



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:12 PM GMT

PDB ID : 4TYV
Title : Ensemble refinement of the E502A variant of sacteLam55A from Streptomyces sp. SirexAA-E in complex with glucose
Authors : Bianchetti, C.M.; Takasuka, T.E.; Yik, E.J.; Bergeman, L.F.; Fox, B.G.
Deposited on : 2014-07-09
Resolution : 1.75 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

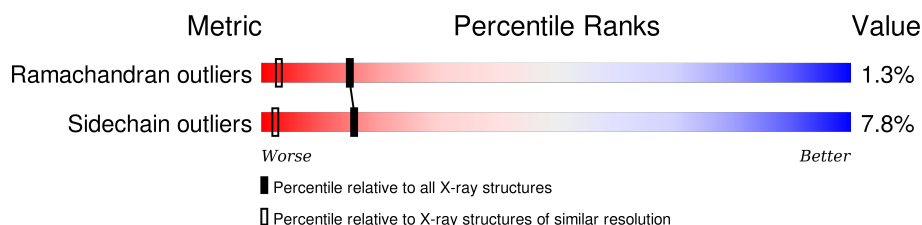
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)














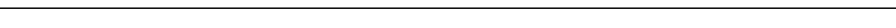


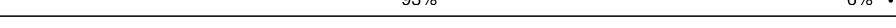








The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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	551	91% 7% ..
1	1-B	551	91% 7% .
1	10-A	551	90% 7% ..
1	10-B	551	90% 8% .
1	11-A	551	92% 7% ..
1	11-B	551	92% 7% .
1	12-A	551	93% 5% ..
1	12-B	551	89% 8% .












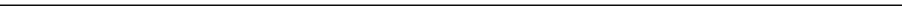





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	13-A	551	 91% 7% ..
1	13-B	551	 91% 7% .
1	14-A	551	 90% 8% ..
1	14-B	551	 90% 7% .
1	15-A	551	 91% 7% ..
1	15-B	551	 90% 9% .
1	16-A	551	 89% 8% ..
1	16-B	551	 92% 7% .
1	17-A	551	 89% 8% ...
1	17-B	551	 91% 8% .
1	18-A	551	 89% 9% ..
1	18-B	551	 91% 8% .
1	19-A	551	 89% 8% ..
1	19-B	551	 91% 8% .
1	2-A	551	 91% 7% ..
1	2-B	551	 93% 6% .
1	20-A	551	 92% 7% ..
1	20-B	551	 92% 6% .
1	21-A	551	 91% 8% ..
1	21-B	551	 91% 7% .
1	22-A	551	 92% 7% ..
1	22-B	551	 90% 8% .
1	23-A	551	 92% 6% ..
1	23-B	551	 91% 8% .
1	24-A	551	 90% 9% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	24-B	551	 91% 9% .
1	25-A	551	 91% 8% .
1	25-B	551	 90% 9% .
1	3-A	551	 92% 7% ..
1	3-B	551	 92% 7% .
1	4-A	551	 92% 7% ..
1	4-B	551	 92% 7% .
1	5-A	551	 93% 6% ..
1	5-B	551	 92% 7% .
1	6-A	551	 92% 6% ..
1	6-B	551	 92% 6% .
1	7-A	551	 92% 6% ..
1	7-B	551	 91% 7% .
1	8-A	551	 89% 9% ..
1	8-B	551	 92% 7% .
1	9-A	551	 91% 7% ..
1	9-B	551	 90% 9% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 418117 atoms, of which 196575 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	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	2-A	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	3-A	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	4-A	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	5-A	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	6-A	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	7-A	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	8-A	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	9-A	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	10-A	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	11-A	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	12-A	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	13-A	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	14-A	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	15-A	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0
1	16-A	548	Total 8059	C 2624	H 3901	N 707	O 822	S 5	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	18-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	19-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	20-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	21-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	22-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	23-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	24-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	25-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	1-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	2-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	3-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	4-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	5-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	6-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	7-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	8-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	9-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	10-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	11-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	12-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	13-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	14-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	15-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	16-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	17-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	18-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	19-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	20-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	21-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	22-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	23-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	24-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			
1	25-B	551	Total	C	H	N	O	S	0	0	0
			8101	2637	3920	711	828	5			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

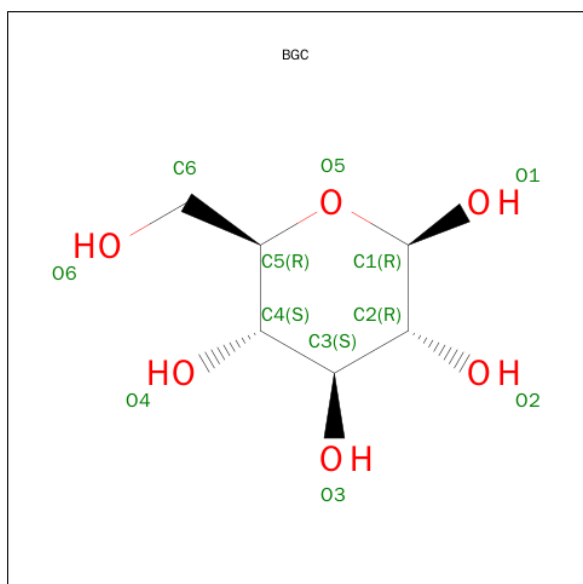
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	24-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	25-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	1-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	2-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	3-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	4-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	5-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	6-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	7-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	8-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	9-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	10-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	11-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	12-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	13-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	14-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	15-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	16-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	17-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	18-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	19-B	1	Total	C	H	O	0	0
			10	2	6	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	20-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	21-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	22-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	23-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	24-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	25-B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is BETA-D-GLUCOSE (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	1-B	1	Total	C	H	O	0	0
			24	6	12	6		
3	2-B	1	Total	C	H	O	0	0
			24	6	12	6		
3	3-B	1	Total	C	H	O	0	0
			24	6	12	6		
3	4-B	1	Total	C	H	O	0	0
			24	6	12	6		
3	5-B	1	Total	C	H	O	0	0
			24	6	12	6		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-A	240	Total O 240 240	0	0
4	2-A	253	Total O 253 253	0	0
4	3-A	262	Total O 262 262	0	0
4	4-A	244	Total O 244 244	0	0
4	5-A	270	Total O 270 270	0	0
4	6-A	247	Total O 247 247	0	0
4	7-A	254	Total O 254 254	0	0
4	8-A	243	Total O 243 243	0	0
4	9-A	237	Total O 237 237	0	0
4	10-A	254	Total O 254 254	0	0
4	11-A	232	Total O 232 232	0	0
4	12-A	239	Total O 239 239	0	0
4	13-A	257	Total O 257 257	0	0
4	14-A	251	Total O 251 251	0	0
4	15-A	246	Total O 246 246	0	0
4	16-A	252	Total O 252 252	0	0
4	17-A	246	Total O 246 246	0	0
4	18-A	258	Total O 258 258	0	0
4	19-A	248	Total O 248 248	0	0
4	20-A	237	Total O 237 237	0	0
4	21-A	242	Total O 242 242	0	0
4	22-A	251	Total O 251 251	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	23-A	248	Total 248	O 248	0	0
4	24-A	239	Total 239	O 239	0	0
4	25-A	240	Total 240	O 240	0	0
4	1-B	263	Total 263	O 263	0	0
4	2-B	236	Total 236	O 236	0	0
4	3-B	224	Total 224	O 224	0	0
4	4-B	246	Total 246	O 246	0	0
4	5-B	233	Total 233	O 233	0	0
4	6-B	243	Total 243	O 243	0	0
4	7-B	236	Total 236	O 236	0	0
4	8-B	242	Total 242	O 242	0	0
4	9-B	240	Total 240	O 240	0	0
4	10-B	252	Total 252	O 252	0	0
4	11-B	252	Total 252	O 252	0	0
4	12-B	263	Total 263	O 263	0	0
4	13-B	231	Total 231	O 231	0	0
4	14-B	246	Total 246	O 246	0	0
4	15-B	239	Total 239	O 239	0	0
4	16-B	246	Total 246	O 246	0	0
4	17-B	238	Total 238	O 238	0	0
4	18-B	251	Total 251	O 251	0	0

Continued on next page...

Continued from previous page...

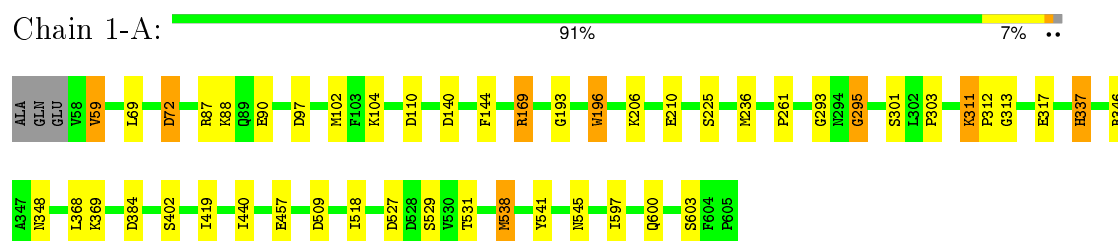
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	19-B	228	Total 228	O 228	0	0
4	20-B	230	Total 230	O 230	0	0
4	21-B	240	Total 240	O 240	0	0
4	22-B	267	Total 267	O 267	0	0
4	23-B	248	Total 248	O 248	0	0
4	24-B	241	Total 241	O 241	0	0
4	25-B	242	Total 242	O 242	0	0

3 Residue-property plots [i](#)

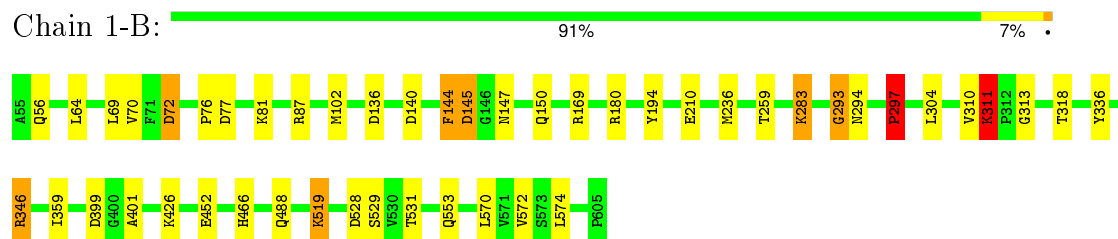
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS failed to run properly.

