



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:51 PM GMT

PDB ID : 4TZ1
Title : Ensemble refinement of the E502A variant of sacteLam55A from Streptomyces sp. SirexAA-E in complex with laminaritriose
Authors : Bianchetti, C.M.; Takasuka, T.E.; Yik, E.J.; Bergeman, L.F.; Fox, B.G.
Deposited on : 2014-07-09
Resolution : 1.50 Å(reported)

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

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

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

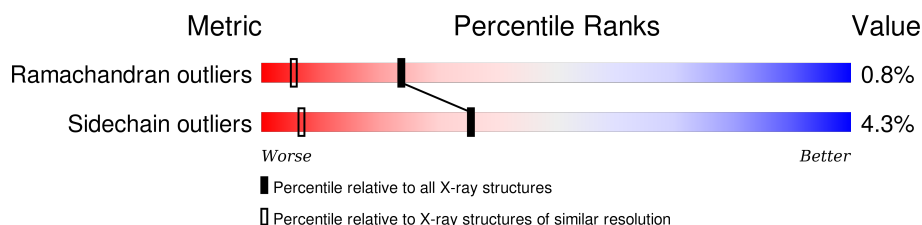
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)

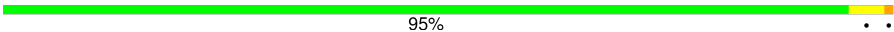
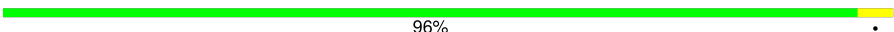
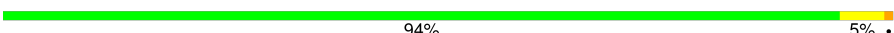









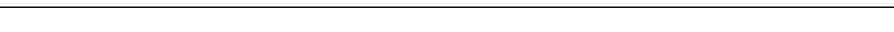

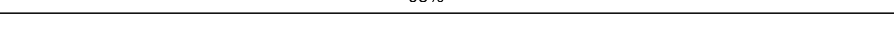
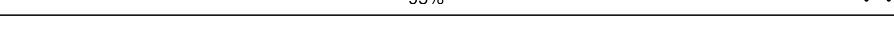
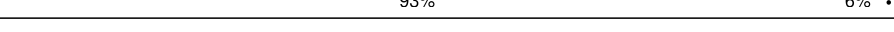
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey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

Note EDS failed to run properly.

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

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 211855 atoms, of which 97675 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative secreted protein.

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

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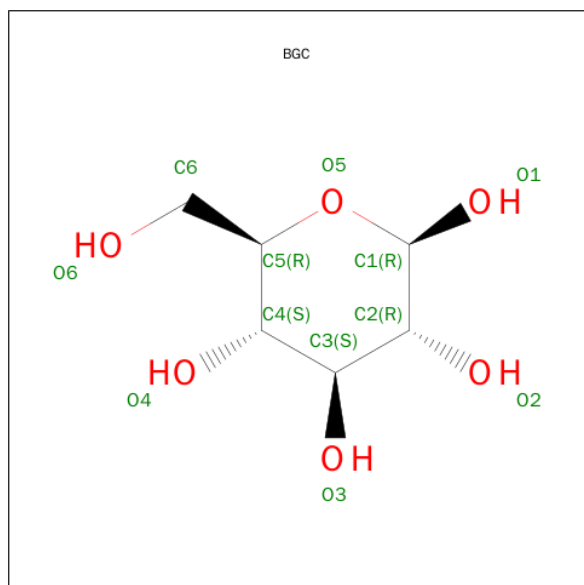
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	18-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	19-A	549	Total	C	H	N	O	S	0	0	0
			8074	2629	3907	708	825	5			
1	20-A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

There is a discrepancy between the modelled and reference sequences:

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

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



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

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

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

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

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

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

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

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

- Molecule 3 is water.

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

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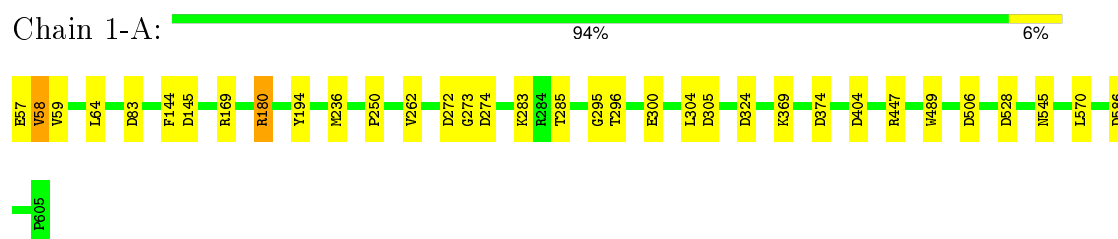
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	18-A	328	Total 328	O 328	0	0
3	19-A	320	Total 320	O 320	0	0
3	20-A	341	Total 341	O 341	0	0
3	21-A	321	Total 321	O 321	0	0
3	22-A	304	Total 304	O 304	0	0
3	23-A	341	Total 341	O 341	0	0
3	24-A	326	Total 326	O 326	0	0
3	25-A	336	Total 336	O 336	0	0

