



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2023 – 03:37 am GMT

PDB ID : 4CBO
Title : Crystal structure of Complement Factor D mutant R202A after ensemble refinement
Authors : Forneris, F.; Burnley, B.T.; Gros, P.
Deposited on : 2013-10-15
Resolution : 1.80 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

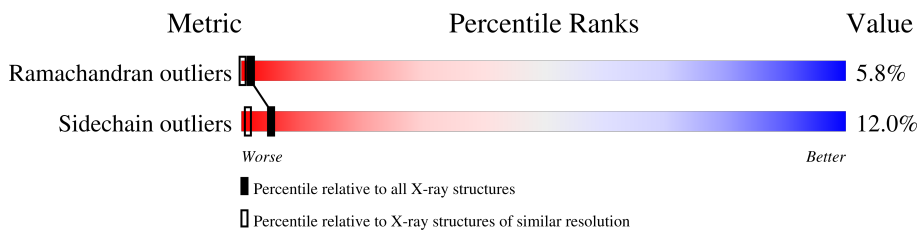
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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	GOL	17-A	1000	-	X	-	-
2	GOL	29-A	1000	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 546299 atoms, of which 263032 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 COMPLEMENT FACTOR D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	1-A	228	3406	1055	1700	322	319	10	0	0	0
1	2-A	228	3406	1055	1700	322	319	10	0	0	0
1	3-A	228	3406	1055	1700	322	319	10	0	0	0
1	4-A	228	3406	1055	1700	322	319	10	0	0	0
1	5-A	228	3406	1055	1700	322	319	10	0	0	0
1	6-A	228	3406	1055	1700	322	319	10	0	0	0
1	7-A	228	3406	1055	1700	322	319	10	0	0	0
1	8-A	228	3406	1055	1700	322	319	10	0	0	0
1	9-A	228	3406	1055	1700	322	319	10	0	0	0
1	10-A	228	3406	1055	1700	322	319	10	0	0	0
1	11-A	228	3406	1055	1700	322	319	10	0	0	0
1	12-A	228	3406	1055	1700	322	319	10	0	0	0
1	13-A	228	3406	1055	1700	322	319	10	0	0	0
1	14-A	228	3406	1055	1700	322	319	10	0	0	0
1	15-A	228	3406	1055	1700	322	319	10	0	0	0
1	16-A	228	3406	1055	1700	322	319	10	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	17-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	18-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	19-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	20-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	21-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	22-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	23-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	24-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	25-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	26-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	27-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	28-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	29-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	30-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	31-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	32-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	33-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	34-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	35-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	36-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	37-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	38-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	39-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	40-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	41-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	42-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	43-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	44-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	45-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	46-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	47-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	48-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	49-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
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			3406	1055	1700	322	319	10			
1	51-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	52-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	53-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	54-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	55-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	56-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	57-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	58-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	59-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	60-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	61-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	62-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	63-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	64-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	65-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	66-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	67-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	68-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	69-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	70-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	71-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	72-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	73-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	74-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	75-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	76-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	77-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	1-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	2-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	3-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	4-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	5-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	6-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	7-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	8-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	9-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	10-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	11-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	12-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	13-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	14-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	15-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	16-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	17-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	18-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	19-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	20-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	21-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	22-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	23-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	24-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	25-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	26-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	27-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	28-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	29-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	30-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	31-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	32-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	33-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	34-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	35-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	36-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	37-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	38-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	39-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	40-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	41-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	42-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	43-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	44-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	45-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	46-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	47-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	48-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	49-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	50-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	51-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	52-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	53-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	54-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	55-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	56-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	57-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	58-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	59-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	60-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	61-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	62-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	63-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	64-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	65-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

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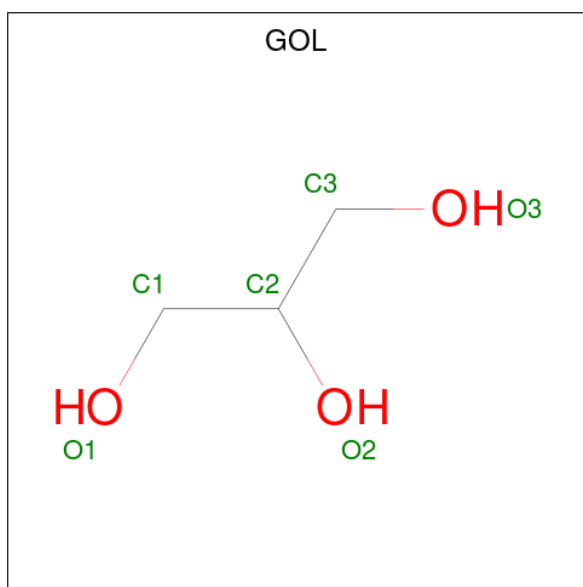
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	66-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	67-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	68-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	69-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	70-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	71-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	72-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	73-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	74-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	75-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	76-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	77-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	ALA	ARG	engineered mutation	UNP P00746
B	202	ALA	ARG	engineered mutation	UNP P00746

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	15-A	1	Total 14	C 3	H 8	O 3	0	0
2	16-A	1	Total 14	C 3	H 8	O 3	0	0
2	17-A	1	Total 14	C 3	H 8	O 3	0	0
2	18-A	1	Total 14	C 3	H 8	O 3	0	0
2	19-A	1	Total 14	C 3	H 8	O 3	0	0
2	20-A	1	Total 14	C 3	H 8	O 3	0	0
2	21-A	1	Total 14	C 3	H 8	O 3	0	0
2	22-A	1	Total 14	C 3	H 8	O 3	0	0
2	23-A	1	Total 14	C 3	H 8	O 3	0	0
2	24-A	1	Total 14	C 3	H 8	O 3	0	0
2	25-A	1	Total 14	C 3	H 8	O 3	0	0
2	26-A	1	Total 14	C 3	H 8	O 3	0	0
2	27-A	1	Total 14	C 3	H 8	O 3	0	0
2	28-A	1	Total 14	C 3	H 8	O 3	0	0
2	29-A	1	Total 14	C 3	H 8	O 3	0	0
2	30-A	1	Total 14	C 3	H 8	O 3	0	0
2	31-A	1	Total 14	C 3	H 8	O 3	0	0
2	32-A	1	Total 14	C 3	H 8	O 3	0	0
2	33-A	1	Total 14	C 3	H 8	O 3	0	0
2	34-A	1	Total 14	C 3	H 8	O 3	0	0
2	35-A	1	Total 14	C 3	H 8	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	36-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	37-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	38-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	39-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	40-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	41-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	42-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	43-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	44-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	45-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	46-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	47-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	48-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	49-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	50-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	51-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	52-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	53-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	54-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	55-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	56-A	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	57-A	1	Total 14	C 3	H 8	O 3	0	0
2	58-A	1	Total 14	C 3	H 8	O 3	0	0
2	59-A	1	Total 14	C 3	H 8	O 3	0	0
2	60-A	1	Total 14	C 3	H 8	O 3	0	0
2	61-A	1	Total 14	C 3	H 8	O 3	0	0
2	62-A	1	Total 14	C 3	H 8	O 3	0	0
2	63-A	1	Total 14	C 3	H 8	O 3	0	0
2	64-A	1	Total 14	C 3	H 8	O 3	0	0
2	65-A	1	Total 14	C 3	H 8	O 3	0	0
2	66-A	1	Total 14	C 3	H 8	O 3	0	0
2	67-A	1	Total 14	C 3	H 8	O 3	0	0
2	68-A	1	Total 14	C 3	H 8	O 3	0	0
2	69-A	1	Total 14	C 3	H 8	O 3	0	0
2	70-A	1	Total 14	C 3	H 8	O 3	0	0
2	71-A	1	Total 14	C 3	H 8	O 3	0	0
2	72-A	1	Total 14	C 3	H 8	O 3	0	0
2	73-A	1	Total 14	C 3	H 8	O 3	0	0
2	74-A	1	Total 14	C 3	H 8	O 3	0	0
2	75-A	1	Total 14	C 3	H 8	O 3	0	0
2	76-A	1	Total 14	C 3	H 8	O 3	0	0
2	77-A	1	Total 14	C 3	H 8	O 3	0	0

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	22-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	23-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	24-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	25-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	26-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	27-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	28-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	29-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	30-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	31-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	32-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	33-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	34-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	35-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	36-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	37-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	38-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	39-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	40-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	41-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	42-B	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	43-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	44-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	45-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	46-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	47-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	48-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	49-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	50-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	51-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	52-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	53-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	54-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	55-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	56-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	57-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	58-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	59-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	60-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	61-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	62-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	63-B	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	64-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	65-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	66-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	67-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	68-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	69-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	70-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	71-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	72-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	73-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	74-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	75-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	76-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	77-B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	148	Total	O	0	0
			148	148		
3	2-A	139	Total	O	0	0
			139	139		
3	3-A	142	Total	O	0	0
			142	142		
3	4-A	129	Total	O	0	0
			129	129		
3	5-A	128	Total	O	0	1
			129	129		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	6-A	135	Total 136	O 136	0	1
3	7-A	134	Total 134	O 134	0	0
3	8-A	136	Total 136	O 136	0	0
3	9-A	138	Total 138	O 138	0	0
3	10-A	135	Total 135	O 135	0	0
3	11-A	123	Total 123	O 123	0	0
3	12-A	145	Total 145	O 145	0	0
3	13-A	164	Total 165	O 165	0	1
3	14-A	157	Total 157	O 157	0	0
3	15-A	142	Total 142	O 142	0	0
3	16-A	135	Total 135	O 135	0	0
3	17-A	142	Total 142	O 142	0	0
3	18-A	147	Total 147	O 147	0	0
3	19-A	127	Total 127	O 127	0	0
3	20-A	131	Total 131	O 131	0	0
3	21-A	144	Total 144	O 144	0	0
3	22-A	142	Total 143	O 143	0	1
3	23-A	142	Total 142	O 142	0	0
3	24-A	127	Total 127	O 127	0	0
3	25-A	136	Total 137	O 137	0	1
3	26-A	144	Total 145	O 145	0	1

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	27-A	139	Total 139	O 139	0	0
3	28-A	136	Total 137	O 137	0	1
3	29-A	134	Total 135	O 135	0	1
3	30-A	149	Total 149	O 149	0	0
3	31-A	146	Total 146	O 146	0	0
3	32-A	135	Total 135	O 135	0	0
3	33-A	133	Total 133	O 133	0	0
3	34-A	139	Total 139	O 139	0	0
3	35-A	125	Total 125	O 125	0	0
3	36-A	130	Total 130	O 130	0	0
3	37-A	138	Total 138	O 138	0	0
3	38-A	133	Total 134	O 134	0	1
3	39-A	130	Total 130	O 130	0	0
3	40-A	127	Total 128	O 128	0	1
3	41-A	139	Total 139	O 139	0	0
3	42-A	128	Total 128	O 128	0	0
3	43-A	154	Total 155	O 155	0	1
3	44-A	143	Total 143	O 143	0	0
3	45-A	140	Total 140	O 140	0	0
3	46-A	131	Total 131	O 131	0	0
3	47-A	127	Total 127	O 127	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	48-A	141	Total 141	O 141	0	0
3	49-A	121	Total 121	O 121	0	0
3	50-A	138	Total 139	O 139	0	1
3	51-A	137	Total 137	O 137	0	0
3	52-A	145	Total 145	O 145	0	0
3	53-A	141	Total 141	O 141	0	0
3	54-A	137	Total 137	O 137	0	0
3	55-A	135	Total 136	O 136	0	1
3	56-A	152	Total 153	O 153	0	1
3	57-A	124	Total 124	O 124	0	0
3	58-A	133	Total 133	O 133	0	0
3	59-A	142	Total 143	O 143	0	1
3	60-A	132	Total 132	O 132	0	0
3	61-A	138	Total 138	O 138	0	0
3	62-A	136	Total 137	O 137	0	1
3	63-A	151	Total 151	O 151	0	0
3	64-A	142	Total 142	O 142	0	0
3	65-A	148	Total 149	O 149	0	1
3	66-A	135	Total 135	O 135	0	0
3	67-A	143	Total 143	O 143	0	0
3	68-A	137	Total 137	O 137	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	69-A	131	Total 131	O 131	0	0
3	70-A	136	Total 136	O 136	0	0
3	71-A	137	Total 138	O 138	0	1
3	72-A	135	Total 135	O 135	0	0
3	73-A	134	Total 134	O 134	0	0
3	74-A	153	Total 153	O 153	0	0
3	75-A	147	Total 147	O 147	0	0
3	76-A	145	Total 145	O 145	0	0
3	77-A	131	Total 131	O 131	0	0
3	1-B	113	Total 113	O 113	0	0
3	2-B	122	Total 122	O 122	0	0
3	3-B	96	Total 96	O 96	0	0
3	4-B	108	Total 108	O 108	0	0
3	5-B	109	Total 109	O 109	0	0
3	6-B	111	Total 111	O 111	0	0
3	7-B	111	Total 111	O 111	0	0
3	8-B	104	Total 104	O 104	0	0
3	9-B	118	Total 119	O 119	0	1
3	10-B	117	Total 117	O 117	0	0
3	11-B	118	Total 118	O 118	0	0
3	12-B	114	Total 115	O 115	0	1

