



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 04:50 AM EDT

PDB ID : 4TYV / pdb_00004tyv
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

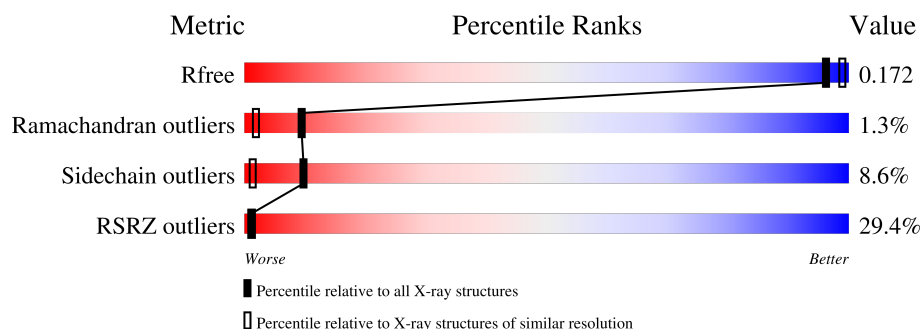
1 Overall quality at a glance

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.



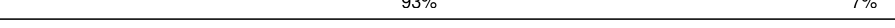
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3183 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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.

Mol	Chain	Length	Quality of chain
1	1-A	551	29% 91% 8%
1	1-B	551	29% 93% 7%
1	10-A	551	90% 10%
1	10-B	551	93% 7%
1	11-A	551	91% 8%
1	11-B	551	92% 8%
1	12-A	551	91% 8%

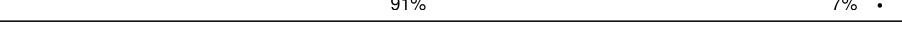
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Mol	Chain	Length	Quality of chain
1	12-B	551	 93% 7%
1	13-A	551	 91% 8% .
1	13-B	551	 93% 7%
1	14-A	551	 91% 9% .
1	14-B	551	 92% 7% .
1	15-A	551	 90% 9% ..
1	15-B	551	 92% 7%
1	16-A	551	 90% 9% ..
1	16-B	551	 93% 7%
1	17-A	551	 89% 10% ..
1	17-B	551	 92% 8%
1	18-A	551	 90% 9% .
1	18-B	551	 92% 7% .
1	19-A	551	 91% 8% .
1	19-B	551	 92% 7% .
1	2-A	551	 90% 9% .
1	2-B	551	 93% 7% .
1	20-A	551	 91% 8% .
1	20-B	551	 92% 7% .
1	21-A	551	 90% 9% .
1	21-B	551	 93% 7%
1	22-A	551	 90% 9% ..
1	22-B	551	 93% 7% .
1	23-A	551	 91% 8% .
1	23-B	551	 92% 7%

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Mol	Chain	Length	Quality of chain
1	24-A	551	 90% 9% ..
1	24-B	551	 93% 7%
1	25-A	551	 90% 9% .
1	25-B	551	 93% 7%
1	3-A	551	 91% 9% .
1	3-B	551	 92% 7%
1	4-A	551	 91% 8% .
1	4-B	551	 93% 7%
1	5-A	551	 90% 10% .
1	5-B	551	 93% 7%
1	6-A	551	 91% 8% ..
1	6-B	551	 93% 7%
1	7-A	551	 90% 9% .
1	7-B	551	 91% 7% .
1	8-A	551	 90% 9% .
1	8-B	551	 93% 7%
1	9-A	551	 90% 9% .
1	9-B	551	 92% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	1-B	704	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 418117 atoms, of which 196575 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Putative secreted protein.

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

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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			

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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 (CCD ID: 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		

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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		

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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		

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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		

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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		

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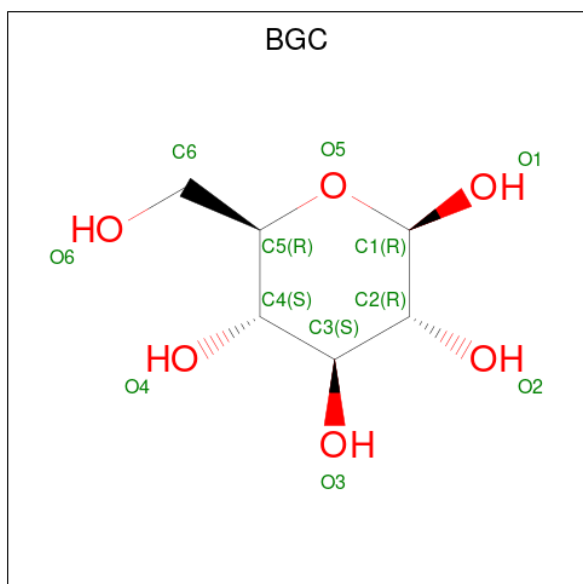
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	24-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	25-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	1-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	2-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	3-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	4-B	1	Total	C	H	O	0	0
			10	2	6	2		
2	5-B	1	Total	C	H	O	0	0
			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		

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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-glucopyranose (CCD ID: 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		

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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

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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

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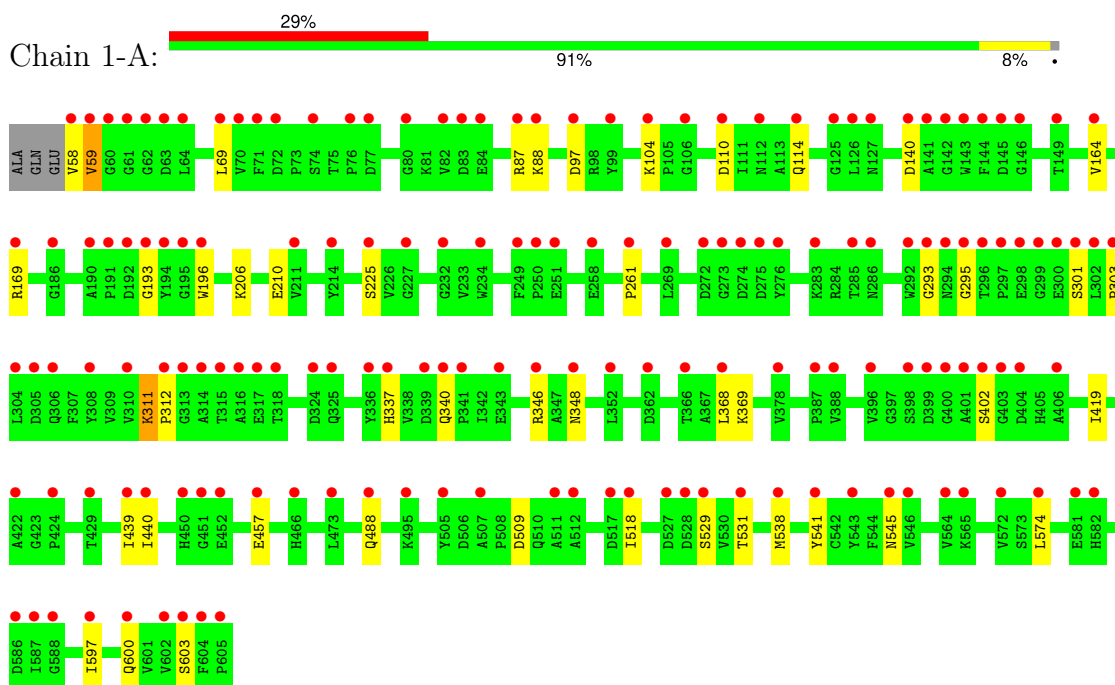
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	19-B	228	Total 228	O 228	0	0
4	20-B	230	Total 230	O 230	0	0
4	21-B	240	Total 240	O 240	0	0
4	22-B	267	Total 267	O 267	0	0
4	23-B	248	Total 248	O 248	0	0
4	24-B	241	Total 241	O 241	0	0
4	25-B	242	Total 242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

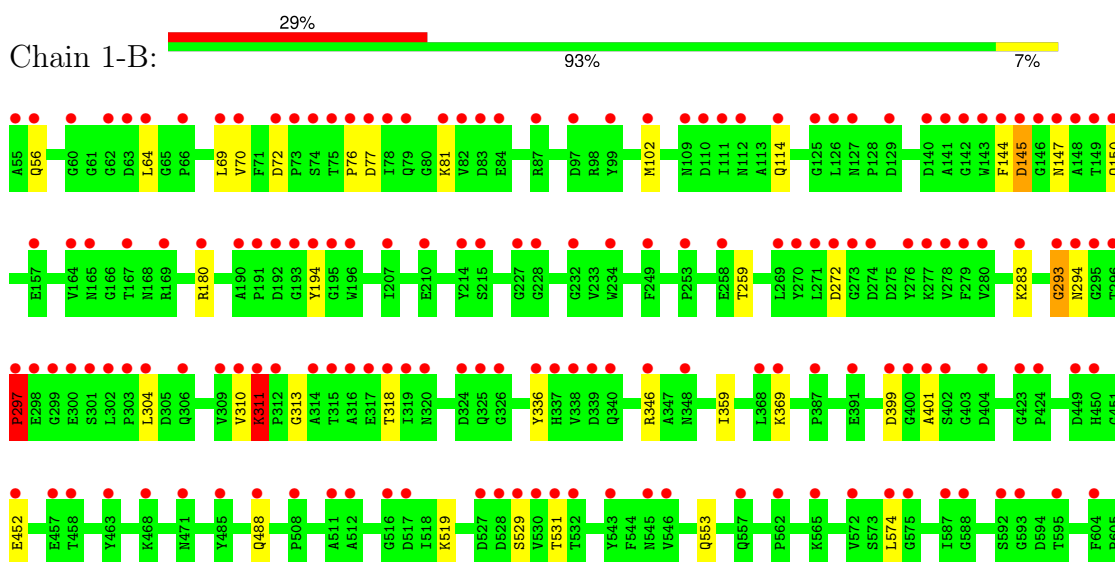
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

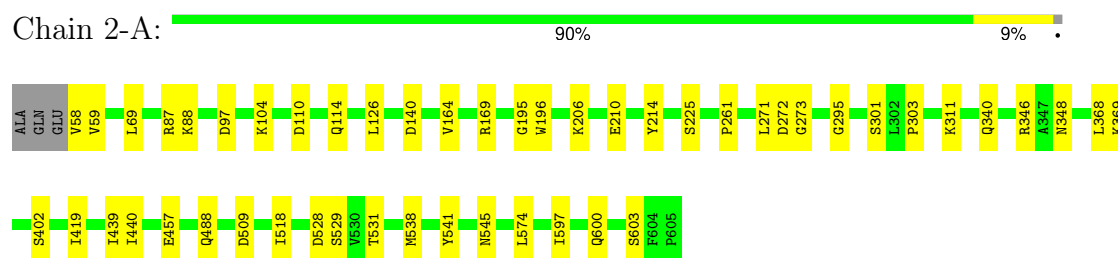
- Molecule 1: Putative secreted protein



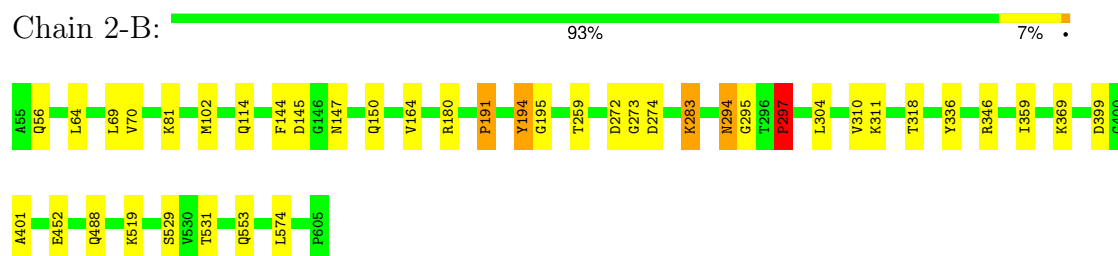
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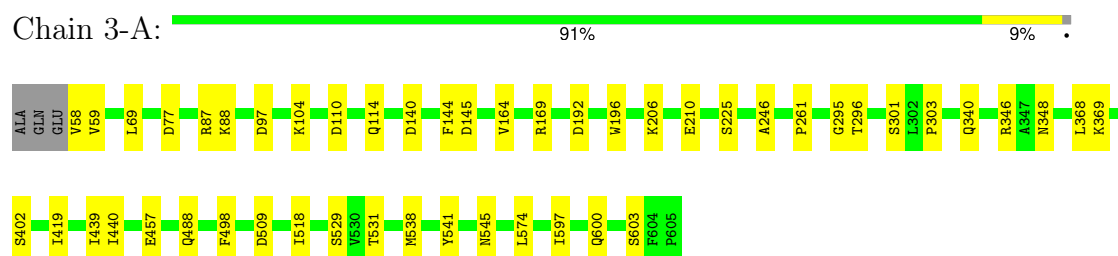
- Molecule 1: Putative secreted protein



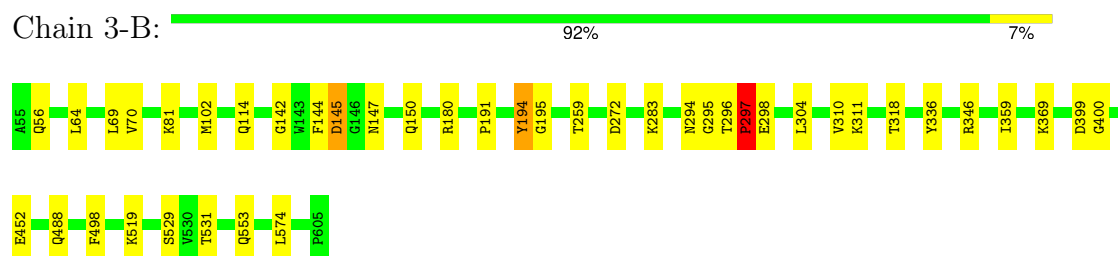
- Molecule 1: Putative secreted protein



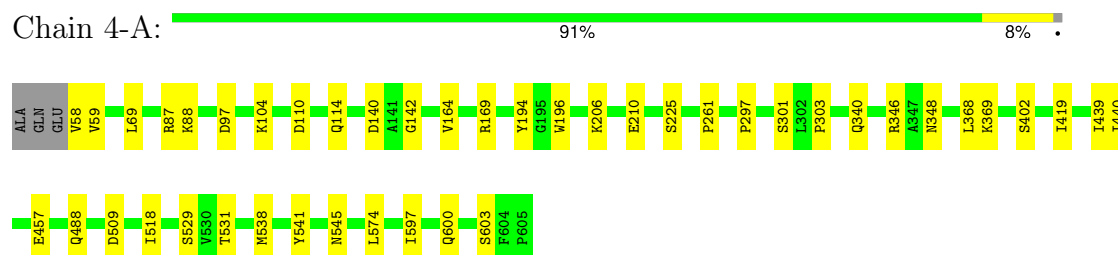
- Molecule 1: Putative secreted protein



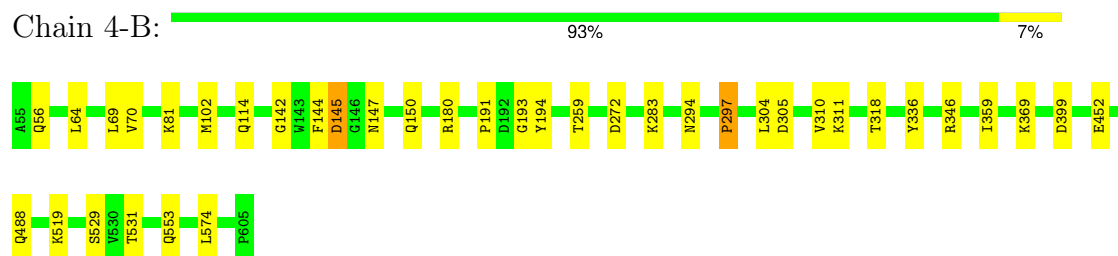
- Molecule 1: Putative secreted protein



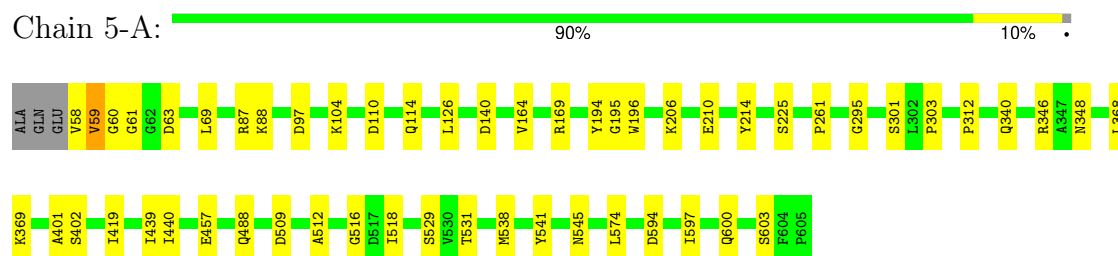
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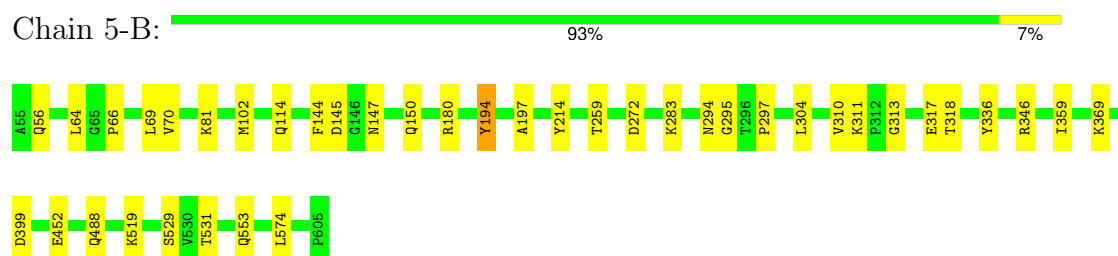
- Molecule 1: Putative secreted protein



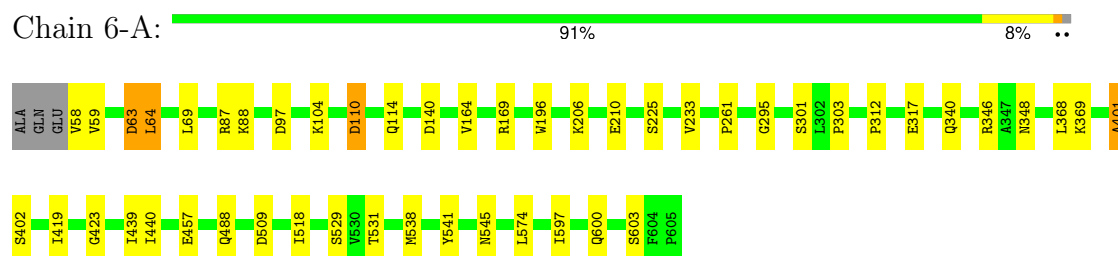
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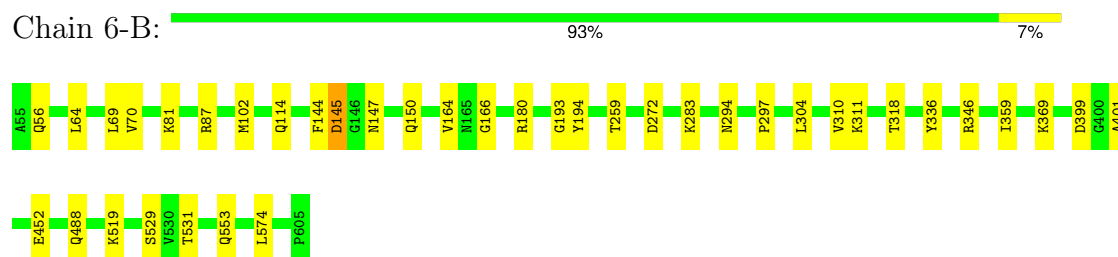
- Molecule 1: Putative secreted protein