3 Residue-property plots

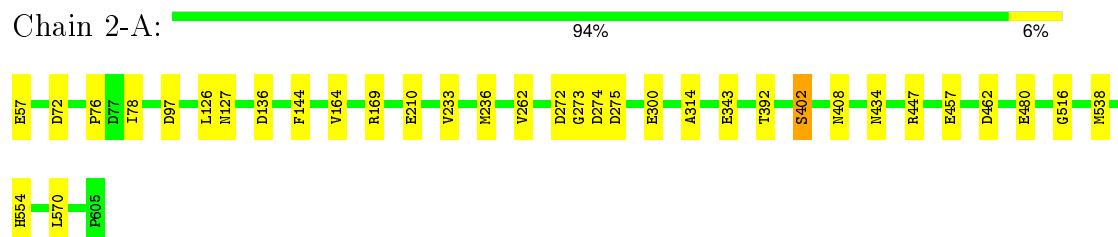
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS failed to run properly.

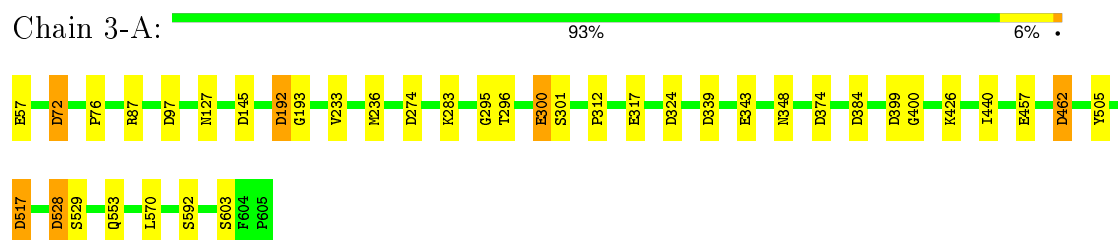
- Molecule 1: Putative secreted protein



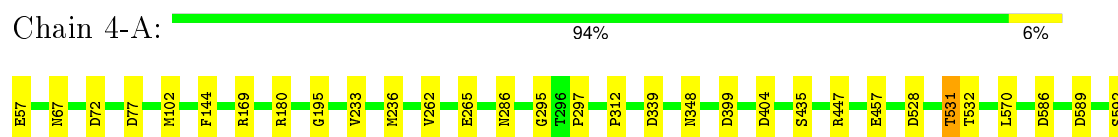
- Molecule 1: Putative secreted protein

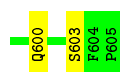


- Molecule 1: Putative secreted protein



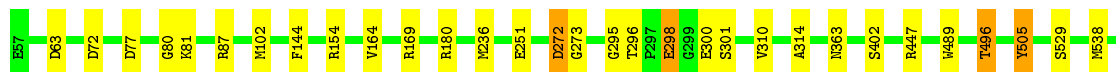
- Molecule 1: Putative secreted protein





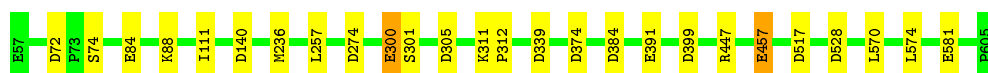
- Molecule 1: Putative secreted protein

Chain 5-A: 94% 5% •



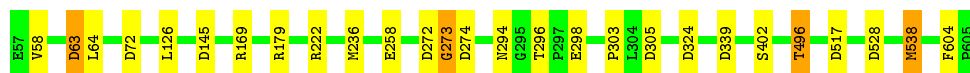
- Molecule 1: Putative secreted protein

Chain 6-A: 95% •



- Molecule 1: Putative secreted protein

Chain 7-A: 95% • •



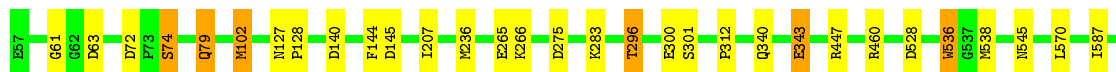
- Molecule 1: Putative secreted protein

Chain 8-A: 93% 6% •



- Molecule 1: Putative secreted protein

Chain 9-A: 94% 5% •



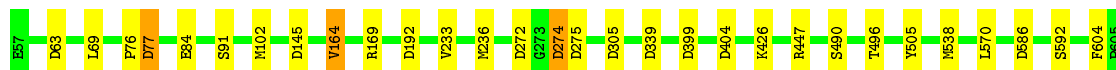
- Molecule 1: Putative secreted protein

Chain 10-A: 96% • •



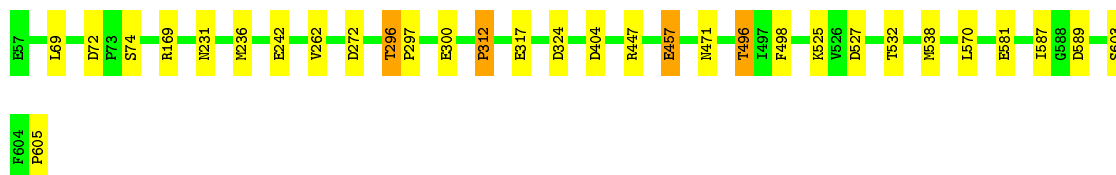
- Molecule 1: Putative secreted protein

Chain 11-A: 95% 5% .



