
2	10-A	703	BGC	C1-C2	-2.28	1.48	1.52
2	5-A	705	BGC	C4-C3	-2.28	1.46	1.52
2	4-A	703	BGC	C1-C2	-2.27	1.48	1.52
2	13-A	703	BGC	C1-C2	-2.27	1.48	1.52
2	11-A	704	BGC	C1-C2	-2.26	1.46	1.52
2	3-A	703	BGC	C1-C2	-2.26	1.48	1.52
2	8-A	703	BGC	C1-C2	-2.26	1.48	1.52
2	10-A	705	BGC	C4-C3	-2.25	1.46	1.52
2	2-A	706	BGC	C1-C2	-2.25	1.48	1.52
2	9-A	705	BGC	C4-C3	-2.24	1.46	1.52
2	22-A	705	BGC	C1-C2	-2.24	1.46	1.52
2	13-A	706	BGC	C1-C2	-2.23	1.48	1.52
2	25-A	705	BGC	C4-C3	-2.23	1.46	1.52
2	2-A	705	BGC	C4-C3	-2.23	1.46	1.52
2	2-A	705	BGC	C1-C2	-2.22	1.46	1.52
2	20-A	702	BGC	C4-C3	-2.21	1.46	1.52
2	18-A	702	BGC	C4-C3	-2.21	1.46	1.52
2	8-A	706	BGC	C4-C3	-2.21	1.46	1.52
2	5-A	703	BGC	C1-C2	-2.21	1.48	1.52
2	6-A	703	BGC	C1-C2	-2.20	1.48	1.52
2	6-A	705	BGC	C4-C3	-2.19	1.46	1.52
2	16-A	703	BGC	C1-C2	-2.18	1.48	1.52
2	3-A	705	BGC	C4-C3	-2.17	1.46	1.52
2	23-A	702	BGC	C4-C3	-2.17	1.46	1.52
2	22-A	703	BGC	C1-C2	-2.16	1.48	1.52
2	2-A	702	BGC	C4-C3	-2.16	1.46	1.52
2	3-A	702	BGC	C1-C2	-2.14	1.47	1.52
2	12-A	703	BGC	C1-C2	-2.13	1.48	1.52
2	5-A	702	BGC	C4-C3	-2.12	1.46	1.52
2	8-A	705	BGC	C4-C3	-2.12	1.46	1.52
2	1-A	703	BGC	C1-C2	-2.11	1.48	1.52
2	20-A	705	BGC	C4-C3	-2.09	1.46	1.52
2	9-A	706	BGC	C4-C3	-2.09	1.46	1.52
2	23-A	704	BGC	C1-C2	-2.09	1.47	1.52
2	17-A	702	BGC	C4-C3	-2.08	1.46	1.52
2	4-A	702	BGC	C4-C3	-2.08	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-A	702	BGC	C4-C3	-2.07	1.47	1.52
2	16-A	706	BGC	C4-C3	-2.07	1.47	1.52
2	14-A	705	BGC	C1-C2	-2.06	1.47	1.52
2	11-A	706	BGC	C4-C3	-2.05	1.47	1.52
2	3-A	702	BGC	C4-C3	-2.05	1.47	1.52
2	9-A	702	BGC	C4-C3	-2.04	1.47	1.52
2	9-A	706	BGC	C1-C2	-2.04	1.49	1.52
2	25-A	706	BGC	C4-C3	-2.03	1.47	1.52
2	21-A	706	BGC	C1-C2	-2.02	1.49	1.52
2	15-A	704	BGC	C1-C2	-2.01	1.47	1.52
2	23-A	706	BGC	C4-C5	2.00	1.57	1.53
2	18-A	706	BGC	O5-C1	2.00	1.46	1.43
2	20-A	701	BGC	O3-C3	2.01	1.47	1.43
2	12-A	701	BGC	O3-C3	2.02	1.47	1.43
2	12-A	704	BGC	O3-C3	2.02	1.47	1.43
2	10-A	704	BGC	O3-C3	2.02	1.47	1.43
2	20-A	704	BGC	O3-C3	2.03	1.47	1.43
2	18-A	705	BGC	O2-C2	2.03	1.47	1.43
2	22-A	702	BGC	O3-C3	2.03	1.47	1.43
2	10-A	701	BGC	O3-C3	2.03	1.47	1.43
2	22-A	701	BGC	O3-C3	2.03	1.47	1.43
2	24-A	703	BGC	O5-C5	2.04	1.49	1.44
2	3-A	701	BGC	O2-C2	2.06	1.48	1.43
2	11-A	705	BGC	O2-C2	2.06	1.48	1.43
2	16-A	701	BGC	O5-C1	2.07	1.47	1.43
2	25-A	703	BGC	O5-C5	2.07	1.49	1.44
2	6-A	706	BGC	O5-C1	2.07	1.47	1.43
2	21-A	704	BGC	O3-C3	2.07	1.47	1.43
2	1-A	706	BGC	O5-C1	2.07	1.47	1.43
2	15-A	701	BGC	O3-C3	2.08	1.47	1.43
2	18-A	701	BGC	O3-C3	2.08	1.47	1.43
2	16-A	701	BGC	O2-C2	2.08	1.48	1.43
2	21-A	701	BGC	O2-C2	2.09	1.48	1.43
2	10-A	705	BGC	O2-C2	2.09	1.48	1.43
2	14-A	703	BGC	O5-C5	2.09	1.49	1.44
2	3-A	703	BGC	O5-C5	2.10	1.49	1.44
2	16-A	706	BGC	O3-C3	2.10	1.48	1.43
2	8-A	701	BGC	O2-C2	2.10	1.48	1.43
2	14-A	705	BGC	O2-C2	2.11	1.48	1.43
2	22-A	706	BGC	O3-C3	2.11	1.48	1.43
2	17-A	701	BGC	O2-C2	2.12	1.48	1.43
2	8-A	701	BGC	O3-C3	2.12	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4-A	705	BGC	O2-C2	2.12	1.48	1.43
2	15-A	701	BGC	O2-C2	2.13	1.48	1.43
2	7-A	704	BGC	O3-C3	2.13	1.48	1.43
2	5-A	701	BGC	O3-C3	2.14	1.48	1.43
2	11-A	701	BGC	O2-C2	2.15	1.48	1.43
2	23-A	705	BGC	O2-C2	2.15	1.48	1.43
2	6-A	705	BGC	O2-C2	2.16	1.48	1.43
2	17-A	702	BGC	O3-C3	2.16	1.48	1.43
2	7-A	701	BGC	O2-C2	2.16	1.48	1.43
2	7-A	701	BGC	O3-C3	2.17	1.48	1.43
2	12-A	701	BGC	O2-C2	2.17	1.48	1.43
2	11-A	703	BGC	O5-C5	2.18	1.49	1.44
2	25-A	701	BGC	O3-C3	2.18	1.48	1.43
2	14-A	706	BGC	O2-C2	2.18	1.48	1.43
2	4-A	706	BGC	O2-C2	2.19	1.48	1.43
2	22-A	701	BGC	O2-C2	2.20	1.48	1.43
2	24-A	705	BGC	O2-C2	2.20	1.48	1.43
2	19-A	701	BGC	O2-C2	2.21	1.48	1.43
2	11-A	704	BGC	O3-C3	2.22	1.48	1.43
2	8-A	704	BGC	O3-C3	2.24	1.48	1.43
2	6-A	701	BGC	O3-C3	2.25	1.48	1.43
2	2-A	702	BGC	O3-C3	2.26	1.48	1.43
2	5-A	701	BGC	O2-C2	2.26	1.48	1.43
2	21-A	703	BGC	O5-C5	2.27	1.50	1.44
2	10-A	702	BGC	O3-C3	2.27	1.48	1.43
2	1-A	701	BGC	O3-C3	2.27	1.48	1.43
2	13-A	701	BGC	O3-C3	2.28	1.48	1.43
2	6-A	701	BGC	O2-C2	2.28	1.48	1.43
2	4-A	701	BGC	O2-C2	2.28	1.48	1.43
2	8-A	703	BGC	O5-C5	2.28	1.50	1.44
2	21-A	701	BGC	O3-C3	2.29	1.48	1.43
