



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

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

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

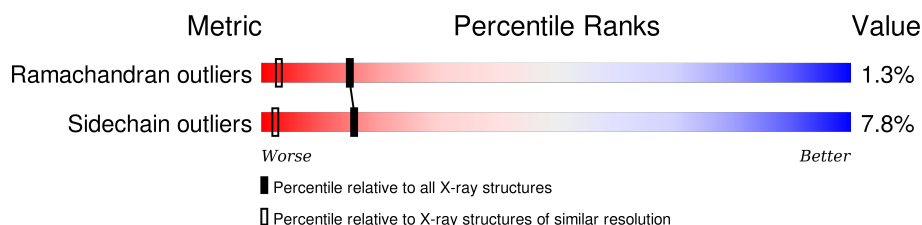
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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)














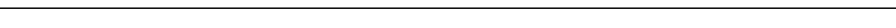


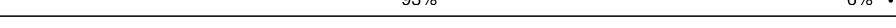








The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey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












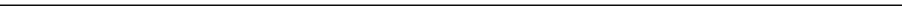





Continued on next page...

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	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	2-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	3-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	4-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	5-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	6-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	7-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	8-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	9-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	10-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	11-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	12-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	13-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	14-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	15-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			
1	16-A	548	Total	C	H	N	O	S	0	0	0
			8059	2624	3901	707	822	5			

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...

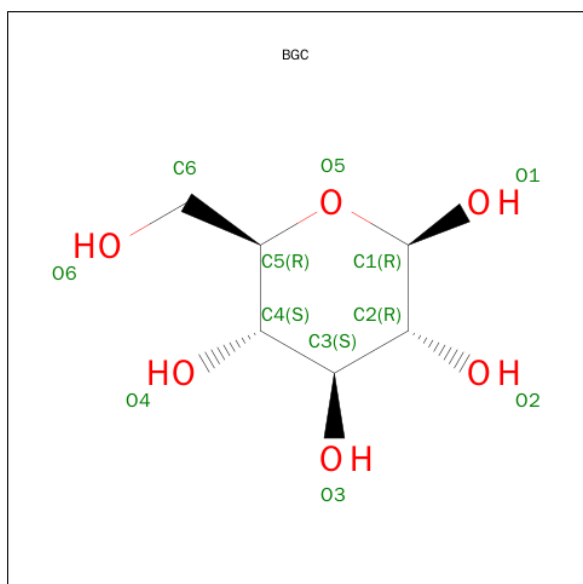
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	24-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	25-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	1-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	2-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	3-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	4-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	5-B	1	Total	C	H	O	0	0
		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

Continued on next page...

Continued from previous page...

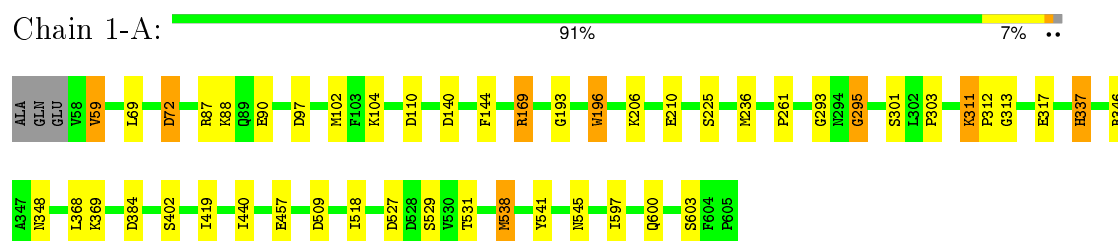
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	19-B	228	Total 228	O 228	0	0
4	20-B	230	Total 230	O 230	0	0
4	21-B	240	Total 240	O 240	0	0
4	22-B	267	Total 267	O 267	0	0
4	23-B	248	Total 248	O 248	0	0
4	24-B	241	Total 241	O 241	0	0
4	25-B	242	Total 242	O 242	0	0

3 Residue-property plots [i](#)

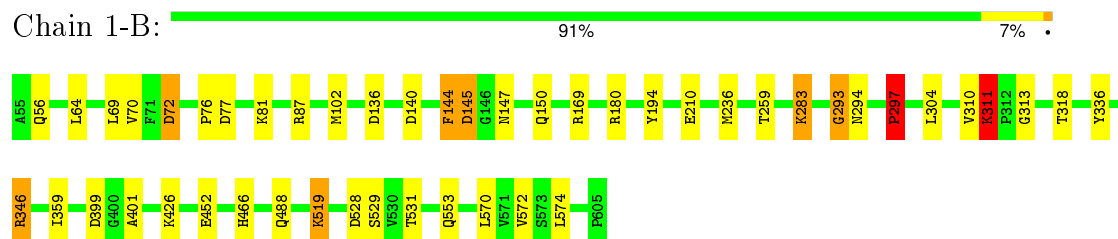
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

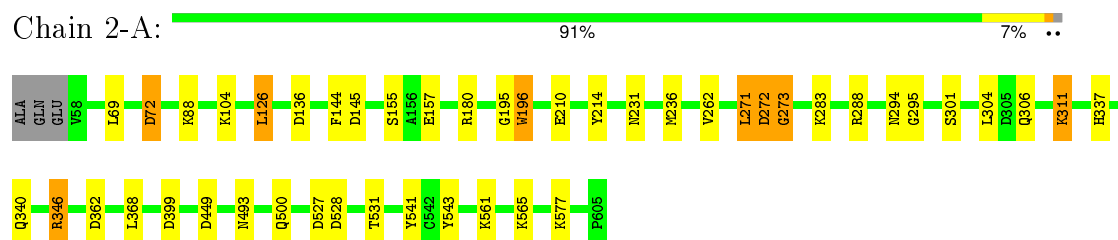
- Molecule 1: Putative secreted protein



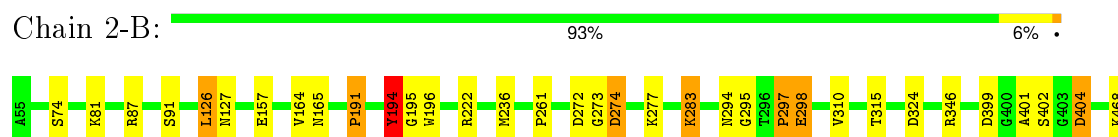
- Molecule 1: Putative secreted protein



- Molecule 1: Putative secreted protein



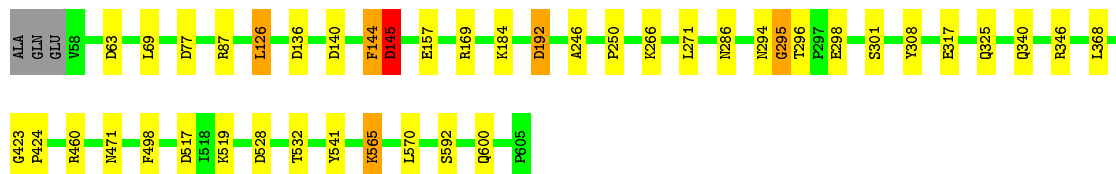
- Molecule 1: Putative secreted protein





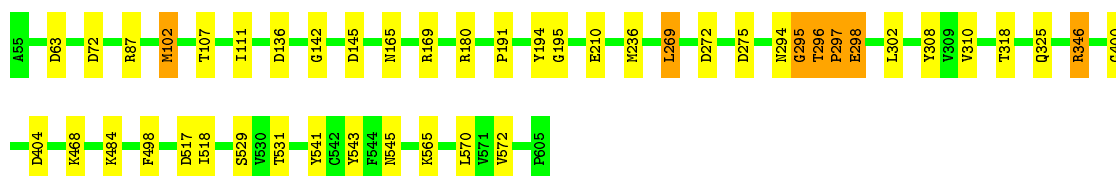
- Molecule 1: Putative secreted protein

Chain 3-A: 92% 7% ..



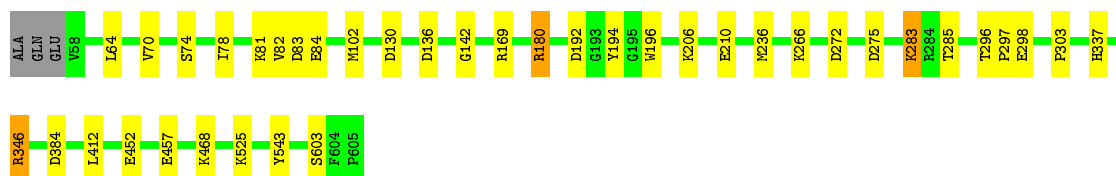
- Molecule 1: Putative secreted protein

Chain 3-B: 92% 7% .



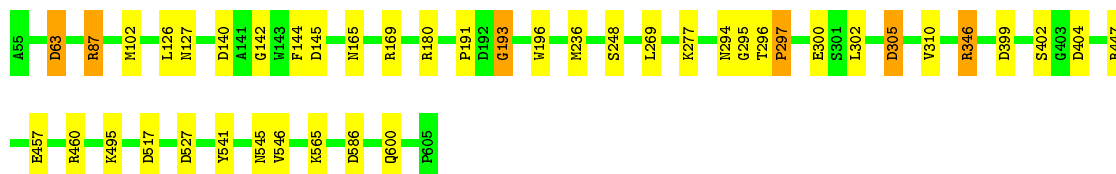
- Molecule 1: Putative secreted protein

Chain 4-A: 92% 7% ..



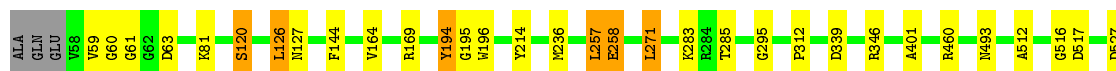
- Molecule 1: Putative secreted protein

Chain 4-B: 92% 7% .



- Molecule 1: Putative secreted protein

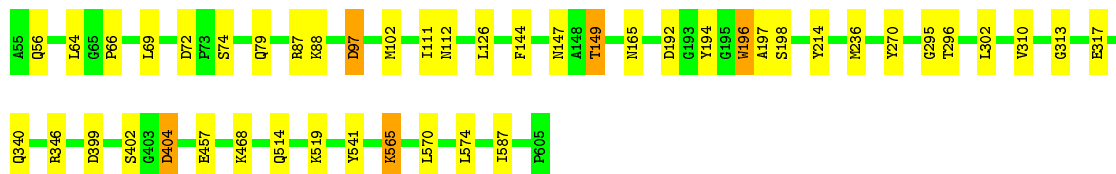
Chain 5-A: 93% 6% ..





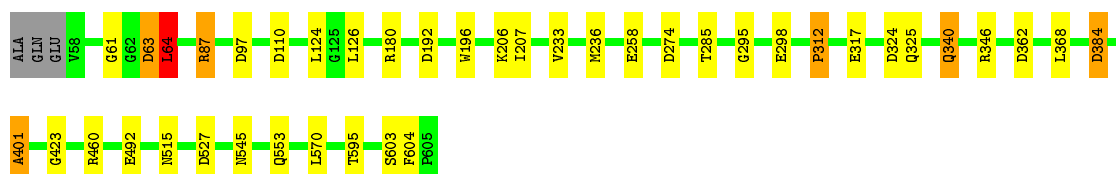
- Molecule 1: Putative secreted protein

Chain 5-B: 92% 7% .



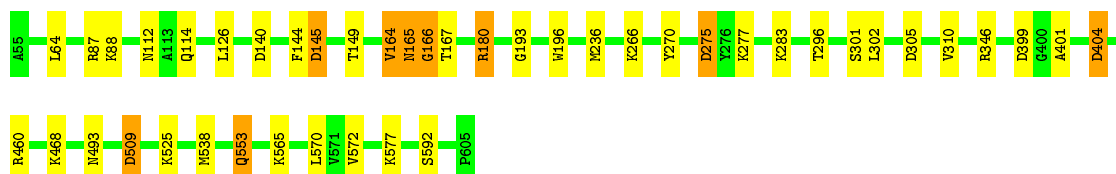
- Molecule 1: Putative secreted protein

Chain 6-A: 92% 6% ..



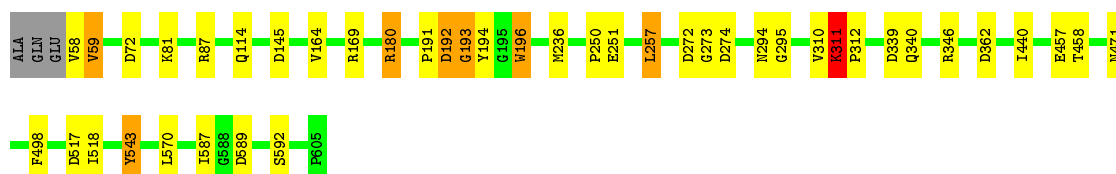
- Molecule 1: Putative secreted protein

Chain 6-B: 92% 6% .



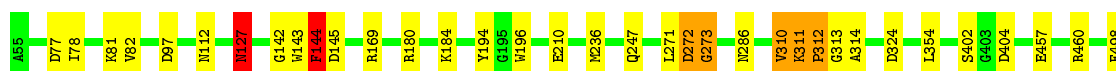
- Molecule 1: Putative secreted protein

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% .



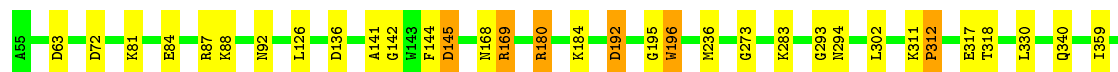
- Molecule 1: Putative secreted protein

Chain 9-A: 91% 7% ..



- Molecule 1: Putative secreted protein

Chain 9-B: 90% 9% .



- Molecule 1: Putative secreted protein

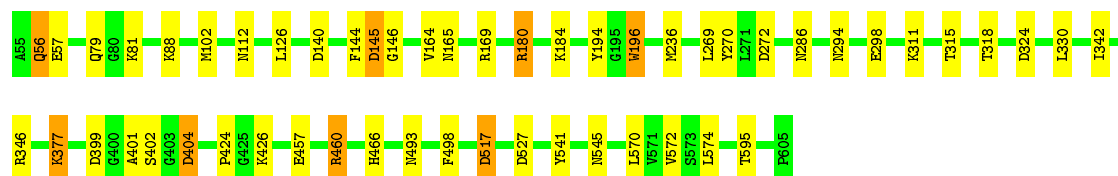
Chain 10-A: 90% 7% ..





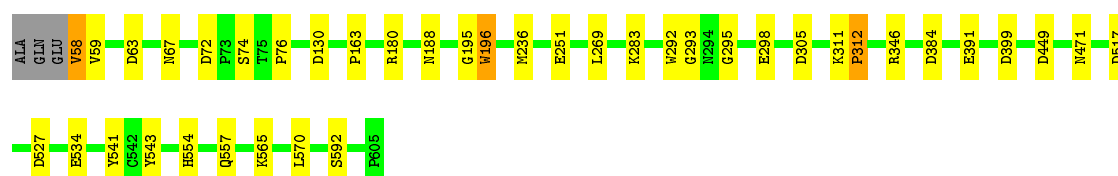
- Molecule 1: Putative secreted protein

Chain 10-B: 90% 8% .



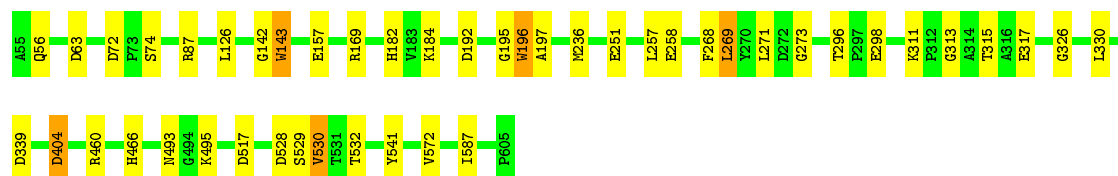
- Molecule 1: Putative secreted protein

Chain 11-A: 92% 7% ..



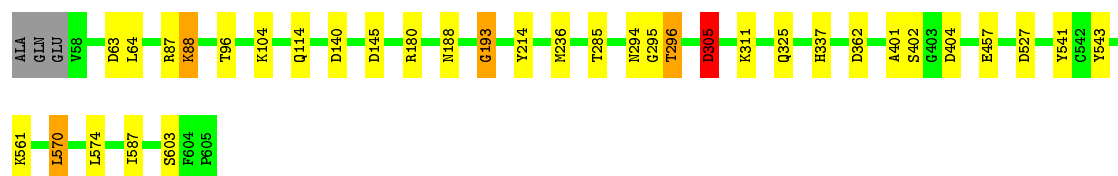
- Molecule 1: Putative secreted protein

Chain 11-B: 92% 7% .



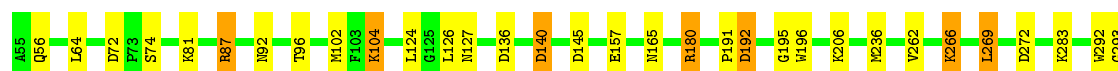
- Molecule 1: Putative secreted protein

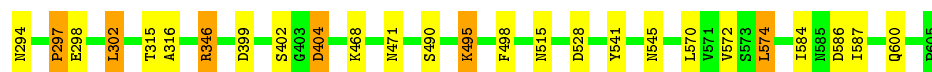
Chain 12-A: 93% 5% ..



- Molecule 1: Putative secreted protein

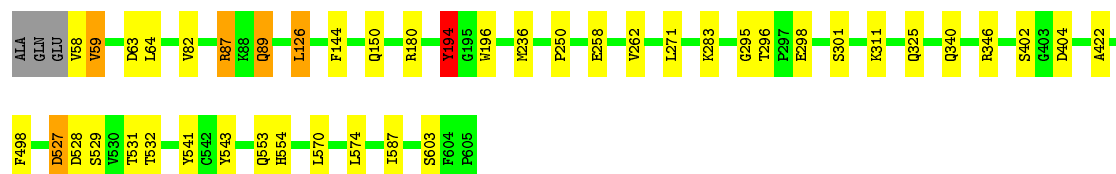
Chain 12-B: 89% 8% .





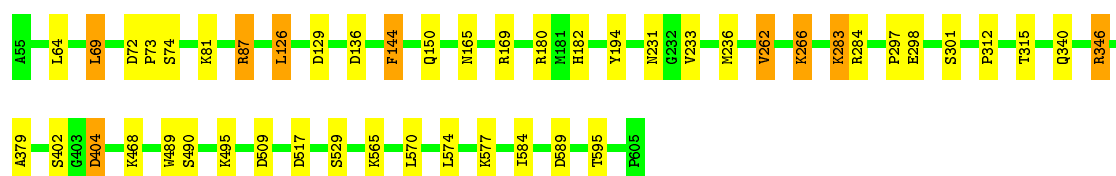
- Molecule 1: Putative secreted protein

Chain 13-A: 91% 7% ..



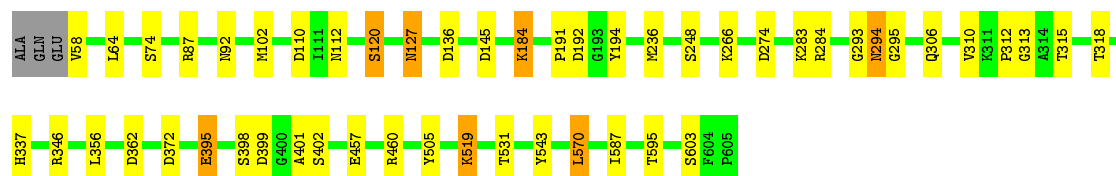
- Molecule 1: Putative secreted protein

Chain 13-B: 91% 7% .



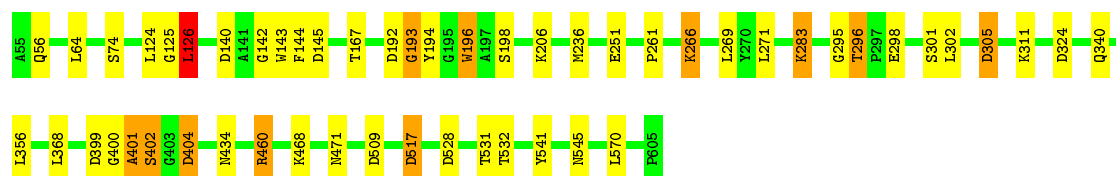
- Molecule 1: Putative secreted protein

Chain 14-A: 90% 8% ..



- Molecule 1: Putative secreted protein

Chain 14-B: 90% 7% .



- Molecule 1: Putative secreted protein

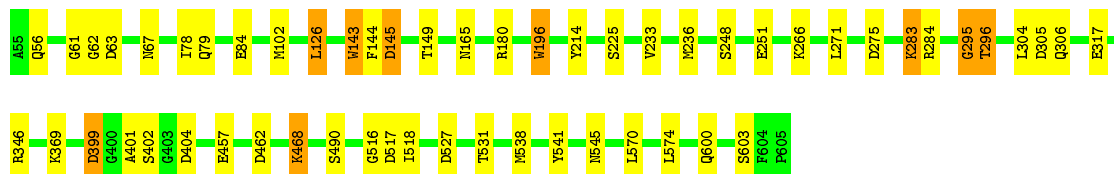
Chain 15-A: 91% 7% ..