- Molecule 1: Putative secreted protein

Chain 12-A: 94% 5% .



- Molecule 1: Putative secreted protein

Chain 13-A: 95% 5% .



- Molecule 1: Putative secreted protein

Chain 14-A: 95% 5% .



- Molecule 1: Putative secreted protein

Chain 15-A: 95% 5% .



- Molecule 1: Putative secreted protein

Chain 16-A: 94% 5% .



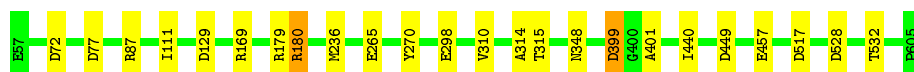
- Molecule 1: Putative secreted protein

Chain 17-A: 95% . .



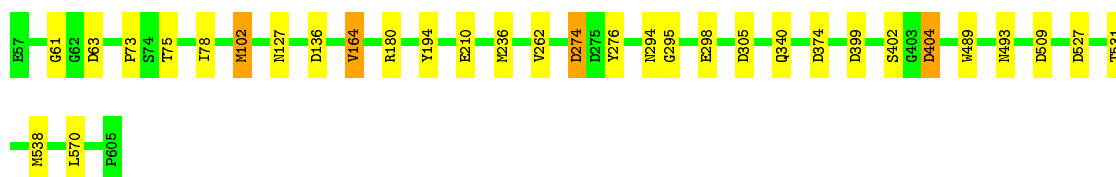
- Molecule 1: Putative secreted protein

Chain 18-A: 96%



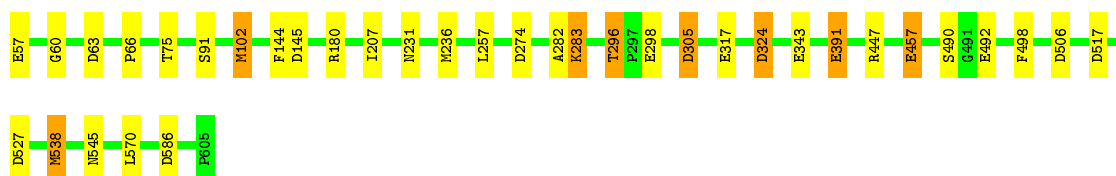
- Molecule 1: Putative secreted protein

Chain 19-A: 94% 5%



- Molecule 1: Putative secreted protein

Chain 20-A: 93% 5%



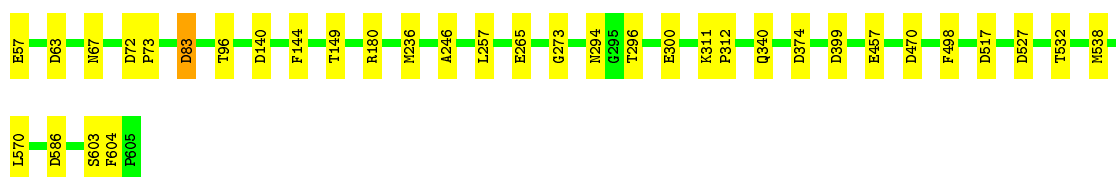
- Molecule 1: Putative secreted protein

Chain 21-A: 94% 5%



- Molecule 1: Putative secreted protein

Chain 22-A: 94% 6%



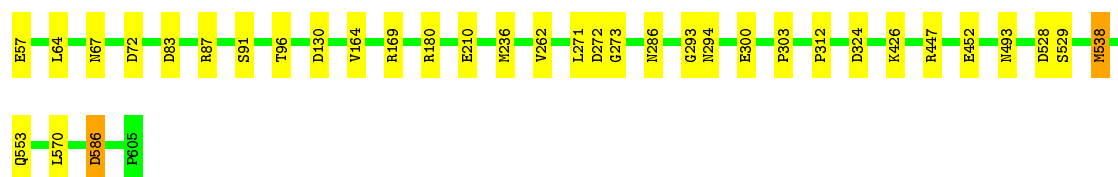
- Molecule 1: Putative secreted protein

Chain 23-A:  95% 5%



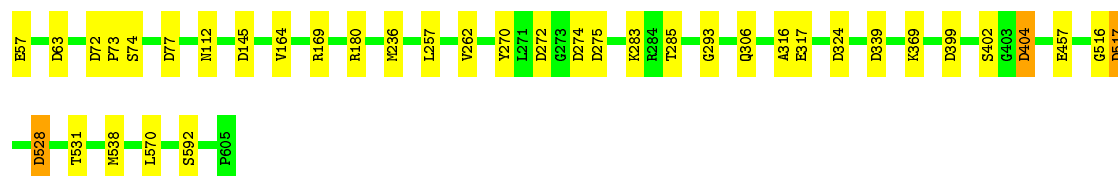
- Molecule 1: Putative secreted protein

Chain 24-A:  94% 6%



- Molecule 1: Putative secreted protein

Chain 25-A:  93% 6%



4 Data and refinement statistics

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

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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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