2	23-A	701	BGC	O3-C3	2.31	1.48	1.43
2	14-A	701	BGC	O2-C2	2.31	1.48	1.43
2	21-A	702	BGC	O3-C3	2.31	1.48	1.43
2	3-A	702	BGC	O3-C3	2.31	1.48	1.43
2	23-A	703	BGC	O5-C5	2.31	1.50	1.44
2	9-A	701	BGC	O2-C2	2.31	1.48	1.43
2	1-A	701	BGC	O2-C2	2.31	1.48	1.43
2	16-A	701	BGC	O3-C3	2.33	1.48	1.43
2	18-A	701	BGC	O2-C2	2.34	1.48	1.43
2	22-A	704	BGC	O2-C2	2.34	1.48	1.43
2	25-A	701	BGC	O2-C2	2.34	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	10-A	705	BGC	O3-C3	2.35	1.48	1.43
2	13-A	701	BGC	O2-C2	2.36	1.48	1.43
2	24-A	701	BGC	O2-C2	2.37	1.48	1.43
2	15-A	705	BGC	O3-C3	2.37	1.48	1.43
2	12-A	702	BGC	O3-C3	2.38	1.48	1.43
2	16-A	702	BGC	O3-C3	2.40	1.48	1.43
2	23-A	701	BGC	O2-C2	2.41	1.48	1.43
2	9-A	702	BGC	O3-C3	2.41	1.48	1.43
2	13-A	702	BGC	O3-C3	2.42	1.48	1.43
2	22-A	705	BGC	O3-C3	2.43	1.48	1.43
2	3-A	704	BGC	O2-C2	2.43	1.48	1.43
2	14-A	705	BGC	O3-C3	2.43	1.48	1.43
2	8-A	702	BGC	O3-C3	2.43	1.48	1.43
2	9-A	706	BGC	O5-C5	2.44	1.50	1.44
2	11-A	705	BGC	O3-C3	2.44	1.48	1.43
2	1-A	702	BGC	O3-C3	2.45	1.48	1.43
2	13-A	704	BGC	O2-C2	2.46	1.48	1.43
2	7-A	706	BGC	C4-C5	2.47	1.58	1.53
2	24-A	701	BGC	O3-C3	2.47	1.48	1.43
2	20-A	701	BGC	O2-C2	2.47	1.48	1.43
2	6-A	704	BGC	O2-C2	2.48	1.48	1.43
2	11-A	701	BGC	O3-C3	2.49	1.48	1.43
2	16-A	704	BGC	O2-C2	2.49	1.49	1.43
2	19-A	703	BGC	O5-C5	2.50	1.50	1.44
2	11-A	702	BGC	O3-C3	2.51	1.49	1.43
2	9-A	705	BGC	O3-C3	2.52	1.49	1.43
2	19-A	706	BGC	O3-C3	2.52	1.49	1.43
2	8-A	704	BGC	O2-C2	2.53	1.49	1.43
2	13-A	706	BGC	O5-C5	2.55	1.50	1.44
2	25-A	702	BGC	O3-C3	2.55	1.49	1.43
2	10-A	701	BGC	O2-C2	2.55	1.49	1.43
2	23-A	702	BGC	O3-C3	2.56	1.49	1.43
2	25-A	706	BGC	O3-C3	2.56	1.49	1.43
2	24-A	704	BGC	O2-C2	2.57	1.49	1.43
2	4-A	702	BGC	O3-C3	2.58	1.49	1.43
2	18-A	702	BGC	O3-C3	2.59	1.49	1.43
2	21-A	704	BGC	O2-C2	2.59	1.49	1.43
2	18-A	701	BGC	O5-C5	2.61	1.49	1.43
2	1-A	704	BGC	O2-C2	2.62	1.49	1.43
2	14-A	704	BGC	O2-C2	2.62	1.49	1.43
2	15-A	702	BGC	O3-C3	2.63	1.49	1.43
2	24-A	705	BGC	O3-C3	2.63	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6-A	701	BGC	O5-C5	2.65	1.49	1.43
2	13-A	705	BGC	O3-C3	2.66	1.49	1.43
2	17-A	704	BGC	O2-C2	2.66	1.49	1.43
2	20-A	702	BGC	O3-C3	2.66	1.49	1.43
2	2-A	701	BGC	O2-C2	2.67	1.49	1.43
2	14-A	702	BGC	O3-C3	2.67	1.49	1.43
2	15-A	701	BGC	O5-C5	2.68	1.49	1.43
2	5-A	702	BGC	O3-C3	2.68	1.49	1.43
2	19-A	704	BGC	O2-C2	2.69	1.49	1.43
2	9-A	704	BGC	O2-C2	2.69	1.49	1.43
2	8-A	705	BGC	O3-C3	2.69	1.49	1.43
2	5-A	704	BGC	O2-C2	2.69	1.49	1.43
2	15-A	704	BGC	O2-C2	2.69	1.49	1.43
2	2-A	705	BGC	O3-C3	2.69	1.49	1.43
2	2-A	704	BGC	O2-C2	2.69	1.49	1.43
2	4-A	705	BGC	O3-C3	2.70	1.49	1.43
2	22-A	701	BGC	O5-C5	2.70	1.49	1.43
2	19-A	705	BGC	O3-C3	2.70	1.49	1.43
2	14-A	706	BGC	O3-C3	2.71	1.49	1.43
2	24-A	701	BGC	O5-C5	2.71	1.49	1.43
2	1-A	705	BGC	O3-C3	2.72	1.49	1.43
2	7-A	704	BGC	O2-C2	2.73	1.49	1.43
2	19-A	706	BGC	O5-C5	2.73	1.51	1.44
2	4-A	706	BGC	O5-C5	2.74	1.51	1.44
2	25-A	704	BGC	O2-C2	2.74	1.49	1.43
2	7-A	702	BGC	O3-C3	2.74	1.49	1.43
2	23-A	705	BGC	O3-C3	2.75	1.49	1.43
2	2-A	706	BGC	O5-C1	2.75	1.48	1.43
2	12-A	704	BGC	O2-C2	2.75	1.49	1.43
2	8-A	706	BGC	C4-C5	2.76	1.58	1.53
2	5-A	705	BGC	O3-C3	2.76	1.49	1.43
2	24-A	706	BGC	O5-C5	2.76	1.51	1.44
2	10-A	704	BGC	O2-C2	2.76	1.49	1.43
2	15-A	706	BGC	O3-C3	2.76	1.49	1.43
2	24-A	702	BGC	O3-C3	2.78	1.49	1.43
2	23-A	704	BGC	O2-C2	2.79	1.49	1.43
2	5-A	701	BGC	O5-C5	2.80	1.49	1.43
2	17-A	705	BGC	O3-C3	2.83	1.49	1.43
2	19-A	702	BGC	O3-C3	2.83	1.49	1.43
2	9-A	701	BGC	O5-C5	2.84	1.49	1.43
2	4-A	701	BGC	O5-C5	2.84	1.49	1.43
2	13-A	701	BGC	O5-C5	2.84	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	17-A	701	BGC	O5-C5	2.85	1.49	1.43
2	11-A	701	BGC	O5-C5	2.87	1.49	1.43
2	23-A	701	BGC	O5-C5	2.87	1.49	1.43
2	11-A	704	BGC	O2-C2	2.87	1.49	1.43
2	18-A	704	BGC	O2-C2	2.88	1.49	1.43
2	20-A	704	BGC	O2-C2	2.88	1.49	1.43
2	25-A	701	BGC	O5-C5	2.91	1.49	1.43
2	16-A	705	BGC	O3-C3	2.91	1.49	1.43
2	19-A	701	BGC	O5-C5	2.91	1.49	1.43
2	5-A	706	BGC	O3-C3	2.92	1.49	1.43
2	14-A	701	BGC	O5-C5	2.92	1.49	1.43
2	18-A	705	BGC	O3-C3	2.92	1.50	1.43
2	1-A	701	BGC	O5-C5	2.93	1.49	1.43
2	20-A	705	BGC	O3-C3	2.93	1.50	1.43