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	13-B	109	Total 109	O 109	0	0
3	14-B	115	Total 115	O 115	0	0
3	15-B	113	Total 113	O 113	0	0
3	16-B	117	Total 117	O 117	0	0
3	17-B	121	Total 122	O 122	0	1
3	18-B	111	Total 111	O 111	0	0
3	19-B	117	Total 117	O 117	0	0
3	20-B	122	Total 123	O 123	0	1
3	21-B	103	Total 103	O 103	0	0
3	22-B	122	Total 122	O 122	0	0
3	23-B	113	Total 113	O 113	0	0
3	24-B	116	Total 116	O 116	0	0
3	25-B	120	Total 120	O 120	0	0
3	26-B	114	Total 114	O 114	0	0
3	27-B	114	Total 114	O 114	0	0
3	28-B	123	Total 123	O 123	0	0
3	29-B	132	Total 132	O 132	0	0
3	30-B	115	Total 115	O 115	0	0
3	31-B	117	Total 117	O 117	0	0
3	32-B	127	Total 127	O 127	0	0
3	33-B	119	Total 119	O 119	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	34-B	109	Total 109	O 109	0	0
3	35-B	102	Total 102	O 102	0	0
3	36-B	119	Total 120	O 120	0	1
3	37-B	110	Total 110	O 110	0	0
3	38-B	118	Total 118	O 118	0	0
3	39-B	112	Total 112	O 112	0	0
3	40-B	118	Total 118	O 118	0	0
3	41-B	106	Total 106	O 106	0	0
3	42-B	123	Total 124	O 124	0	1
3	43-B	125	Total 125	O 125	0	0
3	44-B	118	Total 118	O 118	0	0
3	45-B	108	Total 108	O 108	0	0
3	46-B	105	Total 105	O 105	0	0
3	47-B	117	Total 118	O 118	0	1
3	48-B	128	Total 129	O 129	0	1
3	49-B	109	Total 109	O 109	0	0
3	50-B	111	Total 111	O 111	0	0
3	51-B	130	Total 131	O 131	0	1
3	52-B	119	Total 119	O 119	0	0
3	53-B	113	Total 113	O 113	0	0
3	54-B	109	Total 109	O 109	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	55-B	120	Total 120	O 120	0	0
3	56-B	127	Total 127	O 127	0	0
3	57-B	122	Total 122	O 122	0	0
3	58-B	121	Total 122	O 122	0	1
3	59-B	117	Total 117	O 117	0	0
3	60-B	116	Total 116	O 116	0	0
3	61-B	118	Total 119	O 119	0	1
3	62-B	121	Total 121	O 121	0	0
3	63-B	122	Total 123	O 123	0	1
3	64-B	121	Total 121	O 121	0	0
3	65-B	128	Total 128	O 128	0	0
3	66-B	112	Total 112	O 112	0	0
3	67-B	124	Total 125	O 125	0	1
3	68-B	126	Total 126	O 126	0	0
3	69-B	112	Total 112	O 112	0	0
3	70-B	122	Total 123	O 123	0	1
3	71-B	122	Total 122	O 122	0	0
3	72-B	121	Total 121	O 121	0	0
3	73-B	131	Total 132	O 132	0	1
3	74-B	113	Total 113	O 113	0	0
3	75-B	111	Total 111	O 111	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	76-B	105	Total	O	0	0
			105	105		
3	77-B	119	Total	O	0	0
			119	119		

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.14Å 67.31Å 133.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.33 – 1.80	Depositor
% Data completeness (in resolution range)	98.7 (47.33-1.80)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.79Å)	Xtriage
Refinement program	PHENIX (PHENIX.ENSEMBLE_REFINEMENT: DEV_1259)	Depositor
R, R_{free}	0.163 , 0.212	Depositor
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.319	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	546299	wwPDB-V
Average B, all atoms (Å ²)	26.0	wwPDB-V

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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.

4 Model quality

4.1 Standard geometry

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

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	0.72	0/1741	1.01	5/2370 (0.2%)
1	1-B	0.58	0/1741	0.75	2/2370 (0.1%)
1	2-A	0.77	2/1741 (0.1%)	0.97	2/2370 (0.1%)
1	2-B	0.60	1/1741 (0.1%)	0.82	1/2370 (0.0%)
1	3-A	0.80	1/1741 (0.1%)	0.98	5/2370 (0.2%)
1	3-B	0.54	0/1741	0.79	0/2370
1	4-A	0.79	3/1741 (0.2%)	1.02	7/2370 (0.3%)
1	4-B	0.56	0/1741	0.77	1/2370 (0.0%)
1	5-A	0.77	2/1741 (0.1%)	1.00	8/2370 (0.3%)
1	5-B	0.59	0/1741	0.78	1/2370 (0.0%)
1	6-A	0.74	1/1741 (0.1%)	0.99	3/2370 (0.1%)
1	6-B	0.61	0/1741	0.77	1/2370 (0.0%)
1	7-A	0.74	1/1741 (0.1%)	0.98	7/2370 (0.3%)
1	7-B	0.58	1/1741 (0.1%)	0.82	2/2370 (0.1%)
1	8-A	0.72	0/1741	1.00	6/2370 (0.3%)
1	8-B	0.58	0/1741	0.79	2/2370 (0.1%)
1	9-A	0.76	1/1741 (0.1%)	0.97	6/2370 (0.3%)
1	9-B	0.60	1/1741 (0.1%)	0.81	2/2370 (0.1%)
1	10-A	0.78	5/1741 (0.3%)	1.05	7/2370 (0.3%)
1	10-B	0.59	1/1741 (0.1%)	0.79	0/2370
1	11-A	0.74	2/1741 (0.1%)	1.03	8/2370 (0.3%)
1	11-B	0.62	0/1741	0.80	3/2370 (0.1%)
1	12-A	0.74	1/1741 (0.1%)	1.00	11/2370 (0.5%)
1	12-B	0.59	0/1741	0.80	0/2370
1	13-A	0.75	0/1741	1.00	9/2370 (0.4%)
1	13-B	0.60	1/1741 (0.1%)	0.76	1/2370 (0.0%)
1	14-A	0.73	1/1741 (0.1%)	0.97	6/2370 (0.3%)
1	14-B	0.59	0/1741	0.84	1/2370 (0.0%)
1	15-A	0.70	0/1741	0.96	2/2370 (0.1%)
1	15-B	0.61	0/1741	0.82	2/2370 (0.1%)
1	16-A	0.70	0/1741	0.99	6/2370 (0.3%)
1	16-B	0.62	0/1741	0.81	0/2370