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

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

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

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

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	18-A	180	ARG	CB-CG	-10.28	1.24	1.52
1	20-A	538	MET	CB-CG	-10.08	1.19	1.51
1	3-A	462	ASP	CB-CG	-9.78	1.31	1.51
1	22-A	538	MET	CG-SD	9.54	2.06	1.81
1	1-A	300	GLU	CB-CG	9.27	1.69	1.52

The worst 5 of 257 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16-A	538	MET	CG-SD-CE	-20.07	68.09	100.20
1	10-A	538	MET	CG-SD-CE	-19.51	68.99	100.20
1	21-A	538	MET	CG-SD-CE	-19.04	69.73	100.20
1	22-A	538	MET	CG-SD-CE	-18.99	69.81	100.20
1	23-A	538	MET	CG-SD-CE	-18.91	69.94	100.20

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	57	GLU	Peptide
1	2-A	126	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	3-A	295	GLY	Peptide
1	4-A	295	GLY	Peptide
1	4-A	57	GLU	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	68	0	60	0	0
2	2-A	68	0	60	0	0
2	3-A	68	0	60	0	0
2	4-A	68	0	60	0	0
2	5-A	68	0	59	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	6-A	68	0	60	0	0
2	7-A	68	0	60	0	0
2	8-A	68	0	60	0	0
2	9-A	68	0	60	0	0
2	10-A	68	0	60	0	0
2	11-A	68	0	60	0	0
2	12-A	68	0	60	0	0
2	13-A	68	0	60	0	0
2	14-A	68	0	60	0	0
2	15-A	68	0	60	0	0
2	16-A	68	0	60	0	0
2	17-A	68	0	60	0	0
2	18-A	68	0	59	0	0
2	19-A	68	0	60	0	0
2	20-A	68	0	60	0	0
2	21-A	68	0	59	0	0
2	22-A	68	0	60	0	0
2	23-A	68	0	60	0	0
2	24-A	68	0	60	0	0
2	25-A	68	0	60	0	0
3	1-A	339	0	0	0	0
3	2-A	332	0	0	0	0
3	3-A	343	0	0	0	0
3	4-A	342	0	0	0	0
3	5-A	340	0	0	0	0
3	6-A	340	0	0	0	0
3	7-A	327	0	0	0	0
3	8-A	329	0	0	0	0
3	9-A	329	0	0	0	0
3	10-A	321	0	0	0	0
3	11-A	342	0	0	0	0
3	12-A	315	0	0	0	0
3	13-A	340	0	0	0	0
3	14-A	327	0	0	0	0
3	15-A	354	0	0	0	0
3	16-A	335	0	0	0	0
3	17-A	333	0	0	0	0
3	18-A	328	0	0	0	0
3	19-A	320	0	0	0	0
3	20-A	341	0	0	0	0
3	21-A	321	0	0	0	0
3	22-A	304	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	23-A	341	0	0	0	0
3	24-A	326	0	0	0	0
3	25-A	336	0	0	0	0
All	All	114180	97675	99472	0	0

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

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	547/549 (100%)	510 (93%)	31 (6%)	6 (1%)	17	3
1	2-A	547/549 (100%)	515 (94%)	28 (5%)	4 (1%)	26	6
1	3-A	547/549 (100%)	513 (94%)	27 (5%)	7 (1%)	15	2
1	4-A	547/549 (100%)	510 (93%)	31 (6%)	6 (1%)	17	3
1	5-A	547/549 (100%)	516 (94%)	26 (5%)	5 (1%)	21	4
1	6-A	547/549 (100%)	509 (93%)	37 (7%)	1 (0%)	52	25
1	7-A	547/549 (100%)	517 (94%)	28 (5%)	2 (0%)	39	14
1	8-A	547/549 (100%)	513 (94%)	31 (6%)	3 (0%)	34	10
1	9-A	547/549 (100%)	514 (94%)	28 (5%)	5 (1%)	21	4
1	10-A	547/549 (100%)	512 (94%)	30 (6%)	5 (1%)	21	4
1	11-A	547/549 (100%)	512 (94%)	32 (6%)	3 (0%)	34	10
1	12-A	547/549 (100%)	517 (94%)	25 (5%)	5 (1%)	21	4
1	13-A	547/549 (100%)	513 (94%)	32 (6%)	2 (0%)	39	14
1	14-A	547/549 (100%)	509 (93%)	31 (6%)	7 (1%)	15	2

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

5 of 116 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	58	VAL
1	1-A	194	TYR
1	3-A	400	GLY
1	4-A	77	ASP
1	5-A	80	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	436/436 (100%)	418 (96%)	18 (4%)	37	7
1	2-A	436/436 (100%)	414 (95%)	22 (5%)	30	5
1	3-A	436/436 (100%)	409 (94%)	27 (6%)	23	2
1	4-A	436/436 (100%)	417 (96%)	19 (4%)	35	6
1	5-A	436/436 (100%)	417 (96%)	19 (4%)	35	6