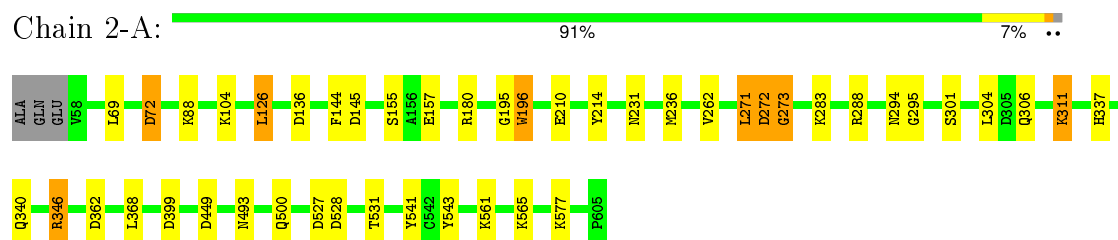
- Molecule 1: Putative secreted protein



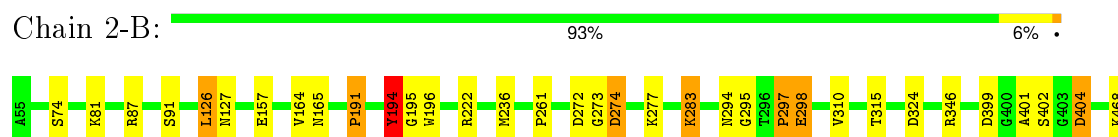
- Molecule 1: Putative secreted protein



- Molecule 1: Putative secreted protein



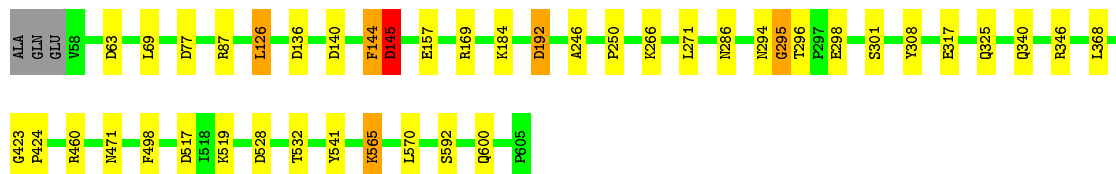
- Molecule 1: Putative secreted protein





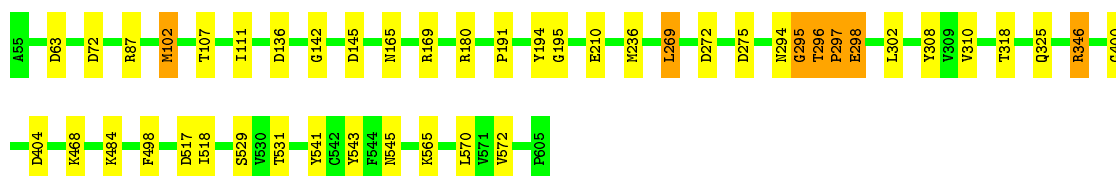
- Molecule 1: Putative secreted protein

Chain 3-A: 92% 7% ..



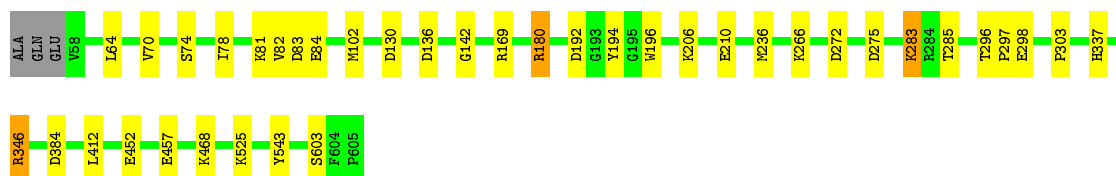
- Molecule 1: Putative secreted protein

Chain 3-B: 92% 7% .



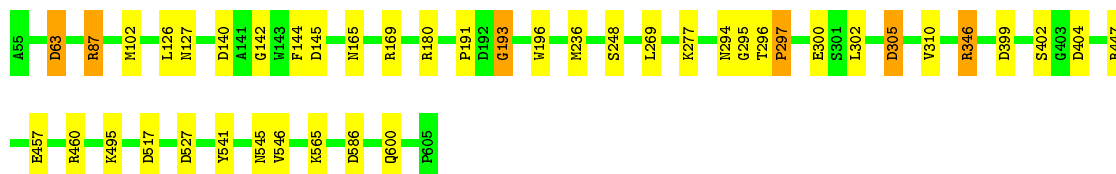
- Molecule 1: Putative secreted protein

Chain 4-A: 92% 7% ..



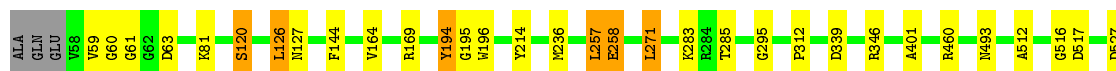
- Molecule 1: Putative secreted protein

Chain 4-B: 92% 7% .



- Molecule 1: Putative secreted protein

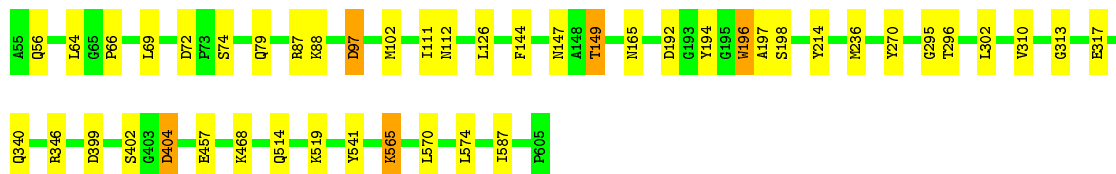
Chain 5-A: 93% 6% ..





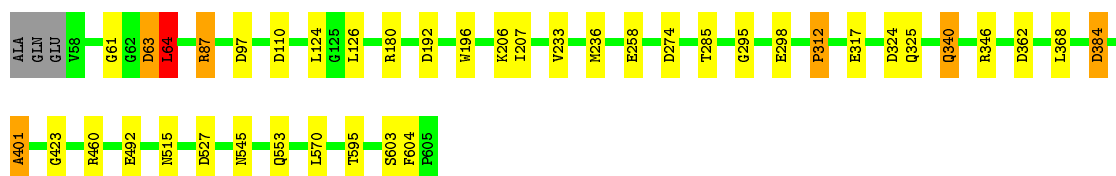
- Molecule 1: Putative secreted protein

Chain 5-B: 92% 7% .



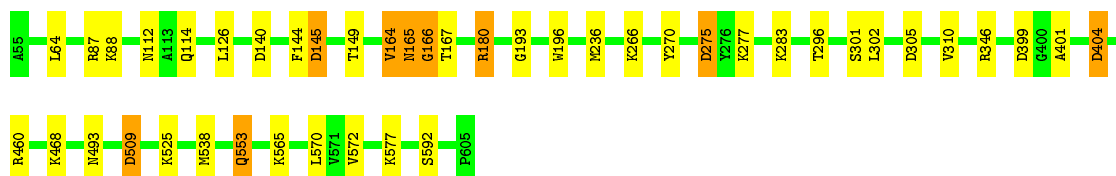
- Molecule 1: Putative secreted protein

Chain 6-A: 92% 6% ..



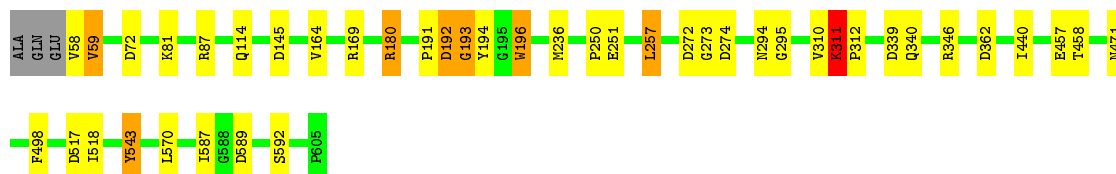
- Molecule 1: Putative secreted protein

Chain 6-B: 92% 6% .



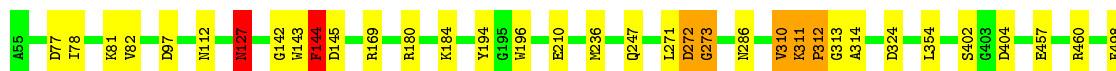
- Molecule 1: Putative secreted protein

Chain 7-A: 92% 6% ..



- Molecule 1: Putative secreted protein

Chain 7-B: 91% 7% .





- Molecule 1: Putative secreted protein

Chain 8-A: 89% 9% ..



- Molecule 1: Putative secreted protein

Chain 8-B: 92% 7% .



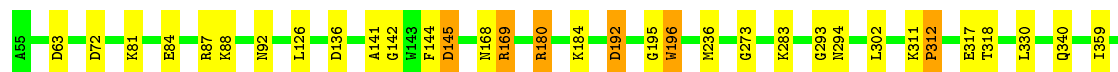
- Molecule 1: Putative secreted protein

Chain 9-A: 91% 7% ..



- Molecule 1: Putative secreted protein

Chain 9-B: 90% 9% .



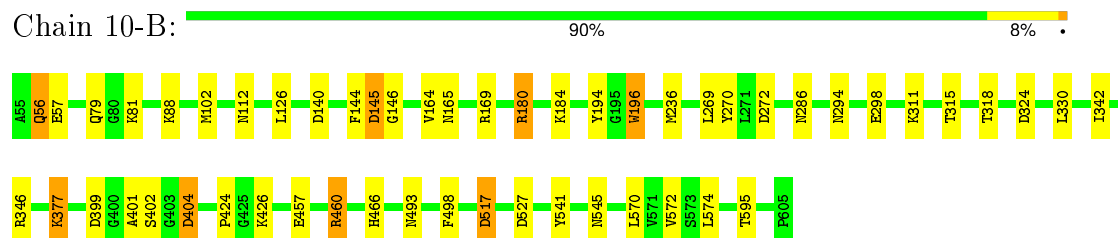
- Molecule 1: Putative secreted protein

Chain 10-A: 90% 7% ..