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	17-A	0.77	1/1741 (0.1%)	1.01	4/2370 (0.2%)
1	17-B	0.62	0/1741	0.83	1/2370 (0.0%)
1	18-A	0.73	2/1741 (0.1%)	0.92	3/2370 (0.1%)
1	18-B	0.60	1/1741 (0.1%)	0.76	1/2370 (0.0%)
1	19-A	0.67	0/1741	0.89	2/2370 (0.1%)
1	19-B	0.62	1/1741 (0.1%)	0.82	0/2370
1	20-A	0.79	2/1741 (0.1%)	0.97	3/2370 (0.1%)
1	20-B	0.69	3/1741 (0.2%)	0.82	1/2370 (0.0%)
1	21-A	0.71	0/1741	0.87	2/2370 (0.1%)
1	21-B	0.57	0/1741	0.76	0/2370
1	22-A	0.75	0/1741	1.02	11/2370 (0.5%)
1	22-B	0.65	1/1741 (0.1%)	0.89	5/2370 (0.2%)
1	23-A	0.70	0/1741	0.99	6/2370 (0.3%)
1	23-B	0.66	1/1741 (0.1%)	0.81	1/2370 (0.0%)
1	24-A	0.83	4/1741 (0.2%)	1.10	9/2370 (0.4%)
1	24-B	0.68	2/1741 (0.1%)	0.83	1/2370 (0.0%)
1	25-A	0.78	0/1741	0.98	4/2370 (0.2%)
1	25-B	0.62	0/1741	0.80	0/2370
1	26-A	0.75	1/1741 (0.1%)	0.98	5/2370 (0.2%)
1	26-B	0.63	0/1741	0.83	1/2370 (0.0%)
1	27-A	0.74	0/1741	0.99	4/2370 (0.2%)
1	27-B	0.58	0/1741	0.78	0/2370
1	28-A	0.83	4/1741 (0.2%)	1.10	12/2370 (0.5%)
1	28-B	0.57	1/1741 (0.1%)	0.77	1/2370 (0.0%)
1	29-A	0.75	1/1741 (0.1%)	0.98	4/2370 (0.2%)
1	29-B	0.57	0/1741	0.77	2/2370 (0.1%)
1	30-A	0.73	0/1741	1.00	5/2370 (0.2%)
1	30-B	0.63	0/1741	0.82	1/2370 (0.0%)
1	31-A	0.73	1/1741 (0.1%)	0.96	4/2370 (0.2%)
1	31-B	0.55	0/1741	0.76	0/2370
1	32-A	0.73	1/1741 (0.1%)	0.92	3/2370 (0.1%)
1	32-B	0.56	0/1741	0.82	5/2370 (0.2%)
1	33-A	0.76	1/1741 (0.1%)	1.00	8/2370 (0.3%)
1	33-B	0.58	0/1741	0.75	0/2370
1	34-A	0.80	5/1741 (0.3%)	0.98	6/2370 (0.3%)
1	34-B	0.59	0/1741	0.78	0/2370
1	35-A	0.70	0/1741	0.99	6/2370 (0.3%)
1	35-B	0.60	1/1741 (0.1%)	0.80	0/2370
1	36-A	0.75	1/1741 (0.1%)	0.99	8/2370 (0.3%)
1	36-B	0.60	0/1741	0.82	2/2370 (0.1%)
1	37-A	0.71	0/1741	0.98	8/2370 (0.3%)
1	37-B	0.61	1/1741 (0.1%)	0.76	1/2370 (0.0%)
1	38-A	0.75	1/1741 (0.1%)	0.97	8/2370 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	38-B	0.62	1/1741 (0.1%)	0.84	3/2370 (0.1%)
1	39-A	0.73	0/1741	0.98	7/2370 (0.3%)
1	39-B	0.57	0/1741	0.77	2/2370 (0.1%)
1	40-A	0.71	1/1741 (0.1%)	0.91	2/2370 (0.1%)
1	40-B	0.58	0/1741	0.80	4/2370 (0.2%)
1	41-A	0.76	1/1741 (0.1%)	1.15	7/2370 (0.3%)
1	41-B	0.61	1/1741 (0.1%)	0.79	1/2370 (0.0%)
1	42-A	0.81	2/1741 (0.1%)	1.09	11/2370 (0.5%)
1	42-B	0.59	0/1741	0.82	1/2370 (0.0%)
1	43-A	0.78	1/1741 (0.1%)	0.98	4/2370 (0.2%)
1	43-B	0.58	0/1741	0.78	2/2370 (0.1%)
1	44-A	0.77	1/1741 (0.1%)	1.10	14/2370 (0.6%)
1	44-B	0.55	0/1741	0.78	1/2370 (0.0%)
1	45-A	0.73	0/1741	0.94	2/2370 (0.1%)
1	45-B	0.76	3/1741 (0.2%)	0.81	2/2370 (0.1%)
1	46-A	0.73	0/1741	1.01	9/2370 (0.4%)
1	46-B	0.57	0/1741	0.78	1/2370 (0.0%)
1	47-A	0.78	0/1741	0.99	5/2370 (0.2%)
1	47-B	0.60	0/1741	0.79	1/2370 (0.0%)
1	48-A	0.70	0/1741	0.97	5/2370 (0.2%)
1	48-B	0.60	1/1741 (0.1%)	0.80	0/2370
1	49-A	0.74	0/1741	1.04	9/2370 (0.4%)
1	49-B	0.61	1/1741 (0.1%)	0.79	1/2370 (0.0%)
1	50-A	0.75	1/1741 (0.1%)	0.94	6/2370 (0.3%)
1	50-B	0.59	0/1741	0.77	3/2370 (0.1%)
1	51-A	0.76	0/1741	0.99	4/2370 (0.2%)
1	51-B	0.61	1/1741 (0.1%)	0.82	3/2370 (0.1%)
1	52-A	0.75	2/1741 (0.1%)	0.97	5/2370 (0.2%)
1	52-B	0.63	1/1741 (0.1%)	0.82	4/2370 (0.2%)
1	53-A	0.79	0/1741	0.96	4/2370 (0.2%)
1	53-B	0.58	1/1741 (0.1%)	0.77	2/2370 (0.1%)
1	54-A	0.74	1/1741 (0.1%)	0.99	6/2370 (0.3%)
1	54-B	0.63	0/1741	0.81	2/2370 (0.1%)
1	55-A	0.72	1/1741 (0.1%)	1.01	6/2370 (0.3%)
1	55-B	0.58	0/1741	0.80	0/2370
1	56-A	0.74	0/1741	0.91	1/2370 (0.0%)
1	56-B	0.68	1/1741 (0.1%)	0.78	0/2370
1	57-A	0.72	0/1741	1.01	7/2370 (0.3%)
1	57-B	0.62	1/1741 (0.1%)	0.81	1/2370 (0.0%)
1	58-A	0.71	0/1741	0.98	5/2370 (0.2%)
1	58-B	0.60	1/1741 (0.1%)	0.84	2/2370 (0.1%)
1	59-A	0.72	1/1741 (0.1%)	0.90	2/2370 (0.1%)
1	59-B	0.64	3/1741 (0.2%)	0.81	2/2370 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	60-A	0.69	0/1741	0.89	3/2370 (0.1%)
1	60-B	0.63	3/1741 (0.2%)	0.81	0/2370
1	61-A	0.71	1/1741 (0.1%)	0.93	3/2370 (0.1%)
1	61-B	0.58	1/1741 (0.1%)	0.77	0/2370
1	62-A	0.71	0/1741	0.98	6/2370 (0.3%)
1	62-B	0.62	1/1741 (0.1%)	0.80	2/2370 (0.1%)
1	63-A	0.79	3/1741 (0.2%)	1.03	8/2370 (0.3%)
1	63-B	0.60	0/1741	0.84	2/2370 (0.1%)
1	64-A	0.73	0/1741	0.97	8/2370 (0.3%)
1	64-B	0.61	0/1741	0.79	2/2370 (0.1%)
1	65-A	0.72	1/1741 (0.1%)	0.94	4/2370 (0.2%)
1	65-B	0.66	1/1741 (0.1%)	0.82	3/2370 (0.1%)
1	66-A	0.73	1/1741 (0.1%)	0.89	3/2370 (0.1%)
1	66-B	0.60	1/1741 (0.1%)	0.78	1/2370 (0.0%)
1	67-A	0.76	1/1741 (0.1%)	0.95	5/2370 (0.2%)
1	67-B	0.59	1/1741 (0.1%)	0.79	2/2370 (0.1%)
1	68-A	0.79	2/1741 (0.1%)	1.01	6/2370 (0.3%)
1	68-B	0.58	1/1741 (0.1%)	0.79	1/2370 (0.0%)
1	69-A	0.79	3/1741 (0.2%)	0.95	6/2370 (0.3%)
1	69-B	0.57	0/1741	0.78	0/2370
1	70-A	0.80	4/1741 (0.2%)	0.98	4/2370 (0.2%)
1	70-B	0.64	0/1741	0.82	1/2370 (0.0%)
1	71-A	0.78	3/1741 (0.2%)	1.05	8/2370 (0.3%)
1	71-B	0.59	1/1741 (0.1%)	0.77	0/2370
1	72-A	0.75	0/1741	1.00	5/2370 (0.2%)
1	72-B	0.65	1/1741 (0.1%)	0.83	1/2370 (0.0%)
1	73-A	0.80	1/1741 (0.1%)	1.00	7/2370 (0.3%)
1	73-B	0.60	0/1741	0.78	1/2370 (0.0%)
1	74-A	0.79	2/1741 (0.1%)	1.06	8/2370 (0.3%)
1	74-B	0.66	3/1741 (0.2%)	0.78	1/2370 (0.0%)
1	75-A	0.70	0/1741	0.92	3/2370 (0.1%)
1	75-B	0.59	0/1741	0.77	0/2370
1	76-A	0.77	1/1741 (0.1%)	0.92	2/2370 (0.1%)
1	76-B	0.62	2/1741 (0.1%)	0.77	1/2370 (0.0%)
1	77-A	0.75	1/1741 (0.1%)	0.93	4/2370 (0.2%)
1	77-B	0.61	3/1741 (0.2%)	0.72	0/2370
All	All	0.68	133/268114 (0.0%)	0.90	535/364980 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	6
1	1-B	0	2
1	2-A	0	5
1	2-B	0	2
1	3-A	0	4
1	3-B	0	1
1	4-A	0	5
1	4-B	0	3
1	5-A	0	4
1	6-A	0	6
1	6-B	0	2
1	7-A	0	6
1	7-B	0	2
1	8-A	0	9
1	8-B	0	1
1	9-A	0	5
1	9-B	0	2
1	10-A	0	9
1	10-B	0	2
1	11-A	0	6
1	11-B	0	4
1	12-A	0	2
1	12-B	0	1
1	13-A	0	4
1	13-B	0	1
1	14-A	0	4
1	14-B	0	1
1	15-A	0	3
1	15-B	0	2
1	16-A	0	5
1	16-B	0	1
1	17-A	0	5
1	17-B	0	5
1	18-A	0	5
1	18-B	0	1
1	19-A	0	6
1	19-B	0	1
1	20-A	0	5
1	20-B	0	3
1	21-A	0	2
1	21-B	0	2
1	22-A	0	8
1	22-B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	23-A	0	3
1	24-A	0	6
1	25-A	0	2
1	26-A	0	4
1	26-B	0	2
1	27-A	0	4
1	27-B	0	2
1	28-A	0	4
1	28-B	0	1
1	29-A	0	4
1	29-B	0	1
1	30-A	0	3
1	30-B	0	1
1	31-A	0	5
1	31-B	0	1
1	32-A	0	10
1	32-B	0	1
1	33-A	0	8
1	34-A	0	4
1	35-A	0	4
1	35-B	0	2
1	36-A	0	3
1	36-B	0	1
1	37-A	0	7
1	37-B	0	1
1	38-A	0	5
1	38-B	0	1
1	39-A	0	5
1	40-A	0	5
1	40-B	0	1
1	41-A	0	6
1	42-A	0	6
1	43-A	0	5
1	43-B	0	3
1	44-A	0	7
1	44-B	0	4
1	45-A	0	5
1	45-B	0	1
1	46-A	0	8
1	46-B	0	1
1	47-A	0	5
1	47-B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	48-A	0	9
1	48-B	0	2
1	49-A	0	5
1	49-B	0	1
1	50-A	0	6
1	51-A	0	7
1	51-B	0	1
1	52-A	0	7
1	53-A	0	3
1	53-B	0	1
1	54-A	0	3
1	54-B	0	4
1	55-A	0	7
1	56-A	0	1
1	57-A	0	7
1	58-A	0	5
1	58-B	0	7
1	59-A	0	4
1	60-A	0	2
1	61-B	0	1
1	62-A	0	2
1	63-A	0	3
1	63-B	0	2
1	64-A	0	6
1	64-B	0	1
1	65-A	0	4
1	65-B	0	1
1	66-A	0	9
1	66-B	0	1
1	67-A	0	9
1	67-B	0	1
1	68-A	0	3
1	69-A	0	7
1	69-B	0	2
1	70-A	0	6
1	70-B	0	3
1	71-A	0	3
1	71-B	0	2
1	72-A	0	7
1	73-A	0	4
1	73-B	0	1
1	74-A	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	74-B	0	1
1	75-A	0	5
1	75-B	0	1
1	76-A	0	2
1	77-A	0	2
1	77-B	0	2
All	All	0	485

