Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:50 PM GMT

PDB ID	:	4TZ3
Title	:	Ensemble refinement of the E502A variant of sacteLam55A from Streptomyces sp. SirexAA-E in complex with laminaritetraose
Authors	:	Bianchetti, C.M.; Takasuka, T.E.; Yik, E.J.; Bergeman, L.F.; Fox, B.G.
Deposited on	:	2014-07-09
Resolution	:	1.90 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 (i) symbol.

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

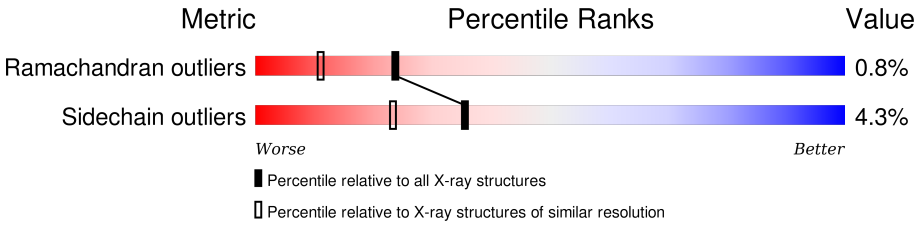
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	FAILED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

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 <=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	95% 5%
1	10-A	549	95% 5%
1	11-A	549	95% 5%
1	12-A	549	95% 5%
1	13-A	549	95%
1	14-A	549	94% 5%
1	15-A	549	94% 5%
1	16-A	549	96%

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 210296 atoms, of which 98125 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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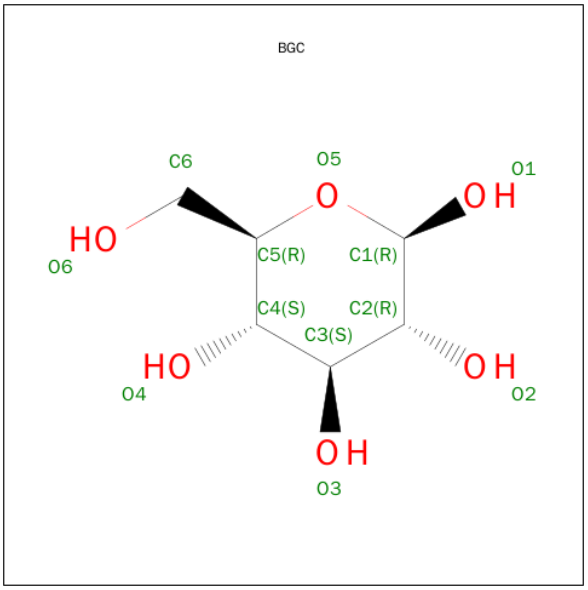
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	18-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	19-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	20-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	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 11 6 5	0	0
2	2-A	1	Total C O 11 6 5	0	0
2	3-A	1	Total C O 11 6 5	0	0
2	4-A	1	Total C O 11 6 5	0	0
2	5-A	1	Total C O 11 6 5	0	0
2	6-A	1	Total C O 11 6 5	0	0
2	7-A	1	Total C O 11 6 5	0	0
2	8-A	1	Total C O 11 6 5	0	0
2	9-A	1	Total C O 11 6 5	0	0
2	10-A	1	Total C O 11 6 5	0	0
2	11-A	1	Total C O 11 6 5	0	0
2	12-A	1	Total C O 11 6 5	0	0
2	13-A	1	Total C O 11 6 5	0	0
2	14-A	1	Total C O 11 6 5	0	0
2	15-A	1	Total C O 11 6 5	0	0
2	16-A	1	Total C O 11 6 5	0	0
2	17-A	1	Total C O 11 6 5	0	0
2	18-A	1	Total C O 11 6 5	0	0
2	19-A	1	Total C O 11 6 5	0	0
2	20-A	1	Total C O 11 6 5	0	0
2	21-A	1	Total C O 11 6 5	0	0
2	22-A	1	Total C O 11 6 5	0	0

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

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

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

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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
			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		

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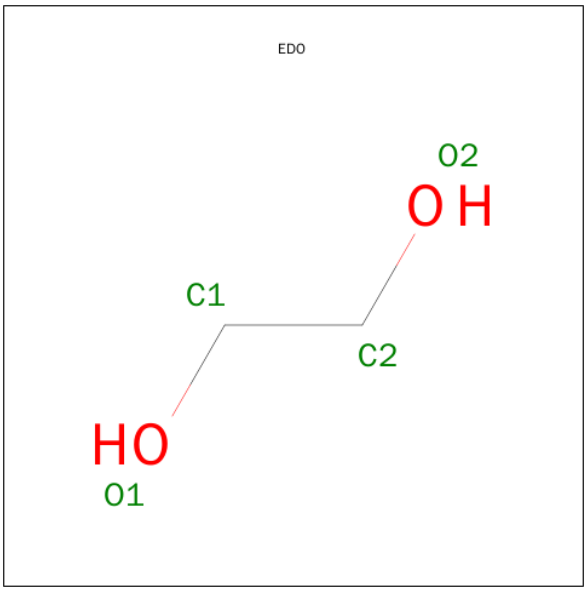
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	7-A	1	Total	C	O	0	0
			12	6	6		
2	8-A	1	Total	C	O	0	0
			12	6	6		
2	9-A	1	Total	C	O	0	0
			12	6	6		
2	10-A	1	Total	C	O	0	0
			12	6	6		
2	11-A	1	Total	C	O	0	0
			12	6	6		
2	12-A	1	Total	C	O	0	0
			12	6	6		
2	13-A	1	Total	C	O	0	0
			12	6	6		
2	14-A	1	Total	C	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		
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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	1-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	2-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	3-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	4-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	5-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	6-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	7-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	8-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	9-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	10-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	11-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	12-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	13-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	14-A	1	Total	C	H	O	0	0
			10	2	6	2		

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	11-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	12-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	13-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	14-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	15-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	16-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	17-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	18-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	19-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	20-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	21-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	22-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	23-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	24-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	25-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	1-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	2-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	3-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	4-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	5-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	6-A	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	7-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	8-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	9-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	10-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	11-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	12-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	13-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	14-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	15-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	16-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	17-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	18-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	19-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	20-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	21-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	22-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	23-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	24-A	1	Total	C	H	O	0	0
			10	2	6	2		
3	25-A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-A	253	Total O 253 253	0	0
4	2-A	248	Total O 248 248	0	0
4	3-A	259	Total O 259 259	0	0
4	4-A	249	Total O 249 249	0	0
4	5-A	246	Total O 246 246	0	0
4	6-A	245	Total O 245 245	0	0
4	7-A	258	Total O 258 258	0	0
4	8-A	264	Total O 264 264	0	0
4	9-A	251	Total O 251 251	0	0
4	10-A	248	Total O 248 248	0	0
4	11-A	264	Total O 264 264	0	0
4	12-A	246	Total O 246 246	0	0
4	13-A	247	Total O 247 247	0	0
4	14-A	242	Total O 242 242	0	0
4	15-A	262	Total O 262 262	0	0
4	16-A	252	Total O 252 252	0	0
4	17-A	243	Total O 243 243	0	0
4	18-A	255	Total O 255 255	0	0
4	19-A	274	Total O 274 274	0	0
4	20-A	242	Total O 242 242	0	0
4	21-A	240	Total O 240 240	0	0
4	22-A	250	Total O 250 250	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	23-A	259	Total O 259 259	0	0
4	24-A	250	Total O 250 250	0	0
4	25-A	249	Total O 249 249	0	0

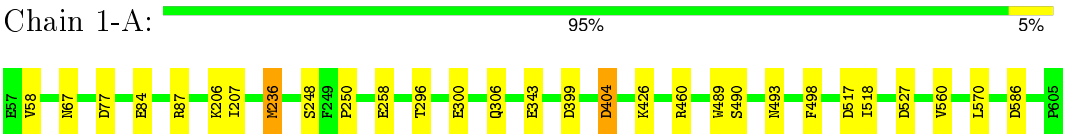
3 Residue-property plots (i)

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

Note EDS failed to run properly.

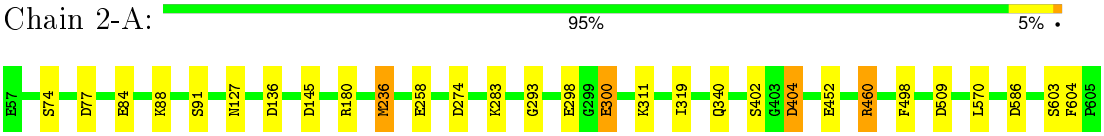
- Molecule 1: Putative secreted protein

Chain 1-A:



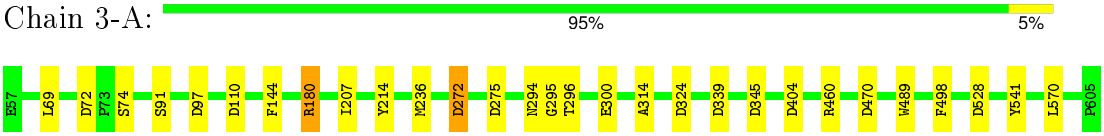
- Molecule 1: Putative secreted protein

Chain 2-A:



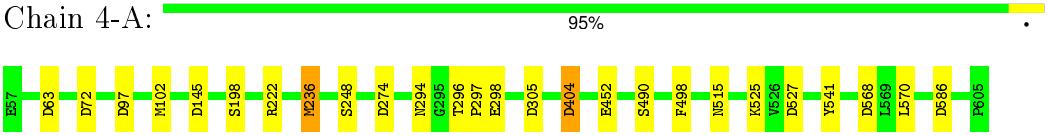
- Molecule 1: Putative secreted protein

Chain 3-A:



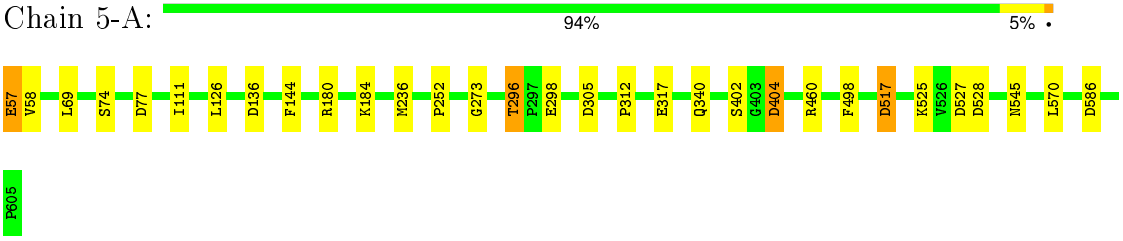
- Molecule 1: Putative secreted protein

Chain 4-A:



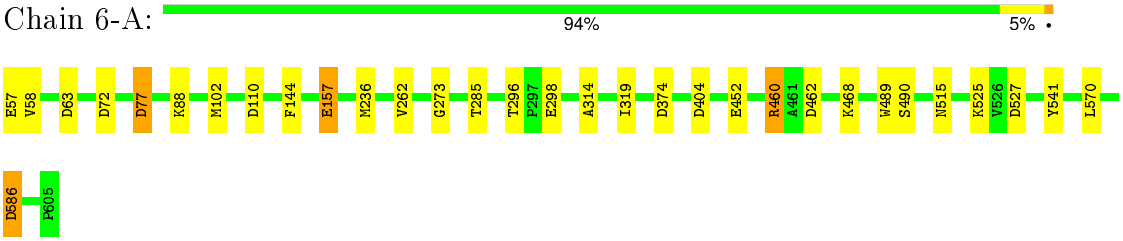
- Molecule 1: Putative secreted protein

Chain 5-A:



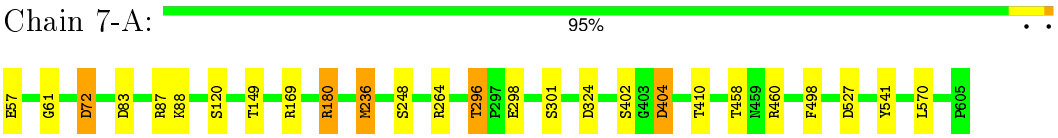
• Molecule 1: Putative secreted protein

Chain 6-A:



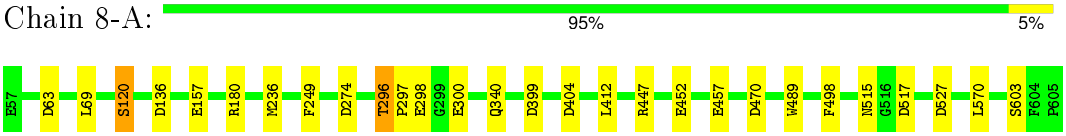
• Molecule 1: Putative secreted protein

Chain 7-A:



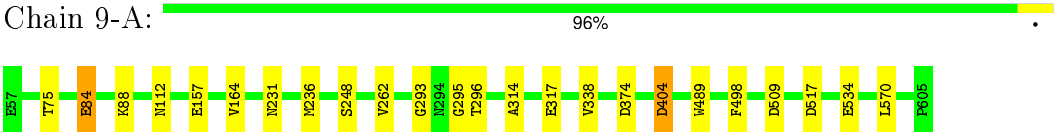
• Molecule 1: Putative secreted protein

Chain 8-A:



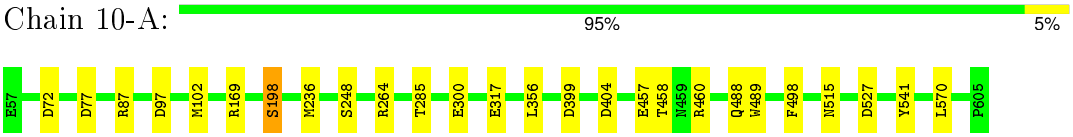
• Molecule 1: Putative secreted protein

Chain 9-A:



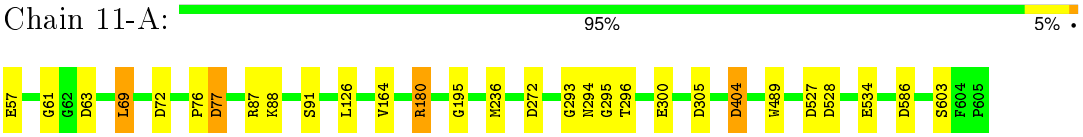
• Molecule 1: Putative secreted protein

Chain 10-A:



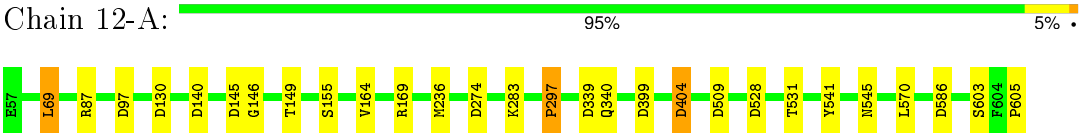
• Molecule 1: Putative secreted protein

Chain 11-A:



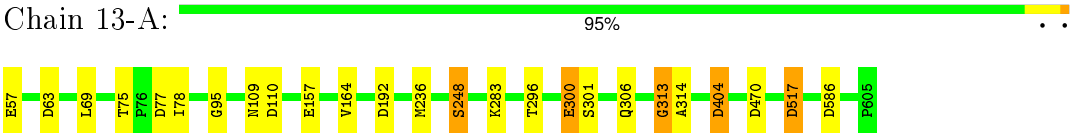
• Molecule 1: Putative secreted protein

Chain 12-A:



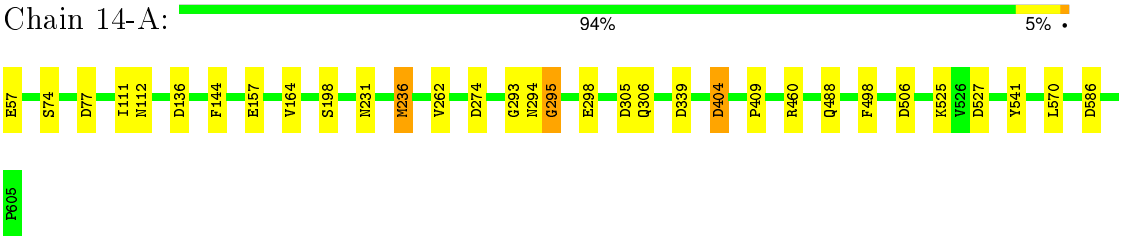
• Molecule 1: Putative secreted protein

Chain 13-A:



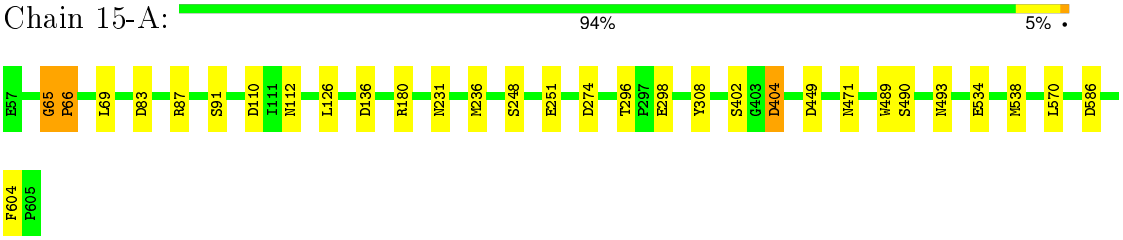
• Molecule 1: Putative secreted protein

Chain 14-A:



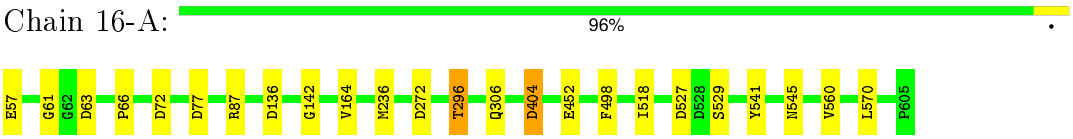
• Molecule 1: Putative secreted protein

Chain 15-A:



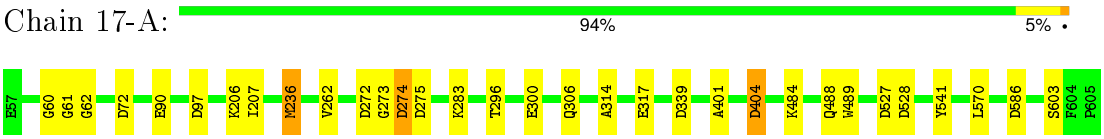
• Molecule 1: Putative secreted protein

Chain 16-A:



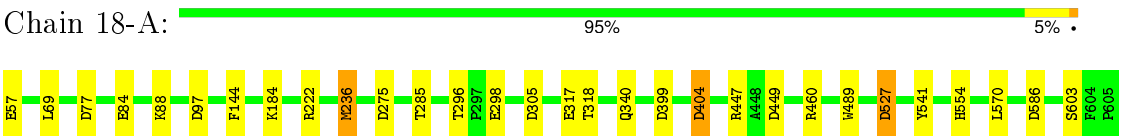
• Molecule 1: Putative secreted protein

Chain 17-A:



• Molecule 1: Putative secreted protein

Chain 18-A:

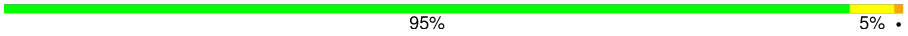


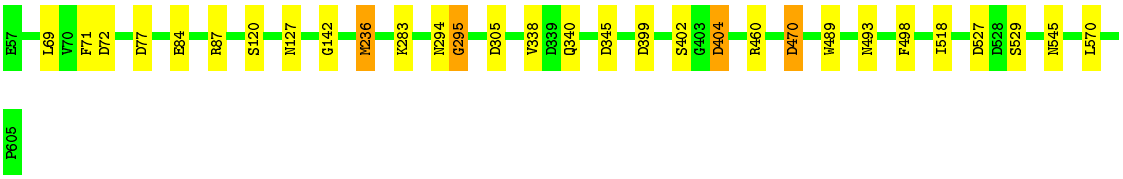
• Molecule 1: Putative secreted protein

Chain 19-A:

• Molecule 1: Putative secreted protein

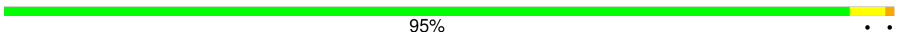
Chain 20-A:

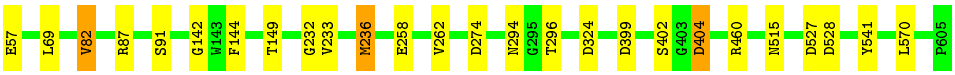




• Molecule 1: Putative secreted protein

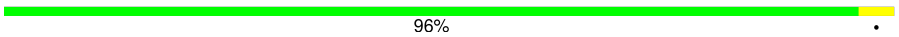
Chain 21-A:

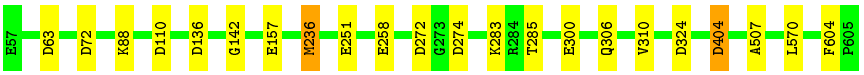




• Molecule 1: Putative secreted protein

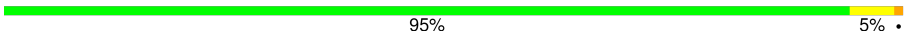
Chain 22-A:

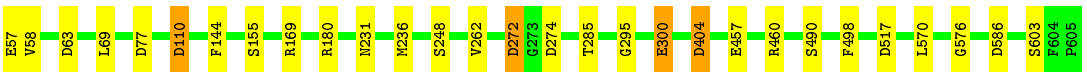




• Molecule 1: Putative secreted protein

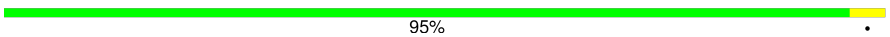
Chain 23-A:

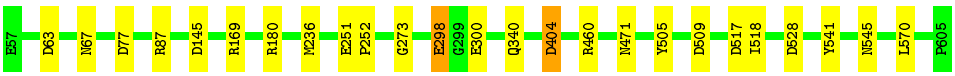




• Molecule 1: Putative secreted protein

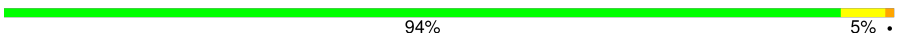
Chain 24-A:





• Molecule 1: Putative secreted protein

Chain 25-A:



4 Data and refinement statistics (i)

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	51.28Å 100.21Å 54.22Å 90.00° 99.46° 90.00°	Depositor
Resolution (Å)	28.33 – 1.90	Depositor
% Data completeness (in resolution range)	93.2 (28.33-1.90)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.33 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement: 1.9_1692)	Depositor
R, R_{free}	0.113 , 0.151	Depositor
Wilson B-factor (Å^2)	19.6	Xtriage
Anisotropy	0.154	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 39632 reflections	Xtriage
Total number of atoms	210296	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, EDO

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	0.85	5/4280 (0.1%)	0.93	11/5848 (0.2%)
1	2-A	0.85	4/4280 (0.1%)	0.91	7/5848 (0.1%)
1	3-A	0.81	1/4280 (0.0%)	0.91	7/5848 (0.1%)
1	4-A	0.83	3/4280 (0.1%)	0.91	7/5848 (0.1%)
1	5-A	0.80	2/4280 (0.0%)	0.89	7/5848 (0.1%)
1	6-A	0.86	5/4280 (0.1%)	0.91	7/5848 (0.1%)
1	7-A	0.83	4/4280 (0.1%)	0.91	7/5848 (0.1%)
1	8-A	0.83	4/4280 (0.1%)	0.86	4/5848 (0.1%)
1	9-A	0.83	5/4280 (0.1%)	0.88	4/5848 (0.1%)
1	10-A	0.85	4/4280 (0.1%)	0.91	6/5848 (0.1%)
1	11-A	0.80	2/4280 (0.0%)	0.90	6/5848 (0.1%)
1	12-A	0.83	2/4280 (0.0%)	0.92	8/5848 (0.1%)
1	13-A	0.83	2/4280 (0.0%)	0.92	7/5848 (0.1%)
1	14-A	0.84	6/4280 (0.1%)	0.92	6/5848 (0.1%)
1	15-A	0.81	1/4280 (0.0%)	0.92	5/5848 (0.1%)
1	16-A	0.82	2/4280 (0.0%)	0.90	5/5848 (0.1%)
1	17-A	0.82	4/4280 (0.1%)	0.91	8/5848 (0.1%)
1	18-A	0.82	4/4280 (0.1%)	0.94	13/5848 (0.2%)
1	19-A	0.87	4/4280 (0.1%)	0.94	9/5848 (0.2%)
1	20-A	0.85	5/4280 (0.1%)	0.92	9/5848 (0.2%)
1	21-A	0.81	2/4280 (0.0%)	0.89	6/5848 (0.1%)
1	22-A	0.82	3/4280 (0.1%)	0.89	3/5848 (0.1%)
1	23-A	0.80	1/4280 (0.0%)	0.90	12/5848 (0.2%)
1	24-A	0.83	3/4280 (0.1%)	0.97	15/5848 (0.3%)
1	25-A	0.86	4/4280 (0.1%)	0.96	13/5848 (0.2%)
All	All	0.83	82/107000 (0.1%)	0.91	192/146200 (0.1%)

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	3-A	0	1
1	14-A	0	1
1	17-A	0	1
1	19-A	0	1
1	24-A	0	1
All	All	0	5

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	236	MET	CB-CG	8.44	1.78	1.51
1	10-A	198	SER	CB-OG	-8.39	1.31	1.42
1	19-A	404	ASP	CB-CG	8.26	1.69	1.51
1	4-A	404	ASP	CB-CG	8.12	1.68	1.51
1	1-A	236	MET	CG-SD	8.07	2.02	1.81
1	20-A	120	SER	CB-OG	-7.91	1.31	1.42
1	6-A	298	GLU	CB-CG	7.88	1.67	1.52
1	17-A	404	ASP	CB-CG	7.79	1.68	1.51
1	20-A	84	GLU	CB-CG	7.75	1.66	1.52
1	7-A	298	GLU	CB-CG	7.73	1.66	1.52
1	6-A	298	GLU	CG-CD	7.67	1.63	1.51
1	23-A	404	ASP	CB-CG	7.67	1.67	1.51
1	4-A	236	MET	CB-CG	7.64	1.75	1.51
1	7-A	404	ASP	CB-CG	-7.58	1.35	1.51
1	19-A	157	GLU	CD-OE2	-7.55	1.17	1.25
1	9-A	317	GLU	CB-CG	7.51	1.66	1.52
1	18-A	236	MET	CG-SD	7.44	2.00	1.81
1	18-A	586	ASP	CB-CG	7.18	1.66	1.51
1	14-A	236	MET	CG-SD	7.15	1.99	1.81
1	18-A	236	MET	CB-CG	7.14	1.74	1.51
1	22-A	258	GLU	CB-CG	7.05	1.65	1.52
1	25-A	236	MET	CB-CG	6.89	1.73	1.51
1	6-A	157	GLU	CG-CD	6.84	1.62	1.51
1	4-A	236	MET	CG-SD	6.81	1.98	1.81
1	14-A	236	MET	CB-CG	6.75	1.73	1.51
1	11-A	180	ARG	CG-CD	6.74	1.68	1.51
1	5-A	57	GLU	CG-CD	-6.72	1.41	1.51
1	3-A	300	GLU	CB-CG	6.62	1.64	1.52
1	14-A	404	ASP	CB-CG	6.53	1.65	1.51
1	25-A	404	ASP	CB-CG	6.45	1.65	1.51
1	9-A	317	GLU	CG-CD	6.43	1.61	1.51
1	6-A	157	GLU	CB-CG	6.39	1.64	1.52
1	16-A	404	ASP	CB-CG	6.33	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	18-A	298	GLU	CB-CG	6.22	1.64	1.52
1	1-A	206	LYS	CD-CE	6.12	1.66	1.51
1	9-A	404	ASP	CB-CG	6.11	1.64	1.51
1	22-A	300	GLU	CG-CD	6.11	1.61	1.51
1	8-A	452	GLU	CG-CD	6.08	1.61	1.51
1	11-A	586	ASP	CB-CG	5.98	1.64	1.51
1	14-A	298	GLU	CB-CG	5.98	1.63	1.52
1	2-A	404	ASP	CB-CG	5.85	1.64	1.51
1	14-A	157	GLU	CB-CG	5.85	1.63	1.52
1	5-A	317	GLU	CB-CG	5.84	1.63	1.52
1	8-A	457	GLU	CG-CD	5.84	1.60	1.51
1	8-A	120	SER	CB-OG	-5.77	1.34	1.42
1	25-A	236	MET	CG-SD	5.74	1.96	1.81
1	2-A	300	GLU	CB-CG	-5.72	1.41	1.52
1	15-A	404	ASP	CB-CG	5.63	1.63	1.51
1	6-A	57	GLU	CG-CD	5.62	1.60	1.51
1	16-A	87	ARG	CG-CD	5.61	1.66	1.51
1	9-A	84	GLU	CG-CD	5.55	1.60	1.51
1	13-A	404	ASP	CB-CG	5.54	1.63	1.51
1	1-A	84	GLU	CB-CG	-5.50	1.41	1.52
1	14-A	198	SER	CB-OG	-5.48	1.35	1.42
1	2-A	298	GLU	CB-CG	5.48	1.62	1.52
1	10-A	317	GLU	CB-CG	5.48	1.62	1.52
1	17-A	488	GLN	CB-CG	-5.48	1.37	1.52
1	10-A	488	GLN	CB-CG	-5.44	1.37	1.52
1	12-A	404	ASP	CB-CG	5.44	1.63	1.51
1	9-A	157	GLU	CD-OE1	5.41	1.31	1.25
1	20-A	404	ASP	CB-CG	5.41	1.63	1.51
1	20-A	87	ARG	CG-CD	5.40	1.65	1.51
1	24-A	87	ARG	CG-CD	5.39	1.65	1.51
1	8-A	157	GLU	CD-OE2	5.37	1.31	1.25
1	20-A	84	GLU	CG-CD	5.35	1.59	1.51
1	13-A	300	GLU	CB-CG	-5.33	1.42	1.52
1	21-A	82	VAL	CB-CG1	-5.30	1.41	1.52
1	12-A	140	ASP	CB-CG	5.28	1.62	1.51
1	10-A	457	GLU	CG-CD	5.28	1.59	1.51
1	17-A	317	GLU	CG-CD	-5.27	1.44	1.51
1	2-A	452	GLU	CG-CD	5.23	1.59	1.51
1	21-A	404	ASP	CB-CG	5.22	1.62	1.51
1	19-A	87	ARG	CG-CD	5.20	1.65	1.51
1	7-A	180	ARG	CG-CD	5.14	1.64	1.51
1	17-A	484	LYS	CD-CE	5.14	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	24-A	298	GLU	CB-CG	5.13	1.61	1.52
1	24-A	505	TYR	CD1-CE1	-5.10	1.31	1.39
1	1-A	404	ASP	CB-CG	5.08	1.62	1.51
1	19-A	84	GLU	CB-CG	-5.08	1.42	1.52
1	22-A	404	ASP	CB-CG	5.07	1.62	1.51
1	7-A	298	GLU	CG-CD	5.07	1.59	1.51
1	25-A	84	GLU	CB-CG	5.07	1.61	1.52

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	4-A	236	MET	CG-SD-CE	-14.71	76.66	100.20
1	18-A	236	MET	CG-SD-CE	-14.68	76.71	100.20
1	1-A	236	MET	CG-SD-CE	-14.32	77.28	100.20
1	24-A	87	ARG	NE-CZ-NH2	-13.75	113.42	120.30
1	14-A	236	MET	CG-SD-CE	-12.86	79.63	100.20
1	20-A	87	ARG	NE-CZ-NH2	-12.77	113.92	120.30
1	19-A	87	ARG	NE-CZ-NH2	-12.67	113.97	120.30
1	24-A	180	ARG	NE-CZ-NH2	12.47	126.53	120.30
1	25-A	460	ARG	NE-CZ-NH2	12.44	126.52	120.30
1	24-A	87	ARG	NE-CZ-NH1	12.28	126.44	120.30
1	7-A	236	MET	CG-SD-CE	11.48	118.58	100.20
1	24-A	180	ARG	NE-CZ-NH1	-11.34	114.63	120.30
1	24-A	169	ARG	NE-CZ-NH2	-10.99	114.80	120.30
1	19-A	87	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	21-A	460	ARG	NE-CZ-NH2	10.63	125.62	120.30
1	25-A	460	ARG	NE-CZ-NH1	-10.47	115.06	120.30
1	16-A	87	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	25-A	236	MET	CG-SD-CE	-9.67	84.73	100.20
1	20-A	87	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	24-A	404	ASP	CB-CG-OD1	-9.53	109.72	118.30
1	25-A	345	ASP	CB-CG-OD1	-9.26	109.97	118.30
1	24-A	460	ARG	NE-CZ-NH2	8.93	124.77	120.30
1	4-A	404	ASP	CB-CG-OD2	8.85	126.26	118.30
1	14-A	460	ARG	NE-CZ-NH1	-8.78	115.91	120.30
1	10-A	236	MET	CG-SD-CE	8.70	114.12	100.20
1	12-A	87	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	16-A	87	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	3-A	180	ARG	NE-CZ-NH2	-8.39	116.10	120.30
1	11-A	404	ASP	CB-CG-OD1	8.38	125.85	118.30
1	7-A	460	ARG	NE-CZ-NH2	8.37	124.48	120.30
1	18-A	460	ARG	NE-CZ-NH2	8.28	124.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	24-A	517	ASP	CB-CG-OD1	8.13	125.62	118.30
1	24-A	169	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	18-A	236	MET	CB-CG-SD	7.91	136.14	112.40
1	1-A	236	MET	CB-CG-SD	7.90	136.11	112.40
1	10-A	460	ARG	NE-CZ-NH2	7.90	124.25	120.30
1	21-A	87	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	22-A	274	ASP	CB-CG-OD1	7.74	125.27	118.30
1	12-A	140	ASP	CB-CG-OD1	7.70	125.23	118.30
1	1-A	460	ARG	NE-CZ-NH2	7.70	124.15	120.30
1	21-A	460	ARG	NE-CZ-NH1	-7.67	116.46	120.30
1	3-A	460	ARG	NE-CZ-NH2	7.59	124.09	120.30
1	12-A	528	ASP	CB-CG-OD1	7.58	125.12	118.30
1	14-A	236	MET	CB-CG-SD	7.52	134.96	112.40
1	14-A	460	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	21-A	87	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	18-A	404	ASP	CB-CG-OD2	7.47	125.02	118.30
1	17-A	339	ASP	CB-CG-OD1	7.44	125.00	118.30
1	24-A	404	ASP	CB-CG-OD2	7.41	124.97	118.30
1	4-A	102	MET	CG-SD-CE	-7.40	88.36	100.20
1	9-A	517	ASP	CB-CG-OD1	7.34	124.91	118.30
1	2-A	180	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	15-A	83	ASP	CB-CG-OD2	7.30	124.87	118.30
1	7-A	87	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	3-A	460	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	21-A	236	MET	CG-SD-CE	7.12	111.60	100.20
1	20-A	236	MET	CG-SD-CE	7.12	111.60	100.20
1	5-A	404	ASP	CB-CG-OD2	7.11	124.70	118.30
1	18-A	586	ASP	CB-CA-C	7.09	124.59	110.40
1	17-A	236	MET	CG-SD-CE	7.04	111.46	100.20
1	4-A	236	MET	CB-CG-SD	7.03	133.49	112.40
1	18-A	404	ASP	CB-CG-OD1	-6.96	112.04	118.30
1	25-A	236	MET	CB-CG-SD	6.96	133.26	112.40
1	23-A	236	MET	CG-SD-CE	-6.89	89.18	100.20
1	1-A	236	MET	CA-CB-CG	6.88	124.99	113.30
1	9-A	509	ASP	CB-CG-OD1	6.87	124.48	118.30
1	1-A	527	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	23-A	272	ASP	CB-CG-OD1	6.67	124.30	118.30
1	3-A	272	ASP	CB-CG-OD1	6.64	124.28	118.30
1	6-A	525	LYS	CD-CE-NZ	-6.61	96.51	111.70
1	25-A	345	ASP	CB-CG-OD2	6.58	124.22	118.30
1	13-A	313	GLY	N-CA-C	-6.48	96.89	113.10
1	25-A	272	ASP	CB-CG-OD1	-6.48	112.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	18-A	305	ASP	CB-CG-OD2	6.47	124.12	118.30
1	11-A	404	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	19-A	236	MET	CG-SD-CE	6.44	110.51	100.20
1	19-A	460	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	12-A	586	ASP	CB-CG-OD1	6.43	124.08	118.30
1	17-A	339	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	2-A	236	MET	CG-SD-CE	6.41	110.46	100.20
1	22-A	236	MET	CG-SD-CE	6.41	110.46	100.20
1	10-A	460	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	13-A	586	ASP	CB-CG-OD1	6.37	124.03	118.30
1	13-A	236	MET	CG-SD-CE	-6.35	90.05	100.20
1	17-A	528	ASP	CB-CG-OD1	6.33	124.00	118.30
1	12-A	87	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	12-A	509	ASP	CB-CG-OD1	6.29	123.96	118.30
1	23-A	404	ASP	CB-CG-OD2	6.29	123.96	118.30
1	19-A	404	ASP	CB-CG-OD2	6.25	123.92	118.30
1	5-A	528	ASP	CB-CG-OD1	6.21	123.89	118.30
1	15-A	449	ASP	CB-CG-OD1	6.15	123.84	118.30
1	10-A	527	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	2-A	404	ASP	CB-CG-OD2	6.10	123.79	118.30
1	20-A	470	ASP	CB-CG-OD1	-6.09	112.82	118.30
1	25-A	272	ASP	CB-CG-OD2	6.03	123.73	118.30
1	17-A	97	ASP	CB-CG-OD1	-6.02	112.88	118.30
1	8-A	447	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	6-A	77	ASP	CB-CG-OD2	-6.02	112.89	118.30
1	7-A	527	ASP	CB-CG-OD1	5.97	123.67	118.30
1	11-A	586	ASP	CB-CA-C	5.96	122.32	110.40
1	16-A	527	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	19-A	495	LYS	CD-CE-NZ	-5.92	98.08	111.70
1	18-A	460	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	25-A	404	ASP	CB-CG-OD2	5.88	123.60	118.30
1	1-A	527	ASP	CB-CG-OD1	5.88	123.59	118.30
1	5-A	69	LEU	CB-CG-CD1	5.88	120.99	111.00
1	18-A	586	ASP	CB-CG-OD1	5.86	123.58	118.30
1	12-A	69	LEU	CB-CG-CD1	5.86	120.96	111.00
1	24-A	300	GLU	OE1-CD-OE2	5.84	130.31	123.30
1	8-A	517	ASP	CB-CG-OD1	5.82	123.54	118.30
1	23-A	586	ASP	CB-CA-C	5.82	122.03	110.40
1	1-A	460	ARG	NE-CZ-NH1	-5.81	117.40	120.30
1	5-A	58	VAL	CB-CA-C	-5.80	100.39	111.40
1	11-A	294	ASN	N-CA-C	5.80	126.65	111.00
1	5-A	517	ASP	CB-CG-OD1	-5.79	113.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	13-A	306	GLN	CA-CB-CG	-5.79	100.67	113.40
1	1-A	399	ASP	CB-CG-OD2	5.78	123.50	118.30
1	22-A	272	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	25-A	58	VAL	CB-CA-C	-5.78	100.42	111.40
1	17-A	527	ASP	CB-CG-OD2	5.75	123.48	118.30
1	23-A	110	ASP	CB-CG-OD1	5.71	123.44	118.30
1	13-A	517	ASP	CB-CG-OD1	5.70	123.43	118.30
1	10-A	87	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	6-A	586	ASP	CB-CG-OD2	5.67	123.40	118.30
1	20-A	305	ASP	CB-CG-OD1	-5.67	113.20	118.30
1	7-A	72	ASP	CB-CG-OD1	5.66	123.40	118.30
1	6-A	462	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	13-A	69	LEU	CB-CG-CD1	5.61	120.54	111.00
1	15-A	65	GLY	C-N-CD	-5.60	108.28	120.60
1	5-A	404	ASP	CB-CG-OD1	-5.60	113.26	118.30
1	20-A	345	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	2-A	460	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	4-A	404	ASP	OD1-CG-OD2	-5.59	112.67	123.30
1	3-A	345	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	6-A	460	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	3-A	180	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	15-A	110	ASP	CB-CG-OD1	5.55	123.29	118.30
1	16-A	272	ASP	CB-CG-OD1	5.54	123.28	118.30
1	23-A	272	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	23-A	460	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	10-A	264	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	19-A	404	ASP	OD1-CG-OD2	-5.44	112.96	123.30
1	5-A	528	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	1-A	206	LYS	CD-CE-NZ	5.42	124.17	111.70
1	23-A	169	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	18-A	447	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	15-A	538	MET	CG-SD-CE	-5.39	91.58	100.20
1	17-A	404	ASP	CB-CG-OD2	5.38	123.15	118.30
1	4-A	236	MET	CA-CB-CG	5.37	122.42	113.30
1	24-A	517	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	8-A	296	THR	C-N-CD	-5.36	108.80	120.60
1	23-A	404	ASP	OD1-CG-OD2	-5.36	113.11	123.30
1	21-A	399	ASP	CB-CG-OD1	5.34	123.11	118.30
1	25-A	374	ASP	CB-CG-OD1	5.33	123.10	118.30
1	19-A	404	ASP	CB-CG-OD1	5.33	123.10	118.30
1	11-A	69	LEU	CB-CG-CD1	5.31	120.03	111.00
1	14-A	236	MET	CA-CB-CG	5.31	122.33	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-A	311	LYS	CD-CE-NZ	5.31	123.92	111.70
1	25-A	305	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	8-A	180	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	18-A	236	MET	CA-CB-CG	5.29	122.28	113.30
1	20-A	120	SER	N-CA-CB	-5.28	102.58	110.50
1	25-A	460	ARG	CD-NE-CZ	5.28	130.99	123.60
1	11-A	295	GLY	N-CA-C	-5.27	99.93	113.10
1	13-A	63	ASP	CB-CG-OD2	5.26	123.04	118.30
1	6-A	298	GLU	OE1-CD-OE2	-5.25	116.99	123.30
1	2-A	293	GLY	N-CA-C	5.25	126.22	113.10
1	19-A	462	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	16-A	518	ILE	CB-CA-C	-5.23	101.13	111.60
1	18-A	449	ASP	CB-CG-OD1	5.23	123.01	118.30
1	9-A	374	ASP	CB-CG-OD1	5.22	123.00	118.30
1	7-A	264	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	24-A	518	ILE	CB-CA-C	-5.20	101.20	111.60
1	18-A	527	ASP	CB-CG-OD1	5.18	122.97	118.30
1	20-A	295	GLY	N-CA-C	5.18	126.04	113.10
1	23-A	517	ASP	CB-CG-OD1	5.17	122.95	118.30
1	14-A	404	ASP	CB-CG-OD2	5.16	122.94	118.30
1	24-A	87	ARG	CD-NE-CZ	5.14	130.80	123.60
1	2-A	586	ASP	CB-CG-OD2	5.13	122.92	118.30
1	4-A	97	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	1-A	426	LYS	CB-CA-C	-5.12	100.16	110.40
1	23-A	404	ASP	CB-CG-OD1	5.12	122.91	118.30
1	1-A	77	ASP	CB-CG-OD2	5.11	122.90	118.30
1	24-A	528	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	7-A	169	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	17-A	275	ASP	CB-CG-OD1	5.07	122.86	118.30
1	6-A	374	ASP	CB-CG-OD1	5.07	122.86	118.30
1	12-A	528	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	23-A	300	GLU	N-CA-C	5.03	124.58	111.00
1	3-A	345	ASP	CB-CG-OD1	5.03	122.83	118.30
1	9-A	404	ASP	CB-CG-OD2	5.03	122.83	118.30
1	20-A	460	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	14-A	295	GLY	Peptide
1	17-A	62	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	19-A	293	GLY	Peptide
1	24-A	251	GLU	Peptide
1	3-A	295	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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
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	56	0	47	0	0
2	2-A	56	0	49	0	0
2	3-A	56	0	49	0	0
2	4-A	56	0	49	0	0
2	5-A	56	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	6-A	56	0	49	0	0
2	7-A	56	0	48	0	0
2	8-A	56	0	48	0	0
2	9-A	56	0	48	0	0
2	10-A	56	0	48	0	0
2	11-A	56	0	49	0	0
2	12-A	56	0	49	0	0
2	13-A	56	0	49	0	0
2	14-A	56	0	49	0	0
2	15-A	56	0	48	0	0
2	16-A	56	0	49	0	0
2	17-A	56	0	49	0	0
2	18-A	56	0	48	0	0
2	19-A	56	0	49	0	0
2	20-A	56	0	48	0	0
2	21-A	56	0	47	0	0
2	22-A	56	0	49	0	0
2	23-A	56	0	48	0	0
2	24-A	56	0	48	0	0
2	25-A	56	0	49	0	0
3	1-A	12	18	18	0	0
3	2-A	12	18	18	0	0
3	3-A	12	18	18	0	0
3	4-A	12	18	18	0	0
3	5-A	12	18	18	0	0
3	6-A	12	18	18	0	0
3	7-A	12	18	18	0	0
3	8-A	12	18	18	0	0
3	9-A	12	18	18	0	0
3	10-A	12	18	18	0	0
3	11-A	12	18	18	0	0
3	12-A	12	18	18	0	0
3	13-A	12	18	18	0	0
3	14-A	12	18	18	0	0
3	15-A	12	18	18	0	0
3	16-A	12	18	18	0	0
3	17-A	12	18	18	0	0
3	18-A	12	18	18	0	0
3	19-A	12	18	18	0	0
3	20-A	12	18	18	0	0
3	21-A	12	18	18	0	0
3	22-A	12	18	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	23-A	12	18	18	0	0
3	24-A	12	18	18	0	0
3	25-A	12	18	18	0	0
4	1-A	253	0	0	0	0
4	2-A	248	0	0	0	0
4	3-A	259	0	0	0	0
4	4-A	249	0	0	0	0
4	5-A	246	0	0	0	0
4	6-A	245	0	0	0	0
4	7-A	258	0	0	0	0
4	8-A	264	0	0	0	0
4	9-A	251	0	0	0	0
4	10-A	248	0	0	0	0
4	11-A	264	0	0	0	0
4	12-A	246	0	0	0	0
4	13-A	247	0	0	0	0
4	14-A	242	0	0	0	0
4	15-A	262	0	0	0	0
4	16-A	252	0	0	0	0
4	17-A	243	0	0	0	0
4	18-A	255	0	0	0	0
4	19-A	274	0	0	0	0
4	20-A	242	0	0	0	0
4	21-A	240	0	0	0	0
4	22-A	250	0	0	0	0
4	23-A	259	0	0	0	0
4	24-A	250	0	0	0	0
4	25-A	249	0	0	0	0
All	All	112171	98125	99634	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%)	508 (93%)	34 (6%)	5 (1%)	21	9
1	2-A	547/549 (100%)	503 (92%)	40 (7%)	4 (1%)	26	14
1	3-A	547/549 (100%)	508 (93%)	34 (6%)	5 (1%)	21	9
1	4-A	547/549 (100%)	512 (94%)	30 (6%)	5 (1%)	21	9
1	5-A	547/549 (100%)	510 (93%)	32 (6%)	5 (1%)	21	9
1	6-A	547/549 (100%)	503 (92%)	40 (7%)	4 (1%)	26	14
1	7-A	547/549 (100%)	506 (92%)	38 (7%)	3 (0%)	34	21
1	8-A	547/549 (100%)	509 (93%)	35 (6%)	3 (0%)	34	21
1	9-A	547/549 (100%)	502 (92%)	40 (7%)	5 (1%)	21	9
1	10-A	547/549 (100%)	501 (92%)	45 (8%)	1 (0%)	52	42
1	11-A	547/549 (100%)	511 (93%)	30 (6%)	6 (1%)	17	6
1	12-A	547/549 (100%)	511 (93%)	32 (6%)	4 (1%)	26	14
1	13-A	547/549 (100%)	505 (92%)	37 (7%)	5 (1%)	21	9
1	14-A	547/549 (100%)	509 (93%)	34 (6%)	4 (1%)	26	14
1	15-A	547/549 (100%)	511 (93%)	29 (5%)	7 (1%)	15	4
1	16-A	547/549 (100%)	499 (91%)	43 (8%)	5 (1%)	21	9
1	17-A	547/549 (100%)	502 (92%)	38 (7%)	7 (1%)	15	4
1	18-A	547/549 (100%)	510 (93%)	35 (6%)	2 (0%)	39	27
1	19-A	547/549 (100%)	503 (92%)	40 (7%)	4 (1%)	26	14
1	20-A	547/549 (100%)	505 (92%)	35 (6%)	7 (1%)	15	4
1	21-A	547/549 (100%)	513 (94%)	31 (6%)	3 (0%)	34	21
1	22-A	547/549 (100%)	507 (93%)	38 (7%)	2 (0%)	39	27
1	23-A	547/549 (100%)	506 (92%)	34 (6%)	7 (1%)	15	4
1	24-A	547/549 (100%)	501 (92%)	43 (8%)	3 (0%)	34	21
1	25-A	547/549 (100%)	501 (92%)	43 (8%)	3 (0%)	34	21
All	All	13675/13725 (100%)	12656 (92%)	910 (7%)	109 (1%)	24	11