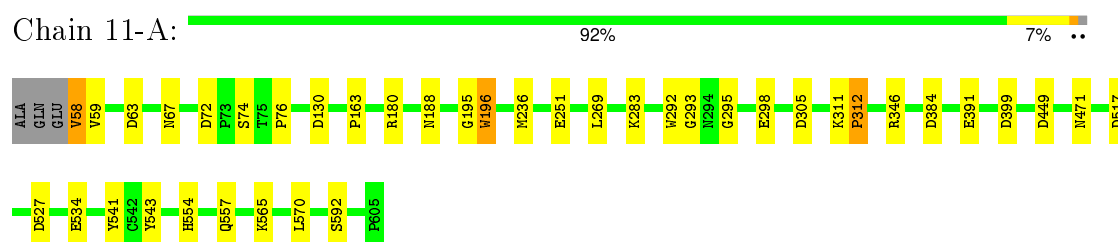




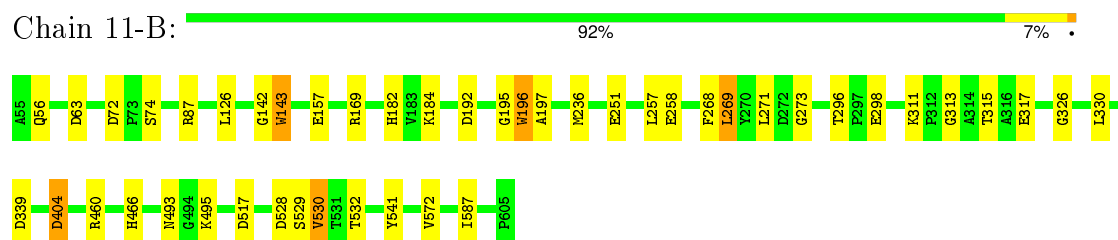
- Molecule 1: Putative secreted protein



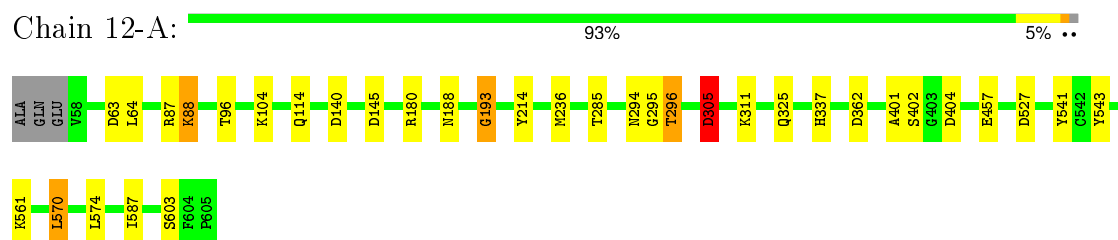
- Molecule 1: Putative secreted protein



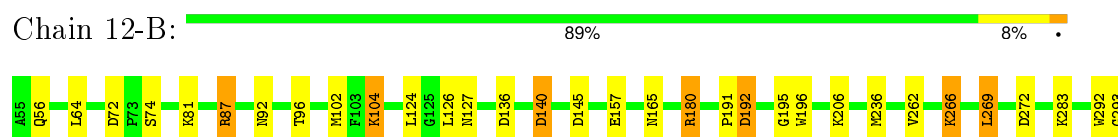
- Molecule 1: Putative secreted protein

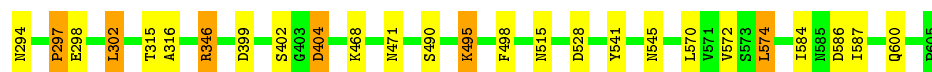


- Molecule 1: Putative secreted protein



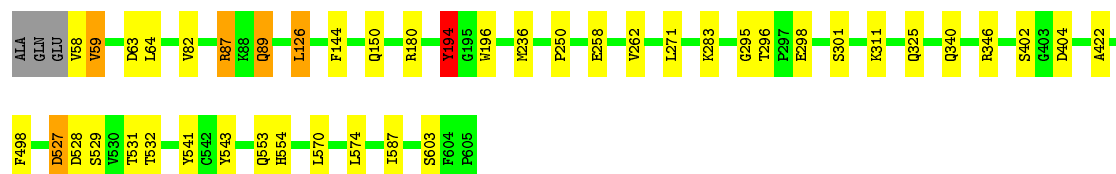
- Molecule 1: Putative secreted protein





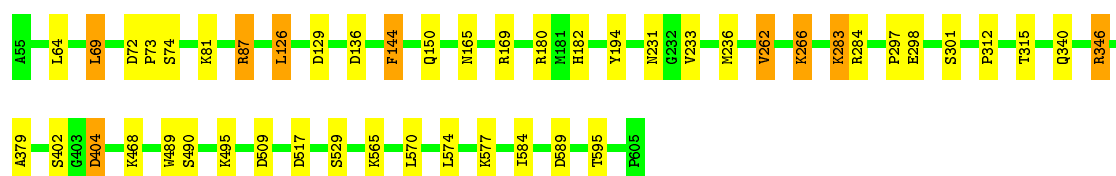
- Molecule 1: Putative secreted protein

Chain 13-A: 91% 7% ..



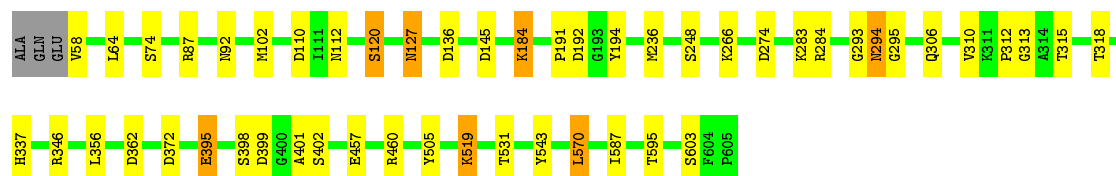
- Molecule 1: Putative secreted protein

Chain 13-B: 91% 7% .



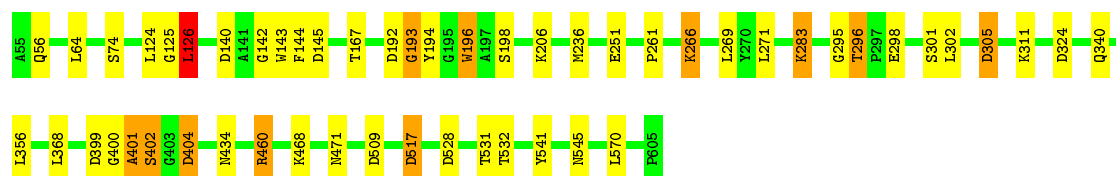
- Molecule 1: Putative secreted protein

Chain 14-A: 90% 8% ..



- Molecule 1: Putative secreted protein

Chain 14-B: 90% 7% .



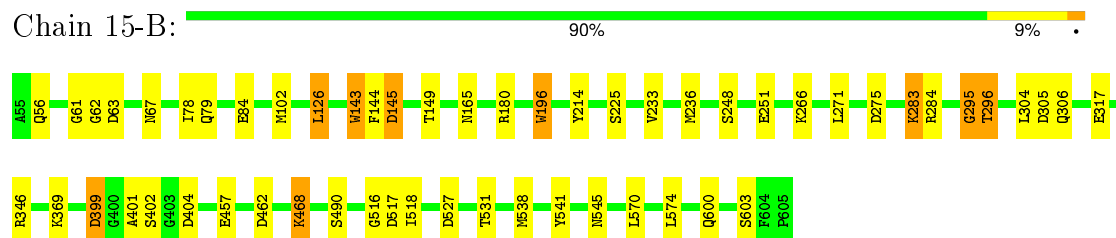
- Molecule 1: Putative secreted protein

Chain 15-A: 91% 7% ..