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	56-B	204	CYS	CB-SG	13.21	2.04	1.82
1	45-B	97	GLU	CG-CD	-12.87	1.32	1.51
1	20-A	97	GLU	CB-CG	-12.81	1.27	1.52
1	65-B	179	CYS	CB-SG	12.24	2.03	1.82
1	23-B	179	CYS	CB-SG	10.94	2.00	1.82
1	62-B	179	CYS	CB-SG	10.74	2.00	1.82
1	45-B	6	GLU	CB-CG	10.66	1.72	1.52
1	24-A	42	CYS	CB-SG	-10.51	1.64	1.82
1	74-B	33	GLU	CB-CG	8.84	1.69	1.52
1	57-B	67	LYS	CB-CG	8.83	1.76	1.52
1	42-A	204	CYS	CB-SG	8.71	1.97	1.82
1	19-B	179	CYS	CB-SG	8.63	1.97	1.82
1	52-B	204	CYS	CB-SG	-8.52	1.67	1.82
1	20-B	62	GLN	CB-CG	-8.26	1.30	1.52
1	24-B	208	LYS	CD-CE	8.02	1.71	1.51
1	59-B	179	CYS	CB-SG	7.96	1.95	1.82
1	3-A	97	GLU	CG-CD	7.76	1.63	1.51
1	33-A	179	CYS	CB-SG	7.48	1.95	1.82
1	35-B	204	CYS	CB-SG	-7.42	1.69	1.82
1	41-B	204	CYS	CB-SG	7.33	1.94	1.82
1	76-B	42	CYS	CB-SG	7.32	1.94	1.82
1	74-B	226	VAL	CB-CG1	-7.26	1.37	1.52
1	20-B	175	ARG	CG-CD	-7.21	1.33	1.51
1	24-A	137	ARG	CB-CG	7.19	1.72	1.52
1	37-B	204	CYS	CB-SG	-7.14	1.70	1.82
1	59-B	204	CYS	CB-SG	7.13	1.94	1.82
1	9-A	42	CYS	CB-SG	7.10	1.94	1.82
1	66-B	204	CYS	CB-SG	6.99	1.94	1.82
1	49-B	204	CYS	CB-SG	-6.97	1.70	1.82
1	51-B	204	CYS	CB-SG	6.97	1.94	1.82
1	24-A	137	ARG	CG-CD	6.96	1.69	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	71-A	226	VAL	CA-CB	6.91	1.69	1.54
1	38-B	204	CYS	CB-SG	6.90	1.94	1.82
1	63-A	204	CYS	CB-SG	6.82	1.93	1.82
1	20-B	62	GLN	CG-CD	6.73	1.66	1.51
1	60-B	42	CYS	CB-SG	6.68	1.93	1.82
1	58-B	204	CYS	CB-SG	6.64	1.93	1.82
1	10-A	204	CYS	CB-SG	6.59	1.93	1.82
1	69-A	172	GLU	CB-CG	6.56	1.64	1.52
1	43-A	226	VAL	CB-CG1	-6.55	1.39	1.52
1	29-A	179	CYS	CB-SG	6.55	1.93	1.82
1	24-B	208	LYS	CE-NZ	6.45	1.65	1.49
1	72-B	227	LEU	CG-CD2	6.41	1.75	1.51
1	34-A	179	CYS	CB-SG	6.40	1.93	1.82
1	63-A	42	CYS	CB-SG	-6.30	1.71	1.82
1	4-A	172	GLU	CB-CG	6.30	1.64	1.52
1	2-A	148	VAL	CB-CG1	-6.25	1.39	1.52
1	42-A	226	VAL	CB-CG2	-6.23	1.39	1.52
1	17-A	179	CYS	CB-SG	6.20	1.92	1.82
1	60-B	33	GLU	CB-CG	6.17	1.63	1.52
1	9-B	226	VAL	CB-CG1	6.16	1.65	1.52
1	68-A	166	GLU	CB-CG	6.07	1.63	1.52
1	48-B	226	VAL	CB-CG1	6.07	1.65	1.52
1	18-B	204	CYS	CB-SG	6.01	1.92	1.82
1	10-A	42	CYS	CB-SG	6.00	1.92	1.82
1	55-A	33	GLU	CB-CG	-5.97	1.40	1.52
1	14-A	172	GLU	CB-CG	5.97	1.63	1.52
1	18-A	172	GLU	CB-CG	5.96	1.63	1.52
1	13-B	33	GLU	CB-CG	5.92	1.63	1.52
1	34-A	215	ARG	CD-NE	-5.91	1.36	1.46
1	71-B	179	CYS	CB-SG	5.89	1.92	1.82
1	73-A	166	GLU	CB-CG	5.89	1.63	1.52
1	26-A	82	GLN	CG-CD	5.89	1.64	1.51
1	74-A	131	VAL	CB-CG1	-5.84	1.40	1.52
1	77-B	204	CYS	CB-SG	-5.83	1.72	1.81
1	59-A	26	CYS	CB-SG	-5.74	1.72	1.81
1	77-B	33	GLU	CD-OE2	5.71	1.31	1.25
1	70-A	48	ASP	CB-CG	-5.71	1.39	1.51
1	66-A	26	CYS	CB-SG	-5.69	1.72	1.81
1	71-A	210	PRO	CA-C	5.66	1.64	1.52
1	77-B	33	GLU	CB-CG	5.64	1.62	1.52
1	11-A	68	ARG	CG-CD	5.64	1.66	1.51
1	71-A	226	VAL	CB-CG2	5.64	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	52-A	166	GLU	CB-CG	5.61	1.62	1.52
1	61-B	204	CYS	CB-SG	-5.61	1.72	1.81
1	74-A	200	GLY	C-O	5.60	1.32	1.23
1	44-A	179	CYS	CB-SG	5.57	1.91	1.82
1	12-A	213	TYR	CD2-CE2	-5.57	1.30	1.39
1	10-A	112	ARG	CG-CD	5.56	1.65	1.51
1	70-A	213	TYR	CD2-CE2	-5.54	1.31	1.39
1	69-A	226	VAL	CB-CG2	-5.53	1.41	1.52
1	74-B	136	ARG	CB-CG	5.51	1.67	1.52
1	63-A	185	GLY	CA-C	5.50	1.60	1.51
1	54-A	42	CYS	CB-SG	5.49	1.91	1.82
1	53-B	204	CYS	CB-SG	-5.48	1.72	1.81
1	76-A	180	LYS	CD-CE	-5.48	1.37	1.51
1	6-A	179	CYS	CB-SG	-5.45	1.73	1.81
1	28-A	53	VAL	CB-CG2	-5.43	1.41	1.52
1	2-A	68	ARG	CG-CD	5.42	1.65	1.51
1	50-A	42	CYS	CB-SG	5.42	1.91	1.82
1	77-A	8	GLU	CB-CG	5.42	1.62	1.52
1	36-A	42	CYS	CB-SG	-5.41	1.73	1.81
1	59-B	137	ARG	CZ-NH2	5.40	1.40	1.33
1	22-B	97	GLU	CB-CG	5.40	1.62	1.52
1	24-A	138	PRO	CG-CD	5.40	1.68	1.50
1	61-A	204	CYS	CB-SG	-5.39	1.73	1.81
1	34-A	172	GLU	CB-CG	5.37	1.62	1.52
1	34-A	182	ASP	N-CA	5.36	1.57	1.46
1	68-B	189	CYS	CB-SG	-5.36	1.73	1.81
1	67-B	47	ALA	CA-CB	5.35	1.63	1.52
1	60-B	204	CYS	CB-SG	5.35	1.91	1.82
1	28-B	204	CYS	CB-SG	5.35	1.91	1.82
1	67-A	15	MET	CB-CG	5.34	1.68	1.51
1	32-A	128	TRP	CB-CG	5.34	1.59	1.50
1	70-A	68	ARG	CZ-NH1	5.32	1.40	1.33
1	5-A	209	LYS	CB-CG	5.31	1.66	1.52
1	41-A	226	VAL	CB-CG2	-5.31	1.41	1.52
1	68-A	179	CYS	CB-SG	5.30	1.91	1.82
1	40-A	166	GLU	CD-OE2	5.25	1.31	1.25
1	18-A	166	GLU	CB-CG	5.23	1.62	1.52
1	70-A	68	ARG	CB-CG	-5.22	1.38	1.52
1	10-B	8	GLU	CG-CD	5.19	1.59	1.51
1	20-A	26	CYS	CB-SG	-5.17	1.73	1.81
1	10-A	8	GLU	CG-CD	5.16	1.59	1.51
1	65-A	44	GLU	CB-CG	5.16	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	31-A	197	VAL	CB-CG1	-5.16	1.42	1.52
1	52-A	179	CYS	CB-SG	5.14	1.91	1.82
1	4-A	215	ARG	CD-NE	-5.13	1.37	1.46
1	4-A	172	GLU	CG-CD	5.13	1.59	1.51
1	5-A	130	ILE	CA-CB	5.11	1.66	1.54
1	45-B	6	GLU	CG-CD	5.11	1.59	1.51
1	34-A	181	GLY	CA-C	5.10	1.60	1.51
1	38-A	204	CYS	CB-SG	5.05	1.90	1.82
1	76-B	33	GLU	CG-CD	5.05	1.59	1.51
1	28-A	180	LYS	N-CA	5.04	1.56	1.46
1	69-A	215	ARG	CD-NE	-5.03	1.38	1.46
1	7-A	185	GLY	C-O	-5.03	1.15	1.23
1	10-A	215	ARG	CD-NE	-5.03	1.38	1.46
1	28-A	204	CYS	CB-SG	5.03	1.90	1.82
1	7-B	8	GLU	CB-CG	5.01	1.61	1.52
1	28-A	210	PRO	CA-C	5.01	1.62	1.52
1	2-B	42	CYS	CB-SG	5.01	1.90	1.82
1	11-A	156	ARG	CZ-NH1	-5.00	1.26	1.33