2	3-A	701	BGC	O5-C5	2.93	1.49	1.43
2	20-A	701	BGC	O5-C5	2.95	1.49	1.43
2	21-A	701	BGC	O5-C5	2.95	1.50	1.43
2	8-A	704	BGC	O5-C5	2.96	1.50	1.43
2	6-A	702	BGC	O3-C3	2.97	1.50	1.43
2	1-A	706	BGC	O3-C3	2.98	1.50	1.43
2	20-A	706	BGC	O5-C5	2.98	1.51	1.44
2	10-A	706	BGC	O5-C5	3.00	1.51	1.44
2	25-A	706	BGC	O5-C5	3.00	1.51	1.44
2	2-A	701	BGC	O5-C5	3.01	1.50	1.43
2	8-A	701	BGC	O5-C5	3.01	1.50	1.43
2	4-A	704	BGC	O2-C2	3.02	1.50	1.43
2	12-A	701	BGC	O5-C5	3.03	1.50	1.43
2	6-A	705	BGC	O3-C3	3.03	1.50	1.43
2	12-A	705	BGC	O3-C3	3.04	1.50	1.43
2	7-A	701	BGC	O5-C5	3.06	1.50	1.43
2	7-A	705	BGC	O3-C3	3.07	1.50	1.43
2	10-A	704	BGC	O5-C5	3.10	1.50	1.43
2	25-A	705	BGC	O3-C3	3.11	1.50	1.43
2	6-A	706	BGC	O3-C3	3.14	1.50	1.43
2	21-A	705	BGC	O3-C3	3.16	1.50	1.43
2	24-A	704	BGC	O5-C5	3.17	1.50	1.43
2	18-A	704	BGC	O5-C5	3.18	1.50	1.43
2	10-A	701	BGC	O5-C5	3.18	1.50	1.43
2	9-A	704	BGC	O5-C5	3.19	1.50	1.43
2	11-A	704	BGC	O5-C5	3.20	1.50	1.43
2	2-A	704	BGC	O5-C5	3.20	1.50	1.43
2	16-A	701	BGC	O5-C5	3.20	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	13-A	704	BGC	O5-C5	3.21	1.50	1.43
2	22-A	704	BGC	O5-C5	3.21	1.50	1.43
2	24-A	702	BGC	O5-C5	3.21	1.50	1.43
2	14-A	704	BGC	O5-C5	3.24	1.50	1.43
2	4-A	704	BGC	O5-C5	3.25	1.50	1.43
2	19-A	704	BGC	O5-C5	3.25	1.50	1.43
2	25-A	704	BGC	O5-C5	3.25	1.50	1.43
2	3-A	704	BGC	O5-C5	3.28	1.50	1.43
2	23-A	702	BGC	O5-C5	3.29	1.50	1.43
2	13-A	706	BGC	O3-C3	3.29	1.50	1.43
2	20-A	704	BGC	O5-C5	3.30	1.50	1.43
2	14-A	706	BGC	O5-C5	3.31	1.52	1.44
2	16-A	706	BGC	O5-C5	3.31	1.52	1.44
2	1-A	704	BGC	O5-C5	3.31	1.50	1.43
2	25-A	702	BGC	O5-C5	3.32	1.50	1.43
2	3-A	702	BGC	O5-C5	3.34	1.50	1.43
2	5-A	704	BGC	O5-C5	3.37	1.50	1.43
2	12-A	706	BGC	O3-C3	3.37	1.51	1.43
2	5-A	706	BGC	O5-C5	3.38	1.52	1.44
2	8-A	702	BGC	O5-C5	3.38	1.50	1.43
2	6-A	704	BGC	O5-C5	3.39	1.50	1.43
2	7-A	704	BGC	O5-C5	3.41	1.51	1.43
2	16-A	704	BGC	O5-C5	3.42	1.51	1.43
2	3-A	705	BGC	O3-C3	3.43	1.51	1.43
2	24-A	706	BGC	O3-C3	3.45	1.51	1.43
2	21-A	704	BGC	O5-C5	3.45	1.51	1.43
2	17-A	704	BGC	O5-C5	3.46	1.51	1.43
2	11-A	706	BGC	O5-C5	3.46	1.53	1.44
2	9-A	706	BGC	O3-C3	3.47	1.51	1.43
2	3-A	706	BGC	O5-C5	3.48	1.53	1.44
2	17-A	706	BGC	O3-C3	3.49	1.51	1.43
2	14-A	702	BGC	O5-C5	3.49	1.51	1.43
2	10-A	706	BGC	O3-C3	3.50	1.51	1.43
2	23-A	704	BGC	O5-C5	3.50	1.51	1.43
2	17-A	702	BGC	O5-C5	3.51	1.51	1.43
2	11-A	702	BGC	O5-C5	3.52	1.51	1.43
2	19-A	702	BGC	O5-C5	3.55	1.51	1.43
2	12-A	704	BGC	O5-C5	3.55	1.51	1.43
2	11-A	703	BGC	O3-C3	3.58	1.51	1.43
2	10-A	702	BGC	O5-C5	3.61	1.51	1.43
2	15-A	704	BGC	O5-C5	3.61	1.51	1.43
2	3-A	703	BGC	O3-C3	3.63	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	23-A	706	BGC	O5-C5	3.65	1.53	1.44
2	12-A	702	BGC	O5-C5	3.65	1.51	1.43
2	22-A	702	BGC	O5-C5	3.68	1.51	1.43
2	12-A	703	BGC	O3-C3	3.68	1.51	1.43
2	16-A	702	BGC	O5-C5	3.69	1.51	1.43
2	12-A	706	BGC	O5-C5	3.69	1.53	1.44
2	13-A	702	BGC	O5-C5	3.70	1.51	1.43
2	21-A	703	BGC	O3-C3	3.71	1.51	1.43
2	20-A	706	BGC	O3-C3	3.72	1.51	1.43
2	14-A	703	BGC	O3-C3	3.75	1.52	1.43
2	20-A	702	BGC	O5-C5	3.76	1.51	1.43
2	8-A	703	BGC	O3-C3	3.76	1.52	1.43
2	5-A	703	BGC	O3-C3	3.76	1.52	1.43
2	20-A	703	BGC	O3-C3	3.76	1.52	1.43
2	19-A	703	BGC	O3-C3	3.77	1.52	1.43
2	5-A	702	BGC	O5-C5	3.78	1.51	1.43
2	15-A	703	BGC	O3-C3	3.78	1.52	1.43
2	4-A	702	BGC	O5-C5	3.82	1.51	1.43
2	17-A	703	BGC	O3-C3	3.82	1.52	1.43
2	9-A	702	BGC	O5-C5	3.83	1.51	1.43
2	1-A	706	BGC	O5-C5	3.84	1.54	1.44
2	7-A	706	BGC	O3-C3	3.84	1.52	1.43
2	18-A	702	BGC	O5-C5	3.85	1.51	1.43
2	6-A	702	BGC	O5-C5	3.85	1.51	1.43
2	1-A	702	BGC	O5-C5	3.85	1.51	1.43
2	1-A	703	BGC	O3-C3	3.87	1.52	1.43
2	2-A	702	BGC	O5-C5	3.87	1.52	1.43
2	7-A	703	BGC	O3-C3	3.87	1.52	1.43
2	4-A	703	BGC	O3-C3	3.88	1.52	1.43
2	8-A	706	BGC	O5-C5	3.88	1.54	1.44
2	2-A	703	BGC	O3-C3	3.88	1.52	1.43
2	23-A	703	BGC	O3-C3	3.91	1.52	1.43
2	2-A	706	BGC	O3-C3	3.91	1.52	1.43
2	21-A	702	BGC	O5-C5	3.92	1.52	1.43
2	16-A	703	BGC	O3-C3	3.94	1.52	1.43
2	10-A	703	BGC	O3-C3	3.95	1.52	1.43
2	2-A	706	BGC	O5-C5	3.95	1.54	1.44
2	22-A	703	BGC	O3-C3	3.96	1.52	1.43
2	6-A	703	BGC	O3-C3	3.97	1.52	1.43
2	9-A	703	BGC	O3-C3	3.98	1.52	1.43