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2-A	509	ASP
1	3-A	314	ALA
1	4-A	297	PRO
1	6-A	77	ASP
1	6-A	319	ILE
1	7-A	61	GLY
1	9-A	293	GLY
1	11-A	77	ASP
1	11-A	293	GLY
1	12-A	146	GLY
1	12-A	297	PRO
1	13-A	77	ASP
1	13-A	314	ALA
1	14-A	77	ASP
1	14-A	295	GLY
1	15-A	126	LEU
1	17-A	274	ASP
1	20-A	493	ASN
1	20-A	518	ILE
1	24-A	145	ASP
1	4-A	568	ASP
1	5-A	273	GLY
1	6-A	314	ALA
1	8-A	297	PRO
1	9-A	295	GLY
1	9-A	314	ALA
1	11-A	61	GLY
1	11-A	195	GLY
1	12-A	145	ASP
1	16-A	61	GLY
1	17-A	273	GLY
1	18-A	77	ASP
1	20-A	77	ASP
1	20-A	142	GLY
1	20-A	295	GLY
1	22-A	142	GLY
1	24-A	273	GLY
1	25-A	295	GLY
1	1-A	67	ASN
1	3-A	294	ASN
1	5-A	77	ASP
1	15-A	66	PRO
1	15-A	248	SER

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Mol	Chain	Res	Type
1	15-A	308	TYR
1	15-A	493	ASN
1	19-A	314	ALA
1	23-A	576	GLY
1	25-A	273	GLY
1	1-A	248	SER
1	1-A	493	ASN
1	4-A	248	SER
1	5-A	296	THR
1	9-A	248	SER
1	12-A	130	ASP
1	13-A	313	GLY
1	15-A	296	THR
1	17-A	61	GLY
1	17-A	314	ALA
1	18-A	296	THR
1	19-A	79	GLN
1	19-A	248	SER
1	20-A	294	ASN
1	23-A	295	GLY
1	1-A	498	PHE
1	2-A	77	ASP
1	3-A	214	TYR
1	3-A	296	THR
1	3-A	498	PHE
1	5-A	498	PHE
1	8-A	498	PHE
1	9-A	498	PHE
1	10-A	498	PHE
1	13-A	248	SER
1	15-A	65	GLY
1	16-A	498	PHE
1	17-A	90	GLU
1	20-A	498	PHE
1	21-A	142	GLY
1	23-A	110	ASP
1	23-A	248	SER
1	23-A	498	PHE
1	2-A	319	ILE
1	2-A	498	PHE
1	4-A	145	ASP
1	4-A	498	PHE

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Mol	Chain	Res	Type
1	7-A	296	THR
1	7-A	498	PHE
1	14-A	498	PHE
1	17-A	401	ALA
1	23-A	77	ASP
1	25-A	498	PHE
1	8-A	249	PHE
1	14-A	293	GLY
1	13-A	95	GLY
1	16-A	142	GLY
1	19-A	233	VAL
1	24-A	252	PRO
1	1-A	58	VAL
1	5-A	312	PRO
1	16-A	296	THR
1	21-A	232	GLY
1	22-A	507	ALA
1	6-A	273	GLY
1	11-A	76	PRO
1	11-A	296	THR
1	16-A	66	PRO
1	17-A	60	GLY
1	21-A	233	VAL
1	23-A	58	VAL

5.3.2 Protein sidechains (i)

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%)	419 (96%)	17 (4%)	39	27
1	2-A	436/436 (100%)	417 (96%)	19 (4%)	35	22
1	3-A	436/436 (100%)	416 (95%)	20 (5%)	33	21
1	4-A	436/436 (100%)	417 (96%)	19 (4%)	35	22
1	5-A	436/436 (100%)	413 (95%)	23 (5%)	28	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	6-A	436/436 (100%)	413 (95%)	23 (5%)	28 16
1	7-A	436/436 (100%)	418 (96%)	18 (4%)	37 25
1	8-A	436/436 (100%)	417 (96%)	19 (4%)	35 22
1	9-A	436/436 (100%)	422 (97%)	14 (3%)	46 35
1	10-A	436/436 (100%)	419 (96%)	17 (4%)	39 27
1	11-A	436/436 (100%)	415 (95%)	21 (5%)	31 19
1	12-A	436/436 (100%)	416 (95%)	20 (5%)	33 21
1	13-A	436/436 (100%)	420 (96%)	16 (4%)	41 29
1	14-A	436/436 (100%)	412 (94%)	24 (6%)	27 14
1	15-A	436/436 (100%)	415 (95%)	21 (5%)	31 19
1	16-A	436/436 (100%)	420 (96%)	16 (4%)	41 29
1	17-A	436/436 (100%)	419 (96%)	17 (4%)	39 27
1	18-A	436/436 (100%)	414 (95%)	22 (5%)	30 18
1	19-A	436/436 (100%)	419 (96%)	17 (4%)	39 27
1	20-A	436/436 (100%)	419 (96%)	17 (4%)	39 27
1	21-A	436/436 (100%)	416 (95%)	20 (5%)	33 21
1	22-A	436/436 (100%)	420 (96%)	16 (4%)	41 29
1	23-A	436/436 (100%)	419 (96%)	17 (4%)	39 27
1	24-A	436/436 (100%)	424 (97%)	12 (3%)	51 41
1	25-A	436/436 (100%)	411 (94%)	25 (6%)	25 13
All	All	10900/10900 (100%)	10430 (96%)	470 (4%)	35 23

All (470) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	87	ARG
1	1-A	207	ILE
1	1-A	236	MET
1	1-A	250	PRO
1	1-A	258	GLU
1	1-A	296	THR
1	1-A	300	GLU
1	1-A	306	GLN
1	1-A	343	GLU
1	1-A	404	ASP

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Mol	Chain	Res	Type
1	1-A	489	TRP
1	1-A	490	SER
1	1-A	517	ASP
1	1-A	518	ILE
1	1-A	560	VAL
1	1-A	570	LEU
1	1-A	586	ASP
1	2-A	74	SER
1	2-A	84	GLU
1	2-A	88	LYS
1	2-A	91	SER
1	2-A	127	ASN
1	2-A	136	ASP
1	2-A	145	ASP
1	2-A	236	MET
1	2-A	258	GLU
1	2-A	274	ASP
1	2-A	283	LYS
1	2-A	300	GLU
1	2-A	340	GLN
1	2-A	402	SER
1	2-A	404	ASP
1	2-A	460	ARG
1	2-A	570	LEU
1	2-A	603	SER
1	2-A	604	PHE
1	3-A	69	LEU
1	3-A	72	ASP
1	3-A	74	SER
1	3-A	91	SER
1	3-A	97	ASP
1	3-A	110	ASP
1	3-A	144	PHE
1	3-A	180	ARG
1	3-A	207	ILE
1	3-A	236	MET
1	3-A	272	ASP
1	3-A	275	ASP
1	3-A	324	ASP
1	3-A	339	ASP
1	3-A	404	ASP
1	3-A	470	ASP

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Mol	Chain	Res	Type
1	3-A	489	TRP
1	3-A	528	ASP
1	3-A	541	TYR
1	3-A	570	LEU
1	4-A	63	ASP
1	4-A	72	ASP
1	4-A	198	SER
1	4-A	222	ARG
1	4-A	236	MET
1	4-A	274	ASP
1	4-A	294	ASN
1	4-A	296	THR
1	4-A	298	GLU
1	4-A	305	ASP
1	4-A	404	ASP
1	4-A	452	GLU
1	4-A	490	SER
1	4-A	515	ASN
1	4-A	525	LYS
1	4-A	527	ASP
1	4-A	541	TYR
1	4-A	570	LEU
1	4-A	586	ASP
1	5-A	57	GLU
1	5-A	74	SER
1	5-A	111	ILE
1	5-A	126	LEU
1	5-A	136	ASP
1	5-A	144	PHE
1	5-A	180	ARG
1	5-A	184	LYS
1	5-A	236	MET
1	5-A	252	PRO
1	5-A	296	THR
1	5-A	298	GLU
1	5-A	305	ASP
1	5-A	340	GLN
1	5-A	402	SER
1	5-A	404	ASP
1	5-A	460	ARG
1	5-A	517	ASP
1	5-A	525	LYS

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Mol	Chain	Res	Type
1	5-A	527	ASP
1	5-A	545	ASN
1	5-A	570	LEU
1	5-A	586	ASP
1	6-A	58	VAL
1	6-A	63	ASP
1	6-A	72	ASP
1	6-A	88	LYS
1	6-A	102	MET
1	6-A	110	ASP
1	6-A	144	PHE
1	6-A	157	GLU
1	6-A	236	MET
1	6-A	262	VAL
1	6-A	285	THR
1	6-A	296	THR
1	6-A	404	ASP
1	6-A	452	GLU
1	6-A	460	ARG
1	6-A	468	LYS
1	6-A	489	TRP
1	6-A	490	SER
1	6-A	515	ASN
1	6-A	527	ASP
1	6-A	541	TYR
1	6-A	570	LEU
1	6-A	586	ASP
1	7-A	57	GLU
1	7-A	72	ASP
1	7-A	83	ASP
1	7-A	88	LYS
1	7-A	120	SER
1	7-A	149	THR
1	7-A	180	ARG
1	7-A	236	MET
1	7-A	248	SER
1	7-A	296	THR
1	7-A	301	SER
1	7-A	324	ASP
1	7-A	402	SER
1	7-A	404	ASP
1	7-A	410	THR

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Mol	Chain	Res	Type
1	7-A	458	THR
1	7-A	541	TYR
1	7-A	570	LEU
1	8-A	63	ASP
1	8-A	69	LEU
1	8-A	120	SER
1	8-A	136	ASP
1	8-A	236	MET
1	8-A	274	ASP
1	8-A	296	THR
1	8-A	298	GLU
1	8-A	300	GLU
1	8-A	340	GLN
1	8-A	399	ASP
1	8-A	404	ASP
1	8-A	412	LEU
1	8-A	470	ASP
1	8-A	489	TRP
1	8-A	515	ASN
1	8-A	527	ASP
1	8-A	570	LEU
1	8-A	603	SER
1	9-A	75	THR
1	9-A	84	GLU
1	9-A	88	LYS
1	9-A	112	ASN
1	9-A	164	VAL
1	9-A	231	ASN
1	9-A	236	MET
1	9-A	262	VAL
1	9-A	296	THR
1	9-A	338	VAL
1	9-A	404	ASP
1	9-A	489	TRP
1	9-A	534	GLU
1	9-A	570	LEU
1	10-A	72	ASP
1	10-A	77	ASP
1	10-A	97	ASP
1	10-A	102	MET
1	10-A	169	ARG
1	10-A	198	SER

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Mol	Chain	Res	Type
1	10-A	248	SER
1	10-A	285	THR
1	10-A	300	GLU
1	10-A	356	LEU
1	10-A	399	ASP
1	10-A	404	ASP
1	10-A	458	THR
1	10-A	489	TRP
1	10-A	515	ASN
1	10-A	541	TYR
1	10-A	570	LEU
1	11-A	57	GLU
1	11-A	63	ASP
1	11-A	69	LEU
1	11-A	72	ASP
1	11-A	77	ASP
1	11-A	87	ARG
1	11-A	88	LYS
1	11-A	91	SER
1	11-A	126	LEU
1	11-A	164	VAL
1	11-A	180	ARG
1	11-A	236	MET
1	11-A	272	ASP
1	11-A	300	GLU
1	11-A	305	ASP
1	11-A	404	ASP
1	11-A	489	TRP
1	11-A	527	ASP
1	11-A	528	ASP
1	11-A	534	GLU
1	11-A	603	SER
1	12-A	69	LEU
1	12-A	97	ASP
1	12-A	149	THR
1	12-A	155	SER
1	12-A	164	VAL
1	12-A	169	ARG
1	12-A	236	MET
1	12-A	274	ASP
1	12-A	283	LYS
1	12-A	297	PRO