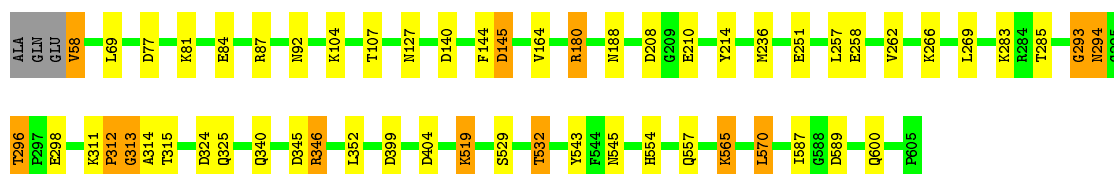
- Molecule 1: Putative secreted protein

Chain 15-B: 90% 9%



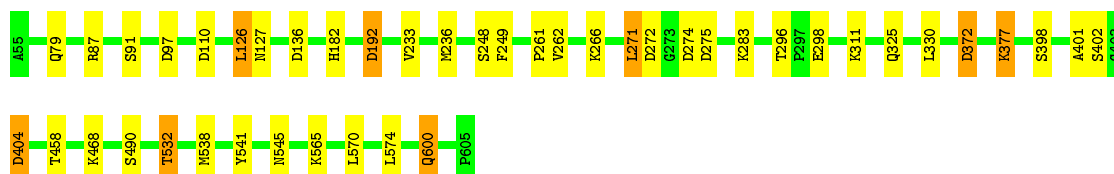
- Molecule 1: Putative secreted protein

Chain 16-A: 89% 8%



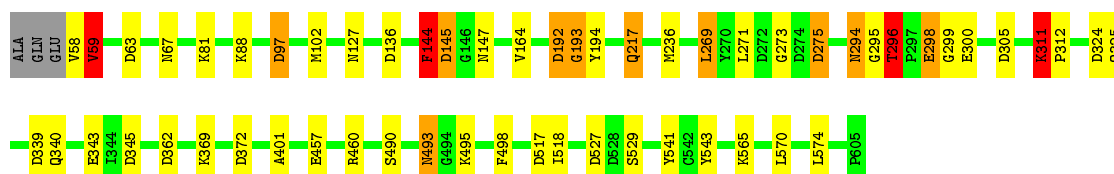
- Molecule 1: Putative secreted protein

Chain 16-B: 92% 7%



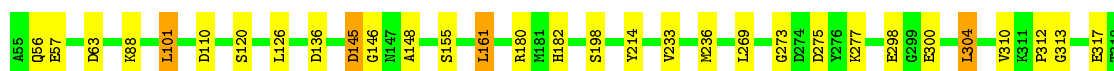
- Molecule 1: Putative secreted protein

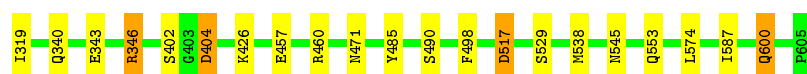
Chain 17-A: 89% 8%



- Molecule 1: Putative secreted protein

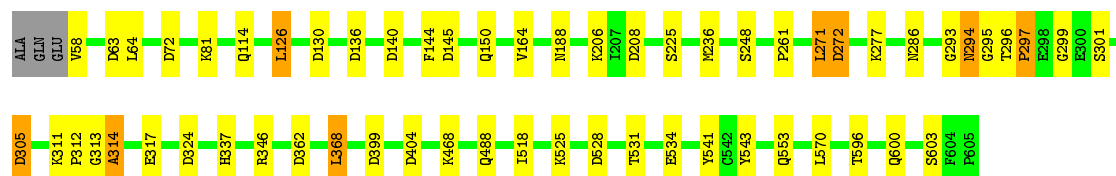
Chain 17-B: 91% 8%





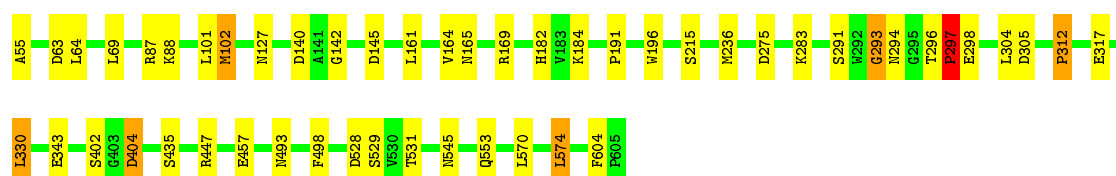
- Molecule 1: Putative secreted protein

Chain 18-A: 89% 9% ..



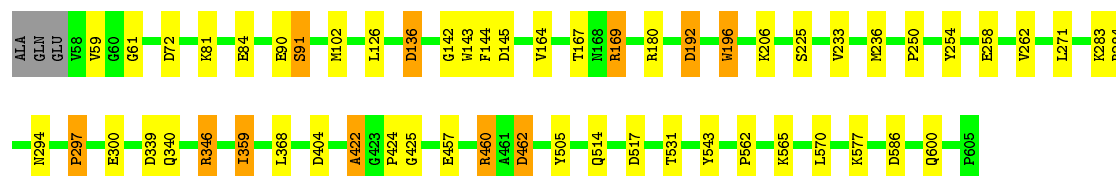
- Molecule 1: Putative secreted protein

Chain 18-B: 91% 8% .



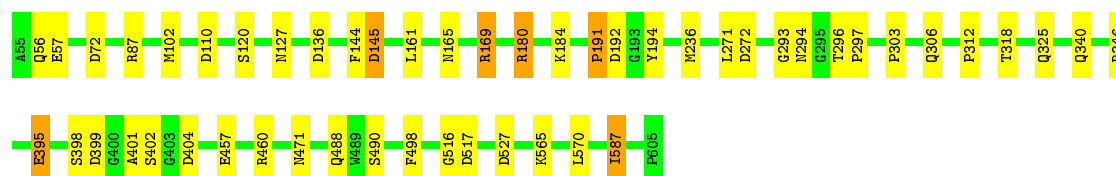
- Molecule 1: Putative secreted protein

Chain 19-A: 89% 8% ..



- Molecule 1: Putative secreted protein

Chain 19-B: 91% 8% .



- Molecule 1: Putative secreted protein

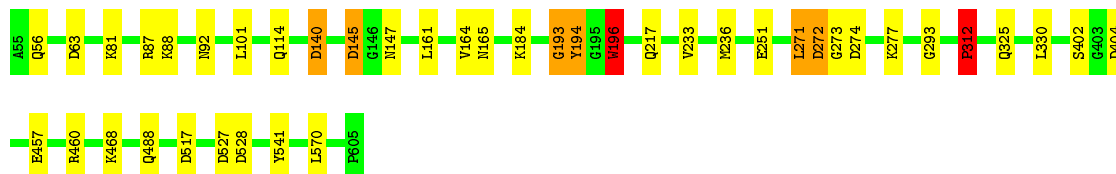
Chain 20-A: 92% 7% ..





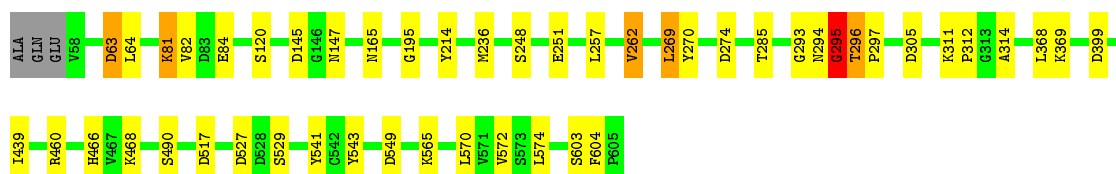
- Molecule 1: Putative secreted protein

Chain 20-B: 92% 6% •



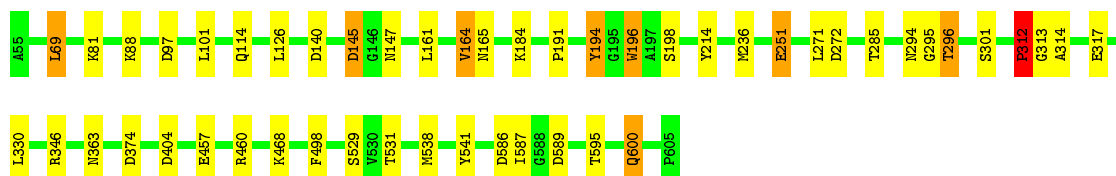
- Molecule 1: Putative secreted protein

Chain 21-A: 91% 8% ••



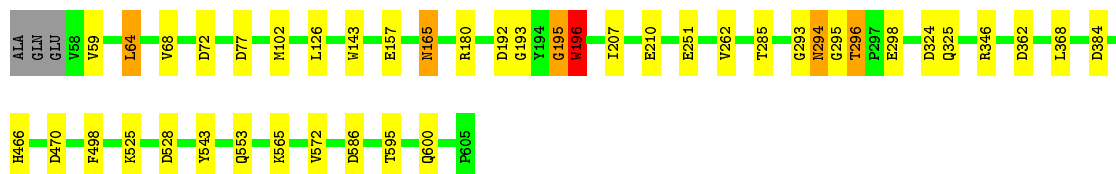
- Molecule 1: Putative secreted protein

Chain 21-B: 91% 7% •



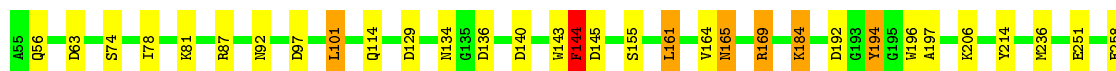
- Molecule 1: Putative secreted protein

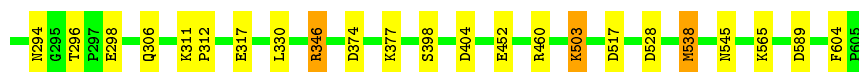
Chain 22-A: 92% 7% ••



- Molecule 1: Putative secreted protein

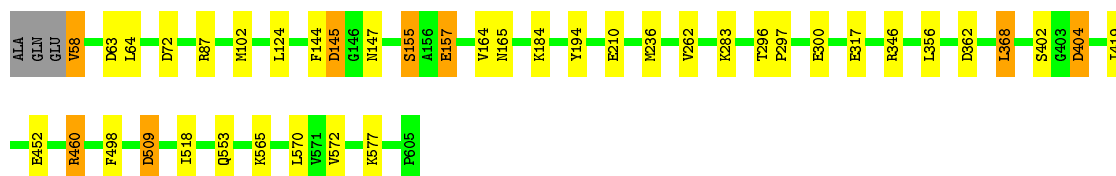
Chain 22-B: 90% 8% •





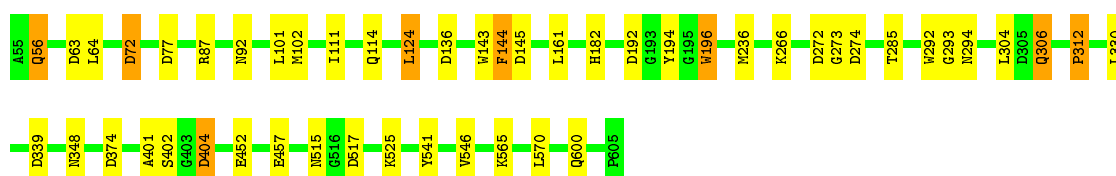
- Molecule 1: Putative secreted protein

Chain 23-A: 92% 6% ..



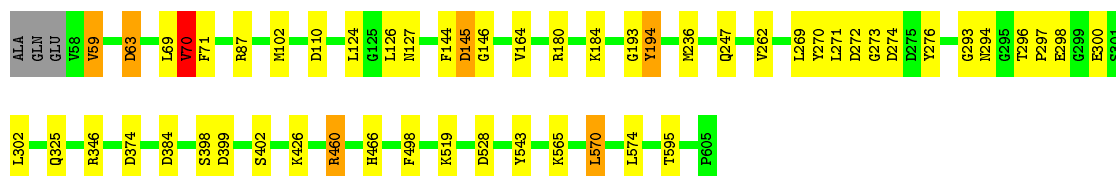
- Molecule 1: Putative secreted protein

Chain 23-B: 91% 8% •



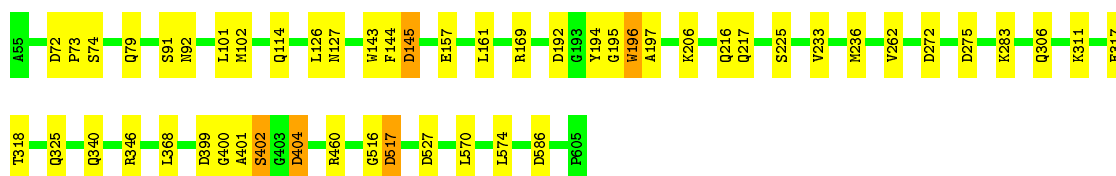
- Molecule 1: Putative secreted protein

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

Chain 25-B:
90% 9%



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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

All (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
1	3-B	310	VAL	CB-CG1	-10.38	1.31	1.52
1	8-B	310	VAL	CB-CG1	-10.29	1.31	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-B	310	VAL	CB-CG2	-10.19	1.31	1.52
1	24-B	196	TRP	CB-CG	9.95	1.68	1.50
1	15-B	196	TRP	CB-CG	9.68	1.67	1.50
1	22-A	572	VAL	CB-CG1	-9.36	1.33	1.52
1	19-A	91	SER	CB-OG	-9.12	1.30	1.42
1	20-B	196	TRP	CB-CG	9.06	1.66	1.50
1	3-A	157	GLU	CD-OE1	8.92	1.35	1.25
1	7-B	196	TRP	CB-CG	8.80	1.66	1.50
1	13-A	194	TYR	CG-CD2	-8.48	1.28	1.39
1	17-A	217	GLN	CB-CG	-8.45	1.29	1.52
1	10-B	572	VAL	CB-CG1	-8.43	1.35	1.52
1	15-B	468	LYS	CB-CG	-8.42	1.29	1.52
1	24-B	143	TRP	CB-CG	-8.35	1.35	1.50
1	3-A	157	GLU	CG-CD	8.25	1.64	1.51
1	14-B	404	ASP	CB-CG	8.06	1.68	1.51
1	7-B	457	GLU	CB-CG	8.04	1.67	1.52
1	14-A	120	SER	CB-OG	-8.03	1.31	1.42
1	14-B	283	LYS	CB-CG	7.88	1.73	1.52
1	11-A	251	GLU	CB-CG	-7.87	1.37	1.52
1	13-B	266	LYS	CD-CE	7.85	1.70	1.51
1	2-B	492	GLU	CB-CG	7.84	1.67	1.52
1	11-B	404	ASP	CB-CG	7.76	1.68	1.51
1	5-B	457	GLU	CG-CD	7.75	1.63	1.51
1	13-A	194	TYR	CD2-CE2	7.73	1.50	1.39
1	7-A	196	TRP	CB-CG	7.70	1.64	1.50
1	5-A	258	GLU	CG-CD	7.66	1.63	1.51
1	6-A	340	GLN	CB-CG	7.66	1.73	1.52
1	23-A	155	SER	CB-OG	-7.65	1.32	1.42
1	20-A	196	TRP	CB-CG	7.61	1.64	1.50
1	4-A	266	LYS	CE-NZ	7.59	1.68	1.49
1	9-B	572	VAL	CB-CG1	-7.55	1.36	1.52
1	4-B	102	MET	CB-CG	7.47	1.75	1.51
1	19-A	457	GLU	CG-CD	7.45	1.63	1.51
1	8-B	572	VAL	CB-CG1	-7.43	1.37	1.52
1	16-A	266	LYS	CE-NZ	7.34	1.67	1.49
1	17-B	485	TYR	CD2-CE2	-7.28	1.28	1.39
1	23-B	404	ASP	CB-CG	7.20	1.66	1.51
1	5-A	120	SER	CB-OG	-7.19	1.32	1.42
1	5-B	310	VAL	CB-CG2	-7.11	1.38	1.52
1	3-B	308	TYR	CD1-CE1	-7.06	1.28	1.39
1	16-B	266	LYS	CE-NZ	6.93	1.66	1.49
1	12-B	404	ASP	CB-CG	6.93	1.66	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16-B	404	ASP	CB-CG	6.93	1.66	1.51
1	19-B	457	GLU	CG-CD	6.86	1.62	1.51
1	1-A	169	ARG	CG-CD	6.85	1.69	1.51
1	4-B	346	ARG	CB-CG	-6.82	1.34	1.52
1	7-B	572	VAL	CB-CG1	-6.80	1.38	1.52
1	10-A	457	GLU	CG-CD	-6.79	1.41	1.51
1	24-B	404	ASP	CB-CG	6.79	1.66	1.51
1	1-B	572	VAL	CB-CG2	-6.78	1.38	1.52
1	8-B	404	ASP	CB-CG	6.74	1.66	1.51
1	19-A	84	GLU	CB-CG	-6.73	1.39	1.52
1	17-A	298	GLU	CB-CG	6.69	1.64	1.52
1	19-B	490	SER	CB-OG	-6.67	1.33	1.42
1	17-B	88	LYS	CB-CG	6.64	1.70	1.52
1	13-A	89	GLN	CB-CG	-6.64	1.34	1.52
1	13-B	404	ASP	CB-CG	6.63	1.65	1.51
1	23-A	157	GLU	CD-OE1	6.63	1.32	1.25
1	18-B	404	ASP	CB-CG	6.63	1.65	1.51
1	19-A	258	GLU	CG-CD	6.62	1.61	1.51
1	2-B	572	VAL	CB-CG1	-6.57	1.39	1.52
1	16-B	377	LYS	CB-CG	-6.57	1.34	1.52
1	6-B	404	ASP	CB-CG	6.56	1.65	1.51
1	9-B	395	GLU	CB-CG	-6.50	1.39	1.52
1	20-A	577	LYS	CD-CE	6.42	1.67	1.51
1	13-A	194	TYR	CE1-CZ	-6.35	1.30	1.38
1	3-B	169	ARG	CB-CG	-6.34	1.35	1.52
1	4-A	266	LYS	CD-CE	6.33	1.67	1.51
1	18-B	164	VAL	CB-CG2	-6.30	1.39	1.52
1	19-B	169	ARG	CB-CG	6.29	1.69	1.52
1	3-B	102	MET	CB-CG	6.23	1.71	1.51
1	14-A	457	GLU	CG-CD	6.22	1.61	1.51
1	22-A	196	TRP	CB-CG	6.21	1.61	1.50
1	14-B	468	LYS	CE-NZ	-6.20	1.33	1.49
1	4-A	169	ARG	CG-CD	6.19	1.67	1.51
1	1-B	519	LYS	CB-CG	-6.18	1.35	1.52
1	17-B	426	LYS	CE-NZ	6.11	1.64	1.49
1	9-B	426	LYS	CD-CE	6.10	1.66	1.51
1	17-B	88	LYS	CD-CE	6.10	1.66	1.51
1	22-B	196	TRP	CB-CG	6.08	1.61	1.50
1	2-B	492	GLU	CG-CD	-6.05	1.42	1.51
1	19-B	395	GLU	CG-CD	-6.04	1.42	1.51
1	10-B	404	ASP	CB-CG	6.04	1.64	1.51
1	18-B	457	GLU	CG-CD	6.03	1.60	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-A	266	LYS	CE-NZ	6.01	1.64	1.49
1	1-B	283	LYS	CG-CD	6.00	1.72	1.52
1	1-B	452	GLU	CB-CG	6.00	1.63	1.52
1	22-B	165	ASN	CB-CG	5.99	1.64	1.51
1	17-A	493	ASN	CB-CG	-5.98	1.37	1.51
1	9-A	346	ARG	CG-CD	-5.98	1.37	1.51
1	17-B	457	GLU	CB-CG	5.95	1.63	1.52
1	8-B	460	ARG	CZ-NH2	5.94	1.40	1.33
1	19-A	254	TYR	CD2-CE2	-5.91	1.30	1.39
1	7-B	457	GLU	CG-CD	5.91	1.60	1.51
1	22-A	68	VAL	CB-CG1	-5.91	1.40	1.52
1	9-A	457	GLU	CG-CD	5.89	1.60	1.51
1	9-A	164	VAL	C-O	5.88	1.34	1.23
1	19-A	462	ASP	CB-CG	-5.87	1.39	1.51
1	24-B	157	GLU	CD-OE1	5.87	1.32	1.25
1	17-A	457	GLU	CG-CD	5.84	1.60	1.51
1	18-B	457	GLU	CB-CG	5.84	1.63	1.52
1	12-B	157	GLU	CB-CG	-5.83	1.41	1.52
1	21-B	251	GLU	CB-CG	5.83	1.63	1.52
1	13-A	258	GLU	CG-CD	5.73	1.60	1.51
1	17-A	343	GLU	CB-CG	5.72	1.63	1.52
1	18-B	196	TRP	CB-CG	5.69	1.60	1.50
1	24-A	426	LYS	CE-NZ	5.67	1.63	1.49
1	14-A	519	LYS	CD-CE	5.66	1.65	1.51
1	16-A	58	VAL	CB-CG1	5.64	1.64	1.52
1	11-B	143	TRP	CB-CG	5.61	1.60	1.50
1	6-A	340	GLN	CG-CD	5.60	1.64	1.51
1	5-A	346	ARG	CG-CD	5.58	1.66	1.51
1	9-B	195	GLY	C-O	-5.58	1.14	1.23
1	8-A	457	GLU	CG-CD	5.56	1.60	1.51
1	10-B	377	LYS	CB-CG	-5.53	1.37	1.52
1	3-B	346	ARG	CB-CG	5.53	1.67	1.52
1	7-A	457	GLU	CG-CD	5.52	1.60	1.51
1	12-A	140	ASP	CB-CG	5.49	1.63	1.51
1	16-A	180	ARG	CG-CD	5.49	1.65	1.51
1	5-A	258	GLU	CB-CG	5.48	1.62	1.52
1	1-B	210	GLU	CG-CD	5.47	1.60	1.51
1	17-A	362	ASP	CB-CG	5.47	1.63	1.51
1	21-B	296	THR	CB-CG2	5.46	1.70	1.52
1	4-A	457	GLU	CG-CD	5.46	1.60	1.51
1	11-B	196	TRP	CB-CG	5.46	1.60	1.50
1	8-A	196	TRP	CB-CG	5.45	1.60	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	24-B	402	SER	CB-OG	5.44	1.49	1.42
1	17-B	600	GLN	CB-CG	5.43	1.67	1.52
1	16-B	266	LYS	CD-CE	5.42	1.64	1.51
1	22-B	306	GLN	CB-CG	5.41	1.67	1.52
1	23-B	457	GLU	CB-CG	5.38	1.62	1.52
1	23-A	577	LYS	CE-NZ	5.37	1.62	1.49
1	9-B	87	ARG	CB-CG	5.36	1.67	1.52
1	2-B	157	GLU	CG-CD	5.36	1.59	1.51
1	10-B	180	ARG	CG-CD	5.35	1.65	1.51
1	10-A	258	GLU	CB-CG	-5.35	1.42	1.52
1	12-B	572	VAL	CB-CG2	-5.34	1.41	1.52
1	22-A	251	GLU	CG-CD	5.34	1.59	1.51
1	16-A	251	GLU	CB-CG	5.33	1.62	1.52
1	17-B	457	GLU	CG-CD	5.32	1.59	1.51
1	9-B	84	GLU	CB-CG	5.32	1.62	1.52
1	5-B	457	GLU	CB-CG	5.32	1.62	1.52
1	22-A	298	GLU	CG-CD	-5.31	1.44	1.51
1	4-A	452	GLU	CB-CG	5.30	1.62	1.52
1	19-A	424	PRO	CA-C	5.30	1.63	1.52
1	4-A	543	TYR	CD2-CE2	-5.30	1.31	1.39
1	12-B	180	ARG	CG-CD	5.29	1.65	1.51
1	13-B	298	GLU	CB-CG	5.28	1.62	1.52
1	8-A	140	ASP	CB-CG	5.28	1.62	1.51
1	21-B	164	VAL	CB-CG2	-5.28	1.41	1.52
1	4-B	295	GLY	CA-C	5.27	1.60	1.51
1	17-B	404	ASP	CB-CG	5.27	1.62	1.51
1	21-A	572	VAL	CB-CG1	-5.25	1.41	1.52
1	2-B	272	ASP	CB-CG	5.25	1.62	1.51
1	20-A	262	VAL	CB-CG2	-5.25	1.41	1.52
1	22-A	251	GLU	CB-CG	5.24	1.62	1.52
1	2-B	404	ASP	CB-CG	5.23	1.62	1.51
1	17-B	485	TYR	CE2-CZ	-5.23	1.31	1.38
1	1-A	317	GLU	CG-CD	5.23	1.59	1.51
1	25-A	196	TRP	CB-CG	5.23	1.59	1.50
1	18-B	402	SER	CB-OG	5.23	1.49	1.42
1	11-B	157	GLU	CD-OE1	5.22	1.31	1.25
1	21-B	457	GLU	CD-OE2	5.21	1.31	1.25
1	23-B	457	GLU	CG-CD	5.18	1.59	1.51
1	19-A	164	VAL	CB-CG1	-5.17	1.42	1.52
1	6-B	114	GLN	CB-CG	5.16	1.66	1.52
1	3-A	140	ASP	CB-CG	5.15	1.62	1.51
1	16-A	314	ALA	CA-C	-5.15	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	18-B	343	GLU	CB-CG	5.15	1.61	1.52
1	14-A	127	ASN	CB-CG	5.14	1.62	1.51
1	10-B	298	GLU	CG-CD	5.14	1.59	1.51
1	15-A	305	ASP	CB-CG	-5.14	1.41	1.51
1	11-A	391	GLU	CB-CG	-5.13	1.42	1.52
1	12-A	457	GLU	CG-CD	5.13	1.59	1.51
1	14-A	266	LYS	CE-NZ	-5.12	1.36	1.49
1	8-B	198	SER	CA-CB	5.11	1.60	1.52
1	7-A	81	LYS	CD-CE	5.10	1.64	1.51
1	14-A	395	GLU	CG-CD	-5.09	1.44	1.51
1	14-A	184	LYS	CD-CE	5.06	1.63	1.51
1	8-B	157	GLU	CD-OE2	-5.06	1.20	1.25
1	10-B	527	ASP	CB-CG	5.04	1.62	1.51
1	16-A	266	LYS	CD-CE	5.04	1.63	1.51
1	25-A	603	SER	CB-OG	-5.04	1.35	1.42
1	20-B	271	LEU	CG-CD2	-5.04	1.33	1.51
1	3-A	266	LYS	CD-CE	5.03	1.63	1.51
1	21-A	369	LYS	CD-CE	5.03	1.63	1.51
1	2-B	196	TRP	CB-CG	5.01	1.59	1.50
1	12-A	104	LYS	CE-NZ	5.01	1.61	1.49
1	13-A	196	TRP	CB-CG	5.00	1.59	1.50