2	8-A	706	BGC	O3-C3	3.98	1.52	1.43
2	21-A	706	BGC	O5-C5	4.01	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7-A	706	BGC	O5-C5	4.01	1.54	1.44
2	24-A	703	BGC	O3-C3	4.02	1.52	1.43
2	15-A	702	BGC	O5-C5	4.05	1.52	1.43
2	25-A	703	BGC	O3-C3	4.06	1.52	1.43
2	1-A	705	BGC	O5-C5	4.09	1.52	1.43
2	6-A	705	BGC	O5-C5	4.10	1.52	1.43
2	12-A	705	BGC	O5-C5	4.12	1.52	1.43
2	17-A	706	BGC	O5-C5	4.13	1.54	1.44
2	7-A	702	BGC	O5-C5	4.15	1.52	1.43
2	25-A	705	BGC	O5-C5	4.15	1.52	1.43
2	17-A	705	BGC	O5-C5	4.20	1.52	1.43
2	18-A	703	BGC	O3-C3	4.21	1.53	1.43
2	15-A	706	BGC	O5-C5	4.21	1.54	1.44
2	13-A	703	BGC	O3-C3	4.23	1.53	1.43
2	22-A	706	BGC	O5-C5	4.25	1.55	1.44
2	11-A	706	BGC	O3-C3	4.27	1.53	1.43
2	6-A	706	BGC	O5-C5	4.29	1.55	1.44
2	21-A	706	BGC	O3-C3	4.31	1.53	1.43
2	15-A	705	BGC	O5-C5	4.34	1.53	1.43
2	23-A	706	BGC	O3-C3	4.36	1.53	1.43
2	13-A	705	BGC	O5-C5	4.39	1.53	1.43
2	7-A	705	BGC	O5-C5	4.39	1.53	1.43
2	19-A	705	BGC	O5-C5	4.40	1.53	1.43
2	14-A	705	BGC	O5-C5	4.42	1.53	1.43
2	10-A	705	BGC	O5-C5	4.48	1.53	1.43
2	18-A	706	BGC	O5-C5	4.50	1.55	1.44
2	9-A	705	BGC	O5-C5	4.53	1.53	1.43
2	22-A	705	BGC	O5-C5	4.54	1.53	1.43
2	18-A	705	BGC	O5-C5	4.58	1.53	1.43
2	24-A	705	BGC	O5-C5	4.58	1.53	1.43
2	3-A	705	BGC	O5-C5	4.60	1.53	1.43
2	2-A	705	BGC	O5-C5	4.67	1.53	1.43
2	16-A	705	BGC	O5-C5	4.71	1.53	1.43
2	23-A	705	BGC	O5-C5	4.72	1.53	1.43
2	5-A	705	BGC	O5-C5	4.77	1.54	1.43
2	4-A	706	BGC	O3-C3	4.84	1.54	1.43
2	11-A	705	BGC	O5-C5	4.85	1.54	1.43
2	20-A	705	BGC	O5-C5	4.89	1.54	1.43
2	18-A	706	BGC	O3-C3	4.90	1.54	1.43
2	3-A	706	BGC	O3-C3	4.91	1.54	1.43
2	4-A	705	BGC	O5-C5	4.99	1.54	1.43
2	8-A	705	BGC	O5-C5	5.16	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	21-A	705	BGC	O5-C5	5.32	1.55	1.43

All (415) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-A	705	BGC	O5-C1-C2	-7.89	98.06	110.86
2	22-A	706	BGC	C1-C2-C3	-7.56	99.18	110.43
2	15-A	706	BGC	C1-C2-C3	-6.94	100.10	110.43
2	2-A	706	BGC	C4-C3-C2	-6.05	99.50	110.79
2	9-A	706	BGC	O5-C5-C4	-5.69	99.00	109.68
2	21-A	705	BGC	C2-C3-C4	-5.45	101.79	111.04
2	8-A	706	BGC	C4-C3-C2	-5.45	100.63	110.79
2	14-A	706	BGC	C1-O5-C5	-5.40	103.48	113.47
2	1-A	706	BGC	C1-C2-C3	-5.33	102.50	110.43
2	23-A	706	BGC	C6-C5-C4	-5.13	100.35	113.02
2	6-A	706	BGC	C1-C2-C3	-4.72	103.41	110.43
2	2-A	706	BGC	O5-C5-C4	-4.67	100.93	109.68
2	8-A	706	BGC	O5-C5-C4	-4.54	101.17	109.68
2	23-A	703	BGC	O5-C5-C4	-4.50	101.23	109.68
2	4-A	706	BGC	C6-C5-C4	-4.47	101.99	113.02
2	21-A	706	BGC	O2-C2-C1	-4.41	100.11	109.82
2	13-A	706	BGC	O5-C5-C4	-4.32	101.58	109.68
2	11-A	703	BGC	O5-C5-C4	-4.27	101.67	109.68
2	8-A	703	BGC	O5-C5-C4	-4.18	101.84	109.68
2	21-A	705	BGC	O5-C1-C2	-4.12	104.18	110.86
2	21-A	703	BGC	O5-C5-C4	-3.89	102.39	109.68
2	10-A	705	BGC	C2-C3-C4	-3.87	104.46	111.04
2	14-A	703	BGC	O5-C5-C4	-3.81	102.53	109.68
2	16-A	703	BGC	O5-C5-C4	-3.62	102.89	109.68
2	19-A	703	BGC	O5-C5-C4	-3.52	103.08	109.68
2	5-A	703	BGC	O5-C5-C4	-3.38	103.33	109.68
2	16-A	706	BGC	O2-C2-C1	-3.38	102.38	109.82
2	4-A	706	BGC	C4-C3-C2	-3.30	104.63	110.79
2	18-A	706	BGC	O5-C5-C4	-3.28	103.52	109.68
2	5-A	706	BGC	O3-C3-C2	-3.28	102.95	110.34
2	21-A	706	BGC	O5-C5-C4	-3.22	103.63	109.68
2	5-A	706	BGC	C1-O5-C5	-3.17	107.60	113.47
2	15-A	703	BGC	O5-C5-C4	-3.16	103.75	109.68
2	3-A	702	BGC	O5-C1-C2	-3.12	105.80	110.86
2	15-A	704	BGC	C6-C5-C4	-3.04	105.51	113.02
2	17-A	702	BGC	O5-C1-C2	-3.02	105.96	110.86
2	2-A	702	BGC	O5-C1-C2	-3.00	105.98	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	24-A	703	BGC	O5-C5-C4	-2.99	104.07	109.68
2	14-A	706	BGC	O3-C3-C2	-2.98	103.62	110.34
2	16-A	705	BGC	O2-C2-C3	-2.96	104.16	110.12
2	3-A	704	BGC	O5-C1-C2	-2.95	106.07	110.86
2	12-A	706	BGC	O2-C2-C1	-2.92	103.39	109.82
2	17-A	703	BGC	O5-C5-C4	-2.92	104.21	109.68
2	3-A	703	BGC	O5-C5-C4	-2.90	104.23	109.68
2	6-A	702	BGC	C1-O5-C5	-2.84	108.64	112.25
2	9-A	703	BGC	O5-C5-C4	-2.81	104.41	109.68
2	10-A	703	BGC	O5-C5-C4	-2.80	104.42	109.68
2	9-A	706	BGC	O2-C2-C3	-2.79	104.05	110.34
2	14-A	706	BGC	O3-C3-C4	-2.77	104.09	110.34
2	9-A	702	BGC	C1-O5-C5	-2.77	108.73	112.25
2	16-A	705	BGC	O4-C4-C3	-2.76	104.12	110.34