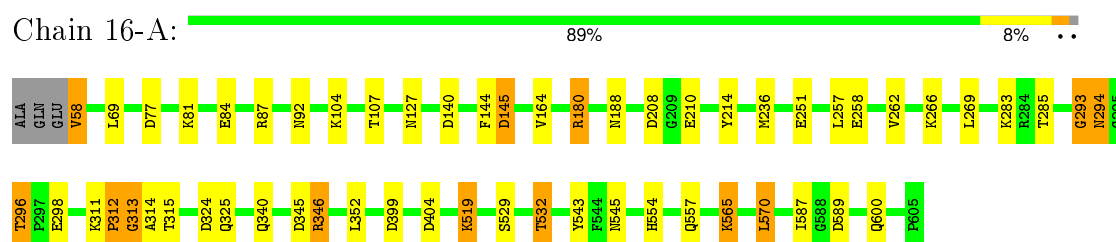




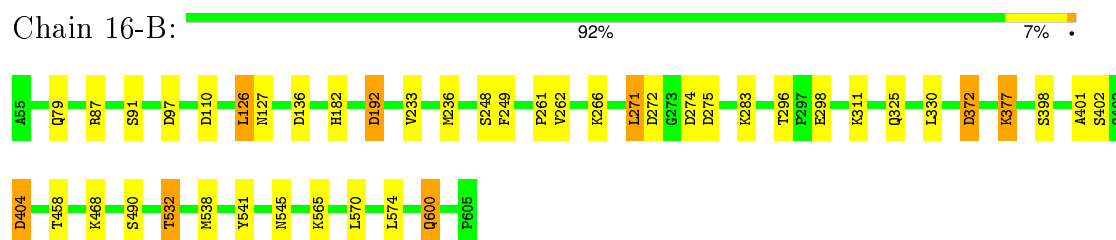
- Molecule 1: Putative secreted protein



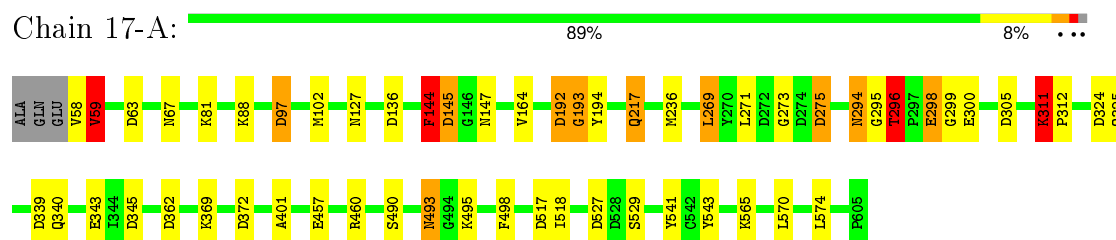
- Molecule 1: Putative secreted protein



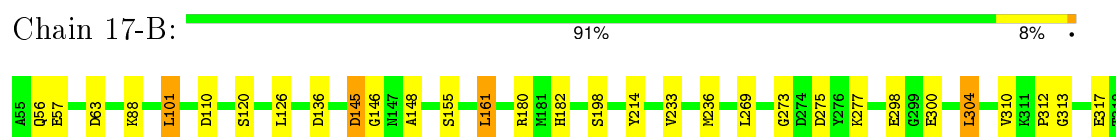
- Molecule 1: Putative secreted protein

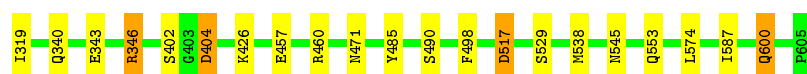


- Molecule 1: Putative secreted protein



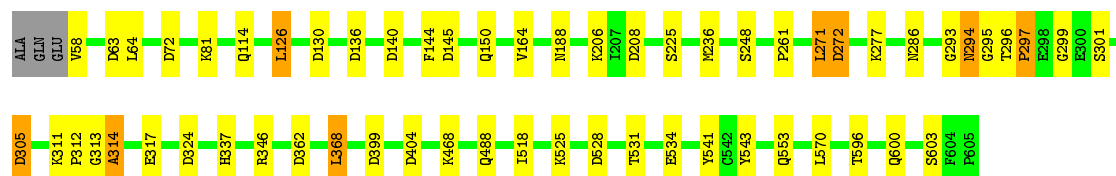
- Molecule 1: Putative secreted protein





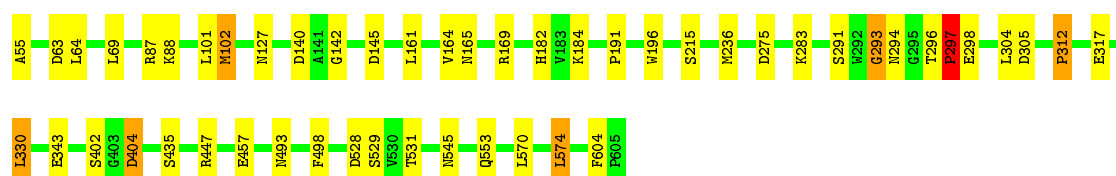
- Molecule 1: Putative secreted protein

Chain 18-A: 89% 9% ..



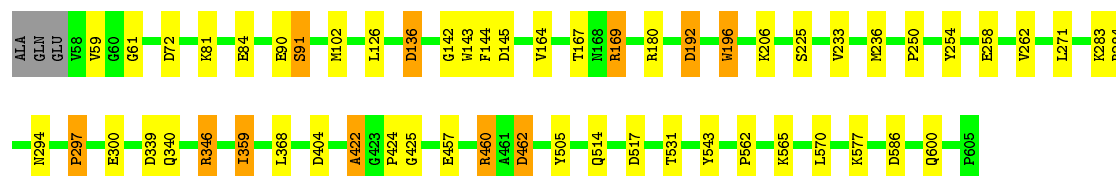
- Molecule 1: Putative secreted protein

Chain 18-B: 91% 8% .



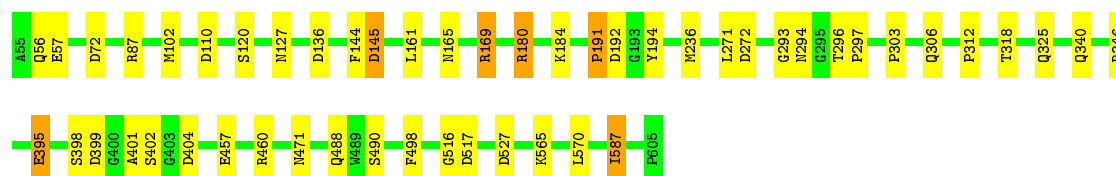
- Molecule 1: Putative secreted protein

Chain 19-A: 89% 8% ..



- Molecule 1: Putative secreted protein

Chain 19-B: 91% 8% .



- Molecule 1: Putative secreted protein

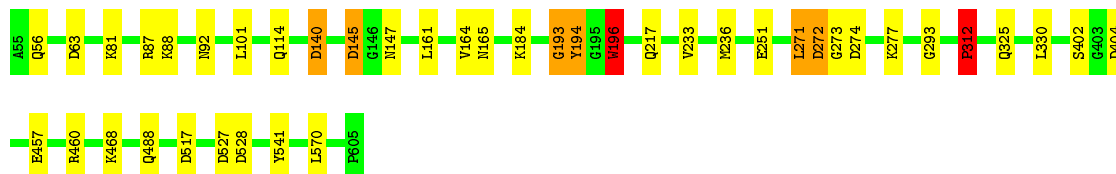
Chain 20-A: 92% 7% ..





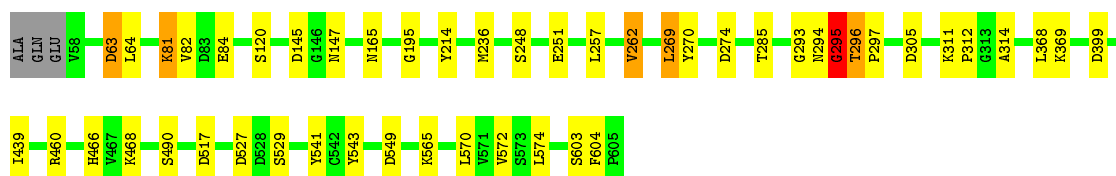
- Molecule 1: Putative secreted protein

Chain 20-B: 92% 6% •



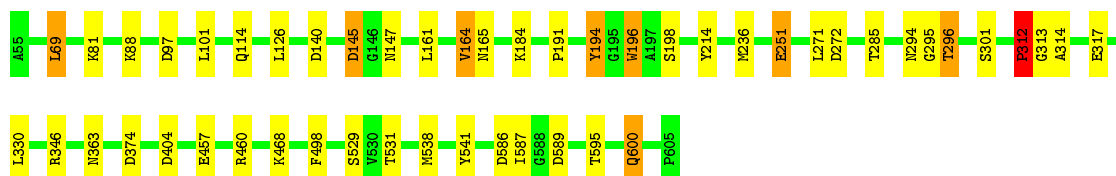
- Molecule 1: Putative secreted protein

Chain 21-A: 91% 8% ••



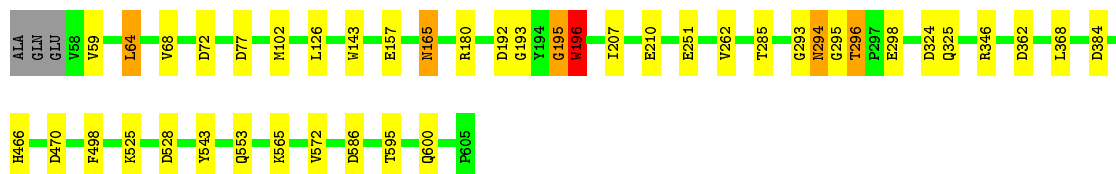
- Molecule 1: Putative secreted protein

Chain 21-B: 91% 7% •



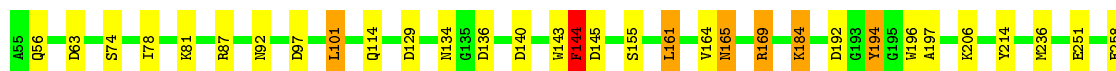
- Molecule 1: Putative secreted protein

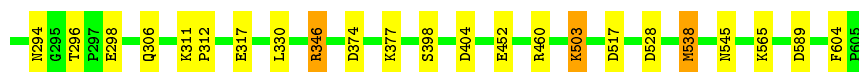
Chain 22-A: 92% 7% ••



- Molecule 1: Putative secreted protein

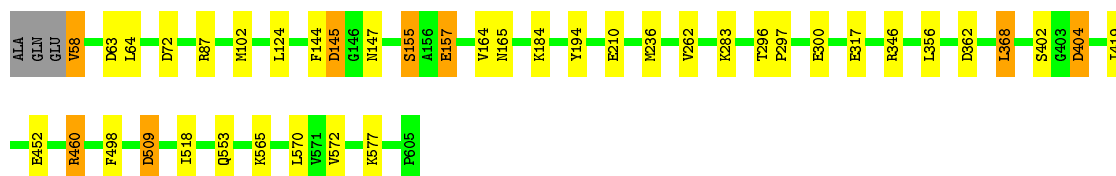
Chain 22-B: 90% 8% •





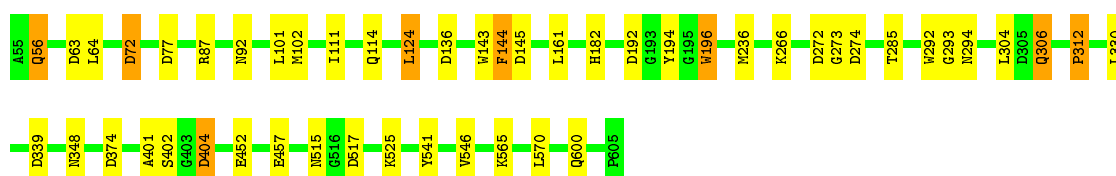
- Molecule 1: Putative secreted protein

Chain 23-A: 92% 6% ..