All (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
1	8-B	87	ARG	NE-CZ-NH1	11.95	126.27	120.30
1	6-A	87	ARG	NE-CZ-NH1	11.85	126.22	120.30
1	7-A	169	ARG	NE-CZ-NH1	-11.41	114.59	120.30
1	3-A	126	LEU	CA-CB-CG	11.15	140.95	115.30
1	13-B	87	ARG	NE-CZ-NH2	-10.88	114.86	120.30
1	3-A	169	ARG	NE-CZ-NH2	10.86	125.73	120.30
1	19-A	462	ASP	CB-CG-OD2	-10.74	108.63	118.30
1	7-B	460	ARG	NE-CZ-NH1	-10.63	114.98	120.30
1	22-B	538	MET	CG-SD-CE	-10.60	83.24	100.20
1	8-B	460	ARG	NE-CZ-NH1	-10.37	115.12	120.30
1	13-B	180	ARG	NE-CZ-NH1	9.95	125.28	120.30
1	3-B	169	ARG	CG-CD-NE	-9.90	91.01	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-B	180	ARG	NE-CZ-NH1	9.89	125.24	120.30
1	14-A	460	ARG	NE-CZ-NH2	9.79	125.20	120.30
1	4-B	193	GLY	N-CA-C	-9.70	88.85	113.10
1	25-B	266	LYS	CD-CE-NZ	9.69	133.98	111.70
1	17-A	460	ARG	NE-CZ-NH2	9.56	125.08	120.30
1	7-B	460	ARG	CG-CD-NE	-9.56	91.72	111.80
1	6-A	340	GLN	N-CA-C	-9.41	85.60	111.00
1	1-A	527	ASP	CB-CG-OD2	9.35	126.71	118.30
1	1-A	538	MET	CG-SD-CE	-9.30	85.32	100.20
1	22-B	169	ARG	NE-CZ-NH1	-9.29	115.65	120.30
1	3-A	126	LEU	CB-CG-CD1	9.27	126.76	111.00
1	17-B	88	LYS	CB-CA-C	9.13	128.67	110.40
1	20-A	102	MET	CG-SD-CE	9.01	114.62	100.20
1	21-A	269	LEU	CA-CB-CG	8.99	135.98	115.30
1	13-B	180	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	25-B	72	ASP	CB-CG-OD2	8.94	126.34	118.30
1	15-A	102	MET	CG-SD-CE	-8.85	86.04	100.20
1	8-B	346	ARG	NE-CZ-NH2	8.80	124.70	120.30
1	22-A	368	LEU	CA-CB-CG	8.77	135.48	115.30
1	15-B	126	LEU	CA-CB-CG	8.72	135.35	115.30
1	13-B	126	LEU	CA-CB-CG	8.69	135.28	115.30
1	22-A	195	GLY	N-CA-C	-8.67	91.44	113.10
1	13-B	346	ARG	NE-CZ-NH2	8.65	124.62	120.30
1	8-B	64	LEU	CA-CB-CG	8.63	135.15	115.30
1	19-A	460	ARG	NE-CZ-NH1	-8.55	116.03	120.30
1	14-B	460	ARG	NE-CZ-NH2	8.54	124.57	120.30
1	1-B	169	ARG	NE-CZ-NH2	8.53	124.57	120.30
1	5-B	102	MET	CG-SD-CE	-8.51	86.58	100.20
1	22-A	525	LYS	CD-CE-NZ	8.43	131.08	111.70
1	23-B	266	LYS	CD-CE-NZ	8.38	130.98	111.70
1	7-A	169	ARG	NE-CZ-NH2	8.36	124.48	120.30
1	22-B	196	TRP	CA-CB-CG	8.33	129.53	113.70
1	3-A	169	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	1-B	311	LYS	C-N-CD	8.32	145.87	128.40
1	3-A	145	ASP	CB-CG-OD2	8.30	125.77	118.30
1	12-B	574	LEU	CA-CB-CG	8.29	134.37	115.30
1	19-B	490	SER	CB-CA-C	-8.23	94.46	110.10
1	2-A	72	ASP	CB-CG-OD1	8.15	125.64	118.30
1	1-B	169	ARG	NE-CZ-NH1	-8.13	116.23	120.30
1	1-A	102	MET	CG-SD-CE	-8.11	87.22	100.20
1	19-B	271	LEU	CA-CB-CG	8.09	133.92	115.30
1	24-A	460	ARG	NE-CZ-NH2	8.09	124.34	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	17-A	144	PHE	N-CA-C	8.08	132.82	111.00
1	25-A	460	ARG	NE-CZ-NH1	-8.08	116.26	120.30
1	22-A	470	ASP	CB-CG-OD1	8.06	125.56	118.30
1	5-B	149	THR	CB-CA-C	-8.03	89.92	111.60
1	8-A	61	GLY	N-CA-C	-8.03	93.03	113.10
1	7-B	169	ARG	NE-CZ-NH1	-8.03	116.29	120.30
1	9-A	460	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	11-A	180	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	11-B	269	LEU	CB-CG-CD2	8.02	124.63	111.00
1	12-B	269	LEU	CA-CB-CG	8.00	133.71	115.30
1	10-A	538	MET	CG-SD-CE	7.96	112.94	100.20
1	14-B	266	LYS	CD-CE-NZ	7.95	129.99	111.70
1	19-A	169	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	24-A	399	ASP	CB-CG-OD1	7.90	125.41	118.30
1	22-B	169	ARG	NE-CZ-NH2	7.88	124.24	120.30
1	7-A	311	LYS	N-CA-C	-7.86	89.78	111.00
1	6-B	538	MET	CG-SD-CE	-7.80	87.71	100.20
1	20-A	460	ARG	NE-CZ-NH1	-7.79	116.41	120.30
1	10-B	460	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	22-A	362	ASP	CB-CG-OD1	-7.74	111.34	118.30
1	4-B	346	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	16-B	538	MET	CG-SD-CE	7.71	112.53	100.20
1	10-A	193	GLY	N-CA-C	-7.66	93.94	113.10
1	12-A	296	THR	N-CA-C	-7.64	90.37	111.00
1	18-A	126	LEU	CA-CB-CG	7.64	132.87	115.30
1	15-B	517	ASP	CB-CG-OD2	7.60	125.14	118.30
1	23-B	196	TRP	CA-CB-CG	7.60	128.14	113.70
1	19-B	102	MET	CG-SD-CE	-7.60	88.04	100.20
1	5-B	196	TRP	N-CA-C	7.59	131.51	111.00
1	19-A	424	PRO	CA-C-N	7.59	131.39	116.20
1	7-A	257	LEU	CA-CB-CG	7.56	132.69	115.30
1	23-B	72	ASP	CB-CG-OD2	7.56	125.11	118.30
1	8-A	59	VAL	N-CA-C	7.54	131.35	111.00
1	23-A	346	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	6-B	266	LYS	CD-CE-NZ	7.49	128.93	111.70
1	15-B	517	ASP	CB-CG-OD1	-7.49	111.56	118.30
1	24-B	143	TRP	CA-CB-CG	-7.48	99.49	113.70
1	11-A	449	ASP	CB-CG-OD2	7.47	125.02	118.30
1	18-B	330	LEU	CA-CB-CG	7.45	132.42	115.30
1	14-A	570	LEU	CA-CB-CG	7.43	132.38	115.30
1	12-A	88	LYS	CA-CB-CG	7.38	129.64	113.40
1	22-B	528	ASP	CB-CG-OD1	7.38	124.94	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	21-A	262	VAL	CB-CA-C	-7.37	97.39	111.40
1	22-B	194	TYR	CB-CG-CD2	7.36	125.42	121.00
1	6-B	166	GLY	N-CA-C	-7.31	94.83	113.10
1	17-B	346	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	6-B	165	ASN	N-CA-C	7.24	130.54	111.00
1	23-A	368	LEU	CB-CG-CD2	7.23	123.29	111.00
1	18-A	399	ASP	CB-CG-OD1	7.21	124.79	118.30
1	21-B	600	GLN	CB-CA-C	7.21	124.81	110.40
1	25-B	72	ASP	CB-CG-OD1	-7.19	111.83	118.30
1	7-B	144	PHE	CB-CG-CD2	7.19	125.83	120.80
1	1-A	72	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	24-A	426	LYS	CD-CE-NZ	7.18	128.22	111.70
1	8-A	308	TYR	CB-CA-C	7.16	124.72	110.40
1	15-B	271	LEU	CA-CB-CG	7.16	131.76	115.30
1	16-B	275	ASP	CB-CA-C	-7.15	96.10	110.40
1	14-B	305	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	12-A	570	LEU	CA-CB-CG	7.12	131.66	115.30
1	23-B	87	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	24-A	63	ASP	CB-CG-OD2	7.08	124.67	118.30
1	21-B	538	MET	CG-SD-CE	-7.07	88.88	100.20
1	25-A	140	ASP	CB-CG-OD2	7.05	124.65	118.30
1	9-A	72	ASP	CB-CA-C	-7.04	96.32	110.40
1	15-A	305	ASP	CB-CG-OD1	-7.04	111.97	118.30
1	9-A	460	ARG	NE-CZ-NH1	-7.03	116.78	120.30
1	14-A	184	LYS	CD-CE-NZ	7.03	127.88	111.70
1	6-B	196	TRP	CA-CB-CG	7.02	127.04	113.70
1	2-B	126	LEU	CA-CB-CG	7.01	131.41	115.30
1	20-B	140	ASP	CB-CA-C	-6.98	96.44	110.40
1	21-B	196	TRP	N-CA-C	6.98	129.84	111.00
1	15-A	197	ALA	N-CA-C	-6.97	92.17	111.00
1	25-A	460	ARG	NE-CZ-NH2	6.97	123.79	120.30
1	21-B	140	ASP	CB-CG-OD1	6.96	124.57	118.30
1	12-B	145	ASP	CB-CG-OD2	6.95	124.55	118.30
1	17-A	296	THR	N-CA-C	-6.93	92.30	111.00
1	12-B	399	ASP	CB-CG-OD2	6.92	124.53	118.30
1	21-B	140	ASP	CB-CG-OD2	-6.89	112.09	118.30
1	16-A	87	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	24-B	197	ALA	N-CA-C	-6.89	92.40	111.00
1	15-A	273	GLY	N-CA-C	-6.87	95.92	113.10
1	7-A	180	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	22-A	180	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	13-A	570	LEU	CB-CA-C	-6.86	97.17	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10-B	272	ASP	CB-CG-OD1	6.84	124.45	118.30
1	16-B	126	LEU	CA-CB-CG	6.83	131.02	115.30
1	16-A	345	ASP	CB-CG-OD1	-6.83	112.15	118.30
1	16-A	589	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	15-B	296	THR	C-N-CD	-6.79	105.65	120.60
1	18-A	272	ASP	CB-CG-OD2	6.79	124.41	118.30
1	2-A	196	TRP	CA-CB-CG	6.75	126.52	113.70
1	4-B	517	ASP	CB-CG-OD1	6.73	124.36	118.30
1	1-B	72	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	2-B	346	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	23-B	196	TRP	CB-CA-C	6.69	123.78	110.40
1	1-B	70	VAL	CB-CA-C	-6.69	98.69	111.40
1	14-A	460	ARG	NE-CZ-NH1	-6.69	116.96	120.30
1	8-B	470	ASP	CB-CG-OD2	6.68	124.31	118.30
1	8-B	87	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	8-A	144	PHE	CB-CA-C	-6.66	97.09	110.40
1	24-A	273	GLY	N-CA-C	-6.65	96.48	113.10
1	22-B	346	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	16-B	600	GLN	CB-CA-C	6.64	123.68	110.40
1	8-A	140	ASP	CB-CG-OD2	6.62	124.26	118.30
1	7-B	509	ASP	CB-CG-OD2	6.59	124.23	118.30
1	20-B	312	PRO	N-CA-C	6.57	129.19	112.10
1	18-A	314	ALA	N-CA-C	6.56	128.71	111.00
1	14-B	460	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	12-B	346	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	18-A	368	LEU	CA-CB-CG	6.51	130.28	115.30
1	10-A	586	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	5-B	565	LYS	CD-CE-NZ	6.50	126.66	111.70
1	11-A	180	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	21-B	312	PRO	CA-C-N	6.48	129.16	116.20
1	22-B	460	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	9-B	169	ARG	N-CA-CB	-6.47	98.96	110.60
1	5-A	346	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	15-A	346	ARG	NE-CZ-NH2	6.47	123.53	120.30
1	15-A	570	LEU	CB-CG-CD1	6.45	121.97	111.00
1	17-A	460	ARG	NE-CZ-NH1	-6.45	117.08	120.30
1	12-A	305	ASP	CB-CG-OD2	6.45	124.10	118.30
1	18-B	528	ASP	CB-CG-OD1	6.43	124.09	118.30
1	4-A	285	THR	CB-CA-C	-6.43	94.25	111.60
1	14-B	401	ALA	N-CA-C	6.42	128.34	111.00
1	16-A	140	ASP	CB-CG-OD1	6.42	124.08	118.30
1	9-A	271	LEU	CB-CG-CD1	6.41	121.90	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	313	GLY	N-CA-C	-6.41	97.08	113.10
1	20-B	468	LYS	CD-CE-NZ	6.40	126.42	111.70
1	1-A	384	ASP	CB-CG-OD1	6.39	124.05	118.30
1	3-B	269	LEU	CA-CB-CG	6.38	129.99	115.30
1	13-A	59	VAL	CB-CA-C	-6.37	99.30	111.40
1	5-B	97	ASP	CB-CG-OD2	6.36	124.02	118.30
1	14-B	296	THR	N-CA-C	-6.34	93.87	111.00
1	18-A	305	ASP	CB-CG-OD1	6.34	124.00	118.30
1	23-B	194	TYR	CA-CB-CG	6.33	125.44	113.40
1	21-B	460	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	4-B	586	ASP	CB-CG-OD2	6.32	123.99	118.30
1	1-A	295	GLY	N-CA-C	6.32	128.89	113.10
1	7-B	517	ASP	CB-CG-OD2	6.30	123.97	118.30
1	24-A	184	LYS	CD-CE-NZ	6.30	126.19	111.70
1	7-A	311	LYS	CA-CB-CG	6.28	127.22	113.40
1	6-B	553	GLN	N-CA-CB	6.26	121.87	110.60
1	23-B	546	VAL	CB-CA-C	-6.26	99.50	111.40
1	4-B	63	ASP	CB-CG-OD2	6.25	123.92	118.30
1	3-A	295	GLY	N-CA-C	6.24	128.69	113.10
1	9-B	449	ASP	CB-CG-OD1	-6.24	112.69	118.30
1	5-B	404	ASP	CB-CG-OD2	6.22	123.90	118.30
1	25-A	126	LEU	CA-CB-CG	6.20	129.56	115.30
1	20-B	271	LEU	CA-CB-CG	6.20	129.55	115.30
1	15-A	180	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	12-A	180	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	25-A	426	LYS	CD-CE-NZ	6.18	125.91	111.70
1	18-B	196	TRP	CB-CA-C	6.17	122.74	110.40
1	25-B	169	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	1-B	283	LYS	CB-CG-CD	6.16	127.61	111.60
1	15-A	404	ASP	CB-CG-OD2	6.16	123.84	118.30
1	6-B	565	LYS	CD-CE-NZ	6.15	125.84	111.70
1	5-A	271	LEU	CB-CG-CD2	-6.11	100.62	111.00
1	7-B	180	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	10-A	384	ASP	CB-CG-OD2	6.09	123.78	118.30
1	7-A	180	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	6-A	384	ASP	CB-CG-OD1	6.09	123.78	118.30
1	23-A	124	LEU	CB-CG-CD1	-6.08	100.67	111.00
1	25-B	87	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	7-B	565	LYS	CD-CE-NZ	-6.05	97.79	111.70
1	13-B	72	ASP	CB-CG-OD1	-6.05	112.86	118.30
1	8-A	368	LEU	CA-CB-CG	6.04	129.21	115.30
1	17-B	538	MET	CG-SD-CE	6.04	109.86	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	12-A	527	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	1-B	426	LYS	CD-CE-NZ	6.01	125.52	111.70
1	22-B	538	MET	CA-CB-CG	6.01	123.51	113.30
1	13-A	570	LEU	CA-CB-CG	5.99	129.09	115.30
1	19-A	586	ASP	CB-CG-OD1	5.99	123.69	118.30
1	3-A	460	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	13-B	266	LYS	CD-CE-NZ	5.97	125.43	111.70
1	18-B	574	LEU	CA-CB-CG	-5.97	101.57	115.30
1	24-B	517	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	13-B	180	ARG	CD-NE-CZ	5.96	131.94	123.60
1	22-B	196	TRP	N-CA-CB	5.95	121.31	110.60
1	13-A	126	LEU	CB-CG-CD2	5.95	121.11	111.00
1	12-B	346	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	4-A	180	ARG	CG-CD-NE	5.94	124.27	111.80
1	2-A	273	GLY	N-CA-C	-5.93	98.26	113.10
1	13-A	527	ASP	CB-CG-OD1	5.93	123.64	118.30
1	16-A	570	LEU	CA-CB-CG	5.93	128.94	115.30
1	3-A	423	GLY	N-CA-C	-5.92	98.30	113.10
1	7-B	457	GLU	CB-CA-C	5.92	122.24	110.40
1	17-B	101	LEU	CB-CG-CD1	-5.92	100.94	111.00
1	8-A	346	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	13-B	517	ASP	CB-CG-OD1	5.90	123.61	118.30
1	15-A	296	THR	C-N-CD	5.89	140.78	128.40
1	19-A	346	ARG	CG-CD-NE	5.89	124.18	111.80
1	17-A	517	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	3-B	296	THR	N-CA-C	-5.89	95.10	111.00
1	6-A	61	GLY	N-CA-C	5.89	127.82	113.10
1	6-A	180	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	24-B	368	LEU	CA-CB-CG	5.88	128.81	115.30
1	2-B	298	GLU	N-CA-C	5.87	126.86	111.00
1	13-A	574	LEU	CB-CA-C	-5.87	99.05	110.20
1	20-A	169	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	12-B	266	LYS	CD-CE-NZ	5.87	125.19	111.70
1	16-A	346	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	9-B	468	LYS	CB-CA-C	-5.86	98.68	110.40
1	15-A	404	ASP	CB-CA-C	5.86	122.12	110.40
1	16-B	87	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	19-A	586	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	6-B	509	ASP	CB-CG-OD1	-5.84	113.04	118.30
1	9-A	140	ASP	CB-CG-OD2	5.83	123.55	118.30
1	15-A	384	ASP	CB-CG-OD1	5.83	123.54	118.30
1	16-A	519	LYS	CA-CB-CG	5.83	126.22	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	11-B	87	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	2-A	346	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	17-B	346	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	24-B	102	MET	CG-SD-CE	-5.81	90.91	100.20
1	14-A	295	GLY	N-CA-C	-5.80	98.61	113.10
1	16-A	313	GLY	N-CA-C	-5.79	98.61	113.10
1	24-A	302	LEU	CA-CB-CG	5.79	128.62	115.30
1	4-B	87	ARG	CB-CA-C	5.78	121.96	110.40
1	25-B	273	GLY	N-CA-C	-5.78	98.65	113.10
1	11-A	130	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	22-B	161	LEU	CA-CB-CG	5.78	128.59	115.30
1	9-A	169	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	4-A	346	ARG	CA-CB-CG	5.77	126.10	113.40
1	6-B	275	ASP	CB-CG-OD1	5.77	123.49	118.30
1	16-B	372	ASP	CB-CG-OD2	5.77	123.49	118.30
1	18-B	196	TRP	CA-CB-CG	-5.76	102.76	113.70
1	5-B	87	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	1-A	313	GLY	N-CA-C	-5.75	98.73	113.10
1	25-B	572	VAL	CB-CA-C	-5.75	100.48	111.40
1	20-A	346	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	16-B	192	ASP	CB-CG-OD1	-5.74	113.13	118.30
1	6-A	274	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	8-A	362	ASP	CB-CG-OD1	5.74	123.46	118.30
1	23-B	77	ASP	CB-CG-OD1	5.73	123.46	118.30
1	10-A	346	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	19-B	87	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	21-B	272	ASP	CB-CG-OD1	5.72	123.45	118.30
1	4-A	346	ARG	CB-CG-CD	5.72	126.47	111.60
1	23-B	56	GLN	N-CA-CB	-5.72	100.31	110.60
1	24-B	402	SER	N-CA-CB	-5.72	101.92	110.50
1	9-B	145	ASP	N-CA-C	5.71	126.43	111.00
1	10-A	169	ARG	NE-CZ-NH1	-5.71	117.44	120.30
1	22-B	194	TYR	CA-CB-CG	5.71	124.26	113.40
1	7-B	517	ASP	CB-CG-OD1	-5.71	113.16	118.30
1	17-A	102	MET	CA-CB-CG	-5.71	103.59	113.30
1	19-A	425	GLY	N-CA-C	5.71	127.36	113.10
1	2-B	157	GLU	CG-CD-OE2	5.70	129.70	118.30
1	4-A	180	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	18-A	140	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	24-A	570	LEU	CB-CG-CD2	5.69	120.67	111.00
1	17-A	269	LEU	CB-CG-CD2	-5.69	101.33	111.00
1	21-A	63	ASP	CB-CA-C	-5.69	99.02	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	15-B	143	TRP	CB-CA-C	5.69	121.77	110.40
1	16-B	91	SER	CB-CA-C	-5.68	99.30	110.10
1	23-A	87	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	12-B	495	LYS	CD-CE-NZ	5.67	124.74	111.70
1	22-A	384	ASP	CB-CG-OD1	5.66	123.40	118.30
1	11-A	384	ASP	CB-CG-OD2	5.66	123.39	118.30