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

5 of 468 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	12-A	72	ASP
1	15-A	57	GLU
1	24-A	96	THR
1	12-A	296	THR
1	13-A	300	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
1	11-A	514	GLN
1	14-A	231	ASN
1	23-A	493	ASN
1	13-A	114	GLN
1	14-A	600	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

150 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BGC	1-A	701	2	11,11,12	2.47	5 (45%)	14,15,17	1.30	1 (7%)
2	BGC	1-A	702	2	11,11,12	2.56	5 (45%)	14,15,17	1.61	2 (14%)
2	BGC	1-A	703	2	12,12,12	2.07	4 (33%)	17,17,17	1.25	2 (11%)
2	BGC	1-A	704	2	11,11,12	3.02	4 (36%)	14,15,17	1.16	1 (7%)
2	BGC	1-A	705	2	11,11,12	3.04	5 (45%)	14,15,17	2.22	3 (21%)
2	BGC	1-A	706	2	12,12,12	2.62	7 (58%)	17,17,17	2.31	6 (35%)
2	BGC	10-A	701	2	11,11,12	2.66	5 (45%)	14,15,17	1.27	2 (14%)
2	BGC	10-A	702	2	11,11,12	2.53	5 (45%)	14,15,17	1.57	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	10-A	703	2	12,12,12	2.08	4 (33%)	17,17,17	1.18	2 (11%)
2	BGC	10-A	704	2	11,11,12	2.97	5 (45%)	14,15,17	1.42	1 (7%)
2	BGC	10-A	705	2	11,11,12	3.07	6 (54%)	14,15,17	1.98	3 (21%)
2	BGC	10-A	706	2	12,12,12	2.40	5 (41%)	17,17,17	1.47	5 (29%)
2	BGC	11-A	701	2	11,11,12	2.54	5 (45%)	14,15,17	1.26	1 (7%)
2	BGC	11-A	702	2	11,11,12	2.52	4 (36%)	14,15,17	1.47	2 (14%)
2	BGC	11-A	703	2	12,12,12	2.04	5 (41%)	17,17,17	1.57	2 (11%)
2	BGC	11-A	704	2	11,11,12	3.06	6 (54%)	14,15,17	1.53	3 (21%)
2	BGC	11-A	705	2	11,11,12	3.09	6 (54%)	14,15,17	1.91	7 (50%)
2	BGC	11-A	706	2	12,12,12	2.43	6 (50%)	17,17,17	1.51	3 (17%)
2	BGC	12-A	701	2	11,11,12	2.66	5 (45%)	14,15,17	1.52	1 (7%)
2	BGC	12-A	702	2	11,11,12	2.47	4 (36%)	14,15,17	1.84	4 (28%)
2	BGC	12-A	703	2	12,12,12	2.05	4 (33%)	17,17,17	1.21	2 (11%)
2	BGC	12-A	704	2	11,11,12	2.96	5 (45%)	14,15,17	1.46	4 (28%)
2	BGC	12-A	705	2	11,11,12	2.94	5 (45%)	14,15,17	1.52	2 (14%)
2	BGC	12-A	706	2	12,12,12	2.50	6 (50%)	17,17,17	1.41	3 (17%)
2	BGC	13-A	701	2	11,11,12	2.54	5 (45%)	14,15,17	1.30	1 (7%)
2	BGC	13-A	702	2	11,11,12	2.42	4 (36%)	14,15,17	1.89	3 (21%)
2	BGC	13-A	703	2	12,12,12	2.18	4 (33%)	17,17,17	1.25	2 (11%)
2	BGC	13-A	704	2	11,11,12	3.09	4 (36%)	14,15,17	1.11	1 (7%)
2	BGC	13-A	705	2	11,11,12	3.00	5 (45%)	14,15,17	1.41	2 (14%)
2	BGC	13-A	706	2	12,12,12	2.14	5 (41%)	17,17,17	2.06	6 (35%)
2	BGC	14-A	701	2	11,11,12	2.63	4 (36%)	14,15,17	1.32	1 (7%)
2	BGC	14-A	702	2	11,11,12	2.45	4 (36%)	14,15,17	1.65	1 (7%)
2	BGC	14-A	703	2	12,12,12	2.05	5 (41%)	17,17,17	1.37	1 (5%)
2	BGC	14-A	704	2	11,11,12	3.05	4 (36%)	14,15,17	1.19	1 (7%)
2	BGC	14-A	705	2	11,11,12	3.07	7 (63%)	14,15,17	1.13	0
2	BGC	14-A	706	2	12,12,12	2.37	6 (50%)	17,17,17	2.65	10 (58%)
2	BGC	15-A	701	2	11,11,12	2.59	5 (45%)	14,15,17	1.39	1 (7%)
2	BGC	15-A	702	2	11,11,12	2.62	5 (45%)	14,15,17	1.62	2 (14%)
2	BGC	15-A	703	2	12,12,12	2.07	4 (33%)	17,17,17	1.32	2 (11%)
2	BGC	15-A	704	2	11,11,12	3.10	5 (45%)	14,15,17	1.92	5 (35%)
2	BGC	15-A	705	2	11,11,12	3.03	5 (45%)	14,15,17	1.87	3 (21%)
2	BGC	15-A	706	2	12,12,12	2.52	6 (50%)	17,17,17	3.04	11 (64%)
2	BGC	16-A	701	2	11,11,12	2.58	6 (54%)	14,15,17	1.23	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	16-A	702	2	11,11,12	2.46	4 (36%)	14,15,17	1.45	2 (14%)
2	BGC	16-A	703	2	12,12,12	2.03	4 (33%)	17,17,17	1.33	2 (11%)
2	BGC	16-A	704	2	11,11,12	3.05	4 (36%)	14,15,17	1.26	1 (7%)
2	BGC	16-A	705	2	11,11,12	3.30	6 (54%)	14,15,17	1.85	5 (35%)
2	BGC	16-A	706	2	12,12,12	2.59	6 (50%)	17,17,17	1.93	6 (35%)
2	BGC	17-A	701	2	11,11,12	2.66	4 (36%)	14,15,17	1.52	2 (14%)
2	BGC	17-A	702	2	11,11,12	2.52	5 (45%)	14,15,17	1.60	2 (14%)
2	BGC	17-A	703	2	12,12,12	2.07	4 (33%)	17,17,17	1.32	2 (11%)
2	BGC	17-A	704	2	11,11,12	3.02	4 (36%)	14,15,17	1.34	2 (14%)
2	BGC	17-A	705	2	11,11,12	2.95	5 (45%)	14,15,17	1.37	2 (14%)
2	BGC	17-A	706	2	12,12,12	2.56	5 (41%)	17,17,17	2.60	7 (41%)
2	BGC	18-A	701	2	11,11,12	2.51	5 (45%)	14,15,17	1.36	1 (7%)
2	BGC	18-A	702	2	11,11,12	2.65	5 (45%)	14,15,17	1.59	2 (14%)
2	BGC	18-A	703	2	12,12,12	2.18	4 (33%)	17,17,17	1.37	2 (11%)
2	BGC	18-A	704	2	11,11,12	3.06	4 (36%)	14,15,17	1.24	1 (7%)
2	BGC	18-A	705	2	11,11,12	2.84	6 (54%)	14,15,17	2.10	3 (21%)
2	BGC	18-A	706	2	12,12,12	2.72	6 (50%)	17,17,17	2.48	8 (47%)
2	BGC	19-A	701	2	11,11,12	2.57	4 (36%)	14,15,17	1.30	1 (7%)