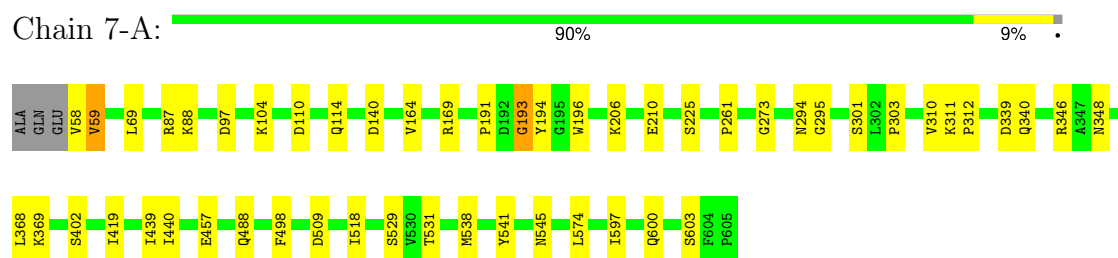
- Molecule 1: Putative secreted protein



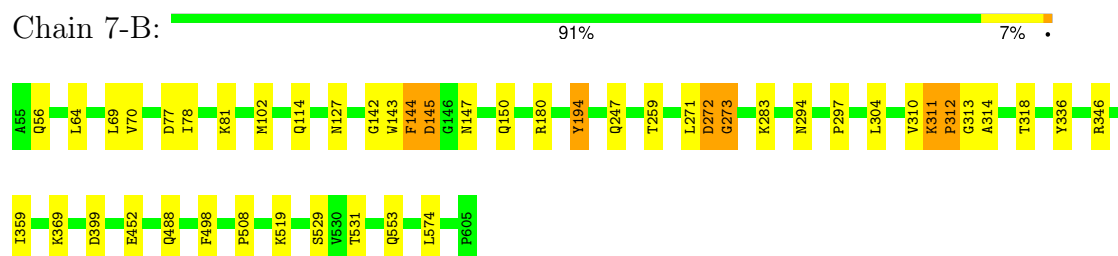
- Molecule 1: Putative secreted protein



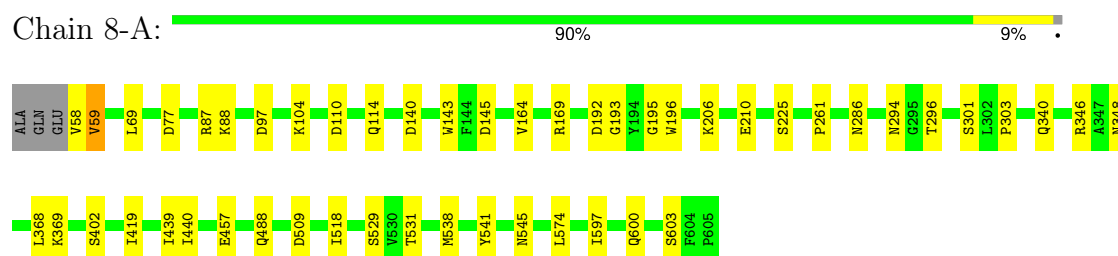
- Molecule 1: Putative secreted protein



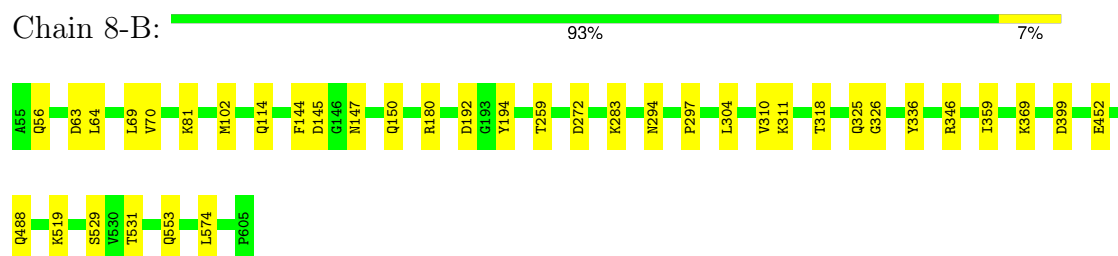
- Molecule 1: Putative secreted protein



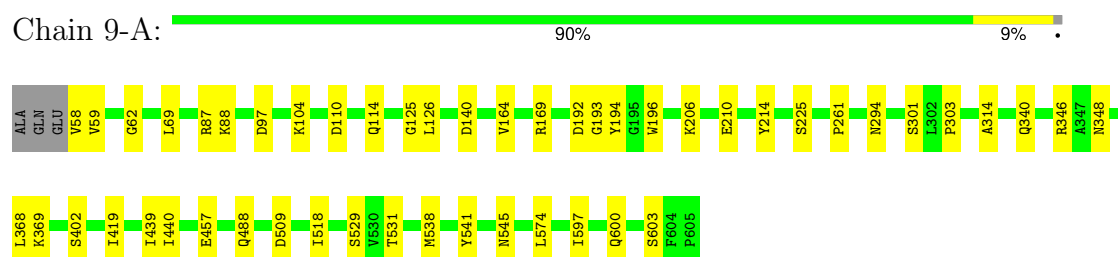
- Molecule 1: Putative secreted protein



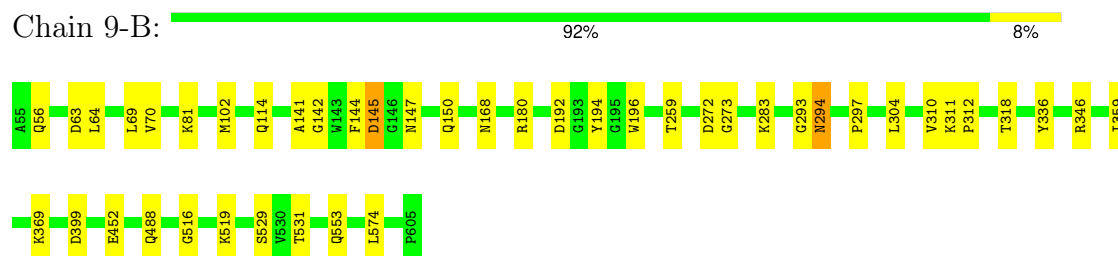
- Molecule 1: Putative secreted protein



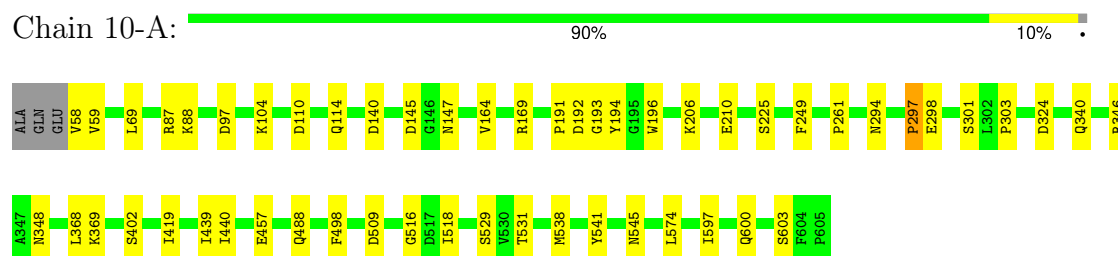
- Molecule 1: Putative secreted protein



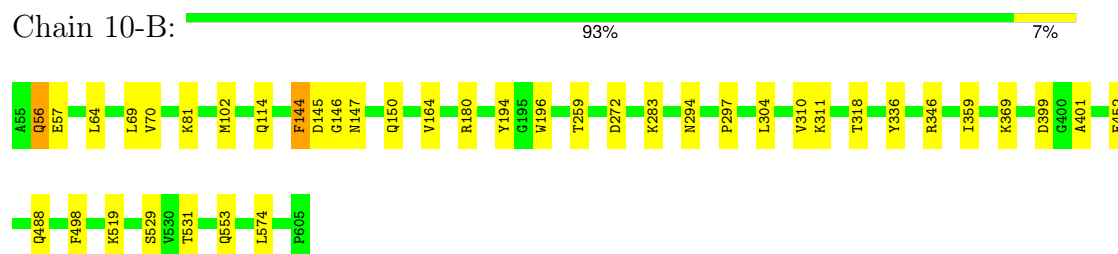
- Molecule 1: Putative secreted protein



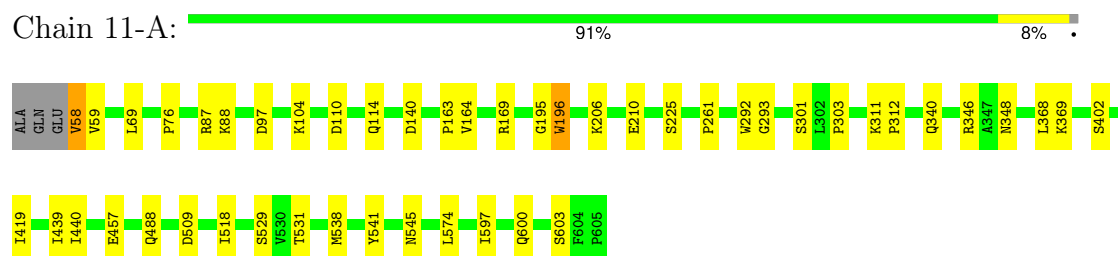
- Molecule 1: Putative secreted protein



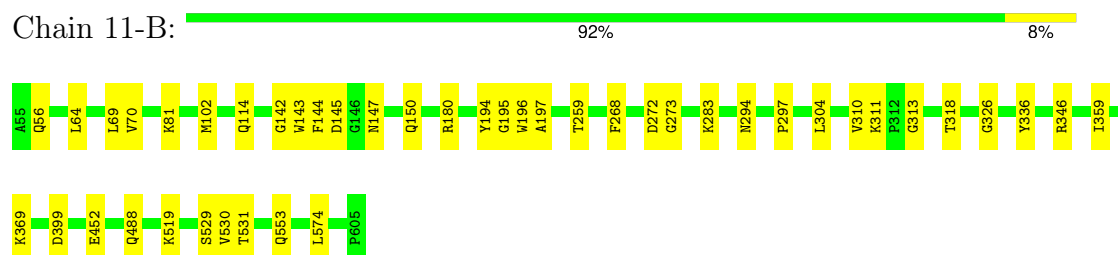
- Molecule 1: Putative secreted protein



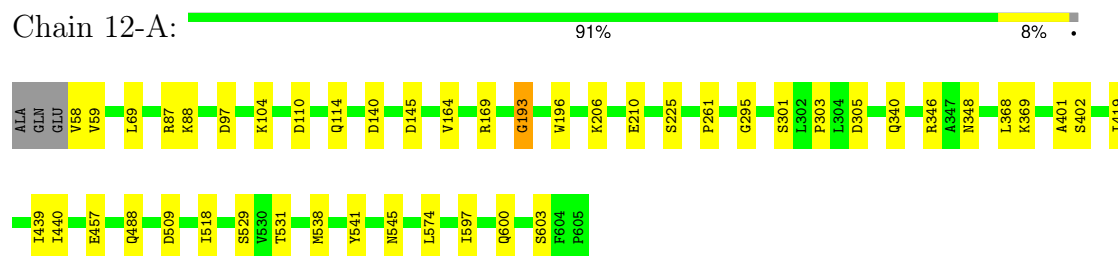
- Molecule 1: Putative secreted protein



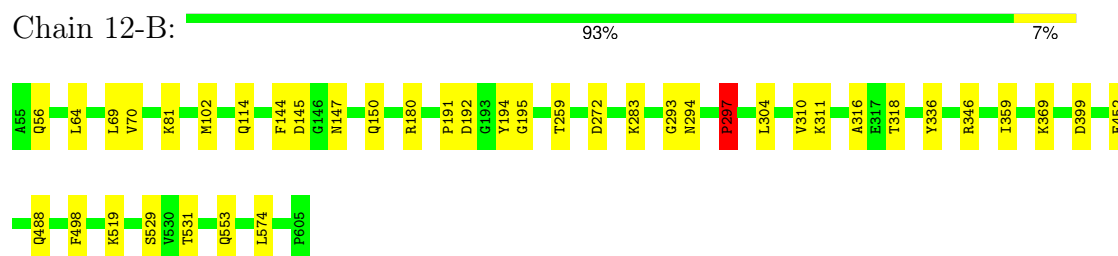
- Molecule 1: Putative secreted protein



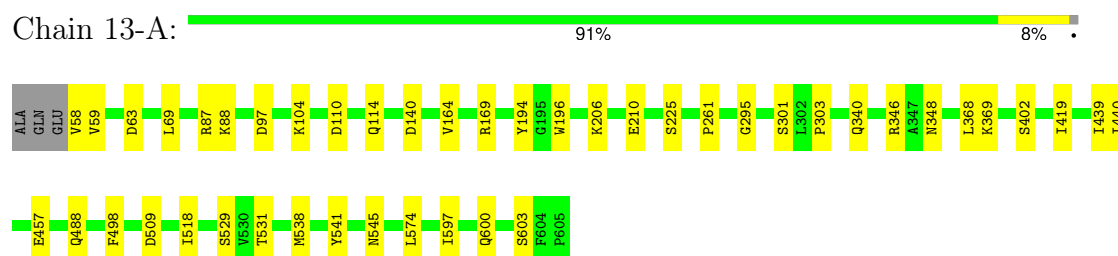
- Molecule 1: Putative secreted protein



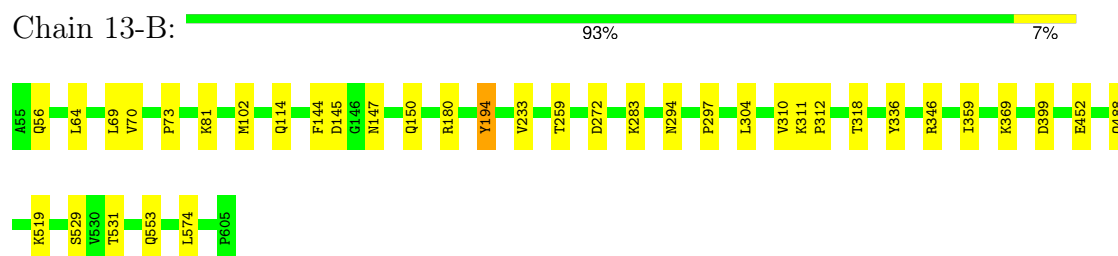
- Molecule 1: Putative secreted protein



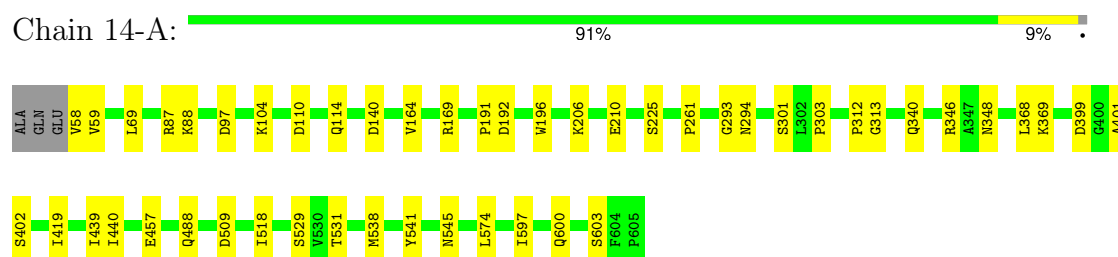
- Molecule 1: Putative secreted protein



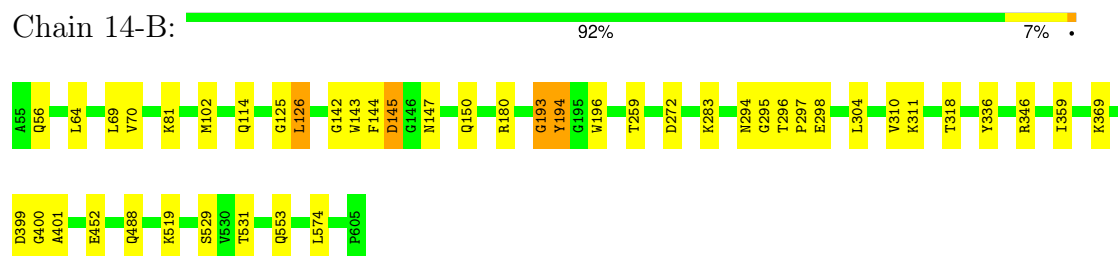
- Molecule 1: Putative secreted protein



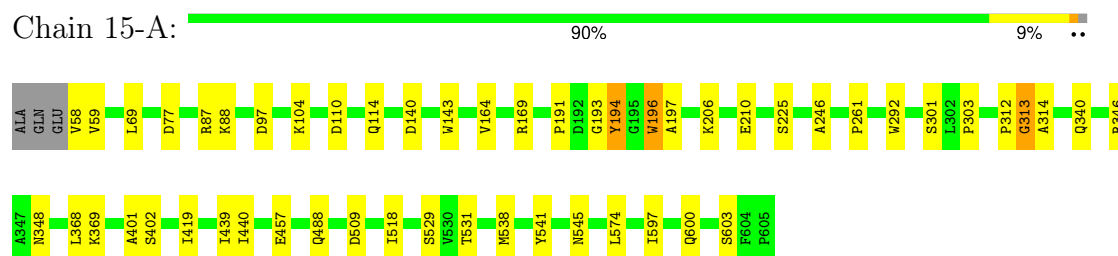
- Molecule 1: Putative secreted protein



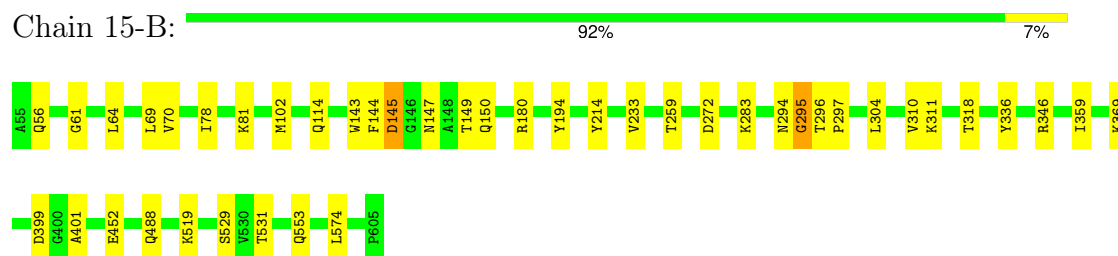
● Molecule 1: Putative secreted protein



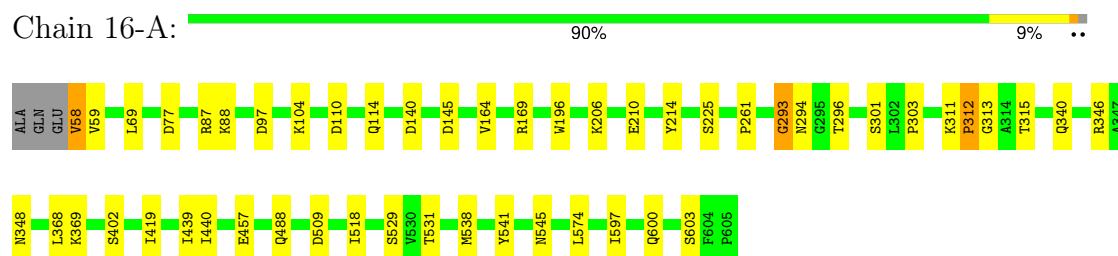
● Molecule 1: Putative secreted protein



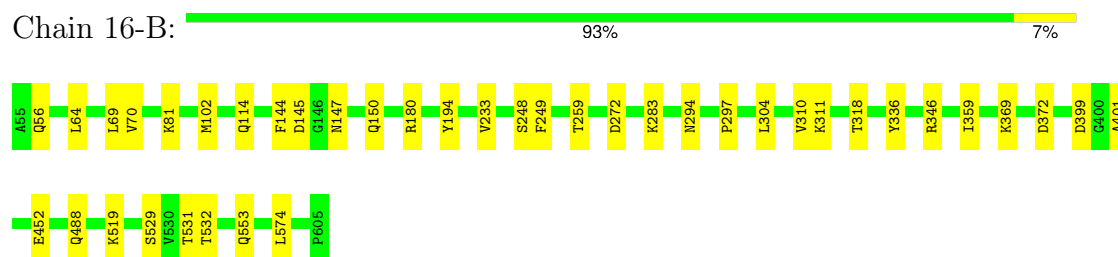
● Molecule 1: Putative secreted protein



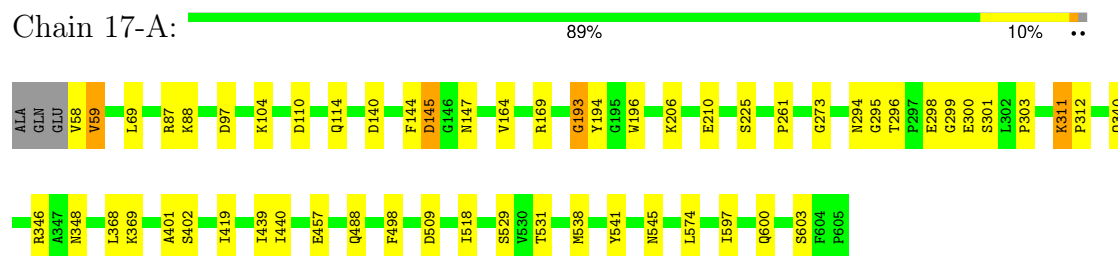
● Molecule 1: Putative secreted protein



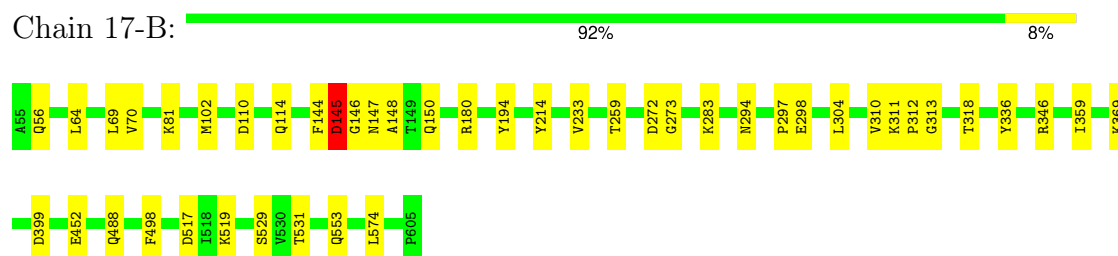
● Molecule 1: Putative secreted protein



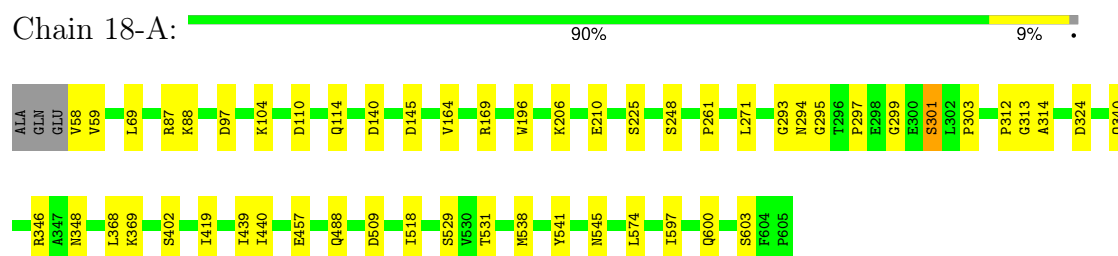
- Molecule 1: Putative secreted protein



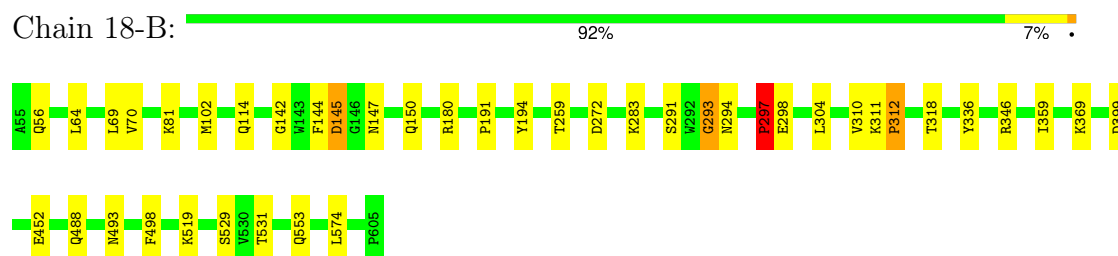
- Molecule 1: Putative secreted protein



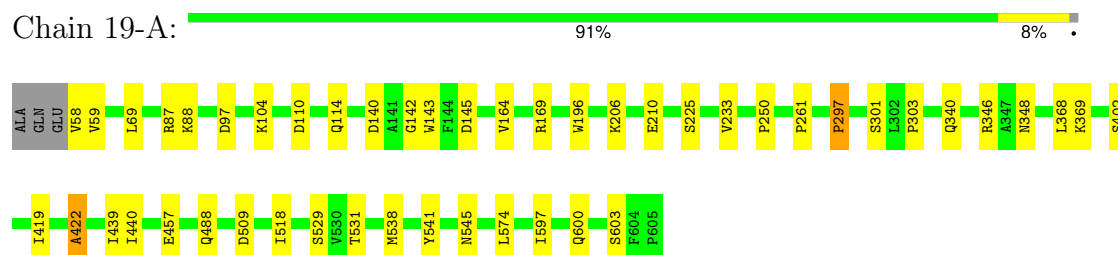
- Molecule 1: Putative secreted protein



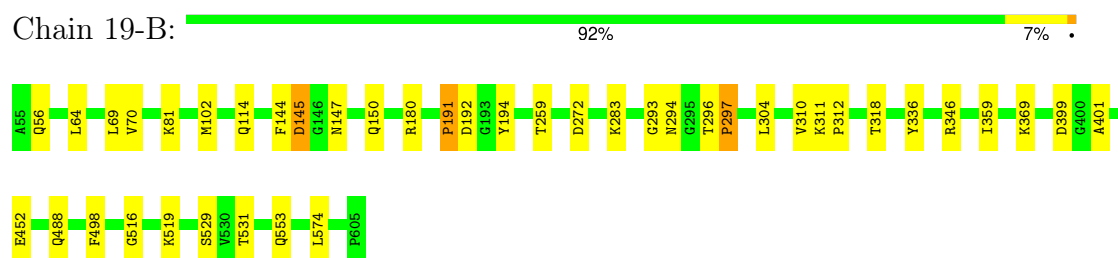
- Molecule 1: Putative secreted protein



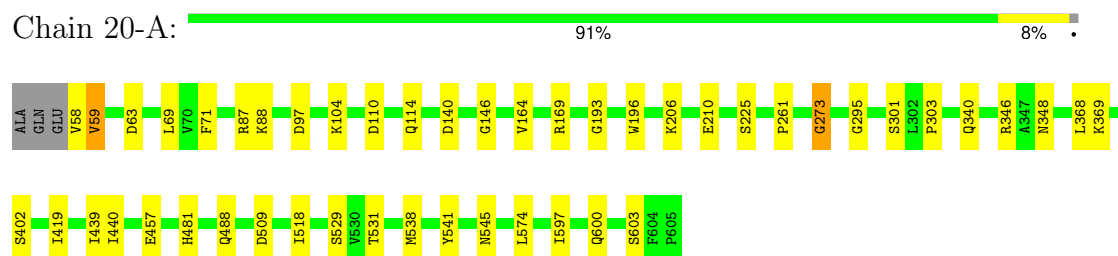
- Molecule 1: Putative secreted protein



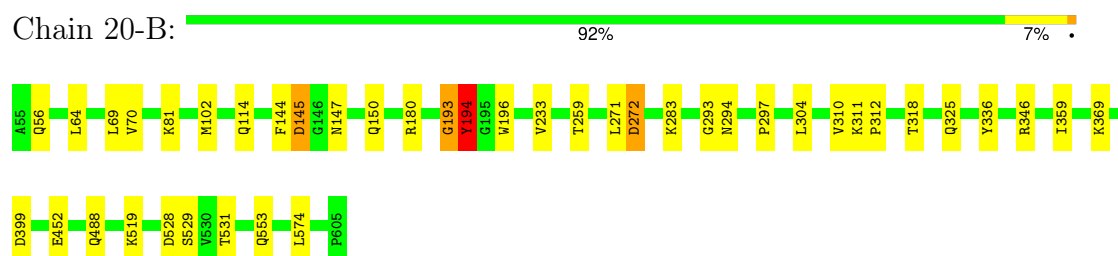
● Molecule 1: Putative secreted protein



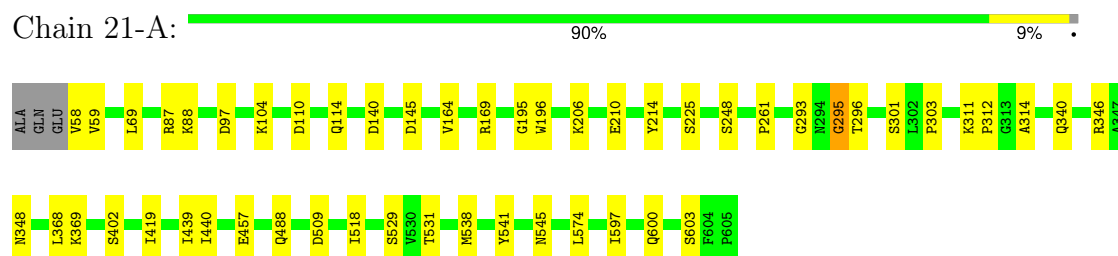
● Molecule 1: Putative secreted protein



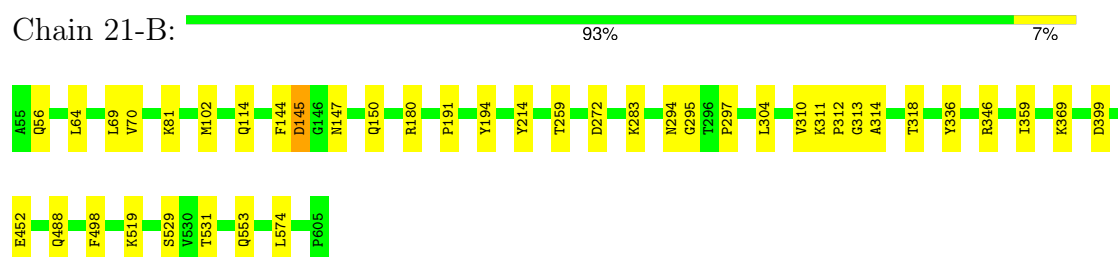
● Molecule 1: Putative secreted protein



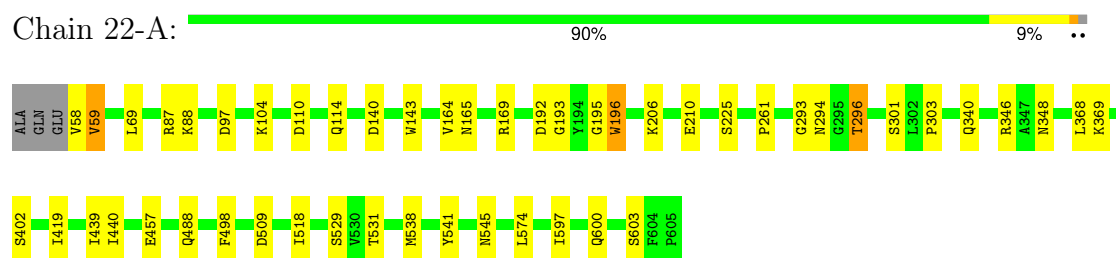
● Molecule 1: Putative secreted protein



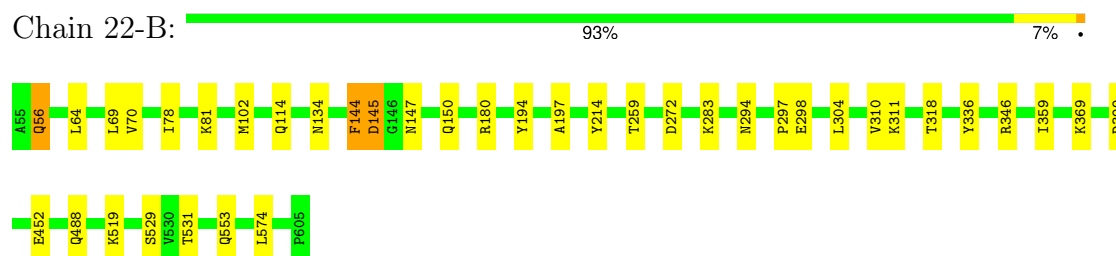
● Molecule 1: Putative secreted protein



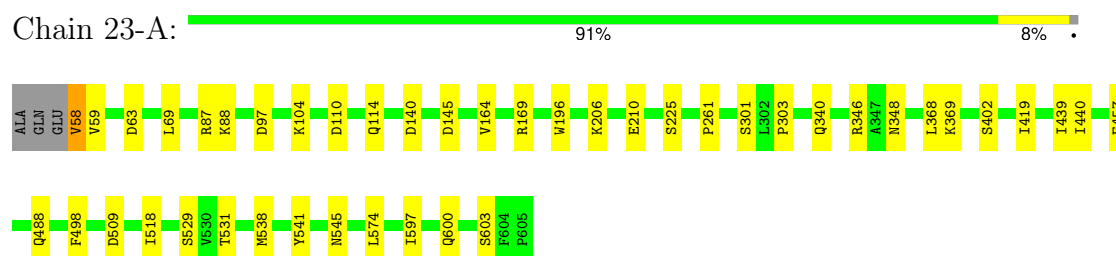
- Molecule 1: Putative secreted protein



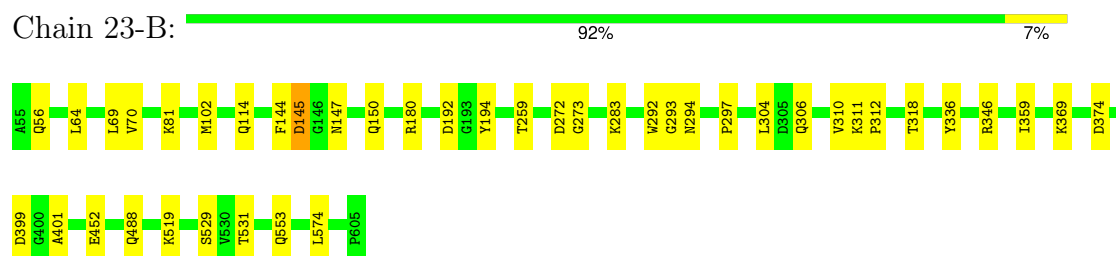
- Molecule 1: Putative secreted protein



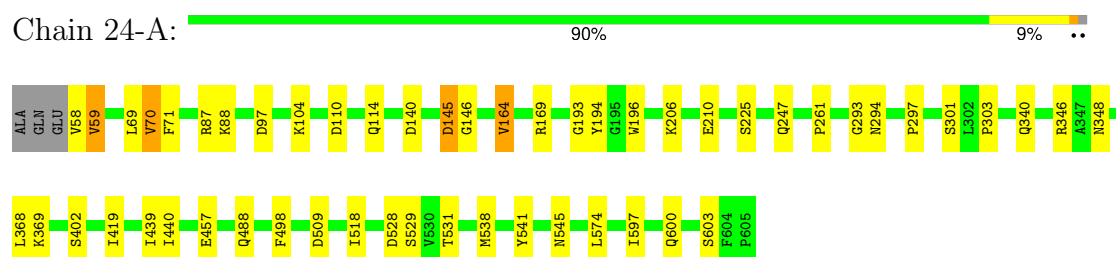
- Molecule 1: Putative secreted protein



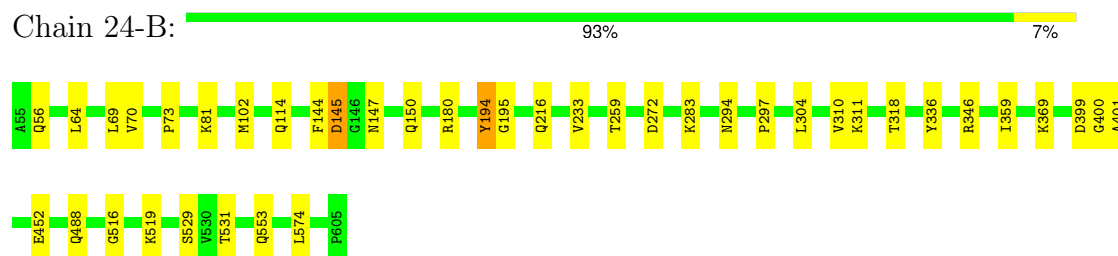
- Molecule 1: Putative secreted protein



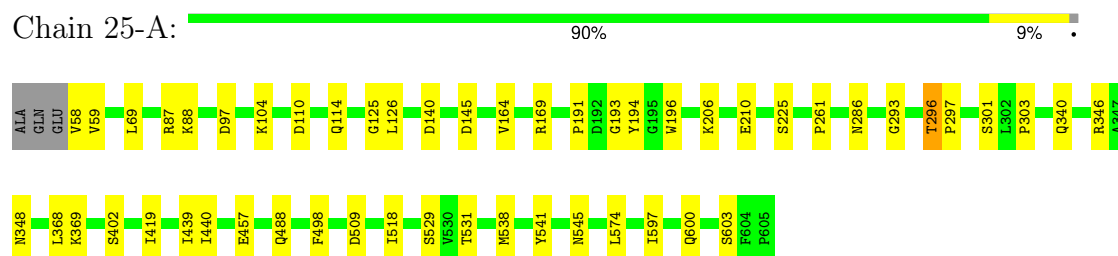
- Molecule 1: Putative secreted protein



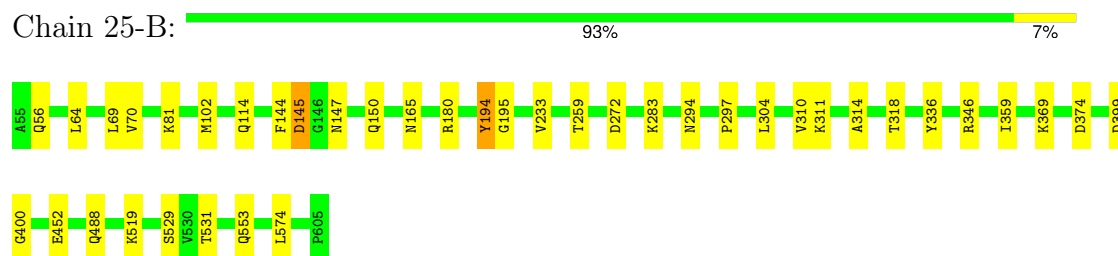
- Molecule 1: Putative secreted protein



- Molecule 1: Putative secreted protein



- Molecule 1: Putative secreted protein



4 Data and refinement statistics

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 24.27 – 1.75	Depositor ED
% Data completeness (in resolution range)	98.8 (24.27-1.75) 92.8 (24.27-1.75)	Depositor ED
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 1.75Å)	Xtriage
Refinement program	PHENIX (PHENIX.ENSEMBLE_REFINEMENT: 1.9_1692)	Depositor
R, R_{free}	0.110 , 0.143 0.139 , 0.172	Depositor DC
R_{free} test set	5256 reflections (4.95%)	wwPDB
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 38.7	ED
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	ED
Total number of atoms	418117	wwPDB
Average B, all atoms (Å ²)	13.0	wwPDB

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 1.4083e-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, 0.333 respectively for untwinned datasets, and 0.375, 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: EDO, BGC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1-A	0.20	0/4271	0.29	0/5836
1	1-B	0.20	0/4294	0.28	0/5867
1	2-A	0.20	0/4271	0.29	0/5836
1	2-B	0.20	0/4294	0.28	0/5867
1	3-A	0.20	0/4271	0.29	0/5836
1	3-B	0.20	0/4294	0.28	0/5867
1	4-A	0.20	0/4271	0.29	0/5836
1	4-B	0.20	0/4294	0.28	0/5867
1	5-A	0.20	0/4271	0.29	0/5836
1	5-B	0.20	0/4294	0.28	0/5867
1	6-A	0.20	0/4271	0.29	0/5836
1	6-B	0.20	0/4294	0.28	0/5867
1	7-A	0.20	0/4271	0.29	0/5836
1	7-B	0.20	0/4294	0.28	0/5867
1	8-A	0.20	0/4271	0.29	0/5836
1	8-B	0.20	0/4294	0.28	0/5867
1	9-A	0.20	0/4271	0.29	0/5836
1	9-B	0.20	0/4294	0.28	0/5867
1	10-A	0.20	0/4271	0.29	0/5836
1	10-B	0.20	0/4294	0.28	0/5867
1	11-A	0.20	0/4271	0.29	0/5836
1	11-B	0.20	0/4294	0.28	0/5867
1	12-A	0.20	0/4271	0.29	0/5836
1	12-B	0.20	0/4294	0.28	0/5867
1	13-A	0.20	0/4271	0.29	0/5836
1	13-B	0.20	0/4294	0.28	0/5867
1	14-A	0.20	0/4271	0.29	0/5836
1	14-B	0.20	0/4294	0.28	0/5867
1	15-A	0.20	0/4271	0.29	0/5836
1	15-B	0.20	0/4294	0.28	0/5867
1	16-A	0.20	0/4271	0.29	0/5836
1	16-B	0.20	0/4294	0.28	0/5867

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	17-A	0.20	0/4271	0.29	0/5836
1	17-B	0.20	0/4294	0.28	0/5867
1	18-A	0.20	0/4271	0.29	0/5836
1	18-B	0.20	0/4294	0.28	0/5867
1	19-A	0.20	0/4271	0.29	0/5836
1	19-B	0.20	0/4294	0.28	0/5867
1	20-A	0.20	0/4271	0.29	0/5836
1	20-B	0.20	0/4294	0.28	0/5867
1	21-A	0.20	0/4271	0.29	0/5836
1	21-B	0.20	0/4294	0.28	0/5867
1	22-A	0.20	0/4271	0.29	0/5836
1	22-B	0.20	0/4294	0.28	0/5867
1	23-A	0.20	0/4271	0.29	0/5836
1	23-B	0.20	0/4294	0.28	0/5867
1	24-A	0.20	0/4271	0.29	0/5836
1	24-B	0.20	0/4294	0.28	0/5867
1	25-A	0.20	0/4271	0.29	0/5836
1	25-B	0.20	0/4294	0.28	0/5867
All	All	0.20	0/214125	0.28	0/292575

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

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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

There are no bond length outliers.

There are no bond angle outliers.

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4-B	4181	3920	3932	0	0
1	5-A	4158	3901	3913	0	0
1	5-B	4181	3920	3932	0	0
1	6-A	4158	3901	3913	0	0
1	6-B	4181	3920	3932	0	0
1	7-A	4158	3901	3913	0	0
1	7-B	4181	3920	3932	0	0
1	8-A	4158	3901	3913	0	0
1	8-B	4181	3920	3932	0	0
1	9-A	4158	3901	3913	0	0
1	9-B	4181	3920	3932	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	25-B	4181	3920	3932	0	0
2	1-A	8	12	12	0	0
2	1-B	12	18	18	0	0
2	2-A	8	12	12	0	0
2	2-B	12	18	18	0	0
2	3-A	8	12	12	0	0
2	3-B	12	18	18	0	0
2	4-A	8	12	12	0	0
2	4-B	12	18	18	0	0
2	5-A	8	12	12	0	0
2	5-B	12	18	18	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	21-B	12	18	18	0	0
2	22-A	8	12	12	0	0
2	22-B	12	18	18	0	0
2	23-A	8	12	12	0	0
2	23-B	12	18	18	0	0
2	24-A	8	12	12	0	0
2	24-B	12	18	18	0	0
2	25-A	8	12	12	0	0
2	25-B	12	18	18	0	0
3	1-B	12	12	12	0	0
3	2-B	12	12	12	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	5-A	270	0	0	0	0
4	5-B	233	0	0	0	0
4	6-A	247	0	0	0	0
4	6-B	243	0	0	0	0
4	7-A	254	0	0	0	0
4	7-B	236	0	0	0	0
4	8-A	243	0	0	0	0
4	8-B	242	0	0	0	0
4	9-A	237	0	0	0	0
4	9-B	240	0	0	0	0
4	10-A	254	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	546/551 (99%)	497 (91%)	45 (8%)	4 (1%)	18	7
1	1-B	549/551 (100%)	504 (92%)	37 (7%)	8 (2%)	8	1
1	2-A	546/551 (99%)	506 (93%)	35 (6%)	5 (1%)	14	4
1	2-B	549/551 (100%)	504 (92%)	37 (7%)	8 (2%)	8	1
1	3-A	546/551 (99%)	507 (93%)	33 (6%)	6 (1%)	11	2
1	3-B	549/551 (100%)	508 (92%)	34 (6%)	7 (1%)	9	2
1	4-A	546/551 (99%)	511 (94%)	33 (6%)	2 (0%)	30	15
1	4-B	549/551 (100%)	508 (92%)	37 (7%)	4 (1%)	18	7
1	5-A	546/551 (99%)	501 (92%)	33 (6%)	12 (2%)	5	1
1	5-B	549/551 (100%)	509 (93%)	33 (6%)	7 (1%)	9	2
1	6-A	546/551 (99%)	500 (92%)	38 (7%)	8 (2%)	8	1
1	6-B	549/551 (100%)	513 (93%)	32 (6%)	4 (1%)	18	7
1	7-A	546/551 (99%)	507 (93%)	31 (6%)	8 (2%)	8	1
1	7-B	549/551 (100%)	494 (90%)	42 (8%)	13 (2%)	4	0
1	8-A	546/551 (99%)	505 (92%)	35 (6%)	6 (1%)	11	2
1	8-B	549/551 (100%)	516 (94%)	30 (6%)	3 (0%)	24	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	9-A	546/551 (99%)	505 (92%)	35 (6%)	6 (1%)	11	2