1	1-B	519	LYS	CB-CA-C	-5.65	99.10	110.40
1	9-A	519	LYS	CD-CE-NZ	5.65	124.69	111.70
1	21-B	586	ASP	CB-CG-OD2	5.65	123.38	118.30
1	2-A	527	ASP	CB-CG-OD1	5.64	123.38	118.30
1	11-B	460	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	21-B	69	LEU	CA-CB-CG	5.64	128.28	115.30
1	4-A	83	ASP	CB-CG-OD1	5.62	123.35	118.30
1	12-B	294	ASN	N-CA-C	-5.61	95.84	111.00
1	10-A	543	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	21-B	271	LEU	CA-CB-CG	5.59	128.16	115.30
1	6-A	362	ASP	CB-CG-OD1	5.59	123.33	118.30
1	22-A	295	GLY	N-CA-C	-5.58	99.14	113.10
1	13-B	129	ASP	CB-CG-OD1	5.57	123.32	118.30
1	22-B	194	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	22-B	503	LYS	CD-CE-NZ	5.57	124.52	111.70
1	9-A	384	ASP	CB-CG-OD2	5.57	123.31	118.30
1	2-A	449	ASP	CB-CG-OD2	5.57	123.31	118.30
1	20-B	145	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	1-A	196	TRP	CA-CB-CG	5.56	124.27	113.70
1	4-A	169	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	9-A	130	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	7-B	127	ASN	C-N-CD	5.55	140.05	128.40
1	15-B	102	MET	CA-CB-CG	5.54	122.72	113.30
1	22-A	368	LEU	CB-CG-CD1	-5.54	101.59	111.00
1	13-B	346	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	19-A	196	TRP	CB-CA-C	-5.53	99.35	110.40
1	12-B	315	THR	CB-CA-C	-5.52	96.69	111.60
1	17-B	304	LEU	CA-CB-CG	5.51	127.96	115.30
1	14-B	532	THR	N-CA-CB	-5.50	99.84	110.30
1	17-B	277	LYS	CD-CE-NZ	5.50	124.36	111.70
1	4-B	460	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	14-B	517	ASP	CB-CG-OD1	5.50	123.25	118.30
1	2-A	72	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	21-A	294	ASN	N-CA-C	-5.50	96.16	111.00
1	8-A	399	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	24-A	194	TYR	CB-CG-CD2	5.49	124.29	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	19-A	136	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	25-A	460	ARG	CG-CD-NE	-5.47	100.30	111.80
1	1-B	87	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	4-B	63	ASP	CB-CG-OD1	-5.47	113.37	118.30
1	22-B	144	PHE	N-CA-C	-5.47	96.24	111.00
1	6-B	180	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	7-A	192	ASP	CB-CG-OD1	5.46	123.22	118.30
1	10-A	296	THR	CB-CA-C	-5.46	96.85	111.60
1	15-B	516	GLY	N-CA-C	-5.46	99.44	113.10
1	19-A	192	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	25-A	130	ASP	CB-CG-OD2	5.46	123.21	118.30
1	3-A	565	LYS	CD-CE-NZ	5.46	124.25	111.70
1	12-A	305	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	19-A	61	GLY	N-CA-C	-5.45	99.48	113.10
1	17-A	59	VAL	CB-CA-C	5.44	121.75	111.40
1	17-A	192	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	11-A	295	GLY	N-CA-C	5.44	126.70	113.10
1	3-A	460	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	9-B	196	TRP	CB-CA-C	5.44	121.27	110.40
1	13-A	422	ALA	N-CA-C	-5.44	96.32	111.00
1	24-A	70	VAL	CB-CA-C	-5.43	101.08	111.40
1	8-A	87	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	8-A	449	ASP	CB-CG-OD1	5.43	123.19	118.30
1	21-B	194	TYR	N-CA-C	-5.43	96.33	111.00
1	23-A	509	ASP	CB-CG-OD2	5.43	123.19	118.30
1	2-A	180	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	12-B	586	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	13-A	87	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	12-B	302	LEU	CA-CB-CG	5.42	127.77	115.30
1	25-B	296	THR	N-CA-C	-5.42	96.36	111.00
1	18-B	55	ALA	N-CA-C	-5.42	96.37	111.00
1	10-A	586	ASP	CB-CG-OD1	5.42	123.17	118.30
1	13-A	574	LEU	CB-CG-CD2	5.42	120.21	111.00
1	22-A	64	LEU	CB-CG-CD2	5.41	120.20	111.00
1	6-B	399	ASP	CB-CG-OD1	5.41	123.17	118.30
1	10-B	426	LYS	CD-CE-NZ	5.41	124.14	111.70
1	4-B	180	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	24-A	63	ASP	CB-CA-C	5.41	121.21	110.40
1	3-B	295	GLY	N-CA-C	5.40	126.61	113.10
1	17-A	296	THR	N-CA-CB	5.40	120.55	110.30
1	15-A	195	GLY	N-CA-C	5.39	126.58	113.10
1	9-A	63	ASP	CB-CG-OD2	5.39	123.15	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-B	165	ASN	N-CA-CB	-5.38	100.91	110.60
1	15-B	399	ASP	CB-CG-OD1	-5.38	113.45	118.30
1	20-A	140	ASP	CB-CG-OD2	5.38	123.14	118.30
1	23-B	144	PHE	N-CA-C	5.38	125.53	111.00
1	13-B	81	LYS	CD-CE-NZ	-5.38	99.32	111.70
1	23-B	124	LEU	CA-CB-CG	5.38	127.67	115.30
1	4-A	82	VAL	CB-CA-C	-5.37	101.19	111.40
1	10-A	97	ASP	CB-CG-OD2	5.37	123.14	118.30
1	11-A	312	PRO	CA-N-CD	-5.37	103.98	111.50
1	7-B	310	VAL	CB-CA-C	5.37	121.60	111.40
1	24-A	374	ASP	CB-CG-OD1	5.37	123.13	118.30
1	16-A	565	LYS	CD-CE-NZ	5.37	124.05	111.70
1	20-B	273	GLY	N-CA-C	-5.36	99.69	113.10
1	13-B	144	PHE	CB-CG-CD2	5.36	124.55	120.80
1	2-B	194	TYR	CB-CA-C	5.35	121.10	110.40
1	17-A	97	ASP	CB-CG-OD2	5.35	123.11	118.30
1	24-A	460	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	15-A	340	GLN	CB-CA-C	5.35	121.09	110.40
1	8-B	64	LEU	CB-CG-CD2	5.34	120.08	111.00
1	21-A	297	PRO	N-CA-C	5.34	125.99	112.10
1	19-A	359	ILE	CB-CA-C	-5.34	100.92	111.60
1	22-A	72	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	25-B	180	ARG	CG-CD-NE	-5.34	100.59	111.80
1	8-A	586	ASP	CB-CG-OD1	5.33	123.10	118.30
1	11-B	126	LEU	CA-CB-CG	5.33	127.56	115.30
1	25-B	400	GLY	N-CA-C	5.33	126.42	113.10
1	5-A	257	LEU	CA-CB-CG	5.32	127.54	115.30
1	21-B	194	TYR	CB-CA-C	5.32	121.04	110.40
1	12-B	87	ARG	N-CA-CB	5.32	120.17	110.60
1	13-B	509	ASP	CB-CG-OD1	5.31	123.08	118.30
1	19-B	346	ARG	CG-CD-NE	-5.31	100.65	111.80
1	22-B	184	LYS	CD-CE-NZ	5.31	123.92	111.70
1	11-B	530	VAL	N-CA-CB	5.31	123.18	111.50
1	1-B	144	PHE	CB-CG-CD1	5.31	124.52	120.80
1	6-B	460	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	13-A	87	ARG	CG-CD-NE	5.29	122.91	111.80
1	19-B	395	GLU	OE1-CD-OE2	5.29	129.65	123.30
1	7-B	169	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	23-A	404	ASP	CB-CG-OD1	5.29	123.06	118.30
1	24-B	272	ASP	N-CA-C	-5.29	96.73	111.00
1	9-B	449	ASP	CB-CG-OD2	5.28	123.05	118.30
1	23-A	194	TYR	CA-CB-CG	-5.28	103.37	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-B	180	ARG	CD-NE-CZ	5.27	130.98	123.60
1	10-B	140	ASP	CB-CG-OD1	5.27	123.05	118.30
1	10-B	145	ASP	CB-CG-OD1	5.27	123.04	118.30
1	19-B	587	ILE	CG1-CB-CG2	-5.27	99.81	111.40
1	25-B	296	THR	N-CA-CB	5.27	120.31	110.30
1	16-A	87	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	3-B	180	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	13-A	574	LEU	N-CA-CB	5.25	120.91	110.40
1	21-B	374	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	18-B	102	MET	CG-SD-CE	-5.25	91.80	100.20
1	14-B	283	LYS	CB-CG-CD	5.25	125.24	111.60
1	25-A	460	ARG	CD-NE-CZ	5.25	130.94	123.60
1	5-B	126	LEU	CB-CG-CD1	-5.24	102.08	111.00
1	14-B	305	ASP	CB-CG-OD1	5.24	123.02	118.30
1	22-B	97	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	17-A	275	ASP	CB-CG-OD2	5.24	123.02	118.30
1	22-B	374	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	13-B	262	VAL	CB-CA-C	-5.24	101.45	111.40
1	10-A	374	ASP	CB-CG-OD1	5.23	123.01	118.30
1	15-A	272	ASP	CB-CG-OD2	5.23	123.01	118.30
1	11-B	56	GLN	CB-CA-C	5.22	120.84	110.40
1	14-A	519	LYS	CD-CE-NZ	5.22	123.70	111.70
1	17-A	102	MET	CG-SD-CE	-5.21	91.86	100.20
1	5-A	194	TYR	N-CA-C	5.21	125.07	111.00
1	10-B	517	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	4-B	447	ARG	CG-CD-NE	5.20	122.72	111.80
1	7-B	144	PHE	CB-CG-CD1	-5.20	117.16	120.80
1	14-A	87	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	23-B	194	TYR	CB-CA-C	-5.20	100.00	110.40
1	22-A	586	ASP	CB-CG-OD1	5.19	122.97	118.30
1	10-A	368	LEU	CA-CB-CG	5.19	127.23	115.30
1	16-A	208	ASP	CB-CG-OD1	5.19	122.97	118.30
1	1-A	196	TRP	CB-CG-CD2	5.18	133.34	126.60
1	19-B	180	ARG	CB-CG-CD	5.18	125.08	111.60
1	4-A	266	LYS	CD-CE-NZ	5.18	123.61	111.70
1	18-A	114	GLN	CB-CA-C	-5.18	100.04	110.40
1	12-A	180	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	22-B	101	LEU	CB-CG-CD2	5.18	119.80	111.00
1	12-A	214	TYR	CA-CB-CG	-5.17	103.58	113.40
1	8-B	369	LYS	CD-CE-NZ	5.16	123.58	111.70
1	7-A	164	VAL	CB-CA-C	-5.16	101.60	111.40
1	7-A	589	ASP	CB-CG-OD1	5.16	122.94	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	15-B	538	MET	CG-SD-CE	5.16	108.45	100.20
1	24-A	126	LEU	CB-CG-CD2	-5.16	102.23	111.00
1	9-A	257	LEU	CA-CB-CG	5.16	127.16	115.30
1	12-B	140	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	18-B	404	ASP	CB-CG-OD1	5.15	122.94	118.30
1	16-B	274	ASP	CB-CG-OD1	5.15	122.93	118.30
1	1-B	528	ASP	CB-CG-OD1	5.14	122.93	118.30
1	6-B	525	LYS	CD-CE-NZ	5.14	123.53	111.70
1	6-A	460	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	11-A	399	ASP	CB-CG-OD1	5.13	122.92	118.30
1	25-A	603	SER	N-CA-CB	-5.13	102.80	110.50
1	19-A	91	SER	N-CA-CB	-5.13	102.81	110.50
1	15-A	70	VAL	CB-CA-C	-5.12	101.66	111.40
1	2-A	288	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	7-A	169	ARG	CG-CD-NE	-5.12	101.04	111.80
1	24-A	274	ASP	CB-CA-C	5.12	120.64	110.40
1	23-A	460	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	23-B	102	MET	CG-SD-CE	-5.11	92.02	100.20
1	14-A	184	LYS	CG-CD-CE	5.11	127.24	111.90
1	7-A	272	ASP	N-CA-C	5.10	124.78	111.00
1	4-A	384	ASP	CB-CG-OD1	5.10	122.89	118.30
1	25-A	302	LEU	CA-CB-CG	5.10	127.03	115.30
1	19-B	169	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	3-A	192	ASP	CB-CA-C	-5.09	100.21	110.40
1	17-A	311	LYS	CD-CE-NZ	5.09	123.42	111.70
1	2-B	468	LYS	CD-CE-NZ	5.09	123.41	111.70
1	4-A	130	ASP	CB-CG-OD2	5.09	122.88	118.30
1	18-A	208	ASP	CB-CG-OD1	5.09	122.88	118.30
1	21-B	296	THR	N-CA-C	-5.09	97.27	111.00
1	13-B	517	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	19-A	339	ASP	CB-CG-OD1	5.08	122.87	118.30
1	3-A	145	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	15-A	272	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	18-A	130	ASP	CB-CG-OD1	5.08	122.87	118.30
1	1-B	346	ARG	CB-CG-CD	5.07	124.79	111.60
1	3-B	169	ARG	CB-CA-C	-5.07	100.25	110.40
1	17-B	161	LEU	CB-CG-CD2	-5.07	102.38	111.00
1	13-B	69	LEU	CA-CB-CG	5.07	126.95	115.30
1	14-A	194	TYR	CB-CA-C	5.06	120.52	110.40
1	14-B	402	SER	N-CA-CB	-5.06	102.91	110.50
1	16-B	271	LEU	CA-CB-CG	5.05	126.93	115.30
1	16-A	58	VAL	CB-CA-C	-5.05	101.80	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-B	275	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	15-B	62	GLY	N-CA-C	-5.05	100.48	113.10
1	13-B	283	LYS	CB-CG-CD	5.04	124.71	111.60
1	14-B	517	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	20-A	468	LYS	CD-CE-NZ	-5.04	100.11	111.70
1	15-B	283	LYS	CD-CE-NZ	5.04	123.29	111.70
1	18-B	447	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	4-A	283	LYS	CD-CE-NZ	5.04	123.28	111.70
1	10-B	194	TYR	CA-CB-CG	5.04	122.97	113.40
1	16-A	532	THR	N-CA-CB	-5.04	100.73	110.30
1	21-A	81	LYS	CD-CE-NZ	5.04	123.28	111.70
1	12-B	104	LYS	CB-CA-C	5.03	120.47	110.40
1	25-B	525	LYS	CD-CE-NZ	5.03	123.27	111.70
1	24-B	586	ASP	CB-CG-OD2	5.03	122.82	118.30
1	23-A	346	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	5-A	120	SER	CB-CA-C	-5.02	100.56	110.10
1	7-A	543	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	13-B	404	ASP	CB-CG-OD1	5.02	122.82	118.30
1	8-A	87	ARG	CG-CD-NE	-5.02	101.26	111.80
1	12-B	269	LEU	CB-CG-CD2	5.02	119.53	111.00
1	21-A	295	GLY	N-CA-C	5.02	125.64	113.10
1	9-B	169	ARG	CA-CB-CG	5.01	124.43	113.40
1	2-B	157	GLU	CG-CD-OE1	-5.01	108.28	118.30
1	22-B	192	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (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	293	GLY	Peptide
1	1-B	297	PRO	Peptide
1	1-B	311	LYS	Peptide
1	1-B	76	PRO	Peptide
1	10-A	191	PRO	Peptide
1	10-A	192	ASP	Peptide
1	10-A	193	GLY	Peptide
1	10-A	194	TYR	Peptide
1	10-A	297	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	10-B	401	ALA	Peptide
1	10-B	56	GLN	Peptide
1	10-B	57	GLU	Peptide
1	11-A	163	PRO	Peptide
1	11-A	195	GLY	Peptide
1	11-A	292	TRP	Peptide
1	11-A	293	GLY	Peptide
1	11-A	311	LYS	Peptide
1	11-A	58	VAL	Peptide
1	11-B	195	GLY	Peptide
1	11-B	268	PHE	Peptide
1	12-A	193	GLY	Peptide
1	12-B	195	GLY	Peptide
1	12-B	297	PRO	Peptide
1	13-A	63	ASP	Peptide
1	14-A	191	PRO	Peptide
1	14-A	313	GLY	Peptide
1	14-A	399	ASP	Peptide
1	14-B	125	GLY	Peptide
1	14-B	126	LEU	Peptide
1	14-B	193	GLY	Peptide
1	14-B	196	TRP	Peptide
1	14-B	296	THR	Peptide
1	15-A	194	TYR	Peptide
1	15-A	196	TRP	Peptide
1	15-A	292	TRP	Peptide
1	15-A	313	GLY	Peptide
1	15-B	143	TRP	Peptide
1	15-B	295	GLY	Peptide
1	16-A	145	ASP	Peptide
1	16-A	293	GLY	Peptide
1	16-A	294	ASN	Peptide
1	16-A	296	THR	Peptide
1	16-A	311	LYS	Peptide
1	16-A	312	PRO	Peptide
1	16-A	313	GLY	Peptide
1	16-A	315	THR	Peptide
1	16-A	58	VAL	Peptide
1	17-A	144	PHE	Peptide
1	17-A	145	ASP	Peptide
1	17-A	193	GLY	Peptide
1	17-A	295	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	17-A	311	LYS	Peptide
1	17-A	401	ALA	Peptide
1	17-B	145	ASP	Peptide
1	17-B	313	GLY	Peptide
1	18-A	271	LEU	Peptide
1	18-A	293	GLY	Peptide
1	18-A	312	PRO	Peptide
1	18-B	291	SER	Peptide
1	18-B	293	GLY	Peptide
1	18-B	297	PRO	Peptide
1	18-B	312	PRO	Peptide
1	19-A	297	PRO	Peptide
1	19-A	422	ALA	Peptide
1	19-B	191	PRO	Peptide
1	19-B	293	GLY	Peptide
1	2-A	271	LEU	Peptide
1	2-A	272	ASP	Peptide
1	2-A	295	GLY	Peptide
1	2-A	311	LYS	Peptide
1	2-B	191	PRO	Peptide
1	2-B	194	TYR	Peptide
1	2-B	273	GLY	Peptide
1	2-B	295	GLY	Peptide
1	2-B	297	PRO	Peptide
1	20-A	193	GLY	Peptide
1	20-A	273	GLY	Peptide
1	20-A	71	PHE	Peptide
1	20-B	193	GLY	Peptide
1	20-B	194	TYR	Peptide
1	20-B	271	LEU	Peptide
1	20-B	272	ASP	Peptide
1	21-A	293	GLY	Peptide
1	21-A	295	GLY	Peptide
1	21-B	295	GLY	Peptide
1	21-B	313	GLY	Peptide
1	22-A	165	ASN	Peptide
1	22-A	193	GLY	Peptide
1	22-A	195	GLY	Peptide
1	22-A	293	GLY	Peptide
1	22-A	296	THR	Peptide
1	22-B	144	PHE	Peptide
1	23-A	58	VAL	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	23-B	192	ASP	Peptide
1	23-B	292	TRP	Peptide
1	23-B	306	GLN	Peptide
1	23-B	374	ASP	Peptide
1	24-A	145	ASP	Peptide
1	24-A	146	GLY	Peptide
1	24-A	193	GLY	Peptide
1	24-A	247	GLN	Peptide
1	24-A	293	GLY	Peptide
1	24-A	59	VAL	Peptide
1	24-A	70	VAL	Peptide
1	25-A	125	GLY	Peptide
1	25-A	193	GLY	Peptide
1	25-A	296	THR	Peptide
1	25-B	165	ASN	Peptide
1	25-B	374	ASP	Peptide
1	3-A	144	PHE	Peptide
1	3-A	295	GLY	Peptide
1	3-B	191	PRO	Peptide
1	3-B	295	GLY	Peptide
1	3-B	296	THR	Peptide
1	3-B	297	PRO	Peptide
1	3-B	400	GLY	Peptide
1	4-A	142	GLY	Peptide
1	4-B	142	GLY	Peptide
1	4-B	193	GLY	Peptide
1	5-A	594	ASP	Peptide
1	5-A	60	GLY	Peptide
1	6-A	295	GLY	Peptide
1	6-A	401	ALA	Peptide
1	6-A	63	ASP	Peptide
1	6-A	64	LEU	Peptide
1	6-B	164	VAL	Peptide
1	6-B	166	GLY	Peptide
1	7-A	193	GLY	Peptide
1	7-A	294	ASN	Peptide
1	7-A	295	GLY	Peptide
1	7-A	310	VAL	Peptide
1	7-A	339	ASP	Peptide
1	7-B	127	ASN	Peptide
1	7-B	144	PHE	Peptide
1	7-B	271	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	7-B	272	ASP	Peptide
1	7-B	273	GLY	Peptide
1	7-B	312	PRO	Peptide
1	7-B	77	ASP	Peptide
1	8-A	143	TRP	Peptide
1	8-A	193	GLY	Peptide
1	8-A	294	ASN	Peptide
1	8-A	296	THR	Peptide
1	8-B	326	GLY	Peptide
1	9-A	125	GLY	Peptide
1	9-A	192	ASP	Peptide
1	9-A	193	GLY	Peptide
1	9-B	142	GLY	Peptide
1	9-B	168	ASN	Peptide
1	9-B	192	ASP	Peptide
1	9-B	294	ASN	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	9-B	4181	3920	3932	0	0
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	5-B	12	18	18	0	0
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2-B	12	12	12	0	0
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	10-A	254	0	0	0	0
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