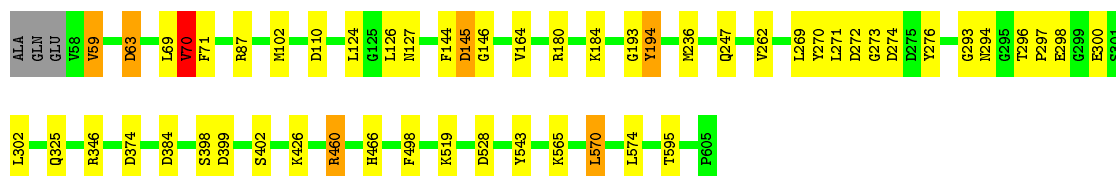
- Molecule 1: Putative secreted protein

Chain 23-B: 91% 8% •



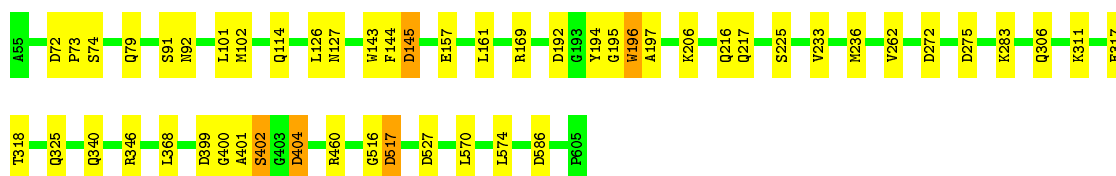
- Molecule 1: Putative secreted protein

Chain 24-A: 90% 9% ..



- Molecule 1: Putative secreted protein

Chain 24-B: 91% 9% •



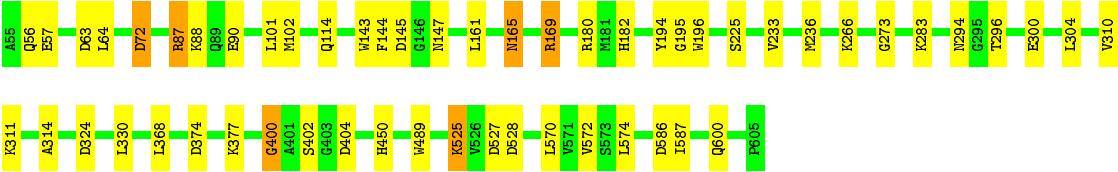
- Molecule 1: Putative secreted protein

Chain 25-A: 91% 8% •





● Molecule 1: Putative secreted protein



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	53.94Å 100.06Å 99.56Å 90.00° 92.31° 90.00°	Depositor
Resolution (Å)	24.27 – 1.75	Depositor
% Data completeness (in resolution range)	98.8 (24.27-1.75)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 1.75Å)	Xtriage
Refinement program	PHENIX (PHENIX.ENSEMBLE_REFINEMENT: 1.9_1692)	Depositor
R, R_{free}	0.110 , 0.143	Depositor
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.063	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.024 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 104913 reflections (0.002%)	Xtriage
Total number of atoms	418117	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.00 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4080e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, 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	0.81	3/4271 (0.1%)	0.93	9/5836 (0.2%)
1	1-B	0.80	5/4294 (0.1%)	0.95	12/5867 (0.2%)
1	2-A	0.77	0/4271	0.91	9/5836 (0.2%)
1	2-B	0.81	8/4294 (0.2%)	0.92	7/5867 (0.1%)
1	3-A	0.79	5/4271 (0.1%)	0.93	12/5836 (0.2%)
1	3-B	0.81	5/4294 (0.1%)	0.91	6/5867 (0.1%)
1	4-A	0.81	6/4271 (0.1%)	0.92	12/5836 (0.2%)
1	4-B	0.79	4/4294 (0.1%)	0.95	12/5867 (0.2%)
1	5-A	0.78	4/4271 (0.1%)	0.90	5/5836 (0.1%)
1	5-B	0.79	3/4294 (0.1%)	0.93	8/5867 (0.1%)
1	6-A	0.78	2/4271 (0.0%)	0.95	8/5836 (0.1%)
1	6-B	0.82	3/4294 (0.1%)	0.96	14/5867 (0.2%)
1	7-A	0.76	3/4271 (0.1%)	0.95	13/5836 (0.2%)
1	7-B	0.80	4/4294 (0.1%)	0.95	14/5867 (0.2%)
1	8-A	0.81	3/4271 (0.1%)	0.98	14/5836 (0.2%)
1	8-B	0.82	6/4294 (0.1%)	0.96	9/5867 (0.2%)
1	9-A	0.77	3/4271 (0.1%)	0.90	11/5836 (0.2%)
1	9-B	0.79	6/4294 (0.1%)	0.94	9/5867 (0.2%)
1	10-A	0.77	2/4271 (0.0%)	0.92	12/5836 (0.2%)
1	10-B	0.83	6/4294 (0.1%)	0.94	7/5867 (0.1%)
1	11-A	0.75	2/4271 (0.0%)	0.91	8/5836 (0.1%)
1	11-B	0.81	4/4294 (0.1%)	0.92	6/5867 (0.1%)
1	12-A	0.76	3/4271 (0.1%)	0.92	9/5836 (0.2%)
1	12-B	0.80	4/4294 (0.1%)	0.96	16/5867 (0.3%)
1	13-A	0.83	7/4271 (0.2%)	0.92	11/5836 (0.2%)
1	13-B	0.84	4/4294 (0.1%)	1.01	20/5867 (0.3%)
1	14-A	0.77	7/4271 (0.2%)	0.94	9/5836 (0.2%)
1	14-B	0.80	3/4294 (0.1%)	0.94	12/5867 (0.2%)
1	15-A	0.75	1/4271 (0.0%)	0.94	16/5836 (0.3%)
1	15-B	0.80	2/4294 (0.0%)	0.95	12/5867 (0.2%)
1	16-A	0.80	6/4271 (0.1%)	0.93	13/5836 (0.2%)
1	16-B	0.79	4/4294 (0.1%)	0.90	10/5867 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	17-A	0.81	6/4271 (0.1%)	0.95	14/5836 (0.2%)
1	17-B	0.80	9/4294 (0.2%)	0.94	8/5867 (0.1%)
1	18-A	0.76	0/4271	0.93	10/5836 (0.2%)
1	18-B	0.80	7/4294 (0.2%)	0.92	9/5867 (0.2%)
1	19-A	0.84	8/4271 (0.2%)	1.01	16/5836 (0.3%)
1	19-B	0.81	4/4294 (0.1%)	0.94	9/5867 (0.2%)
1	20-A	0.76	3/4271 (0.1%)	0.89	6/5836 (0.1%)
1	20-B	0.77	2/4294 (0.0%)	0.90	6/5867 (0.1%)
1	21-A	0.77	2/4271 (0.0%)	0.92	7/5836 (0.1%)
1	21-B	0.79	4/4294 (0.1%)	0.95	15/5867 (0.3%)
1	22-A	0.78	6/4271 (0.1%)	0.94	12/5836 (0.2%)
1	22-B	0.78	3/4294 (0.1%)	0.97	21/5867 (0.4%)
1	23-A	0.76	3/4271 (0.1%)	0.91	9/5836 (0.2%)
1	23-B	0.76	3/4294 (0.1%)	0.94	13/5867 (0.2%)
1	24-A	0.78	1/4271 (0.0%)	0.97	15/5836 (0.3%)
1	24-B	0.79	5/4294 (0.1%)	0.92	8/5867 (0.1%)
1	25-A	0.79	2/4271 (0.0%)	0.93	10/5836 (0.2%)
1	25-B	0.75	0/4294	0.95	12/5867 (0.2%)
All	All	0.79	196/214125 (0.1%)	0.94	545/292575 (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	4
1	1-B	0	4
1	2-A	0	4
1	2-B	0	5
1	3-A	0	2
1	3-B	0	5
1	4-A	0	1
1	4-B	0	2
1	5-A	0	2
1	6-A	0	4
1	6-B	0	2
1	7-A	0	5
1	7-B	0	7
1	8-A	0	4
1	8-B	0	1
1	9-A	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	9-B	0	4
1	10-A	0	5
1	10-B	0	3
1	11-A	0	6
1	11-B	0	2
1	12-A	0	1
1	12-B	0	2
1	13-A	0	1
1	14-A	0	3
1	14-B	0	5
1	15-A	0	4
1	15-B	0	2
1	16-A	0	9
1	17-A	0	6
1	17-B	0	2
1	18-A	0	3
1	18-B	0	4
1	19-A	0	2
1	19-B	0	2
1	20-A	0	3
1	20-B	0	4
1	21-A	0	2
1	21-B	0	2
1	22-A	0	5
1	22-B	0	1
1	23-A	0	1
1	23-B	0	4
1	24-A	0	7
1	25-A	0	3
1	25-B	0	2
All	All	0	155

The worst 5 of 196 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	13-A	194	TYR	CE2-CZ	-12.36	1.22	1.38
1	6-B	310	VAL	CB-CG2	-11.58	1.28	1.52
1	13-B	379	ALA	CA-CB	-11.38	1.28	1.52
1	4-B	310	VAL	CB-CG2	-10.93	1.29	1.52
1	1-A	196	TRP	CB-CG	10.82	1.69	1.50

The worst 5 of 545 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	13-B	87	ARG	NE-CZ-NH1	16.90	128.75	120.30
1	19-A	460	ARG	NE-CZ-NH2	13.89	127.24	120.30
1	4-B	346	ARG	NE-CZ-NH2	13.10	126.85	120.30
1	8-B	460	ARG	NE-CZ-NH2	12.66	126.63	120.30
1	22-B	346	ARG	NE-CZ-NH2	12.33	126.46	120.30

There are no chirality outliers.