1	9-B	549/551 (100%)	505 (92%)	36 (7%)	8 (2%)	8	1
1	10-A	546/551 (99%)	499 (91%)	38 (7%)	9 (2%)	7	1
1	10-B	549/551 (100%)	507 (92%)	37 (7%)	5 (1%)	14	4
1	11-A	546/551 (99%)	509 (93%)	34 (6%)	3 (0%)	24	11
1	11-B	549/551 (100%)	508 (92%)	33 (6%)	8 (2%)	8	1
1	12-A	546/551 (99%)	504 (92%)	37 (7%)	5 (1%)	14	4
1	12-B	549/551 (100%)	507 (92%)	36 (7%)	6 (1%)	11	2
1	13-A	546/551 (99%)	502 (92%)	41 (8%)	3 (0%)	24	11
1	13-B	549/551 (100%)	514 (94%)	31 (6%)	4 (1%)	18	7
1	14-A	546/551 (99%)	505 (92%)	36 (7%)	5 (1%)	14	4
1	14-B	549/551 (100%)	504 (92%)	35 (6%)	10 (2%)	6	1
1	15-A	546/551 (99%)	496 (91%)	39 (7%)	11 (2%)	6	1
1	15-B	549/551 (100%)	505 (92%)	35 (6%)	9 (2%)	7	1
1	16-A	546/551 (99%)	503 (92%)	39 (7%)	4 (1%)	18	7
1	16-B	549/551 (100%)	515 (94%)	28 (5%)	6 (1%)	11	2
1	17-A	546/551 (99%)	500 (92%)	32 (6%)	14 (3%)	4	0
1	17-B	549/551 (100%)	510 (93%)	28 (5%)	11 (2%)	6	1
1	18-A	546/551 (99%)	487 (89%)	49 (9%)	10 (2%)	6	1
1	18-B	549/551 (100%)	506 (92%)	34 (6%)	9 (2%)	7	1
1	19-A	546/551 (99%)	505 (92%)	34 (6%)	7 (1%)	9	2
1	19-B	549/551 (100%)	508 (92%)	32 (6%)	9 (2%)	7	1
1	20-A	546/551 (99%)	508 (93%)	32 (6%)	6 (1%)	11	2
1	20-B	549/551 (100%)	513 (93%)	27 (5%)	9 (2%)	7	1
1	21-A	546/551 (99%)	510 (93%)	27 (5%)	9 (2%)	7	1
1	21-B	549/551 (100%)	510 (93%)	33 (6%)	6 (1%)	11	2
1	22-A	546/551 (99%)	505 (92%)	34 (6%)	7 (1%)	9	2
1	22-B	549/551 (100%)	513 (93%)	29 (5%)	7 (1%)	9	2
1	23-A	546/551 (99%)	510 (93%)	33 (6%)	3 (0%)	24	11
1	23-B	549/551 (100%)	508 (92%)	36 (7%)	5 (1%)	14	4
1	24-A	546/551 (99%)	499 (91%)	38 (7%)	9 (2%)	7	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	24-B	549/551 (100%)	505 (92%)	35 (6%)	9 (2%)	7	1
1	25-A	546/551 (99%)	505 (92%)	32 (6%)	9 (2%)	7	1
1	25-B	549/551 (100%)	509 (93%)	34 (6%)	6 (1%)	11	2
All	All	27375/27550 (99%)	25289 (92%)	1734 (6%)	352 (1%)	9	2

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	394 (91%)	41 (9%)	8	1
1	1-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	2-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	2-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	3-A	435/437 (100%)	394 (91%)	41 (9%)	8	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	4-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	4-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	5-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	5-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	6-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	6-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	7-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	7-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	8-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	8-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	9-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	9-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	10-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	10-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	11-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	11-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	12-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	12-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	13-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	13-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	14-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	14-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	15-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	15-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	16-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	16-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	17-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	17-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	18-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	18-B	437/437 (100%)	403 (92%)	34 (8%)	11	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	19-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	19-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	20-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	20-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	21-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	21-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	22-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	22-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	23-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	23-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	24-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	24-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
1	25-A	435/437 (100%)	394 (91%)	41 (9%)	8	1
1	25-B	437/437 (100%)	403 (92%)	34 (8%)	11	2
All	All	21800/21850 (100%)	19925 (91%)	1875 (9%)	10	1

All (1875) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	58	VAL
1	1-A	59	VAL
1	1-A	69	LEU
1	1-A	87	ARG
1	1-A	88	LYS
1	1-A	97	ASP
1	1-A	104	LYS
1	1-A	110	ASP
1	1-A	114	GLN
1	1-A	140	ASP
1	1-A	164	VAL
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	261	PRO
1	1-A	301	SER

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Mol	Chain	Res	Type
1	1-A	303	PRO
1	1-A	340	GLN
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	439	ILE
1	1-A	440	ILE
1	1-A	457	GLU
1	1-A	488	GLN
1	1-A	509	ASP
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	574	LEU
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	70	VAL
1	1-B	81	LYS
1	1-B	102	MET
1	1-B	114	GLN
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	259	THR
1	1-B	272	ASP
1	1-B	283	LYS
1	1-B	294	ASN
1	1-B	297	PRO
1	1-B	304	LEU

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Mol	Chain	Res	Type
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	369	LYS
1	1-B	399	ASP
1	1-B	452	GLU
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	574	LEU
1	2-A	58	VAL
1	2-A	59	VAL
1	2-A	69	LEU
1	2-A	87	ARG
1	2-A	88	LYS
1	2-A	97	ASP
1	2-A	104	LYS
1	2-A	110	ASP
1	2-A	114	GLN
1	2-A	140	ASP
1	2-A	164	VAL
1	2-A	169	ARG
1	2-A	196	TRP
1	2-A	206	LYS
1	2-A	210	GLU
1	2-A	225	SER
1	2-A	261	PRO
1	2-A	301	SER
1	2-A	303	PRO
1	2-A	340	GLN
1	2-A	346	ARG
1	2-A	348	ASN
1	2-A	368	LEU
1	2-A	369	LYS
1	2-A	402	SER
1	2-A	419	ILE
1	2-A	439	ILE

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Mol	Chain	Res	Type
1	2-A	440	ILE
1	2-A	457	GLU
1	2-A	488	GLN
1	2-A	509	ASP
1	2-A	518	ILE
1	2-A	529	SER
1	2-A	531	THR
1	2-A	538	MET
1	2-A	541	TYR
1	2-A	545	ASN
1	2-A	574	LEU
1	2-A	597	ILE
1	2-A	600	GLN
1	2-A	603	SER
1	2-B	56	GLN
1	2-B	64	LEU
1	2-B	69	LEU
1	2-B	70	VAL
1	2-B	81	LYS
1	2-B	102	MET
1	2-B	114	GLN
1	2-B	144	PHE
1	2-B	145	ASP
1	2-B	147	ASN
1	2-B	150	GLN
1	2-B	180	ARG
1	2-B	194	TYR
1	2-B	259	THR
1	2-B	272	ASP
1	2-B	283	LYS
1	2-B	294	ASN
1	2-B	297	PRO
1	2-B	304	LEU
1	2-B	310	VAL
1	2-B	311	LYS
1	2-B	318	THR
1	2-B	336	TYR
1	2-B	346	ARG
1	2-B	359	ILE
1	2-B	369	LYS
1	2-B	399	ASP
1	2-B	452	GLU

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Mol	Chain	Res	Type
1	2-B	488	GLN
1	2-B	519	LYS
1	2-B	529	SER
1	2-B	531	THR
1	2-B	553	GLN
1	2-B	574	LEU
1	3-A	58	VAL
1	3-A	59	VAL
1	3-A	69	LEU
1	3-A	87	ARG
1	3-A	88	LYS
1	3-A	97	ASP
1	3-A	104	LYS
1	3-A	110	ASP
1	3-A	114	GLN
1	3-A	140	ASP
1	3-A	164	VAL
1	3-A	169	ARG
1	3-A	196	TRP
1	3-A	206	LYS
1	3-A	210	GLU
1	3-A	225	SER
1	3-A	261	PRO
1	3-A	301	SER
1	3-A	303	PRO
1	3-A	340	GLN
1	3-A	346	ARG
1	3-A	348	ASN
1	3-A	368	LEU
1	3-A	369	LYS
1	3-A	402	SER
1	3-A	419	ILE
1	3-A	439	ILE
1	3-A	440	ILE
1	3-A	457	GLU
1	3-A	488	GLN
1	3-A	509	ASP
1	3-A	518	ILE
1	3-A	529	SER
1	3-A	531	THR
1	3-A	538	MET
1	3-A	541	TYR

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Mol	Chain	Res	Type
1	3-A	545	ASN
1	3-A	574	LEU
1	3-A	597	ILE
1	3-A	600	GLN
1	3-A	603	SER
1	3-B	56	GLN
1	3-B	64	LEU
1	3-B	69	LEU
1	3-B	70	VAL
1	3-B	81	LYS
1	3-B	102	MET
1	3-B	114	GLN
1	3-B	144	PHE
1	3-B	145	ASP
1	3-B	147	ASN
1	3-B	150	GLN
1	3-B	180	ARG
1	3-B	194	TYR
1	3-B	259	THR
1	3-B	272	ASP
1	3-B	283	LYS
1	3-B	294	ASN
1	3-B	297	PRO
1	3-B	304	LEU
1	3-B	310	VAL
1	3-B	311	LYS
1	3-B	318	THR
1	3-B	336	TYR
1	3-B	346	ARG
1	3-B	359	ILE
1	3-B	369	LYS
1	3-B	399	ASP
1	3-B	452	GLU
1	3-B	488	GLN
1	3-B	519	LYS
1	3-B	529	SER
1	3-B	531	THR
1	3-B	553	GLN
1	3-B	574	LEU
1	4-A	58	VAL
1	4-A	59	VAL
1	4-A	69	LEU