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Mol	Chain	Res	Type
1	12-A	339	ASP
1	12-A	340	GLN
1	12-A	399	ASP
1	12-A	404	ASP
1	12-A	531	THR
1	12-A	541	TYR
1	12-A	545	ASN
1	12-A	570	LEU
1	12-A	603	SER
1	12-A	605	PRO
1	13-A	57	GLU
1	13-A	75	THR
1	13-A	78	ILE
1	13-A	109	ASN
1	13-A	110	ASP
1	13-A	157	GLU
1	13-A	164	VAL
1	13-A	192	ASP
1	13-A	248	SER
1	13-A	283	LYS
1	13-A	296	THR
1	13-A	300	GLU
1	13-A	301	SER
1	13-A	404	ASP
1	13-A	470	ASP
1	13-A	517	ASP
1	14-A	57	GLU
1	14-A	74	SER
1	14-A	111	ILE
1	14-A	112	ASN
1	14-A	136	ASP
1	14-A	144	PHE
1	14-A	164	VAL
1	14-A	231	ASN
1	14-A	236	MET
1	14-A	262	VAL
1	14-A	274	ASP
1	14-A	294	ASN
1	14-A	305	ASP
1	14-A	306	GLN
1	14-A	339	ASP
1	14-A	404	ASP

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Mol	Chain	Res	Type
1	14-A	409	PRO
1	14-A	488	GLN
1	14-A	506	ASP
1	14-A	525	LYS
1	14-A	527	ASP
1	14-A	541	TYR
1	14-A	570	LEU
1	14-A	586	ASP
1	15-A	66	PRO
1	15-A	69	LEU
1	15-A	87	ARG
1	15-A	91	SER
1	15-A	112	ASN
1	15-A	136	ASP
1	15-A	180	ARG
1	15-A	231	ASN
1	15-A	236	MET
1	15-A	251	GLU
1	15-A	274	ASP
1	15-A	298	GLU
1	15-A	402	SER
1	15-A	404	ASP
1	15-A	471	ASN
1	15-A	489	TRP
1	15-A	490	SER
1	15-A	534	GLU
1	15-A	570	LEU
1	15-A	586	ASP
1	15-A	604	PHE
1	16-A	57	GLU
1	16-A	63	ASP
1	16-A	72	ASP
1	16-A	77	ASP
1	16-A	136	ASP
1	16-A	164	VAL
1	16-A	236	MET
1	16-A	296	THR
1	16-A	306	GLN
1	16-A	404	ASP
1	16-A	452	GLU
1	16-A	529	SER
1	16-A	541	TYR

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Mol	Chain	Res	Type
1	16-A	545	ASN
1	16-A	560	VAL
1	16-A	570	LEU
1	17-A	72	ASP
1	17-A	206	LYS
1	17-A	207	ILE
1	17-A	236	MET
1	17-A	262	VAL
1	17-A	272	ASP
1	17-A	274	ASP
1	17-A	283	LYS
1	17-A	296	THR
1	17-A	300	GLU
1	17-A	306	GLN
1	17-A	404	ASP
1	17-A	489	TRP
1	17-A	541	TYR
1	17-A	570	LEU
1	17-A	586	ASP
1	17-A	603	SER
1	18-A	57	GLU
1	18-A	69	LEU
1	18-A	84	GLU
1	18-A	88	LYS
1	18-A	97	ASP
1	18-A	144	PHE
1	18-A	184	LYS
1	18-A	222	ARG
1	18-A	236	MET
1	18-A	275	ASP
1	18-A	285	THR
1	18-A	317	GLU
1	18-A	318	THR
1	18-A	340	GLN
1	18-A	399	ASP
1	18-A	404	ASP
1	18-A	489	TRP
1	18-A	527	ASP
1	18-A	541	TYR
1	18-A	554	HIS
1	18-A	570	LEU
1	18-A	603	SER

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Mol	Chain	Res	Type
1	19-A	71	PHE
1	19-A	136	ASP
1	19-A	180	ARG
1	19-A	236	MET
1	19-A	274	ASP
1	19-A	275	ASP
1	19-A	283	LYS
1	19-A	296	THR
1	19-A	300	GLU
1	19-A	306	GLN
1	19-A	404	ASP
1	19-A	527	ASP
1	19-A	528	ASP
1	19-A	531	THR
1	19-A	541	TYR
1	19-A	570	LEU
1	19-A	586	ASP
1	20-A	69	LEU
1	20-A	71	PHE
1	20-A	72	ASP
1	20-A	127	ASN
1	20-A	236	MET
1	20-A	283	LYS
1	20-A	338	VAL
1	20-A	340	GLN
1	20-A	399	ASP
1	20-A	402	SER
1	20-A	404	ASP
1	20-A	470	ASP
1	20-A	489	TRP
1	20-A	527	ASP
1	20-A	529	SER
1	20-A	545	ASN
1	20-A	570	LEU
1	21-A	57	GLU
1	21-A	69	LEU
1	21-A	82	VAL
1	21-A	91	SER
1	21-A	144	PHE
1	21-A	149	THR
1	21-A	236	MET
1	21-A	258	GLU

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Mol	Chain	Res	Type
1	21-A	262	VAL
1	21-A	274	ASP
1	21-A	294	ASN
1	21-A	296	THR
1	21-A	324	ASP
1	21-A	402	SER
1	21-A	404	ASP
1	21-A	515	ASN
1	21-A	527	ASP
1	21-A	528	ASP
1	21-A	541	TYR
1	21-A	570	LEU
1	22-A	63	ASP
1	22-A	72	ASP
1	22-A	88	LYS
1	22-A	110	ASP
1	22-A	136	ASP
1	22-A	157	GLU
1	22-A	236	MET
1	22-A	251	GLU
1	22-A	283	LYS
1	22-A	285	THR
1	22-A	306	GLN
1	22-A	310	VAL
1	22-A	324	ASP
1	22-A	404	ASP
1	22-A	570	LEU
1	22-A	604	PHE
1	23-A	57	GLU
1	23-A	63	ASP
1	23-A	69	LEU
1	23-A	144	PHE
1	23-A	155	SER
1	23-A	180	ARG
1	23-A	231	ASN
1	23-A	262	VAL
1	23-A	272	ASP
1	23-A	274	ASP
1	23-A	285	THR
1	23-A	300	GLU
1	23-A	404	ASP
1	23-A	457	GLU

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Mol	Chain	Res	Type
1	23-A	490	SER
1	23-A	570	LEU
1	23-A	603	SER
1	24-A	63	ASP
1	24-A	67	ASN
1	24-A	77	ASP
1	24-A	236	MET
1	24-A	298	GLU
1	24-A	340	GLN
1	24-A	404	ASP
1	24-A	471	ASN
1	24-A	509	ASP
1	24-A	541	TYR
1	24-A	545	ASN
1	24-A	570	LEU
1	25-A	58	VAL
1	25-A	69	LEU
1	25-A	74	SER
1	25-A	97	ASP
1	25-A	111	ILE
1	25-A	144	PHE
1	25-A	184	LYS
1	25-A	236	MET
1	25-A	258	GLU
1	25-A	271	LEU
1	25-A	285	THR
1	25-A	296	THR
1	25-A	305	ASP
1	25-A	306	GLN
1	25-A	340	GLN
1	25-A	345	ASP
1	25-A	348	ASN
1	25-A	402	SER
1	25-A	404	ASP
1	25-A	488	GLN
1	25-A	518	ILE
1	25-A	527	ASP
1	25-A	541	TYR
1	25-A	549	ASP
1	25-A	570	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	2-A	112	ASN
1	2-A	127	ASN
1	2-A	306	GLN
1	2-A	471	ASN
1	2-A	547	ASN
1	2-A	553	GLN
1	3-A	127	ASN
1	4-A	89	GLN
1	4-A	109	ASN
1	4-A	325	GLN
1	4-A	488	GLN
1	5-A	89	GLN
1	5-A	109	ASN
1	5-A	466	HIS
1	5-A	488	GLN
1	6-A	286	ASN
1	6-A	325	GLN
1	7-A	306	GLN
1	7-A	325	GLN
1	7-A	488	GLN
1	8-A	93	GLN
1	8-A	127	ASN
1	8-A	165	ASN
1	10-A	127	ASN
1	10-A	217	GLN
1	10-A	218	GLN
1	10-A	286	ASN
1	10-A	294	ASN
1	10-A	306	GLN
1	11-A	127	ASN
1	11-A	553	GLN
1	12-A	127	ASN
1	12-A	286	ASN
1	12-A	325	GLN
1	12-A	515	ASN
1	13-A	286	ASN
1	13-A	325	GLN
1	13-A	553	GLN
1	13-A	600	GLN
1	14-A	286	ASN
1	15-A	553	GLN
1	16-A	79	GLN
1	16-A	114	GLN

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Mol	Chain	Res	Type
1	16-A	127	ASN
1	16-A	306	GLN
1	17-A	127	ASN
1	17-A	286	ASN
1	18-A	165	ASN
1	18-A	340	GLN
1	18-A	515	ASN
1	18-A	600	GLN
1	19-A	93	GLN
1	19-A	286	ASN
1	19-A	306	GLN
1	20-A	600	GLN
1	21-A	127	ASN
1	22-A	127	ASN
1	22-A	306	GLN
1	22-A	567	HIS
1	23-A	466	HIS
1	23-A	553	GLN
1	24-A	325	GLN
1	24-A	483	ASN
1	25-A	93	GLN
1	25-A	127	ASN
1	25-A	150	GLN
1	25-A	348	ASN
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 (i)

200 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	-	11,11,12	0.72	0	14,15,17	1.30	2 (14%)
3	EDO	1-A	702	-	3,3,3	0.48	0	2,2,2	0.41	0
3	EDO	1-A	703	-	3,3,3	0.40	0	2,2,2	0.30	0
3	EDO	1-A	704	-	3,3,3	0.43	0	2,2,2	0.13	0
2	BGC	1-A	705	2	11,11,12	2.82	4 (36%)	14,15,17	3.25	5 (35%)
2	BGC	1-A	706	2	11,11,12	3.06	5 (45%)	14,15,17	1.98	4 (28%)
2	BGC	1-A	707	2	11,11,12	2.77	4 (36%)	14,15,17	1.79	1 (7%)
2	BGC	1-A	708	2	12,12,12	2.49	5 (41%)	17,17,17	3.25	7 (41%)
2	BGC	10-A	701	-	11,11,12	1.18	1 (9%)	14,15,17	2.29	7 (50%)
3	EDO	10-A	702	-	3,3,3	0.42	0	2,2,2	0.26	0
3	EDO	10-A	703	-	3,3,3	0.50	0	2,2,2	0.12	0
3	EDO	10-A	704	-	3,3,3	0.60	0	2,2,2	0.17	0
2	BGC	10-A	705	2	11,11,12	2.61	5 (45%)	14,15,17	2.14	4 (28%)
2	BGC	10-A	706	2	11,11,12	3.29	6 (54%)	14,15,17	1.94	3 (21%)
2	BGC	10-A	707	2	11,11,12	2.98	5 (45%)	14,15,17	2.26	5 (35%)
2	BGC	10-A	708	2	12,12,12	2.29	5 (41%)	17,17,17	1.43	3 (17%)
2	BGC	11-A	701	-	11,11,12	1.06	1 (9%)	14,15,17	2.38	6 (42%)
3	EDO	11-A	702	-	3,3,3	0.48	0	2,2,2	0.48	0
3	EDO	11-A	703	-	3,3,3	0.57	0	2,2,2	0.09	0
3	EDO	11-A	704	-	3,3,3	0.54	0	2,2,2	0.56	0
2	BGC	11-A	705	2	11,11,12	2.64	5 (45%)	14,15,17	2.45	3 (21%)
2	BGC	11-A	706	2	11,11,12	2.97	5 (45%)	14,15,17	1.85	3 (21%)
2	BGC	11-A	707	2	11,11,12	2.89	4 (36%)	14,15,17	1.74	2 (14%)
2	BGC	11-A	708	2	12,12,12	2.33	5 (41%)	17,17,17	1.28	2 (11%)
2	BGC	12-A	701	-	11,11,12	0.86	0	14,15,17	2.26	6 (42%)
3	EDO	12-A	702	-	3,3,3	0.45	0	2,2,2	0.40	0
3	EDO	12-A	703	-	3,3,3	0.57	0	2,2,2	0.07	0
3	EDO	12-A	704	-	3,3,3	0.57	0	2,2,2	0.56	0