5 of 155 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	193	GLY	Peptide
1	1-A	311	LYS	Peptide
1	1-A	312	PRO	Peptide
1	1-A	337	HIS	Peptide
1	1-B	76	PRO	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	4158	3901	3913	0	0
1	1-B	4181	3920	3932	0	0
1	2-A	4158	3901	3913	0	0
1	2-B	4181	3920	3932	0	0
1	3-A	4158	3901	3913	0	0
1	3-B	4181	3920	3932	0	0
1	4-A	4158	3901	3913	0	0
1	4-B	4181	3920	3932	0	0
1	5-A	4158	3901	3913	0	0
1	5-B	4181	3920	3932	0	0
1	6-A	4158	3901	3913	0	0
1	6-B	4181	3920	3932	0	0
1	7-A	4158	3901	3913	0	0
1	7-B	4181	3920	3932	0	0
1	8-A	4158	3901	3913	0	0
1	8-B	4181	3920	3932	0	0
1	9-A	4158	3901	3913	0	0
1	9-B	4181	3920	3932	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	10-A	4158	3901	3913	0	0
1	10-B	4181	3920	3932	0	0
1	11-A	4158	3901	3913	0	0
1	11-B	4181	3920	3932	0	0
1	12-A	4158	3901	3913	0	0
1	12-B	4181	3920	3932	0	0
1	13-A	4158	3901	3913	0	0
1	13-B	4181	3920	3932	0	0
1	14-A	4158	3901	3913	0	0
1	14-B	4181	3920	3932	0	0
1	15-A	4158	3901	3913	0	0
1	15-B	4181	3920	3932	0	0
1	16-A	4158	3901	3913	0	0
1	16-B	4181	3920	3932	0	0
1	17-A	4158	3901	3913	0	0
1	17-B	4181	3920	3932	0	0
1	18-A	4158	3901	3913	0	0
1	18-B	4181	3920	3932	0	0
1	19-A	4158	3901	3913	0	0
1	19-B	4181	3920	3932	0	0
1	20-A	4158	3901	3913	0	0
1	20-B	4181	3920	3932	0	0
1	21-A	4158	3901	3913	0	0
1	21-B	4181	3920	3932	0	0
1	22-A	4158	3901	3913	0	0
1	22-B	4181	3920	3932	0	0
1	23-A	4158	3901	3913	0	0
1	23-B	4181	3920	3932	0	0
1	24-A	4158	3901	3913	0	0
1	24-B	4181	3920	3932	0	0
1	25-A	4158	3901	3913	0	0
1	25-B	4181	3920	3932	0	0
2	1-A	8	12	12	0	0
2	1-B	12	18	18	0	0
2	2-A	8	12	12	0	0
2	2-B	12	18	18	0	0
2	3-A	8	12	12	0	0
2	3-B	12	18	18	0	0
2	4-A	8	12	12	0	0
2	4-B	12	18	18	0	0
2	5-A	8	12	12	0	0
2	5-B	12	18	18	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3-B	12	12	11	0	0
3	4-B	12	12	12	0	0
3	5-B	12	12	12	0	0
3	6-B	12	12	12	0	0
3	7-B	12	12	12	0	0
3	8-B	12	12	12	0	0
3	9-B	12	12	12	0	0
3	10-B	12	12	12	0	0
3	11-B	12	12	12	0	0
3	12-B	12	12	12	0	0
3	13-B	12	12	12	0	0
3	14-B	12	12	12	0	0
3	15-B	12	12	12	0	0
3	16-B	12	12	12	0	0
3	17-B	12	12	12	0	0
3	18-B	12	12	12	0	0
3	19-B	12	12	12	0	0
3	20-B	12	12	12	0	0
3	21-B	12	12	12	0	0
3	22-B	12	12	12	0	0
3	23-B	12	12	12	0	0
3	24-B	12	12	12	0	0
3	25-B	12	12	12	0	0
4	1-A	240	0	0	0	0
4	1-B	263	0	0	0	0
4	2-A	253	0	0	0	0
4	2-B	236	0	0	0	0
4	3-A	262	0	0	0	0
4	3-B	224	0	0	0	0
4	4-A	244	0	0	0	0
4	4-B	246	0	0	0	0
4	5-A	270	0	0	0	0
4	5-B	233	0	0	0	0
4	6-A	247	0	0	0	0
4	6-B	243	0	0	0	0
4	7-A	254	0	0	0	0
4	7-B	236	0	0	0	0
4	8-A	243	0	0	0	0
4	8-B	242	0	0	0	0
4	9-A	237	0	0	0	0
4	9-B	240	0	0	0	0
4	10-A	254	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	10-B	252	0	0	0	0
4	11-A	232	0	0	0	0
4	11-B	252	0	0	0	0
4	12-A	239	0	0	0	0
4	12-B	263	0	0	0	0
4	13-A	257	0	0	0	0
4	13-B	231	0	0	0	0
4	14-A	251	0	0	0	0
4	14-B	246	0	0	0	0
4	15-A	246	0	0	0	0
4	15-B	239	0	0	0	0
4	16-A	252	0	0	0	0
4	16-B	246	0	0	0	0
4	17-A	246	0	0	0	0
4	17-B	238	0	0	0	0
4	18-A	258	0	0	0	0
4	18-B	251	0	0	0	0
4	19-A	248	0	0	0	0
4	19-B	228	0	0	0	0
4	20-A	237	0	0	0	0
4	20-B	230	0	0	0	0
4	21-A	242	0	0	0	0
4	21-B	240	0	0	0	0
4	22-A	251	0	0	0	0
4	22-B	267	0	0	0	0
4	23-A	248	0	0	0	0
4	23-B	248	0	0	0	0
4	24-A	239	0	0	0	0
4	24-B	241	0	0	0	0
4	25-A	240	0	0	0	0
4	25-B	242	0	0	0	0
All	All	221542	196575	197174	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

5.3.1 Protein backbone

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	546/551 (99%)	497 (91%)	45 (8%)	4 (1%)	26	10
1	1-B	549/551 (100%)	504 (92%)	37 (7%)	8 (2%)	13	2
1	2-A	546/551 (99%)	506 (93%)	35 (6%)	5 (1%)	21	6
1	2-B	549/551 (100%)	504 (92%)	37 (7%)	8 (2%)	13	2
1	3-A	546/551 (99%)	507 (93%)	33 (6%)	6 (1%)	17	4
1	3-B	549/551 (100%)	508 (92%)	34 (6%)	7 (1%)	15	3
1	4-A	546/551 (99%)	511 (94%)	33 (6%)	2 (0%)	39	19
1	4-B	549/551 (100%)	508 (92%)	37 (7%)	4 (1%)	26	10
1	5-A	546/551 (99%)	501 (92%)	33 (6%)	12 (2%)	8	1
1	5-B	549/551 (100%)	509 (93%)	33 (6%)	7 (1%)	15	3
1	6-A	546/551 (99%)	500 (92%)	38 (7%)	8 (2%)	13	2
1	6-B	549/551 (100%)	513 (93%)	32 (6%)	4 (1%)	26	10
1	7-A	546/551 (99%)	507 (93%)	31 (6%)	8 (2%)	13	2
1	7-B	549/551 (100%)	494 (90%)	42 (8%)	13 (2%)	7	1
1	8-A	546/551 (99%)	505 (92%)	35 (6%)	6 (1%)	17	4
1	8-B	549/551 (100%)	516 (94%)	30 (6%)	3 (0%)	34	14
1	9-A	546/551 (99%)	505 (92%)	35 (6%)	6 (1%)	17	4
1	9-B	549/551 (100%)	505 (92%)	36 (7%)	8 (2%)	13	2
1	10-A	546/551 (99%)	499 (91%)	38 (7%)	9 (2%)	12	2
1	10-B	549/551 (100%)	507 (92%)	37 (7%)	5 (1%)	21	6
1	11-A	546/551 (99%)	509 (93%)	34 (6%)	3 (0%)	34	14
1	11-B	549/551 (100%)	508 (92%)	33 (6%)	8 (2%)	13	2
1	12-A	546/551 (99%)	504 (92%)	37 (7%)	5 (1%)	21	6
1	12-B	549/551 (100%)	507 (92%)	36 (7%)	6 (1%)	17	4
1	13-A	546/551 (99%)	502 (92%)	41 (8%)	3 (0%)	34	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	13-B	549/551 (100%)	514 (94%)	31 (6%)	4 (1%)	26	10
1	14-A	546/551 (99%)	505 (92%)	36 (7%)	5 (1%)	21	6
1	14-B	549/551 (100%)	504 (92%)	35 (6%)	10 (2%)	11	1
1	15-A	546/551 (99%)	496 (91%)	39 (7%)	11 (2%)	9	1
1	15-B	549/551 (100%)	505 (92%)	35 (6%)	9 (2%)	12	2
1	16-A	546/551 (99%)	503 (92%)	39 (7%)	4 (1%)	26	10
1	16-B	549/551 (100%)	515 (94%)	28 (5%)	6 (1%)	17	4
1	17-A	546/551 (99%)	500 (92%)	32 (6%)	14 (3%)	7	0
1	17-B	549/551 (100%)	510 (93%)	28 (5%)	11 (2%)	9	1
1	18-A	546/551 (99%)	487 (89%)	49 (9%)	10 (2%)	11	1
1	18-B	549/551 (100%)	506 (92%)	34 (6%)	9 (2%)	12	2
1	19-A	546/551 (99%)	505 (92%)	34 (6%)	7 (1%)	15	3
1	19-B	549/551 (100%)	508 (92%)	32 (6%)	9 (2%)	12	2
1	20-A	546/551 (99%)	508 (93%)	32 (6%)	6 (1%)	17	4
1	20-B	549/551 (100%)	513 (93%)	27 (5%)	9 (2%)	12	2
1	21-A	546/551 (99%)	510 (93%)	27 (5%)	9 (2%)	12	2
1	21-B	549/551 (100%)	510 (93%)	33 (6%)	6 (1%)	17	4
1	22-A	546/551 (99%)	505 (92%)	34 (6%)	7 (1%)	15	3
1	22-B	549/551 (100%)	513 (93%)	29 (5%)	7 (1%)	15	3
1	23-A	546/551 (99%)	510 (93%)	33 (6%)	3 (0%)	34	14
1	23-B	549/551 (100%)	508 (92%)	36 (7%)	5 (1%)	21	6
1	24-A	546/551 (99%)	499 (91%)	38 (7%)	9 (2%)	12	2
1	24-B	549/551 (100%)	505 (92%)	35 (6%)	9 (2%)	12	2
1	25-A	546/551 (99%)	505 (92%)	32 (6%)	9 (2%)	12	2
1	25-B	549/551 (100%)	509 (93%)	34 (6%)	6 (1%)	17	4
All	All	27375/27550 (99%)	25289 (92%)	1734 (6%)	352 (1%)	15	3