All (535) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	41-A	115	ARG	NE-CZ-NH2	-18.51	111.04	120.30
1	41-A	215	ARG	NE-CZ-NH1	16.22	128.41	120.30
1	24-A	137	ARG	NE-CZ-NH1	15.96	128.28	120.30
1	74-A	215	ARG	NE-CZ-NH2	-14.64	112.98	120.30
1	41-A	215	ARG	NE-CZ-NH2	-14.54	113.03	120.30
1	44-A	215	ARG	NE-CZ-NH2	-14.12	113.24	120.30
1	26-A	215	ARG	NE-CZ-NH2	-13.72	113.44	120.30
1	44-A	215	ARG	NE-CZ-NH1	13.60	127.10	120.30
1	28-A	215	ARG	NE-CZ-NH2	-13.34	113.63	120.30
1	63-A	215	ARG	NE-CZ-NH2	-13.29	113.65	120.30
1	30-A	215	ARG	NE-CZ-NH2	-13.23	113.68	120.30
1	10-A	215	ARG	NE-CZ-NH2	-13.22	113.69	120.30
1	35-A	215	ARG	NE-CZ-NH2	-12.77	113.92	120.30
1	63-A	215	ARG	NE-CZ-NH1	12.75	126.67	120.30
1	10-A	215	ARG	NE-CZ-NH1	12.40	126.50	120.30
1	28-A	215	ARG	NE-CZ-NH1	12.39	126.50	120.30
1	29-A	215	ARG	NE-CZ-NH2	-12.28	114.16	120.30
1	8-A	215	ARG	NE-CZ-NH2	-11.74	114.43	120.30
1	42-A	209	LYS	C-N-CD	-11.52	95.27	120.60
1	41-A	209	LYS	C-N-CD	-11.51	95.29	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	24-A	215	ARG	NE-CZ-NH2	-11.46	114.57	120.30
1	57-A	215	ARG	NE-CZ-NH2	-11.42	114.59	120.30
1	18-A	215	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	55-A	215	ARG	NE-CZ-NH2	-11.03	114.79	120.30
1	26-A	215	ARG	NE-CZ-NH1	10.71	125.65	120.30
1	46-A	112	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	49-A	112	ARG	NE-CZ-NH1	10.63	125.61	120.30
1	48-A	215	ARG	NE-CZ-NH2	-10.63	114.98	120.30
1	62-A	215	ARG	NE-CZ-NH2	-10.60	115.00	120.30
1	33-A	215	ARG	NE-CZ-NH2	-10.58	115.01	120.30
1	27-A	215	ARG	NE-CZ-NH2	-10.54	115.03	120.30
1	55-A	215	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	13-A	2	LEU	CA-CB-CG	9.68	137.57	115.30
1	27-A	215	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	4-A	215	ARG	NE-CZ-NH2	-9.51	115.55	120.30
1	36-A	43	LEU	CA-CB-CG	9.37	136.84	115.30
1	24-A	137	ARG	NE-CZ-NH2	-9.35	115.63	120.30
1	70-A	68	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	36-A	215	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	41-A	115	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	49-A	112	ARG	NE-CZ-NH2	-9.15	115.73	120.30
1	23-A	112	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	9-A	215	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	72-A	215	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	74-A	74	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	74-A	179	CYS	CA-CB-SG	8.95	130.12	114.00
1	71-A	215	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	44-A	112	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	28-A	5	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	42-B	205	GLY	N-CA-C	-8.79	91.14	113.10
1	42-A	106	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	43-A	215	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	66-B	5	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	65-A	112	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	49-A	15	MET	CG-SD-CE	8.64	114.02	100.20
1	57-A	215	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	42-A	115	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	73-A	215	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	74-A	215	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	24-A	215	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	77-A	43	LEU	CB-CG-CD2	8.56	125.56	111.00
1	67-A	129	GLY	N-CA-C	8.51	134.38	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	33-A	215	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	1-A	215	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	55-A	157	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	48-A	215	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	8-A	215	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	60-A	68	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	13-A	106	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	30-A	215	ARG	NE-CZ-NH1	8.17	124.38	120.30
1	70-A	227	LEU	CB-CG-CD1	8.16	124.88	111.00
1	7-A	179	CYS	N-CA-C	-8.08	89.18	111.00
1	23-A	182	ASP	N-CA-C	8.07	132.80	111.00
1	73-A	226	VAL	CB-CA-C	7.99	126.57	111.40
1	54-A	106	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	9-A	215	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	16-A	200	GLY	N-CA-C	7.97	133.03	113.10
1	23-A	182	ASP	CB-CG-OD2	-7.97	111.13	118.30
1	58-A	112	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	29-A	129	GLY	N-CA-C	7.82	132.64	113.10
1	25-A	45	ASP	N-CA-C	7.79	132.02	111.00
1	61-A	73	LEU	CA-CB-CG	7.76	133.16	115.30
1	26-A	43	LEU	CA-CB-CG	7.74	133.10	115.30
1	72-A	227	LEU	CA-CB-CG	7.73	133.07	115.30
1	22-A	43	LEU	CB-CG-CD1	7.70	124.09	111.00
1	35-A	215	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	71-A	49	GLY	N-CA-C	-7.66	93.95	113.10
1	68-B	205	GLY	N-CA-C	-7.61	94.07	113.10
1	47-B	175	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	22-B	5	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	22-A	215	ARG	CG-CD-NE	-7.52	96.01	111.80
1	62-A	215	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	22-A	68	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	22-A	43	LEU	CA-CB-CG	7.50	132.56	115.30
1	29-A	215	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	22-B	167	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	39-A	199	SER	N-CA-CB	-7.40	99.40	110.50
1	42-A	2	LEU	CA-CB-CG	7.38	132.28	115.30
1	57-B	136	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	24-A	182	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	40-A	112	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	63-B	115	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	7-A	182	ASP	CB-CA-C	7.34	125.09	110.40
1	22-A	179	CYS	CA-CB-SG	7.33	127.19	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	46-A	68	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	38-B	175	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	71-A	209	LYS	C-N-CD	-7.29	104.57	120.60
1	1-A	137	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	16-A	175	ARG	N-CA-C	-7.26	91.41	111.00
1	28-A	182	ASP	CB-CG-OD2	7.26	124.83	118.30
1	64-A	215	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	64-A	15	MET	CG-SD-CE	7.20	111.72	100.20
1	11-B	5	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	11-B	5	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	6-A	137	ARG	C-N-CD	7.16	143.44	128.40
1	23-A	200	GLY	N-CA-C	-7.15	95.23	113.10
1	61-A	68	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	54-A	106	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	55-A	106	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	32-B	227	LEU	CA-CB-CG	7.11	131.66	115.30
1	53-B	74	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	71-A	210	PRO	N-CA-C	7.10	130.57	112.10
1	65-A	137	ARG	C-N-CD	7.10	143.31	128.40
1	37-A	182	ASP	CB-CG-OD2	7.08	124.67	118.30
1	35-A	115	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	38-A	115	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	34-A	215	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	11-A	156	ARG	NE-CZ-NH2	7.05	123.83	120.30
1	23-A	112	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	4-A	137	ARG	C-N-CD	7.03	143.17	128.40
1	1-B	227	LEU	CA-CB-CG	7.02	131.45	115.30
1	28-A	5	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	44-A	112	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	49-A	177	ASP	CB-CG-OD1	6.98	124.58	118.30
1	22-B	45	ASP	CB-CG-OD2	6.98	124.58	118.30
1	13-A	112	ARG	NE-CZ-NH2	6.97	123.78	120.30
1	46-A	136	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	12-A	182	ASP	CB-CG-OD1	-6.93	112.06	118.30
1	13-A	49	GLY	N-CA-C	-6.93	95.76	113.10
1	38-A	3	GLY	N-CA-C	-6.92	95.80	113.10
1	12-A	115	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	63-A	185	GLY	N-CA-C	6.91	130.38	113.10
1	28-A	179	CYS	N-CA-C	6.91	129.65	111.00
1	7-A	227	LEU	CA-CB-CG	6.89	131.15	115.30
1	76-B	41	HIS	CB-CA-C	-6.89	96.62	110.40
1	50-B	68	ARG	NE-CZ-NH2	-6.88	116.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	39-A	215	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	18-B	204	CYS	CA-CB-SG	6.84	126.32	114.00
1	42-A	74	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	54-A	112	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	25-A	180	LYS	N-CA-C	6.78	129.32	111.00
1	44-A	227	LEU	CA-CB-CG	6.76	130.85	115.30
1	37-A	2	LEU	CA-CB-CG	6.76	130.84	115.30
1	24-A	43	LEU	CA-CB-CG	6.73	130.78	115.30
1	44-B	226	VAL	N-CA-C	-6.73	92.84	111.00
1	28-A	106	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	40-B	204	CYS	CA-CB-SG	-6.69	101.95	114.00
1	45-B	112	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	22-A	224	ASP	CB-CG-OD1	6.68	124.31	118.30
1	20-A	112	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	69-A	129	GLY	N-CA-C	6.67	129.76	113.10
1	38-A	115	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	73-A	215	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	27-A	182	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	50-B	68	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	40-A	174	ASN	N-CA-C	-6.60	93.17	111.00
1	52-B	5	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	45-A	68	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	58-A	183	SER	N-CA-C	6.56	128.71	111.00
1	74-A	129	GLY	N-CA-C	6.55	129.49	113.10
1	46-B	5	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	46-A	138	PRO	N-CA-C	6.52	129.06	112.10
1	64-A	215	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	75-A	215	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	11-A	215	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	37-A	85	THR	N-CA-C	-6.51	93.43	111.00
1	55-A	106	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	50-B	204	CYS	N-CA-C	-6.48	93.51	111.00
1	15-B	5	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	38-B	68	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	5-A	181	GLY	N-CA-C	6.47	129.27	113.10
1	71-A	68	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	8-A	227	LEU	CA-CB-CG	6.46	130.15	115.30
1	47-A	112	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	75-A	215	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	52-A	199	SER	N-CA-C	6.44	128.39	111.00
1	22-A	182	ASP	N-CA-C	6.44	128.39	111.00
1	30-B	200	GLY	N-CA-C	-6.43	97.02	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	14-B	115	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	58-A	129	GLY	N-CA-C	-6.41	97.08	113.10
1	51-A	199	SER	N-CA-CB	6.40	120.10	110.50
1	36-B	176	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	65-B	137	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	33-A	199	SER	N-CA-C	-6.38	93.78	111.00
1	35-A	181	GLY	N-CA-C	6.38	129.04	113.10
1	32-A	199	SER	N-CA-C	-6.37	93.81	111.00
1	44-A	181	GLY	N-CA-C	6.36	129.00	113.10
1	14-A	198	THR	N-CA-C	6.36	128.17	111.00
1	34-A	137	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	7-A	68	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	61-A	68	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	28-A	112	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	32-B	227	LEU	CB-CG-CD1	6.30	121.71	111.00
1	9-B	226	VAL	CG1-CB-CG2	6.30	120.97	110.90
1	24-A	182	ASP	CB-CG-OD1	6.30	123.97	118.30
1	3-A	198	THR	CB-CA-C	-6.28	94.63	111.60
1	33-A	209	LYS	C-N-CD	6.26	141.54	128.40
1	17-A	129	GLY	N-CA-C	6.24	128.70	113.10
1	39-B	74	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	68-A	84	ASP	CB-CG-OD2	6.24	123.91	118.30
1	66-A	204	CYS	CA-CB-SG	6.24	125.22	114.00
1	13-A	2	LEU	CB-CG-CD2	6.23	121.59	111.00
1	37-B	204	CYS	CA-CB-SG	-6.23	102.78	114.00
1	17-A	176	ARG	N-CA-C	6.23	127.81	111.00
1	18-A	135	GLY	N-CA-C	-6.23	97.53	113.10
1	63-B	115	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	71-A	215	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	12-A	215	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	57-A	15	MET	CG-SD-CE	6.20	110.12	100.20
1	4-B	137	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	12-A	115	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	46-A	205	GLY	N-CA-C	-6.18	97.65	113.10
1	41-A	215	ARG	CD-NE-CZ	6.18	132.25	123.60
1	58-B	204	CYS	CA-CB-SG	6.17	125.11	114.00
1	69-A	68	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	32-A	215	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	39-B	74	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	34-A	207	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	53-B	74	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	11-A	130	ILE	N-CA-C	6.14	127.57	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	76-A	129	GLY	N-CA-C	6.14	128.44	113.10
1	3-A	129	GLY	N-CA-C	6.13	128.44	113.10
1	30-A	227	LEU	CA-CB-CG	6.13	129.41	115.30
1	22-A	203	VAL	N-CA-C	-6.13	94.45	111.00
1	7-B	227	LEU	CB-CG-CD2	-6.12	100.59	111.00
1	28-A	156	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	63-A	139	ASP	CB-CG-OD1	-6.12	112.80	118.30
1	26-A	49	GLY	N-CA-C	-6.12	97.81	113.10
1	11-B	205	GLY	N-CA-C	-6.11	97.82	113.10
1	14-A	5	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	39-A	2	LEU	N-CA-C	-6.10	94.52	111.00
1	20-B	25	LEU	CA-CB-CG	6.10	129.33	115.30
1	59-A	43	LEU	CA-CB-CG	6.09	129.30	115.30
1	36-B	44	GLU	OE1-CD-OE2	-6.08	116.00	123.30
1	73-A	227	LEU	CA-CB-CG	6.08	129.28	115.30
1	67-B	68	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	71-A	106	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	6-A	182	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	72-A	4	GLY	N-CA-C	-6.05	97.97	113.10
1	31-A	2	LEU	CA-CB-CG	6.05	129.21	115.30
1	44-A	15	MET	CG-SD-CE	-6.04	90.53	100.20
1	63-A	15	MET	CG-SD-CE	-6.04	90.53	100.20
1	42-A	209	LYS	C-N-CA	6.03	147.31	122.00
1	35-A	115	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	22-B	5	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	6-A	115	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	31-A	106	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	12-A	15	MET	CG-SD-CE	-6.01	90.59	100.20