All (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
1	2-B	164	VAL
1	2-B	294	ASN
1	2-B	297	PRO
1	3-A	145	ASP
1	3-B	145	ASP
1	3-B	195	GLY
1	3-B	297	PRO
1	4-A	194	TYR
1	4-B	145	ASP
1	5-A	59	VAL
1	5-A	194	TYR
1	5-A	195	GLY
1	5-A	401	ALA
1	5-B	197	ALA
1	6-A	63	ASP
1	6-A	64	LEU
1	6-B	145	ASP
1	6-B	401	ALA
1	7-A	194	TYR
1	7-A	311	LYS
1	7-B	78	ILE
1	7-B	143	TRP
1	7-B	145	ASP
1	7-B	194	TYR
1	7-B	314	ALA
1	8-A	59	VAL
1	8-A	77	ASP
1	8-A	145	ASP
1	8-B	63	ASP
1	9-A	126	LEU
1	9-A	194	TYR
1	9-B	63	ASP
1	9-B	196	TRP
1	9-B	312	PRO
1	10-A	145	ASP
1	10-A	147	ASN
1	10-A	249	PHE
1	10-A	297	PRO
1	10-A	298	GLU
1	10-B	196	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	11-A	76	PRO
1	11-A	312	PRO
1	11-B	143	TRP
1	11-B	196	TRP
1	12-A	145	ASP
1	12-B	191	PRO
1	12-B	192	ASP
1	12-B	297	PRO
1	12-B	316	ALA
1	14-A	192	ASP
1	14-B	126	LEU
1	14-B	143	TRP
1	14-B	145	ASP
1	14-B	194	TYR
1	14-B	295	GLY
1	15-A	77	ASP
1	15-A	194	TYR
1	15-A	197	ALA
1	15-A	312	PRO
1	15-B	233	VAL
1	15-B	295	GLY
1	16-A	293	GLY
1	16-A	312	PRO
1	17-A	145	ASP
1	17-A	294	ASN
1	17-A	296	THR
1	17-A	298	GLU
1	17-A	299	GLY
1	17-A	300	GLU
1	17-B	145	ASP
1	17-B	312	PRO
1	18-A	297	PRO
1	18-A	314	ALA
1	18-B	142	GLY
1	18-B	297	PRO
1	18-B	493	ASN
1	19-A	145	ASP
1	19-A	422	ALA
1	19-B	192	ASP
1	19-B	296	THR
1	19-B	312	PRO
1	19-B	401	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	20-A	273	GLY
1	20-B	145	ASP
1	20-B	312	PRO
1	21-A	295	GLY
1	21-A	311	LYS
1	21-A	314	ALA
1	21-B	191	PRO
1	21-B	312	PRO
1	22-A	294	ASN
1	22-A	296	THR
1	22-B	145	ASP
1	23-A	63	ASP
1	23-A	145	ASP
1	23-B	293	GLY
1	23-B	312	PRO
1	24-A	70	VAL
1	24-A	145	ASP
1	24-A	164	VAL
1	24-A	294	ASN
1	24-A	297	PRO
1	24-B	145	ASP
1	24-B	194	TYR
1	24-B	401	ALA
1	25-A	126	LEU
1	25-A	145	ASP
1	25-A	191	PRO
1	25-A	194	TYR
1	25-B	194	TYR
1	25-B	195	GLY
1	1-A	293	GLY
1	1-A	295	GLY
1	1-B	72	ASP
1	1-B	145	ASP
1	1-B	313	GLY
1	1-B	401	ALA
1	2-A	195	GLY
1	2-A	273	GLY
1	2-B	195	GLY
1	2-B	274	ASP
1	3-A	77	ASP
1	3-A	192	ASP
1	3-A	246	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-B	142	GLY
1	3-B	298	GLU
1	5-A	61	GLY
1	5-A	512	ALA
1	5-A	516	GLY
1	5-B	194	TYR
1	5-B	317	GLU
1	7-B	142	GLY
1	7-B	273	GLY
1	7-B	313	GLY
1	9-A	62	GLY
1	9-A	314	ALA
1	9-B	273	GLY
1	10-A	294	ASN
1	10-B	164	VAL
1	11-A	196	TRP
1	11-B	142	GLY
1	11-B	197	ALA
1	12-A	305	ASP
1	12-A	401	ALA
1	12-B	293	GLY
1	14-A	293	GLY
1	14-A	312	PRO
1	14-A	401	ALA
1	14-B	142	GLY
1	14-B	400	GLY
1	14-B	401	ALA
1	15-B	78	ILE
1	17-A	193	GLY
1	17-B	148	ALA
1	17-B	273	GLY
1	17-B	517	ASP
1	18-A	145	ASP
1	18-A	295	GLY
1	18-A	313	GLY
1	18-B	145	ASP
1	18-B	298	GLU
1	19-B	297	PRO
1	20-A	295	GLY
1	20-B	193	GLY
1	20-B	233	VAL
1	20-B	325	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	21-A	145	ASP
1	21-A	312	PRO
1	22-A	59	VAL
1	22-B	134	ASN
1	23-B	145	ASP
1	23-B	273	GLY
1	23-B	401	ALA
1	24-A	71	PHE
1	24-A	194	TYR
1	24-B	400	GLY
1	25-A	286	ASN
1	25-B	145	ASP
1	25-B	233	VAL
1	25-B	314	ALA
1	25-B	400	GLY
1	2-A	528	ASP
1	5-A	63	ASP
1	5-A	126	LEU
1	5-A	295	GLY
1	5-A	312	PRO
1	5-B	313	GLY
1	6-A	317	GLU
1	7-A	191	PRO
1	7-A	193	GLY
1	7-B	247	GLN
1	7-B	311	LYS
1	8-B	192	ASP
1	9-A	214	TYR
1	10-A	324	ASP
1	10-B	144	PHE
1	10-B	146	GLY
1	11-B	326	GLY
1	11-B	530	VAL
1	12-A	295	GLY
1	13-A	194	TYR
1	13-B	194	TYR
1	13-B	233	VAL
1	14-A	294	ASN
1	14-B	298	GLU
1	15-A	143	TRP
1	15-A	191	PRO
1	15-A	193	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	15-A	246	ALA
1	15-A	313	GLY
1	15-A	314	ALA
1	15-A	401	ALA
1	15-B	61	GLY
1	15-B	145	ASP
1	15-B	401	ALA
1	16-B	372	ASP
1	16-B	401	ALA
1	17-A	147	ASN
1	17-A	194	TYR
1	17-A	311	LYS
1	17-A	312	PRO
1	17-B	110	ASP
1	17-B	146	GLY
1	17-B	214	TYR
1	17-B	298	GLU
1	18-A	324	ASP
1	18-B	312	PRO
1	19-A	233	VAL
1	20-A	59	VAL
1	20-B	194	TYR
1	22-B	197	ALA
1	22-B	298	GLU
1	24-B	195	GLY
1	2-A	126	LEU
1	2-A	214	TYR
1	4-A	297	PRO
1	4-B	297	PRO
1	6-A	110	ASP
1	6-A	312	PRO
1	7-A	59	VAL
1	8-A	192	ASP
1	8-A	286	ASN
1	8-B	325	GLN
1	11-B	273	GLY
1	11-B	313	GLY
1	12-A	193	GLY
1	15-B	214	TYR
1	15-B	296	THR
1	18-A	294	ASN
1	18-B	293	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	20-A	63	ASP
1	20-B	196	TRP
1	20-B	528	ASP
1	21-B	145	ASP
1	21-B	214	TYR
1	22-A	143	TRP
1	22-A	192	ASP
1	22-A	196	TRP
1	22-B	56	GLN
1	22-B	78	ILE
1	22-B	214	TYR
1	24-A	528	ASP
1	24-B	216	GLN
1	2-B	283	LYS
1	2-B	401	ALA
1	3-A	296	THR
1	3-B	194	TYR
1	4-B	305	ASP
1	5-A	214	TYR
1	5-B	214	TYR
1	5-B	295	GLY
1	6-A	401	ALA
1	6-B	87	ARG
1	6-B	193	GLY
1	9-A	294	ASN
1	9-B	141	ALA
1	9-B	145	ASP
1	10-A	498	PHE
1	10-A	516	GLY
1	13-B	73	PRO
1	15-B	149	THR
1	16-A	214	TYR
1	16-B	248	SER
1	16-B	249	PHE
1	16-B	532	THR
1	17-A	59	VAL
1	17-A	498	PHE
1	18-A	248	SER
1	18-A	299	GLY
1	18-A	301	SER
1	19-A	143	TRP
1	19-A	297	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	19-B	145	ASP
1	20-A	146	GLY
1	20-A	481	HIS
1	21-A	214	TYR
1	21-B	314	ALA
1	21-B	498	PHE
1	22-A	498	PHE
1	24-A	498	PHE
1	24-B	73	PRO
1	24-B	516	GLY
1	25-A	293	GLY
1	25-A	297	PRO
1	3-A	498	PHE
1	3-B	498	PHE
1	4-B	191	PRO
1	7-A	498	PHE
1	7-B	498	PHE
1	8-A	195	GLY
1	9-B	516	GLY
1	10-B	498	PHE
1	12-B	498	PHE
1	13-A	295	GLY
1	13-A	498	PHE
1	16-A	77	ASP
1	17-B	498	PHE
1	18-B	498	PHE
1	19-B	498	PHE
1	21-A	248	SER
1	21-A	296	THR
1	23-A	498	PHE
1	25-A	296	THR
1	25-A	498	PHE
1	5-B	66	PRO
1	19-B	191	PRO
1	6-A	233	VAL
1	7-B	508	PRO
1	24-B	233	VAL
1	7-A	312	PRO
1	16-B	233	VAL
1	17-B	233	VAL
1	19-A	142	GLY
1	20-B	293	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-B	191	PRO
1	6-A	423	GLY
1	7-A	273	GLY
1	9-B	293	GLY
1	13-B	312	PRO
1	14-B	193	GLY
1	18-B	191	PRO
1	21-A	195	GLY
1	1-B	293	GLY
1	7-B	312	PRO
1	17-A	273	GLY
1	19-B	516	GLY
1	19-A	250	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (1693) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	59	VAL
1	1-A	69	LEU
1	1-A	72	ASP
1	1-A	87	ARG
1	1-A	88	LYS
1	1-A	90	GLU
1	1-A	97	ASP
1	1-A	104	LYS
1	1-A	110	ASP
1	1-A	140	ASP
1	1-A	144	PHE
1	1-A	169	ARG
1	1-A	196	TRP
1	1-A	206	LYS
1	1-A	210	GLU
1	1-A	225	SER
1	1-A	236	MET
1	1-A	261	PRO
1	1-A	301	SER
1	1-A	303	PRO
1	1-A	337	HIS
1	1-A	346	ARG
1	1-A	348	ASN
1	1-A	368	LEU
1	1-A	369	LYS
1	1-A	402	SER
1	1-A	419	ILE
1	1-A	440	ILE
1	1-A	457	GLU
1	1-A	509	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-A	518	ILE
1	1-A	529	SER
1	1-A	531	THR
1	1-A	538	MET
1	1-A	541	TYR
1	1-A	545	ASN
1	1-A	597	ILE
1	1-A	600	GLN
1	1-A	603	SER
1	1-B	56	GLN
1	1-B	64	LEU
1	1-B	69	LEU
1	1-B	81	LYS
1	1-B	102	MET
1	1-B	136	ASP
1	1-B	140	ASP
1	1-B	144	PHE
1	1-B	145	ASP
1	1-B	147	ASN
1	1-B	150	GLN
1	1-B	180	ARG
1	1-B	194	TYR
1	1-B	236	MET
1	1-B	259	THR
1	1-B	283	LYS
1	1-B	294	ASN
1	1-B	297	PRO
1	1-B	304	LEU
1	1-B	310	VAL
1	1-B	311	LYS
1	1-B	318	THR
1	1-B	336	TYR
1	1-B	346	ARG
1	1-B	359	ILE
1	1-B	399	ASP
1	1-B	466	HIS
1	1-B	488	GLN
1	1-B	519	LYS
1	1-B	529	SER
1	1-B	531	THR
1	1-B	553	GLN
1	1-B	570	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-B	574	LEU
1	2-A	69	LEU
1	2-A	72	ASP
1	2-A	88	LYS
1	2-A	104	LYS
1	2-A	126	LEU
1	2-A	136	ASP
1	2-A	144	PHE
1	2-A	145	ASP
1	2-A	155	SER
1	2-A	157	GLU
1	2-A	196	TRP
1	2-A	210	GLU
1	2-A	231	ASN
1	2-A	236	MET
1	2-A	262	VAL
1	2-A	271	LEU
1	2-A	272	ASP
1	2-A	283	LYS
1	2-A	294	ASN
1	2-A	301	SER
1	2-A	304	LEU
1	2-A	306	GLN
1	2-A	311	LYS
1	2-A	337	HIS
1	2-A	340	GLN
1	2-A	346	ARG
1	2-A	362	ASP
1	2-A	368	LEU
1	2-A	399	ASP
1	2-A	493	ASN
1	2-A	500	GLN
1	2-A	531	THR
1	2-A	541	TYR
1	2-A	543	TYR
1	2-A	561	LYS
1	2-A	565	LYS
1	2-A	577	LYS
1	2-B	74	SER
1	2-B	81	LYS
1	2-B	87	ARG
1	2-B	91	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-B	126	LEU
1	2-B	127	ASN
1	2-B	165	ASN
1	2-B	194	TYR
1	2-B	222	ARG
1	2-B	236	MET
1	2-B	261	PRO
1	2-B	274	ASP
1	2-B	277	LYS
1	2-B	283	LYS
1	2-B	298	GLU
1	2-B	315	THR
1	2-B	324	ASP
1	2-B	399	ASP
1	2-B	402	SER
1	2-B	404	ASP
1	2-B	492	GLU
1	2-B	517	ASP
1	2-B	531	THR
1	2-B	565	LYS
1	2-B	600	GLN
1	3-A	63	ASP
1	3-A	69	LEU
1	3-A	87	ARG
1	3-A	126	LEU
1	3-A	136	ASP
1	3-A	144	PHE
1	3-A	145	ASP
1	3-A	184	LYS
1	3-A	250	PRO
1	3-A	271	LEU
1	3-A	286	ASN
1	3-A	294	ASN
1	3-A	298	GLU
1	3-A	301	SER
1	3-A	308	TYR
1	3-A	317	GLU
1	3-A	325	GLN
1	3-A	340	GLN
1	3-A	346	ARG
1	3-A	368	LEU
1	3-A	424	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-A	471	ASN
1	3-A	517	ASP
1	3-A	519	LYS
1	3-A	528	ASP
1	3-A	532	THR
1	3-A	541	TYR
1	3-A	565	LYS
1	3-A	570	LEU
1	3-A	592	SER
1	3-A	600	GLN
1	3-B	63	ASP
1	3-B	72	ASP
1	3-B	87	ARG
1	3-B	102	MET
1	3-B	107	THR
1	3-B	111	ILE
1	3-B	136	ASP
1	3-B	165	ASN
1	3-B	210	GLU
1	3-B	236	MET
1	3-B	269	LEU
1	3-B	272	ASP
1	3-B	275	ASP
1	3-B	294	ASN
1	3-B	298	GLU
1	3-B	302	LEU
1	3-B	318	THR
1	3-B	325	GLN
1	3-B	346	ARG
1	3-B	404	ASP
1	3-B	468	LYS
1	3-B	484	LYS
1	3-B	517	ASP
1	3-B	518	ILE
1	3-B	529	SER
1	3-B	531	THR
1	3-B	541	TYR
1	3-B	543	TYR
1	3-B	545	ASN
1	3-B	565	LYS
1	3-B	570	LEU
1	3-B	572	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-A	64	LEU
1	4-A	70	VAL
1	4-A	74	SER
1	4-A	78	ILE
1	4-A	81	LYS
1	4-A	84	GLU
1	4-A	102	MET
1	4-A	136	ASP
1	4-A	180	ARG
1	4-A	192	ASP
1	4-A	196	TRP
1	4-A	206	LYS
1	4-A	210	GLU
1	4-A	236	MET
1	4-A	272	ASP
1	4-A	275	ASP
1	4-A	283	LYS
1	4-A	296	THR
1	4-A	298	GLU
1	4-A	303	PRO
1	4-A	337	HIS
1	4-A	346	ARG
1	4-A	412	LEU
1	4-A	468	LYS
1	4-A	525	LYS
1	4-A	603	SER
1	4-B	63	ASP
1	4-B	87	ARG
1	4-B	126	LEU
1	4-B	127	ASN
1	4-B	140	ASP
1	4-B	144	PHE
1	4-B	169	ARG
1	4-B	196	TRP
1	4-B	236	MET
1	4-B	248	SER
1	4-B	269	LEU
1	4-B	277	LYS
1	4-B	294	ASN
1	4-B	296	THR
1	4-B	297	PRO
1	4-B	300	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-B	302	LEU
1	4-B	305	ASP
1	4-B	346	ARG
1	4-B	399	ASP
1	4-B	402	SER
1	4-B	404	ASP
1	4-B	457	GLU
1	4-B	495	LYS
1	4-B	527	ASP
1	4-B	541	TYR
1	4-B	545	ASN
1	4-B	546	VAL
1	4-B	565	LYS
1	4-B	600	GLN
1	5-A	81	LYS
1	5-A	120	SER
1	5-A	126	LEU
1	5-A	127	ASN
1	5-A	144	PHE
1	5-A	164	VAL
1	5-A	169	ARG
1	5-A	196	TRP
1	5-A	236	MET
1	5-A	257	LEU
1	5-A	258	GLU
1	5-A	271	LEU
1	5-A	283	LYS
1	5-A	285	THR
1	5-A	339	ASP
1	5-A	460	ARG
1	5-A	493	ASN
1	5-A	517	ASP
1	5-A	527	ASP
1	5-A	543	TYR
1	5-A	553	GLN
1	5-A	577	LYS
1	5-A	586	ASP
1	5-A	603	SER
1	5-B	56	GLN
1	5-B	64	LEU
1	5-B	69	LEU
1	5-B	72	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-B	74	SER
1	5-B	79	GLN
1	5-B	88	LYS
1	5-B	97	ASP
1	5-B	111	ILE
1	5-B	112	ASN
1	5-B	144	PHE
1	5-B	147	ASN
1	5-B	149	THR
1	5-B	165	ASN
1	5-B	192	ASP
1	5-B	196	TRP
1	5-B	198	SER
1	5-B	236	MET
1	5-B	270	TYR
1	5-B	296	THR
1	5-B	302	LEU
1	5-B	340	GLN
1	5-B	346	ARG
1	5-B	399	ASP
1	5-B	402	SER
1	5-B	404	ASP
1	5-B	468	LYS
1	5-B	514	GLN
1	5-B	519	LYS
1	5-B	541	TYR
1	5-B	565	LYS
1	5-B	570	LEU
1	5-B	574	LEU
1	5-B	587	ILE
1	6-A	64	LEU
1	6-A	87	ARG
1	6-A	97	ASP
1	6-A	124	LEU
1	6-A	126	LEU
1	6-A	192	ASP
1	6-A	196	TRP
1	6-A	206	LYS
1	6-A	207	ILE
1	6-A	236	MET
1	6-A	258	GLU
1	6-A	285	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-A	298	GLU
1	6-A	312	PRO
1	6-A	324	ASP
1	6-A	325	GLN
1	6-A	340	GLN
1	6-A	346	ARG
1	6-A	368	LEU
1	6-A	384	ASP
1	6-A	492	GLU
1	6-A	515	ASN
1	6-A	527	ASP
1	6-A	545	ASN
1	6-A	553	GLN
1	6-A	570	LEU
1	6-A	595	THR
1	6-A	603	SER
1	6-A	604	PHE
1	6-B	64	LEU
1	6-B	88	LYS
1	6-B	112	ASN
1	6-B	126	LEU
1	6-B	140	ASP
1	6-B	144	PHE
1	6-B	145	ASP
1	6-B	149	THR
1	6-B	164	VAL
1	6-B	165	ASN
1	6-B	167	THR
1	6-B	180	ARG
1	6-B	236	MET
1	6-B	270	TYR
1	6-B	275	ASP
1	6-B	277	LYS
1	6-B	283	LYS
1	6-B	296	THR
1	6-B	301	SER
1	6-B	302	LEU
1	6-B	305	ASP
1	6-B	346	ARG
1	6-B	404	ASP
1	6-B	468	LYS
1	6-B	493	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-B	509	ASP
1	6-B	553	GLN
1	6-B	570	LEU
1	6-B	572	VAL
1	6-B	577	LYS
1	6-B	592	SER
1	7-A	58	VAL
1	7-A	59	VAL
1	7-A	72	ASP
1	7-A	87	ARG
1	7-A	114	GLN
1	7-A	145	ASP
1	7-A	180	ARG
1	7-A	192	ASP
1	7-A	196	TRP
1	7-A	236	MET
1	7-A	250	PRO
1	7-A	251	GLU
1	7-A	257	LEU
1	7-A	274	ASP
1	7-A	311	LYS
1	7-A	340	GLN
1	7-A	346	ARG
1	7-A	362	ASP
1	7-A	440	ILE
1	7-A	458	THR
1	7-A	471	ASN
1	7-A	517	ASP
1	7-A	518	ILE
1	7-A	543	TYR
1	7-A	570	LEU
1	7-A	587	ILE
1	7-A	592	SER
1	7-B	81	LYS
1	7-B	82	VAL
1	7-B	97	ASP
1	7-B	112	ASN
1	7-B	127	ASN
1	7-B	144	PHE
1	7-B	184	LYS
1	7-B	210	GLU
1	7-B	236	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-B	272	ASP
1	7-B	286	ASN
1	7-B	310	VAL
1	7-B	311	LYS
1	7-B	324	ASP
1	7-B	354	LEU
1	7-B	402	SER
1	7-B	404	ASP
1	7-B	517	ASP
1	7-B	527	ASP
1	7-B	529	SER
1	7-B	532	THR
1	7-B	541	TYR
1	7-B	546	VAL
1	7-B	570	LEU
1	7-B	574	LEU
1	8-A	59	VAL
1	8-A	69	LEU
1	8-A	77	ASP
1	8-A	78	ILE
1	8-A	81	LYS
1	8-A	87	ARG
1	8-A	88	LYS
1	8-A	97	ASP
1	8-A	102	MET
1	8-A	114	GLN
1	8-A	147	ASN
1	8-A	155	SER
1	8-A	157	GLU
1	8-A	169	ARG
1	8-A	180	ARG
1	8-A	194	TYR
1	8-A	207	ILE
1	8-A	231	ASN
1	8-A	236	MET
1	8-A	270	TYR
1	8-A	283	LYS
1	8-A	285	THR
1	8-A	294	ASN
1	8-A	305	ASP
1	8-A	306	GLN
1	8-A	308	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-A	339	ASP
1	8-A	340	GLN
1	8-A	369	LYS
1	8-A	384	ASP
1	8-A	404	ASP
1	8-A	449	ASP
1	8-A	517	ASP
1	8-A	527	ASP
1	8-A	531	THR
1	8-A	541	TYR
1	8-A	543	TYR
1	8-A	570	LEU
1	8-A	603	SER
1	8-B	64	LEU
1	8-B	69	LEU
1	8-B	74	SER
1	8-B	81	LYS
1	8-B	112	ASN
1	8-B	114	GLN
1	8-B	140	ASP
1	8-B	180	ARG
1	8-B	196	TRP
1	8-B	222	ARG
1	8-B	231	ASN
1	8-B	236	MET
1	8-B	257	LEU
1	8-B	262	VAL
1	8-B	274	ASP
1	8-B	277	LYS
1	8-B	283	LYS
1	8-B	300	GLU
1	8-B	310	VAL
1	8-B	311	LYS
1	8-B	330	LEU
1	8-B	402	SER
1	8-B	404	ASP
1	8-B	458	THR
1	8-B	460	ARG
1	8-B	468	LYS
1	8-B	508	PRO
1	8-B	527	ASP
1	8-B	529	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-B	531	THR
1	8-B	541	TYR
1	8-B	545	ASN
1	8-B	574	LEU
1	8-B	605	PRO
1	9-A	58	VAL
1	9-A	81	LYS
1	9-A	114	GLN
1	9-A	126	LEU
1	9-A	136	ASP
1	9-A	144	PHE
1	9-A	147	ASN
1	9-A	169	ARG
1	9-A	180	ARG
1	9-A	194	TYR
1	9-A	236	MET