5 of 352 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	59	VAL
1	1-A	311	LYS
1	1-B	77	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-B	297	PRO
1	1-B	311	LYS

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	435/437 (100%)	396 (91%)	39 (9%)	12	1
1	1-B	437/437 (100%)	403 (92%)	34 (8%)	16	2
1	2-A	435/437 (100%)	398 (92%)	37 (8%)	13	2
1	2-B	437/437 (100%)	412 (94%)	25 (6%)	25	6
1	3-A	435/437 (100%)	404 (93%)	31 (7%)	18	3
1	3-B	437/437 (100%)	405 (93%)	32 (7%)	17	3
1	4-A	435/437 (100%)	409 (94%)	26 (6%)	24	5
1	4-B	437/437 (100%)	407 (93%)	30 (7%)	19	3
1	5-A	435/437 (100%)	411 (94%)	24 (6%)	27	7
1	5-B	437/437 (100%)	403 (92%)	34 (8%)	16	2
1	6-A	435/437 (100%)	406 (93%)	29 (7%)	20	4
1	6-B	437/437 (100%)	406 (93%)	31 (7%)	18	3
1	7-A	435/437 (100%)	408 (94%)	27 (6%)	23	5
1	7-B	437/437 (100%)	412 (94%)	25 (6%)	25	6
1	8-A	435/437 (100%)	396 (91%)	39 (9%)	12	1
1	8-B	437/437 (100%)	403 (92%)	34 (8%)	16	2
1	9-A	435/437 (100%)	402 (92%)	33 (8%)	16	3
1	9-B	437/437 (100%)	399 (91%)	38 (9%)	13	1
1	10-A	435/437 (100%)	400 (92%)	35 (8%)	15	2
1	10-B	437/437 (100%)	397 (91%)	40 (9%)	11	1
1	11-A	435/437 (100%)	410 (94%)	25 (6%)	25	6
1	11-B	437/437 (100%)	406 (93%)	31 (7%)	18	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	12-A	435/437 (100%)	410 (94%)	25 (6%)	25	6
1	12-B	437/437 (100%)	392 (90%)	45 (10%)	9	1
1	13-A	435/437 (100%)	399 (92%)	36 (8%)	14	2
1	13-B	437/437 (100%)	401 (92%)	36 (8%)	14	2
1	14-A	435/437 (100%)	397 (91%)	38 (9%)	13	1
1	14-B	437/437 (100%)	397 (91%)	40 (9%)	11	1
1	15-A	435/437 (100%)	412 (95%)	23 (5%)	28	7
1	15-B	437/437 (100%)	396 (91%)	41 (9%)	11	1
1	16-A	435/437 (100%)	394 (91%)	41 (9%)	11	1
1	16-B	437/437 (100%)	404 (92%)	33 (8%)	16	3
1	17-A	435/437 (100%)	396 (91%)	39 (9%)	12	1
1	17-B	437/437 (100%)	402 (92%)	35 (8%)	15	2
1	18-A	435/437 (100%)	391 (90%)	44 (10%)	9	1
1	18-B	437/437 (100%)	403 (92%)	34 (8%)	16	2
1	19-A	435/437 (100%)	395 (91%)	40 (9%)	11	1
1	19-B	437/437 (100%)	401 (92%)	36 (8%)	14	2
1	20-A	435/437 (100%)	408 (94%)	27 (6%)	23	5
1	20-B	437/437 (100%)	405 (93%)	32 (7%)	17	3
1	21-A	435/437 (100%)	399 (92%)	36 (8%)	14	2
1	21-B	437/437 (100%)	401 (92%)	36 (8%)	14	2
1	22-A	435/437 (100%)	413 (95%)	22 (5%)	29	8
1	22-B	437/437 (100%)	396 (91%)	41 (9%)	11	1
1	23-A	435/437 (100%)	401 (92%)	34 (8%)	16	2
1	23-B	437/437 (100%)	401 (92%)	36 (8%)	14	2
1	24-A	435/437 (100%)	401 (92%)	34 (8%)	16	2
1	24-B	437/437 (100%)	400 (92%)	37 (8%)	13	2
1	25-A	435/437 (100%)	405 (93%)	30 (7%)	19	3
1	25-B	437/437 (100%)	394 (90%)	43 (10%)	10	1
All	All	21800/21850 (100%)	20107 (92%)	1693 (8%)	16	2

5 of 1693 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	12-B	574	LEU
1	15-B	126	LEU
1	24-A	271	LEU
1	13-A	311	LYS
1	14-A	306	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 465 such sidechains are listed below:

Mol	Chain	Res	Type
1	12-B	67	ASN
1	15-B	337	HIS
1	24-A	337	HIS
1	12-B	450	HIS
1	14-A	92	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](#)