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	2.69	5 (45%)	14,15,17	1.96	4 (28%)
2	BGC	12-A	706	2	11,11,12	3.06	5 (45%)	14,15,17	1.96	3 (21%)
2	BGC	12-A	707	2	11,11,12	2.89	4 (36%)	14,15,17	1.69	1 (7%)
2	BGC	12-A	708	2	12,12,12	2.46	6 (50%)	17,17,17	0.85	0
2	BGC	13-A	701	-	11,11,12	0.75	0	14,15,17	1.91	4 (28%)
3	EDO	13-A	702	-	3,3,3	0.43	0	2,2,2	0.61	0
3	EDO	13-A	703	-	3,3,3	0.62	0	2,2,2	0.07	0
3	EDO	13-A	704	-	3,3,3	0.59	0	2,2,2	0.42	0
2	BGC	13-A	705	2	11,11,12	2.62	5 (45%)	14,15,17	2.26	3 (21%)
2	BGC	13-A	706	2	11,11,12	3.09	6 (54%)	14,15,17	1.76	3 (21%)
2	BGC	13-A	707	2	11,11,12	2.91	4 (36%)	14,15,17	1.61	2 (14%)
2	BGC	13-A	708	2	12,12,12	2.40	5 (41%)	17,17,17	1.28	2 (11%)
2	BGC	14-A	701	-	11,11,12	0.90	1 (9%)	14,15,17	3.22	7 (50%)
3	EDO	14-A	702	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	14-A	703	-	3,3,3	0.53	0	2,2,2	0.11	0
3	EDO	14-A	704	-	3,3,3	0.55	0	2,2,2	0.60	0
2	BGC	14-A	705	2	11,11,12	2.66	4 (36%)	14,15,17	2.38	5 (35%)
2	BGC	14-A	706	2	11,11,12	3.12	5 (45%)	14,15,17	1.91	2 (14%)
2	BGC	14-A	707	2	11,11,12	2.95	5 (45%)	14,15,17	1.77	3 (21%)
2	BGC	14-A	708	2	12,12,12	2.35	5 (41%)	17,17,17	1.04	1 (5%)
2	BGC	15-A	701	-	11,11,12	1.07	1 (9%)	14,15,17	2.76	5 (35%)
3	EDO	15-A	702	-	3,3,3	0.43	0	2,2,2	0.51	0
3	EDO	15-A	703	-	3,3,3	0.52	0	2,2,2	0.18	0
3	EDO	15-A	704	-	3,3,3	0.56	0	2,2,2	0.14	0
2	BGC	15-A	705	2	11,11,12	2.60	4 (36%)	14,15,17	2.47	5 (35%)
2	BGC	15-A	706	2	11,11,12	2.91	6 (54%)	14,15,17	1.86	3 (21%)
2	BGC	15-A	707	2	11,11,12	2.97	4 (36%)	14,15,17	2.07	6 (42%)
2	BGC	15-A	708	2	12,12,12	2.27	5 (41%)	17,17,17	1.69	5 (29%)
2	BGC	16-A	701	-	11,11,12	0.88	0	14,15,17	2.92	7 (50%)
3	EDO	16-A	702	-	3,3,3	0.41	0	2,2,2	0.50	0
3	EDO	16-A	703	-	3,3,3	0.53	0	2,2,2	0.18	0
3	EDO	16-A	704	-	3,3,3	0.61	0	2,2,2	0.16	0
2	BGC	16-A	705	2	11,11,12	2.77	5 (45%)	14,15,17	2.34	4 (28%)
2	BGC	16-A	706	2	11,11,12	3.19	6 (54%)	14,15,17	2.07	3 (21%)
2	BGC	16-A	707	2	11,11,12	2.97	5 (45%)	14,15,17	1.56	3 (21%)
2	BGC	16-A	708	2	12,12,12	2.22	5 (41%)	17,17,17	1.72	3 (17%)
2	BGC	17-A	701	-	11,11,12	0.79	0	14,15,17	2.41	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	17-A	702	-	3,3,3	0.50	0	2,2,2	0.46	0
3	EDO	17-A	703	-	3,3,3	0.66	0	2,2,2	0.11	0
3	EDO	17-A	704	-	3,3,3	0.64	0	2,2,2	0.29	0
2	BGC	17-A	705	2	11,11,12	2.58	5 (45%)	14,15,17	2.26	4 (28%)
2	BGC	17-A	706	2	11,11,12	2.98	6 (54%)	14,15,17	1.69	1 (7%)
2	BGC	17-A	707	2	11,11,12	3.10	5 (45%)	14,15,17	1.67	2 (14%)
2	BGC	17-A	708	2	12,12,12	2.53	5 (41%)	17,17,17	1.42	4 (23%)
2	BGC	18-A	701	-	11,11,12	0.68	0	14,15,17	1.50	3 (21%)
3	EDO	18-A	702	-	3,3,3	0.47	0	2,2,2	0.36	0
3	EDO	18-A	703	-	3,3,3	0.49	0	2,2,2	0.12	0
3	EDO	18-A	704	-	3,3,3	0.63	0	2,2,2	0.20	0
2	BGC	18-A	705	2	11,11,12	2.67	5 (45%)	14,15,17	2.56	7 (50%)
2	BGC	18-A	706	2	11,11,12	2.89	5 (45%)	14,15,17	2.07	2 (14%)
2	BGC	18-A	707	2	11,11,12	2.98	4 (36%)	14,15,17	1.92	1 (7%)
2	BGC	18-A	708	2	12,12,12	2.35	5 (41%)	17,17,17	1.21	2 (11%)
2	BGC	19-A	701	-	11,11,12	0.74	0	14,15,17	1.99	5 (35%)
3	EDO	19-A	702	-	3,3,3	0.42	0	2,2,2	0.30	0
3	EDO	19-A	703	-	3,3,3	0.37	0	2,2,2	0.48	0
3	EDO	19-A	704	-	3,3,3	0.64	0	2,2,2	0.28	0
2	BGC	19-A	705	2	11,11,12	2.74	4 (36%)	14,15,17	2.92	4 (28%)
2	BGC	19-A	706	2	11,11,12	3.10	6 (54%)	14,15,17	2.00	4 (28%)
2	BGC	19-A	707	2	11,11,12	2.97	4 (36%)	14,15,17	1.72	3 (21%)
2	BGC	19-A	708	2	12,12,12	2.28	5 (41%)	17,17,17	1.84	6 (35%)
2	BGC	2-A	701	-	11,11,12	0.86	0	14,15,17	3.59	8 (57%)
3	EDO	2-A	702	-	3,3,3	0.41	0	2,2,2	0.47	0
3	EDO	2-A	703	-	3,3,3	0.51	0	2,2,2	0.17	0
3	EDO	2-A	704	-	3,3,3	0.65	0	2,2,2	0.18	0
2	BGC	2-A	705	2	11,11,12	2.75	5 (45%)	14,15,17	2.48	4 (28%)
2	BGC	2-A	706	2	11,11,12	3.16	5 (45%)	14,15,17	1.80	3 (21%)
2	BGC	2-A	707	2	11,11,12	3.10	6 (54%)	14,15,17	2.01	2 (14%)
2	BGC	2-A	708	2	12,12,12	2.40	5 (41%)	17,17,17	1.13	2 (11%)
2	BGC	20-A	701	-	11,11,12	0.76	0	14,15,17	2.41	6 (42%)
3	EDO	20-A	702	-	3,3,3	0.43	0	2,2,2	0.31	0
3	EDO	20-A	703	-	3,3,3	0.42	0	2,2,2	0.28	0
3	EDO	20-A	704	-	3,3,3	0.36	0	2,2,2	0.62	0
2	BGC	20-A	705	2	11,11,12	2.77	5 (45%)	14,15,17	3.26	5 (35%)
2	BGC	20-A	706	2	11,11,12	2.98	6 (54%)	14,15,17	1.73	1 (7%)
2	BGC	20-A	707	2	11,11,12	3.02	5 (45%)	14,15,17	1.89	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BGC	20-A	708	2	12,12,12	2.47	5 (41%)	17,17,17	1.21	1 (5%)
2	BGC	21-A	701	-	11,11,12	0.85	0	14,15,17	2.39	4 (28%)
3	EDO	21-A	702	-	3,3,3	0.44	0	2,2,2	0.76	0
3	EDO	21-A	703	-	3,3,3	0.56	0	2,2,2	0.18	0
3	EDO	21-A	704	-	3,3,3	0.57	0	2,2,2	0.25	0
2	BGC	21-A	705	2	11,11,12	2.71	5 (45%)	14,15,17	2.49	3 (21%)
2	BGC	21-A	706	2	11,11,12	3.05	6 (54%)	14,15,17	1.49	1 (7%)
2	BGC	21-A	707	2	11,11,12	3.04	5 (45%)	14,15,17	2.10	6 (42%)
2	BGC	21-A	708	2	12,12,12	2.35	5 (41%)	17,17,17	1.17	1 (5%)
2	BGC	22-A	701	-	11,11,12	1.03	0	14,15,17	3.86	10 (71%)
3	EDO	22-A	702	-	3,3,3	0.38	0	2,2,2	0.39	0
3	EDO	22-A	703	-	3,3,3	0.53	0	2,2,2	0.13	0
3	EDO	22-A	704	-	3,3,3	0.62	0	2,2,2	0.31	0
2	BGC	22-A	705	2	11,11,12	2.70	4 (36%)	14,15,17	2.61	5 (35%)
2	BGC	22-A	706	2	11,11,12	3.21	5 (45%)	14,15,17	1.31	2 (14%)
2	BGC	22-A	707	2	11,11,12	2.84	4 (36%)	14,15,17	2.29	2 (14%)
2	BGC	22-A	708	2	12,12,12	2.35	5 (41%)	17,17,17	1.14	0
2	BGC	23-A	701	-	11,11,12	0.73	0	14,15,17	1.64	4 (28%)
3	EDO	23-A	702	-	3,3,3	0.51	0	2,2,2	0.25	0
3	EDO	23-A	703	-	3,3,3	0.49	0	2,2,2	0.32	0
3	EDO	23-A	704	-	3,3,3	0.41	0	2,2,2	0.39	0
2	BGC	23-A	705	2	11,11,12	2.60	4 (36%)	14,15,17	2.32	4 (28%)
2	BGC	23-A	706	2	11,11,12	3.08	5 (45%)	14,15,17	2.26	3 (21%)
2	BGC	23-A	707	2	11,11,12	3.11	5 (45%)	14,15,17	2.14	3 (21%)
2	BGC	23-A	708	2	12,12,12	2.44	6 (50%)	17,17,17	2.01	6 (35%)
2	BGC	24-A	701	-	11,11,12	1.16	1 (9%)	14,15,17	1.84	3 (21%)
3	EDO	24-A	702	-	3,3,3	0.44	0	2,2,2	0.10	0
3	EDO	24-A	703	-	3,3,3	0.53	0	2,2,2	0.09	0
3	EDO	24-A	704	-	3,3,3	0.64	0	2,2,2	0.14	0
2	BGC	24-A	705	2	11,11,12	2.67	4 (36%)	14,15,17	2.49	4 (28%)
2	BGC	24-A	706	2	11,11,12	3.19	6 (54%)	14,15,17	1.54	1 (7%)
2	BGC	24-A	707	2	11,11,12	3.08	5 (45%)	14,15,17	1.76	2 (14%)
2	BGC	24-A	708	2	12,12,12	2.26	5 (41%)	17,17,17	1.54	2 (11%)
2	BGC	25-A	701	-	11,11,12	0.56	0	14,15,17	2.18	4 (28%)
3	EDO	25-A	702	-	3,3,3	0.47	0	2,2,2	0.26	0
3	EDO	25-A	703	-	3,3,3	0.45	0	2,2,2	0.40	0
3	EDO	25-A	704	-	3,3,3	0.33	0	2,2,2	0.38	0
2	BGC	25-A	705	2	11,11,12	2.58	5 (45%)	14,15,17	2.10	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BGC	25-A	706	2	11,11,12	3.08	5 (45%)	14,15,17	1.73	2 (14%)
2	BGC	25-A	707	2	11,11,12	3.06	5 (45%)	14,15,17	1.87	4 (28%)
2	BGC	25-A	708	2	12,12,12	2.39	5 (41%)	17,17,17	1.39	4 (23%)
2	BGC	3-A	701	-	11,11,12	1.15	1 (9%)	14,15,17	2.93	6 (42%)
3	EDO	3-A	702	-	3,3,3	0.42	0	2,2,2	0.26	0
3	EDO	3-A	703	-	3,3,3	0.50	0	2,2,2	0.18	0
3	EDO	3-A	704	-	3,3,3	0.61	0	2,2,2	0.17	0
2	BGC	3-A	705	2	11,11,12	2.64	4 (36%)	14,15,17	2.23	5 (35%)
2	BGC	3-A	706	2	11,11,12	2.98	6 (54%)	14,15,17	1.70	1 (7%)
2	BGC	3-A	707	2	11,11,12	2.94	4 (36%)	14,15,17	1.76	2 (14%)
2	BGC	3-A	708	2	12,12,12	2.42	6 (50%)	17,17,17	1.18	1 (5%)
2	BGC	4-A	701	-	11,11,12	0.65	0	14,15,17	0.90	0
3	EDO	4-A	702	-	3,3,3	0.42	0	2,2,2	0.22	0
3	EDO	4-A	703	-	3,3,3	0.51	0	2,2,2	0.12	0
3	EDO	4-A	704	-	3,3,3	0.65	0	2,2,2	0.16	0
2	BGC	4-A	705	2	11,11,12	2.61	5 (45%)	14,15,17	2.17	3 (21%)
2	BGC	4-A	706	2	11,11,12	2.97	6 (54%)	14,15,17	1.56	1 (7%)
2	BGC	4-A	707	2	11,11,12	2.93	4 (36%)	14,15,17	2.06	2 (14%)
2	BGC	4-A	708	2	12,12,12	2.26	5 (41%)	17,17,17	1.61	4 (23%)
2	BGC	5-A	701	-	11,11,12	0.75	0	14,15,17	1.71	3 (21%)
3	EDO	5-A	702	-	3,3,3	0.52	0	2,2,2	0.18	0
3	EDO	5-A	703	-	3,3,3	0.49	0	2,2,2	0.16	0
3	EDO	5-A	704	-	3,3,3	0.63	0	2,2,2	0.20	0
2	BGC	5-A	705	2	11,11,12	2.70	6 (54%)	14,15,17	2.28	4 (28%)
2	BGC	5-A	706	2	11,11,12	3.24	5 (45%)	14,15,17	1.68	2 (14%)
2	BGC	5-A	707	2	11,11,12	3.08	4 (36%)	14,15,17	2.47	7 (50%)
2	BGC	5-A	708	2	12,12,12	2.36	5 (41%)	17,17,17	1.49	4 (23%)
2	BGC	6-A	701	-	11,11,12	0.76	0	14,15,17	1.36	2 (14%)
3	EDO	6-A	702	-	3,3,3	0.45	0	2,2,2	0.44	0
3	EDO	6-A	703	-	3,3,3	0.54	0	2,2,2	0.05	0
3	EDO	6-A	704	-	3,3,3	0.68	0	2,2,2	0.15	0
2	BGC	6-A	705	2	11,11,12	2.75	4 (36%)	14,15,17	3.05	5 (35%)
2	BGC	6-A	706	2	11,11,12	3.02	5 (45%)	14,15,17	1.55	2 (14%)
2	BGC	6-A	707	2	11,11,12	2.89	4 (36%)	14,15,17	1.63	2 (14%)
2	BGC	6-A	708	2	12,12,12	2.33	5 (41%)	17,17,17	1.26	1 (5%)
2	BGC	7-A	701	-	11,11,12	0.82	0	14,15,17	1.68	3 (21%)
3	EDO	7-A	702	-	3,3,3	0.62	0	2,2,2	0.19	0
3	EDO	7-A	703	-	3,3,3	0.38	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	7-A	704	-	3,3,3	0.54	0	2,2,2	0.07	0
2	BGC	7-A	705	2	11,11,12	2.77	5 (45%)	14,15,17	2.09	5 (35%)
2	BGC	7-A	706	2	11,11,12	3.14	6 (54%)	14,15,17	2.45	5 (35%)
2	BGC	7-A	707	2	11,11,12	2.91	4 (36%)	14,15,17	1.53	1 (7%)
2	BGC	7-A	708	2	12,12,12	2.54	5 (41%)	17,17,17	1.35	3 (17%)
2	BGC	8-A	701	-	11,11,12	1.04	1 (9%)	14,15,17	2.06	5 (35%)
3	EDO	8-A	702	-	3,3,3	0.47	0	2,2,2	0.17	0
3	EDO	8-A	703	-	3,3,3	0.51	0	2,2,2	0.44	0
3	EDO	8-A	704	-	3,3,3	0.62	0	2,2,2	0.39	0
2	BGC	8-A	705	2	11,11,12	2.63	5 (45%)	14,15,17	2.81	3 (21%)
2	BGC	8-A	706	2	11,11,12	3.02	6 (54%)	14,15,17	1.48	1 (7%)
2	BGC	8-A	707	2	11,11,12	2.99	5 (45%)	14,15,17	2.19	2 (14%)
2	BGC	8-A	708	2	12,12,12	2.35	5 (41%)	17,17,17	1.48	4 (23%)
2	BGC	9-A	701	-	11,11,12	0.66	0	14,15,17	1.94	3 (21%)
3	EDO	9-A	702	-	3,3,3	0.62	0	2,2,2	0.16	0
3	EDO	9-A	703	-	3,3,3	0.55	0	2,2,2	0.21	0
3	EDO	9-A	704	-	3,3,3	0.62	0	2,2,2	0.26	0
2	BGC	9-A	705	2	11,11,12	2.85	4 (36%)	14,15,17	2.58	5 (35%)
2	BGC	9-A	706	2	11,11,12	3.20	5 (45%)	14,15,17	1.69	1 (7%)
2	BGC	9-A	707	2	11,11,12	3.15	4 (36%)	14,15,17	2.09	2 (14%)
2	BGC	9-A	708	2	12,12,12	2.51	5 (41%)	17,17,17	1.30	2 (11%)

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	-	-	0/2/19/22	0/1/1/1
3	EDO	1-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	1-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	1-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	1-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	1-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	1-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	10-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	10-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	10-A	703	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	10-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	10-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	10-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	10-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	10-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	11-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	11-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	11-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	11-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	11-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	11-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	11-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	11-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	12-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	12-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	12-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	12-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	12-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	12-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	12-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	12-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	13-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	13-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	13-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	13-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	13-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	13-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	13-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	13-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	14-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	14-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	14-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	14-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	14-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	14-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	14-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	14-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	15-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	15-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	15-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	15-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	15-A	705	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	15-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	15-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	15-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	16-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	16-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	16-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	16-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	16-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	16-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	16-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	16-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	17-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	17-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	17-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	17-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	17-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	17-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	17-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	17-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	18-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	18-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	18-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	18-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	18-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	18-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	18-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	18-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	19-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	19-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	19-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	19-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	19-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	19-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	19-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	19-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	2-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	2-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	2-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	2-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	2-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	2-A	707	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	2-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	20-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	20-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	20-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	20-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	20-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	20-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	20-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	20-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	21-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	21-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	21-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	21-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	21-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	21-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	21-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	21-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	22-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	22-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	22-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	22-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	22-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	22-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	22-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	22-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	23-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	23-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	23-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	23-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	23-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	23-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	23-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	23-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	24-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	24-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	24-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	24-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	24-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	24-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	24-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	24-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	25-A	701	-	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	25-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	25-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	25-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	25-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	25-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	25-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	25-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	3-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	3-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	3-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	3-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	3-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	3-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	3-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	4-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	4-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	4-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	4-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	4-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	4-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	4-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	5-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	5-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	5-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	5-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	5-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	5-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	5-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	6-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	6-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	6-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	6-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	6-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	6-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	6-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	7-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	7-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	7-A	703	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	7-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	7-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	7-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	7-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	7-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	8-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	8-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	8-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	8-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	8-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	8-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	8-A	708	2	-	0/2/22/22	0/1/1/1
2	BGC	9-A	701	-	-	0/2/19/22	0/1/1/1
3	EDO	9-A	702	-	-	0/1/1/1	0/0/0/0
3	EDO	9-A	703	-	-	0/1/1/1	0/0/0/0
3	EDO	9-A	704	-	-	0/1/1/1	0/0/0/0
2	BGC	9-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	9-A	706	2	-	0/2/19/22	0/1/1/1
2	BGC	9-A	707	2	-	0/2/19/22	0/1/1/1
2	BGC	9-A	708	2	-	0/2/22/22	0/1/1/1