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Mol	Chain	Res	Type
1	4-A	87	ARG
1	4-A	88	LYS
1	4-A	97	ASP
1	4-A	104	LYS
1	4-A	110	ASP
1	4-A	114	GLN
1	4-A	140	ASP
1	4-A	164	VAL
1	4-A	169	ARG
1	4-A	196	TRP
1	4-A	206	LYS
1	4-A	210	GLU
1	4-A	225	SER
1	4-A	261	PRO
1	4-A	301	SER
1	4-A	303	PRO
1	4-A	340	GLN
1	4-A	346	ARG
1	4-A	348	ASN
1	4-A	368	LEU
1	4-A	369	LYS
1	4-A	402	SER
1	4-A	419	ILE
1	4-A	439	ILE
1	4-A	440	ILE
1	4-A	457	GLU
1	4-A	488	GLN
1	4-A	509	ASP
1	4-A	518	ILE
1	4-A	529	SER
1	4-A	531	THR
1	4-A	538	MET
1	4-A	541	TYR
1	4-A	545	ASN
1	4-A	574	LEU
1	4-A	597	ILE
1	4-A	600	GLN
1	4-A	603	SER
1	4-B	56	GLN
1	4-B	64	LEU
1	4-B	69	LEU
1	4-B	70	VAL

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Mol	Chain	Res	Type
1	4-B	81	LYS
1	4-B	102	MET
1	4-B	114	GLN
1	4-B	144	PHE
1	4-B	145	ASP
1	4-B	147	ASN
1	4-B	150	GLN
1	4-B	180	ARG
1	4-B	194	TYR
1	4-B	259	THR
1	4-B	272	ASP
1	4-B	283	LYS
1	4-B	294	ASN
1	4-B	297	PRO
1	4-B	304	LEU
1	4-B	310	VAL
1	4-B	311	LYS
1	4-B	318	THR
1	4-B	336	TYR
1	4-B	346	ARG
1	4-B	359	ILE
1	4-B	369	LYS
1	4-B	399	ASP
1	4-B	452	GLU
1	4-B	488	GLN
1	4-B	519	LYS
1	4-B	529	SER
1	4-B	531	THR
1	4-B	553	GLN
1	4-B	574	LEU
1	5-A	58	VAL
1	5-A	59	VAL
1	5-A	69	LEU
1	5-A	87	ARG
1	5-A	88	LYS
1	5-A	97	ASP
1	5-A	104	LYS
1	5-A	110	ASP
1	5-A	114	GLN
1	5-A	140	ASP
1	5-A	164	VAL
1	5-A	169	ARG

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Mol	Chain	Res	Type
1	5-A	196	TRP
1	5-A	206	LYS
1	5-A	210	GLU
1	5-A	225	SER
1	5-A	261	PRO
1	5-A	301	SER
1	5-A	303	PRO
1	5-A	340	GLN
1	5-A	346	ARG
1	5-A	348	ASN
1	5-A	368	LEU
1	5-A	369	LYS
1	5-A	402	SER
1	5-A	419	ILE
1	5-A	439	ILE
1	5-A	440	ILE
1	5-A	457	GLU
1	5-A	488	GLN
1	5-A	509	ASP
1	5-A	518	ILE
1	5-A	529	SER
1	5-A	531	THR
1	5-A	538	MET
1	5-A	541	TYR
1	5-A	545	ASN
1	5-A	574	LEU
1	5-A	597	ILE
1	5-A	600	GLN
1	5-A	603	SER
1	5-B	56	GLN
1	5-B	64	LEU
1	5-B	69	LEU
1	5-B	70	VAL
1	5-B	81	LYS
1	5-B	102	MET
1	5-B	114	GLN
1	5-B	144	PHE
1	5-B	145	ASP
1	5-B	147	ASN
1	5-B	150	GLN
1	5-B	180	ARG
1	5-B	194	TYR

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Mol	Chain	Res	Type
1	5-B	259	THR
1	5-B	272	ASP
1	5-B	283	LYS
1	5-B	294	ASN
1	5-B	297	PRO
1	5-B	304	LEU
1	5-B	310	VAL
1	5-B	311	LYS
1	5-B	318	THR
1	5-B	336	TYR
1	5-B	346	ARG
1	5-B	359	ILE
1	5-B	369	LYS
1	5-B	399	ASP
1	5-B	452	GLU
1	5-B	488	GLN
1	5-B	519	LYS
1	5-B	529	SER
1	5-B	531	THR
1	5-B	553	GLN
1	5-B	574	LEU
1	6-A	58	VAL
1	6-A	59	VAL
1	6-A	69	LEU
1	6-A	87	ARG
1	6-A	88	LYS
1	6-A	97	ASP
1	6-A	104	LYS
1	6-A	110	ASP
1	6-A	114	GLN
1	6-A	140	ASP
1	6-A	164	VAL
1	6-A	169	ARG
1	6-A	196	TRP
1	6-A	206	LYS
1	6-A	210	GLU
1	6-A	225	SER
1	6-A	261	PRO
1	6-A	301	SER
1	6-A	303	PRO
1	6-A	340	GLN
1	6-A	346	ARG

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Mol	Chain	Res	Type
1	6-A	348	ASN
1	6-A	368	LEU
1	6-A	369	LYS
1	6-A	402	SER
1	6-A	419	ILE
1	6-A	439	ILE
1	6-A	440	ILE
1	6-A	457	GLU
1	6-A	488	GLN
1	6-A	509	ASP
1	6-A	518	ILE
1	6-A	529	SER
1	6-A	531	THR
1	6-A	538	MET
1	6-A	541	TYR
1	6-A	545	ASN
1	6-A	574	LEU
1	6-A	597	ILE
1	6-A	600	GLN
1	6-A	603	SER
1	6-B	56	GLN
1	6-B	64	LEU
1	6-B	69	LEU
1	6-B	70	VAL
1	6-B	81	LYS
1	6-B	102	MET
1	6-B	114	GLN
1	6-B	144	PHE
1	6-B	145	ASP
1	6-B	147	ASN
1	6-B	150	GLN
1	6-B	180	ARG
1	6-B	194	TYR
1	6-B	259	THR
1	6-B	272	ASP
1	6-B	283	LYS
1	6-B	294	ASN
1	6-B	297	PRO
1	6-B	304	LEU
1	6-B	310	VAL
1	6-B	311	LYS
1	6-B	318	THR

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Mol	Chain	Res	Type
1	6-B	336	TYR
1	6-B	346	ARG
1	6-B	359	ILE
1	6-B	369	LYS
1	6-B	399	ASP
1	6-B	452	GLU
1	6-B	488	GLN
1	6-B	519	LYS
1	6-B	529	SER
1	6-B	531	THR
1	6-B	553	GLN
1	6-B	574	LEU
1	7-A	58	VAL
1	7-A	59	VAL
1	7-A	69	LEU
1	7-A	87	ARG
1	7-A	88	LYS
1	7-A	97	ASP
1	7-A	104	LYS
1	7-A	110	ASP
1	7-A	114	GLN
1	7-A	140	ASP
1	7-A	164	VAL
1	7-A	169	ARG
1	7-A	196	TRP
1	7-A	206	LYS
1	7-A	210	GLU
1	7-A	225	SER
1	7-A	261	PRO
1	7-A	301	SER
1	7-A	303	PRO
1	7-A	340	GLN
1	7-A	346	ARG
1	7-A	348	ASN
1	7-A	368	LEU
1	7-A	369	LYS
1	7-A	402	SER
1	7-A	419	ILE
1	7-A	439	ILE
1	7-A	440	ILE
1	7-A	457	GLU
1	7-A	488	GLN

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Mol	Chain	Res	Type
1	7-A	509	ASP
1	7-A	518	ILE
1	7-A	529	SER
1	7-A	531	THR
1	7-A	538	MET
1	7-A	541	TYR
1	7-A	545	ASN
1	7-A	574	LEU
1	7-A	597	ILE
1	7-A	600	GLN
1	7-A	603	SER
1	7-B	56	GLN
1	7-B	64	LEU
1	7-B	69	LEU
1	7-B	70	VAL
1	7-B	81	LYS
1	7-B	102	MET
1	7-B	114	GLN
1	7-B	144	PHE
1	7-B	145	ASP
1	7-B	147	ASN
1	7-B	150	GLN
1	7-B	180	ARG
1	7-B	194	TYR
1	7-B	259	THR
1	7-B	272	ASP
1	7-B	283	LYS
1	7-B	294	ASN
1	7-B	297	PRO
1	7-B	304	LEU
1	7-B	310	VAL
1	7-B	311	LYS
1	7-B	318	THR
1	7-B	336	TYR
1	7-B	346	ARG
1	7-B	359	ILE
1	7-B	369	LYS
1	7-B	399	ASP
1	7-B	452	GLU
1	7-B	488	GLN
1	7-B	519	LYS
1	7-B	529	SER

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Mol	Chain	Res	Type
1	7-B	531	THR
1	7-B	553	GLN
1	7-B	574	LEU
1	8-A	58	VAL
1	8-A	59	VAL
1	8-A	69	LEU
1	8-A	87	ARG
1	8-A	88	LYS
1	8-A	97	ASP
1	8-A	104	LYS
1	8-A	110	ASP
1	8-A	114	GLN
1	8-A	140	ASP
1	8-A	164	VAL
1	8-A	169	ARG
1	8-A	196	TRP
1	8-A	206	LYS
1	8-A	210	GLU
1	8-A	225	SER
1	8-A	261	PRO
1	8-A	301	SER
1	8-A	303	PRO
1	8-A	340	GLN
1	8-A	346	ARG
1	8-A	348	ASN
1	8-A	368	LEU
1	8-A	369	LYS
1	8-A	402	SER
1	8-A	419	ILE
1	8-A	439	ILE
1	8-A	440	ILE
1	8-A	457	GLU
1	8-A	488	GLN
1	8-A	509	ASP
1	8-A	518	ILE
1	8-A	529	SER
1	8-A	531	THR
1	8-A	538	MET
1	8-A	541	TYR
1	8-A	545	ASN
1	8-A	574	LEU
1	8-A	597	ILE

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Mol	Chain	Res	Type
1	8-A	600	GLN
1	8-A	603	SER
1	8-B	56	GLN
1	8-B	64	LEU
1	8-B	69	LEU
1	8-B	70	VAL
1	8-B	81	LYS
1	8-B	102	MET
1	8-B	114	GLN
1	8-B	144	PHE
1	8-B	145	ASP
1	8-B	147	ASN
1	8-B	150	GLN
1	8-B	180	ARG
1	8-B	194	TYR
1	8-B	259	THR
1	8-B	272	ASP
1	8-B	283	LYS
1	8-B	294	ASN
1	8-B	297	PRO
1	8-B	304	LEU
1	8-B	310	VAL
1	8-B	311	LYS
1	8-B	318	THR
1	8-B	336	TYR
1	8-B	346	ARG
1	8-B	359	ILE
1	8-B	369	LYS
1	8-B	399	ASP
1	8-B	452	GLU
1	8-B	488	GLN
1	8-B	519	LYS
1	8-B	529	SER
1	8-B	531	THR
1	8-B	553	GLN
1	8-B	574	LEU
1	9-A	58	VAL
1	9-A	59	VAL
1	9-A	69	LEU
1	9-A	87	ARG
1	9-A	88	LYS
1	9-A	97	ASP

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Mol	Chain	Res	Type
1	9-A	104	LYS
1	9-A	110	ASP
1	9-A	114	GLN
1	9-A	140	ASP
1	9-A	164	VAL
1	9-A	169	ARG
1	9-A	196	TRP
1	9-A	206	LYS
1	9-A	210	GLU
1	9-A	225	SER
1	9-A	261	PRO
1	9-A	301	SER
1	9-A	303	PRO
1	9-A	340	GLN
1	9-A	346	ARG
1	9-A	348	ASN
1	9-A	368	LEU
1	9-A	369	LYS
1	9-A	402	SER
1	9-A	419	ILE
1	9-A	439	ILE
1	9-A	440	ILE
1	9-A	457	GLU
1	9-A	488	GLN
1	9-A	509	ASP
1	9-A	518	ILE
1	9-A	529	SER
1	9-A	531	THR
1	9-A	538	MET
1	9-A	541	TYR
1	9-A	545	ASN
1	9-A	574	LEU
1	9-A	597	ILE
1	9-A	600	GLN
1	9-A	603	SER
1	9-B	56	GLN
1	9-B	64	LEU
1	9-B	69	LEU
1	9-B	70	VAL
1	9-B	81	LYS
1	9-B	102	MET
1	9-B	114	GLN

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Mol	Chain	Res	Type
1	9-B	144	PHE
1	9-B	145	ASP
1	9-B	147	ASN
1	9-B	150	GLN
1	9-B	180	ARG
1	9-B	194	TYR
1	9-B	259	THR
1	9-B	272	ASP
1	9-B	283	LYS
1	9-B	294	ASN
1	9-B	297	PRO
1	9-B	304	LEU
1	9-B	310	VAL
1	9-B	311	LYS
1	9-B	318	THR
1	9-B	336	TYR
1	9-B	346	ARG
1	9-B	359	ILE
1	9-B	369	LYS
1	9-B	399	ASP
1	9-B	452	GLU
1	9-B	488	GLN
1	9-B	519	LYS
1	9-B	529	SER
1	9-B	531	THR
1	9-B	553	GLN
1	9-B	574	LEU
1	10-A	58	VAL
1	10-A	59	VAL
1	10-A	69	LEU
1	10-A	87	ARG
1	10-A	88	LYS
1	10-A	97	ASP
1	10-A	104	LYS
1	10-A	110	ASP
1	10-A	114	GLN
1	10-A	140	ASP
1	10-A	164	VAL
1	10-A	169	ARG
1	10-A	196	TRP
1	10-A	206	LYS
1	10-A	210	GLU

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Mol	Chain	Res	Type
1	10-A	225	SER
1	10-A	261	PRO
1	10-A	301	SER
1	10-A	303	PRO
1	10-A	340	GLN
1	10-A	346	ARG
1	10-A	348	ASN
1	10-A	368	LEU
1	10-A	369	LYS
1	10-A	402	SER
1	10-A	419	ILE
1	10-A	439	ILE
1	10-A	440	ILE
1	10-A	457	GLU
1	10-A	488	GLN
1	10-A	509	ASP
1	10-A	518	ILE
1	10-A	529	SER
1	10-A	531	THR
1	10-A	538	MET
1	10-A	541	TYR
1	10-A	545	ASN
1	10-A	574	LEU
1	10-A	597	ILE
1	10-A	600	GLN
1	10-A	603	SER
1	10-B	56	GLN
1	10-B	64	LEU
1	10-B	69	LEU
1	10-B	70	VAL
1	10-B	81	LYS
1	10-B	102	MET
1	10-B	114	GLN
1	10-B	144	PHE
1	10-B	145	ASP
1	10-B	147	ASN
1	10-B	150	GLN
1	10-B	180	ARG
1	10-B	194	TYR
1	10-B	259	THR
1	10-B	272	ASP
1	10-B	283	LYS

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Mol	Chain	Res	Type
1	10-B	294	ASN
1	10-B	297	PRO
1	10-B	304	LEU
1	10-B	310	VAL
1	10-B	311	LYS
1	10-B	318	THR
1	10-B	336	TYR
1	10-B	346	ARG
1	10-B	359	ILE
1	10-B	369	LYS
1	10-B	399	ASP
1	10-B	452	GLU
1	10-B	488	GLN
1	10-B	519	LYS
1	10-B	529	SER
1	10-B	531	THR
1	10-B	553	GLN
1	10-B	574	LEU
1	11-A	58	VAL
1	11-A	59	VAL
1	11-A	69	LEU
1	11-A	87	ARG
1	11-A	88	LYS
1	11-A	97	ASP
1	11-A	104	LYS
1	11-A	110	ASP
1	11-A	114	GLN
1	11-A	140	ASP
1	11-A	164	VAL
1	11-A	169	ARG
1	11-A	196	TRP
1	11-A	206	LYS
1	11-A	210	GLU
1	11-A	225	SER
1	11-A	261	PRO
1	11-A	301	SER
1	11-A	303	PRO
1	11-A	340	GLN
1	11-A	346	ARG
1	11-A	348	ASN
1	11-A	368	LEU
1	11-A	369	LYS

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Mol	Chain	Res	Type
1	11-A	402	SER
1	11-A	419	ILE
1	11-A	439	ILE
1	11-A	440	ILE
1	11-A	457	GLU
1	11-A	488	GLN
1	11-A	509	ASP
1	11-A	518	ILE
1	11-A	529	SER
1	11-A	531	THR
1	11-A	538	MET
1	11-A	541	TYR
1	11-A	545	ASN
1	11-A	574	LEU
1	11-A	597	ILE
1	11-A	600	GLN
1	11-A	603	SER
1	11-B	56	GLN
1	11-B	64	LEU
1	11-B	69	LEU
1	11-B	70	VAL
1	11-B	81	LYS
1	11-B	102	MET
1	11-B	114	GLN
1	11-B	144	PHE
1	11-B	145	ASP
1	11-B	147	ASN
1	11-B	150	GLN
1	11-B	180	ARG
1	11-B	194	TYR
1	11-B	259	THR
1	11-B	272	ASP
1	11-B	283	LYS
1	11-B	294	ASN
1	11-B	297	PRO
1	11-B	304	LEU
1	11-B	310	VAL
1	11-B	311	LYS
1	11-B	318	THR
1	11-B	336	TYR
1	11-B	346	ARG
1	11-B	359	ILE

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Mol	Chain	Res	Type
1	11-B	369	LYS
1	11-B	399	ASP
1	11-B	452	GLU
1	11-B	488	GLN
1	11-B	519	LYS
1	11-B	529	SER
1	11-B	531	THR
1	11-B	553	GLN
1	11-B	574	LEU
1	12-A	58	VAL
1	12-A	59	VAL
1	12-A	69	LEU
1	12-A	87	ARG
1	12-A	88	LYS
1	12-A	97	ASP
1	12-A	104	LYS
1	12-A	110	ASP
1	12-A	114	GLN
1	12-A	140	ASP
1	12-A	164	VAL
1	12-A	169	ARG
1	12-A	196	TRP
1	12-A	206	LYS
1	12-A	210	GLU
1	12-A	225	SER
1	12-A	261	PRO
1	12-A	301	SER
1	12-A	303	PRO
1	12-A	340	GLN
1	12-A	346	ARG
1	12-A	348	ASN
1	12-A	368	LEU
1	12-A	369	LYS
1	12-A	402	SER
1	12-A	419	ILE
1	12-A	439	ILE
1	12-A	440	ILE
1	12-A	457	GLU
1	12-A	488	GLN
1	12-A	509	ASP
1	12-A	518	ILE
1	12-A	529	SER

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Mol	Chain	Res	Type
1	12-A	531	THR
1	12-A	538	MET
1	12-A	541	TYR
1	12-A	545	ASN
1	12-A	574	LEU
1	12-A	597	ILE
1	12-A	600	GLN
1	12-A	603	SER
1	12-B	56	GLN
1	12-B	64	LEU
1	12-B	69	LEU
1	12-B	70	VAL
1	12-B	81	LYS
1	12-B	102	MET
1	12-B	114	GLN
1	12-B	144	PHE
1	12-B	145	ASP
1	12-B	147	ASN
1	12-B	150	GLN
1	12-B	180	ARG
1	12-B	194	TYR
1	12-B	259	THR
1	12-B	272	ASP
1	12-B	283	LYS
1	12-B	294	ASN
1	12-B	297	PRO
1	12-B	304	LEU
1	12-B	310	VAL
1	12-B	311	LYS
1	12-B	318	THR
1	12-B	336	TYR
1	12-B	346	ARG
1	12-B	359	ILE
1	12-B	369	LYS
1	12-B	399	ASP
1	12-B	452	GLU
1	12-B	488	GLN
1	12-B	519	LYS
1	12-B	529	SER
1	12-B	531	THR
1	12-B	553	GLN
1	12-B	574	LEU

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Mol	Chain	Res	Type
1	13-A	58	VAL
1	13-A	59	VAL
1	13-A	69	LEU
1	13-A	87	ARG
1	13-A	88	LYS
1	13-A	97	ASP
1	13-A	104	LYS
1	13-A	110	ASP
1	13-A	114	GLN
1	13-A	140	ASP
1	13-A	164	VAL
1	13-A	169	ARG
1	13-A	196	TRP
1	13-A	206	LYS
1	13-A	210	GLU
1	13-A	225	SER
1	13-A	261	PRO
1	13-A	301	SER
1	13-A	303	PRO
1	13-A	340	GLN
1	13-A	346	ARG
1	13-A	348	ASN
1	13-A	368	LEU
1	13-A	369	LYS
1	13-A	402	SER
1	13-A	419	ILE
1	13-A	439	ILE
1	13-A	440	ILE
1	13-A	457	GLU
1	13-A	488	GLN
1	13-A	509	ASP
1	13-A	518	ILE
1	13-A	529	SER
1	13-A	531	THR
1	13-A	538	MET
1	13-A	541	TYR
1	13-A	545	ASN
1	13-A	574	LEU
1	13-A	597	ILE
1	13-A	600	GLN
1	13-A	603	SER
1	13-B	56	GLN

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Mol	Chain	Res	Type
1	13-B	64	LEU
1	13-B	69	LEU
1	13-B	70	VAL
1	13-B	81	LYS
1	13-B	102	MET
1	13-B	114	GLN
1	13-B	144	PHE
1	13-B	145	ASP
1	13-B	147	ASN
1	13-B	150	GLN
1	13-B	180	ARG
1	13-B	194	TYR
1	13-B	259	THR
1	13-B	272	ASP
1	13-B	283	LYS
1	13-B	294	ASN
1	13-B	297	PRO
1	13-B	304	LEU
1	13-B	310	VAL
1	13-B	311	LYS
1	13-B	318	THR
1	13-B	336	TYR
1	13-B	346	ARG
1	13-B	359	ILE
1	13-B	369	LYS
1	13-B	399	ASP
1	13-B	452	GLU
1	13-B	488	GLN
1	13-B	519	LYS
1	13-B	529	SER
1	13-B	531	THR
1	13-B	553	GLN
1	13-B	574	LEU
1	14-A	58	VAL
1	14-A	59	VAL
1	14-A	69	LEU
1	14-A	87	ARG
1	14-A	88	LYS
1	14-A	97	ASP
1	14-A	104	LYS
1	14-A	110	ASP
1	14-A	114	GLN

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Mol	Chain	Res	Type
1	14-A	140	ASP
1	14-A	164	VAL
1	14-A	169	ARG
1	14-A	196	TRP
1	14-A	206	LYS
1	14-A	210	GLU
1	14-A	225	SER
1	14-A	261	PRO
1	14-A	301	SER
1	14-A	303	PRO
1	14-A	340	GLN
1	14-A	346	ARG
1	14-A	348	ASN
1	14-A	368	LEU
1	14-A	369	LYS
1	14-A	402	SER
1	14-A	419	ILE
1	14-A	439	ILE
1	14-A	440	ILE
1	14-A	457	GLU
1	14-A	488	GLN
1	14-A	509	ASP
1	14-A	518	ILE
1	14-A	529	SER
1	14-A	531	THR
1	14-A	538	MET
1	14-A	541	TYR
1	14-A	545	ASN
1	14-A	574	LEU
1	14-A	597	ILE
1	14-A	600	GLN
1	14-A	603	SER
1	14-B	56	GLN
1	14-B	64	LEU
1	14-B	69	LEU
1	14-B	70	VAL
1	14-B	81	LYS
1	14-B	102	MET
1	14-B	114	GLN
1	14-B	144	PHE
1	14-B	145	ASP
1	14-B	147	ASN

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Mol	Chain	Res	Type
1	14-B	150	GLN
1	14-B	180	ARG
1	14-B	194	TYR
1	14-B	259	THR
1	14-B	272	ASP
1	14-B	283	LYS
1	14-B	294	ASN
1	14-B	297	PRO
1	14-B	304	LEU
1	14-B	310	VAL
1	14-B	311	LYS
1	14-B	318	THR
1	14-B	336	TYR
1	14-B	346	ARG
1	14-B	359	ILE
1	14-B	369	LYS
1	14-B	399	ASP
1	14-B	452	GLU
1	14-B	488	GLN
1	14-B	519	LYS
1	14-B	529	SER
1	14-B	531	THR
1	14-B	553	GLN
1	14-B	574	LEU
1	15-A	58	VAL
1	15-A	59	VAL
1	15-A	69	LEU
1	15-A	87	ARG
1	15-A	88	LYS
1	15-A	97	ASP
1	15-A	104	LYS
1	15-A	110	ASP
1	15-A	114	GLN
1	15-A	140	ASP
1	15-A	164	VAL
1	15-A	169	ARG
1	15-A	196	TRP
1	15-A	206	LYS
1	15-A	210	GLU
1	15-A	225	SER
1	15-A	261	PRO
1	15-A	301	SER