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	EDO	1-A	701	-	3,3,3	0.66	0	2,2,2	0.34	0
2	EDO	1-A	702	-	3,3,3	0.55	0	2,2,2	0.61	0
3	BGC	1-B	701	-	12,12,12	0.84	0	17,17,17	2.17	7 (41%)
2	EDO	1-B	702	-	3,3,3	0.37	0	2,2,2	0.19	0
2	EDO	1-B	703	-	3,3,3	0.46	0	2,2,2	0.36	0
2	EDO	1-B	704	-	3,3,3	0.91	0	2,2,2	0.47	0
2	EDO	10-A	701	-	3,3,3	0.49	0	2,2,2	0.29	0
2	EDO	10-A	702	-	3,3,3	0.65	0	2,2,2	0.43	0
3	BGC	10-B	701	-	12,12,12	0.66	0	17,17,17	2.20	8 (47%)
2	EDO	10-B	702	-	3,3,3	0.40	0	2,2,2	0.42	0
2	EDO	10-B	703	-	3,3,3	0.47	0	2,2,2	0.36	0
2	EDO	10-B	704	-	3,3,3	0.51	0	2,2,2	0.59	0
2	EDO	11-A	701	-	3,3,3	0.52	0	2,2,2	0.23	0
2	EDO	11-A	702	-	3,3,3	0.68	0	2,2,2	0.52	0
3	BGC	11-B	701	-	12,12,12	0.91	0	17,17,17	2.50	4 (23%)
2	EDO	11-B	702	-	3,3,3	0.38	0	2,2,2	0.36	0
2	EDO	11-B	703	-	3,3,3	0.50	0	2,2,2	0.24	0
2	EDO	11-B	704	-	3,3,3	0.50	0	2,2,2	0.79	0
2	EDO	12-A	701	-	3,3,3	0.51	0	2,2,2	0.33	0
2	EDO	12-A	702	-	3,3,3	0.64	0	2,2,2	0.53	0
3	BGC	12-B	701	-	12,12,12	0.74	0	17,17,17	1.96	5 (29%)
2	EDO	12-B	702	-	3,3,3	0.35	0	2,2,2	0.13	0
2	EDO	12-B	703	-	3,3,3	0.47	0	2,2,2	0.25	0
2	EDO	12-B	704	-	3,3,3	0.51	0	2,2,2	0.49	0
2	EDO	13-A	701	-	3,3,3	0.49	0	2,2,2	0.35	0
2	EDO	13-A	702	-	3,3,3	0.62	0	2,2,2	0.43	0
3	BGC	13-B	701	-	12,12,12	1.12	2 (16%)	17,17,17	1.31	2 (11%)
2	EDO	13-B	702	-	3,3,3	0.48	0	2,2,2	0.63	0
2	EDO	13-B	703	-	3,3,3	0.47	0	2,2,2	0.40	0
2	EDO	13-B	704	-	3,3,3	0.50	0	2,2,2	0.31	0
2	EDO	14-A	701	-	3,3,3	0.49	0	2,2,2	0.40	0
2	EDO	14-A	702	-	3,3,3	0.58	0	2,2,2	0.44	0
3	BGC	14-B	701	-	12,12,12	1.16	1 (8%)	17,17,17	2.41	8 (47%)
2	EDO	14-B	702	-	3,3,3	0.48	0	2,2,2	0.33	0
2	EDO	14-B	703	-	3,3,3	0.46	0	2,2,2	0.39	0
2	EDO	14-B	704	-	3,3,3	0.47	0	2,2,2	0.24	0
2	EDO	15-A	701	-	3,3,3	0.56	0	2,2,2	0.37	0
2	EDO	15-A	702	-	3,3,3	0.61	0	2,2,2	0.55	0
3	BGC	15-B	701	-	12,12,12	0.88	0	17,17,17	2.29	4 (23%)
2	EDO	15-B	702	-	3,3,3	0.41	0	2,2,2	0.44	0
2	EDO	15-B	703	-	3,3,3	0.49	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	15-B	704	-	3,3,3	0.26	0	2,2,2	1.00	0
2	EDO	16-A	701	-	3,3,3	0.52	0	2,2,2	0.58	0
2	EDO	16-A	702	-	3,3,3	0.68	0	2,2,2	0.52	0
3	BGC	16-B	701	-	12,12,12	0.83	0	17,17,17	1.70	4 (23%)
2	EDO	16-B	702	-	3,3,3	0.47	0	2,2,2	0.42	0
2	EDO	16-B	703	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	16-B	704	-	3,3,3	0.61	0	2,2,2	0.23	0
2	EDO	17-A	701	-	3,3,3	0.47	0	2,2,2	0.43	0
2	EDO	17-A	702	-	3,3,3	0.64	0	2,2,2	0.49	0
3	BGC	17-B	701	-	12,12,12	1.30	2 (16%)	17,17,17	2.91	9 (52%)
2	EDO	17-B	702	-	3,3,3	0.43	0	2,2,2	0.59	0
2	EDO	17-B	703	-	3,3,3	0.57	0	2,2,2	0.26	0
2	EDO	17-B	704	-	3,3,3	0.61	0	2,2,2	0.86	0
2	EDO	18-A	701	-	3,3,3	0.47	0	2,2,2	0.23	0
2	EDO	18-A	702	-	3,3,3	0.60	0	2,2,2	0.49	0
3	BGC	18-B	701	-	12,12,12	0.64	0	17,17,17	2.40	9 (52%)
2	EDO	18-B	702	-	3,3,3	0.44	0	2,2,2	0.46	0
2	EDO	18-B	703	-	3,3,3	0.47	0	2,2,2	0.27	0
2	EDO	18-B	704	-	3,3,3	0.55	0	2,2,2	0.16	0
2	EDO	19-A	701	-	3,3,3	0.54	0	2,2,2	0.28	0
2	EDO	19-A	702	-	3,3,3	0.63	0	2,2,2	0.64	0
3	BGC	19-B	701	-	12,12,12	0.80	0	17,17,17	1.92	5 (29%)
2	EDO	19-B	702	-	3,3,3	0.45	0	2,2,2	0.61	0
2	EDO	19-B	703	-	3,3,3	0.51	0	2,2,2	0.49	0
2	EDO	19-B	704	-	3,3,3	0.46	0	2,2,2	1.71	0
2	EDO	2-A	701	-	3,3,3	0.46	0	2,2,2	0.33	0
2	EDO	2-A	702	-	3,3,3	0.62	0	2,2,2	0.53	0
3	BGC	2-B	701	-	12,12,12	1.01	0	17,17,17	2.38	8 (47%)
2	EDO	2-B	702	-	3,3,3	0.42	0	2,2,2	0.18	0
2	EDO	2-B	703	-	3,3,3	0.48	0	2,2,2	0.26	0
2	EDO	2-B	704	-	3,3,3	0.94	0	2,2,2	0.74	0
2	EDO	20-A	701	-	3,3,3	0.49	0	2,2,2	0.43	0
2	EDO	20-A	702	-	3,3,3	0.65	0	2,2,2	0.52	0
3	BGC	20-B	701	-	12,12,12	1.04	0	17,17,17	2.31	5 (29%)
2	EDO	20-B	702	-	3,3,3	0.48	0	2,2,2	0.77	0
2	EDO	20-B	703	-	3,3,3	0.45	0	2,2,2	0.41	0
2	EDO	20-B	704	-	3,3,3	0.49	0	2,2,2	0.79	0
2	EDO	21-A	701	-	3,3,3	0.53	0	2,2,2	0.37	0
2	EDO	21-A	702	-	3,3,3	0.62	0	2,2,2	0.60	0
3	BGC	21-B	701	-	12,12,12	0.82	0	17,17,17	2.73	11 (64%)
2	EDO	21-B	702	-	3,3,3	0.42	0	2,2,2	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	21-B	703	-	3,3,3	0.46	0	2,2,2	0.22	0
2	EDO	21-B	704	-	3,3,3	0.42	0	2,2,2	0.32	0
2	EDO	22-A	701	-	3,3,3	0.52	0	2,2,2	0.43	0
2	EDO	22-A	702	-	3,3,3	0.69	0	2,2,2	0.51	0
3	BGC	22-B	701	-	12,12,12	0.77	0	17,17,17	2.34	4 (23%)
2	EDO	22-B	702	-	3,3,3	0.45	0	2,2,2	0.28	0
2	EDO	22-B	703	-	3,3,3	0.49	0	2,2,2	0.39	0
2	EDO	22-B	704	-	3,3,3	0.45	0	2,2,2	0.95	0
2	EDO	23-A	701	-	3,3,3	0.55	0	2,2,2	0.46	0
2	EDO	23-A	702	-	3,3,3	0.58	0	2,2,2	0.58	0
3	BGC	23-B	701	-	12,12,12	0.67	0	17,17,17	2.03	5 (29%)
2	EDO	23-B	702	-	3,3,3	0.51	0	2,2,2	0.08	0
2	EDO	23-B	703	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	23-B	704	-	3,3,3	0.58	0	2,2,2	0.07	0
2	EDO	24-A	701	-	3,3,3	0.55	0	2,2,2	0.36	0
2	EDO	24-A	702	-	3,3,3	0.61	0	2,2,2	0.47	0
3	BGC	24-B	701	-	12,12,12	0.71	0	17,17,17	1.74	4 (23%)
2	EDO	24-B	702	-	3,3,3	0.34	0	2,2,2	0.50	0
2	EDO	24-B	703	-	3,3,3	0.45	0	2,2,2	0.36	0
2	EDO	24-B	704	-	3,3,3	0.49	0	2,2,2	1.24	0
2	EDO	25-A	701	-	3,3,3	0.60	0	2,2,2	0.29	0
2	EDO	25-A	702	-	3,3,3	0.65	0	2,2,2	0.44	0
3	BGC	25-B	701	-	12,12,12	0.91	1 (8%)	17,17,17	2.43	7 (41%)
2	EDO	25-B	702	-	3,3,3	0.41	0	2,2,2	0.42	0
2	EDO	25-B	703	-	3,3,3	0.48	0	2,2,2	0.45	0
2	EDO	25-B	704	-	3,3,3	0.41	0	2,2,2	0.23	0
2	EDO	3-A	701	-	3,3,3	0.53	0	2,2,2	0.38	0
2	EDO	3-A	702	-	3,3,3	0.63	0	2,2,2	0.39	0
3	BGC	3-B	701	-	12,12,12	1.08	1 (8%)	17,17,17	1.93	6 (35%)
2	EDO	3-B	702	-	3,3,3	0.31	0	2,2,2	0.41	0
2	EDO	3-B	703	-	3,3,3	0.48	0	2,2,2	0.31	0
2	EDO	3-B	704	-	3,3,3	0.54	0	2,2,2	0.63	0
2	EDO	4-A	701	-	3,3,3	0.51	0	2,2,2	0.38	0
2	EDO	4-A	702	-	3,3,3	0.67	0	2,2,2	0.40	0
3	BGC	4-B	701	-	12,12,12	0.98	0	17,17,17	1.43	2 (11%)
2	EDO	4-B	702	-	3,3,3	0.45	0	2,2,2	0.54	0
2	EDO	4-B	703	-	3,3,3	0.44	0	2,2,2	0.44	0
2	EDO	4-B	704	-	3,3,3	0.43	0	2,2,2	0.86	0
2	EDO	5-A	701	-	3,3,3	0.54	0	2,2,2	0.48	0
2	EDO	5-A	702	-	3,3,3	0.68	0	2,2,2	0.43	0
3	BGC	5-B	701	-	12,12,12	0.77	0	17,17,17	2.27	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	5-B	702	-	3,3,3	0.36	0	2,2,2	0.38	0
2	EDO	5-B	703	-	3,3,3	0.48	0	2,2,2	0.49	0
2	EDO	5-B	704	-	3,3,3	0.61	0	2,2,2	0.40	0
2	EDO	6-A	701	-	3,3,3	0.58	0	2,2,2	0.48	0
2	EDO	6-A	702	-	3,3,3	0.66	0	2,2,2	0.49	0
3	BGC	6-B	701	-	12,12,12	0.91	0	17,17,17	1.94	4 (23%)
2	EDO	6-B	702	-	3,3,3	0.29	0	2,2,2	0.62	0
2	EDO	6-B	703	-	3,3,3	0.51	0	2,2,2	0.32	0
2	EDO	6-B	704	-	3,3,3	0.52	0	2,2,2	0.53	0
2	EDO	7-A	701	-	3,3,3	0.50	0	2,2,2	0.27	0
2	EDO	7-A	702	-	3,3,3	0.62	0	2,2,2	0.54	0
3	BGC	7-B	701	-	12,12,12	0.96	0	17,17,17	1.52	4 (23%)
2	EDO	7-B	702	-	3,3,3	0.35	0	2,2,2	0.56	0
2	EDO	7-B	703	-	3,3,3	0.43	0	2,2,2	0.37	0
2	EDO	7-B	704	-	3,3,3	0.52	0	2,2,2	0.47	0
2	EDO	8-A	701	-	3,3,3	0.63	0	2,2,2	0.31	0
2	EDO	8-A	702	-	3,3,3	0.64	0	2,2,2	0.44	0
3	BGC	8-B	701	-	12,12,12	0.77	0	17,17,17	1.92	5 (29%)
2	EDO	8-B	702	-	3,3,3	0.39	0	2,2,2	0.26	0
2	EDO	8-B	703	-	3,3,3	0.41	0	2,2,2	0.51	0
2	EDO	8-B	704	-	3,3,3	0.62	0	2,2,2	0.18	0
2	EDO	9-A	701	-	3,3,3	0.50	0	2,2,2	0.35	0
2	EDO	9-A	702	-	3,3,3	0.62	0	2,2,2	0.52	0
3	BGC	9-B	701	-	12,12,12	0.56	0	17,17,17	3.33	9 (52%)
2	EDO	9-B	702	-	3,3,3	0.40	0	2,2,2	0.19	0
2	EDO	9-B	703	-	3,3,3	0.44	0	2,2,2	0.29	0
2	EDO	9-B	704	-	3,3,3	0.48	0	2,2,2	0.82	0

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	EDO	1-A	701	-	-	0/1/1/1	0/0/0/0
2	EDO	1-A	702	-	-	0/1/1/1	0/0/0/0
3	BGC	1-B	701	-	-	0/2/22/22	0/1/1/1
2	EDO	1-B	702	-	-	0/1/1/1	0/0/0/0
2	EDO	1-B	703	-	-	0/1/1/1	0/0/0/0
2	EDO	1-B	704	-	-	0/1/1/1	0/0/0/0
2	EDO	10-A	701	-	-	0/1/1/1	0/0/0/0
2	EDO	10-A	702	-	-	0/1/1/1	0/0/0/0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-B	701	BGC	O3-C3	-3.07	1.35	1.43
3	17-B	701	BGC	C1-C2	2.02	1.56	1.52
3	25-B	701	BGC	C1-C2	2.03	1.56	1.52
3	13-B	701	BGC	C4-C3	2.04	1.57	1.52
3	17-B	701	BGC	C4-C5	2.04	1.57	1.53

The worst 5 of 145 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-B	701	BGC	O4-C4-C3	-8.43	91.36	110.34
3	9-B	701	BGC	C1-O5-C5	-5.61	103.10	113.47
3	8-B	701	BGC	C1-C2-C3	-5.43	102.36	110.43
3	11-B	701	BGC	C1-C2-C3	-5.28	102.58	110.43
3	17-B	701	BGC	C4-C3-C2	-4.96	101.54	110.79

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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