All (501) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	10-A	706	BGC	C2-C3	-7.79	1.41	1.52
2	23-A	707	BGC	C2-C3	-7.62	1.42	1.52
2	22-A	706	BGC	C2-C3	-7.55	1.42	1.52
2	9-A	707	BGC	C2-C3	-7.49	1.42	1.52
2	2-A	707	BGC	C2-C3	-7.47	1.42	1.52
2	9-A	706	BGC	C2-C3	-7.45	1.42	1.52
2	24-A	707	BGC	C2-C3	-7.32	1.42	1.52
2	5-A	706	BGC	C2-C3	-7.32	1.42	1.52
2	24-A	706	BGC	C2-C3	-7.24	1.42	1.52
2	25-A	707	BGC	C2-C3	-7.16	1.42	1.52
2	5-A	707	BGC	C2-C3	-7.13	1.42	1.52
2	17-A	707	BGC	C2-C3	-7.10	1.42	1.52
2	2-A	706	BGC	C2-C3	-7.10	1.42	1.52
2	13-A	706	BGC	C2-C3	-7.07	1.42	1.52
2	16-A	706	BGC	C2-C3	-7.07	1.42	1.52
2	7-A	706	BGC	C2-C3	-7.02	1.42	1.52
2	12-A	706	BGC	C2-C3	-6.98	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	19-A	707	BGC	C2-C3	-6.95	1.43	1.52
2	6-A	706	BGC	C2-C3	-6.94	1.43	1.52
2	14-A	706	BGC	C2-C3	-6.92	1.43	1.52
2	20-A	707	BGC	C2-C3	-6.91	1.43	1.52
2	8-A	706	BGC	C2-C3	-6.89	1.43	1.52
2	11-A	706	BGC	C2-C3	-6.89	1.43	1.52
2	21-A	707	BGC	C2-C3	-6.86	1.43	1.52
2	18-A	707	BGC	C2-C3	-6.86	1.43	1.52
2	16-A	707	BGC	C2-C3	-6.85	1.43	1.52
2	13-A	707	BGC	C2-C3	-6.83	1.43	1.52
2	7-A	707	BGC	C2-C3	-6.80	1.43	1.52
2	8-A	707	BGC	C2-C3	-6.79	1.43	1.52
2	10-A	707	BGC	C2-C3	-6.79	1.43	1.52
2	4-A	706	BGC	C2-C3	-6.78	1.43	1.52
2	21-A	706	BGC	C2-C3	-6.77	1.43	1.52
2	3-A	706	BGC	C2-C3	-6.75	1.43	1.52
2	3-A	707	BGC	C2-C3	-6.70	1.43	1.52
2	1-A	706	BGC	C2-C3	-6.67	1.43	1.52
2	14-A	707	BGC	C2-C3	-6.66	1.43	1.52
2	25-A	706	BGC	C2-C3	-6.65	1.43	1.52
2	19-A	706	BGC	C2-C3	-6.64	1.43	1.52
2	15-A	706	BGC	C2-C3	-6.62	1.43	1.52
2	15-A	707	BGC	C2-C3	-6.61	1.43	1.52
2	12-A	707	BGC	C2-C3	-6.60	1.43	1.52
2	6-A	707	BGC	C2-C3	-6.58	1.43	1.52
2	23-A	706	BGC	C2-C3	-6.57	1.43	1.52
2	4-A	707	BGC	C2-C3	-6.54	1.43	1.52
2	11-A	707	BGC	C2-C3	-6.44	1.43	1.52
2	18-A	706	BGC	C2-C3	-6.44	1.43	1.52
2	17-A	706	BGC	C2-C3	-6.37	1.43	1.52
2	1-A	707	BGC	C2-C3	-6.28	1.43	1.52
2	22-A	707	BGC	C2-C3	-6.24	1.44	1.52
2	20-A	706	BGC	C2-C3	-6.23	1.44	1.52
2	7-A	705	BGC	C2-C3	-5.87	1.44	1.52
2	16-A	705	BGC	C2-C3	-5.83	1.44	1.52
2	19-A	705	BGC	C2-C3	-5.82	1.44	1.52
2	2-A	705	BGC	C2-C3	-5.78	1.44	1.52
2	1-A	705	BGC	C2-C3	-5.69	1.44	1.52
2	20-A	705	BGC	C2-C3	-5.48	1.45	1.52
2	24-A	705	BGC	C2-C3	-5.48	1.45	1.52
2	12-A	705	BGC	C2-C3	-5.47	1.45	1.52
2	14-A	705	BGC	C2-C3	-5.38	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	18-A	705	BGC	C2-C3	-5.37	1.45	1.52
2	6-A	705	BGC	C2-C3	-5.35	1.45	1.52
2	9-A	705	BGC	C2-C3	-5.34	1.45	1.52
2	8-A	705	BGC	C2-C3	-5.29	1.45	1.52
2	5-A	705	BGC	C2-C3	-5.21	1.45	1.52
2	22-A	705	BGC	C2-C3	-5.20	1.45	1.52
2	15-A	705	BGC	C2-C3	-5.18	1.45	1.52
2	23-A	705	BGC	C2-C3	-5.12	1.45	1.52
2	11-A	705	BGC	C2-C3	-5.11	1.45	1.52
2	4-A	705	BGC	C2-C3	-5.10	1.45	1.52
2	21-A	708	BGC	C6-C5	-5.07	1.33	1.51
2	13-A	705	BGC	C2-C3	-5.06	1.45	1.52
2	21-A	705	BGC	C2-C3	-5.06	1.45	1.52
2	9-A	708	BGC	C6-C5	-5.03	1.34	1.51
2	5-A	708	BGC	C6-C5	-4.98	1.34	1.51
2	9-A	705	BGC	C6-C5	-4.98	1.34	1.51
2	18-A	708	BGC	C6-C5	-4.97	1.34	1.51
2	11-A	708	BGC	C6-C5	-4.95	1.34	1.51
2	2-A	708	BGC	C6-C5	-4.94	1.34	1.51
2	6-A	708	BGC	C6-C5	-4.92	1.34	1.51
2	3-A	705	BGC	C2-C3	-4.86	1.45	1.52
2	22-A	708	BGC	C6-C5	-4.84	1.34	1.51
2	25-A	705	BGC	C2-C3	-4.84	1.45	1.52
2	20-A	708	BGC	C6-C5	-4.83	1.34	1.51
2	14-A	708	BGC	C6-C5	-4.82	1.34	1.51
2	19-A	708	BGC	C6-C5	-4.81	1.34	1.51
2	14-A	706	BGC	C6-C5	-4.79	1.34	1.51
2	17-A	705	BGC	C2-C3	-4.79	1.46	1.52
2	25-A	708	BGC	C6-C5	-4.78	1.34	1.51
2	25-A	706	BGC	C6-C5	-4.75	1.35	1.51
2	24-A	708	BGC	C6-C5	-4.75	1.35	1.51
2	12-A	708	BGC	C6-C5	-4.75	1.35	1.51
2	10-A	708	BGC	C6-C5	-4.75	1.35	1.51
2	10-A	705	BGC	C2-C3	-4.74	1.46	1.52
2	23-A	708	BGC	C6-C5	-4.74	1.35	1.51
2	16-A	708	BGC	C6-C5	-4.74	1.35	1.51
2	7-A	706	BGC	C6-C5	-4.70	1.35	1.51
2	1-A	708	BGC	C6-C5	-4.70	1.35	1.51
2	7-A	708	BGC	C6-C5	-4.69	1.35	1.51
2	3-A	708	BGC	C6-C5	-4.69	1.35	1.51
2	12-A	705	BGC	C6-C5	-4.68	1.35	1.51
2	17-A	708	BGC	C6-C5	-4.68	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	13-A	706	BGC	C6-C5	-4.64	1.35	1.51
2	10-A	706	BGC	C6-C5	-4.62	1.35	1.51
2	2-A	706	BGC	C6-C5	-4.62	1.35	1.51
2	5-A	706	BGC	C6-C5	-4.61	1.35	1.51
2	18-A	706	BGC	C6-C5	-4.61	1.35	1.51
2	16-A	706	BGC	C6-C5	-4.61	1.35	1.51
2	19-A	706	BGC	C6-C5	-4.60	1.35	1.51
2	20-A	705	BGC	C6-C5	-4.59	1.35	1.51
2	22-A	706	BGC	C6-C5	-4.57	1.35	1.51
2	13-A	708	BGC	C6-C5	-4.57	1.35	1.51
2	4-A	708	BGC	C6-C5	-4.56	1.35	1.51
2	1-A	706	BGC	C6-C5	-4.55	1.35	1.51
2	15-A	708	BGC	C6-C5	-4.54	1.35	1.51
2	4-A	707	BGC	C6-C5	-4.54	1.35	1.51
2	6-A	706	BGC	C6-C5	-4.53	1.35	1.51
2	3-A	705	BGC	C6-C5	-4.53	1.35	1.51
2	8-A	708	BGC	C6-C5	-4.52	1.35	1.51
2	24-A	706	BGC	C6-C5	-4.49	1.36	1.51
2	9-A	707	BGC	C6-C5	-4.46	1.36	1.51
2	3-A	706	BGC	C6-C5	-4.45	1.36	1.51
2	25-A	707	BGC	C6-C5	-4.44	1.36	1.51
2	21-A	707	BGC	C6-C5	-4.44	1.36	1.51
2	8-A	706	BGC	C6-C5	-4.43	1.36	1.51
2	15-A	707	BGC	C6-C5	-4.41	1.36	1.51
2	16-A	707	BGC	C6-C5	-4.41	1.36	1.51
2	21-A	706	BGC	C6-C5	-4.41	1.36	1.51
2	20-A	707	BGC	C6-C5	-4.40	1.36	1.51
2	3-A	707	BGC	C6-C5	-4.39	1.36	1.51
2	5-A	707	BGC	C6-C5	-4.39	1.36	1.51
2	12-A	706	BGC	C6-C5	-4.39	1.36	1.51
2	20-A	706	BGC	C6-C5	-4.37	1.36	1.51
2	21-A	705	BGC	C6-C5	-4.36	1.36	1.51
2	9-A	706	BGC	C6-C5	-4.35	1.36	1.51
2	10-A	707	BGC	C6-C5	-4.34	1.36	1.51
2	24-A	707	BGC	C6-C5	-4.34	1.36	1.51
2	8-A	707	BGC	C6-C5	-4.34	1.36	1.51
2	17-A	706	BGC	C6-C5	-4.34	1.36	1.51
2	23-A	707	BGC	C6-C5	-4.33	1.36	1.51
2	16-A	705	BGC	C6-C5	-4.32	1.36	1.51
2	23-A	706	BGC	C6-C5	-4.32	1.36	1.51
2	15-A	706	BGC	C6-C5	-4.30	1.36	1.51
2	11-A	707	BGC	C6-C5	-4.30	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	15-A	705	BGC	C6-C5	-4.29	1.36	1.51
2	17-A	707	BGC	C6-C5	-4.27	1.36	1.51
2	1-A	705	BGC	C6-C5	-4.26	1.36	1.51
2	4-A	706	BGC	C6-C5	-4.26	1.36	1.51
2	7-A	707	BGC	C6-C5	-4.25	1.36	1.51
2	1-A	707	BGC	C6-C5	-4.24	1.36	1.51
2	6-A	707	BGC	C6-C5	-4.24	1.36	1.51
2	11-A	706	BGC	C6-C5	-4.23	1.36	1.51
2	24-A	705	BGC	C6-C5	-4.22	1.36	1.51
2	22-A	707	BGC	C6-C5	-4.22	1.36	1.51
2	13-A	707	BGC	C6-C5	-4.21	1.37	1.51
2	12-A	707	BGC	C6-C5	-4.21	1.37	1.51
2	2-A	707	BGC	C6-C5	-4.20	1.37	1.51
2	6-A	705	BGC	C6-C5	-4.20	1.37	1.51
2	19-A	707	BGC	C6-C5	-4.19	1.37	1.51
2	18-A	707	BGC	C6-C5	-4.19	1.37	1.51
2	7-A	705	BGC	C6-C5	-4.18	1.37	1.51
2	17-A	705	BGC	C6-C5	-4.17	1.37	1.51
2	14-A	705	BGC	C6-C5	-4.17	1.37	1.51
2	11-A	705	BGC	C6-C5	-4.17	1.37	1.51
2	14-A	707	BGC	C6-C5	-4.16	1.37	1.51
2	13-A	705	BGC	C6-C5	-4.14	1.37	1.51
2	25-A	705	BGC	C6-C5	-4.13	1.37	1.51
2	2-A	705	BGC	C6-C5	-4.09	1.37	1.51
2	17-A	708	BGC	C1-C2	-4.01	1.45	1.52
2	22-A	705	BGC	C6-C5	-4.00	1.37	1.51
2	10-A	705	BGC	C6-C5	-3.99	1.37	1.51
2	4-A	705	BGC	C6-C5	-3.98	1.37	1.51
2	19-A	705	BGC	C6-C5	-3.98	1.37	1.51
2	5-A	705	BGC	C6-C5	-3.93	1.38	1.51
2	23-A	705	BGC	C6-C5	-3.92	1.38	1.51
2	7-A	708	BGC	C1-C2	-3.85	1.45	1.52
2	8-A	705	BGC	C6-C5	-3.70	1.38	1.51
2	2-A	708	BGC	C1-C2	-3.65	1.45	1.52
2	13-A	708	BGC	C1-C2	-3.65	1.45	1.52
2	18-A	705	BGC	C6-C5	-3.53	1.39	1.51
2	20-A	708	BGC	C1-C2	-3.53	1.46	1.52
2	10-A	701	BGC	O5-C1	-3.49	1.37	1.43
2	1-A	708	BGC	C3-C2	-3.46	1.43	1.52
2	21-A	708	BGC	C1-C2	-3.41	1.46	1.52
2	14-A	708	BGC	C1-C2	-3.39	1.46	1.52
2	7-A	708	BGC	C3-C2	-3.39	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	23-A	708	BGC	C1-C2	-3.38	1.46	1.52
2	25-A	708	BGC	C1-C2	-3.33	1.46	1.52
2	9-A	708	BGC	C1-C2	-3.33	1.46	1.52
2	17-A	708	BGC	C3-C2	-3.28	1.43	1.52
2	10-A	708	BGC	C1-C2	-3.24	1.46	1.52
2	12-A	708	BGC	C1-C2	-3.23	1.46	1.52
2	5-A	708	BGC	C1-C2	-3.22	1.46	1.52
2	13-A	708	BGC	C3-C2	-3.20	1.44	1.52
2	3-A	708	BGC	C1-C2	-3.17	1.46	1.52
2	3-A	708	BGC	C3-C2	-3.10	1.44	1.52
2	8-A	708	BGC	C1-C2	-3.07	1.47	1.52
2	21-A	708	BGC	C3-C2	-3.06	1.44	1.52
2	20-A	708	BGC	C3-C2	-3.06	1.44	1.52
2	9-A	708	BGC	C3-C2	-3.05	1.44	1.52
2	22-A	708	BGC	C3-C2	-3.03	1.44	1.52
2	8-A	708	BGC	C3-C2	-3.03	1.44	1.52
2	19-A	708	BGC	C1-C2	-3.01	1.47	1.52
2	22-A	708	BGC	C1-C2	-3.01	1.47	1.52
2	11-A	708	BGC	C1-C2	-3.00	1.47	1.52
2	12-A	708	BGC	C3-C2	-2.99	1.44	1.52
2	6-A	708	BGC	C1-C2	-2.97	1.47	1.52
2	15-A	708	BGC	C1-C2	-2.92	1.47	1.52
2	18-A	708	BGC	C1-C2	-2.91	1.47	1.52
2	2-A	708	BGC	C3-C2	-2.89	1.44	1.52
2	24-A	708	BGC	C1-C2	-2.89	1.47	1.52
2	4-A	708	BGC	C1-C2	-2.87	1.47	1.52
2	4-A	708	BGC	C3-C2	-2.86	1.44	1.52
2	14-A	708	BGC	C3-C2	-2.85	1.44	1.52
2	16-A	708	BGC	C1-C2	-2.81	1.47	1.52
2	25-A	708	BGC	C3-C2	-2.81	1.45	1.52
2	6-A	708	BGC	C3-C2	-2.78	1.45	1.52
2	25-A	706	BGC	C4-C3	-2.78	1.45	1.52
2	24-A	708	BGC	C3-C2	-2.76	1.45	1.52
2	10-A	708	BGC	C3-C2	-2.72	1.45	1.52
2	16-A	708	BGC	C3-C2	-2.72	1.45	1.52
2	1-A	708	BGC	C1-C2	-2.68	1.47	1.52
2	15-A	708	BGC	C3-C2	-2.66	1.45	1.52
2	3-A	701	BGC	O5-C1	-2.65	1.39	1.43
2	24-A	706	BGC	C4-C3	-2.60	1.45	1.52
2	5-A	706	BGC	C4-C3	-2.59	1.45	1.52
2	11-A	708	BGC	C3-C2	-2.58	1.45	1.52
2	14-A	706	BGC	C4-C3	-2.56	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5-A	708	BGC	C3-C2	-2.55	1.45	1.52
2	6-A	706	BGC	C4-C3	-2.54	1.45	1.52
2	2-A	706	BGC	C4-C3	-2.53	1.45	1.52
2	1-A	706	BGC	C4-C3	-2.49	1.45	1.52
2	23-A	708	BGC	C3-C2	-2.47	1.45	1.52
2	10-A	706	BGC	C4-C3	-2.46	1.45	1.52
2	9-A	706	BGC	C4-C3	-2.45	1.46	1.52
2	18-A	708	BGC	C3-C2	-2.45	1.46	1.52
2	22-A	706	BGC	C4-C3	-2.44	1.46	1.52
2	19-A	708	BGC	C3-C2	-2.37	1.46	1.52
2	15-A	706	BGC	C4-C3	-2.35	1.46	1.52
2	3-A	706	BGC	C4-C3	-2.28	1.46	1.52
2	19-A	706	BGC	C4-C3	-2.26	1.46	1.52
2	7-A	706	BGC	C4-C3	-2.25	1.46	1.52
2	23-A	707	BGC	C1-C2	-2.20	1.46	1.52
2	18-A	706	BGC	C4-C3	-2.19	1.46	1.52
2	21-A	706	BGC	C4-C3	-2.17	1.46	1.52
2	24-A	701	BGC	O2-C2	-2.15	1.38	1.43
2	17-A	706	BGC	C4-C3	-2.12	1.46	1.52