1	9-A	257	LEU
1	9-A	262	VAL
1	9-A	266	LYS
1	9-A	271	LEU
1	9-A	274	ASP
1	9-A	277	LYS
1	9-A	294	ASN
1	9-A	300	GLU
1	9-A	317	GLU
1	9-A	337	HIS
1	9-A	340	GLN
1	9-A	346	ARG
1	9-A	389	ASN
1	9-A	399	ASP
1	9-A	493	ASN
1	9-A	531	THR
1	9-A	541	TYR
1	9-A	543	TYR
1	9-A	553	GLN
1	9-A	565	LYS
1	9-A	570	LEU
1	9-A	600	GLN
1	9-B	72	ASP
1	9-B	81	LYS
1	9-B	88	LYS
1	9-B	92	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-B	126	LEU
1	9-B	136	ASP
1	9-B	144	PHE
1	9-B	169	ARG
1	9-B	180	ARG
1	9-B	184	LYS
1	9-B	192	ASP
1	9-B	236	MET
1	9-B	283	LYS
1	9-B	302	LEU
1	9-B	311	LYS
1	9-B	312	PRO
1	9-B	317	GLU
1	9-B	318	THR
1	9-B	330	LEU
1	9-B	340	GLN
1	9-B	359	ILE
1	9-B	368	LEU
1	9-B	391	GLU
1	9-B	404	ASP
1	9-B	458	THR
1	9-B	468	LYS
1	9-B	493	ASN
1	9-B	509	ASP
1	9-B	517	ASP
1	9-B	531	THR
1	9-B	541	TYR
1	9-B	565	LYS
1	9-B	570	LEU
1	9-B	586	ASP
1	9-B	587	ILE
1	9-B	589	ASP
1	9-B	592	SER
1	9-B	600	GLN
1	10-A	59	VAL
1	10-A	102	MET
1	10-A	110	ASP
1	10-A	112	ASN
1	10-A	126	LEU
1	10-A	144	PHE
1	10-A	169	ARG
1	10-A	188	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-A	192	ASP
1	10-A	194	TYR
1	10-A	198	SER
1	10-A	236	MET
1	10-A	259	THR
1	10-A	269	LEU
1	10-A	277	LYS
1	10-A	283	LYS
1	10-A	286	ASN
1	10-A	294	ASN
1	10-A	296	THR
1	10-A	298	GLU
1	10-A	306	GLN
1	10-A	311	LYS
1	10-A	324	ASP
1	10-A	339	ASP
1	10-A	362	ASP
1	10-A	399	ASP
1	10-A	402	SER
1	10-A	457	GLU
1	10-A	460	ARG
1	10-A	489	TRP
1	10-A	543	TYR
1	10-A	570	LEU
1	10-A	574	LEU
1	10-A	587	ILE
1	10-A	595	THR
1	10-B	56	GLN
1	10-B	79	GLN
1	10-B	81	LYS
1	10-B	88	LYS
1	10-B	102	MET
1	10-B	112	ASN
1	10-B	126	LEU
1	10-B	145	ASP
1	10-B	165	ASN
1	10-B	169	ARG
1	10-B	180	ARG
1	10-B	184	LYS
1	10-B	196	TRP
1	10-B	236	MET
1	10-B	269	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-B	270	TYR
1	10-B	286	ASN
1	10-B	294	ASN
1	10-B	311	LYS
1	10-B	315	THR
1	10-B	318	THR
1	10-B	324	ASP
1	10-B	330	LEU
1	10-B	342	ILE
1	10-B	346	ARG
1	10-B	377	LYS
1	10-B	399	ASP
1	10-B	402	SER
1	10-B	404	ASP
1	10-B	424	PRO
1	10-B	457	GLU
1	10-B	460	ARG
1	10-B	466	HIS
1	10-B	493	ASN
1	10-B	517	ASP
1	10-B	541	TYR
1	10-B	545	ASN
1	10-B	570	LEU
1	10-B	574	LEU
1	10-B	595	THR
1	11-A	58	VAL
1	11-A	59	VAL
1	11-A	63	ASP
1	11-A	67	ASN
1	11-A	72	ASP
1	11-A	74	SER
1	11-A	188	ASN
1	11-A	196	TRP
1	11-A	236	MET
1	11-A	269	LEU
1	11-A	283	LYS
1	11-A	298	GLU
1	11-A	305	ASP
1	11-A	346	ARG
1	11-A	471	ASN
1	11-A	517	ASP
1	11-A	527	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	11-A	534	GLU
1	11-A	541	TYR
1	11-A	543	TYR
1	11-A	554	HIS
1	11-A	557	GLN
1	11-A	565	LYS
1	11-A	570	LEU
1	11-A	592	SER
1	11-B	63	ASP
1	11-B	72	ASP
1	11-B	74	SER
1	11-B	169	ARG
1	11-B	182	HIS
1	11-B	184	LYS
1	11-B	192	ASP
1	11-B	236	MET
1	11-B	251	GLU
1	11-B	257	LEU
1	11-B	258	GLU
1	11-B	269	LEU
1	11-B	271	LEU
1	11-B	296	THR
1	11-B	298	GLU
1	11-B	311	LYS
1	11-B	315	THR
1	11-B	317	GLU
1	11-B	330	LEU
1	11-B	339	ASP
1	11-B	404	ASP
1	11-B	466	HIS
1	11-B	493	ASN
1	11-B	495	LYS
1	11-B	517	ASP
1	11-B	528	ASP
1	11-B	529	SER
1	11-B	532	THR
1	11-B	541	TYR
1	11-B	572	VAL
1	11-B	587	ILE
1	12-A	63	ASP
1	12-A	64	LEU
1	12-A	87	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	12-A	88	LYS
1	12-A	96	THR
1	12-A	114	GLN
1	12-A	188	ASN
1	12-A	236	MET
1	12-A	285	THR
1	12-A	294	ASN
1	12-A	296	THR
1	12-A	305	ASP
1	12-A	311	LYS
1	12-A	325	GLN
1	12-A	337	HIS
1	12-A	362	ASP
1	12-A	402	SER
1	12-A	404	ASP
1	12-A	541	TYR
1	12-A	543	TYR
1	12-A	561	LYS
1	12-A	570	LEU
1	12-A	574	LEU
1	12-A	587	ILE
1	12-A	603	SER
1	12-B	56	GLN
1	12-B	64	LEU
1	12-B	72	ASP
1	12-B	74	SER
1	12-B	81	LYS
1	12-B	87	ARG
1	12-B	92	ASN
1	12-B	96	THR
1	12-B	102	MET
1	12-B	104	LYS
1	12-B	124	LEU
1	12-B	126	LEU
1	12-B	127	ASN
1	12-B	136	ASP
1	12-B	140	ASP
1	12-B	165	ASN
1	12-B	180	ARG
1	12-B	192	ASP
1	12-B	196	TRP
1	12-B	206	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	12-B	236	MET
1	12-B	262	VAL
1	12-B	266	LYS
1	12-B	269	LEU
1	12-B	272	ASP
1	12-B	283	LYS
1	12-B	292	TRP
1	12-B	298	GLU
1	12-B	302	LEU
1	12-B	346	ARG
1	12-B	402	SER
1	12-B	404	ASP
1	12-B	468	LYS
1	12-B	471	ASN
1	12-B	490	SER
1	12-B	495	LYS
1	12-B	515	ASN
1	12-B	528	ASP
1	12-B	541	TYR
1	12-B	545	ASN
1	12-B	570	LEU
1	12-B	574	LEU
1	12-B	584	ILE
1	12-B	587	ILE
1	12-B	600	GLN
1	13-A	58	VAL
1	13-A	59	VAL
1	13-A	64	LEU
1	13-A	82	VAL
1	13-A	87	ARG
1	13-A	89	GLN
1	13-A	126	LEU
1	13-A	144	PHE
1	13-A	150	GLN
1	13-A	180	ARG
1	13-A	194	TYR
1	13-A	236	MET
1	13-A	250	PRO
1	13-A	262	VAL
1	13-A	271	LEU
1	13-A	283	LYS
1	13-A	296	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	13-A	298	GLU
1	13-A	301	SER
1	13-A	311	LYS
1	13-A	325	GLN
1	13-A	340	GLN
1	13-A	346	ARG
1	13-A	402	SER
1	13-A	404	ASP
1	13-A	527	ASP
1	13-A	528	ASP
1	13-A	529	SER
1	13-A	531	THR
1	13-A	532	THR
1	13-A	541	TYR
1	13-A	543	TYR
1	13-A	553	GLN
1	13-A	554	HIS
1	13-A	587	ILE
1	13-A	603	SER
1	13-B	64	LEU
1	13-B	69	LEU
1	13-B	74	SER
1	13-B	87	ARG
1	13-B	126	LEU
1	13-B	136	ASP
1	13-B	144	PHE
1	13-B	150	GLN
1	13-B	165	ASN
1	13-B	169	ARG
1	13-B	182	HIS
1	13-B	231	ASN
1	13-B	236	MET
1	13-B	262	VAL
1	13-B	266	LYS
1	13-B	283	LYS
1	13-B	284	ARG
1	13-B	297	PRO
1	13-B	301	SER
1	13-B	315	THR
1	13-B	340	GLN
1	13-B	346	ARG
1	13-B	402	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	13-B	404	ASP
1	13-B	468	LYS
1	13-B	489	TRP
1	13-B	490	SER
1	13-B	495	LYS
1	13-B	529	SER
1	13-B	565	LYS
1	13-B	570	LEU
1	13-B	574	LEU
1	13-B	577	LYS
1	13-B	584	ILE
1	13-B	589	ASP
1	13-B	595	THR
1	14-A	58	VAL
1	14-A	64	LEU
1	14-A	74	SER
1	14-A	92	ASN
1	14-A	102	MET
1	14-A	110	ASP
1	14-A	112	ASN
1	14-A	120	SER
1	14-A	127	ASN
1	14-A	136	ASP
1	14-A	145	ASP
1	14-A	184	LYS
1	14-A	236	MET
1	14-A	248	SER
1	14-A	274	ASP
1	14-A	283	LYS
1	14-A	284	ARG
1	14-A	294	ASN
1	14-A	306	GLN
1	14-A	310	VAL
1	14-A	315	THR
1	14-A	318	THR
1	14-A	337	HIS
1	14-A	346	ARG
1	14-A	356	LEU
1	14-A	362	ASP
1	14-A	372	ASP
1	14-A	395	GLU
1	14-A	398	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	14-A	402	SER
1	14-A	505	TYR
1	14-A	519	LYS
1	14-A	531	THR
1	14-A	543	TYR
1	14-A	570	LEU
1	14-A	587	ILE
1	14-A	595	THR
1	14-A	603	SER
1	14-B	56	GLN
1	14-B	64	LEU
1	14-B	74	SER
1	14-B	124	LEU
1	14-B	126	LEU
1	14-B	140	ASP
1	14-B	144	PHE
1	14-B	167	THR
1	14-B	192	ASP
1	14-B	196	TRP
1	14-B	198	SER
1	14-B	206	LYS
1	14-B	236	MET
1	14-B	251	GLU
1	14-B	261	PRO
1	14-B	266	LYS
1	14-B	269	LEU
1	14-B	271	LEU
1	14-B	283	LYS
1	14-B	301	SER
1	14-B	302	LEU
1	14-B	305	ASP
1	14-B	311	LYS
1	14-B	324	ASP
1	14-B	340	GLN
1	14-B	356	LEU
1	14-B	368	LEU
1	14-B	399	ASP
1	14-B	402	SER
1	14-B	404	ASP
1	14-B	434	ASN
1	14-B	460	ARG
1	14-B	471	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	14-B	509	ASP
1	14-B	517	ASP
1	14-B	528	ASP
1	14-B	531	THR
1	14-B	541	TYR
1	14-B	545	ASN
1	14-B	570	LEU
1	15-A	69	LEU
1	15-A	92	ASN
1	15-A	102	MET
1	15-A	114	GLN
1	15-A	144	PHE
1	15-A	192	ASP
1	15-A	196	TRP
1	15-A	271	LEU
1	15-A	285	THR
1	15-A	300	GLU
1	15-A	301	SER
1	15-A	311	LYS
1	15-A	340	GLN
1	15-A	346	ARG
1	15-A	348	ASN
1	15-A	468	LYS
1	15-A	488	GLN
1	15-A	517	ASP
1	15-A	565	LYS
1	15-A	570	LEU
1	15-A	577	LYS
1	15-A	587	ILE
1	15-A	592	SER
1	15-B	56	GLN
1	15-B	63	ASP
1	15-B	67	ASN
1	15-B	79	GLN
1	15-B	84	GLU
1	15-B	126	LEU
1	15-B	144	PHE
1	15-B	145	ASP
1	15-B	165	ASN
1	15-B	180	ARG
1	15-B	196	TRP
1	15-B	225	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	15-B	236	MET
1	15-B	248	SER
1	15-B	251	GLU
1	15-B	266	LYS
1	15-B	275	ASP
1	15-B	283	LYS
1	15-B	284	ARG
1	15-B	304	LEU
1	15-B	305	ASP
1	15-B	306	GLN
1	15-B	317	GLU
1	15-B	346	ARG
1	15-B	369	LYS
1	15-B	399	ASP
1	15-B	402	SER
1	15-B	404	ASP
1	15-B	457	GLU
1	15-B	462	ASP
1	15-B	468	LYS
1	15-B	490	SER
1	15-B	518	ILE
1	15-B	527	ASP
1	15-B	531	THR
1	15-B	541	TYR
1	15-B	545	ASN
1	15-B	570	LEU
1	15-B	574	LEU
1	15-B	600	GLN
1	15-B	603	SER
1	16-A	69	LEU
1	16-A	81	LYS
1	16-A	84	GLU
1	16-A	92	ASN
1	16-A	104	LYS
1	16-A	107	THR
1	16-A	127	ASN
1	16-A	144	PHE
1	16-A	145	ASP
1	16-A	164	VAL
1	16-A	180	ARG
1	16-A	188	ASN
1	16-A	210	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16-A	236	MET
1	16-A	257	LEU
1	16-A	258	GLU
1	16-A	262	VAL
1	16-A	269	LEU
1	16-A	283	LYS
1	16-A	285	THR
1	16-A	294	ASN
1	16-A	296	THR
1	16-A	298	GLU
1	16-A	324	ASP
1	16-A	325	GLN
1	16-A	340	GLN
1	16-A	346	ARG
1	16-A	352	LEU
1	16-A	399	ASP
1	16-A	404	ASP
1	16-A	519	LYS
1	16-A	529	SER
1	16-A	532	THR
1	16-A	543	TYR
1	16-A	545	ASN
1	16-A	554	HIS
1	16-A	557	GLN
1	16-A	565	LYS
1	16-A	570	LEU
1	16-A	587	ILE
1	16-A	600	GLN
1	16-B	79	GLN
1	16-B	97	ASP
1	16-B	110	ASP
1	16-B	126	LEU
1	16-B	127	ASN
1	16-B	136	ASP
1	16-B	182	HIS
1	16-B	192	ASP
1	16-B	236	MET
1	16-B	261	PRO
1	16-B	262	VAL
1	16-B	271	LEU
1	16-B	272	ASP
1	16-B	283	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16-B	296	THR
1	16-B	298	GLU
1	16-B	311	LYS
1	16-B	325	GLN
1	16-B	330	LEU
1	16-B	377	LYS
1	16-B	398	SER
1	16-B	402	SER
1	16-B	404	ASP
1	16-B	458	THR
1	16-B	468	LYS
1	16-B	490	SER
1	16-B	532	THR
1	16-B	541	TYR
1	16-B	545	ASN
1	16-B	565	LYS
1	16-B	570	LEU
1	16-B	574	LEU
1	16-B	600	GLN
1	17-A	58	VAL
1	17-A	59	VAL
1	17-A	63	ASP
1	17-A	67	ASN
1	17-A	81	LYS
1	17-A	88	LYS
1	17-A	97	ASP
1	17-A	127	ASN
1	17-A	136	ASP
1	17-A	144	PHE
1	17-A	164	VAL
1	17-A	192	ASP
1	17-A	217	GLN
1	17-A	236	MET
1	17-A	269	LEU
1	17-A	271	LEU
1	17-A	275	ASP
1	17-A	294	ASN
1	17-A	296	THR
1	17-A	305	ASP
1	17-A	311	LYS
1	17-A	324	ASP
1	17-A	325	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	17-A	339	ASP
1	17-A	340	GLN
1	17-A	345	ASP
1	17-A	369	LYS
1	17-A	372	ASP
1	17-A	490	SER
1	17-A	493	ASN
1	17-A	495	LYS
1	17-A	518	ILE
1	17-A	527	ASP
1	17-A	529	SER
1	17-A	541	TYR
1	17-A	543	TYR
1	17-A	565	LYS
1	17-A	570	LEU
1	17-A	574	LEU
1	17-B	56	GLN
1	17-B	57	GLU
1	17-B	63	ASP
1	17-B	101	LEU
1	17-B	120	SER
1	17-B	126	LEU
1	17-B	136	ASP
1	17-B	155	SER
1	17-B	161	LEU
1	17-B	180	ARG
1	17-B	182	HIS
1	17-B	198	SER
1	17-B	236	MET
1	17-B	269	LEU
1	17-B	275	ASP
1	17-B	300	GLU
1	17-B	304	LEU
1	17-B	310	VAL
1	17-B	317	GLU
1	17-B	319	ILE
1	17-B	340	GLN
1	17-B	343	GLU
1	17-B	346	ARG
1	17-B	402	SER
1	17-B	404	ASP
1	17-B	460	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	17-B	471	ASN
1	17-B	490	SER
1	17-B	517	ASP
1	17-B	529	SER
1	17-B	545	ASN
1	17-B	553	GLN
1	17-B	574	LEU
1	17-B	587	ILE
1	17-B	600	GLN
1	18-A	58	VAL
1	18-A	63	ASP
1	18-A	64	LEU
1	18-A	72	ASP
1	18-A	81	LYS
1	18-A	126	LEU
1	18-A	136	ASP
1	18-A	144	PHE
1	18-A	150	GLN
1	18-A	164	VAL
1	18-A	188	ASN
1	18-A	206	LYS
1	18-A	225	SER
1	18-A	236	MET
1	18-A	261	PRO
1	18-A	271	LEU
1	18-A	272	ASP
1	18-A	277	LYS
1	18-A	286	ASN
1	18-A	294	ASN
1	18-A	296	THR
1	18-A	297	PRO
1	18-A	305	ASP
1	18-A	311	LYS
1	18-A	317	GLU
1	18-A	337	HIS
1	18-A	346	ARG
1	18-A	362	ASP
1	18-A	368	LEU
1	18-A	404	ASP
1	18-A	468	LYS
1	18-A	488	GLN
1	18-A	518	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	18-A	525	LYS
1	18-A	528	ASP
1	18-A	531	THR
1	18-A	534	GLU
1	18-A	541	TYR
1	18-A	543	TYR
1	18-A	553	GLN
1	18-A	570	LEU
1	18-A	596	THR
1	18-A	600	GLN
1	18-A	603	SER
1	18-B	63	ASP
1	18-B	64	LEU
1	18-B	69	LEU
1	18-B	87	ARG
1	18-B	88	LYS
1	18-B	101	LEU
1	18-B	102	MET
1	18-B	127	ASN
1	18-B	140	ASP
1	18-B	161	LEU
1	18-B	165	ASN
1	18-B	169	ARG
1	18-B	182	HIS
1	18-B	184	LYS
1	18-B	215	SER
1	18-B	236	MET
1	18-B	275	ASP
1	18-B	283	LYS
1	18-B	294	ASN
1	18-B	296	THR
1	18-B	297	PRO
1	18-B	304	LEU
1	18-B	305	ASP
1	18-B	317	GLU
1	18-B	330	LEU
1	18-B	404	ASP
1	18-B	435	SER
1	18-B	529	SER
1	18-B	531	THR
1	18-B	545	ASN
1	18-B	553	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	18-B	570	LEU
1	18-B	574	LEU
1	18-B	604	PHE
1	19-A	59	VAL
1	19-A	72	ASP
1	19-A	81	LYS
1	19-A	90	GLU
1	19-A	91	SER
1	19-A	102	MET
1	19-A	126	LEU
1	19-A	136	ASP
1	19-A	144	PHE
1	19-A	167	THR
1	19-A	169	ARG
1	19-A	180	ARG
1	19-A	192	ASP
1	19-A	196	TRP
1	19-A	206	LYS
1	19-A	225	SER
1	19-A	236	MET
1	19-A	262	VAL
1	19-A	271	LEU
1	19-A	283	LYS
1	19-A	284	ARG
1	19-A	294	ASN
1	19-A	300	GLU
1	19-A	340	GLN
1	19-A	346	ARG
1	19-A	359	ILE
1	19-A	368	LEU
1	19-A	404	ASP
1	19-A	460	ARG
1	19-A	462	ASP
1	19-A	505	TYR
1	19-A	514	GLN
1	19-A	517	ASP
1	19-A	531	THR
1	19-A	543	TYR
1	19-A	562	PRO
1	19-A	565	LYS
1	19-A	570	LEU
1	19-A	577	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	19-A	600	GLN
1	19-B	56	GLN
1	19-B	57	GLU
1	19-B	72	ASP
1	19-B	110	ASP
1	19-B	120	SER
1	19-B	127	ASN
1	19-B	136	ASP
1	19-B	144	PHE
1	19-B	145	ASP
1	19-B	161	LEU
1	19-B	165	ASN
1	19-B	169	ARG
1	19-B	180	ARG
1	19-B	184	LYS
1	19-B	194	TYR
1	19-B	236	MET
1	19-B	272	ASP
1	19-B	294	ASN
1	19-B	303	PRO
1	19-B	306	GLN
1	19-B	318	THR
1	19-B	325	GLN
1	19-B	340	GLN
1	19-B	395	GLU
1	19-B	398	SER
1	19-B	399	ASP
1	19-B	402	SER
1	19-B	404	ASP
1	19-B	460	ARG
1	19-B	471	ASN
1	19-B	488	GLN
1	19-B	517	ASP
1	19-B	527	ASP
1	19-B	565	LYS
1	19-B	570	LEU
1	19-B	587	ILE
1	20-A	92	ASN
1	20-A	147	ASN
1	20-A	164	VAL
1	20-A	165	ASN
1	20-A	169	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	20-A	214	TYR
1	20-A	217	GLN
1	20-A	236	MET
1	20-A	257	LEU
1	20-A	258	GLU
1	20-A	269	LEU
1	20-A	283	LYS
1	20-A	294	ASN
1	20-A	296	THR
1	20-A	300	GLU
1	20-A	305	ASP
1	20-A	306	GLN
1	20-A	340	GLN
1	20-A	402	SER
1	20-A	439	ILE
1	20-A	470	ASP
1	20-A	495	LYS
1	20-A	517	ASP
1	20-A	543	TYR
1	20-A	565	LYS
1	20-A	577	LYS
1	20-A	597	ILE
1	20-B	56	GLN
1	20-B	63	ASP
1	20-B	81	LYS
1	20-B	87	ARG
1	20-B	88	LYS
1	20-B	92	ASN
1	20-B	101	LEU
1	20-B	114	GLN
1	20-B	140	ASP
1	20-B	147	ASN
1	20-B	161	LEU
1	20-B	164	VAL
1	20-B	165	ASN
1	20-B	184	LYS
1	20-B	196	TRP
1	20-B	217	GLN
1	20-B	236	MET
1	20-B	251	GLU
1	20-B	272	ASP
1	20-B	274	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	20-B	277	LYS
1	20-B	312	PRO
1	20-B	330	LEU