2	BGC	19-A	702	2	11,11,12	2.55	4 (36%)	14,15,17	1.66	1 (7%)
2	BGC	19-A	703	2	12,12,12	2.14	5 (41%)	17,17,17	1.34	2 (11%)
2	BGC	19-A	704	2	11,11,12	3.04	4 (36%)	14,15,17	1.20	1 (7%)
2	BGC	19-A	705	2	11,11,12	3.05	5 (45%)	14,15,17	1.22	3 (21%)
2	BGC	19-A	706	2	12,12,12	2.34	5 (41%)	17,17,17	1.39	3 (17%)
2	BGC	2-A	701	2	11,11,12	2.60	4 (36%)	14,15,17	1.16	1 (7%)
2	BGC	2-A	702	2	11,11,12	2.56	5 (45%)	14,15,17	1.68	2 (14%)
2	BGC	2-A	703	2	12,12,12	2.15	4 (33%)	17,17,17	1.19	1 (5%)
2	BGC	2-A	704	2	11,11,12	3.00	4 (36%)	14,15,17	1.20	2 (14%)
2	BGC	2-A	705	2	11,11,12	3.19	6 (54%)	14,15,17	1.07	0
2	BGC	2-A	706	2	12,12,12	2.64	6 (50%)	17,17,17	3.32	7 (41%)
2	BGC	20-A	701	2	11,11,12	2.63	5 (45%)	14,15,17	1.58	2 (14%)
2	BGC	20-A	702	2	11,11,12	2.53	5 (45%)	14,15,17	1.48	1 (7%)
2	BGC	20-A	703	2	12,12,12	2.10	4 (33%)	17,17,17	1.17	1 (5%)
2	BGC	20-A	704	2	11,11,12	3.05	5 (45%)	14,15,17	1.74	3 (21%)
2	BGC	20-A	705	2	11,11,12	3.03	5 (45%)	14,15,17	2.14	2 (14%)
2	BGC	20-A	706	2	12,12,12	2.34	5 (41%)	17,17,17	1.46	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	21-A	701	2	11,11,12	2.52	5 (45%)	14,15,17	1.24	1 (7%)
2	BGC	21-A	702	2	11,11,12	2.65	5 (45%)	14,15,17	1.42	1 (7%)
2	BGC	21-A	703	2	12,12,12	2.10	5 (41%)	17,17,17	1.35	1 (5%)
2	BGC	21-A	704	2	11,11,12	3.05	5 (45%)	14,15,17	1.80	3 (21%)
2	BGC	21-A	705	2	11,11,12	3.09	5 (45%)	14,15,17	2.88	8 (57%)
2	BGC	21-A	706	2	12,12,12	2.44	6 (50%)	17,17,17	2.76	11 (64%)
2	BGC	22-A	701	2	11,11,12	2.66	5 (45%)	14,15,17	1.34	1 (7%)
2	BGC	22-A	702	2	11,11,12	2.50	5 (45%)	14,15,17	1.48	2 (14%)
2	BGC	22-A	703	2	12,12,12	2.11	4 (33%)	17,17,17	1.21	1 (5%)
2	BGC	22-A	704	2	11,11,12	3.02	4 (36%)	14,15,17	1.25	1 (7%)
2	BGC	22-A	705	2	11,11,12	3.07	6 (54%)	14,15,17	1.25	2 (14%)
2	BGC	22-A	706	2	12,12,12	2.70	6 (50%)	17,17,17	2.70	6 (35%)
2	BGC	23-A	701	2	11,11,12	2.57	5 (45%)	14,15,17	1.24	1 (7%)
2	BGC	23-A	702	2	11,11,12	2.50	5 (45%)	14,15,17	1.55	1 (7%)
2	BGC	23-A	703	2	12,12,12	2.10	5 (41%)	17,17,17	1.50	1 (5%)
2	BGC	23-A	704	2	11,11,12	3.23	5 (45%)	14,15,17	1.73	6 (42%)
2	BGC	23-A	705	2	11,11,12	2.99	6 (54%)	14,15,17	1.42	3 (21%)
2	BGC	23-A	706	2	12,12,12	2.69	6 (50%)	17,17,17	2.18	5 (29%)
2	BGC	24-A	701	2	11,11,12	2.58	5 (45%)	14,15,17	1.51	1 (7%)
2	BGC	24-A	702	2	11,11,12	2.42	4 (36%)	14,15,17	1.73	2 (14%)
2	BGC	24-A	703	2	12,12,12	2.11	5 (41%)	17,17,17	1.32	2 (11%)
2	BGC	24-A	704	2	11,11,12	3.02	4 (36%)	14,15,17	1.24	1 (7%)
2	BGC	24-A	705	2	11,11,12	3.19	6 (54%)	14,15,17	1.22	2 (14%)
2	BGC	24-A	706	2	12,12,12	2.43	5 (41%)	17,17,17	1.45	4 (23%)
2	BGC	25-A	701	2	11,11,12	2.54	5 (45%)	14,15,17	1.33	1 (7%)
2	BGC	25-A	702	2	11,11,12	2.41	4 (36%)	14,15,17	1.77	2 (14%)
2	BGC	25-A	703	2	12,12,12	2.22	5 (41%)	17,17,17	1.25	1 (5%)
2	BGC	25-A	704	2	11,11,12	2.86	4 (36%)	14,15,17	1.47	3 (21%)
2	BGC	25-A	705	2	11,11,12	3.07	5 (45%)	14,15,17	1.23	2 (14%)
2	BGC	25-A	706	2	12,12,12	2.56	6 (50%)	17,17,17	2.07	8 (47%)
2	BGC	3-A	701	2	11,11,12	2.57	4 (36%)	14,15,17	1.12	1 (7%)
2	BGC	3-A	702	2	11,11,12	2.46	6 (54%)	14,15,17	1.77	3 (21%)
2	BGC	3-A	703	2	12,12,12	2.02	5 (41%)	17,17,17	1.15	1 (5%)
2	BGC	3-A	704	2	11,11,12	2.91	4 (36%)	14,15,17	1.39	2 (14%)
2	BGC	3-A	705	2	11,11,12	2.88	5 (45%)	14,15,17	1.58	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	3-A	706	2	12,12,12	2.57	5 (41%)	17,17,17	2.14	7 (41%)
2	BGC	4-A	701	2	11,11,12	2.51	4 (36%)	14,15,17	1.27	1 (7%)
2	BGC	4-A	702	2	11,11,12	2.58	5 (45%)	14,15,17	1.64	2 (14%)
2	BGC	4-A	703	2	12,12,12	2.11	4 (33%)	17,17,17	1.37	3 (17%)
2	BGC	4-A	704	2	11,11,12	3.09	4 (36%)	14,15,17	1.44	3 (21%)
2	BGC	4-A	705	2	11,11,12	3.19	6 (54%)	14,15,17	2.88	5 (35%)
2	BGC	4-A	706	2	12,12,12	2.59	6 (50%)	17,17,17	2.54	8 (47%)
2	BGC	5-A	701	2	11,11,12	2.61	5 (45%)	14,15,17	1.26	1 (7%)
2	BGC	5-A	702	2	11,11,12	2.58	5 (45%)	14,15,17	1.66	2 (14%)
2	BGC	5-A	703	2	12,12,12	2.01	4 (33%)	17,17,17	1.27	1 (5%)
2	BGC	5-A	704	2	11,11,12	2.99	4 (36%)	14,15,17	1.34	2 (14%)
2	BGC	5-A	705	2	11,11,12	3.23	6 (54%)	14,15,17	1.32	2 (14%)
2	BGC	5-A	706	2	12,12,12	2.56	5 (41%)	17,17,17	2.17	8 (47%)
2	BGC	6-A	701	2	11,11,12	2.50	5 (45%)	14,15,17	1.61	2 (14%)
2	BGC	6-A	702	2	11,11,12	2.62	4 (36%)	14,15,17	1.76	2 (14%)
2	BGC	6-A	703	2	12,12,12	2.04	4 (33%)	17,17,17	1.21	2 (11%)
2	BGC	6-A	704	2	11,11,12	2.97	4 (36%)	14,15,17	1.29	2 (14%)
