



# wwPDB X-ray Structure Validation Summary Report ⓘ

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

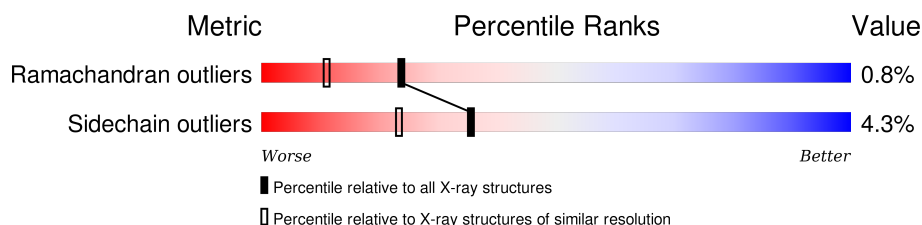
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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)





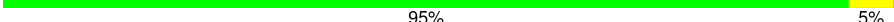


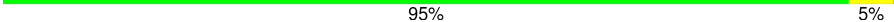
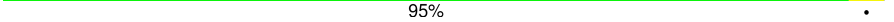

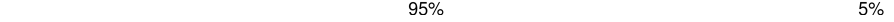
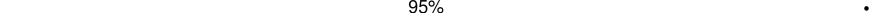


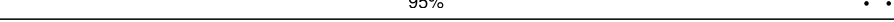
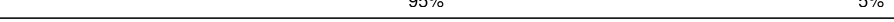
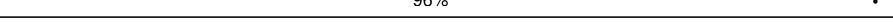
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS failed to run properly.

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

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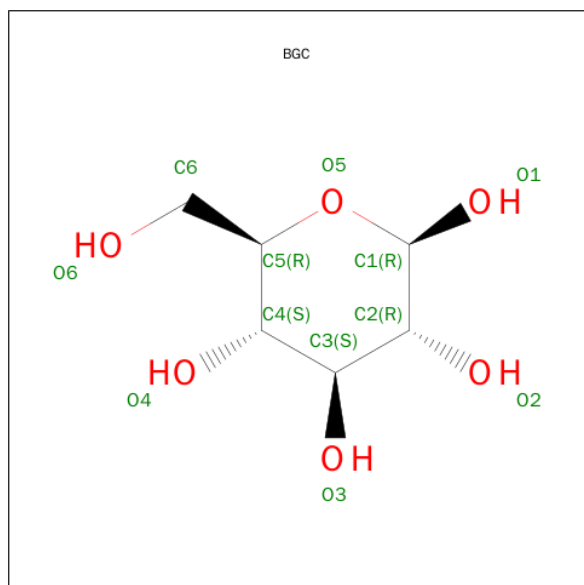
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	18-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	19-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	20-A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

There is a discrepancy between the modelled and reference sequences:

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

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



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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	11-A	1	Total	C	O	0	0
			11	6	5		
2	12-A	1	Total	C	O	0	0
			11	6	5		
2	13-A	1	Total	C	O	0	0
			11	6	5		
2	14-A	1	Total	C	O	0	0
			11	6	5		
2	15-A	1	Total	C	O	0	0
			11	6	5		
2	16-A	1	Total	C	O	0	0
			11	6	5		
2	17-A	1	Total	C	O	0	0
			11	6	5		
2	18-A	1	Total	C	O	0	0
			11	6	5		
2	19-A	1	Total	C	O	0	0
			11	6	5		
2	20-A	1	Total	C	O	0	0
			11	6	5		
2	21-A	1	Total	C	O	0	0
			11	6	5		
2	22-A	1	Total	C	O	0	0
			11	6	5		
2	23-A	1	Total	C	O	0	0
			11	6	5		
2	24-A	1	Total	C	O	0	0
			11	6	5		
2	25-A	1	Total	C	O	0	0
			11	6	5		
2	1-A	1	Total	C	O	0	0
			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<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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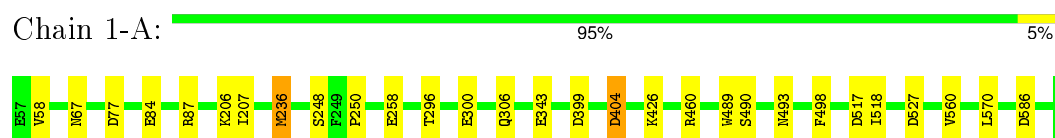
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	23-A	259	Total 259	O 259	0	0
4	24-A	250	Total 250	O 250	0	0
4	25-A	249	Total 249	O 249	0	0