2	11-A	701	BGC	O5-C1	-2.12	1.40	1.43
2	16-A	706	BGC	C4-C3	-2.08	1.46	1.52
2	8-A	706	BGC	C4-C3	-2.07	1.47	1.52
2	8-A	701	BGC	O3-C3	-2.06	1.38	1.43
2	8-A	707	BGC	C1-C2	-2.05	1.47	1.52
2	13-A	706	BGC	C4-C3	-2.04	1.47	1.52
2	4-A	706	BGC	C4-C3	-2.03	1.47	1.52
2	24-A	707	BGC	C1-C2	-2.03	1.47	1.52
2	20-A	706	BGC	C4-C3	-2.03	1.47	1.52
2	2-A	707	BGC	C1-C2	-2.01	1.47	1.52
2	14-A	707	BGC	C4-C5	2.00	1.57	1.53
2	16-A	707	BGC	O2-C2	2.01	1.47	1.43
2	2-A	705	BGC	O2-C2	2.02	1.47	1.43
2	13-A	705	BGC	O2-C2	2.03	1.47	1.43
2	20-A	707	BGC	O2-C2	2.03	1.47	1.43
2	12-A	708	BGC	O2-C2	2.03	1.47	1.43
2	17-A	705	BGC	O2-C2	2.04	1.48	1.43
2	11-A	705	BGC	O2-C2	2.06	1.48	1.43
2	12-A	705	BGC	O3-C3	2.06	1.47	1.43
2	16-A	705	BGC	O2-C2	2.06	1.48	1.43
2	3-A	708	BGC	O2-C2	2.07	1.47	1.43
2	20-A	705	BGC	O2-C2	2.10	1.48	1.43
2	18-A	705	BGC	C4-C5	2.10	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	14-A	701	BGC	C2-C3	2.10	1.55	1.52
2	23-A	707	BGC	O3-C3	2.11	1.48	1.43
2	7-A	705	BGC	O3-C3	2.12	1.48	1.43
2	15-A	706	BGC	C4-C5	2.14	1.57	1.53
2	24-A	706	BGC	C4-C5	2.14	1.57	1.53
2	10-A	706	BGC	C4-C5	2.16	1.57	1.53
2	2-A	707	BGC	O2-C2	2.17	1.48	1.43
2	3-A	706	BGC	C4-C5	2.18	1.57	1.53
2	7-A	706	BGC	C4-C5	2.19	1.57	1.53
2	21-A	708	BGC	O5-C5	2.20	1.49	1.44
2	21-A	707	BGC	O2-C2	2.21	1.48	1.43
2	4-A	705	BGC	O2-C2	2.22	1.48	1.43
2	12-A	705	BGC	O2-C2	2.24	1.48	1.43
2	10-A	707	BGC	O2-C2	2.25	1.48	1.43
2	13-A	706	BGC	C4-C5	2.27	1.57	1.53
2	5-A	705	BGC	O2-C2	2.27	1.48	1.43
2	25-A	705	BGC	O2-C2	2.28	1.48	1.43
2	17-A	707	BGC	O2-C2	2.30	1.48	1.43
2	25-A	707	BGC	O2-C2	2.31	1.48	1.43
2	1-A	705	BGC	O3-C3	2.32	1.48	1.43
2	5-A	705	BGC	C4-C5	2.32	1.58	1.53
2	16-A	705	BGC	O3-C3	2.33	1.48	1.43
2	10-A	708	BGC	O5-C5	2.33	1.50	1.44
2	10-A	705	BGC	C4-C5	2.33	1.58	1.53
2	16-A	707	BGC	O3-C3	2.35	1.48	1.43
2	8-A	705	BGC	C4-C5	2.35	1.58	1.53
2	4-A	706	BGC	C4-C5	2.35	1.58	1.53
2	21-A	707	BGC	O3-C3	2.37	1.48	1.43
2	11-A	706	BGC	C4-C5	2.37	1.58	1.53
2	24-A	707	BGC	O3-C3	2.37	1.48	1.43
2	25-A	705	BGC	O3-C3	2.38	1.48	1.43
2	12-A	706	BGC	C4-C5	2.38	1.58	1.53
2	20-A	708	BGC	O3-C3	2.39	1.48	1.43
2	8-A	707	BGC	O3-C3	2.41	1.48	1.43
2	25-A	707	BGC	O3-C3	2.41	1.48	1.43
2	20-A	705	BGC	O3-C3	2.41	1.48	1.43
2	15-A	707	BGC	O3-C3	2.41	1.48	1.43
2	19-A	708	BGC	O5-C5	2.42	1.50	1.44
2	1-A	708	BGC	O5-C5	2.43	1.50	1.44
2	2-A	705	BGC	O3-C3	2.43	1.48	1.43
2	4-A	707	BGC	O3-C3	2.43	1.48	1.43
2	15-A	701	BGC	C2-C3	2.44	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	24-A	708	BGC	O5-C5	2.44	1.50	1.44
2	21-A	705	BGC	O2-C2	2.44	1.48	1.43
2	6-A	707	BGC	O3-C3	2.45	1.48	1.43
2	3-A	707	BGC	O3-C3	2.45	1.48	1.43
2	22-A	707	BGC	O3-C3	2.45	1.48	1.43
2	14-A	708	BGC	O5-C5	2.47	1.50	1.44
2	6-A	708	BGC	O5-C5	2.48	1.50	1.44
2	19-A	707	BGC	O3-C3	2.48	1.48	1.43
2	21-A	708	BGC	O3-C3	2.48	1.48	1.43
2	2-A	707	BGC	O3-C3	2.50	1.49	1.43
2	13-A	707	BGC	O3-C3	2.51	1.49	1.43
2	15-A	708	BGC	O5-C5	2.52	1.50	1.44
2	9-A	707	BGC	O3-C3	2.54	1.49	1.43
2	17-A	705	BGC	O3-C3	2.54	1.49	1.43
2	8-A	706	BGC	C4-C5	2.55	1.58	1.53
2	14-A	705	BGC	O3-C3	2.56	1.49	1.43
2	16-A	706	BGC	C4-C5	2.56	1.58	1.53
2	23-A	708	BGC	C4-C5	2.57	1.58	1.53
2	13-A	708	BGC	O3-C3	2.59	1.49	1.43
2	21-A	706	BGC	C4-C5	2.60	1.58	1.53
2	22-A	708	BGC	O5-C5	2.61	1.50	1.44
2	17-A	708	BGC	O3-C3	2.62	1.49	1.43
2	10-A	707	BGC	O3-C3	2.62	1.49	1.43
2	7-A	707	BGC	O3-C3	2.63	1.49	1.43
2	16-A	708	BGC	O5-C5	2.64	1.51	1.44
2	11-A	708	BGC	O5-C5	2.65	1.51	1.44
2	2-A	708	BGC	O5-C5	2.65	1.51	1.44
2	9-A	705	BGC	O3-C3	2.65	1.49	1.43
2	12-A	707	BGC	O3-C3	2.67	1.49	1.43
2	23-A	705	BGC	O3-C3	2.67	1.49	1.43
2	13-A	705	BGC	O3-C3	2.68	1.49	1.43
2	16-A	708	BGC	O3-C3	2.68	1.49	1.43
2	7-A	705	BGC	O2-C2	2.68	1.49	1.43
2	2-A	708	BGC	O3-C3	2.69	1.49	1.43
2	25-A	708	BGC	O3-C3	2.69	1.49	1.43
2	18-A	708	BGC	O5-C5	2.69	1.51	1.44
2	11-A	705	BGC	O3-C3	2.69	1.49	1.43
2	19-A	706	BGC	C4-C5	2.73	1.58	1.53
2	15-A	706	BGC	O3-C3	2.73	1.49	1.43
2	6-A	706	BGC	O3-C3	2.74	1.49	1.43
2	17-A	706	BGC	C4-C5	2.74	1.58	1.53
2	19-A	705	BGC	O3-C3	2.74	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3-A	708	BGC	O5-C5	2.74	1.51	1.44
2	4-A	705	BGC	O3-C3	2.76	1.49	1.43
2	22-A	705	BGC	O3-C3	2.76	1.49	1.43
2	3-A	705	BGC	O3-C3	2.76	1.49	1.43
2	7-A	708	BGC	O3-C3	2.76	1.49	1.43
2	20-A	706	BGC	C4-C5	2.77	1.59	1.53
2	5-A	707	BGC	O3-C3	2.77	1.49	1.43
2	15-A	705	BGC	O3-C3	2.77	1.49	1.43
2	11-A	707	BGC	O3-C3	2.78	1.49	1.43
2	24-A	708	BGC	O3-C3	2.79	1.49	1.43
2	3-A	706	BGC	O3-C3	2.79	1.49	1.43
2	18-A	706	BGC	O3-C3	2.79	1.49	1.43
2	14-A	707	BGC	O3-C3	2.80	1.49	1.43
2	4-A	708	BGC	O5-C5	2.82	1.51	1.44
2	10-A	705	BGC	O3-C3	2.83	1.49	1.43
2	20-A	707	BGC	O3-C3	2.83	1.49	1.43
2	17-A	707	BGC	O3-C3	2.85	1.49	1.43
2	1-A	707	BGC	O3-C3	2.85	1.49	1.43
2	23-A	708	BGC	O5-C5	2.87	1.51	1.44
2	24-A	706	BGC	O3-C3	2.87	1.49	1.43
2	5-A	708	BGC	O3-C3	2.87	1.49	1.43
2	8-A	706	BGC	O3-C3	2.88	1.49	1.43
2	8-A	708	BGC	O3-C3	2.89	1.49	1.43
2	5-A	708	BGC	O5-C5	2.90	1.51	1.44
2	4-A	708	BGC	O3-C3	2.90	1.49	1.43
2	14-A	708	BGC	O3-C3	2.91	1.49	1.43
2	21-A	705	BGC	O3-C3	2.91	1.49	1.43
2	10-A	708	BGC	O3-C3	2.92	1.49	1.43
2	5-A	705	BGC	O3-C3	2.93	1.50	1.43
2	8-A	705	BGC	O3-C3	2.93	1.50	1.43
2	13-A	708	BGC	O5-C5	2.93	1.51	1.44
2	24-A	705	BGC	O3-C3	2.94	1.50	1.43
2	6-A	705	BGC	O3-C3	2.94	1.50	1.43
2	18-A	707	BGC	O3-C3	2.95	1.50	1.43
2	12-A	708	BGC	O3-C3	2.98	1.50	1.43
2	22-A	708	BGC	O3-C3	2.99	1.50	1.43
2	22-A	706	BGC	O3-C3	3.04	1.50	1.43
2	25-A	706	BGC	O3-C3	3.04	1.50	1.43
2	18-A	705	BGC	O3-C3	3.05	1.50	1.43
2	11-A	706	BGC	O5-C5	3.05	1.50	1.43
2	11-A	708	BGC	O3-C3	3.06	1.50	1.43
2	7-A	708	BGC	O5-C5	3.07	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	9-A	708	BGC	O3-C3	3.08	1.50	1.43
2	4-A	706	BGC	O3-C3	3.09	1.50	1.43
2	23-A	706	BGC	O5-C5	3.13	1.50	1.43
2	8-A	708	BGC	O5-C5	3.13	1.52	1.44
2	3-A	708	BGC	O3-C3	3.15	1.50	1.43
2	21-A	706	BGC	O3-C3	3.15	1.50	1.43
2	25-A	708	BGC	O5-C5	3.19	1.52	1.44
2	15-A	708	BGC	O3-C3	3.22	1.50	1.43
2	12-A	708	BGC	O5-C5	3.22	1.52	1.44
2	10-A	706	BGC	O3-C3	3.23	1.50	1.43
2	9-A	708	BGC	O5-C5	3.24	1.52	1.44
2	23-A	708	BGC	O3-C3	3.25	1.50	1.43
2	18-A	708	BGC	O3-C3	3.25	1.50	1.43
2	1-A	706	BGC	O3-C3	3.25	1.50	1.43
2	13-A	707	BGC	O5-C5	3.26	1.50	1.43
2	6-A	706	BGC	O5-C5	3.27	1.50	1.43
2	20-A	708	BGC	O5-C5	3.28	1.52	1.44
2	8-A	706	BGC	O5-C5	3.29	1.50	1.43
2	17-A	708	BGC	O5-C5	3.29	1.52	1.44
2	6-A	708	BGC	O3-C3	3.29	1.50	1.43
2	11-A	706	BGC	O3-C3	3.30	1.50	1.43
2	1-A	707	BGC	O5-C5	3.30	1.50	1.43
2	4-A	706	BGC	O5-C5	3.30	1.50	1.43
2	14-A	706	BGC	O3-C3	3.30	1.50	1.43
2	18-A	706	BGC	O5-C5	3.30	1.50	1.43
2	23-A	706	BGC	C4-C5	3.32	1.60	1.53
2	13-A	706	BGC	O5-C5	3.33	1.50	1.43
2	5-A	706	BGC	O3-C3	3.33	1.50	1.43
2	17-A	706	BGC	O5-C5	3.35	1.50	1.43
2	2-A	706	BGC	O3-C3	3.35	1.51	1.43
2	19-A	708	BGC	O3-C3	3.36	1.51	1.43
2	9-A	706	BGC	O3-C3	3.37	1.51	1.43
2	22-A	706	BGC	O5-C5	3.38	1.50	1.43
2	17-A	706	BGC	O3-C3	3.38	1.51	1.43
2	16-A	706	BGC	O5-C5	3.39	1.50	1.43
2	12-A	706	BGC	O3-C3	3.40	1.51	1.43
2	19-A	706	BGC	O3-C3	3.41	1.51	1.43
2	13-A	706	BGC	O3-C3	3.42	1.51	1.43
2	7-A	707	BGC	O5-C5	3.43	1.51	1.43
2	3-A	706	BGC	O5-C5	3.45	1.51	1.43
2	7-A	706	BGC	O5-C5	3.45	1.51	1.43
2	20-A	706	BGC	O3-C3	3.46	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	15-A	706	BGC	O5-C5	3.46	1.51	1.43
2	16-A	707	BGC	O5-C5	3.48	1.51	1.43
2	14-A	707	BGC	O5-C5	3.48	1.51	1.43
2	12-A	706	BGC	O5-C5	3.48	1.51	1.43
2	25-A	706	BGC	O5-C5	3.50	1.51	1.43
2	2-A	706	BGC	O5-C5	3.51	1.51	1.43
2	10-A	706	BGC	O5-C5	3.51	1.51	1.43
2	9-A	706	BGC	O5-C5	3.52	1.51	1.43
2	2-A	707	BGC	O5-C5	3.55	1.51	1.43
2	21-A	706	BGC	O5-C5	3.57	1.51	1.43
2	23-A	707	BGC	O5-C5	3.57	1.51	1.43
2	10-A	707	BGC	O5-C5	3.58	1.51	1.43
2	7-A	706	BGC	O3-C3	3.58	1.51	1.43
2	15-A	705	BGC	O5-C5	3.59	1.51	1.43
2	12-A	707	BGC	O5-C5	3.61	1.51	1.43
2	14-A	706	BGC	O5-C5	3.63	1.51	1.43
2	5-A	706	BGC	O5-C5	3.65	1.51	1.43
2	23-A	706	BGC	O3-C3	3.66	1.51	1.43
2	11-A	707	BGC	O5-C5	3.66	1.51	1.43
2	24-A	705	BGC	O5-C5	3.66	1.51	1.43
2	24-A	706	BGC	O5-C5	3.66	1.51	1.43
2	6-A	707	BGC	O5-C5	3.68	1.51	1.43
2	8-A	705	BGC	O5-C5	3.69	1.51	1.43
2	3-A	707	BGC	O5-C5	3.71	1.51	1.43
2	20-A	707	BGC	O5-C5	3.73	1.51	1.43
2	25-A	707	BGC	O5-C5	3.74	1.51	1.43
2	5-A	707	BGC	O5-C5	3.75	1.51	1.43
2	18-A	707	BGC	O5-C5	3.75	1.51	1.43
2	24-A	707	BGC	O5-C5	3.75	1.51	1.43
2	20-A	706	BGC	O5-C5	3.77	1.51	1.43
2	22-A	707	BGC	O5-C5	3.78	1.51	1.43
2	19-A	707	BGC	O5-C5	3.79	1.51	1.43
2	19-A	706	BGC	O5-C5	3.80	1.51	1.43
2	8-A	707	BGC	O5-C5	3.82	1.51	1.43
2	9-A	707	BGC	O5-C5	3.82	1.51	1.43
2	12-A	705	BGC	O5-C5	3.85	1.51	1.43
2	4-A	707	BGC	O5-C5	3.87	1.52	1.43
2	23-A	705	BGC	O5-C5	3.92	1.52	1.43
2	17-A	707	BGC	O5-C5	3.96	1.52	1.43
2	10-A	705	BGC	O5-C5	3.97	1.52	1.43
2	19-A	705	BGC	O5-C5	4.00	1.52	1.43
2	4-A	705	BGC	O5-C5	4.01	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-A	706	BGC	O5-C5	4.01	1.52	1.43
2	15-A	707	BGC	O5-C5	4.03	1.52	1.43
2	14-A	705	BGC	O5-C5	4.04	1.52	1.43
2	3-A	705	BGC	O5-C5	4.04	1.52	1.43
2	21-A	707	BGC	O5-C5	4.07	1.52	1.43
2	16-A	706	BGC	O3-C3	4.09	1.52	1.43
2	7-A	705	BGC	O5-C5	4.10	1.52	1.43
2	2-A	705	BGC	O5-C5	4.11	1.52	1.43
2	18-A	705	BGC	O5-C5	4.11	1.52	1.43
2	5-A	705	BGC	O5-C5	4.11	1.52	1.43
2	17-A	705	BGC	O5-C5	4.14	1.52	1.43
2	25-A	705	BGC	O5-C5	4.16	1.52	1.43
2	13-A	705	BGC	O5-C5	4.16	1.52	1.43
2	16-A	705	BGC	O5-C5	4.26	1.52	1.43
2	11-A	705	BGC	O5-C5	4.27	1.52	1.43
2	9-A	705	BGC	O5-C5	4.29	1.52	1.43
2	1-A	708	BGC	O3-C3	4.31	1.53	1.43
2	21-A	705	BGC	O5-C5	4.33	1.53	1.43
2	20-A	705	BGC	O5-C5	4.37	1.53	1.43
2	22-A	705	BGC	O5-C5	4.47	1.53	1.43
2	1-A	705	BGC	O5-C5	4.53	1.53	1.43
2	6-A	705	BGC	O5-C5	4.57	1.53	1.43