1	36-A	85	THR	N-CA-C	-6.00	94.79	111.00
1	54-B	74	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	50-A	2	LEU	CA-CB-CG	5.99	129.07	115.30
1	37-A	106	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	8-A	68	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	75-A	128	TRP	N-CA-C	-5.97	94.89	111.00
1	77-A	182	ASP	CB-CG-OD2	5.97	123.67	118.30
1	36-A	15	MET	CG-SD-CE	5.96	109.74	100.20
1	36-A	2	LEU	CA-CB-CG	5.96	129.00	115.30
1	62-A	43	LEU	CA-CB-CG	5.96	129.00	115.30
1	28-B	136	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	22-B	45	ASP	CB-CG-OD1	-5.95	112.94	118.30
1	46-A	73	LEU	CA-CB-CG	5.94	128.97	115.30
1	4-A	224	ASP	CB-CG-OD1	-5.94	112.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	13-A	215	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	17-A	183	SER	N-CA-C	-5.93	94.98	111.00
1	34-A	112	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	18-A	215	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	53-A	182	ASP	N-CA-C	5.91	126.96	111.00
1	59-B	156	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	47-A	200	GLY	N-CA-C	-5.91	98.33	113.10
1	38-A	200	GLY	N-CA-C	5.91	127.86	113.10
1	72-B	227	LEU	CD1-CG-CD2	5.90	128.21	110.50
1	60-A	43	LEU	CA-CB-CG	5.90	128.87	115.30
1	37-A	227	LEU	CA-CB-CG	5.89	128.85	115.30
1	74-A	178	SER	N-CA-C	5.87	126.86	111.00
1	22-A	68	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	44-A	106	ARG	NE-CZ-NH2	5.87	123.24	120.30
1	13-A	106	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	14-A	68	ARG	CB-CG-CD	5.87	126.85	111.60
1	32-B	108	LEU	CA-CB-CG	5.86	128.77	115.30
1	66-A	129	GLY	N-CA-C	5.85	127.73	113.10
1	9-B	45	ASP	CB-CG-OD1	5.85	123.56	118.30
1	17-B	43	LEU	CA-CB-CG	5.84	128.74	115.30
1	63-A	215	ARG	CD-NE-CZ	5.84	131.78	123.60
1	39-A	5	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	10-A	182	ASP	CB-CA-C	-5.83	98.75	110.40
1	77-A	43	LEU	CA-CB-CG	5.83	128.70	115.30
1	22-A	43	LEU	CB-CG-CD2	-5.82	101.10	111.00
1	52-A	215	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	2-A	15	MET	CG-SD-CE	-5.79	90.93	100.20
1	3-A	137	ARG	C-N-CD	5.79	140.55	128.40
1	44-A	178	SER	N-CA-C	5.78	126.61	111.00
1	57-A	8	GLU	CA-CB-CG	5.78	126.12	113.40
1	39-A	182	ASP	N-CA-C	-5.78	95.40	111.00
1	19-A	215	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	44-A	215	ARG	CD-NE-CZ	5.77	131.68	123.60
1	74-A	183	SER	N-CA-C	5.76	126.56	111.00
1	53-A	184	GLY	N-CA-C	5.76	127.51	113.10
1	77-A	15	MET	CG-SD-CE	-5.76	90.99	100.20
1	20-A	183	SER	C-N-CA	-5.75	110.22	122.30
1	1-A	187	LEU	CA-CB-CG	5.72	128.46	115.30
1	71-A	68	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	37-A	106	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	57-A	128	TRP	N-CA-C	5.72	126.44	111.00
1	33-A	228	ALA	N-CA-C	5.71	126.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	28-A	43	LEU	CA-CB-CG	5.71	128.43	115.30
1	5-A	224	ASP	N-CA-CB	5.70	120.86	110.60
1	11-A	115	ARG	CB-CG-CD	5.70	126.42	111.60
1	52-B	113	VAL	CG1-CB-CG2	5.70	120.02	110.90
1	68-A	115	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	69-A	215	ARG	CG-CD-NE	-5.70	99.84	111.80
1	11-A	209	LYS	N-CA-C	5.69	126.37	111.00
1	41-B	68	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	4-A	181	GLY	N-CA-C	5.68	127.30	113.10
1	51-B	50	LYS	N-CA-C	-5.68	95.67	111.00
1	53-A	224	ASP	CB-CG-OD1	5.68	123.41	118.30
1	67-B	68	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	73-A	181	GLY	N-CA-C	-5.67	98.92	113.10
1	69-A	49	GLY	N-CA-C	-5.66	98.95	113.10
1	36-A	106	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	17-A	175	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	32-A	48	ASP	N-CA-C	5.66	126.27	111.00
1	38-A	215	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	9-A	209	LYS	N-CA-C	-5.65	95.75	111.00
1	64-A	106	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	45-A	68	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	47-A	2	LEU	CA-CB-CG	5.64	128.26	115.30
1	10-A	112	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	14-A	49	GLY	N-CA-C	-5.63	99.01	113.10
1	51-A	112	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	42-A	3	GLY	N-CA-C	5.63	127.17	113.10
1	54-A	204	CYS	N-CA-C	5.63	126.20	111.00
1	7-B	68	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	34-A	201	SER	CB-CA-C	-5.61	99.45	110.10
1	73-A	68	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	34-A	201	SER	N-CA-C	5.60	126.11	111.00
1	70-A	215	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	46-A	137	ARG	N-CA-C	5.59	126.11	111.00
1	12-A	227	LEU	CA-CB-CG	5.58	128.14	115.30
1	14-A	68	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	67-A	48	ASP	N-CA-C	-5.58	95.93	111.00
1	39-A	174	ASN	N-CA-C	-5.58	95.95	111.00
1	44-A	49	GLY	N-CA-C	-5.58	99.16	113.10
1	68-A	115	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	49-A	215	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	51-A	3	GLY	N-CA-C	-5.57	99.17	113.10
1	12-A	73	LEU	CB-CG-CD1	-5.56	101.54	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	49-A	3	GLY	N-CA-C	-5.56	99.20	113.10
1	1-A	137	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	44-A	224	ASP	CB-CG-OD2	5.56	123.30	118.30
1	64-B	46	ALA	N-CA-C	-5.56	95.99	111.00
1	11-A	201	SER	N-CA-C	-5.56	95.99	111.00
1	65-A	112	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	52-A	49	GLY	N-CA-C	5.54	126.95	113.10
1	8-B	45	ASP	CB-CG-OD1	-5.54	113.32	118.30
1	25-A	15	MET	CG-SD-CE	-5.54	91.34	100.20
1	29-B	108	LEU	CA-CB-CG	5.53	128.03	115.30
1	54-B	5	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	64-A	203	VAL	N-CA-C	-5.53	96.06	111.00
1	62-A	201	SER	N-CA-CB	5.53	118.79	110.50
1	10-A	74	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	27-A	182	ASP	CB-CG-OD1	5.53	123.27	118.30
1	54-A	112	ARG	CB-CA-C	-5.53	99.35	110.40
1	15-A	48	ASP	N-CA-C	5.52	125.91	111.00
1	7-A	215	ARG	CG-CD-NE	-5.52	100.21	111.80
1	49-A	209	LYS	C-N-CD	5.51	139.98	128.40
1	68-A	84	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	38-A	2	LEU	CA-CB-CG	5.51	127.96	115.30
1	9-A	42	CYS	CB-CA-C	5.50	121.40	110.40
1	51-B	204	CYS	CA-CB-SG	5.50	123.89	114.00
1	68-A	125	VAL	CB-CA-C	-5.50	100.96	111.40
1	8-A	115	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	43-B	226	VAL	N-CA-C	-5.48	96.19	111.00
1	9-A	68	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	24-A	200	GLY	N-CA-C	5.47	126.78	113.10
1	49-A	182	ASP	N-CA-C	5.47	125.77	111.00
1	58-B	137	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	10-A	15	MET	CG-SD-CE	5.47	108.95	100.20
1	50-A	183	SER	N-CA-C	5.47	125.77	111.00
1	13-A	128	TRP	CB-CA-C	5.46	121.32	110.40
1	11-A	49	GLY	N-CA-C	-5.45	99.47	113.10
1	42-A	112	ARG	CG-CD-NE	5.45	123.25	111.80
1	48-A	4	GLY	N-CA-C	-5.45	99.47	113.10
1	7-A	182	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	63-A	3	GLY	N-CA-C	-5.44	99.49	113.10
1	38-B	108	LEU	CA-CB-CG	5.44	127.81	115.30
1	23-B	5	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	11-A	68	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	33-A	15	MET	CG-SD-CE	-5.43	91.51	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	64-A	132	ASN	N-CA-C	-5.43	96.34	111.00
1	8-B	137	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	26-B	227	LEU	CA-CB-CG	5.43	127.78	115.30
1	42-A	199	SER	N-CA-C	5.42	125.64	111.00
1	42-A	198	THR	N-CA-C	5.42	125.63	111.00
1	48-A	200	GLY	N-CA-C	5.42	126.64	113.10
1	4-A	174	ASN	N-CA-C	-5.41	96.38	111.00
1	72-A	139	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	60-A	115	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	9-A	200	GLY	N-CA-C	-5.40	99.61	113.10
1	64-B	112	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	37-A	209	LYS	N-CA-C	5.39	125.56	111.00
1	16-A	198	THR	CB-CA-C	-5.39	97.05	111.60
1	68-A	68	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	70-B	5	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	58-A	43	LEU	CA-CB-CG	5.38	127.67	115.30
1	67-A	179	CYS	CA-CB-SG	5.37	123.67	114.00
1	19-A	124	ASP	CB-CG-OD2	5.37	123.14	118.30
1	73-B	5	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	66-A	68	ARG	CG-CD-NE	5.37	123.08	111.80
1	28-A	215	ARG	CD-NE-CZ	5.36	131.11	123.60
1	49-A	115	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	3-A	182	ASP	N-CA-C	-5.36	96.53	111.00
1	40-B	200	GLY	N-CA-C	-5.36	99.70	113.10
1	43-A	215	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	53-A	156	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	73-A	175	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	20-A	129	GLY	N-CA-C	5.34	126.45	113.10
1	62-B	108	LEU	CA-CB-CG	5.34	127.58	115.30
1	52-A	227	LEU	CB-CG-CD2	5.34	120.08	111.00
1	44-A	182	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	13-B	108	LEU	CA-CB-CG	5.33	127.55	115.30
1	37-A	131	VAL	N-CA-C	5.32	125.38	111.00
1	67-A	2	LEU	CB-CG-CD2	-5.32	101.95	111.00
1	13-A	200	GLY	N-CA-C	5.32	126.40	113.10
1	1-A	115	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	42-A	106	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	65-B	179	CYS	CB-CA-C	5.30	121.00	110.40
1	30-A	43	LEU	CA-CB-CG	5.29	127.47	115.30
1	25-A	199	SER	N-CA-C	5.29	125.28	111.00
1	41-A	2	LEU	CA-CB-CG	5.29	127.47	115.30
1	5-A	198	THR	N-CA-C	5.29	125.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	36-A	4	GLY	N-CA-C	5.29	126.32	113.10
1	29-B	43	LEU	CA-CB-CG	5.29	127.46	115.30
1	28-A	50	LYS	N-CA-C	5.28	125.25	111.00
1	50-A	199	SER	N-CA-C	5.28	125.25	111.00
1	32-B	68	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	54-A	2	LEU	CB-CG-CD1	-5.27	102.04	111.00
1	63-A	184	GLY	N-CA-C	5.26	126.26	113.10
1	70-A	49	GLY	N-CA-C	-5.26	99.95	113.10
1	76-A	48	ASP	CB-CG-OD1	5.25	123.03	118.30
1	38-A	182	ASP	CB-CA-C	-5.24	99.92	110.40
1	55-A	157	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	31-A	68	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	16-A	179	CYS	N-CA-C	5.23	125.13	111.00
1	38-A	203	VAL	N-CA-C	5.23	125.11	111.00
1	57-A	129	GLY	N-CA-C	5.23	126.17	113.10
1	5-A	224	ASP	CB-CG-OD1	5.22	123.00	118.30
1	62-B	177	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	16-A	45	ASP	N-CA-C	-5.22	96.91	111.00
1	52-B	206	ASN	N-CA-C	5.22	125.08	111.00
1	62-A	139	ASP	N-CA-C	5.21	125.06	111.00
1	22-A	68	ARG	CG-CD-NE	5.21	122.73	111.80
1	59-A	45	ASP	N-CA-C	5.20	125.05	111.00
1	36-A	179	CYS	N-CA-C	5.20	125.04	111.00
1	16-A	112	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	33-A	2	LEU	CB-CG-CD1	-5.19	102.17	111.00
1	14-A	180	LYS	N-CA-C	5.19	125.00	111.00
1	52-A	202	ALA	N-CA-C	-5.18	97.03	111.00
1	26-A	74	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	29-A	106	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	65-B	179	CYS	CA-CB-SG	5.17	123.30	114.00
1	47-A	115	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	5-B	227	LEU	CA-CB-CG	5.16	127.17	115.30
1	44-A	198	THR	N-CA-C	5.16	124.93	111.00
1	62-A	106	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	5-A	115	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	40-B	204	CYS	N-CA-C	5.16	124.92	111.00
1	23-A	182	ASP	CA-C-N	-5.15	105.87	117.20
1	74-B	200	GLY	N-CA-C	5.15	125.97	113.10
1	46-A	198	THR	N-CA-C	5.15	124.89	111.00
1	32-B	227	LEU	N-CA-C	-5.14	97.11	111.00
1	5-A	224	ASP	CB-CA-C	-5.14	100.12	110.40
1	10-A	74	ARG	NE-CZ-NH1	5.14	122.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	64-A	179	CYS	N-CA-C	5.14	124.88	111.00
1	69-A	176	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	74-A	179	CYS	N-CA-CB	5.14	119.85	110.60
1	50-A	112	ARG	CB-CG-CD	5.14	124.95	111.60
1	12-A	215	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	67-A	227	LEU	CA-CB-CG	5.13	127.10	115.30
1	2-A	156	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	15-B	43	LEU	CA-CB-CG	5.13	127.09	115.30
1	5-A	74	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	46-A	112	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	3-A	15	MET	CG-SD-CE	-5.12	92.00	100.20
1	31-A	182	ASP	N-CA-C	-5.12	97.17	111.00
1	12-A	181	GLY	N-CA-C	5.12	125.90	113.10
1	43-B	137	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	51-A	183	SER	N-CA-C	5.12	124.81	111.00
1	5-A	115	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	57-A	15	MET	CA-CB-CG	5.11	121.98	113.30
1	65-A	3	GLY	N-CA-C	-5.10	100.34	113.10
1	51-B	177	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	24-B	208	LYS	CD-CE-NZ	5.10	123.43	111.70
1	39-A	199	SER	N-CA-C	5.10	124.77	111.00
1	4-A	2	LEU	CB-CG-CD1	5.10	119.67	111.00
1	47-A	86	ILE	CG1-CB-CG2	-5.09	100.19	111.40
1	49-B	74	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	12-A	50	LYS	N-CA-C	5.08	124.72	111.00
1	69-A	199	SER	N-CA-C	5.08	124.72	111.00
1	64-A	74	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	2-B	154	CYS	CA-CB-SG	5.08	123.14	114.00
1	21-A	204	CYS	CA-CB-SG	-5.07	104.87	114.00
1	48-A	130	ILE	CB-CA-C	5.06	121.73	111.60
1	43-A	198	THR	N-CA-C	5.06	124.65	111.00
1	12-A	175	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	30-A	108	LEU	CB-CG-CD2	-5.04	102.44	111.00
1	33-A	183	SER	N-CA-C	5.03	124.58	111.00
1	43-A	179	CYS	CB-CA-C	-5.03	100.34	110.40
1	7-A	182	ASP	CB-CG-OD2	5.03	122.82	118.30
1	50-A	215	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	56-A	179	CYS	N-CA-C	5.03	124.57	111.00
1	21-A	129	GLY	N-CA-C	5.02	125.66	113.10
1	45-B	140	SER	CB-CA-C	-5.02	100.56	110.10
1	59-B	176	ARG	N-CA-C	-5.02	97.44	111.00
1	40-B	43	LEU	CA-CB-CG	5.02	126.85	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	58-A	174	ASN	N-CA-C	5.02	124.56	111.00
1	72-A	134	ALA	N-CA-C	-5.02	97.45	111.00
1	4-A	112	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	15-A	179	CYS	CA-CB-SG	-5.01	104.97	114.00
1	24-A	112	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	6-B	226	VAL	N-CA-C	-5.01	97.47	111.00
1	50-A	174	ASN	N-CA-C	-5.01	97.47	111.00
1	52-B	5	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	1-B	198	THR	CB-CA-C	-5.00	98.09	111.60
1	8-A	68	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	35-A	137	ARG	C-N-CD	-5.00	109.60	120.60