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

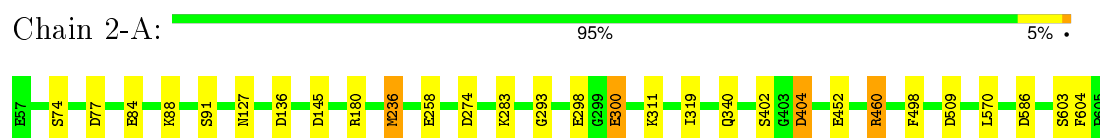
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

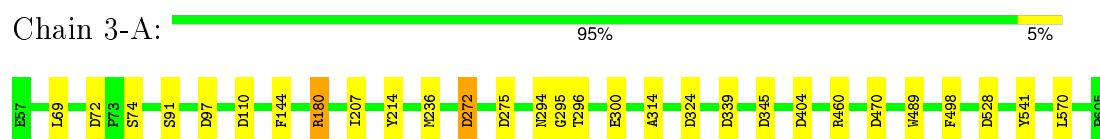
- Molecule 1: Putative secreted protein



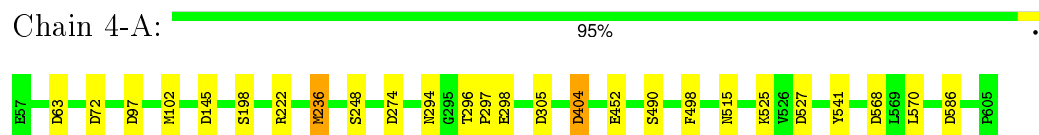
- Molecule 1: Putative secreted protein



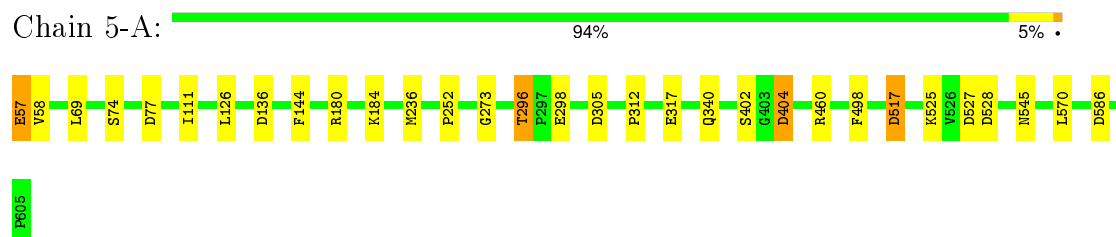
- Molecule 1: Putative secreted protein



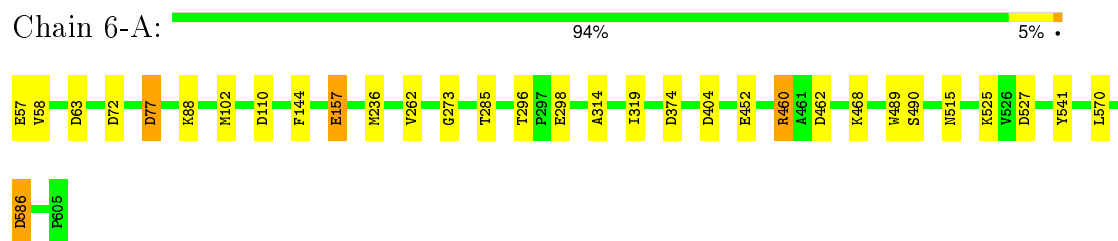
- Molecule 1: Putative secreted protein



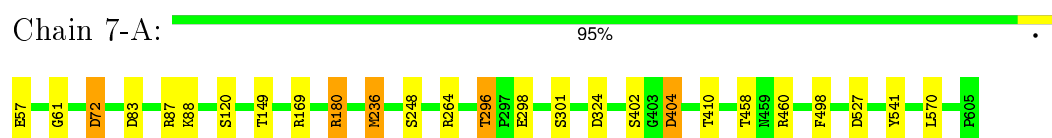
- Molecule 1: Putative secreted protein



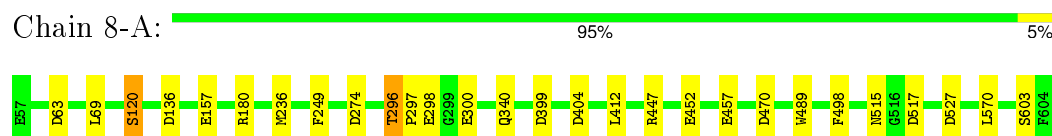
- Molecule 1: Putative secreted protein



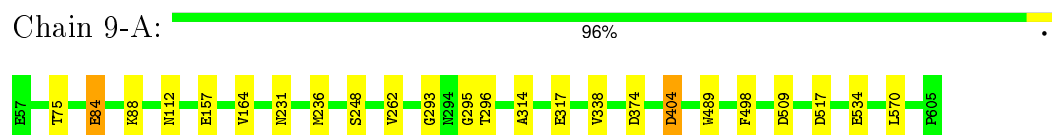
- Molecule 1: Putative secreted protein



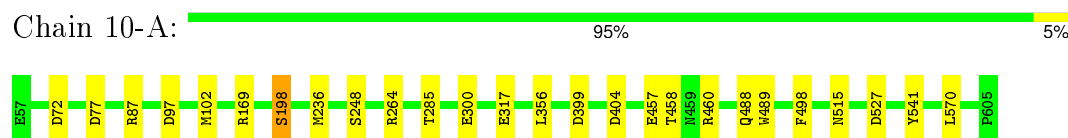
- Molecule 1: Putative secreted protein



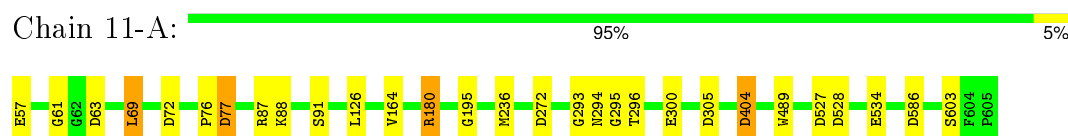
- Molecule 1: Putative secreted protein



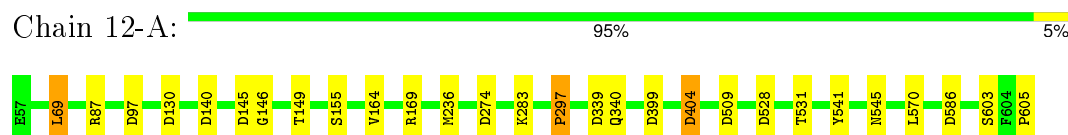
- Molecule 1: Putative secreted protein



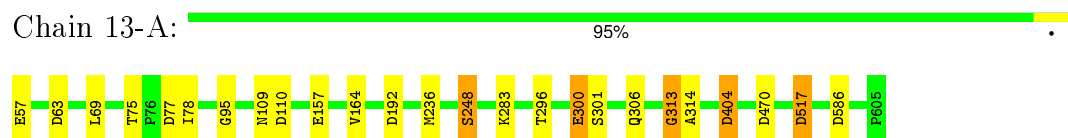
- Molecule 1: Putative secreted protein



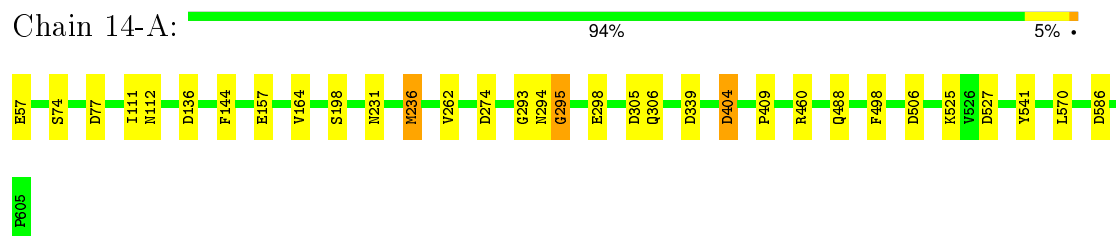
- Molecule 1: Putative secreted protein



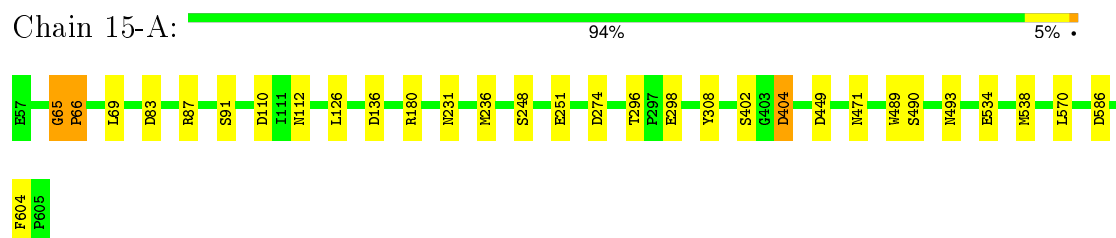
- Molecule 1: Putative secreted protein