All (419) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1-A	708	BGC	O4-C4-C5	-7.24	90.05	109.24
2	3-A	701	BGC	C3-C4-C5	-6.24	99.32	110.20
2	2-A	701	BGC	C1-O5-C5	-5.82	104.86	112.25
2	23-A	707	BGC	O3-C3-C2	-4.89	101.16	110.00
2	15-A	701	BGC	C6-C5-C4	-4.81	101.15	113.02
2	24-A	701	BGC	O2-C2-C3	-4.55	100.96	110.12
2	19-A	708	BGC	O5-C5-C4	-4.51	101.22	109.68
2	2-A	707	BGC	O3-C3-C2	-4.31	102.21	110.00
2	16-A	708	BGC	O5-C5-C4	-4.25	101.71	109.68
2	22-A	707	BGC	O3-C3-C2	-4.24	102.34	110.00
2	23-A	708	BGC	O2-C2-C1	-4.17	100.64	109.82
2	5-A	701	BGC	C1-O5-C5	-4.03	107.14	112.25
2	24-A	708	BGC	O5-C5-C4	-4.02	102.13	109.68
2	23-A	706	BGC	C1-O5-C5	-3.96	107.22	112.25
2	8-A	707	BGC	O3-C3-C2	-3.91	102.93	110.00
2	20-A	701	BGC	O5-C1-C2	-3.85	104.61	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	9-A	707	BGC	O3-C3-C2	-3.70	103.31	110.00
2	11-A	701	BGC	O5-C1-C2	-3.66	104.92	110.86
2	8-A	701	BGC	O3-C3-C4	-3.63	102.17	110.34
2	1-A	708	BGC	O2-C2-C3	-3.59	102.26	110.34
2	11-A	701	BGC	C1-C2-C3	-3.52	105.38	109.54
2	24-A	707	BGC	O3-C3-C2	-3.48	103.71	110.00
2	11-A	701	BGC	C1-O5-C5	-3.45	107.87	112.25
2	6-A	706	BGC	O3-C3-C4	-3.41	102.66	110.34
2	18-A	706	BGC	O3-C3-C4	-3.39	102.70	110.34
2	2-A	701	BGC	C3-C4-C5	-3.34	104.37	110.20
2	25-A	701	BGC	C1-C2-C3	-3.30	105.64	109.54
2	8-A	701	BGC	O5-C1-C2	-3.27	105.55	110.86
2	16-A	701	BGC	O3-C3-C2	-3.27	104.10	110.00
2	14-A	701	BGC	C3-C4-C5	-3.26	104.51	110.20
2	9-A	705	BGC	O3-C3-C4	-3.26	103.00	110.34
2	21-A	707	BGC	C1-O5-C5	-3.24	108.14	112.25
2	5-A	707	BGC	O3-C3-C2	-3.21	104.19	110.00
2	2-A	701	BGC	O4-C4-C3	-3.17	103.20	110.34
2	5-A	708	BGC	C1-O5-C5	-3.17	107.61	113.47
2	9-A	705	BGC	C6-C5-C4	-3.15	105.25	113.02
2	22-A	701	BGC	O4-C4-C3	-3.10	103.35	110.34
2	12-A	706	BGC	O3-C3-C2	-3.05	104.50	110.00
2	11-A	701	BGC	O2-C2-C1	-3.02	103.15	109.21
2	18-A	705	BGC	O2-C2-C1	-3.02	103.16	109.21
2	17-A	701	BGC	C6-C5-C4	-3.01	105.60	113.02
2	15-A	708	BGC	O5-C5-C4	-2.99	104.06	109.68
2	20-A	705	BGC	O3-C3-C4	-2.97	103.66	110.34
2	19-A	706	BGC	C1-O5-C5	-2.94	108.51	112.25
2	10-A	706	BGC	O3-C3-C2	-2.92	104.72	110.00
2	5-A	708	BGC	O2-C2-C1	-2.91	103.40	109.82
2	4-A	707	BGC	O3-C3-C2	-2.88	104.80	110.00
2	16-A	708	BGC	C1-O5-C5	-2.85	108.20	113.47
2	8-A	708	BGC	C6-C5-C4	-2.79	106.14	113.02
2	25-A	707	BGC	C1-O5-C5	-2.79	108.71	112.25
2	12-A	701	BGC	O2-C2-C3	-2.78	104.54	110.12
2	10-A	708	BGC	O2-C2-C1	-2.77	103.71	109.82
2	10-A	707	BGC	O3-C3-C2	-2.73	105.06	110.00
2	20-A	701	BGC	O6-C6-C5	-2.70	102.41	111.33
2	15-A	707	BGC	C1-O5-C5	-2.69	108.83	112.25
2	1-A	705	BGC	O3-C3-C4	-2.68	104.31	110.34
2	7-A	705	BGC	O3-C3-C4	-2.66	104.34	110.34
2	2-A	708	BGC	O2-C2-C1	-2.66	103.96	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	15-A	708	BGC	C1-O5-C5	-2.65	108.56	113.47
2	17-A	708	BGC	O5-C1-C2	-2.65	105.57	109.80
2	20-A	707	BGC	O3-C3-C2	-2.61	105.29	110.00
2	10-A	701	BGC	O3-C3-C2	-2.59	105.32	110.00
2	7-A	708	BGC	O2-C2-C1	-2.58	104.14	109.82
2	23-A	701	BGC	C6-C5-C4	-2.58	106.66	113.02
2	19-A	708	BGC	C1-O5-C5	-2.57	108.72	113.47
2	19-A	706	BGC	O2-C2-C1	-2.57	104.06	109.21
2	12-A	705	BGC	O3-C3-C4	-2.56	104.57	110.34
2	20-A	701	BGC	C6-C5-C4	-2.56	106.71	113.02
2	12-A	701	BGC	C3-C4-C5	-2.52	105.80	110.20
2	2-A	701	BGC	O2-C2-C3	-2.51	105.08	110.12
2	5-A	707	BGC	C1-O5-C5	-2.50	109.08	112.25
2	17-A	707	BGC	O3-C3-C2	-2.49	105.49	110.00
2	13-A	707	BGC	O3-C3-C2	-2.49	105.50	110.00
2	1-A	706	BGC	O3-C3-C4	-2.48	104.75	110.34
2	22-A	701	BGC	C6-C5-C4	-2.47	106.92	113.02
2	6-A	707	BGC	O3-C3-C2	-2.45	105.57	110.00
2	25-A	706	BGC	O3-C3-C4	-2.45	104.83	110.34
2	22-A	701	BGC	O2-C2-C3	-2.42	105.25	110.12
2	3-A	705	BGC	O3-C3-C4	-2.42	104.89	110.34
2	7-A	706	BGC	O3-C3-C2	-2.41	105.64	110.00
2	13-A	701	BGC	C6-C5-C4	-2.41	107.08	113.02
2	18-A	708	BGC	C1-O5-C5	-2.38	109.08	113.47
2	10-A	701	BGC	C6-C5-C4	-2.37	107.17	113.02
2	9-A	701	BGC	C6-C5-C4	-2.37	107.17	113.02
2	3-A	707	BGC	O3-C3-C2	-2.36	105.73	110.00
2	19-A	707	BGC	O3-C3-C2	-2.36	105.73	110.00
2	4-A	708	BGC	C6-C5-C4	-2.35	107.22	113.02
2	11-A	706	BGC	O3-C3-C2	-2.34	105.77	110.00
2	1-A	708	BGC	O4-C4-C3	-2.33	105.08	110.34
2	16-A	706	BGC	O3-C3-C2	-2.33	105.78	110.00
2	3-A	701	BGC	O2-C2-C3	-2.33	105.44	110.12
2	17-A	708	BGC	C1-O5-C5	-2.32	109.18	113.47
2	19-A	708	BGC	O2-C2-C1	-2.30	104.74	109.82
2	25-A	708	BGC	O5-C1-C2	-2.29	106.15	109.80
2	15-A	706	BGC	O3-C3-C2	-2.29	105.87	110.00
2	24-A	701	BGC	C1-O5-C5	-2.26	109.39	112.25
2	2-A	706	BGC	O2-C2-C3	-2.25	105.59	110.12
2	25-A	701	BGC	O4-C4-C5	-2.24	103.30	109.24
2	2-A	705	BGC	O3-C3-C4	-2.24	105.29	110.34
2	14-A	707	BGC	O3-C3-C2	-2.24	105.96	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	17-A	708	BGC	O2-C2-C1	-2.23	104.92	109.82
2	1-A	701	BGC	C6-C5-C4	-2.22	107.53	113.02
2	13-A	708	BGC	C6-C5-C4	-2.20	107.59	113.02
2	7-A	708	BGC	C6-C5-C4	-2.20	107.59	113.02
2	25-A	707	BGC	O3-C3-C2	-2.20	106.03	110.00
2	1-A	706	BGC	C6-C5-C4	-2.19	107.60	113.02
2	15-A	707	BGC	O3-C3-C2	-2.19	106.04	110.00
2	12-A	701	BGC	O5-C1-C2	-2.18	107.32	110.86
2	15-A	705	BGC	O2-C2-C1	-2.15	104.90	109.21
2	8-A	701	BGC	C6-C5-C4	-2.14	107.74	113.02
2	11-A	707	BGC	O3-C3-C2	-2.14	106.14	110.00
2	21-A	707	BGC	C3-C4-C5	-2.12	106.50	110.20
2	21-A	708	BGC	O5-C5-C4	-2.12	105.71	109.68
2	21-A	707	BGC	O3-C3-C2	-2.11	106.19	110.00
2	1-A	701	BGC	C2-C3-C4	-2.08	107.50	111.04
2	22-A	706	BGC	C1-O5-C5	-2.04	109.66	112.25
2	25-A	708	BGC	C6-C5-C4	-2.03	108.02	113.02
2	5-A	707	BGC	C3-C4-C5	-2.02	106.67	110.20
2	15-A	707	BGC	C3-C4-C5	-2.01	106.69	110.20
2	15-A	701	BGC	O3-C3-C4	-2.01	105.82	110.34
2	8-A	708	BGC	O4-C4-C3	2.01	114.86	110.34
2	14-A	707	BGC	C6-C5-C4	2.01	117.97	113.02
2	22-A	705	BGC	C3-C4-C5	2.01	113.70	110.20
2	1-A	705	BGC	O5-C1-C2	2.03	114.14	110.86
2	22-A	705	BGC	O2-C2-C3	2.03	114.20	110.12
2	7-A	705	BGC	C3-C4-C5	2.04	113.75	110.20
2	19-A	701	BGC	O5-C5-C6	2.04	111.77	107.35
2	25-A	708	BGC	O4-C4-C3	2.04	114.94	110.34
2	15-A	706	BGC	O4-C4-C3	2.05	114.95	110.34
2	18-A	705	BGC	O5-C1-C2	2.05	114.19	110.86
2	5-A	708	BGC	C1-C2-C3	2.05	113.48	110.43
2	18-A	708	BGC	C1-C2-C3	2.06	113.49	110.43
2	6-A	701	BGC	O5-C1-C2	2.06	114.20	110.86
2	24-A	705	BGC	O6-C6-C5	2.06	118.14	111.33
2	3-A	705	BGC	O5-C5-C6	2.06	111.81	107.35
2	19-A	708	BGC	O4-C4-C3	2.06	114.98	110.34
2	2-A	708	BGC	C4-C3-C2	2.06	114.64	110.79
2	2-A	706	BGC	O5-C5-C6	2.07	111.82	107.35
2	6-A	705	BGC	O5-C1-C2	2.07	114.21	110.86
2	14-A	705	BGC	O2-C2-C3	2.08	114.30	110.12
2	14-A	705	BGC	C6-C5-C4	2.08	118.14	113.02
2	14-A	708	BGC	C3-C4-C5	2.08	113.83	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	16-A	707	BGC	O6-C6-C5	2.09	118.22	111.33
2	3-A	701	BGC	O4-C4-C5	2.09	114.78	109.24
2	23-A	708	BGC	O1-C1-C2	2.09	114.82	109.21
2	13-A	701	BGC	C2-C3-C4	2.10	114.60	111.04
2	10-A	701	BGC	O3-C3-C4	2.10	115.06	110.34
2	1-A	708	BGC	O1-C1-C2	2.10	114.84	109.21
2	8-A	708	BGC	O6-C6-C5	2.11	118.30	111.33
2	15-A	708	BGC	O1-C1-C2	2.11	114.86	109.21
2	15-A	705	BGC	C6-C5-C4	2.11	118.23	113.02
2	14-A	701	BGC	O4-C4-C3	2.12	115.10	110.34
2	20-A	701	BGC	O5-C5-C6	2.13	111.97	107.35
2	23-A	708	BGC	O6-C6-C5	2.15	118.43	111.33
2	19-A	707	BGC	O6-C6-C5	2.15	118.45	111.33
2	5-A	706	BGC	O5-C5-C6	2.16	112.02	107.35
2	5-A	707	BGC	O3-C3-C4	2.16	115.19	110.34
2	1-A	706	BGC	O4-C4-C3	2.17	115.22	110.34
2	19-A	701	BGC	O2-C2-C1	2.18	113.57	109.21
2	3-A	701	BGC	O3-C3-C2	2.18	113.94	110.00
2	3-A	705	BGC	O2-C2-C3	2.18	114.51	110.12
2	10-A	707	BGC	C2-C3-C4	2.19	114.76	111.04
2	13-A	706	BGC	O6-C6-C5	2.19	118.56	111.33
2	9-A	708	BGC	C1-C2-C3	2.19	113.69	110.43
2	7-A	706	BGC	O6-C6-C5	2.19	118.58	111.33
2	16-A	708	BGC	C1-C2-C3	2.21	113.71	110.43
2	20-A	708	BGC	C1-C2-C3	2.21	113.71	110.43
2	17-A	705	BGC	C6-C5-C4	2.21	118.46	113.02
2	17-A	708	BGC	C3-C4-C5	2.21	114.06	110.20
2	18-A	701	BGC	C3-C4-C5	2.22	114.06	110.20
2	20-A	705	BGC	O2-C2-C3	2.22	114.59	110.12
2	11-A	708	BGC	C1-C2-C3	2.23	113.75	110.43
2	5-A	701	BGC	C1-C2-C3	2.24	112.19	109.54
2	10-A	706	BGC	O4-C4-C3	2.25	115.39	110.34
2	10-A	705	BGC	O4-C4-C5	2.25	115.19	109.24
2	23-A	701	BGC	C1-C2-C3	2.26	112.21	109.54
2	15-A	705	BGC	C2-C3-C4	2.26	114.88	111.04
2	4-A	708	BGC	O4-C4-C3	2.26	115.43	110.34
2	24-A	701	BGC	C3-C4-C5	2.27	114.16	110.20
2	3-A	708	BGC	C3-C4-C5	2.28	114.17	110.20
2	22-A	701	BGC	C2-C3-C4	2.28	114.92	111.04
2	16-A	707	BGC	O2-C2-C3	2.31	114.76	110.12
2	25-A	707	BGC	O6-C6-C5	2.31	118.97	111.33
2	22-A	705	BGC	O4-C4-C3	2.33	115.58	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	23-A	708	BGC	O4-C4-C5	2.33	115.42	109.24
2	4-A	708	BGC	O6-C6-C5	2.34	119.05	111.33
2	4-A	705	BGC	O4-C4-C3	2.34	115.60	110.34
2	11-A	708	BGC	O1-C1-C2	2.34	115.48	109.21
2	19-A	705	BGC	O4-C4-C3	2.34	115.61	110.34
2	5-A	708	BGC	O1-C1-C2	2.35	115.51	109.21
2	24-A	708	BGC	C1-C2-C3	2.36	113.93	110.43
2	10-A	708	BGC	O4-C4-C3	2.37	115.67	110.34
2	20-A	707	BGC	O6-C6-C5	2.37	119.16	111.33
2	5-A	705	BGC	O2-C2-C3	2.39	114.93	110.12
2	5-A	705	BGC	O4-C4-C3	2.40	115.73	110.34
2	19-A	708	BGC	O1-C1-C2	2.40	115.65	109.21
2	19-A	706	BGC	O4-C4-C3	2.41	115.77	110.34
2	12-A	706	BGC	O4-C4-C3	2.43	115.80	110.34
2	5-A	701	BGC	O5-C5-C6	2.44	112.64	107.35
2	13-A	708	BGC	C3-C4-C5	2.45	114.46	110.20
2	11-A	701	BGC	O4-C4-C3	2.45	115.85	110.34
2	12-A	705	BGC	C1-O5-C5	2.47	115.38	112.25
2	20-A	701	BGC	C2-C3-C4	2.47	115.24	111.04
2	9-A	705	BGC	O4-C4-C3	2.47	115.90	110.34
2	2-A	705	BGC	O4-C4-C3	2.47	115.91	110.34
2	12-A	701	BGC	C2-C3-C4	2.48	115.25	111.04
2	7-A	701	BGC	C1-O5-C5	2.48	115.39	112.25
2	18-A	701	BGC	C1-C2-C3	2.48	112.47	109.54
2	23-A	707	BGC	C1-O5-C5	2.49	115.41	112.25
2	16-A	706	BGC	O4-C4-C3	2.50	115.96	110.34
2	21-A	707	BGC	O6-C6-C5	2.51	119.62	111.33
2	10-A	705	BGC	O2-C2-C3	2.51	115.17	110.12
2	6-A	708	BGC	C1-C2-C3	2.52	114.17	110.43
2	10-A	701	BGC	O4-C4-C3	2.52	116.01	110.34
2	23-A	705	BGC	O4-C4-C3	2.52	116.01	110.34
2	16-A	705	BGC	O6-C6-C5	2.57	119.81	111.33
2	1-A	708	BGC	O5-C5-C6	2.57	112.85	106.36
2	15-A	708	BGC	O6-C6-C5	2.57	119.83	111.33
2	11-A	706	BGC	O4-C4-C3	2.58	116.14	110.34
2	9-A	708	BGC	C4-C3-C2	2.58	115.61	110.79
2	21-A	707	BGC	O5-C5-C6	2.59	112.95	107.35
2	5-A	707	BGC	O5-C5-C6	2.59	112.95	107.35
2	7-A	708	BGC	C3-C4-C5	2.61	114.75	110.20
2	19-A	708	BGC	C1-C2-C3	2.61	114.31	110.43
2	3-A	705	BGC	O4-C4-C3	2.62	116.23	110.34
2	7-A	706	BGC	O4-C4-C3	2.63	116.27	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	10-A	708	BGC	C1-C2-C3	2.64	114.35	110.43
2	14-A	701	BGC	O2-C2-C3	2.64	115.43	110.12
2	15-A	708	BGC	C3-C4-C5	2.66	114.83	110.20
2	14-A	705	BGC	O4-C4-C3	2.66	116.33	110.34
2	25-A	705	BGC	O4-C4-C3	2.67	116.35	110.34
2	12-A	705	BGC	O4-C4-C3	2.68	116.37	110.34
2	22-A	701	BGC	O5-C5-C6	2.69	113.16	107.35
2	15-A	707	BGC	O6-C6-C5	2.70	120.25	111.33
2	10-A	707	BGC	C6-C5-C4	2.71	119.69	113.02
2	15-A	707	BGC	O5-C5-C6	2.71	113.22	107.35
2	8-A	701	BGC	C1-C2-C3	2.72	112.75	109.54
2	17-A	705	BGC	O4-C4-C3	2.74	116.51	110.34
2	23-A	701	BGC	C2-C3-C4	2.75	115.70	111.04
2	10-A	701	BGC	O5-C5-C6	2.76	113.32	107.35
2	6-A	705	BGC	O6-C6-C5	2.76	120.47	111.33
2	18-A	705	BGC	C2-C3-C4	2.77	115.74	111.04
2	13-A	706	BGC	O4-C4-C3	2.77	116.56	110.34
2	6-A	701	BGC	C1-C2-C3	2.80	112.85	109.54
2	14-A	706	BGC	O4-C4-C3	2.80	116.64	110.34
2	10-A	707	BGC	C1-O5-C5	2.81	115.81	112.25
2	7-A	705	BGC	O4-C4-C3	2.81	116.67	110.34
2	19-A	701	BGC	C1-O5-C5	2.83	115.84	112.25
2	18-A	701	BGC	C1-O5-C5	2.84	115.85	112.25
2	22-A	701	BGC	O4-C4-C5	2.84	116.78	109.24
2	21-A	701	BGC	C2-C3-C4	2.85	115.87	111.04
2	24-A	705	BGC	O4-C4-C3	2.86	116.77	110.34
2	23-A	708	BGC	C4-C3-C2	2.87	116.15	110.79
2	15-A	701	BGC	O5-C5-C6	2.88	113.58	107.35
2	16-A	701	BGC	O5-C5-C6	2.89	113.59	107.35
2	22-A	701	BGC	O5-C1-C2	2.89	115.54	110.86
2	16-A	701	BGC	O2-C2-C1	2.94	115.09	109.21
2	8-A	708	BGC	C3-C4-C5	2.96	115.35	110.20
2	1-A	705	BGC	C3-C4-C5	2.97	115.37	110.20
2	5-A	707	BGC	O6-C6-C5	2.98	121.17	111.33
2	6-A	705	BGC	O4-C4-C3	2.99	117.07	110.34
2	25-A	705	BGC	C1-O5-C5	3.01	116.07	112.25
2	14-A	701	BGC	O3-C3-C2	3.02	115.45	110.00
2	21-A	705	BGC	O4-C4-C3	3.03	117.16	110.34
2	9-A	705	BGC	O5-C5-C6	3.06	113.97	107.35
2	25-A	708	BGC	C3-C4-C5	3.06	115.54	110.20
2	2-A	701	BGC	O3-C3-C2	3.07	115.55	110.00
2	20-A	705	BGC	O4-C4-C3	3.08	117.28	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	12-A	701	BGC	O5-C5-C6	3.09	114.05	107.35
2	13-A	705	BGC	O4-C4-C3	3.13	117.38	110.34
2	16-A	701	BGC	C3-C4-C5	3.14	115.67	110.20
2	23-A	701	BGC	O5-C5-C6	3.14	114.14	107.35
2	23-A	705	BGC	C6-C5-C4	3.16	120.81	113.02
2	22-A	706	BGC	C1-C2-C3	3.17	113.29	109.54
2	7-A	701	BGC	C1-C2-C3	3.20	113.32	109.54
2	16-A	701	BGC	O2-C2-C3	3.24	116.63	110.12
2	7-A	701	BGC	O5-C5-C6	3.25	114.39	107.35
2	22-A	701	BGC	O3-C3-C2	3.28	115.93	110.00
2	13-A	705	BGC	C1-O5-C5	3.30	116.44	112.25
2	13-A	701	BGC	C3-C4-C5	3.32	115.98	110.20
2	23-A	705	BGC	C1-O5-C5	3.32	116.47	112.25
2	23-A	706	BGC	C6-C5-C4	3.35	121.29	113.02
2	16-A	705	BGC	C1-O5-C5	3.39	116.55	112.25
2	8-A	701	BGC	C2-C3-C4	3.44	116.88	111.04
2	4-A	708	BGC	C3-C4-C5	3.51	116.32	110.20
2	19-A	705	BGC	C3-C4-C5	3.55	116.39	110.20
2	19-A	701	BGC	C2-C3-C4	3.57	117.11	111.04
2	21-A	701	BGC	C1-O5-C5	3.60	116.81	112.25
2	18-A	705	BGC	C1-O5-C5	3.65	116.88	112.25
2	18-A	705	BGC	C1-C2-C3	3.66	113.87	109.54
2	14-A	701	BGC	O5-C1-C2	3.70	116.86	110.86
2	11-A	705	BGC	O4-C4-C3	3.74	118.75	110.34
2	16-A	707	BGC	C1-C2-C3	3.74	113.97	109.54
2	17-A	701	BGC	C1-C2-C3	3.77	114.00	109.54
2	2-A	701	BGC	C6-C5-C4	3.81	122.41	113.02
2	23-A	708	BGC	C1-C2-C3	3.81	116.10	110.43
2	25-A	701	BGC	C3-C4-C5	3.87	116.94	110.20
2	16-A	705	BGC	O4-C4-C3	3.96	119.26	110.34
2	4-A	705	BGC	C1-O5-C5	4.03	117.36	112.25
2	6-A	706	BGC	C1-C2-C3	4.05	114.34	109.54
2	8-A	706	BGC	C1-C2-C3	4.06	114.34	109.54
2	1-A	708	BGC	O3-C3-C4	4.09	119.54	110.34
2	18-A	705	BGC	O6-C6-C5	4.09	124.85	111.33
2	5-A	705	BGC	C6-C5-C4	4.10	123.14	113.02
2	7-A	706	BGC	C1-O5-C5	4.12	117.48	112.25
2	10-A	705	BGC	C6-C5-C4	4.12	123.18	113.02
2	4-A	706	BGC	C1-C2-C3	4.13	114.42	109.54
2	15-A	701	BGC	C1-C2-C3	4.16	114.46	109.54
2	19-A	701	BGC	C1-C2-C3	4.17	114.48	109.54
2	10-A	701	BGC	C1-O5-C5	4.18	117.55	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	7-A	705	BGC	C1-C2-C3	4.20	114.51	109.54
2	7-A	705	BGC	C1-O5-C5	4.25	117.65	112.25
2	2-A	701	BGC	O3-C3-C4	4.30	120.01	110.34
2	25-A	707	BGC	C1-C2-C3	4.33	114.67	109.54
2	10-A	701	BGC	C1-C2-C3	4.34	114.68	109.54
2	17-A	701	BGC	C2-C3-C4	4.37	118.46	111.04
2	9-A	701	BGC	C1-O5-C5	4.46	117.90	112.25
2	21-A	706	BGC	C1-C2-C3	4.46	114.81	109.54
2	24-A	705	BGC	C1-O5-C5	4.47	117.92	112.25
2	2-A	705	BGC	C1-O5-C5	4.49	117.95	112.25
2	24-A	706	BGC	C1-C2-C3	4.49	114.86	109.54
2	9-A	701	BGC	C1-C2-C3	4.50	114.86	109.54
2	8-A	705	BGC	C6-C5-C4	4.52	124.16	113.02
2	17-A	705	BGC	C1-O5-C5	4.54	118.00	112.25
2	11-A	701	BGC	O2-C2-C3	4.56	119.28	110.12
2	21-A	701	BGC	O5-C5-C6	4.57	117.24	107.35
2	13-A	707	BGC	C1-C2-C3	4.57	114.95	109.54
2	18-A	705	BGC	C6-C5-C4	4.58	124.31	113.02
2	21-A	707	BGC	C1-C2-C3	4.60	114.98	109.54
2	14-A	701	BGC	C1-C2-C3	4.65	115.04	109.54
2	13-A	701	BGC	C1-O5-C5	4.67	118.18	112.25
2	19-A	707	BGC	C1-C2-C3	4.68	115.08	109.54
2	3-A	701	BGC	O5-C5-C6	4.71	117.55	107.35
2	24-A	707	BGC	C1-C2-C3	4.77	115.18	109.54
2	7-A	707	BGC	C1-C2-C3	4.79	115.20	109.54
2	23-A	707	BGC	C1-C2-C3	4.82	115.24	109.54
2	12-A	701	BGC	C1-C2-C3	4.82	115.25	109.54
2	5-A	706	BGC	C1-C2-C3	4.86	115.28	109.54
2	21-A	701	BGC	C1-C2-C3	4.88	115.32	109.54
2	13-A	706	BGC	C1-C2-C3	4.91	115.35	109.54
2	10-A	705	BGC	C1-C2-C3	4.91	115.35	109.54
2	3-A	706	BGC	C1-C2-C3	4.98	115.43	109.54
2	20-A	707	BGC	C1-C2-C3	5.00	115.46	109.54
2	15-A	707	BGC	C1-C2-C3	5.01	115.46	109.54
2	25-A	701	BGC	C1-O5-C5	5.02	118.61	112.25
2	6-A	707	BGC	C1-C2-C3	5.02	115.48	109.54
2	2-A	706	BGC	C1-C2-C3	5.03	115.49	109.54
2	25-A	706	BGC	C1-C2-C3	5.08	115.55	109.54
2	17-A	707	BGC	C1-C2-C3	5.10	115.58	109.54
2	17-A	701	BGC	C1-O5-C5	5.11	118.73	112.25
2	10-A	706	BGC	C1-C2-C3	5.13	115.61	109.54
2	14-A	705	BGC	C1-C2-C3	5.15	115.63	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	9-A	706	BGC	C1-C2-C3	5.16	115.64	109.54
2	11-A	706	BGC	C1-C2-C3	5.17	115.66	109.54
2	11-A	707	BGC	C1-C2-C3	5.18	115.67	109.54
2	14-A	707	BGC	C1-C2-C3	5.18	115.67	109.54
2	11-A	705	BGC	C1-O5-C5	5.20	118.85	112.25
2	12-A	705	BGC	C1-C2-C3	5.25	115.75	109.54
2	18-A	706	BGC	C1-C2-C3	5.26	115.76	109.54
2	15-A	706	BGC	C1-C2-C3	5.30	115.81	109.54
2	19-A	706	BGC	C1-C2-C3	5.34	115.86	109.54
2	16-A	701	BGC	O5-C1-C2	5.34	119.53	110.86
2	21-A	705	BGC	C1-O5-C5	5.38	119.08	112.25
2	15-A	705	BGC	C1-C2-C3	5.39	115.92	109.54
2	16-A	705	BGC	C1-C2-C3	5.43	115.96	109.54
2	17-A	705	BGC	C1-C2-C3	5.44	115.98	109.54
2	1-A	705	BGC	C1-C2-C3	5.52	116.07	109.54
2	2-A	707	BGC	C1-C2-C3	5.56	116.12	109.54
2	1-A	706	BGC	C1-C2-C3	5.57	116.13	109.54
2	20-A	706	BGC	C1-C2-C3	5.57	116.14	109.54
2	22-A	705	BGC	C1-O5-C5	5.58	119.34	112.25
2	17-A	706	BGC	C1-C2-C3	5.59	116.16	109.54
2	14-A	705	BGC	C1-O5-C5	5.61	119.37	112.25
2	12-A	707	BGC	C1-C2-C3	5.64	116.22	109.54
2	23-A	706	BGC	C1-C2-C3	5.65	116.22	109.54
2	14-A	706	BGC	C1-C2-C3	5.69	116.27	109.54
2	12-A	706	BGC	C1-C2-C3	5.71	116.29	109.54
2	4-A	705	BGC	C1-C2-C3	5.71	116.30	109.54
2	25-A	705	BGC	C1-C2-C3	5.71	116.30	109.54
2	19-A	705	BGC	C1-C2-C3	5.74	116.33	109.54
2	3-A	707	BGC	C1-C2-C3	5.76	116.35	109.54
2	5-A	705	BGC	C1-C2-C3	5.77	116.37	109.54
2	3-A	701	BGC	C1-C2-C3	5.82	116.43	109.54
2	20-A	701	BGC	C1-C2-C3	5.83	116.44	109.54
2	8-A	705	BGC	C1-C2-C3	5.88	116.50	109.54
2	11-A	705	BGC	C1-C2-C3	5.91	116.53	109.54
2	1-A	707	BGC	C1-C2-C3	5.92	116.54	109.54
2	9-A	705	BGC	C1-C2-C3	6.01	116.66	109.54
2	15-A	705	BGC	C1-O5-C5	6.10	120.00	112.25
2	16-A	701	BGC	C1-O5-C5	6.13	120.02	112.25
2	8-A	705	BGC	C1-O5-C5	6.13	120.03	112.25
2	23-A	705	BGC	C1-C2-C3	6.15	116.81	109.54
2	13-A	705	BGC	C1-C2-C3	6.22	116.90	109.54
2	21-A	705	BGC	C1-C2-C3	6.26	116.95	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	3-A	705	BGC	C1-C2-C3	6.27	116.96	109.54
2	15-A	701	BGC	C1-O5-C5	6.29	120.24	112.25
2	10-A	707	BGC	C1-C2-C3	6.34	117.04	109.54
2	8-A	707	BGC	C1-C2-C3	6.35	117.06	109.54
2	5-A	707	BGC	C1-C2-C3	6.37	117.08	109.54
2	9-A	707	BGC	C1-C2-C3	6.45	117.17	109.54
2	16-A	706	BGC	C1-C2-C3	6.46	117.19	109.54
2	22-A	707	BGC	C1-C2-C3	6.48	117.21	109.54
2	4-A	707	BGC	C1-C2-C3	6.49	117.22	109.54
2	22-A	705	BGC	C1-C2-C3	6.59	117.33	109.54
2	2-A	705	BGC	C1-C2-C3	6.60	117.35	109.54
2	18-A	707	BGC	C1-C2-C3	6.65	117.41	109.54
2	24-A	705	BGC	C1-C2-C3	6.68	117.44	109.54
2	6-A	705	BGC	C1-O5-C5	6.70	120.76	112.25
2	7-A	706	BGC	C1-C2-C3	6.71	117.47	109.54
2	22-A	701	BGC	C1-C2-C3	6.94	117.76	109.54
2	6-A	705	BGC	C1-C2-C3	7.11	117.95	109.54
2	20-A	705	BGC	C1-O5-C5	7.55	121.83	112.25
2	19-A	705	BGC	C1-O5-C5	7.73	122.05	112.25
2	20-A	705	BGC	C1-C2-C3	8.09	119.11	109.54
2	1-A	708	BGC	C3-C4-C5	8.27	124.61	110.20
2	2-A	701	BGC	C1-C2-C3	8.43	119.52	109.54
2	14-A	701	BGC	C1-O5-C5	8.56	123.11	112.25
2	1-A	705	BGC	C1-O5-C5	9.04	123.72	112.25
2	22-A	701	BGC	C1-O5-C5	9.57	124.39	112.25

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.