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Mol	Chain	Res	Type
1	15-A	303	PRO
1	15-A	340	GLN
1	15-A	346	ARG
1	15-A	348	ASN
1	15-A	368	LEU
1	15-A	369	LYS
1	15-A	402	SER
1	15-A	419	ILE
1	15-A	439	ILE
1	15-A	440	ILE
1	15-A	457	GLU
1	15-A	488	GLN
1	15-A	509	ASP
1	15-A	518	ILE
1	15-A	529	SER
1	15-A	531	THR
1	15-A	538	MET
1	15-A	541	TYR
1	15-A	545	ASN
1	15-A	574	LEU
1	15-A	597	ILE
1	15-A	600	GLN
1	15-A	603	SER
1	15-B	56	GLN
1	15-B	64	LEU
1	15-B	69	LEU
1	15-B	70	VAL
1	15-B	81	LYS
1	15-B	102	MET
1	15-B	114	GLN
1	15-B	144	PHE
1	15-B	145	ASP
1	15-B	147	ASN
1	15-B	150	GLN
1	15-B	180	ARG
1	15-B	194	TYR
1	15-B	259	THR
1	15-B	272	ASP
1	15-B	283	LYS
1	15-B	294	ASN
1	15-B	297	PRO
1	15-B	304	LEU

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Mol	Chain	Res	Type
1	15-B	310	VAL
1	15-B	311	LYS
1	15-B	318	THR
1	15-B	336	TYR
1	15-B	346	ARG
1	15-B	359	ILE
1	15-B	369	LYS
1	15-B	399	ASP
1	15-B	452	GLU
1	15-B	488	GLN
1	15-B	519	LYS
1	15-B	529	SER
1	15-B	531	THR
1	15-B	553	GLN
1	15-B	574	LEU
1	16-A	58	VAL
1	16-A	59	VAL
1	16-A	69	LEU
1	16-A	87	ARG
1	16-A	88	LYS
1	16-A	97	ASP
1	16-A	104	LYS
1	16-A	110	ASP
1	16-A	114	GLN
1	16-A	140	ASP
1	16-A	164	VAL
1	16-A	169	ARG
1	16-A	196	TRP
1	16-A	206	LYS
1	16-A	210	GLU
1	16-A	225	SER
1	16-A	261	PRO
1	16-A	301	SER
1	16-A	303	PRO
1	16-A	340	GLN
1	16-A	346	ARG
1	16-A	348	ASN
1	16-A	368	LEU
1	16-A	369	LYS
1	16-A	402	SER
1	16-A	419	ILE
1	16-A	439	ILE

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Mol	Chain	Res	Type
1	16-A	440	ILE
1	16-A	457	GLU
1	16-A	488	GLN
1	16-A	509	ASP
1	16-A	518	ILE
1	16-A	529	SER
1	16-A	531	THR
1	16-A	538	MET
1	16-A	541	TYR
1	16-A	545	ASN
1	16-A	574	LEU
1	16-A	597	ILE
1	16-A	600	GLN
1	16-A	603	SER
1	16-B	56	GLN
1	16-B	64	LEU
1	16-B	69	LEU
1	16-B	70	VAL
1	16-B	81	LYS
1	16-B	102	MET
1	16-B	114	GLN
1	16-B	144	PHE
1	16-B	145	ASP
1	16-B	147	ASN
1	16-B	150	GLN
1	16-B	180	ARG
1	16-B	194	TYR
1	16-B	259	THR
1	16-B	272	ASP
1	16-B	283	LYS
1	16-B	294	ASN
1	16-B	297	PRO
1	16-B	304	LEU
1	16-B	310	VAL
1	16-B	311	LYS
1	16-B	318	THR
1	16-B	336	TYR
1	16-B	346	ARG
1	16-B	359	ILE
1	16-B	369	LYS
1	16-B	399	ASP
1	16-B	452	GLU

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Mol	Chain	Res	Type
1	16-B	488	GLN
1	16-B	519	LYS
1	16-B	529	SER
1	16-B	531	THR
1	16-B	553	GLN
1	16-B	574	LEU
1	17-A	58	VAL
1	17-A	59	VAL
1	17-A	69	LEU
1	17-A	87	ARG
1	17-A	88	LYS
1	17-A	97	ASP
1	17-A	104	LYS
1	17-A	110	ASP
1	17-A	114	GLN
1	17-A	140	ASP
1	17-A	164	VAL
1	17-A	169	ARG
1	17-A	196	TRP
1	17-A	206	LYS
1	17-A	210	GLU
1	17-A	225	SER
1	17-A	261	PRO
1	17-A	301	SER
1	17-A	303	PRO
1	17-A	340	GLN
1	17-A	346	ARG
1	17-A	348	ASN
1	17-A	368	LEU
1	17-A	369	LYS
1	17-A	402	SER
1	17-A	419	ILE
1	17-A	439	ILE
1	17-A	440	ILE
1	17-A	457	GLU
1	17-A	488	GLN
1	17-A	509	ASP
1	17-A	518	ILE
1	17-A	529	SER
1	17-A	531	THR
1	17-A	538	MET
1	17-A	541	TYR

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Mol	Chain	Res	Type
1	17-A	545	ASN
1	17-A	574	LEU
1	17-A	597	ILE
1	17-A	600	GLN
1	17-A	603	SER
1	17-B	56	GLN
1	17-B	64	LEU
1	17-B	69	LEU
1	17-B	70	VAL
1	17-B	81	LYS
1	17-B	102	MET
1	17-B	114	GLN
1	17-B	144	PHE
1	17-B	145	ASP
1	17-B	147	ASN
1	17-B	150	GLN
1	17-B	180	ARG
1	17-B	194	TYR
1	17-B	259	THR
1	17-B	272	ASP
1	17-B	283	LYS
1	17-B	294	ASN
1	17-B	297	PRO
1	17-B	304	LEU
1	17-B	310	VAL
1	17-B	311	LYS
1	17-B	318	THR
1	17-B	336	TYR
1	17-B	346	ARG
1	17-B	359	ILE
1	17-B	369	LYS
1	17-B	399	ASP
1	17-B	452	GLU
1	17-B	488	GLN
1	17-B	519	LYS
1	17-B	529	SER
1	17-B	531	THR
1	17-B	553	GLN
1	17-B	574	LEU
1	18-A	58	VAL
1	18-A	59	VAL
1	18-A	69	LEU

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Mol	Chain	Res	Type
1	18-A	87	ARG
1	18-A	88	LYS
1	18-A	97	ASP
1	18-A	104	LYS
1	18-A	110	ASP
1	18-A	114	GLN
1	18-A	140	ASP
1	18-A	164	VAL
1	18-A	169	ARG
1	18-A	196	TRP
1	18-A	206	LYS
1	18-A	210	GLU
1	18-A	225	SER
1	18-A	261	PRO
1	18-A	301	SER
1	18-A	303	PRO
1	18-A	340	GLN
1	18-A	346	ARG
1	18-A	348	ASN
1	18-A	368	LEU
1	18-A	369	LYS
1	18-A	402	SER
1	18-A	419	ILE
1	18-A	439	ILE
1	18-A	440	ILE
1	18-A	457	GLU
1	18-A	488	GLN
1	18-A	509	ASP
1	18-A	518	ILE
1	18-A	529	SER
1	18-A	531	THR
1	18-A	538	MET
1	18-A	541	TYR
1	18-A	545	ASN
1	18-A	574	LEU
1	18-A	597	ILE
1	18-A	600	GLN
1	18-A	603	SER
1	18-B	56	GLN
1	18-B	64	LEU
1	18-B	69	LEU
1	18-B	70	VAL

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Mol	Chain	Res	Type
1	18-B	81	LYS
1	18-B	102	MET
1	18-B	114	GLN
1	18-B	144	PHE
1	18-B	145	ASP
1	18-B	147	ASN
1	18-B	150	GLN
1	18-B	180	ARG
1	18-B	194	TYR
1	18-B	259	THR
1	18-B	272	ASP
1	18-B	283	LYS
1	18-B	294	ASN
1	18-B	297	PRO
1	18-B	304	LEU
1	18-B	310	VAL
1	18-B	311	LYS
1	18-B	318	THR
1	18-B	336	TYR
1	18-B	346	ARG
1	18-B	359	ILE
1	18-B	369	LYS
1	18-B	399	ASP
1	18-B	452	GLU
1	18-B	488	GLN
1	18-B	519	LYS
1	18-B	529	SER
1	18-B	531	THR
1	18-B	553	GLN
1	18-B	574	LEU
1	19-A	58	VAL
1	19-A	59	VAL
1	19-A	69	LEU
1	19-A	87	ARG
1	19-A	88	LYS
1	19-A	97	ASP
1	19-A	104	LYS
1	19-A	110	ASP
1	19-A	114	GLN
1	19-A	140	ASP
1	19-A	164	VAL
1	19-A	169	ARG

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Mol	Chain	Res	Type
1	19-A	196	TRP
1	19-A	206	LYS
1	19-A	210	GLU
1	19-A	225	SER
1	19-A	261	PRO
1	19-A	301	SER
1	19-A	303	PRO
1	19-A	340	GLN
1	19-A	346	ARG
1	19-A	348	ASN
1	19-A	368	LEU
1	19-A	369	LYS
1	19-A	402	SER
1	19-A	419	ILE
1	19-A	439	ILE
1	19-A	440	ILE
1	19-A	457	GLU
1	19-A	488	GLN
1	19-A	509	ASP
1	19-A	518	ILE
1	19-A	529	SER
1	19-A	531	THR
1	19-A	538	MET
1	19-A	541	TYR
1	19-A	545	ASN
1	19-A	574	LEU
1	19-A	597	ILE
1	19-A	600	GLN
1	19-A	603	SER
1	19-B	56	GLN
1	19-B	64	LEU
1	19-B	69	LEU
1	19-B	70	VAL
1	19-B	81	LYS
1	19-B	102	MET
1	19-B	114	GLN
1	19-B	144	PHE
1	19-B	145	ASP
1	19-B	147	ASN
1	19-B	150	GLN
1	19-B	180	ARG
1	19-B	194	TYR

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Mol	Chain	Res	Type
1	19-B	259	THR
1	19-B	272	ASP
1	19-B	283	LYS
1	19-B	294	ASN
1	19-B	297	PRO
1	19-B	304	LEU
1	19-B	310	VAL
1	19-B	311	LYS
1	19-B	318	THR
1	19-B	336	TYR
1	19-B	346	ARG
1	19-B	359	ILE
1	19-B	369	LYS
1	19-B	399	ASP
1	19-B	452	GLU
1	19-B	488	GLN
1	19-B	519	LYS
1	19-B	529	SER
1	19-B	531	THR
1	19-B	553	GLN
1	19-B	574	LEU
1	20-A	58	VAL
1	20-A	59	VAL
1	20-A	69	LEU
1	20-A	87	ARG
1	20-A	88	LYS
1	20-A	97	ASP
1	20-A	104	LYS
1	20-A	110	ASP
1	20-A	114	GLN
1	20-A	140	ASP
1	20-A	164	VAL
1	20-A	169	ARG
1	20-A	196	TRP
1	20-A	206	LYS
1	20-A	210	GLU
1	20-A	225	SER
1	20-A	261	PRO
1	20-A	301	SER
1	20-A	303	PRO
1	20-A	340	GLN
1	20-A	346	ARG

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Mol	Chain	Res	Type
1	20-A	348	ASN
1	20-A	368	LEU
1	20-A	369	LYS
1	20-A	402	SER
1	20-A	419	ILE
1	20-A	439	ILE
1	20-A	440	ILE
1	20-A	457	GLU
1	20-A	488	GLN
1	20-A	509	ASP
1	20-A	518	ILE
1	20-A	529	SER
1	20-A	531	THR
1	20-A	538	MET
1	20-A	541	TYR
1	20-A	545	ASN
1	20-A	574	LEU
1	20-A	597	ILE
1	20-A	600	GLN
1	20-A	603	SER
1	20-B	56	GLN
1	20-B	64	LEU
1	20-B	69	LEU
1	20-B	70	VAL
1	20-B	81	LYS
1	20-B	102	MET
1	20-B	114	GLN
1	20-B	144	PHE
1	20-B	145	ASP
1	20-B	147	ASN
1	20-B	150	GLN
1	20-B	180	ARG
1	20-B	194	TYR
1	20-B	259	THR
1	20-B	272	ASP
1	20-B	283	LYS
1	20-B	294	ASN
1	20-B	297	PRO
1	20-B	304	LEU
1	20-B	310	VAL
1	20-B	311	LYS
1	20-B	318	THR

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Mol	Chain	Res	Type
1	20-B	336	TYR
1	20-B	346	ARG
1	20-B	359	ILE
1	20-B	369	LYS
1	20-B	399	ASP
1	20-B	452	GLU
1	20-B	488	GLN
1	20-B	519	LYS
1	20-B	529	SER
1	20-B	531	THR
1	20-B	553	GLN
1	20-B	574	LEU
1	21-A	58	VAL
1	21-A	59	VAL
1	21-A	69	LEU
1	21-A	87	ARG
1	21-A	88	LYS
1	21-A	97	ASP
1	21-A	104	LYS
1	21-A	110	ASP
1	21-A	114	GLN
1	21-A	140	ASP
1	21-A	164	VAL
1	21-A	169	ARG
1	21-A	196	TRP
1	21-A	206	LYS
1	21-A	210	GLU
1	21-A	225	SER
1	21-A	261	PRO
1	21-A	301	SER
1	21-A	303	PRO
1	21-A	340	GLN
1	21-A	346	ARG
1	21-A	348	ASN
1	21-A	368	LEU
1	21-A	369	LYS
1	21-A	402	SER
1	21-A	419	ILE
1	21-A	439	ILE
1	21-A	440	ILE
1	21-A	457	GLU
1	21-A	488	GLN

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Mol	Chain	Res	Type
1	21-A	509	ASP
1	21-A	518	ILE
1	21-A	529	SER
1	21-A	531	THR
1	21-A	538	MET
1	21-A	541	TYR
1	21-A	545	ASN
1	21-A	574	LEU
1	21-A	597	ILE
1	21-A	600	GLN
1	21-A	603	SER
1	21-B	56	GLN
1	21-B	64	LEU
1	21-B	69	LEU
1	21-B	70	VAL
1	21-B	81	LYS
1	21-B	102	MET
1	21-B	114	GLN
1	21-B	144	PHE
1	21-B	145	ASP
1	21-B	147	ASN
1	21-B	150	GLN
1	21-B	180	ARG
1	21-B	194	TYR
1	21-B	259	THR
1	21-B	272	ASP
1	21-B	283	LYS
1	21-B	294	ASN
1	21-B	297	PRO
1	21-B	304	LEU
1	21-B	310	VAL
1	21-B	311	LYS
1	21-B	318	THR
1	21-B	336	TYR
1	21-B	346	ARG
1	21-B	359	ILE
1	21-B	369	LYS
1	21-B	399	ASP
1	21-B	452	GLU
1	21-B	488	GLN
1	21-B	519	LYS
1	21-B	529	SER

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Mol	Chain	Res	Type
1	21-B	531	THR
1	21-B	553	GLN
1	21-B	574	LEU
1	22-A	58	VAL
1	22-A	59	VAL
1	22-A	69	LEU
1	22-A	87	ARG
1	22-A	88	LYS
1	22-A	97	ASP
1	22-A	104	LYS
1	22-A	110	ASP
1	22-A	114	GLN
1	22-A	140	ASP
1	22-A	164	VAL
1	22-A	169	ARG
1	22-A	196	TRP
1	22-A	206	LYS
1	22-A	210	GLU
1	22-A	225	SER
1	22-A	261	PRO
1	22-A	301	SER
1	22-A	303	PRO
1	22-A	340	GLN
1	22-A	346	ARG
1	22-A	348	ASN
1	22-A	368	LEU
1	22-A	369	LYS
1	22-A	402	SER
1	22-A	419	ILE
1	22-A	439	ILE
1	22-A	440	ILE
1	22-A	457	GLU
1	22-A	488	GLN
1	22-A	509	ASP
1	22-A	518	ILE
1	22-A	529	SER
1	22-A	531	THR
1	22-A	538	MET
1	22-A	541	TYR
1	22-A	545	ASN
1	22-A	574	LEU
1	22-A	597	ILE

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Mol	Chain	Res	Type
1	22-A	600	GLN
1	22-A	603	SER
1	22-B	56	GLN
1	22-B	64	LEU
1	22-B	69	LEU
1	22-B	70	VAL
1	22-B	81	LYS
1	22-B	102	MET
1	22-B	114	GLN
1	22-B	144	PHE
1	22-B	145	ASP
1	22-B	147	ASN
1	22-B	150	GLN
1	22-B	180	ARG
1	22-B	194	TYR
1	22-B	259	THR
1	22-B	272	ASP
1	22-B	283	LYS
1	22-B	294	ASN
1	22-B	297	PRO
1	22-B	304	LEU
1	22-B	310	VAL
1	22-B	311	LYS
1	22-B	318	THR
1	22-B	336	TYR
1	22-B	346	ARG
1	22-B	359	ILE
1	22-B	369	LYS
1	22-B	399	ASP
1	22-B	452	GLU
1	22-B	488	GLN
1	22-B	519	LYS
1	22-B	529	SER
1	22-B	531	THR
1	22-B	553	GLN
1	22-B	574	LEU
1	23-A	58	VAL
1	23-A	59	VAL
1	23-A	69	LEU
1	23-A	87	ARG
1	23-A	88	LYS
1	23-A	97	ASP

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Mol	Chain	Res	Type
1	23-A	104	LYS
1	23-A	110	ASP
1	23-A	114	GLN
1	23-A	140	ASP
1	23-A	164	VAL
1	23-A	169	ARG
1	23-A	196	TRP
1	23-A	206	LYS
1	23-A	210	GLU
1	23-A	225	SER
1	23-A	261	PRO
1	23-A	301	SER
1	23-A	303	PRO
1	23-A	340	GLN
1	23-A	346	ARG
1	23-A	348	ASN
1	23-A	368	LEU
1	23-A	369	LYS
1	23-A	402	SER
1	23-A	419	ILE
1	23-A	439	ILE
1	23-A	440	ILE
1	23-A	457	GLU
1	23-A	488	GLN
1	23-A	509	ASP
1	23-A	518	ILE
1	23-A	529	SER
1	23-A	531	THR
1	23-A	538	MET
1	23-A	541	TYR
1	23-A	545	ASN
1	23-A	574	LEU
1	23-A	597	ILE
1	23-A	600	GLN
1	23-A	603	SER
1	23-B	56	GLN
1	23-B	64	LEU
1	23-B	69	LEU
1	23-B	70	VAL
1	23-B	81	LYS
1	23-B	102	MET
1	23-B	114	GLN

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Mol	Chain	Res	Type
1	23-B	144	PHE
1	23-B	145	ASP
1	23-B	147	ASN
1	23-B	150	GLN
1	23-B	180	ARG
1	23-B	194	TYR
1	23-B	259	THR
1	23-B	272	ASP
1	23-B	283	LYS
1	23-B	294	ASN
1	23-B	297	PRO
1	23-B	304	LEU
1	23-B	310	VAL
1	23-B	311	LYS
1	23-B	318	THR
1	23-B	336	TYR
1	23-B	346	ARG
1	23-B	359	ILE
1	23-B	369	LYS
1	23-B	399	ASP
1	23-B	452	GLU
1	23-B	488	GLN
1	23-B	519	LYS
1	23-B	529	SER
1	23-B	531	THR
1	23-B	553	GLN
1	23-B	574	LEU
1	24-A	58	VAL
1	24-A	59	VAL
1	24-A	69	LEU
1	24-A	87	ARG
1	24-A	88	LYS
1	24-A	97	ASP
1	24-A	104	LYS
1	24-A	110	ASP
1	24-A	114	GLN
1	24-A	140	ASP
1	24-A	164	VAL
1	24-A	169	ARG
1	24-A	196	TRP
1	24-A	206	LYS
1	24-A	210	GLU

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Mol	Chain	Res	Type
1	24-A	225	SER
1	24-A	261	PRO
1	24-A	301	SER
1	24-A	303	PRO
1	24-A	340	GLN
1	24-A	346	ARG
1	24-A	348	ASN
1	24-A	368	LEU
1	24-A	369	LYS
1	24-A	402	SER
1	24-A	419	ILE
1	24-A	439	ILE
1	24-A	440	ILE
1	24-A	457	GLU
1	24-A	488	GLN
1	24-A	509	ASP
1	24-A	518	ILE
1	24-A	529	SER
1	24-A	531	THR
1	24-A	538	MET
1	24-A	541	TYR
1	24-A	545	ASN
1	24-A	574	LEU
1	24-A	597	ILE
1	24-A	600	GLN
1	24-A	603	SER
1	24-B	56	GLN
1	24-B	64	LEU
1	24-B	69	LEU
1	24-B	70	VAL
1	24-B	81	LYS
1	24-B	102	MET
1	24-B	114	GLN
1	24-B	144	PHE
1	24-B	145	ASP
1	24-B	147	ASN
1	24-B	150	GLN
1	24-B	180	ARG
1	24-B	194	TYR
1	24-B	259	THR
1	24-B	272	ASP
1	24-B	283	LYS

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Mol	Chain	Res	Type
1	24-B	294	ASN
1	24-B	297	PRO
1	24-B	304	LEU
1	24-B	310	VAL
1	24-B	311	LYS
1	24-B	318	THR
1	24-B	336	TYR
1	24-B	346	ARG
1	24-B	359	ILE
1	24-B	369	LYS
1	24-B	399	ASP
1	24-B	452	GLU
1	24-B	488	GLN
1	24-B	519	LYS
1	24-B	529	SER
1	24-B	531	THR
1	24-B	553	GLN
1	24-B	574	LEU
1	25-A	58	VAL
1	25-A	59	VAL
1	25-A	69	LEU
1	25-A	87	ARG
1	25-A	88	LYS
1	25-A	97	ASP
1	25-A	104	LYS
1	25-A	110	ASP
1	25-A	114	GLN
1	25-A	140	ASP
1	25-A	164	VAL
1	25-A	169	ARG
1	25-A	196	TRP
1	25-A	206	LYS
1	25-A	210	GLU
1	25-A	225	SER
1	25-A	261	PRO
1	25-A	301	SER
1	25-A	303	PRO
1	25-A	340	GLN
1	25-A	346	ARG
1	25-A	348	ASN
1	25-A	368	LEU
1	25-A	369	LYS

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Mol	Chain	Res	Type
1	25-A	402	SER
1	25-A	419	ILE
1	25-A	439	ILE
1	25-A	440	ILE
1	25-A	457	GLU
1	25-A	488	GLN
1	25-A	509	ASP
1	25-A	518	ILE
1	25-A	529	SER
1	25-A	531	THR
1	25-A	538	MET
1	25-A	541	TYR
1	25-A	545	ASN
1	25-A	574	LEU
1	25-A	597	ILE
1	25-A	600	GLN
1	25-A	603	SER
1	25-B	56	GLN
1	25-B	64	LEU
1	25-B	69	LEU
1	25-B	70	VAL
1	25-B	81	LYS
1	25-B	102	MET
1	25-B	114	GLN
1	25-B	144	PHE
1	25-B	145	ASP
1	25-B	147	ASN
1	25-B	150	GLN
1	25-B	180	ARG
1	25-B	194	TYR
1	25-B	259	THR
1	25-B	272	ASP
1	25-B	283	LYS
1	25-B	294	ASN
1	25-B	297	PRO
1	25-B	304	LEU
1	25-B	310	VAL
1	25-B	311	LYS
1	25-B	318	THR
1	25-B	336	TYR
1	25-B	346	ARG
1	25-B	359	ILE

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Mol	Chain	Res	Type
1	25-B	369	LYS
1	25-B	399	ASP
1	25-B	452	GLU
1	25-B	488	GLN
1	25-B	519	LYS
1	25-B	529	SER
1	25-B	531	THR
1	25-B	553	GLN
1	25-B	574	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (591) 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	340	GLN
1	1-A	348	ASN
1	1-A	408	ASN
1	1-A	471	ASN
1	1-A	501	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	93	GLN
1	1-B	150	GLN
1	1-B	294	ASN
1	1-B	450	HIS
1	1-B	471	ASN
1	1-B	488	GLN
1	1-B	553	GLN
1	1-B	582	HIS
1	2-A	93	GLN
1	2-A	114	GLN
1	2-A	363	ASN
1	2-A	471	ASN
1	2-B	67	ASN
1	2-B	79	GLN

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Mol	Chain	Res	Type
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	501	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	348	ASN
1	3-A	389	ASN
1	3-A	493	ASN
1	3-A	501	ASN
1	3-A	553	GLN
1	3-A	600	GLN
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	348	ASN
1	3-B	434	ASN
1	3-B	450	HIS
1	3-B	501	ASN
1	3-B	545	ASN
1	4-A	67	ASN
1	4-A	158	ASN
1	4-A	286	ASN
1	4-A	306	GLN
1	4-A	434	ASN
1	4-A	493	ASN
1	4-A	553	GLN
1	4-A	579	GLN
1	4-B	79	GLN