2	11-A	705	BGC	O3-C3-C2	-2.75	105.04	110.00
2	13-A	702	BGC	O5-C1-C2	-2.72	106.44	110.86
2	3-A	706	BGC	O2-C2-C1	-2.70	103.87	109.82
2	21-A	706	BGC	O3-C3-C4	-2.69	104.27	110.34
2	1-A	703	BGC	O5-C5-C4	-2.69	104.63	109.68
2	6-A	703	BGC	O5-C5-C4	-2.68	104.64	109.68
2	4-A	702	BGC	O5-C1-C2	-2.68	106.52	110.86
2	25-A	706	BGC	O1-C1-C2	-2.67	102.05	109.21
2	13-A	702	BGC	C1-O5-C5	-2.63	108.92	112.25
2	12-A	703	BGC	O5-C5-C4	-2.61	104.78	109.68
2	24-A	706	BGC	O3-C3-C2	-2.61	104.46	110.34
2	7-A	702	BGC	C1-O5-C5	-2.61	108.94	112.25
2	5-A	702	BGC	O5-C1-C2	-2.61	106.62	110.86
2	12-A	702	BGC	C1-O5-C5	-2.60	108.94	112.25
2	18-A	706	BGC	O4-C4-C3	-2.60	104.48	110.34
2	4-A	704	BGC	O5-C1-C2	-2.58	106.66	110.86
2	11-A	704	BGC	O5-C1-C2	-2.58	106.66	110.86
2	21-A	706	BGC	C3-C4-C5	-2.56	105.74	110.20
2	11-A	702	BGC	O5-C1-C2	-2.56	106.71	110.86
2	18-A	706	BGC	O4-C4-C5	-2.55	102.48	109.24
2	11-A	705	BGC	O3-C3-C4	-2.55	104.61	110.34
2	16-A	702	BGC	O5-C1-C2	-2.55	106.73	110.86
2	16-A	705	BGC	O5-C1-C2	-2.54	106.73	110.86
2	8-A	704	BGC	O4-C4-C5	-2.53	102.54	109.24
2	4-A	705	BGC	C2-C3-C4	-2.51	106.77	111.04
2	2-A	706	BGC	C6-C5-C4	-2.47	106.92	113.02
2	4-A	704	BGC	O4-C4-C5	-2.43	102.80	109.24
2	7-A	706	BGC	C1-C2-C3	-2.42	106.83	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-A	703	BGC	O1-C1-O5	-2.40	103.69	110.25
2	22-A	702	BGC	O5-C1-C2	-2.33	107.08	110.86
2	15-A	702	BGC	O5-C1-C2	-2.33	107.08	110.86
2	25-A	702	BGC	O5-C1-C2	-2.33	107.08	110.86
2	10-A	702	BGC	O5-C1-C2	-2.32	107.10	110.86
2	15-A	706	BGC	C6-C5-C4	-2.32	107.30	113.02
2	12-A	702	BGC	O5-C1-C2	-2.31	107.11	110.86
2	21-A	705	BGC	C3-C4-C5	-2.31	106.17	110.20
2	25-A	706	BGC	O2-C2-C1	-2.30	104.75	109.82
2	8-A	702	BGC	O5-C1-C2	-2.30	107.13	110.86
2	25-A	706	BGC	C1-C2-C3	-2.28	107.03	110.43
2	18-A	702	BGC	O5-C1-C2	-2.27	107.17	110.86
2	1-A	703	BGC	C1-O5-C5	-2.27	109.28	113.47
2	18-A	705	BGC	O5-C1-C2	-2.25	107.21	110.86
2	4-A	703	BGC	O5-C5-C4	-2.24	105.47	109.68
2	12-A	702	BGC	O4-C4-C5	-2.24	103.30	109.24
2	3-A	702	BGC	O3-C3-C2	-2.24	105.96	110.00
2	9-A	703	BGC	O5-C1-C2	-2.24	106.23	109.80
2	4-A	705	BGC	O3-C3-C4	-2.22	105.34	110.34
2	11-A	706	BGC	O2-C2-C1	-2.19	104.99	109.82
2	10-A	706	BGC	O3-C3-C2	-2.19	105.41	110.34
2	9-A	703	BGC	O1-C1-O5	-2.19	104.27	110.25
2	6-A	704	BGC	O5-C1-C2	-2.18	107.32	110.86
2	24-A	706	BGC	O5-C5-C4	-2.18	105.60	109.68
2	25-A	706	BGC	O5-C5-C4	-2.17	105.61	109.68
2	15-A	706	BGC	O4-C4-C5	-2.16	103.52	109.24
2	5-A	706	BGC	O4-C4-C5	-2.16	103.52	109.24
2	7-A	702	BGC	C6-C5-C4	-2.15	107.71	113.02
2	20-A	706	BGC	O2-C2-C1	-2.15	105.08	109.82
2	23-A	704	BGC	O5-C1-C2	-2.14	107.39	110.86
2	11-A	703	BGC	O3-C3-C2	-2.14	105.53	110.34
2	13-A	703	BGC	O5-C5-C4	-2.12	105.70	109.68
2	17-A	706	BGC	C4-C3-C2	-2.11	106.85	110.79
2	18-A	703	BGC	O1-C1-O5	-2.11	104.48	110.25
2	25-A	704	BGC	O4-C4-C5	-2.10	103.68	109.24
2	7-A	703	BGC	O5-C5-C4	-2.09	105.76	109.68
2	8-A	705	BGC	O3-C3-C2	-2.08	106.23	110.00
2	19-A	706	BGC	O3-C3-C2	-2.05	105.72	110.34
2	1-A	702	BGC	O2-C2-C3	-2.03	106.04	110.12
2	5-A	706	BGC	O5-C5-C4	-2.03	105.88	109.68
2	24-A	702	BGC	O4-C4-C5	-2.02	103.87	109.24
2	12-A	704	BGC	C1-O5-C5	-2.01	109.69	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	8-A	706	BGC	C1-C2-C3	-2.01	107.43	110.43
2	9-A	702	BGC	O5-C1-C2	-2.01	107.60	110.86
2	4-A	706	BGC	O5-C5-C4	-2.00	105.92	109.68
2	23-A	704	BGC	C6-C5-C4	-2.00	108.08	113.02
2	20-A	704	BGC	O6-C6-C5	2.00	117.96	111.33
2	7-A	705	BGC	C1-C2-C3	2.01	111.92	109.54
2	8-A	704	BGC	O6-C6-C5	2.01	117.96	111.33
2	10-A	706	BGC	O6-C6-C5	2.01	117.98	111.33
2	16-A	705	BGC	C1-C2-C3	2.01	111.92	109.54
2	20-A	706	BGC	O1-C1-C2	2.01	114.60	109.21
2	3-A	706	BGC	C1-O5-C5	2.02	117.20	113.47
2	21-A	706	BGC	O1-C1-O5	2.02	115.78	110.25
2	19-A	705	BGC	O5-C5-C6	2.03	111.74	107.35
2	25-A	704	BGC	C2-C3-C4	2.03	114.49	111.04
2	12-A	704	BGC	O6-C6-C5	2.03	118.05	111.33
2	15-A	706	BGC	C3-C4-C5	2.05	113.77	110.20
2	19-A	706	BGC	O2-C2-C3	2.05	114.95	110.34
2	11-A	706	BGC	C1-O5-C5	2.06	117.28	113.47
2	10-A	701	BGC	C2-C3-C4	2.06	114.55	111.04
2	19-A	705	BGC	O6-C6-C5	2.07	118.17	111.33