There are no chirality outliers.

All (485) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	1	ILE	Peptide
1	1-A	131	VAL	Peptide
1	1-A	137	ARG	Peptide
1	1-A	178	SER	Peptide
1	1-A	179	CYS	Peptide
1	1-A	49	GLY	Peptide
1	1-B	226	VAL	Peptide
1	1-B	46	ALA	Peptide
1	10-A	131	VAL	Peptide
1	10-A	136	ARG	Peptide
1	10-A	137	ARG	Peptide
1	10-A	178	SER	Peptide
1	10-A	181	GLY	Peptide
1	10-A	201	SER	Peptide
1	10-A	204	CYS	Peptide
1	10-A	227	LEU	Peptide
1	10-A	4	GLY	Peptide
1	10-B	199	SER	Peptide
1	10-B	202	ALA	Peptide
1	11-A	1	ILE	Peptide
1	11-A	137	ARG	Peptide
1	11-A	181	GLY	Peptide
1	11-A	182	ASP	Peptide
1	11-A	45	ASP	Peptide
1	11-A	48	ASP	Peptide
1	11-B	202	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	11-B	203	VAL	Peptide
1	11-B	226	VAL	Peptide
1	11-B	45	ASP	Peptide
1	12-A	178	SER	Peptide
1	12-A	49	GLY	Peptide
1	12-B	225	SER	Peptide
1	13-A	200	GLY	Peptide
1	13-A	205	GLY	Peptide
1	13-A	227	LEU	Peptide
1	13-A	48	ASP	Peptide
1	13-B	44	GLU	Peptide
1	14-A	128	TRP	Peptide
1	14-A	179	CYS	Peptide
1	14-A	199	SER	Peptide
1	14-A	227	LEU	Peptide
1	14-B	204	CYS	Peptide
1	15-A	198	THR	Peptide
1	15-A	206	ASN	Peptide
1	15-A	47	ALA	Peptide
1	15-B	174	ASN	Peptide
1	15-B	202	ALA	Peptide
1	16-A	128	TRP	Peptide
1	16-A	178	SER	Peptide
1	16-A	184	GLY	Peptide
1	16-A	3	GLY	Peptide
1	16-A	44	GLU	Peptide
1	16-B	202	ALA	Peptide
1	17-A	1	ILE	Peptide
1	17-A	136	ARG	Peptide
1	17-A	182	ASP	Peptide
1	17-A	183	SER	Peptide
1	17-A	185	GLY	Peptide
1	17-B	199	SER	Peptide
1	17-B	203	VAL	Peptide
1	17-B	204	CYS	Peptide
1	17-B	32	ALA	Peptide
1	17-B	44	GLU	Peptide
1	18-A	1	ILE	Peptide
1	18-A	130	ILE	Peptide
1	18-A	134	ALA	Peptide
1	18-A	179	CYS	Peptide
1	18-A	201	SER	Peptide

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Mol	Chain	Res	Type	Group
1	18-B	49	GLY	Peptide
1	19-A	130	ILE	Peptide
1	19-A	172	GLU	Peptide
1	19-A	175	ARG	Peptide
1	19-A	176	ARG	Peptide
1	19-A	178	SER	Peptide
1	19-A	182	ASP	Peptide
1	19-B	44	GLU	Peptide
1	2-A	137	ARG	Peptide
1	2-A	173	SER	Peptide
1	2-A	180	LYS	Peptide
1	2-A	181	GLY	Peptide
1	2-A	198	THR	Peptide
1	2-B	226	VAL	Peptide
1	2-B	42	CYS	Peptide
1	20-A	175	ARG	Peptide
1	20-A	176	ARG	Peptide
1	20-A	198	THR	Peptide
1	20-A	202	ALA	Peptide
1	20-A	43	LEU	Peptide
1	20-B	198	THR	Peptide
1	20-B	202	ALA	Peptide
1	20-B	226	VAL	Peptide
1	21-A	178	SER	Peptide
1	21-A	44	GLU	Peptide
1	21-B	133	HIS	Peptide
1	21-B	198	THR	Peptide
1	22-A	1	ILE	Peptide
1	22-A	132	ASN	Peptide
1	22-A	173	SER	Peptide
1	22-A	174	ASN	Peptide
1	22-A	178	SER	Peptide
1	22-A	199	SER	Peptide
1	22-A	203	VAL	Peptide
1	22-A	48	ASP	Peptide
1	22-B	226	VAL	Peptide
1	23-A	182	ASP	Peptide
1	23-A	199	SER	Peptide
1	23-A	203	VAL	Peptide
1	24-A	133	HIS	Peptide
1	24-A	181	GLY	Peptide
1	24-A	197	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	24-A	209	LYS	Peptide
1	24-A	46	ALA	Peptide
1	24-A	83	PRO	Peptide
1	25-A	136	ARG	Peptide
1	25-A	197	VAL	Peptide
1	26-A	136	ARG	Peptide
1	26-A	198	THR	Peptide
1	26-A	43	LEU	Peptide
1	26-A	48	ASP	Peptide
1	26-B	199	SER	Peptide
1	26-B	84	ASP	Mainchain
1	27-A	129	GLY	Peptide
1	27-A	132	ASN	Peptide
1	27-A	135	GLY	Peptide
1	27-A	138	PRO	Peptide
1	27-B	175	ARG	Peptide
1	27-B	201	SER	Peptide
1	28-A	135	GLY	Peptide
1	28-A	176	ARG	Peptide
1	28-A	180	LYS	Peptide
1	28-A	200	GLY	Peptide
1	28-B	45	ASP	Peptide
1	29-A	173	SER	Peptide
1	29-A	2	LEU	Peptide
1	29-A	203	VAL	Peptide
1	29-A	47	ALA	Peptide
1	29-B	50	LYS	Peptide
1	3-A	114	ASP	Peptide
1	3-A	132	ASN	Peptide
1	3-A	173	SER	Peptide
1	3-A	197	VAL	Peptide
1	3-B	46	ALA	Peptide
1	30-A	129	GLY	Peptide
1	30-A	176	ARG	Peptide
1	30-A	209	LYS	Peptide
1	30-B	43	LEU	Peptide
1	31-A	172	GLU	Peptide
1	31-A	173	SER	Peptide
1	31-A	175	ARG	Peptide
1	31-A	179	CYS	Peptide
1	31-A	209	LYS	Peptide
1	31-B	227	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	32-A	1	ILE	Peptide
1	32-A	128	TRP	Peptide
1	32-A	131	VAL	Peptide
1	32-A	172	GLU	Peptide
1	32-A	175	ARG	Peptide
1	32-A	176	ARG	Peptide
1	32-A	180	LYS	Peptide
1	32-A	182	ASP	Peptide
1	32-A	44	GLU	Peptide
1	32-A	48	ASP	Peptide
1	32-B	226	VAL	Peptide
1	33-A	179	CYS	Peptide
1	33-A	180	LYS	Peptide
1	33-A	198	THR	Peptide
1	33-A	202	ALA	Peptide
1	33-A	207	ARG	Peptide
1	33-A	209	LYS	Peptide
1	33-A	226	VAL	Peptide
1	33-A	227	LEU	Peptide
1	34-A	130	ILE	Peptide
1	34-A	179	CYS	Peptide
1	34-A	209	LYS	Peptide
1	34-A	226	VAL	Peptide
1	35-A	128	TRP	Peptide
1	35-A	137	ARG	Peptide
1	35-A	206	ASN	Peptide
1	35-A	209	LYS	Peptide
1	35-B	201	SER	Peptide
1	35-B	204	CYS	Peptide
1	36-A	131	VAL	Peptide
1	36-A	181	GLY	Peptide
1	36-A	46	ALA	Peptide
1	36-B	45	ASP	Peptide
1	37-A	131	VAL	Peptide
1	37-A	175	ARG	Peptide
1	37-A	179	CYS	Peptide
1	37-A	208	LYS	Peptide
1	37-A	226	VAL	Peptide
1	37-A	83	PRO	Peptide
1	37-A	84	ASP	Peptide
1	37-B	204	CYS	Peptide
1	38-A	177	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	38-A	178	SER	Peptide
1	38-A	198	THR	Peptide
1	38-A	209	LYS	Peptide
1	38-A	46	ALA	Peptide
1	38-B	204	CYS	Peptide
1	39-A	1	ILE	Peptide
1	39-A	173	SER	Peptide
1	39-A	198	THR	Peptide
1	39-A	209	LYS	Peptide
1	39-A	225	SER	Peptide
1	4-A	173	SER	Peptide
1	4-A	180	LYS	Peptide
1	4-A	198	THR	Peptide
1	4-A	204	CYS	Peptide
1	4-A	42	CYS	Peptide
1	4-B	202	ALA	Peptide
1	4-B	204	CYS	Peptide
1	4-B	205	GLY	Peptide
1	40-A	1	ILE	Peptide
1	40-A	132	ASN	Peptide
1	40-A	182	ASP	Peptide
1	40-A	209	LYS	Peptide
1	40-A	43	LEU	Peptide
1	40-B	203	VAL	Peptide
1	41-A	1	ILE	Peptide
1	41-A	173	SER	Peptide
1	41-A	178	SER	Peptide
1	41-A	209	LYS	Peptide
1	41-A	225	SER	Peptide
1	41-A	4	GLY	Peptide
1	42-A	1	ILE	Peptide
1	42-A	128	TRP	Peptide
1	42-A	201	SER	Peptide
1	42-A	204	CYS	Peptide
1	42-A	209	LYS	Peptide
1	42-A	227	LEU	Peptide
1	43-A	174	ASN	Peptide
1	43-A	177	ASP	Peptide
1	43-A	179	CYS	Peptide
1	43-A	180	LYS	Peptide
1	43-A	209	LYS	Peptide
1	43-B	132	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	43-B	225	SER	Peptide
1	43-B	227	LEU	Peptide
1	44-A	136	ARG	Peptide
1	44-A	173	SER	Peptide
1	44-A	174	ASN	Peptide
1	44-A	175	ARG	Peptide
1	44-A	181	GLY	Peptide
1	44-A	209	LYS	Peptide
1	44-A	226	VAL	Peptide
1	44-B	198	THR	Peptide
1	44-B	204	CYS	Peptide
1	44-B	224	ASP	Peptide
1	44-B	225	SER	Peptide
1	45-A	137	ARG	Peptide
1	45-A	175	ARG	Peptide
1	45-A	197	VAL	Peptide
1	45-A	43	LEU	Peptide
1	45-A	45	ASP	Peptide
1	45-B	203	VAL	Peptide
1	46-A	138	PRO	Peptide
1	46-A	183	SER	Peptide
1	46-A	197	VAL	Peptide
1	46-A	198	THR	Peptide
1	46-A	203	VAL	Peptide
1	46-A	208	LYS	Peptide
1	46-A	83	PRO	Peptide
1	46-A	85	THR	Peptide
1	46-B	225	SER	Peptide
1	47-A	1	ILE	Peptide
1	47-A	129	GLY	Peptide
1	47-A	138	PRO	Peptide
1	47-A	2	LEU	Peptide
1	47-A	47	ALA	Peptide
1	47-B	225	SER	Peptide
1	48-A	128	TRP	Peptide
1	48-A	138	PRO	Peptide
1	48-A	172	GLU	Peptide
1	48-A	174	ASN	Peptide
1	48-A	177	ASP	Peptide
1	48-A	184	GLY	Peptide
1	48-A	200	GLY	Peptide
1	48-A	205	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	48-A	3	GLY	Peptide
1	48-B	197	VAL	Peptide
1	48-B	225	SER	Peptide
1	49-A	138	PRO	Peptide
1	49-A	182	ASP	Peptide
1	49-A	207	ARG	Peptide
1	49-A	43	LEU	Peptide
1	49-A	47	ALA	Peptide
1	49-B	45	ASP	Peptide
1	5-A	174	ASN	Peptide
1	5-A	2	LEU	Peptide
1	5-A	208	LYS	Peptide
1	5-A	43	LEU	Peptide
1	50-A	129	GLY	Peptide
1	50-A	138	PRO	Peptide
1	50-A	175	ARG	Peptide
1	50-A	181	GLY	Peptide
1	50-A	198	THR	Peptide
1	50-A	42	CYS	Peptide
1	51-A	175	ARG	Peptide
1	51-A	182	ASP	Peptide
1	51-A	183	SER	Peptide
1	51-A	2	LEU	Peptide
1	51-A	206	ASN	Peptide
1	51-A	81	SER	Peptide
1	51-A	84	ASP	Peptide
1	51-B	175	ARG	Peptide
1	52-A	176	ARG	Peptide
1	52-A	181	GLY	Peptide
1	52-A	183	SER	Peptide
1	52-A	198	THR	Peptide
1	52-A	3	GLY	Peptide
1	52-A	42	CYS	Peptide
1	52-A	46	ALA	Peptide
1	53-A	182	ASP	Peptide
1	53-A	202	ALA	Peptide
1	53-A	206	ASN	Peptide
1	53-B	45	ASP	Peptide
1	54-A	177	ASP	Peptide
1	54-A	199	SER	Peptide
1	54-A	203	VAL	Peptide
1	54-B	201	SER	Peptide