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Mol	Chain	Res	Type
1	4-B	93	GLN
1	4-B	127	ASN
1	4-B	286	ASN
1	4-B	325	GLN
1	4-B	337	HIS
1	4-B	450	HIS
1	4-B	493	ASN
1	4-B	501	ASN
1	4-B	515	ASN
1	4-B	545	ASN
1	5-A	67	ASN
1	5-A	109	ASN
1	5-A	217	GLN
1	5-A	501	ASN
1	5-A	514	GLN
1	5-A	545	ASN
1	5-A	553	GLN
1	5-A	557	GLN
1	5-B	93	GLN
1	5-B	147	ASN
1	5-B	150	GLN
1	5-B	165	ASN
1	5-B	218	GLN
1	5-B	286	ASN
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	501	ASN
1	6-A	515	ASN
1	6-A	545	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	114	GLN
1	6-B	286	ASN
1	6-B	337	HIS

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Mol	Chain	Res	Type
1	6-B	436	ASN
1	6-B	450	HIS
1	6-B	501	ASN
1	6-B	514	GLN
1	6-B	515	ASN
1	6-B	557	GLN
1	7-A	89	GLN
1	7-A	114	GLN
1	7-A	147	ASN
1	7-A	306	GLN
1	7-A	337	HIS
1	7-A	340	GLN
1	7-A	557	GLN
1	7-B	93	GLN
1	7-B	112	ASN
1	7-B	127	ASN
1	7-B	182	HIS
1	7-B	217	GLN
1	7-B	306	GLN
1	7-B	434	ASN
1	7-B	436	ASN
1	7-B	450	HIS
1	7-B	471	ASN
1	7-B	514	GLN
1	7-B	515	ASN
1	7-B	557	GLN
1	8-A	89	GLN
1	8-A	147	ASN
1	8-A	165	ASN
1	8-A	217	GLN
1	8-A	294	ASN
1	8-A	348	ASN
1	8-A	450	HIS
1	8-A	514	GLN
1	8-A	582	HIS
1	8-B	92	ASN
1	8-B	93	GLN
1	8-B	114	GLN
1	8-B	150	GLN
1	8-B	182	HIS
1	8-B	218	GLN
1	8-B	340	GLN

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Mol	Chain	Res	Type
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	89	GLN
1	9-A	112	ASN
1	9-A	127	ASN
1	9-A	306	GLN
1	9-A	493	ASN
1	9-A	501	ASN
1	9-A	514	GLN
1	9-A	579	GLN
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	389	ASN
1	9-B	434	ASN
1	9-B	436	ASN
1	9-B	466	HIS
1	9-B	493	ASN
1	9-B	515	ASN
1	9-B	553	GLN
1	9-B	557	GLN
1	9-B	579	GLN
1	10-A	67	ASN
1	10-A	93	GLN
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	337	HIS
1	10-A	340	GLN
1	10-A	348	ASN
1	10-A	363	ASN
1	10-A	389	ASN
1	10-A	466	HIS

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Mol	Chain	Res	Type
1	10-A	471	ASN
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	150	GLN
1	10-B	182	HIS
1	10-B	217	GLN
1	10-B	286	ASN
1	10-B	325	GLN
1	10-B	337	HIS
1	10-B	434	ASN
1	10-B	436	ASN
1	10-B	450	HIS
1	10-B	466	HIS
1	10-B	501	ASN
1	10-B	545	ASN
1	11-A	112	ASN
1	11-A	114	GLN
1	11-A	147	ASN
1	11-A	188	ASN
1	11-A	325	GLN
1	11-A	337	HIS
1	11-A	340	GLN
1	11-A	348	ASN
1	11-A	363	ASN
1	11-A	408	ASN
1	11-A	450	HIS
1	11-A	493	ASN
1	11-B	92	ASN
1	11-B	93	GLN
1	11-B	112	ASN
1	11-B	162	ASN
1	11-B	165	ASN
1	11-B	182	HIS
1	11-B	218	GLN
1	11-B	286	ASN
1	11-B	337	HIS
1	11-B	436	ASN
1	11-B	450	HIS

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Mol	Chain	Res	Type
1	11-B	471	ASN
1	11-B	488	GLN
1	11-B	493	ASN
1	11-B	501	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	150	GLN
1	12-A	286	ASN
1	12-A	363	ASN
1	12-A	389	ASN
1	12-A	434	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	93	GLN
1	12-B	127	ASN
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	557	GLN
1	12-B	579	GLN
1	13-A	67	ASN
1	13-A	92	ASN
1	13-A	93	GLN
1	13-A	114	GLN
1	13-A	150	GLN
1	13-A	325	GLN
1	13-A	501	ASN
1	13-A	567	HIS
1	13-A	579	GLN
1	13-B	93	GLN
1	13-B	109	ASN
1	13-B	114	GLN

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Mol	Chain	Res	Type
1	13-B	134	ASN
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	340	GLN
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	109	ASN
1	14-A	112	ASN
1	14-A	134	ASN
1	14-A	162	ASN
1	14-A	348	ASN
1	14-A	408	ASN
1	14-A	450	HIS
1	14-A	471	ASN
1	14-A	493	ASN
1	14-A	553	GLN
1	14-A	579	GLN
1	14-A	600	GLN
1	14-B	67	ASN
1	14-B	158	ASN
1	14-B	182	HIS
1	14-B	217	GLN
1	14-B	218	GLN
1	14-B	294	ASN
1	14-B	337	HIS
1	14-B	434	ASN
1	14-B	450	HIS
1	14-B	501	ASN
1	14-B	545	ASN
1	14-B	557	GLN
1	15-A	92	ASN
1	15-A	93	GLN
1	15-A	114	GLN
1	15-A	127	ASN
1	15-A	294	ASN

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Mol	Chain	Res	Type
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	363	ASN
1	15-B	434	ASN
1	15-B	450	HIS
1	15-B	481	HIS
1	15-B	514	GLN
1	15-B	515	ASN
1	15-B	545	ASN
1	16-A	67	ASN
1	16-A	92	ASN
1	16-A	150	GLN
1	16-A	294	ASN
1	16-A	450	HIS
1	16-A	557	GLN
1	16-A	579	GLN
1	16-B	67	ASN
1	16-B	150	GLN
1	16-B	182	HIS
1	16-B	389	ASN
1	16-B	434	ASN
1	16-B	501	ASN
1	16-B	515	ASN
1	16-B	545	ASN
1	16-B	579	GLN
1	16-B	600	GLN
1	17-A	67	ASN
1	17-A	89	GLN
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	514	GLN
1	17-A	545	ASN
1	17-A	554	HIS

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Mol	Chain	Res	Type
1	17-A	600	GLN
1	17-B	56	GLN
1	17-B	93	GLN
1	17-B	150	GLN
1	17-B	182	HIS
1	17-B	217	GLN
1	17-B	306	GLN
1	17-B	337	HIS
1	17-B	340	GLN
1	17-B	348	ASN
1	17-B	450	HIS
1	17-B	501	ASN
1	17-B	545	ASN
1	17-B	579	GLN
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	501	ASN
1	18-A	579	GLN
1	18-A	600	GLN
1	18-B	114	GLN
1	18-B	182	HIS
1	18-B	286	ASN
1	18-B	306	GLN
1	18-B	348	ASN
1	18-B	450	HIS
1	18-B	493	ASN
1	18-B	501	ASN
1	18-B	545	ASN
1	18-B	554	HIS
1	18-B	557	GLN
1	18-B	579	GLN
1	19-A	89	GLN
1	19-A	93	GLN
1	19-A	150	GLN
1	19-A	306	GLN
1	19-A	450	HIS

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Mol	Chain	Res	Type
1	19-A	466	HIS
1	19-A	471	ASN
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	150	GLN
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	488	GLN
1	19-B	557	GLN
1	19-B	579	GLN
1	20-A	93	GLN
1	20-A	217	GLN
1	20-A	218	GLN
1	20-A	231	ASN
1	20-A	294	ASN
1	20-A	306	GLN
1	20-A	434	ASN
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	582	HIS
1	20-B	67	ASN
1	20-B	79	GLN
1	20-B	92	ASN
1	20-B	93	GLN
1	20-B	114	GLN
1	20-B	127	ASN
1	20-B	147	ASN
1	20-B	165	ASN
1	20-B	182	HIS
1	20-B	306	GLN
1	20-B	434	ASN
1	20-B	450	HIS

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Mol	Chain	Res	Type
1	20-B	466	HIS
1	20-B	471	ASN
1	20-B	488	GLN
1	20-B	493	ASN
1	20-B	514	GLN
1	21-A	93	GLN
1	21-A	147	ASN
1	21-A	165	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-A	579	GLN
1	21-A	582	HIS
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	501	ASN
1	21-B	515	ASN
1	21-B	553	GLN
1	22-A	93	GLN
1	22-A	109	ASN
1	22-A	127	ASN
1	22-A	150	GLN
1	22-A	165	ASN
1	22-A	217	GLN
1	22-A	286	ASN
1	22-A	294	ASN
1	22-A	389	ASN

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Mol	Chain	Res	Type
1	22-A	434	ASN
1	22-A	450	HIS
1	22-A	466	HIS
1	22-A	493	ASN
1	22-A	501	ASN
1	22-A	514	GLN
1	22-A	553	GLN
1	22-A	567	HIS
1	22-B	92	ASN
1	22-B	127	ASN
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	493	ASN
1	22-B	514	GLN
1	22-B	545	ASN
1	22-B	582	HIS
1	22-B	600	GLN
1	23-A	67	ASN
1	23-A	93	GLN
1	23-A	112	ASN
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	413	GLN
1	23-A	450	HIS
1	23-A	501	ASN
1	23-A	579	GLN
1	23-A	600	GLN
1	23-B	92	ASN
1	23-B	93	GLN
1	23-B	114	GLN
1	23-B	150	GLN
1	23-B	182	HIS
1	23-B	286	ASN
1	23-B	306	GLN

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Mol	Chain	Res	Type
1	23-B	348	ASN
1	23-B	450	HIS
1	23-B	471	ASN
1	23-B	501	ASN
1	23-B	515	ASN
1	23-B	557	GLN
1	23-B	579	GLN
1	23-B	600	GLN
1	24-A	114	GLN
1	24-A	127	ASN
1	24-A	188	ASN
1	24-A	217	GLN
1	24-A	231	ASN
1	24-A	325	GLN
1	24-A	337	HIS
1	24-A	348	ASN
1	24-A	389	ASN
1	24-A	450	HIS
1	24-A	471	ASN
1	24-A	488	GLN
1	24-A	493	ASN
1	24-B	56	GLN
1	24-B	79	GLN
1	24-B	92	ASN
1	24-B	93	GLN
1	24-B	127	ASN
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	24-B	554	HIS
1	24-B	579	GLN
1	25-A	79	GLN
1	25-A	93	GLN
1	25-A	112	ASN
1	25-A	127	ASN
1	25-A	286	ASN
1	25-A	294	ASN

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Mol	Chain	Res	Type
1	25-A	306	GLN
1	25-A	325	GLN
1	25-A	389	ASN
1	25-A	434	ASN
1	25-A	450	HIS
1	25-A	501	ASN
1	25-A	515	ASN
1	25-A	557	GLN
1	25-B	92	ASN
1	25-B	93	GLN
1	25-B	165	ASN
1	25-B	182	HIS
1	25-B	471	ASN
1	25-B	501	ASN
1	25-B	557	GLN
1	25-B	600	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

150 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	1-B	704	-	3,3,3	0.86	0	2,2,2	0.44	0
2	EDO	3-A	702	-	3,3,3	0.59	0	2,2,2	0.34	0
2	EDO	11-B	704	-	3,3,3	0.46	0	2,2,2	0.73	0
2	EDO	25-B	704	-	3,3,3	0.37	0	2,2,2	0.21	0
2	EDO	21-B	702	-	3,3,3	0.38	0	2,2,2	0.52	0
3	BGC	19-B	701	-	12,12,12	0.83	0	17,17,17	1.87	4 (23%)
2	EDO	6-B	704	-	3,3,3	0.49	0	2,2,2	0.48	0
2	EDO	7-B	704	-	3,3,3	0.51	0	2,2,2	0.44	0
3	BGC	5-B	701	-	12,12,12	0.79	0	17,17,17	2.16	6 (35%)
2	EDO	6-A	702	-	3,3,3	0.62	0	2,2,2	0.44	0
2	EDO	25-B	702	-	3,3,3	0.38	0	2,2,2	0.37	0
2	EDO	18-B	703	-	3,3,3	0.42	0	2,2,2	0.24	0
2	EDO	15-B	702	-	3,3,3	0.38	0	2,2,2	0.40	0
2	EDO	24-B	703	-	3,3,3	0.40	0	2,2,2	0.32	0
2	EDO	16-B	703	-	3,3,3	0.39	0	2,2,2	0.34	0
3	BGC	22-B	701	-	12,12,12	0.76	0	17,17,17	2.10	4 (23%)
2	EDO	17-A	702	-	3,3,3	0.61	0	2,2,2	0.44	0
2	EDO	18-B	704	-	3,3,3	0.51	0	2,2,2	0.17	0
2	EDO	2-B	703	-	3,3,3	0.42	0	2,2,2	0.24	0
2	EDO	7-B	703	-	3,3,3	0.38	0	2,2,2	0.33	0
2	EDO	12-B	704	-	3,3,3	0.46	0	2,2,2	0.46	0
2	EDO	15-B	703	-	3,3,3	0.44	0	2,2,2	0.25	0
2	EDO	19-A	701	-	3,3,3	0.50	0	2,2,2	0.25	0
2	EDO	6-B	702	-	3,3,3	0.26	0	2,2,2	0.56	0
3	BGC	15-B	701	-	12,12,12	0.87	0	17,17,17	2.15	4 (23%)
2	EDO	24-B	702	-	3,3,3	0.31	0	2,2,2	0.45	0
2	EDO	15-A	701	-	3,3,3	0.53	0	2,2,2	0.34	0
2	EDO	5-A	701	-	3,3,3	0.50	0	2,2,2	0.43	0
2	EDO	23-A	702	-	3,3,3	0.54	0	2,2,2	0.52	0
2	EDO	3-B	702	-	3,3,3	0.27	0	2,2,2	0.37	0
2	EDO	12-A	702	-	3,3,3	0.60	0	2,2,2	0.48	0
2	EDO	4-B	702	-	3,3,3	0.43	0	2,2,2	0.49	0
2	EDO	22-A	701	-	3,3,3	0.49	0	2,2,2	0.39	0
2	EDO	20-B	704	-	3,3,3	0.47	0	2,2,2	0.72	0
2	EDO	11-A	701	-	3,3,3	0.48	0	2,2,2	0.21	0
2	EDO	14-A	701	-	3,3,3	0.45	0	2,2,2	0.36	0
2	EDO	2-B	702	-	3,3,3	0.38	0	2,2,2	0.15	0
2	EDO	11-B	702	-	3,3,3	0.35	0	2,2,2	0.32	0
2	EDO	12-A	701	-	3,3,3	0.46	0	2,2,2	0.29	0
2	EDO	10-B	704	-	3,3,3	0.49	0	2,2,2	0.54	0
2	EDO	19-B	703	-	3,3,3	0.46	0	2,2,2	0.44	0
3	BGC	3-B	701	-	12,12,12	1.07	1 (8%)	17,17,17	1.95	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	16-A	702	-	3,3,3	0.65	0	2,2,2	0.47	0
2	EDO	10-A	701	-	3,3,3	0.44	0	2,2,2	0.25	0
2	EDO	13-B	703	-	3,3,3	0.42	0	2,2,2	0.36	0
2	EDO	16-B	702	-	3,3,3	0.44	0	2,2,2	0.38	0
3	BGC	1-B	701	-	12,12,12	0.85	0	17,17,17	2.00	7 (41%)
3	BGC	25-B	701	-	12,12,12	0.91	0	17,17,17	2.23	7 (41%)
2	EDO	9-B	702	-	3,3,3	0.36	0	2,2,2	0.16	0
2	EDO	6-A	701	-	3,3,3	0.54	0	2,2,2	0.46	0
2	EDO	18-A	702	-	3,3,3	0.56	0	2,2,2	0.44	0
2	EDO	24-B	704	-	3,3,3	0.49	0	2,2,2	1.14	0
2	EDO	14-B	702	-	3,3,3	0.45	0	2,2,2	0.29	0
2	EDO	17-A	701	-	3,3,3	0.42	0	2,2,2	0.38	0
2	EDO	2-A	702	-	3,3,3	0.59	0	2,2,2	0.48	0
2	EDO	17-B	702	-	3,3,3	0.40	0	2,2,2	0.54	0
2	EDO	9-A	701	-	3,3,3	0.46	0	2,2,2	0.31	0
3	BGC	21-B	701	-	12,12,12	0.82	0	17,17,17	2.55	11 (64%)
2	EDO	1-A	702	-	3,3,3	0.53	0	2,2,2	0.55	0
2	EDO	6-B	703	-	3,3,3	0.46	0	2,2,2	0.29	0
2	EDO	19-B	702	-	3,3,3	0.43	0	2,2,2	0.55	0
2	EDO	10-B	703	-	3,3,3	0.42	0	2,2,2	0.33	0
2	EDO	15-A	702	-	3,3,3	0.58	0	2,2,2	0.50	0
2	EDO	23-B	703	-	3,3,3	0.40	0	2,2,2	0.33	0
3	BGC	6-B	701	-	12,12,12	0.92	0	17,17,17	1.90	4 (23%)
3	BGC	24-B	701	-	12,12,12	0.72	0	17,17,17	1.74	4 (23%)
2	EDO	4-B	703	-	3,3,3	0.38	0	2,2,2	0.40	0
2	EDO	21-B	703	-	3,3,3	0.42	0	2,2,2	0.20	0
2	EDO	18-A	701	-	3,3,3	0.42	0	2,2,2	0.20	0
3	BGC	10-B	701	-	12,12,12	0.70	0	17,17,17	2.03	4 (23%)
2	EDO	20-B	702	-	3,3,3	0.45	0	2,2,2	0.70	0
2	EDO	7-B	702	-	3,3,3	0.31	0	2,2,2	0.51	0
3	BGC	14-B	701	-	12,12,12	1.12	1 (8%)	17,17,17	2.22	8 (47%)
3	BGC	12-B	701	-	12,12,12	0.76	0	17,17,17	1.92	4 (23%)
2	EDO	14-B	704	-	3,3,3	0.43	0	2,2,2	0.21	0
2	EDO	23-A	701	-	3,3,3	0.49	0	2,2,2	0.42	0
2	EDO	1-B	702	-	3,3,3	0.32	0	2,2,2	0.16	0
3	BGC	9-B	701	-	12,12,12	0.57	0	17,17,17	3.08	9 (52%)
2	EDO	5-B	703	-	3,3,3	0.42	0	2,2,2	0.44	0
2	EDO	8-B	703	-	3,3,3	0.36	0	2,2,2	0.47	0
2	EDO	12-B	702	-	3,3,3	0.31	0	2,2,2	0.11	0
3	BGC	17-B	701	-	12,12,12	1.31	1 (8%)	17,17,17	2.77	9 (52%)
2	EDO	24-A	702	-	3,3,3	0.57	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	4-B	704	-	3,3,3	0.40	0	2,2,2	0.79	0
2	EDO	11-B	703	-	3,3,3	0.44	0	2,2,2	0.21	0
2	EDO	21-B	704	-	3,3,3	0.38	0	2,2,2	0.29	0
2	EDO	20-B	703	-	3,3,3	0.40	0	2,2,2	0.37	0
2	EDO	16-A	701	-	3,3,3	0.47	0	2,2,2	0.52	0
2	EDO	8-A	702	-	3,3,3	0.60	0	2,2,2	0.40	0
2	EDO	13-A	701	-	3,3,3	0.45	0	2,2,2	0.31	0
2	EDO	7-A	701	-	3,3,3	0.45	0	2,2,2	0.24	0
2	EDO	25-A	701	-	3,3,3	0.56	0	2,2,2	0.27	0
2	EDO	9-B	703	-	3,3,3	0.38	0	2,2,2	0.25	0
2	EDO	19-A	702	-	3,3,3	0.60	0	2,2,2	0.58	0
2	EDO	20-A	701	-	3,3,3	0.45	0	2,2,2	0.38	0
2	EDO	15-B	704	-	3,3,3	0.24	0	2,2,2	0.92	0
2	EDO	21-A	702	-	3,3,3	0.58	0	2,2,2	0.55	0
2	EDO	2-A	701	-	3,3,3	0.41	0	2,2,2	0.30	0
3	BGC	16-B	701	-	12,12,12	0.84	0	17,17,17	1.68	4 (23%)
2	EDO	9-B	704	-	3,3,3	0.46	0	2,2,2	0.75	0
2	EDO	17-B	703	-	3,3,3	0.50	0	2,2,2	0.23	0
2	EDO	4-A	701	-	3,3,3	0.47	0	2,2,2	0.34	0
2	EDO	18-B	702	-	3,3,3	0.42	0	2,2,2	0.41	0
2	EDO	3-A	701	-	3,3,3	0.48	0	2,2,2	0.35	0
2	EDO	23-B	704	-	3,3,3	0.54	0	2,2,2	0.04	0
3	BGC	7-B	701	-	12,12,12	0.98	0	17,17,17	1.50	4 (23%)
2	EDO	5-B	704	-	3,3,3	0.58	0	2,2,2	0.40	0
2	EDO	22-B	703	-	3,3,3	0.43	0	2,2,2	0.35	0
2	EDO	13-B	704	-	3,3,3	0.46	0	2,2,2	0.28	0
2	EDO	17-B	704	-	3,3,3	0.59	0	2,2,2	0.79	0
3	BGC	23-B	701	-	12,12,12	0.68	0	17,17,17	1.94	5 (29%)
2	EDO	21-A	701	-	3,3,3	0.48	0	2,2,2	0.33	0
2	EDO	1-A	701	-	3,3,3	0.62	0	2,2,2	0.33	0
2	EDO	2-B	704	-	3,3,3	0.94	0	2,2,2	0.72	0
2	EDO	22-B	704	-	3,3,3	0.42	0	2,2,2	0.88	0
2	EDO	8-B	702	-	3,3,3	0.36	0	2,2,2	0.25	0
2	EDO	10-A	702	-	3,3,3	0.62	0	2,2,2	0.39	0
2	EDO	5-A	702	-	3,3,3	0.64	0	2,2,2	0.38	0
2	EDO	24-A	701	-	3,3,3	0.50	0	2,2,2	0.34	0
3	BGC	4-B	701	-	12,12,12	1.00	0	17,17,17	1.41	3 (17%)
3	BGC	8-B	701	-	12,12,12	0.79	0	17,17,17	1.70	5 (29%)
2	EDO	22-B	702	-	3,3,3	0.41	0	2,2,2	0.25	0
2	EDO	22-A	702	-	3,3,3	0.66	0	2,2,2	0.46	0
2	EDO	3-B	703	-	3,3,3	0.43	0	2,2,2	0.28	0
2	EDO	13-A	702	-	3,3,3	0.59	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	23-B	702	-	3,3,3	0.49	0	2,2,2	0.06	0
2	EDO	5-B	702	-	3,3,3	0.31	0	2,2,2	0.34	0
3	BGC	11-B	701	-	12,12,12	0.93	0	17,17,17	2.32	4 (23%)
2	EDO	19-B	704	-	3,3,3	0.46	0	2,2,2	1.59	0
2	EDO	16-B	704	-	3,3,3	0.56	0	2,2,2	0.23	0
2	EDO	9-A	702	-	3,3,3	0.59	0	2,2,2	0.47	0
2	EDO	13-B	702	-	3,3,3	0.45	0	2,2,2	0.57	0
3	BGC	18-B	701	-	12,12,12	0.66	0	17,17,17	2.28	9 (52%)
2	EDO	10-B	702	-	3,3,3	0.36	0	2,2,2	0.38	0
2	EDO	4-A	702	-	3,3,3	0.64	0	2,2,2	0.36	0
3	BGC	2-B	701	-	12,12,12	1.01	0	17,17,17	2.27	8 (47%)
2	EDO	1-B	703	-	3,3,3	0.41	0	2,2,2	0.32	0
2	EDO	25-A	702	-	3,3,3	0.61	0	2,2,2	0.39	0
2	EDO	25-B	703	-	3,3,3	0.43	0	2,2,2	0.41	0
3	BGC	13-B	701	-	12,12,12	1.08	2 (16%)	17,17,17	1.30	3 (17%)
2	EDO	11-A	702	-	3,3,3	0.65	0	2,2,2	0.47	0
2	EDO	14-B	703	-	3,3,3	0.41	0	2,2,2	0.35	0
2	EDO	8-B	704	-	3,3,3	0.59	0	2,2,2	0.16	0
2	EDO	3-B	704	-	3,3,3	0.51	0	2,2,2	0.61	0
2	EDO	7-A	702	-	3,3,3	0.58	0	2,2,2	0.49	0
2	EDO	20-A	702	-	3,3,3	0.61	0	2,2,2	0.47	0
3	BGC	20-B	701	-	12,12,12	1.07	0	17,17,17	2.26	5 (29%)
2	EDO	8-A	701	-	3,3,3	0.59	0	2,2,2	0.29	0
2	EDO	14-A	702	-	3,3,3	0.56	0	2,2,2	0.39	0
2	EDO	12-B	703	-	3,3,3	0.41	0	2,2,2	0.22	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-B	704	-	-	1/1/1/1	-
2	EDO	3-A	702	-	-	0/1/1/1	-
2	EDO	11-B	704	-	-	1/1/1/1	-
2	EDO	25-B	704	-	-	1/1/1/1	-
2	EDO	21-B	702	-	-	0/1/1/1	-
3	BGC	19-B	701	-	-	0/2/22/22	0/1/1/1
2	EDO	6-B	704	-	-	0/1/1/1	-
2	EDO	7-B	704	-	-	0/1/1/1	-
3	BGC	5-B	701	-	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	6-A	702	-	-	0/1/1/1	-
2	EDO	25-B	702	-	-	0/1/1/1	-
2	EDO	18-B	703	-	-	1/1/1/1	-
2	EDO	15-B	702	-	-	0/1/1/1	-
2	EDO	24-B	703	-	-	0/1/1/1	-
2	EDO	16-B	703	-	-	0/1/1/1	-
3	BGC	22-B	701	-	-	0/2/22/22	0/1/1/1
2	EDO	17-A	702	-	-	0/1/1/1	-
2	EDO	18-B	704	-	-	1/1/1/1	-
2	EDO	2-B	703	-	-	0/1/1/1	-
2	EDO	7-B	703	-	-	0/1/1/1	-
2	EDO	12-B	704	-	-	1/1/1/1	-
2	EDO	15-B	703	-	-	0/1/1/1	-
2	EDO	19-A	701	-	-	1/1/1/1	-
2	EDO	6-B	702	-	-	0/1/1/1	-
3	BGC	15-B	701	-	-	0/2/22/22	0/1/1/1
2	EDO	24-B	702	-	-	0/1/1/1	-
2	EDO	15-A	701	-	-	0/1/1/1	-
2	EDO	5-A	701	-	-	0/1/1/1	-
2	EDO	23-A	702	-	-	0/1/1/1	-
2	EDO	3-B	702	-	-	0/1/1/1	-
2	EDO	12-A	702	-	-	0/1/1/1	-
2	EDO	4-B	702	-	-	0/1/1/1	-
2	EDO	22-A	701	-	-	0/1/1/1	-
2	EDO	20-B	704	-	-	1/1/1/1	-
2	EDO	11-A	701	-	-	1/1/1/1	-
2	EDO	14-A	701	-	-	0/1/1/1	-
2	EDO	2-B	702	-	-	0/1/1/1	-
2	EDO	11-B	702	-	-	0/1/1/1	-
2	EDO	12-A	701	-	-	0/1/1/1	-
2	EDO	10-B	704	-	-	0/1/1/1	-
2	EDO	19-B	703	-	-	0/1/1/1	-
3	BGC	3-B	701	-	-	2/2/22/22	0/1/1/1
2	EDO	16-A	702	-	-	0/1/1/1	-
2	EDO	10-A	701	-	-	0/1/1/1	-
2	EDO	13-B	703	-	-	0/1/1/1	-
2	EDO	16-B	702	-	-	0/1/1/1	-
3	BGC	1-B	701	-	-	2/2/22/22	0/1/1/1
3	BGC	25-B	701	-	-	0/2/22/22	0/1/1/1
2	EDO	9-B	702	-	-	0/1/1/1	-
2	EDO	6-A	701	-	-	1/1/1/1	-
2	EDO	18-A	702	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	24-B	704	-	-	1/1/1/1	-
2	EDO	14-B	702	-	-	0/1/1/1	-
2	EDO	17-A	701	-	-	1/1/1/1	-
2	EDO	2-A	702	-	-	0/1/1/1	-
2	EDO	17-B	702	-	-	0/1/1/1	-
2	EDO	9-A	701	-	-	1/1/1/1	-
3	BGC	21-B	701	-	-	2/2/22/22	0/1/1/1
2	EDO	1-A	702	-	-	0/1/1/1	-
2	EDO	6-B	703	-	-	0/1/1/1	-
2	EDO	19-B	702	-	-	0/1/1/1	-
2	EDO	10-B	703	-	-	0/1/1/1	-
2	EDO	15-A	702	-	-	0/1/1/1	-
2	EDO	23-B	703	-	-	0/1/1/1	-
3	BGC	6-B	701	-	-	2/2/22/22	0/1/1/1
3	BGC	24-B	701	-	-	1/2/22/22	0/1/1/1
2	EDO	4-B	703	-	-	0/1/1/1	-
2	EDO	21-B	703	-	-	0/1/1/1	-
2	EDO	18-A	701	-	-	1/1/1/1	-
3	BGC	10-B	701	-	-	1/2/22/22	0/1/1/1
2	EDO	20-B	702	-	-	0/1/1/1	-
2	EDO	7-B	702	-	-	0/1/1/1	-
3	BGC	14-B	701	-	-	0/2/22/22	0/1/1/1
3	BGC	12-B	701	-	-	0/2/22/22	0/1/1/1
2	EDO	14-B	704	-	-	1/1/1/1	-
2	EDO	23-A	701	-	-	0/1/1/1	-
2	EDO	1-B	702	-	-	0/1/1/1	-
3	BGC	9-B	701	-	-	2/2/22/22	0/1/1/1
2	EDO	5-B	703	-	-	0/1/1/1	-
2	EDO	8-B	703	-	-	0/1/1/1	-
2	EDO	12-B	702	-	-	1/1/1/1	-
3	BGC	17-B	701	-	-	1/2/22/22	0/1/1/1
2	EDO	24-A	702	-	-	0/1/1/1	-
2	EDO	4-B	704	-	-	0/1/1/1	-
2	EDO	11-B	703	-	-	0/1/1/1	-
2	EDO	21-B	704	-	-	0/1/1/1	-
2	EDO	20-B	703	-	-	0/1/1/1	-
2	EDO	16-A	701	-	-	0/1/1/1	-
2	EDO	8-A	702	-	-	0/1/1/1	-
2	EDO	13-A	701	-	-	0/1/1/1	-
2	EDO	7-A	701	-	-	0/1/1/1	-
2	EDO	25-A	701	-	-	1/1/1/1	-
2	EDO	9-B	703	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	19-A	702	-	-	0/1/1/1	-
2	EDO	20-A	701	-	-	0/1/1/1	-
2	EDO	15-B	704	-	-	0/1/1/1	-
2	EDO	21-A	702	-	-	0/1/1/1	-
2	EDO	2-A	701	-	-	1/1/1/1	-
3	BGC	16-B	701	-	-	0/2/22/22	0/1/1/1
2	EDO	9-B	704	-	-	1/1/1/1	-
2	EDO	17-B	703	-	-	0/1/1/1	-
2	EDO	4-A	701	-	-	0/1/1/1	-
2	EDO	18-B	702	-	-	0/1/1/1	-
2	EDO	3-A	701	-	-	0/1/1/1	-
2	EDO	23-B	704	-	-	1/1/1/1	-
3	BGC	7-B	701	-	-	2/2/22/22	0/1/1/1
2	EDO	5-B	704	-	-	0/1/1/1	-
2	EDO	22-B	703	-	-	0/1/1/1	-
2	EDO	13-B	704	-	-	0/1/1/1	-
2	EDO	17-B	704	-	-	1/1/1/1	-
3	BGC	23-B	701	-	-	2/2/22/22	0/1/1/1
2	EDO	21-A	701	-	-	0/1/1/1	-
2	EDO	1-A	701	-	-	1/1/1/1	-
2	EDO	2-B	704	-	-	0/1/1/1	-
2	EDO	22-B	704	-	-	1/1/1/1	-
2	EDO	8-B	702	-	-	1/1/1/1	-
2	EDO	10-A	702	-	-	0/1/1/1	-
2	EDO	5-A	702	-	-	0/1/1/1	-
2	EDO	24-A	701	-	-	1/1/1/1	-
3	BGC	4-B	701	-	-	2/2/22/22	0/1/1/1
3	BGC	8-B	701	-	-	0/2/22/22	0/1/1/1
2	EDO	22-B	702	-	-	0/1/1/1	-
2	EDO	22-A	702	-	-	0/1/1/1	-
2	EDO	3-B	703	-	-	0/1/1/1	-
2	EDO	13-A	702	-	-	0/1/1/1	-
2	EDO	23-B	702	-	-	0/1/1/1	-
2	EDO	5-B	702	-	-	0/1/1/1	-
3	BGC	11-B	701	-	-	1/2/22/22	0/1/1/1
2	EDO	19-B	704	-	-	1/1/1/1	-
2	EDO	16-B	704	-	-	1/1/1/1	-
2	EDO	9-A	702	-	-	0/1/1/1	-
2	EDO	13-B	702	-	-	0/1/1/1	-
3	BGC	18-B	701	-	-	2/2/22/22	0/1/1/1
2	EDO	10-B	702	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	4-A	702	-	-	0/1/1/1	-
3	BGC	2-B	701	-	-	0/2/22/22	0/1/1/1
2	EDO	1-B	703	-	-	0/1/1/1	-
2	EDO	25-A	702	-	-	0/1/1/1	-
2	EDO	25-B	703	-	-	0/1/1/1	-
3	BGC	13-B	701	-	-	0/2/22/22	0/1/1/1
2	EDO	11-A	702	-	-	0/1/1/1	-
2	EDO	14-B	703	-	-	0/1/1/1	-
2	EDO	8-B	704	-	-	1/1/1/1	-
2	EDO	3-B	704	-	-	1/1/1/1	-
2	EDO	7-A	702	-	-	0/1/1/1	-
2	EDO	20-A	702	-	-	0/1/1/1	-
3	BGC	20-B	701	-	-	2/2/22/22	0/1/1/1
2	EDO	8-A	701	-	-	1/1/1/1	-
2	EDO	14-A	702	-	-	0/1/1/1	-
2	EDO	12-B	703	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-B	701	BGC	O3-C3	-2.97	1.35	1.43
3	14-B	701	BGC	C1-C2	2.79	1.58	1.52
3	13-B	701	BGC	C1-C2	2.53	1.58	1.52
3	13-B	701	BGC	C4-C3	2.08	1.57	1.52
3	17-B	701	BGC	C4-C5	2.06	1.57	1.53