2	15-A	706	BGC	O5-C5-C4	2.07	113.58	109.68
2	14-A	706	BGC	O2-C2-C1	2.08	114.40	109.82
2	16-A	706	BGC	O3-C3-C4	2.08	115.02	110.34
2	7-A	704	BGC	C2-C3-C4	2.09	114.59	111.04
2	7-A	702	BGC	O5-C5-C6	2.09	111.87	107.35
2	16-A	703	BGC	C1-C2-C3	2.10	113.55	110.43
2	5-A	704	BGC	C1-C2-C3	2.10	112.02	109.54
2	2-A	704	BGC	O4-C4-C3	2.11	115.08	110.34
2	4-A	706	BGC	C3-C4-C5	2.11	113.88	110.20
2	11-A	705	BGC	O2-C2-C1	2.11	113.44	109.21
2	9-A	704	BGC	C1-C2-C3	2.12	112.04	109.54
2	11-A	704	BGC	C3-C4-C5	2.12	113.89	110.20
2	7-A	706	BGC	C1-O5-C5	2.13	117.41	113.47
2	8-A	703	BGC	O4-C4-C3	2.13	115.13	110.34
2	23-A	704	BGC	C2-C3-C4	2.13	114.67	111.04
2	19-A	704	BGC	C2-C3-C4	2.14	114.68	111.04
2	9-A	701	BGC	O6-C6-C5	2.15	118.44	111.33
2	6-A	705	BGC	O6-C6-C5	2.16	118.46	111.33
2	19-A	706	BGC	C1-O5-C5	2.16	117.47	113.47
2	1-A	705	BGC	O5-C1-C2	2.16	114.36	110.86
2	17-A	701	BGC	O4-C4-C3	2.16	115.20	110.34
2	16-A	706	BGC	O2-C2-C3	2.17	115.22	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	8-A	706	BGC	C6-C5-C4	2.18	118.39	113.02
2	5-A	706	BGC	C6-C5-C4	2.19	118.42	113.02
2	11-A	706	BGC	C1-C2-C3	2.20	113.69	110.43
2	12-A	706	BGC	O5-C5-C6	2.21	111.94	106.36
2	8-A	703	BGC	C1-C2-C3	2.21	113.72	110.43
2	10-A	706	BGC	C1-C2-C3	2.21	113.72	110.43
2	21-A	704	BGC	C1-O5-C5	2.22	115.06	112.25
2	10-A	706	BGC	C4-C3-C2	2.22	114.94	110.79
2	8-A	705	BGC	O6-C6-C5	2.22	118.67	111.33
2	21-A	705	BGC	O4-C4-C3	2.23	115.35	110.34
2	6-A	704	BGC	C2-C3-C4	2.23	114.83	111.04
2	24-A	705	BGC	O5-C5-C6	2.23	112.19	107.35
2	23-A	705	BGC	O6-C6-C5	2.24	118.72	111.33
2	17-A	706	BGC	C1-O5-C5	2.24	117.62	113.47
2	17-A	704	BGC	O6-C6-C5	2.26	118.80	111.33
2	10-A	705	BGC	C1-C2-C3	2.27	112.23	109.54
2	20-A	706	BGC	C4-C3-C2	2.28	115.04	110.79
2	21-A	706	BGC	O5-C1-C2	2.30	113.46	109.80
2	9-A	705	BGC	O6-C6-C5	2.31	118.97	111.33
2	23-A	706	BGC	O4-C4-C3	2.31	115.55	110.34
2	25-A	706	BGC	O5-C1-C2	2.32	113.49	109.80
2	19-A	703	BGC	C1-C2-C3	2.32	113.88	110.43
2	3-A	701	BGC	C1-C2-C3	2.32	112.28	109.54
2	6-A	706	BGC	O4-C4-C3	2.33	115.57	110.34
2	3-A	705	BGC	O6-C6-C5	2.33	119.02	111.33
2	2-A	704	BGC	C2-C3-C4	2.33	114.99	111.04
2	22-A	706	BGC	O3-C3-C4	2.33	115.58	110.34
2	12-A	704	BGC	O5-C5-C6	2.33	112.39	107.35
2	10-A	703	BGC	C1-C2-C3	2.33	113.90	110.43
2	22-A	704	BGC	C2-C3-C4	2.33	115.00	111.04
2	13-A	706	BGC	O4-C4-C3	2.35	115.62	110.34
2	22-A	706	BGC	O3-C3-C2	2.36	115.65	110.34
2	11-A	705	BGC	O5-C5-C6	2.36	112.46	107.35
2	7-A	706	BGC	O5-C1-C2	2.36	113.57	109.80
2	24-A	705	BGC	O6-C6-C5	2.37	119.15	111.33
2	7-A	706	BGC	O1-C1-C2	2.38	115.58	109.21
2	11-A	705	BGC	C3-C4-C5	2.38	114.34	110.20
2	15-A	706	BGC	C1-O5-C5	2.38	117.88	113.47
2	2-A	701	BGC	C1-C2-C3	2.39	112.36	109.54
2	24-A	704	BGC	C2-C3-C4	2.39	115.10	111.04
2	14-A	706	BGC	O5-C1-C2	2.39	113.61	109.80
2	9-A	705	BGC	C1-C2-C3	2.40	112.38	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	22-A	705	BGC	C1-O5-C5	2.40	115.30	112.25
2	4-A	705	BGC	O2-C2-C3	2.41	114.96	110.12
2	17-A	703	BGC	C1-C2-C3	2.41	114.01	110.43
2	21-A	705	BGC	O5-C5-C6	2.42	112.58	107.35
2	24-A	706	BGC	O6-C6-C5	2.43	119.35	111.33
2	8-A	703	BGC	O5-C5-C6	2.44	112.51	106.36
2	23-A	705	BGC	C3-C4-C5	2.44	114.45	110.20
2	16-A	706	BGC	O5-C1-C2	2.47	113.74	109.80
2	20-A	701	BGC	O6-C6-C5	2.48	119.54	111.33
2	21-A	705	BGC	O3-C3-C2	2.48	114.49	110.00
2	7-A	704	BGC	C1-C2-C3	2.49	112.49	109.54
2	18-A	704	BGC	C2-C3-C4	2.50	115.28	111.04
2	21-A	706	BGC	O6-C6-C5	2.50	119.58	111.33
2	12-A	703	BGC	C1-C2-C3	2.52	114.17	110.43
2	9-A	703	BGC	C1-C2-C3	2.53	114.19	110.43
2	8-A	705	BGC	C3-C4-C5	2.54	114.62	110.20
2	6-A	706	BGC	O2-C2-C1	2.54	115.42	109.82
2	10-A	706	BGC	C1-O5-C5	2.55	118.19	113.47
2	25-A	705	BGC	C1-C2-C3	2.55	112.56	109.54
2	24-A	706	BGC	C1-C2-C3	2.56	114.23	110.43
2	21-A	705	BGC	C1-O5-C5	2.56	115.50	112.25
2	23-A	705	BGC	O5-C5-C6	2.56	112.90	107.35
2	23-A	704	BGC	O6-C6-C5	2.57	119.82	111.33
2	12-A	704	BGC	C2-C3-C4	2.57	115.41	111.04
2	19-A	705	BGC	C1-C2-C3	2.57	112.59	109.54
2	25-A	706	BGC	C1-O5-C5	2.58	118.23	113.47
2	6-A	706	BGC	O5-C1-C2	2.58	113.91	109.80
2	4-A	706	BGC	O2-C2-C3	2.58	116.14	110.34