1	20-B	402	SER
1	20-B	404	ASP
1	20-B	457	GLU
1	20-B	460	ARG
1	20-B	488	GLN
1	20-B	517	ASP
1	20-B	527	ASP
1	20-B	541	TYR
1	20-B	570	LEU
1	21-A	63	ASP
1	21-A	64	LEU
1	21-A	81	LYS
1	21-A	82	VAL
1	21-A	84	GLU
1	21-A	120	SER
1	21-A	147	ASN
1	21-A	165	ASN
1	21-A	236	MET
1	21-A	251	GLU
1	21-A	257	LEU
1	21-A	262	VAL
1	21-A	269	LEU
1	21-A	270	TYR
1	21-A	274	ASP
1	21-A	285	THR
1	21-A	296	THR
1	21-A	305	ASP
1	21-A	368	LEU
1	21-A	399	ASP
1	21-A	439	ILE
1	21-A	460	ARG
1	21-A	466	HIS
1	21-A	468	LYS
1	21-A	490	SER
1	21-A	517	ASP
1	21-A	527	ASP
1	21-A	529	SER
1	21-A	541	TYR
1	21-A	543	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	21-A	549	ASP
1	21-A	565	LYS
1	21-A	570	LEU
1	21-A	574	LEU
1	21-A	603	SER
1	21-A	604	PHE
1	21-B	69	LEU
1	21-B	81	LYS
1	21-B	88	LYS
1	21-B	97	ASP
1	21-B	101	LEU
1	21-B	114	GLN
1	21-B	126	LEU
1	21-B	145	ASP
1	21-B	147	ASN
1	21-B	161	LEU
1	21-B	164	VAL
1	21-B	165	ASN
1	21-B	184	LYS
1	21-B	194	TYR
1	21-B	196	TRP
1	21-B	198	SER
1	21-B	236	MET
1	21-B	251	GLU
1	21-B	285	THR
1	21-B	294	ASN
1	21-B	296	THR
1	21-B	301	SER
1	21-B	312	PRO
1	21-B	317	GLU
1	21-B	330	LEU
1	21-B	346	ARG
1	21-B	363	ASN
1	21-B	404	ASP
1	21-B	468	LYS
1	21-B	529	SER
1	21-B	531	THR
1	21-B	541	TYR
1	21-B	587	ILE
1	21-B	589	ASP
1	21-B	595	THR
1	21-B	600	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	22-A	64	LEU
1	22-A	77	ASP
1	22-A	102	MET
1	22-A	126	LEU
1	22-A	157	GLU
1	22-A	165	ASN
1	22-A	196	TRP
1	22-A	207	ILE
1	22-A	210	GLU
1	22-A	262	VAL
1	22-A	285	THR
1	22-A	294	ASN
1	22-A	324	ASP
1	22-A	325	GLN
1	22-A	346	ARG
1	22-A	466	HIS
1	22-A	528	ASP
1	22-A	543	TYR
1	22-A	553	GLN
1	22-A	565	LYS
1	22-A	595	THR
1	22-A	600	GLN
1	22-B	63	ASP
1	22-B	74	SER
1	22-B	81	LYS
1	22-B	87	ARG
1	22-B	92	ASN
1	22-B	101	LEU
1	22-B	114	GLN
1	22-B	129	ASP
1	22-B	136	ASP
1	22-B	140	ASP
1	22-B	143	TRP
1	22-B	144	PHE
1	22-B	155	SER
1	22-B	161	LEU
1	22-B	164	VAL
1	22-B	165	ASN
1	22-B	169	ARG
1	22-B	184	LYS
1	22-B	194	TYR
1	22-B	206	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	22-B	236	MET
1	22-B	251	GLU
1	22-B	258	GLU
1	22-B	294	ASN
1	22-B	296	THR
1	22-B	311	LYS
1	22-B	312	PRO
1	22-B	317	GLU
1	22-B	330	LEU
1	22-B	346	ARG
1	22-B	377	LYS
1	22-B	398	SER
1	22-B	404	ASP
1	22-B	452	GLU
1	22-B	503	LYS
1	22-B	517	ASP
1	22-B	538	MET
1	22-B	545	ASN
1	22-B	565	LYS
1	22-B	589	ASP
1	22-B	604	PHE
1	23-A	58	VAL
1	23-A	64	LEU
1	23-A	72	ASP
1	23-A	102	MET
1	23-A	144	PHE
1	23-A	145	ASP
1	23-A	147	ASN
1	23-A	155	SER
1	23-A	157	GLU
1	23-A	164	VAL
1	23-A	165	ASN
1	23-A	184	LYS
1	23-A	210	GLU
1	23-A	236	MET
1	23-A	262	VAL
1	23-A	283	LYS
1	23-A	296	THR
1	23-A	297	PRO
1	23-A	300	GLU
1	23-A	317	GLU
1	23-A	356	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	23-A	362	ASP
1	23-A	368	LEU
1	23-A	402	SER
1	23-A	404	ASP
1	23-A	419	ILE
1	23-A	452	GLU
1	23-A	460	ARG
1	23-A	509	ASP
1	23-A	518	ILE
1	23-A	553	GLN
1	23-A	565	LYS
1	23-A	570	LEU
1	23-A	572	VAL
1	23-B	56	GLN
1	23-B	63	ASP
1	23-B	64	LEU
1	23-B	72	ASP
1	23-B	92	ASN
1	23-B	101	LEU
1	23-B	111	ILE
1	23-B	114	GLN
1	23-B	124	LEU
1	23-B	136	ASP
1	23-B	143	TRP
1	23-B	144	PHE
1	23-B	161	LEU
1	23-B	182	HIS
1	23-B	196	TRP
1	23-B	236	MET
1	23-B	272	ASP
1	23-B	274	ASP
1	23-B	285	THR
1	23-B	294	ASN
1	23-B	304	LEU
1	23-B	306	GLN
1	23-B	312	PRO
1	23-B	330	LEU
1	23-B	339	ASP
1	23-B	348	ASN
1	23-B	402	SER
1	23-B	404	ASP
1	23-B	452	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	23-B	515	ASN
1	23-B	517	ASP
1	23-B	525	LYS
1	23-B	541	TYR
1	23-B	565	LYS
1	23-B	570	LEU
1	23-B	600	GLN
1	24-A	59	VAL
1	24-A	63	ASP
1	24-A	69	LEU
1	24-A	70	VAL
1	24-A	87	ARG
1	24-A	102	MET
1	24-A	110	ASP
1	24-A	124	LEU
1	24-A	127	ASN
1	24-A	144	PHE
1	24-A	180	ARG
1	24-A	236	MET
1	24-A	262	VAL
1	24-A	269	LEU
1	24-A	270	TYR
1	24-A	271	LEU
1	24-A	272	ASP
1	24-A	276	TYR
1	24-A	296	THR
1	24-A	298	GLU
1	24-A	300	GLU
1	24-A	325	GLN
1	24-A	346	ARG
1	24-A	384	ASP
1	24-A	398	SER
1	24-A	402	SER
1	24-A	460	ARG
1	24-A	466	HIS
1	24-A	519	LYS
1	24-A	543	TYR
1	24-A	565	LYS
1	24-A	570	LEU
1	24-A	574	LEU
1	24-A	595	THR
1	24-B	72	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	24-B	74	SER
1	24-B	79	GLN
1	24-B	91	SER
1	24-B	92	ASN
1	24-B	101	LEU
1	24-B	114	GLN
1	24-B	126	LEU
1	24-B	127	ASN
1	24-B	144	PHE
1	24-B	145	ASP
1	24-B	161	LEU
1	24-B	169	ARG
1	24-B	192	ASP
1	24-B	196	TRP
1	24-B	206	LYS
1	24-B	217	GLN
1	24-B	225	SER
1	24-B	236	MET
1	24-B	262	VAL
1	24-B	275	ASP
1	24-B	283	LYS
1	24-B	306	GLN
1	24-B	311	LYS
1	24-B	317	GLU
1	24-B	318	THR
1	24-B	325	GLN
1	24-B	340	GLN
1	24-B	346	ARG
1	24-B	399	ASP
1	24-B	402	SER
1	24-B	404	ASP
1	24-B	460	ARG
1	24-B	517	ASP
1	24-B	527	ASP
1	24-B	570	LEU
1	24-B	574	LEU
1	25-A	72	ASP
1	25-A	79	GLN
1	25-A	88	LYS
1	25-A	112	ASN
1	25-A	124	LEU
1	25-A	126	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	25-A	144	PHE
1	25-A	192	ASP
1	25-A	236	MET
1	25-A	248	SER
1	25-A	269	LEU
1	25-A	272	ASP
1	25-A	283	LYS
1	25-A	294	ASN
1	25-A	296	THR
1	25-A	301	SER
1	25-A	312	PRO
1	25-A	325	GLN
1	25-A	337	HIS
1	25-A	340	GLN
1	25-A	368	LEU
1	25-A	399	ASP
1	25-A	493	ASN
1	25-A	514	GLN
1	25-A	517	ASP
1	25-A	528	ASP
1	25-A	543	TYR
1	25-A	565	LYS
1	25-A	572	VAL
1	25-A	592	SER
1	25-B	56	GLN
1	25-B	57	GLU
1	25-B	63	ASP
1	25-B	64	LEU
1	25-B	72	ASP
1	25-B	87	ARG
1	25-B	88	LYS
1	25-B	90	GLU
1	25-B	101	LEU
1	25-B	102	MET
1	25-B	114	GLN
1	25-B	143	TRP
1	25-B	144	PHE
1	25-B	147	ASN
1	25-B	161	LEU
1	25-B	165	ASN
1	25-B	169	ARG
1	25-B	182	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	25-B	196	TRP
1	25-B	225	SER
1	25-B	236	MET
1	25-B	283	LYS
1	25-B	294	ASN
1	25-B	300	GLU
1	25-B	304	LEU
1	25-B	310	VAL
1	25-B	311	LYS
1	25-B	324	ASP
1	25-B	330	LEU
1	25-B	368	LEU
1	25-B	377	LYS
1	25-B	402	SER
1	25-B	404	ASP
1	25-B	450	HIS
1	25-B	489	TRP
1	25-B	525	LYS
1	25-B	527	ASP
1	25-B	528	ASP
1	25-B	570	LEU
1	25-B	574	LEU
1	25-B	586	ASP
1	25-B	587	ILE
1	25-B	600	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (465) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	67	ASN
1	1-A	93	GLN
1	1-A	114	GLN
1	1-A	217	GLN
1	1-A	306	GLN
1	1-A	471	ASN
1	1-A	514	GLN
1	1-A	553	GLN
1	1-A	557	GLN
1	1-A	600	GLN
1	1-B	67	ASN
1	1-B	150	GLN
1	1-B	294	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-B	450	HIS
1	1-B	488	GLN
1	1-B	553	GLN
1	2-A	93	GLN
1	2-A	363	ASN
1	2-A	471	ASN
1	2-B	67	ASN
1	2-B	79	GLN
1	2-B	93	GLN
1	2-B	127	ASN
1	2-B	150	GLN
1	2-B	325	GLN
1	2-B	337	HIS
1	2-B	340	GLN
1	2-B	471	ASN
1	2-B	488	GLN
1	2-B	493	ASN
1	2-B	600	GLN
1	3-A	93	GLN
1	3-A	150	GLN
1	3-A	286	ASN
1	3-A	294	ASN
1	3-A	493	ASN
1	3-B	79	GLN
1	3-B	93	GLN
1	3-B	114	GLN
1	3-B	150	GLN
1	3-B	294	ASN
1	3-B	306	GLN
1	3-B	337	HIS
1	3-B	450	HIS
1	3-B	545	ASN
1	4-A	67	ASN
1	4-A	286	ASN
1	4-A	488	GLN
1	4-A	493	ASN
1	4-B	79	GLN
1	4-B	93	GLN
1	4-B	150	GLN
1	4-B	286	ASN
1	4-B	294	ASN
1	4-B	337	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-B	450	HIS
1	4-B	493	ASN
1	4-B	515	ASN
1	4-B	545	ASN
1	5-A	67	ASN
1	5-A	109	ASN
1	5-A	150	GLN
1	5-A	514	GLN
1	5-A	553	GLN
1	5-A	557	GLN
1	5-B	147	ASN
1	5-B	150	GLN
1	5-B	218	GLN
1	5-B	337	HIS
1	5-B	436	ASN
1	5-B	450	HIS
1	5-B	493	ASN
1	6-A	325	GLN
1	6-A	340	GLN
1	6-A	408	ASN
1	6-A	515	ASN
1	6-A	553	GLN
1	6-A	557	GLN
1	6-B	56	GLN
1	6-B	109	ASN
1	6-B	112	ASN
1	6-B	165	ASN
1	6-B	337	HIS
1	6-B	436	ASN
1	6-B	450	HIS
1	6-B	466	HIS
1	6-B	514	GLN
1	7-A	89	GLN
1	7-A	114	GLN
1	7-A	127	ASN
1	7-A	147	ASN
1	7-A	217	GLN
1	7-A	306	GLN
1	7-A	340	GLN
1	7-A	557	GLN
1	7-B	93	GLN
1	7-B	112	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-B	114	GLN
1	7-B	127	ASN
1	7-B	150	GLN
1	7-B	182	HIS
1	7-B	217	GLN
1	7-B	306	GLN
1	7-B	436	ASN
1	7-B	450	HIS
1	7-B	471	ASN
1	7-B	488	GLN
1	7-B	493	ASN
1	7-B	514	GLN
1	8-A	89	GLN
1	8-A	112	ASN
1	8-A	114	GLN
1	8-A	147	ASN
1	8-A	165	ASN
1	8-A	286	ASN
1	8-A	294	ASN
1	8-A	348	ASN
1	8-A	450	HIS
1	8-B	92	ASN
1	8-B	93	GLN
1	8-B	112	ASN
1	8-B	114	GLN
1	8-B	150	GLN
1	8-B	182	HIS
1	8-B	337	HIS
1	8-B	340	GLN
1	8-B	436	ASN
1	8-B	450	HIS
1	8-B	471	ASN
1	8-B	493	ASN
1	8-B	514	GLN
1	9-A	67	ASN
1	9-A	89	GLN
1	9-A	112	ASN
1	9-A	127	ASN
1	9-A	306	GLN
1	9-A	337	HIS
1	9-A	493	ASN
1	9-A	514	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-A	600	GLN
1	9-B	56	GLN
1	9-B	92	ASN
1	9-B	112	ASN
1	9-B	151	ASN
1	9-B	182	HIS
1	9-B	217	GLN
1	9-B	436	ASN
1	9-B	466	HIS
1	9-B	493	ASN
1	9-B	557	GLN
1	10-A	67	ASN
1	10-A	112	ASN
1	10-A	127	ASN
1	10-A	165	ASN
1	10-A	188	ASN
1	10-A	286	ASN
1	10-A	348	ASN
1	10-A	363	ASN
1	10-A	450	HIS
1	10-A	466	HIS
1	10-A	488	GLN
1	10-A	553	GLN
1	10-A	600	GLN
1	10-B	92	ASN
1	10-B	93	GLN
1	10-B	112	ASN
1	10-B	114	GLN
1	10-B	150	GLN
1	10-B	182	HIS
1	10-B	286	ASN
1	10-B	325	GLN
1	10-B	337	HIS
1	10-B	436	ASN
1	10-B	450	HIS
1	10-B	493	ASN
1	10-B	545	ASN
1	11-A	112	ASN
1	11-A	114	GLN
1	11-A	147	ASN
1	11-A	165	ASN
1	11-A	188	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	11-A	325	GLN
1	11-A	340	GLN
1	11-A	450	HIS
1	11-A	493	ASN
1	11-B	92	ASN
1	11-B	165	ASN
1	11-B	182	HIS
1	11-B	286	ASN
1	11-B	337	HIS
1	11-B	436	ASN
1	11-B	450	HIS
1	11-B	466	HIS
1	11-B	471	ASN
1	11-B	488	GLN
1	11-B	493	ASN
1	11-B	515	ASN
1	12-A	67	ASN
1	12-A	93	GLN
1	12-A	112	ASN
1	12-A	114	GLN
1	12-A	127	ASN
1	12-A	188	ASN
1	12-A	286	ASN
1	12-A	363	ASN
1	12-A	450	HIS
1	12-A	488	GLN
1	12-A	553	GLN
1	12-A	600	GLN
1	12-B	56	GLN
1	12-B	67	ASN
1	12-B	92	ASN
1	12-B	150	GLN
1	12-B	182	HIS
1	12-B	286	ASN
1	12-B	436	ASN
1	12-B	450	HIS
1	12-B	493	ASN
1	12-B	515	ASN
1	12-B	557	GLN
1	13-A	67	ASN
1	13-A	92	ASN
1	13-A	93	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	13-A	150	GLN
1	13-A	325	GLN
1	13-A	493	ASN
1	13-B	114	GLN
1	13-B	150	GLN
1	13-B	165	ASN
1	13-B	306	GLN
1	13-B	325	GLN
1	13-B	337	HIS
1	13-B	450	HIS
1	13-B	481	HIS
1	13-B	514	GLN
1	13-B	557	GLN
1	14-A	92	ASN
1	14-A	93	GLN
1	14-A	112	ASN
1	14-A	348	ASN
1	14-A	408	ASN
1	14-A	450	HIS
1	14-A	567	HIS
1	14-B	158	ASN
1	14-B	182	HIS
1	14-B	337	HIS
1	14-B	434	ASN
1	14-B	450	HIS
1	14-B	545	ASN
1	14-B	557	GLN
1	15-A	92	ASN
1	15-A	112	ASN
1	15-A	127	ASN
1	15-A	306	GLN
1	15-A	434	ASN
1	15-A	450	HIS
1	15-A	553	GLN
1	15-B	114	GLN
1	15-B	182	HIS
1	15-B	217	GLN
1	15-B	337	HIS
1	15-B	363	ASN
1	15-B	434	ASN
1	15-B	450	HIS
1	15-B	481	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	15-B	514	GLN
1	15-B	545	ASN
1	16-A	67	ASN
1	16-A	92	ASN
1	16-A	93	GLN
1	16-A	294	ASN
1	16-A	450	HIS
1	16-A	557	GLN
1	16-B	67	ASN
1	16-B	150	GLN
1	16-B	182	HIS
1	16-B	434	ASN
1	16-B	450	HIS
1	16-B	545	ASN
1	16-B	600	GLN
1	17-A	67	ASN
1	17-A	93	GLN
1	17-A	127	ASN
1	17-A	188	ASN
1	17-A	217	GLN
1	17-A	294	ASN
1	17-A	363	ASN
1	17-A	493	ASN
1	17-A	514	GLN
1	17-A	545	ASN
1	17-A	554	HIS
1	17-B	56	GLN
1	17-B	182	HIS
1	17-B	337	HIS
1	17-B	348	ASN
1	17-B	450	HIS
1	17-B	545	ASN
1	18-A	109	ASN
1	18-A	188	ASN
1	18-A	306	GLN
1	18-A	325	GLN
1	18-A	337	HIS
1	18-A	348	ASN
1	18-A	363	ASN
1	18-A	450	HIS
1	18-A	600	GLN
1	18-B	114	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	18-B	182	HIS
1	18-B	286	ASN
1	18-B	306	GLN
1	18-B	348	ASN
1	18-B	408	ASN
1	18-B	450	HIS
1	18-B	493	ASN
1	18-B	545	ASN
1	18-B	557	GLN
1	19-A	89	GLN
1	19-A	306	GLN
1	19-A	450	HIS
1	19-A	466	HIS
1	19-A	488	GLN
1	19-A	600	GLN
1	19-B	56	GLN
1	19-B	93	GLN
1	19-B	127	ASN
1	19-B	147	ASN
1	19-B	325	GLN
1	19-B	337	HIS
1	19-B	348	ASN
1	19-B	450	HIS
1	19-B	471	ASN
1	19-B	557	GLN
1	20-A	217	GLN
1	20-A	306	GLN
1	20-A	450	HIS
1	20-A	493	ASN
1	20-A	514	GLN
1	20-A	545	ASN
1	20-A	553	GLN
1	20-A	567	HIS
1	20-A	582	HIS
1	20-B	67	ASN
1	20-B	79	GLN
1	20-B	92	ASN
1	20-B	114	GLN
1	20-B	127	ASN
1	20-B	147	ASN
1	20-B	150	GLN
1	20-B	165	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	20-B	182	HIS
1	20-B	306	GLN
1	20-B	450	HIS
1	20-B	466	HIS
1	20-B	471	ASN
1	20-B	488	GLN
1	20-B	514	GLN
1	21-A	93	GLN
1	21-A	114	GLN
1	21-A	147	ASN
1	21-A	217	GLN
1	21-A	286	ASN
1	21-A	450	HIS
1	21-A	488	GLN
1	21-A	545	ASN
1	21-A	553	GLN
1	21-B	79	GLN
1	21-B	92	ASN
1	21-B	109	ASN
1	21-B	147	ASN
1	21-B	150	GLN
1	21-B	165	ASN
1	21-B	182	HIS
1	21-B	217	GLN
1	21-B	218	GLN
1	21-B	306	GLN
1	21-B	348	ASN
1	21-B	363	ASN
1	21-B	408	ASN
1	21-B	450	HIS
1	21-B	515	ASN
1	21-B	553	GLN
1	22-A	109	ASN
1	22-A	165	ASN
1	22-A	217	GLN
1	22-A	294	ASN
1	22-A	325	GLN
1	22-A	389	ASN
1	22-A	450	HIS
1	22-A	466	HIS
1	22-A	493	ASN
1	22-A	514	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	22-A	553	GLN
1	22-A	567	HIS
1	22-B	92	ASN
1	22-B	127	ASN
1	22-B	150	GLN
1	22-B	182	HIS
1	22-B	325	GLN
1	22-B	348	ASN
1	22-B	450	HIS
1	22-B	488	GLN
1	22-B	545	ASN
1	22-B	600	GLN
1	23-A	67	ASN
1	23-A	93	GLN
1	23-A	114	GLN
1	23-A	127	ASN
1	23-A	147	ASN
1	23-A	150	GLN
1	23-A	165	ASN
1	23-A	217	GLN
1	23-A	218	GLN
1	23-A	389	ASN
1	23-A	450	HIS
1	23-A	600	GLN
1	23-B	92	ASN
1	23-B	182	HIS
1	23-B	286	ASN
1	23-B	306	GLN
1	23-B	348	ASN
1	23-B	450	HIS
1	23-B	515	ASN
1	23-B	557	GLN
1	23-B	600	GLN
1	24-A	93	GLN
1	24-A	114	GLN
1	24-A	127	ASN
1	24-A	182	HIS
1	24-A	217	GLN
1	24-A	337	HIS
1	24-A	348	ASN
1	24-A	389	ASN
1	24-A	450	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	24-A	471	ASN
1	24-A	488	GLN
1	24-A	493	ASN
1	24-A	514	GLN
1	24-B	56	GLN
1	24-B	79	GLN
1	24-B	92	ASN
1	24-B	93	GLN
1	24-B	182	HIS
1	24-B	217	GLN
1	24-B	325	GLN
1	24-B	340	GLN
1	24-B	348	ASN
1	24-B	450	HIS
1	24-B	481	HIS
1	24-B	515	ASN
1	25-A	93	GLN
1	25-A	114	GLN
1	25-A	127	ASN
1	25-A	217	GLN
1	25-A	294	ASN
1	25-A	306	GLN
1	25-A	389	ASN
1	25-A	450	HIS
1	25-A	557	GLN
1	25-B	92	ASN
1	25-B	165	ASN
1	25-B	182	HIS
1	25-B	471	ASN
1	25-B	488	GLN
1	25-B	557	GLN
1	25-B	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	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