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-B	701	BGC	O4-C4-C3	-8.07	91.36	110.38
3	20-B	701	BGC	C3-C4-C5	6.02	121.14	110.23
3	9-B	701	BGC	C1-O5-C5	-5.45	103.10	113.65
3	17-B	701	BGC	C4-C3-C2	-5.29	101.54	110.83
3	22-B	701	BGC	O5-C1-C2	5.07	119.22	110.30
3	17-B	701	BGC	C3-C4-C5	5.05	119.40	110.23
3	21-B	701	BGC	C4-C3-C2	-5.00	102.05	110.83
3	11-B	701	BGC	O3-C3-C2	4.96	122.08	110.38
3	11-B	701	BGC	O5-C5-C6	4.92	118.64	106.44
3	15-B	701	BGC	O3-C3-C2	4.81	121.71	110.38
3	24-B	701	BGC	C4-C3-C2	-4.67	102.64	110.83
3	25-B	701	BGC	C4-C3-C2	-4.66	102.64	110.83
3	5-B	701	BGC	C3-C4-C5	4.39	118.19	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	15-B	701	BGC	O2-C2-C3	4.33	120.59	110.38
3	12-B	701	BGC	O2-C2-C3	4.32	120.57	110.38
3	6-B	701	BGC	C3-C4-C5	4.25	117.94	110.23
3	1-B	701	BGC	C3-C4-C5	4.21	117.87	110.23
3	10-B	701	BGC	O5-C1-C2	4.18	117.64	110.30
3	2-B	701	BGC	C4-C3-C2	-4.11	103.61	110.83
3	9-B	701	BGC	O3-C3-C2	4.08	120.00	110.38
3	5-B	701	BGC	C1-O5-C5	4.05	121.49	113.65
3	18-B	701	BGC	O3-C3-C2	-4.04	100.85	110.38
3	23-B	701	BGC	C4-C3-C2	-4.01	103.78	110.83
3	3-B	701	BGC	O4-C4-C5	3.99	119.15	109.32
3	8-B	701	BGC	C1-C2-C3	-3.92	102.36	110.36
3	3-B	701	BGC	C4-C3-C2	-3.90	103.98	110.83
3	9-B	701	BGC	C1-C2-C3	3.89	118.29	110.36
3	20-B	701	BGC	O4-C4-C3	3.86	119.47	110.38
3	14-B	701	BGC	O5-C5-C6	3.84	115.95	106.44
3	11-B	701	BGC	C1-C2-C3	-3.81	102.58	110.36
3	18-B	701	BGC	O5-C5-C4	-3.80	102.85	109.70
3	18-B	701	BGC	C3-C4-C5	3.76	117.05	110.23
3	21-B	701	BGC	O5-C1-C2	3.69	116.78	110.30
3	19-B	701	BGC	C3-C4-C5	3.66	116.87	110.23
3	22-B	701	BGC	C1-O5-C5	3.63	120.67	113.65
3	14-B	701	BGC	C1-C2-C3	3.59	117.68	110.36
3	12-B	701	BGC	C4-C3-C2	-3.56	104.59	110.83
3	2-B	701	BGC	O3-C3-C4	-3.55	102.01	110.38
3	25-B	701	BGC	C1-C2-C3	3.54	117.58	110.36
3	10-B	701	BGC	C3-C4-C5	3.53	116.63	110.23
3	25-B	701	BGC	O5-C1-C2	3.52	116.50	110.30
3	19-B	701	BGC	C4-C3-C2	-3.52	104.66	110.83
3	23-B	701	BGC	O2-C2-C3	3.46	118.54	110.38
3	5-B	701	BGC	O3-C3-C4	-3.42	102.31	110.38
3	21-B	701	BGC	O3-C3-C4	-3.41	102.34	110.38
3	6-B	701	BGC	O3-C3-C4	-3.38	102.41	110.38
3	20-B	701	BGC	O4-C4-C5	-3.35	101.08	109.32
3	21-B	701	BGC	C1-C2-C3	3.33	117.15	110.36
3	21-B	701	BGC	C6-C5-C4	-3.31	104.90	113.02
3	2-B	701	BGC	O2-C2-C1	3.30	116.87	109.25
3	17-B	701	BGC	O5-C1-C2	3.29	116.08	110.30
3	16-B	701	BGC	C4-C3-C2	-3.22	105.18	110.83
3	14-B	701	BGC	C4-C3-C2	-3.16	105.28	110.83
3	5-B	701	BGC	C4-C3-C2	-3.15	105.29	110.83
3	14-B	701	BGC	C3-C4-C5	3.14	115.93	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-B	701	BGC	C4-C3-C2	-3.13	105.33	110.83
3	17-B	701	BGC	C1-O5-C5	3.13	119.70	113.65
3	14-B	701	BGC	C6-C5-C4	-3.07	105.49	113.02
3	11-B	701	BGC	O2-C2-C3	3.07	117.60	110.38
3	2-B	701	BGC	C1-O5-C5	3.06	119.56	113.65
3	17-B	701	BGC	O5-C5-C4	3.01	115.13	109.70
3	7-B	701	BGC	O5-C5-C6	3.01	113.89	106.44
3	19-B	701	BGC	O2-C2-C3	2.99	117.43	110.38
3	16-B	701	BGC	O2-C2-C3	2.97	117.39	110.38
3	22-B	701	BGC	C1-C2-C3	2.97	116.42	110.36
3	17-B	701	BGC	C1-C2-C3	2.96	116.39	110.36
3	13-B	701	BGC	O5-C5-C6	2.95	113.74	106.44
3	3-B	701	BGC	O4-C4-C3	2.92	117.27	110.38
3	12-B	701	BGC	C3-C4-C5	2.90	115.50	110.23
3	10-B	701	BGC	C4-C3-C2	-2.82	105.88	110.83
3	23-B	701	BGC	C1-C2-C3	-2.81	104.63	110.36
3	16-B	701	BGC	C3-C4-C5	2.80	115.30	110.23
3	18-B	701	BGC	O3-C3-C4	-2.79	103.80	110.38
3	21-B	701	BGC	C3-C4-C5	2.79	115.29	110.23
3	17-B	701	BGC	C6-C5-C4	-2.76	106.24	113.02
3	13-B	701	BGC	O1-C1-C2	2.75	116.96	108.98
3	1-B	701	BGC	C1-C2-C3	2.75	115.96	110.36
3	15-B	701	BGC	C1-C2-C3	-2.75	104.75	110.36
3	2-B	701	BGC	C1-C2-C3	-2.70	104.84	110.36
3	17-B	701	BGC	O2-C2-C3	2.69	116.71	110.38
3	1-B	701	BGC	O4-C4-C3	2.68	116.69	110.38
3	20-B	701	BGC	O5-C5-C6	2.66	113.03	106.44
3	17-B	701	BGC	O6-C6-C5	2.66	120.38	111.33
3	25-B	701	BGC	O1-C1-O5	-2.64	102.56	110.41
3	9-B	701	BGC	O5-C5-C6	2.64	112.98	106.44
3	18-B	701	BGC	O2-C2-C3	2.62	116.56	110.38
3	15-B	701	BGC	O5-C1-C2	-2.60	105.73	110.30
3	20-B	701	BGC	C1-O5-C5	-2.59	108.64	113.65
3	18-B	701	BGC	O5-C5-C6	2.59	112.85	106.44
3	24-B	701	BGC	O2-C2-C3	2.50	116.28	110.38
3	8-B	701	BGC	O2-C2-C1	2.50	115.02	109.25
3	24-B	701	BGC	O2-C2-C1	2.49	114.99	109.25
3	1-B	701	BGC	O3-C3-C4	-2.48	104.53	110.38
3	4-B	701	BGC	C4-C3-C2	-2.46	106.51	110.83
3	7-B	701	BGC	O4-C4-C5	2.45	115.35	109.32
3	22-B	701	BGC	O5-C5-C6	2.44	112.49	106.44
3	23-B	701	BGC	O3-C3-C2	2.44	116.12	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	10-B	701	BGC	C1-O5-C5	2.43	118.36	113.65
3	19-B	701	BGC	O3-C3-C4	-2.42	104.68	110.38
3	23-B	701	BGC	O4-C4-C5	2.38	115.20	109.32
3	1-B	701	BGC	C4-C3-C2	-2.38	106.64	110.83
3	25-B	701	BGC	C1-O5-C5	2.38	118.26	113.65
3	8-B	701	BGC	O5-C5-C6	2.38	112.34	106.44
3	5-B	701	BGC	O5-C1-C2	2.36	114.44	110.30
3	2-B	701	BGC	O4-C4-C5	2.33	115.05	109.32
3	16-B	701	BGC	O2-C2-C1	2.31	114.57	109.25
3	7-B	701	BGC	O5-C1-C2	2.30	114.34	110.30
3	21-B	701	BGC	O5-C5-C6	2.30	112.13	106.44
3	14-B	701	BGC	C1-O5-C5	2.28	118.07	113.65
3	5-B	701	BGC	O1-C1-O5	-2.28	103.64	110.41
3	14-B	701	BGC	O5-C1-C2	2.26	114.27	110.30
3	14-B	701	BGC	O4-C4-C3	2.25	115.67	110.38
3	4-B	701	BGC	O5-C5-C6	2.24	111.99	106.44
3	2-B	701	BGC	C6-C5-C4	-2.23	107.53	113.02
3	18-B	701	BGC	C1-C2-C3	2.23	114.91	110.36
3	21-B	701	BGC	O2-C2-C3	2.20	115.57	110.38
3	3-B	701	BGC	O5-C5-C4	-2.20	105.73	109.70
3	3-B	701	BGC	O3-C3-C4	-2.18	105.23	110.38
3	6-B	701	BGC	C4-C3-C2	-2.17	107.01	110.83
3	1-B	701	BGC	O2-C2-C3	2.16	115.47	110.38
3	9-B	701	BGC	O2-C2-C1	-2.16	104.26	109.25
3	21-B	701	BGC	O1-C1-O5	-2.15	104.02	110.41
3	2-B	701	BGC	O4-C4-C3	2.15	115.44	110.38
3	9-B	701	BGC	O6-C6-C5	-2.15	104.02	111.33
3	9-B	701	BGC	O2-C2-C3	2.14	115.42	110.38
3	9-B	701	BGC	C3-C4-C5	2.13	114.10	110.23
3	25-B	701	BGC	O2-C2-C3	2.13	115.39	110.38
3	8-B	701	BGC	C4-C3-C2	-2.13	107.09	110.83
3	21-B	701	BGC	C1-O5-C5	2.12	117.75	113.65
3	21-B	701	BGC	O5-C5-C4	2.12	113.51	109.70
3	1-B	701	BGC	O5-C1-C2	2.10	113.98	110.30
3	18-B	701	BGC	O5-C1-C2	2.08	113.96	110.30
3	8-B	701	BGC	O1-C1-C2	2.07	115.00	108.98
3	12-B	701	BGC	C6-C5-C4	-2.06	107.95	113.02
3	4-B	701	BGC	O4-C4-C5	2.06	114.40	109.32
3	25-B	701	BGC	C3-C4-C5	2.06	113.97	110.23
3	24-B	701	BGC	O5-C5-C6	2.06	111.54	106.44
3	6-B	701	BGC	O5-C5-C4	-2.04	106.01	109.70
3	13-B	701	BGC	O2-C2-C1	2.04	113.96	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	18-B	701	BGC	O1-C1-C2	-2.03	103.10	108.98
3	3-B	701	BGC	O5-C5-C6	2.01	111.42	106.44

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	23-B	701	BGC	O5-C5-C6-O6
3	1-B	701	BGC	O5-C5-C6-O6
3	18-B	701	BGC	O5-C5-C6-O6
3	3-B	701	BGC	O5-C5-C6-O6
3	1-B	701	BGC	C4-C5-C6-O6
3	18-B	701	BGC	C4-C5-C6-O6
3	7-B	701	BGC	C4-C5-C6-O6
3	9-B	701	BGC	C4-C5-C6-O6
3	3-B	701	BGC	C4-C5-C6-O6
3	20-B	701	BGC	C4-C5-C6-O6
3	21-B	701	BGC	O5-C5-C6-O6
3	17-B	701	BGC	O5-C5-C6-O6
3	6-B	701	BGC	O5-C5-C6-O6
3	6-B	701	BGC	C4-C5-C6-O6
3	4-B	701	BGC	C4-C5-C6-O6
3	23-B	701	BGC	C4-C5-C6-O6
2	11-A	701	EDO	O1-C1-C2-O2
2	18-B	704	EDO	O1-C1-C2-O2
2	19-B	704	EDO	O1-C1-C2-O2
2	22-B	704	EDO	O1-C1-C2-O2
3	7-B	701	BGC	O5-C5-C6-O6
2	1-B	704	EDO	O1-C1-C2-O2
2	8-B	704	EDO	O1-C1-C2-O2
2	14-B	704	EDO	O1-C1-C2-O2
2	25-B	704	EDO	O1-C1-C2-O2
2	16-B	704	EDO	O1-C1-C2-O2
3	9-B	701	BGC	O5-C5-C6-O6
3	20-B	701	BGC	O5-C5-C6-O6
3	24-B	701	BGC	O5-C5-C6-O6
2	17-A	701	EDO	O1-C1-C2-O2
3	4-B	701	BGC	O5-C5-C6-O6
2	1-A	701	EDO	O1-C1-C2-O2
2	12-B	702	EDO	O1-C1-C2-O2
2	9-B	704	EDO	O1-C1-C2-O2
3	21-B	701	BGC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	6-A	701	EDO	O1-C1-C2-O2
2	24-B	704	EDO	O1-C1-C2-O2
3	11-B	701	BGC	C4-C5-C6-O6
2	19-A	701	EDO	O1-C1-C2-O2
2	24-A	701	EDO	O1-C1-C2-O2
2	18-B	703	EDO	O1-C1-C2-O2
2	12-B	704	EDO	O1-C1-C2-O2
2	17-B	704	EDO	O1-C1-C2-O2
2	23-B	704	EDO	O1-C1-C2-O2
3	10-B	701	BGC	O5-C5-C6-O6
2	2-A	701	EDO	O1-C1-C2-O2
2	8-A	701	EDO	O1-C1-C2-O2
2	9-A	701	EDO	O1-C1-C2-O2
2	18-A	701	EDO	O1-C1-C2-O2
2	8-B	702	EDO	O1-C1-C2-O2
2	3-B	704	EDO	O1-C1-C2-O2
2	11-B	704	EDO	O1-C1-C2-O2
2	20-B	704	EDO	O1-C1-C2-O2
2	25-A	701	EDO	O1-C1-C2-O2