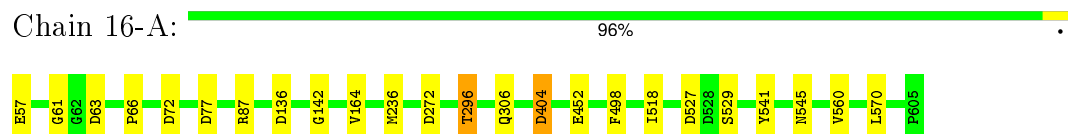
- Molecule 1: Putative secreted protein



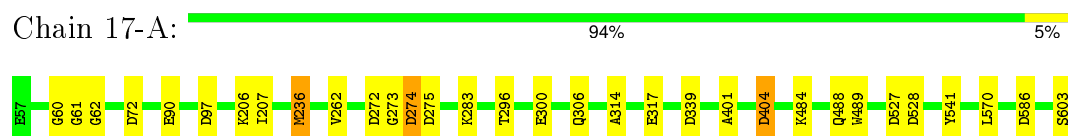
- Molecule 1: Putative secreted protein



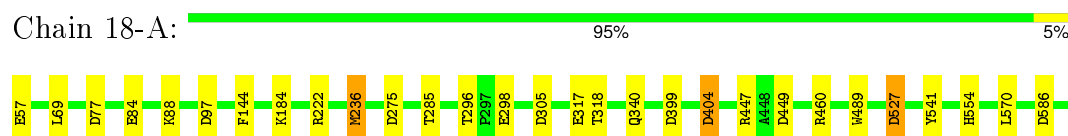
- Molecule 1: Putative secreted protein



- Molecule 1: Putative secreted protein



- Molecule 1: Putative secreted protein



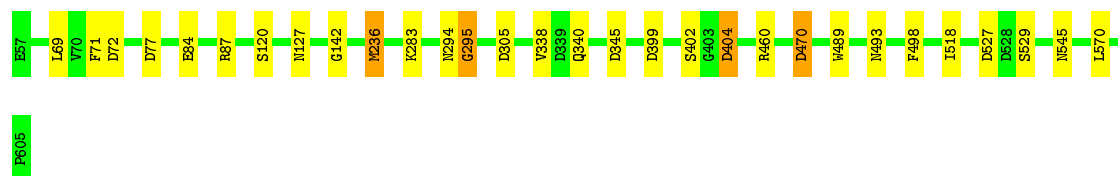
- Molecule 1: Putative secreted protein





- Molecule 1: Putative secreted protein

Chain 20-A: 95% 5% .



- Molecule 1: Putative secreted protein

Chain 21-A: 95% . .



- Molecule 1: Putative secreted protein

Chain 22-A: 96% .



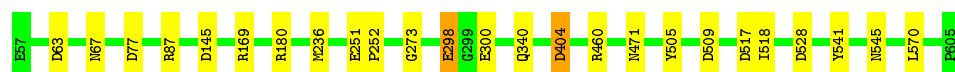
- Molecule 1: Putative secreted protein

Chain 23-A: 95% 5% .



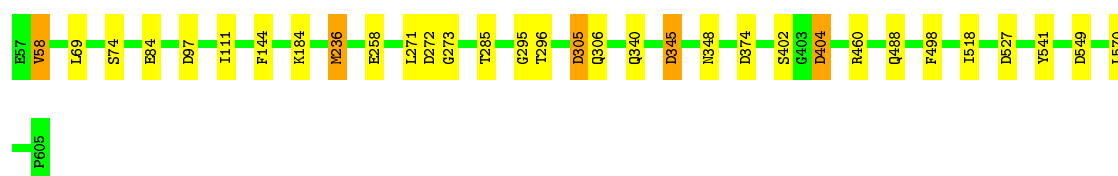
- Molecule 1: Putative secreted protein

Chain 24-A: 95% .



- Molecule 1: Putative secreted protein

Chain 25-A: 94% 5% .



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.154	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 39632 reflections	Xtriage
Total number of atoms	210296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

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

## 5 Model quality ⓘ

### 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

The worst 5 of 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

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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
1	19-A	293	GLY	Peptide
1	24-A	251	GLU	Peptide
1	3-A	295	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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



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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 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

### 5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	436/436 (100%)	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
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

5 of 470 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	12-A	149	THR
1	14-A	488	GLN
1	24-A	67	ASN
1	12-A	283	LYS
1	13-A	248	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	11-A	553	GLN
1	13-A	600	GLN
1	24-A	483	ASN
1	12-A	127	ASN
1	12-A	515	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 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

The worst 5 of 419 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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