2	14-A	706	BGC	C1-C2-C3	2.58	114.27	110.43
2	5-A	706	BGC	O5-C5-C6	2.58	112.89	106.36
2	15-A	704	BGC	O6-C6-C5	2.59	119.90	111.33
2	1-A	706	BGC	O5-C5-C6	2.60	112.92	106.36
2	18-A	706	BGC	C6-C5-C4	2.60	119.42	113.02
2	15-A	703	BGC	C1-C2-C3	2.61	114.31	110.43
2	17-A	704	BGC	C2-C3-C4	2.64	115.52	111.04
2	7-A	703	BGC	C1-C2-C3	2.64	114.35	110.43
2	14-A	706	BGC	O5-C5-C6	2.65	113.04	106.36
2	6-A	701	BGC	O6-C6-C5	2.65	120.07	111.33
2	8-A	706	BGC	O2-C2-C3	2.67	116.36	110.34
2	23-A	706	BGC	O5-C5-C4	2.67	114.70	109.68
2	18-A	706	BGC	O5-C1-C2	2.68	114.06	109.80
2	15-A	705	BGC	O5-C1-C2	2.68	115.20	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	11-A	705	BGC	O6-C6-C5	2.68	120.19	111.33
2	20-A	703	BGC	C1-C2-C3	2.68	114.42	110.43
2	13-A	704	BGC	C2-C3-C4	2.69	115.61	111.04
2	11-A	704	BGC	O2-C2-C3	2.69	115.53	110.12
2	23-A	704	BGC	C1-O5-C5	2.70	115.68	112.25
2	5-A	705	BGC	O6-C6-C5	2.70	120.27	111.33
2	9-A	701	BGC	O5-C1-C2	2.72	115.27	110.86
2	1-A	704	BGC	C2-C3-C4	2.72	115.67	111.04
2	13-A	703	BGC	C1-C2-C3	2.73	114.49	110.43
2	9-A	705	BGC	O5-C5-C6	2.74	113.28	107.35
2	6-A	703	BGC	C1-C2-C3	2.75	114.51	110.43
2	15-A	704	BGC	C2-C3-C4	2.75	115.71	111.04
2	13-A	705	BGC	C1-C2-C3	2.78	112.83	109.54
2	8-A	705	BGC	C1-O5-C5	2.79	115.79	112.25
2	17-A	705	BGC	C1-O5-C5	2.80	115.80	112.25
2	12-A	706	BGC	O6-C6-C5	2.80	120.59	111.33
2	15-A	704	BGC	C3-C4-C5	2.80	115.08	110.20
2	20-A	704	BGC	C2-C3-C4	2.82	115.83	111.04
2	4-A	704	BGC	C2-C3-C4	2.82	115.83	111.04
2	9-A	704	BGC	C2-C3-C4	2.83	115.84	111.04
2	13-A	706	BGC	O5-C5-C6	2.83	113.50	106.36
2	1-A	706	BGC	O2-C2-C3	2.83	116.71	110.34
2	13-A	706	BGC	C1-O5-C5	2.83	118.71	113.47
2	3-A	706	BGC	O6-C6-C5	2.83	120.70	111.33
2	3-A	704	BGC	C2-C3-C4	2.83	115.86	111.04
2	22-A	706	BGC	O5-C5-C6	2.84	113.52	106.36
2	16-A	704	BGC	C2-C3-C4	2.84	115.87	111.04
2	10-A	701	BGC	C1-C2-C3	2.86	112.92	109.54
2	25-A	704	BGC	O4-C4-C3	2.86	116.78	110.34
2	13-A	705	BGC	C1-O5-C5	2.87	115.89	112.25
2	2-A	703	BGC	C1-C2-C3	2.89	114.72	110.43
2	22-A	703	BGC	C1-C2-C3	2.90	114.74	110.43
2	24-A	703	BGC	C1-C2-C3	2.91	114.75	110.43
2	13-A	706	BGC	O5-C1-C2	2.91	114.44	109.80
2	5-A	705	BGC	O5-C5-C6	2.92	113.66	107.35
2	22-A	705	BGC	C1-C2-C3	2.93	113.01	109.54
2	16-A	706	BGC	O5-C5-C6	2.94	113.79	106.36
2	14-A	706	BGC	O1-C1-C2	2.94	117.10	109.21
2	1-A	706	BGC	O3-C3-C2	2.94	116.97	110.34
2	9-A	701	BGC	C1-C2-C3	2.95	113.03	109.54
2	14-A	704	BGC	C2-C3-C4	2.95	116.05	111.04
2	17-A	705	BGC	C1-C2-C3	2.95	113.04	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	21-A	704	BGC	C2-C3-C4	2.99	116.12	111.04
2	8-A	706	BGC	O6-C6-C5	3.03	121.33	111.33
2	10-A	704	BGC	C1-C2-C3	3.06	113.16	109.54
2	4-A	703	BGC	C1-C2-C3	3.06	114.97	110.43
2	15-A	706	BGC	O5-C5-C6	3.06	114.09	106.36
2	25-A	703	BGC	C1-C2-C3	3.07	114.99	110.43
2	20-A	706	BGC	O6-C6-C5	3.07	121.47	111.33
2	25-A	705	BGC	C1-O5-C5	3.08	116.16	112.25
2	23-A	704	BGC	C3-C4-C5	3.10	115.60	110.20
2	3-A	706	BGC	C1-C2-C3	3.15	115.11	110.43
2	5-A	704	BGC	C2-C3-C4	3.17	116.43	111.04
2	6-A	705	BGC	C1-C2-C3	3.24	113.37	109.54
2	17-A	706	BGC	O4-C4-C3	3.26	117.67	110.34
2	3-A	706	BGC	C4-C3-C2	3.28	116.92	110.79
2	16-A	701	BGC	C1-C2-C3	3.29	113.43	109.54
2	23-A	706	BGC	O5-C1-C2	3.29	115.05	109.80
2	1-A	706	BGC	C1-O5-C5	3.31	119.59	113.47
2	11-A	705	BGC	C1-C2-C3	3.32	113.47	109.54
2	3-A	706	BGC	O5-C1-C2	3.32	115.10	109.80
2	21-A	701	BGC	C1-C2-C3	3.33	113.48	109.54
2	9-A	706	BGC	O5-C1-C2	3.34	115.12	109.80
2	15-A	704	BGC	C1-O5-C5	3.35	116.50	112.25
2	1-A	701	BGC	C1-C2-C3	3.38	113.54	109.54
2	8-A	705	BGC	C1-C2-C3	3.40	113.56	109.54
2	13-A	701	BGC	C1-C2-C3	3.41	113.57	109.54
2	4-A	701	BGC	C1-C2-C3	3.44	113.61	109.54
2	5-A	706	BGC	O6-C6-C5	3.45	122.72	111.33
2	25-A	706	BGC	O5-C5-C6	3.45	115.07	106.36
2	22-A	706	BGC	C1-O5-C5	3.47	119.89	113.47
2	16-A	706	BGC	C1-O5-C5	3.49	119.93	113.47
2	4-A	706	BGC	O3-C3-C4	3.51	118.23	110.34
2	14-A	706	BGC	C3-C4-C5	3.52	116.34	110.20
2	12-A	705	BGC	C1-C2-C3	3.53	113.71	109.54
2	5-A	701	BGC	C1-C2-C3	3.53	113.72	109.54
2	21-A	706	BGC	C1-C2-C3	3.53	115.68	110.43