2	BGC	6-A	705	2	11,11,12	2.81	6 (54%)	14,15,17	1.23	2 (14%)
2	BGC	6-A	706	2	12,12,12	2.77	7 (58%)	17,17,17	2.43	6 (35%)
2	BGC	7-A	701	2	11,11,12	2.44	5 (45%)	14,15,17	1.43	1 (7%)
2	BGC	7-A	702	2	11,11,12	2.57	4 (36%)	14,15,17	1.85	4 (28%)
2	BGC	7-A	703	2	12,12,12	2.09	4 (33%)	17,17,17	1.18	2 (11%)
2	BGC	7-A	704	2	11,11,12	2.90	5 (45%)	14,15,17	1.23	2 (14%)
2	BGC	7-A	705	2	11,11,12	2.98	4 (36%)	14,15,17	0.81	1 (7%)
2	BGC	7-A	706	2	12,12,12	2.60	6 (50%)	17,17,17	2.08	6 (35%)
2	BGC	8-A	701	2	11,11,12	2.54	5 (45%)	14,15,17	1.40	1 (7%)
2	BGC	8-A	702	2	11,11,12	2.49	4 (36%)	14,15,17	1.52	2 (14%)
2	BGC	8-A	703	2	12,12,12	2.07	5 (41%)	17,17,17	1.68	4 (23%)
2	BGC	8-A	704	2	11,11,12	3.00	5 (45%)	14,15,17	1.43	2 (14%)
2	BGC	8-A	705	2	11,11,12	3.28	6 (54%)	14,15,17	1.82	5 (35%)
2	BGC	8-A	706	2	12,12,12	2.71	7 (58%)	17,17,17	2.42	7 (41%)
2	BGC	9-A	701	2	11,11,12	2.59	4 (36%)	14,15,17	1.43	3 (21%)
2	BGC	9-A	702	2	11,11,12	2.48	5 (45%)	14,15,17	1.69	3 (21%)
2	BGC	9-A	703	2	12,12,12	2.10	4 (33%)	17,17,17	1.41	4 (23%)
2	BGC	9-A	704	2	11,11,12	2.97	4 (36%)	14,15,17	1.16	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	9-A	705	2	11,11,12	2.97	5 (45%)	14,15,17	1.32	3 (21%)
2	BGC	9-A	706	2	12,12,12	2.29	6 (50%)	17,17,17	2.38	4 (23%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	14-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	14-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	14-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	15-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	15-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	15-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	15-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	15-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	15-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	16-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	16-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	16-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	16-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	16-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	16-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	17-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	17-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	17-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	17-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	17-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	17-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	18-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	18-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	18-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	18-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	18-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	18-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	19-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	19-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	19-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	19-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	19-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	19-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	2-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	2-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	2-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	2-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	2-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	2-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	20-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	20-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	20-A	703	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	20-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	20-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	20-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	21-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	21-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	21-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	21-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	21-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	21-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	