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

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

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

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (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
3	13-B	701	BGC	C1-C2	2.75	1.58	1.52
3	14-B	701	BGC	C1-C2	3.05	1.58	1.52

All (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
3	21-B	701	BGC	C4-C3-C2	-4.68	102.05	110.79
3	24-B	701	BGC	C4-C3-C2	-4.37	102.64	110.79
3	25-B	701	BGC	C4-C3-C2	-4.37	102.64	110.79
3	18-B	701	BGC	O3-C3-C2	-4.22	100.85	110.34
3	23-B	701	BGC	C1-C2-C3	-3.90	104.63	110.43
3	2-B	701	BGC	C4-C3-C2	-3.85	103.61	110.79
3	15-B	701	BGC	C1-C2-C3	-3.82	104.75	110.43
3	23-B	701	BGC	C4-C3-C2	-3.76	103.78	110.79
3	2-B	701	BGC	C1-C2-C3	-3.75	104.84	110.43
3	2-B	701	BGC	O3-C3-C4	-3.70	102.01	110.34
3	3-B	701	BGC	C4-C3-C2	-3.65	103.98	110.79
3	18-B	701	BGC	O5-C5-C4	-3.64	102.85	109.68
3	5-B	701	BGC	O3-C3-C4	-3.57	102.31	110.34
3	21-B	701	BGC	O3-C3-C4	-3.55	102.34	110.34
3	6-B	701	BGC	O3-C3-C4	-3.52	102.41	110.34
3	12-B	701	BGC	C4-C3-C2	-3.32	104.59	110.79
3	21-B	701	BGC	C6-C5-C4	-3.29	104.90	113.02
3	19-B	701	BGC	C4-C3-C2	-3.29	104.66	110.79
3	20-B	701	BGC	O4-C4-C5	-3.08	101.08	109.24
3	14-B	701	BGC	C6-C5-C4	-3.05	105.49	113.02
3	16-B	701	BGC	C4-C3-C2	-3.01	105.18	110.79
3	14-B	701	BGC	C4-C3-C2	-2.95	105.28	110.79
3	5-B	701	BGC	C4-C3-C2	-2.95	105.29	110.79
3	7-B	701	BGC	C4-C3-C2	-2.93	105.33	110.79
3	18-B	701	BGC	O3-C3-C4	-2.91	103.80	110.34
3	25-B	701	BGC	O1-C1-O5	-2.81	102.56	110.25
3	17-B	701	BGC	C6-C5-C4	-2.74	106.24	113.02
3	10-B	701	BGC	C4-C3-C2	-2.63	105.88	110.79
3	20-B	701	BGC	C1-O5-C5	-2.61	108.64	113.47
3	1-B	701	BGC	O3-C3-C4	-2.58	104.53	110.34
3	15-B	701	BGC	O5-C1-C2	-2.55	105.73	109.80
3	9-B	701	BGC	O2-C2-C1	-2.52	104.26	109.82
3	19-B	701	BGC	O3-C3-C4	-2.51	104.68	110.34
3	5-B	701	BGC	O1-C1-O5	-2.42	103.64	110.25
3	4-B	701	BGC	C4-C3-C2	-2.29	106.51	110.79
3	18-B	701	BGC	O1-C1-C2	-2.28	103.10	109.21
3	21-B	701	BGC	O1-C1-O5	-2.28	104.02	110.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-B	701	BGC	O3-C3-C4	-2.27	105.23	110.34
3	1-B	701	BGC	C4-C3-C2	-2.22	106.64	110.79
3	2-B	701	BGC	C6-C5-C4	-2.22	107.53	113.02
3	9-B	701	BGC	O6-C6-C5	-2.21	104.02	111.33
3	3-B	701	BGC	O5-C5-C4	-2.10	105.73	109.68
3	10-B	701	BGC	O1-C1-O5	-2.08	104.56	110.25
3	12-B	701	BGC	C6-C5-C4	-2.05	107.95	113.02
3	6-B	701	BGC	C4-C3-C2	-2.02	107.01	110.79
3	10-B	701	BGC	O1-C1-C2	-2.01	103.82	109.21
3	10-B	701	BGC	O3-C3-C4	-2.01	105.82	110.34
3	3-B	701	BGC	O5-C5-C6	2.01	111.42	106.36
3	8-B	701	BGC	O3-C3-C2	2.01	114.87	110.34
3	21-B	701	BGC	O5-C5-C4	2.04	113.51	109.68
3	24-B	701	BGC	O5-C5-C6	2.05	111.54	106.36
3	6-B	701	BGC	O4-C4-C3	2.08	115.02	110.34
3	12-B	701	BGC	O4-C4-C3	2.09	115.05	110.34
3	16-B	701	BGC	O2-C2-C1	2.16	114.57	109.82
3	8-B	701	BGC	O1-C1-C2	2.16	115.00	109.21
3	25-B	701	BGC	C3-C4-C5	2.16	113.97	110.20
3	2-B	701	BGC	O4-C4-C5	2.19	115.05	109.24
3	10-B	701	BGC	C1-C2-C3	2.19	113.69	110.43
3	4-B	701	BGC	O5-C5-C6	2.23	111.99	106.36
3	9-B	701	BGC	C3-C4-C5	2.24	114.10	110.20
3	25-B	701	BGC	O2-C2-C3	2.25	115.39	110.34
3	23-B	701	BGC	O4-C4-C5	2.25	115.20	109.24
3	9-B	701	BGC	O2-C2-C3	2.26	115.42	110.34
3	2-B	701	BGC	O4-C4-C3	2.27	115.44	110.34
3	1-B	701	BGC	O2-C2-C3	2.28	115.47	110.34
3	21-B	701	BGC	O5-C5-C6	2.28	112.13	106.36
3	7-B	701	BGC	O4-C4-C5	2.31	115.35	109.24
3	21-B	701	BGC	C1-O5-C5	2.31	117.75	113.47
3	21-B	701	BGC	O2-C2-C3	2.33	115.57	110.34
3	24-B	701	BGC	O2-C2-C1	2.35	114.99	109.82
3	8-B	701	BGC	O2-C2-C1	2.36	115.02	109.82
3	8-B	701	BGC	O5-C5-C6	2.37	112.34	106.36
3	14-B	701	BGC	O4-C4-C3	2.37	115.67	110.34
3	22-B	701	BGC	O5-C5-C6	2.43	112.49	106.36
3	19-B	701	BGC	C1-C2-C3	2.43	114.05	110.43
3	14-B	701	BGC	C1-O5-C5	2.49	118.07	113.47
3	18-B	701	BGC	O5-C5-C6	2.57	112.85	106.36
3	23-B	701	BGC	O3-C3-C2	2.57	116.12	110.34
3	25-B	701	BGC	C1-O5-C5	2.59	118.26	113.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	18-B	701	BGC	O5-C1-C2	2.61	113.96	109.80
3	9-B	701	BGC	O5-C5-C6	2.62	112.98	106.36
3	1-B	701	BGC	O5-C1-C2	2.62	113.98	109.80
3	24-B	701	BGC	O2-C2-C3	2.64	116.28	110.34
3	20-B	701	BGC	O5-C5-C6	2.64	113.03	106.36
3	10-B	701	BGC	C1-O5-C5	2.64	118.36	113.47
3	17-B	701	BGC	O6-C6-C5	2.74	120.38	111.33
3	18-B	701	BGC	O2-C2-C3	2.77	116.56	110.34
3	14-B	701	BGC	O5-C1-C2	2.80	114.27	109.80
3	1-B	701	BGC	O4-C4-C3	2.82	116.69	110.34
3	17-B	701	BGC	O2-C2-C3	2.83	116.71	110.34
3	7-B	701	BGC	O5-C1-C2	2.85	114.34	109.80
3	13-B	701	BGC	O1-C1-C2	2.89	116.96	109.21
3	17-B	701	BGC	O5-C5-C4	2.90	115.13	109.68
3	5-B	701	BGC	O5-C1-C2	2.91	114.44	109.80
3	21-B	701	BGC	C3-C4-C5	2.92	115.29	110.20
3	13-B	701	BGC	O5-C5-C6	2.92	113.74	106.36
3	16-B	701	BGC	C3-C4-C5	2.93	115.30	110.20
3	7-B	701	BGC	O5-C5-C6	2.98	113.89	106.36
3	18-B	701	BGC	C1-C2-C3	3.01	114.91	110.43
3	12-B	701	BGC	C3-C4-C5	3.04	115.50	110.20
3	3-B	701	BGC	O4-C4-C3	3.08	117.27	110.34
3	16-B	701	BGC	O2-C2-C3	3.13	117.39	110.34
3	19-B	701	BGC	O2-C2-C3	3.15	117.43	110.34
3	2-B	701	BGC	O2-C2-C1	3.20	116.87	109.82
3	11-B	701	BGC	O2-C2-C3	3.23	117.60	110.34
3	14-B	701	BGC	C3-C4-C5	3.29	115.93	110.20
3	2-B	701	BGC	C1-O5-C5	3.29	119.56	113.47
3	17-B	701	BGC	C1-O5-C5	3.37	119.70	113.47
3	23-B	701	BGC	O2-C2-C3	3.64	118.54	110.34
3	10-B	701	BGC	C3-C4-C5	3.69	116.63	110.20
3	1-B	701	BGC	C1-C2-C3	3.72	115.96	110.43
3	3-B	701	BGC	O4-C4-C5	3.74	119.15	109.24
3	14-B	701	BGC	O5-C5-C6	3.80	115.95	106.36
3	19-B	701	BGC	C3-C4-C5	3.83	116.87	110.20
3	22-B	701	BGC	C1-O5-C5	3.89	120.67	113.47
3	18-B	701	BGC	C3-C4-C5	3.93	117.05	110.20
3	17-B	701	BGC	O5-C1-C2	3.94	116.08	109.80
3	17-B	701	BGC	C1-C2-C3	4.01	116.39	110.43
3	22-B	701	BGC	C1-C2-C3	4.03	116.42	110.43
3	20-B	701	BGC	O4-C4-C3	4.06	119.47	110.34
3	25-B	701	BGC	O5-C1-C2	4.20	116.50	109.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-B	701	BGC	O3-C3-C2	4.29	120.00	110.34
3	5-B	701	BGC	C1-O5-C5	4.34	121.49	113.47
3	21-B	701	BGC	O5-C1-C2	4.38	116.78	109.80
3	1-B	701	BGC	C3-C4-C5	4.40	117.87	110.20
3	6-B	701	BGC	C3-C4-C5	4.44	117.94	110.20
3	21-B	701	BGC	C1-C2-C3	4.52	117.15	110.43
3	12-B	701	BGC	O2-C2-C3	4.54	120.57	110.34
3	15-B	701	BGC	O2-C2-C3	4.55	120.59	110.34
3	5-B	701	BGC	C3-C4-C5	4.59	118.19	110.20
3	25-B	701	BGC	C1-C2-C3	4.81	117.58	110.43
3	11-B	701	BGC	O5-C5-C6	4.86	118.64	106.36
3	14-B	701	BGC	C1-C2-C3	4.88	117.68	110.43
3	10-B	701	BGC	O5-C1-C2	4.92	117.64	109.80
3	15-B	701	BGC	O3-C3-C2	5.05	121.71	110.34
3	11-B	701	BGC	O3-C3-C2	5.21	122.08	110.34
3	17-B	701	BGC	C3-C4-C5	5.28	119.40	110.20
3	9-B	701	BGC	C1-C2-C3	5.29	118.29	110.43
3	22-B	701	BGC	O5-C1-C2	5.91	119.22	109.80
3	20-B	701	BGC	C3-C4-C5	6.28	121.14	110.20

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.