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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	548/551 (99%)	1.75	161 (29%) ⓘ ⓘ	0, 1, 1, 1	548 (100%)
1	1-B	551/551 (100%)	1.75	162 (29%) ⓘ ⓘ	0, 1, 1, 1	551 (100%)
1	2-A	0/551	-	-	-	-
1	2-B	0/551	-	-	-	-
1	3-A	0/551	-	-	-	-
1	3-B	0/551	-	-	-	-
1	4-A	0/551	-	-	-	-
1	4-B	0/551	-	-	-	-
1	5-A	0/551	-	-	-	-
1	5-B	0/551	-	-	-	-
1	6-A	0/551	-	-	-	-
1	6-B	0/551	-	-	-	-
1	7-A	0/551	-	-	-	-
1	7-B	0/551	-	-	-	-
1	8-A	0/551	-	-	-	-
1	8-B	0/551	-	-	-	-
1	9-A	0/551	-	-	-	-
1	9-B	0/551	-	-	-	-
1	10-A	0/551	-	-	-	-
1	10-B	0/551	-	-	-	-
1	11-A	0/551	-	-	-	-
1	11-B	0/551	-	-	-	-
1	12-A	0/551	-	-	-	-
1	12-B	0/551	-	-	-	-
1	13-A	0/551	-	-	-	-
1	13-B	0/551	-	-	-	-
1	14-A	0/551	-	-	-	-
1	14-B	0/551	-	-	-	-
1	15-A	0/551	-	-	-	-
1	15-B	0/551	-	-	-	-
1	16-A	0/551	-	-	-	-
1	16-B	0/551	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	17-A	0/551	-	-	-	-
1	17-B	0/551	-	-	-	-
1	18-A	0/551	-	-	-	-
1	18-B	0/551	-	-	-	-
1	19-A	0/551	-	-	-	-
1	19-B	0/551	-	-	-	-
1	20-A	0/551	-	-	-	-
1	20-B	0/551	-	-	-	-
1	21-A	0/551	-	-	-	-
1	21-B	0/551	-	-	-	-
1	22-A	0/551	-	-	-	-
1	22-B	0/551	-	-	-	-
1	23-A	0/551	-	-	-	-
1	23-B	0/551	-	-	-	-
1	24-A	0/551	-	-	-	-
1	24-B	0/551	-	-	-	-
1	25-A	0/551	-	-	-	-
1	25-B	0/551	-	-	-	-
All	All	1099/27550 (3%)	1.75	323 (29%) 1 1	0, 1, 1, 1	1099 (100%)

All (323) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	312	PRO	16.4
1	1-A	196	TRP	12.6
1	1-B	295	GLY	12.0
1	1-B	194	TYR	11.9
1	1-B	297	PRO	11.7
1	1-A	312	PRO	11.4
1	1-B	296	THR	11.3
1	1-A	295	GLY	10.1
1	1-B	141	ALA	10.1
1	1-B	196	TRP	9.5
1	1-A	58	VAL	9.0
1	1-A	194	TYR	8.8
1	1-A	59	VAL	8.3
1	1-B	126	LEU	8.2
1	1-B	294	ASN	8.2
1	1-B	193	GLY	8.2
1	1-A	296	THR	8.1
1	1-A	297	PRO	8.0
1	1-B	402	SER	7.9

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Mol	Chain	Res	Type	RSRZ
1	1-A	191	PRO	7.8
1	1-A	60	GLY	7.8
1	1-A	192	ASP	7.7
1	1-B	399	ASP	7.5
1	1-B	144	PHE	7.0
1	1-A	274	ASP	6.8
1	1-B	192	ASP	6.7
1	1-A	400	GLY	6.7
1	1-A	169	ARG	6.7
1	1-A	337	HIS	6.5
1	1-B	102	MET	6.5
1	1-B	400	GLY	6.3
1	1-B	401	ALA	6.2
1	1-B	76	PRO	6.2
1	1-B	298	GLU	6.2
1	1-B	143	TRP	6.1
1	1-A	424	PRO	6.1
1	1-B	73	PRO	6.0
1	1-A	143	TRP	5.9
1	1-A	348	ASN	5.8
1	1-B	87	ARG	5.8
1	1-B	145	ASP	5.8
1	1-A	298	GLU	5.7
1	1-B	62	GLY	5.7
1	1-A	76	PRO	5.7
1	1-A	293	GLY	5.6
1	1-A	586	ASP	5.5
1	1-A	126	LEU	5.4
1	1-A	538	MET	5.4
1	1-A	340	GLN	5.4
1	1-A	144	PHE	5.3
1	1-B	293	GLY	5.3
1	1-A	305	ASP	5.3
1	1-B	531	THR	5.3
1	1-A	399	ASP	5.3
1	1-A	366	THR	5.2
1	1-A	104	LYS	5.1
1	1-A	402	SER	5.1
1	1-A	251	GLU	5.1
1	1-A	529	SER	5.1
1	1-A	543	TYR	5.1
1	1-B	81	LYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	1-A	346	ARG	5.0
1	1-B	302	LEU	5.0
1	1-B	340	GLN	5.0
1	1-B	56	GLN	4.9
1	1-A	517	ASP	4.9
1	1-B	72	ASP	4.9
1	1-B	272	ASP	4.9
1	1-B	326	GLY	4.9
1	1-A	324	ASP	4.9
1	1-A	306	GLN	4.8
1	1-B	164	VAL	4.8
1	1-B	75	THR	4.8
1	1-A	422	ALA	4.7
1	1-B	227	GLY	4.7
1	1-A	294	ASN	4.7
1	1-B	140	ASP	4.7
1	1-B	149	THR	4.7
1	1-B	574	LEU	4.6
1	1-A	193	GLY	4.6
1	1-A	587	ILE	4.6
1	1-A	80	GLY	4.6
1	1-A	313	GLY	4.5
1	1-A	401	ALA	4.5
1	1-B	74	SER	4.5
1	1-B	346	ARG	4.5
1	1-B	452	GLU	4.4
1	1-B	147	ASN	4.4
1	1-B	369	LYS	4.4
1	1-A	276	TYR	4.4
1	1-A	368	LEU	4.4
1	1-B	63	ASP	4.4
1	1-A	398	SER	4.3
1	1-A	314	ALA	4.3
1	1-B	311	LYS	4.3
1	1-B	325	GLN	4.3
1	1-B	195	GLY	4.3
1	1-B	55	ALA	4.3
1	1-B	66	PRO	4.3
1	1-A	597	ILE	4.3
1	1-B	167	THR	4.2
1	1-A	64	LEU	4.2
1	1-B	587	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	1-A	285	THR	4.2
1	1-B	512	ALA	4.2
1	1-B	109	ASN	4.2
1	1-A	273	GLY	4.2
1	1-B	318	THR	4.2
1	1-B	274	ASP	4.1
1	1-B	64	LEU	4.1
1	1-B	142	GLY	4.1
1	1-B	588	GLY	4.0
1	1-A	145	ASP	4.0
1	1-B	70	VAL	4.0
1	1-B	114	GLN	3.9
1	1-A	451	GLY	3.9
1	1-A	466	HIS	3.9
1	1-B	300	GLU	3.9
1	1-B	336	TYR	3.9
1	1-A	343	GLU	3.9
1	1-B	304	LEU	3.8
1	1-A	63	ASP	3.8
1	1-A	574	LEU	3.8
1	1-B	77	ASP	3.8
1	1-A	190	ALA	3.7
1	1-B	306	GLN	3.7
1	1-B	148	ALA	3.7
1	1-A	339	ASP	3.6
1	1-A	286	ASN	3.6
1	1-B	348	ASN	3.6
1	1-B	545	ASN	3.6
1	1-B	232	GLY	3.6
1	1-A	605	PRO	3.5
1	1-B	319	ILE	3.5
1	1-A	452	GLU	3.5
1	1-A	269	LEU	3.5
1	1-A	404	ASP	3.5
1	1-B	528	ASP	3.5
1	1-A	457	GLU	3.5
1	1-B	207	ILE	3.4
1	1-A	87	ARG	3.4
1	1-B	299	GLY	3.4
1	1-B	516	GLY	3.4
1	1-A	88	LYS	3.4
1	1-A	388	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	1-A	258	GLU	3.4
1	1-B	150	GLN	3.3
1	1-A	518	ILE	3.3
1	1-A	61	GLY	3.3
1	1-B	125	GLY	3.3
1	1-B	423	GLY	3.3
1	1-A	225	SER	3.3
1	1-B	314	ALA	3.3
1	1-B	527	ASP	3.3
1	1-B	592	SER	3.3
1	1-A	300	GLU	3.3
1	1-A	250	PRO	3.2
1	1-B	317	GLU	3.2
1	1-A	512	ALA	3.2
1	1-B	572	VAL	3.2
1	1-B	165	ASN	3.2
1	1-A	304	LEU	3.2
1	1-A	83	ASP	3.2
1	1-A	315	THR	3.2
1	1-A	341	PRO	3.1
1	1-B	303	PRO	3.1
1	1-A	299	GLY	3.1
1	1-B	60	GLY	3.1
1	1-A	527	ASP	3.1
1	1-B	557	GLN	3.1
1	1-A	317	GLU	3.1
1	1-A	272	ASP	3.1
1	1-B	276	TYR	3.1
1	1-B	273	GLY	3.1
1	1-A	545	ASN	3.1
1	1-A	149	THR	3.1
1	1-B	471	ASN	3.0
1	1-B	316	ALA	3.0
1	1-B	404	ASP	3.0
1	1-B	529	SER	3.0
1	1-A	604	PHE	3.0
1	1-B	279	PHE	3.0
1	1-A	164	VAL	3.0
1	1-B	99	TYR	3.0
1	1-A	69	LEU	3.0
1	1-A	325	GLN	3.0
1	1-A	495	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	1-B	593	GLY	3.0
1	1-A	308	TYR	3.0
1	1-B	458	THR	3.0
1	1-A	302	LEU	3.0
1	1-A	546	VAL	2.9
1	1-B	339	ASP	2.9
1	1-B	215	SER	2.9
1	1-B	565	LYS	2.9
1	1-B	78	ILE	2.9
1	1-A	301	SER	2.9
1	1-B	214	TYR	2.9
1	1-A	362	ASP	2.9
1	1-B	301	SER	2.9
1	1-A	403	GLY	2.9
1	1-A	565	LYS	2.9
1	1-B	391	GLU	2.9
1	1-B	488	GLN	2.8
1	1-A	141	ALA	2.8
1	1-B	310	VAL	2.8
1	1-B	511	ALA	2.8
1	1-A	77	ASP	2.8
1	1-B	277	LYS	2.8
1	1-A	261	PRO	2.8
1	1-B	368	LEU	2.8
1	1-B	79	GLN	2.8
1	1-B	283	LYS	2.8
1	1-A	336	TYR	2.8
1	1-B	387	PRO	2.8
1	1-B	111	ILE	2.8
1	1-A	450	HIS	2.8
1	1-B	169	ARG	2.8
1	1-A	114	GLN	2.8
1	1-A	600	GLN	2.8
1	1-B	84	GLU	2.8
1	1-A	74	SER	2.8
1	1-A	488	GLN	2.7
1	1-A	511	ALA	2.7
1	1-A	303	PRO	2.7
1	1-B	543	TYR	2.7
1	1-A	429	THR	2.7
1	1-B	449	ASP	2.7
1	1-A	214	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	1-B	575	GLY	2.7
1	1-B	508	PRO	2.6
1	1-B	309	VAL	2.6
1	1-A	112	ASN	2.6
1	1-B	129	ASP	2.6
1	1-A	572	VAL	2.6
1	1-A	507	ALA	2.6
1	1-A	283	LYS	2.6
1	1-B	517	ASP	2.6
1	1-B	69	LEU	2.6
1	1-A	602	VAL	2.6
1	1-B	463	TYR	2.6
1	1-A	234	TRP	2.6
1	1-A	528	ASP	2.5
1	1-A	249	PHE	2.5
1	1-B	127	ASN	2.5
1	1-A	82	VAL	2.5
1	1-B	97	ASP	2.5
1	1-B	324	ASP	2.5
1	1-A	186	GLY	2.5
1	1-A	195	GLY	2.5
1	1-B	337	HIS	2.5
1	1-B	604	PHE	2.5
1	1-B	338	VAL	2.5
1	1-B	146	GLY	2.5
1	1-B	110	ASP	2.5
1	1-A	142	GLY	2.5
1	1-B	595	THR	2.5
1	1-A	127	ASN	2.4
1	1-A	292	TRP	2.4
1	1-B	210	GLU	2.4
1	1-A	125	GLY	2.4
1	1-A	406	ALA	2.4
1	1-A	440	ILE	2.4
1	1-A	110	ASP	2.4
1	1-A	99	TYR	2.4
1	1-B	82	VAL	2.4
1	1-B	530	VAL	2.4
1	1-B	258	GLU	2.4
1	1-B	253	PRO	2.4
1	1-A	140	ASP	2.4
1	1-B	191	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	1-B	83	ASP	2.3
1	1-A	541	TYR	2.3
1	1-B	546	VAL	2.3
1	1-A	62	GLY	2.3
1	1-A	439	ILE	2.3
1	1-A	227	GLY	2.3
1	1-A	275	ASP	2.3
1	1-A	310	VAL	2.3
1	1-B	234	TRP	2.2
1	1-A	473	LEU	2.2
1	1-A	72	ASP	2.2
1	1-B	450	HIS	2.2
1	1-A	564	VAL	2.2
1	1-B	280	VAL	2.2
1	1-A	97	ASP	2.2
1	1-B	269	LEU	2.2
1	1-B	271	LEU	2.2
1	1-A	581	GLU	2.2
1	1-B	270	TYR	2.2
1	1-B	424	PRO	2.2
1	1-B	562	PRO	2.2
1	1-A	232	GLY	2.2
1	1-A	71	PHE	2.2
1	1-B	320	ASN	2.2
1	1-A	505	TYR	2.2
1	1-A	318	THR	2.2
1	1-B	190	ALA	2.1
1	1-B	228	GLY	2.1
1	1-A	387	PRO	2.1
1	1-A	531	THR	2.1
1	1-B	532	THR	2.1
1	1-A	378	VAL	2.1
1	1-B	278	VAL	2.1
1	1-A	588	GLY	2.1
1	1-A	84	GLU	2.1
1	1-B	315	THR	2.1
1	1-A	106	GLY	2.1
1	1-A	70	VAL	2.1
1	1-B	157	GLU	2.1
1	1-B	457	GLU	2.1
1	1-A	603	SER	2.1
1	1-A	352	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-B	468	LYS	2.1
1	1-B	485	TYR	2.1
1	1-A	146	GLY	2.0
1	1-B	112	ASN	2.0
1	1-A	211	VAL	2.0
1	1-A	396	VAL	2.0
1	1-B	180	ARG	2.0
1	1-B	249	PHE	2.0
1	1-A	316	ALA	2.0
1	1-A	582	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	1-B	704	4/4	0.08	0.49	13,14,29,30	10
2	EDO	2-A	701	4/4	-	-	13,26,27,27	10
2	EDO	3-A	701	4/4	-	-	13,26,27,27	10
2	EDO	4-A	701	4/4	-	-	13,26,27,27	10
2	EDO	5-A	701	4/4	-	-	13,26,27,27	10
2	EDO	6-A	701	4/4	-	-	13,26,27,27	10
2	EDO	7-A	701	4/4	-	-	13,26,27,27	10
2	EDO	8-A	701	4/4	-	-	13,26,27,27	10
2	EDO	9-A	701	4/4	-	-	13,26,27,27	10
2	EDO	10-A	701	4/4	-	-	13,26,27,27	10
2	EDO	11-A	701	4/4	-	-	13,26,27,27	10
2	EDO	12-A	701	4/4	-	-	13,26,27,27	10
2	EDO	13-A	701	4/4	-	-	13,26,27,27	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	14-A	701	4/4	-	-	13,26,27,27	10
2	EDO	15-A	701	4/4	-	-	13,26,27,27	10
2	EDO	16-A	701	4/4	-	-	13,26,27,27	10
2	EDO	17-A	701	4/4	-	-	13,26,27,27	10
2	EDO	18-A	701	4/4	-	-	13,26,27,27	10
2	EDO	19-A	701	4/4	-	-	13,26,27,27	10
2	EDO	20-A	701	4/4	-	-	13,26,27,27	10
2	EDO	21-A	701	4/4	-	-	13,26,27,27	10
2	EDO	22-A	701	4/4	-	-	13,26,27,27	10
2	EDO	23-A	701	4/4	-	-	13,26,27,27	10
2	EDO	24-A	701	4/4	-	-	13,26,27,27	10
2	EDO	25-A	701	4/4	-	-	13,26,27,27	10
2	EDO	1-A	701	4/4	0.76	0.17	13,26,27,27	10
2	EDO	2-A	702	4/4	-	-	13,20,20,21	10
2	EDO	3-A	702	4/4	-	-	13,20,20,21	10
2	EDO	4-A	702	4/4	-	-	13,20,20,21	10
2	EDO	5-A	702	4/4	-	-	13,20,20,21	10
2	EDO	6-A	702	4/4	-	-	13,20,20,21	10
2	EDO	7-A	702	4/4	-	-	13,20,20,21	10
2	EDO	8-A	702	4/4	-	-	13,20,20,21	10
2	EDO	9-A	702	4/4	-	-	13,20,20,21	10
2	EDO	10-A	702	4/4	-	-	13,20,20,21	10
2	EDO	11-A	702	4/4	-	-	13,20,20,21	10
2	EDO	12-A	702	4/4	-	-	13,20,20,21	10
2	EDO	13-A	702	4/4	-	-	13,20,20,21	10
2	EDO	14-A	702	4/4	-	-	13,20,20,21	10
2	EDO	15-A	702	4/4	-	-	13,20,20,21	10
2	EDO	16-A	702	4/4	-	-	13,20,20,21	10
2	EDO	17-A	702	4/4	-	-	13,20,20,21	10
2	EDO	18-A	702	4/4	-	-	13,20,20,21	10
2	EDO	19-A	702	4/4	-	-	13,20,20,21	10
2	EDO	20-A	702	4/4	-	-	13,20,20,21	10
2	EDO	21-A	702	4/4	-	-	13,20,20,21	10
2	EDO	22-A	702	4/4	-	-	13,20,20,21	10
2	EDO	23-A	702	4/4	-	-	13,20,20,21	10
2	EDO	24-A	702	4/4	-	-	13,20,20,21	10
2	EDO	25-A	702	4/4	-	-	13,20,20,21	10
2	EDO	1-B	702	4/4	0.78	0.14	13,13,16,16	10
2	EDO	2-B	702	4/4	-	-	13,13,16,16	10
2	EDO	3-B	702	4/4	-	-	13,13,16,16	10
2	EDO	4-B	702	4/4	-	-	13,13,16,16	10
2	EDO	5-B	702	4/4	-	-	13,13,16,16	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	6-B	702	4/4	-	-	13,13,16,16	10
2	EDO	7-B	702	4/4	-	-	13,13,16,16	10
2	EDO	8-B	702	4/4	-	-	13,13,16,16	10
2	EDO	9-B	702	4/4	-	-	13,13,16,16	10
2	EDO	10-B	702	4/4	-	-	13,13,16,16	10
2	EDO	11-B	702	4/4	-	-	13,13,16,16	10
2	EDO	12-B	702	4/4	-	-	13,13,16,16	10
2	EDO	13-B	702	4/4	-	-	13,13,16,16	10
2	EDO	14-B	702	4/4	-	-	13,13,16,16	10
2	EDO	15-B	702	4/4	-	-	13,13,16,16	10
2	EDO	16-B	702	4/4	-	-	13,13,16,16	10
2	EDO	17-B	702	4/4	-	-	13,13,16,16	10
2	EDO	18-B	702	4/4	-	-	13,13,16,16	10
2	EDO	19-B	702	4/4	-	-	13,13,16,16	10
2	EDO	20-B	702	4/4	-	-	13,13,16,16	10
2	EDO	21-B	702	4/4	-	-	13,13,16,16	10
2	EDO	22-B	702	4/4	-	-	13,13,16,16	10
2	EDO	23-B	702	4/4	-	-	13,13,16,16	10
2	EDO	24-B	702	4/4	-	-	13,13,16,16	10
2	EDO	25-B	702	4/4	-	-	13,13,16,16	10
3	BGC	1-B	701	12/12	0.83	0.13	10,16,32,38	24
2	EDO	2-B	703	4/4	-	-	12,21,22,22	10
2	EDO	3-B	703	4/4	-	-	12,21,22,22	10
2	EDO	4-B	703	4/4	-	-	12,21,22,22	10
2	EDO	5-B	703	4/4	-	-	12,21,22,22	10
2	EDO	6-B	703	4/4	-	-	12,21,22,22	10
2	EDO	7-B	703	4/4	-	-	12,21,22,22	10
2	EDO	8-B	703	4/4	-	-	12,21,22,22	10
2	EDO	9-B	703	4/4	-	-	12,21,22,22	10
2	EDO	10-B	703	4/4	-	-	12,21,22,22	10
2	EDO	11-B	703	4/4	-	-	12,21,22,22	10
2	EDO	12-B	703	4/4	-	-	12,21,22,22	10
2	EDO	13-B	703	4/4	-	-	12,21,22,22	10
2	EDO	14-B	703	4/4	-	-	12,21,22,22	10
2	EDO	15-B	703	4/4	-	-	12,21,22,22	10
2	EDO	16-B	703	4/4	-	-	12,21,22,22	10
2	EDO	17-B	703	4/4	-	-	12,21,22,22	10
2	EDO	18-B	703	4/4	-	-	12,21,22,22	10
2	EDO	19-B	703	4/4	-	-	12,21,22,22	10
2	EDO	20-B	703	4/4	-	-	12,21,22,22	10
2	EDO	21-B	703	4/4	-	-	12,21,22,22	10
2	EDO	22-B	703	4/4	-	-	12,21,22,22	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	23-B	703	4/4	-	-	12,21,22,22	10
2	EDO	24-B	703	4/4	-	-	12,21,22,22	10
2	EDO	25-B	703	4/4	-	-	12,21,22,22	10
2	EDO	1-A	702	4/4	0.84	0.14	13,20,20,21	10
2	EDO	2-B	704	4/4	-	-	13,14,29,30	10
2	EDO	3-B	704	4/4	-	-	13,14,29,30	10
2	EDO	4-B	704	4/4	-	-	13,14,29,30	10
2	EDO	5-B	704	4/4	-	-	13,14,29,30	10
2	EDO	6-B	704	4/4	-	-	13,14,29,30	10
2	EDO	7-B	704	4/4	-	-	13,14,29,30	10
2	EDO	8-B	704	4/4	-	-	13,14,29,30	10
2	EDO	9-B	704	4/4	-	-	13,14,29,30	10
2	EDO	10-B	704	4/4	-	-	13,14,29,30	10
2	EDO	11-B	704	4/4	-	-	13,14,29,30	10
2	EDO	12-B	704	4/4	-	-	13,14,29,30	10
2	EDO	13-B	704	4/4	-	-	13,14,29,30	10
2	EDO	14-B	704	4/4	-	-	13,14,29,30	10
2	EDO	15-B	704	4/4	-	-	13,14,29,30	10
2	EDO	16-B	704	4/4	-	-	13,14,29,30	10
2	EDO	17-B	704	4/4	-	-	13,14,29,30	10
2	EDO	18-B	704	4/4	-	-	13,14,29,30	10
2	EDO	19-B	704	4/4	-	-	13,14,29,30	10
2	EDO	20-B	704	4/4	-	-	13,14,29,30	10
2	EDO	21-B	704	4/4	-	-	13,14,29,30	10
2	EDO	22-B	704	4/4	-	-	13,14,29,30	10
2	EDO	23-B	704	4/4	-	-	13,14,29,30	10
2	EDO	24-B	704	4/4	-	-	13,14,29,30	10
2	EDO	25-B	704	4/4	-	-	13,14,29,30	10
2	EDO	1-B	703	4/4	0.93	0.13	12,21,22,22	10
3	BGC	2-B	701	12/12	-	-	10,16,32,38	24
3	BGC	3-B	701	12/12	-	-	10,16,32,38	24
3	BGC	4-B	701	12/12	-	-	10,16,32,38	24
3	BGC	5-B	701	12/12	-	-	10,16,32,38	24
3	BGC	6-B	701	12/12	-	-	10,16,32,38	24
3	BGC	7-B	701	12/12	-	-	10,16,32,38	24
3	BGC	8-B	701	12/12	-	-	10,16,32,38	24
3	BGC	9-B	701	12/12	-	-	10,16,32,38	24
3	BGC	10-B	701	12/12	-	-	10,16,32,38	24
3	BGC	11-B	701	12/12	-	-	10,16,32,38	24
3	BGC	12-B	701	12/12	-	-	10,16,32,38	24
3	BGC	13-B	701	12/12	-	-	10,16,32,38	24
3	BGC	14-B	701	12/12	-	-	10,16,32,38	24

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BGC	15-B	701	12/12	-	-	10,16,32,38	24
3	BGC	16-B	701	12/12	-	-	10,16,32,38	24
3	BGC	17-B	701	12/12	-	-	10,16,32,38	24
3	BGC	18-B	701	12/12	-	-	10,16,32,38	24
3	BGC	19-B	701	12/12	-	-	10,16,32,38	24
3	BGC	20-B	701	12/12	-	-	10,16,32,38	24
3	BGC	21-B	701	12/12	-	-	10,16,32,38	24
3	BGC	22-B	701	12/12	-	-	10,16,32,38	24
3	BGC	23-B	701	12/12	-	-	10,16,32,38	24
3	BGC	24-B	701	12/12	-	-	10,16,32,38	24
3	BGC	25-B	701	12/12	-	-	10,16,32,38	24

6.5 Other polymers [i](#)

There are no such residues in this entry.