22-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	22-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	22-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	22-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	22-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	22-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	23-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	23-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	23-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	23-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	23-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	23-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	24-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	24-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	24-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	24-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	24-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	24-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	25-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	25-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	25-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	25-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	25-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	25-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	3-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	3-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	3-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	3-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	3-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	3-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	4-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	4-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	4-A	703	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	4-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	4-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	4-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	5-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	5-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	5-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	5-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	5-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	5-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	6-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	6-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	6-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	6-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	6-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	6-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	7-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	7-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	7-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	7-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	7-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	7-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	8-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	8-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	8-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	8-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	8-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	8-A	706	2	-	0/2/22/22	0/1/1/1
2	BGC	9-A	701	2	-	0/2/19/22	0/1/1/1
2	BGC	9-A	702	2	-	0/2/19/22	0/1/1/1
2	BGC	9-A	703	2	-	0/2/22/22	0/1/1/1
2	BGC	9-A	704	2	-	0/2/19/22	0/1/1/1
2	BGC	9-A	705	2	-	0/2/19/22	0/1/1/1
2	BGC	9-A	706	2	-	0/2/22/22	0/1/1/1

The worst 5 of 736 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	23-A	704	BGC	C2-C3	-8.07	1.41	1.52
2	13-A	704	BGC	C2-C3	-7.91	1.41	1.52
2	14-A	704	BGC	C2-C3	-7.61	1.42	1.52
2	15-A	704	BGC	C2-C3	-7.58	1.42	1.52
2	18-A	704	BGC	C2-C3	-7.57	1.42	1.52

The worst 5 of 415 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-A	705	BGC	O5-C1-C2	-7.89	98.06	110.86
2	22-A	706	BGC	C1-C2-C3	-7.56	99.18	110.43
2	15-A	706	BGC	C1-C2-C3	-6.94	100.10	110.43
2	2-A	706	BGC	C4-C3-C2	-6.05	99.50	110.79
2	9-A	706	BGC	O5-C5-C4	-5.69	99.00	109.68

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.