2	18-A	703	BGC	C1-C2-C3	3.54	115.69	110.43
2	7-A	706	BGC	C3-C4-C5	3.55	116.39	110.20
2	17-A	706	BGC	C1-C2-C3	3.56	115.72	110.43
2	15-A	706	BGC	O2-C2-C3	3.58	118.39	110.34
2	12-A	705	BGC	C1-O5-C5	3.63	116.86	112.25
2	1-A	706	BGC	C3-C4-C5	3.64	116.55	110.20
2	17-A	706	BGC	O5-C5-C6	3.65	115.58	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	15-A	706	BGC	O2-C2-C1	3.69	117.94	109.82
2	11-A	701	BGC	C1-C2-C3	3.73	113.95	109.54
2	21-A	706	BGC	O3-C3-C2	3.74	118.75	110.34
2	1-A	705	BGC	C1-C2-C3	3.74	113.96	109.54
2	2-A	706	BGC	O3-C3-C4	3.76	118.79	110.34
2	18-A	701	BGC	C1-C2-C3	3.78	114.01	109.54
2	19-A	701	BGC	C1-C2-C3	3.78	114.01	109.54
2	15-A	706	BGC	O1-C1-C2	3.79	119.36	109.21
2	6-A	706	BGC	O5-C5-C6	3.83	116.04	106.36
2	16-A	705	BGC	C2-C3-C4	3.87	117.61	111.04
2	13-A	706	BGC	O6-C6-C5	3.89	124.18	111.33
2	15-A	705	BGC	C1-O5-C5	3.90	117.19	112.25
2	14-A	701	BGC	C1-C2-C3	3.92	114.18	109.54
2	16-A	702	BGC	C1-C2-C3	3.93	114.19	109.54
2	22-A	701	BGC	C1-C2-C3	3.94	114.20	109.54
2	11-A	702	BGC	C1-C2-C3	3.95	114.21	109.54
2	15-A	705	BGC	C1-C2-C3	3.95	114.22	109.54
2	23-A	701	BGC	C1-C2-C3	3.97	114.24	109.54
2	2-A	706	BGC	O5-C5-C6	4.00	116.46	106.36
2	15-A	701	BGC	C1-C2-C3	4.02	114.30	109.54
2	25-A	706	BGC	O2-C2-C3	4.04	119.43	110.34
2	25-A	701	BGC	C1-C2-C3	4.08	114.37	109.54
2	7-A	701	BGC	C1-C2-C3	4.12	114.41	109.54
2	22-A	702	BGC	C1-C2-C3	4.13	114.43	109.54
2	17-A	701	BGC	C1-C2-C3	4.13	114.43	109.54
2	21-A	706	BGC	O2-C2-C3	4.18	119.74	110.34
2	21-A	706	BGC	O5-C5-C6	4.18	116.93	106.36
2	23-A	702	BGC	C1-C2-C3	4.22	114.53	109.54
2	8-A	701	BGC	C1-C2-C3	4.25	114.57	109.54
2	8-A	702	BGC	C1-C2-C3	4.28	114.60	109.54
2	17-A	706	BGC	O3-C3-C4	4.28	119.98	110.34
2	9-A	702	BGC	C1-C2-C3	4.30	114.63	109.54
2	7-A	702	BGC	C1-C2-C3	4.30	114.63	109.54
2	5-A	706	BGC	O3-C3-C4	4.30	120.03	110.34
2	22-A	706	BGC	O2-C2-C3	4.32	120.07	110.34
2	21-A	704	BGC	C1-C2-C3	4.35	114.68	109.54
2	3-A	702	BGC	C1-C2-C3	4.35	114.69	109.54
2	12-A	702	BGC	C1-C2-C3	4.36	114.70	109.54
2	10-A	702	BGC	C1-C2-C3	4.36	114.70	109.54
2	17-A	702	BGC	C1-C2-C3	4.36	114.70	109.54
2	4-A	706	BGC	O5-C1-C2	4.38	116.78	109.80
2	21-A	702	BGC	C1-C2-C3	4.39	114.73	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	23-A	706	BGC	C3-C4-C5	4.39	117.85	110.20
2	18-A	706	BGC	O6-C6-C5	4.41	125.90	111.33
2	8-A	706	BGC	O4-C4-C5	4.42	120.96	109.24
2	14-A	702	BGC	C1-C2-C3	4.44	114.79	109.54
2	20-A	701	BGC	C1-C2-C3	4.44	114.80	109.54
2	18-A	706	BGC	C3-C4-C5	4.45	117.96	110.20
2	3-A	705	BGC	C1-C2-C3	4.48	114.83	109.54
2	18-A	706	BGC	O5-C5-C6	4.48	117.67	106.36
2	10-A	705	BGC	C1-O5-C5	4.48	117.93	112.25
2	18-A	705	BGC	C1-C2-C3	4.59	114.97	109.54
2	20-A	704	BGC	C1-O5-C5	4.60	118.08	112.25
2	4-A	702	BGC	C1-C2-C3	4.60	114.99	109.54
2	6-A	702	BGC	C1-C2-C3	4.63	115.02	109.54
2	15-A	702	BGC	C1-C2-C3	4.65	115.04	109.54
2	20-A	702	BGC	C1-C2-C3	4.66	115.05	109.54
2	18-A	705	BGC	C1-O5-C5	4.68	118.19	112.25
2	2-A	702	BGC	C1-C2-C3	4.69	115.09	109.54
2	6-A	701	BGC	C1-C2-C3	4.70	115.10	109.54
2	7-A	706	BGC	C4-C3-C2	4.73	119.62	110.79
2	24-A	702	BGC	C1-C2-C3	4.74	115.15	109.54
2	5-A	702	BGC	C1-C2-C3	4.76	115.17	109.54
2	24-A	701	BGC	C1-C2-C3	4.78	115.20	109.54
2	3-A	706	BGC	C3-C4-C5	4.80	118.57	110.20
2	4-A	706	BGC	O4-C4-C3	4.82	121.20	110.34
2	12-A	701	BGC	C1-C2-C3	4.83	115.25	109.54
2	18-A	702	BGC	C1-C2-C3	4.84	115.26	109.54
2	1-A	702	BGC	C1-C2-C3	4.87	115.30	109.54
2	2-A	706	BGC	O4-C4-C3	4.91	121.40	110.34
2	19-A	702	BGC	C1-C2-C3	5.04	115.51	109.54
2	4-A	705	BGC	O2-C2-C1	5.09	119.41	109.21
2	14-A	706	BGC	C4-C3-C2	5.09	120.29	110.79
2	15-A	706	BGC	O3-C3-C2	5.10	121.83	110.34
2	25-A	702	BGC	C1-C2-C3	5.12	115.59	109.54
2	20-A	705	BGC	C1-O5-C5	5.13	118.76	112.25
2	20-A	705	BGC	C1-C2-C3	5.22	115.71	109.54
2	6-A	706	BGC	C1-O5-C5	5.27	123.22	113.47
2	9-A	706	BGC	C1-C2-C3	5.30	118.31	110.43
2	13-A	702	BGC	C1-C2-C3	5.31	115.83	109.54
2	21-A	705	BGC	O2-C2-C1	5.37	119.98	109.21
2	1-A	705	BGC	C1-O5-C5	5.51	119.24	112.25
2	17-A	706	BGC	O5-C1-C2	6.09	119.50	109.80
2	2-A	706	BGC	O5-C1-C2	7.55	121.84	109.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.