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Mol	Chain	Res	Type	Group
1	54-B	204	CYS	Peptide
1	54-B	4	GLY	Peptide
1	54-B	49	GLY	Peptide
1	55-A	1	ILE	Peptide
1	55-A	129	GLY	Peptide
1	55-A	130	ILE	Peptide
1	55-A	181	GLY	Peptide
1	55-A	198	THR	Peptide
1	55-A	199	SER	Peptide
1	55-A	43	LEU	Peptide
1	56-A	178	SER	Peptide
1	57-A	137	ARG	Peptide
1	57-A	138	PRO	Peptide
1	57-A	172	GLU	Peptide
1	57-A	177	ASP	Peptide
1	57-A	198	THR	Peptide
1	57-A	209	LYS	Peptide
1	57-A	47	ALA	Peptide
1	58-A	132	ASN	Peptide
1	58-A	137	ARG	Peptide
1	58-A	178	SER	Peptide
1	58-A	179	CYS	Peptide
1	58-A	4	GLY	Peptide
1	58-B	197	VAL	Peptide
1	58-B	202	ALA	Peptide
1	58-B	204	CYS	Peptide
1	58-B	206	ASN	Peptide
1	58-B	226	VAL	Peptide
1	58-B	49	GLY	Peptide
1	58-B	86	ILE	Peptide
1	59-A	128	TRP	Peptide
1	59-A	133	HIS	Peptide
1	59-A	182	ASP	Peptide
1	59-A	198	THR	Peptide
1	6-A	1	ILE	Peptide
1	6-A	136	ARG	Peptide
1	6-A	137	ARG	Peptide
1	6-A	185	GLY	Peptide
1	6-A	2	LEU	Peptide
1	6-A	3	GLY	Peptide
1	6-B	198	THR	Peptide
1	6-B	225	SER	Peptide

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Mol	Chain	Res	Type	Group
1	60-A	135	GLY	Peptide
1	60-A	45	ASP	Peptide
1	61-B	203	VAL	Peptide
1	62-A	138	PRO	Peptide
1	62-A	203	VAL	Peptide
1	63-A	129	GLY	Peptide
1	63-A	138	PRO	Peptide
1	63-A	2	LEU	Peptide
1	63-B	202	ALA	Peptide
1	63-B	47	ALA	Peptide
1	64-A	114	ASP	Peptide
1	64-A	131	VAL	Peptide
1	64-A	138	PRO	Peptide
1	64-A	185	GLY	Peptide
1	64-A	203	VAL	Peptide
1	64-A	43	LEU	Peptide
1	64-B	226	VAL	Peptide
1	65-A	128	TRP	Peptide
1	65-A	181	GLY	Peptide
1	65-A	44	GLU	Peptide
1	65-A	96	SER	Peptide
1	65-B	198	THR	Peptide
1	66-A	129	GLY	Peptide
1	66-A	132	ASN	Peptide
1	66-A	176	ARG	Peptide
1	66-A	179	CYS	Peptide
1	66-A	182	ASP	Peptide
1	66-A	184	GLY	Peptide
1	66-A	208	LYS	Peptide
1	66-A	49	GLY	Peptide
1	66-A	83	PRO	Peptide
1	66-B	47	ALA	Peptide
1	67-A	129	GLY	Peptide
1	67-A	175	ARG	Peptide
1	67-A	176	ARG	Peptide
1	67-A	182	ASP	Peptide
1	67-A	184	GLY	Peptide
1	67-A	197	VAL	Peptide
1	67-A	2	LEU	Peptide
1	67-A	44	GLU	Peptide
1	67-A	49	GLY	Peptide
1	67-B	203	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	68-A	137	ARG	Peptide
1	68-A	207	ARG	Peptide
1	68-A	3	GLY	Peptide
1	69-A	138	PRO	Peptide
1	69-A	175	ARG	Peptide
1	69-A	178	SER	Peptide
1	69-A	227	LEU	Peptide
1	69-A	43	LEU	Peptide
1	69-A	45	ASP	Peptide
1	69-A	48	ASP	Peptide
1	69-B	132	ASN	Peptide
1	69-B	205	GLY	Peptide
1	7-A	174	ASN	Peptide
1	7-A	184	GLY	Peptide
1	7-A	201	SER	Peptide
1	7-A	3	GLY	Peptide
1	7-A	4	GLY	Peptide
1	7-A	85	THR	Peptide
1	7-B	200	GLY	Peptide
1	7-B	203	VAL	Peptide
1	70-A	132	ASN	Peptide
1	70-A	135	GLY	Peptide
1	70-A	175	ARG	Peptide
1	70-A	176	ARG	Peptide
1	70-A	203	VAL	Peptide
1	70-A	48	ASP	Peptide
1	70-B	134	ALA	Peptide
1	70-B	204	CYS	Peptide
1	70-B	225	SER	Peptide
1	71-A	202	ALA	Peptide
1	71-A	44	GLU	Peptide
1	71-A	46	ALA	Peptide
1	71-B	197	VAL	Peptide
1	71-B	225	SER	Peptide
1	72-A	138	PRO	Peptide
1	72-A	173	SER	Peptide
1	72-A	179	CYS	Peptide
1	72-A	182	ASP	Peptide
1	72-A	201	SER	Peptide
1	72-A	226	VAL	Peptide
1	72-A	45	ASP	Peptide
1	73-A	179	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	73-A	202	ALA	Peptide
1	73-A	226	VAL	Peptide
1	73-A	46	ALA	Peptide
1	73-B	225	SER	Peptide
1	74-A	129	GLY	Peptide
1	74-A	131	VAL	Peptide
1	74-A	132	ASN	Peptide
1	74-A	178	SER	Peptide
1	74-A	226	VAL	Peptide
1	74-B	226	VAL	Peptide
1	75-A	136	ARG	Peptide
1	75-A	138	PRO	Peptide
1	75-A	181	GLY	Peptide
1	75-A	206	ASN	Peptide
1	75-A	226	VAL	Peptide
1	75-B	226	VAL	Peptide
1	76-A	138	PRO	Peptide
1	76-A	179	CYS	Peptide
1	77-A	138	PRO	Peptide
1	77-A	2	LEU	Peptide
1	77-B	227	LEU	Peptide
1	77-B	47	ALA	Peptide
1	8-A	131	VAL	Peptide
1	8-A	175	ARG	Peptide
1	8-A	202	ALA	Peptide
1	8-A	203	VAL	Peptide
1	8-A	205	GLY	Peptide
1	8-A	207	ARG	Peptide
1	8-A	227	LEU	Peptide
1	8-A	4	GLY	Peptide
1	8-A	46	ALA	Peptide
1	8-B	226	VAL	Peptide
1	9-A	135	GLY	Peptide
1	9-A	138	PRO	Peptide
1	9-A	208	LYS	Peptide
1	9-A	43	LEU	Peptide
1	9-A	46	ALA	Peptide
1	9-B	199	SER	Peptide
1	9-B	83	PRO	Peptide

4.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	1706	1700	1690	0	0
1	1-B	1706	1700	1690	0	0
1	2-A	1706	1700	1690	0	0
1	2-B	1706	1700	1690	0	0
1	3-A	1706	1700	1690	0	0
1	3-B	1706	1700	1690	0	0
1	4-A	1706	1700	1690	0	0
1	4-B	1706	1700	1690	0	0
1	5-A	1706	1700	1690	0	0
1	5-B	1706	1700	1690	0	0
1	6-A	1706	1700	1690	0	0
1	6-B	1706	1700	1690	0	0
1	7-A	1706	1700	1690	0	0
1	7-B	1706	1700	1690	0	0
1	8-A	1706	1700	1690	0	0
1	8-B	1706	1700	1690	0	0
1	9-A	1706	1700	1690	0	0
1	9-B	1706	1700	1690	0	0
1	10-A	1706	1700	1690	0	0
1	10-B	1706	1700	1690	0	0
1	11-A	1706	1700	1690	0	0
1	11-B	1706	1700	1690	0	0
1	12-A	1706	1700	1690	0	0
1	12-B	1706	1700	1690	0	0
1	13-A	1706	1700	1690	0	0
1	13-B	1706	1700	1690	0	0
1	14-A	1706	1700	1690	0	0
1	14-B	1706	1700	1690	0	0
1	15-A	1706	1700	1690	0	0
1	15-B	1706	1700	1690	0	0
1	16-A	1706	1700	1690	0	0
1	16-B	1706	1700	1690	0	0
1	17-A	1706	1700	1690	0	0
1	17-B	1706	1700	1690	0	0
1	18-A	1706	1700	1690	0	0
1	18-B	1706	1700	1690	0	0
1	19-A	1706	1700	1690	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	19-B	1706	1700	1690	0	0
1	20-A	1706	1700	1690	0	0
1	20-B	1706	1700	1690	0	0
1	21-A	1706	1700	1690	0	0
1	21-B	1706	1700	1690	0	0
1	22-A	1706	1700	1690	0	0
1	22-B	1706	1700	1690	0	0
1	23-A	1706	1700	1690	0	0
1	23-B	1706	1700	1690	0	0
1	24-A	1706	1700	1690	0	0
1	24-B	1706	1700	1690	0	0
1	25-A	1706	1700	1690	0	0
1	25-B	1706	1700	1690	0	0
1	26-A	1706	1700	1690	0	0
1	26-B	1706	1700	1690	0	0
1	27-A	1706	1700	1690	0	0
1	27-B	1706	1700	1690	0	0
1	28-A	1706	1700	1690	0	0
1	28-B	1706	1700	1690	0	0
1	29-A	1706	1700	1690	0	0
1	29-B	1706	1700	1690	0	0
1	30-A	1706	1700	1690	0	0
1	30-B	1706	1700	1690	0	0
1	31-A	1706	1700	1690	0	0
1	31-B	1706	1700	1690	0	0
1	32-A	1706	1700	1690	0	0
1	32-B	1706	1700	1690	0	0
1	33-A	1706	1700	1690	0	0
1	33-B	1706	1700	1690	0	0
1	34-A	1706	1700	1690	0	0
1	34-B	1706	1700	1690	0	0
1	35-A	1706	1700	1690	0	0
1	35-B	1706	1700	1690	0	0
1	36-A	1706	1700	1690	0	0
1	36-B	1706	1700	1690	0	0
1	37-A	1706	1700	1690	0	0
1	37-B	1706	1700	1690	0	0
1	38-A	1706	1700	1690	0	0
1	38-B	1706	1700	1690	0	0
1	39-A	1706	1700	1690	0	0
1	39-B	1706	1700	1690	0	0
1	40-A	1706	1700	1690	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	40-B	1706	1700	1690	0	0
1	41-A	1706	1700	1690	0	0
1	41-B	1706	1700	1690	0	0
1	42-A	1706	1700	1690	0	0
1	42-B	1706	1700	1690	0	0
1	43-A	1706	1700	1690	0	0
1	43-B	1706	1700	1690	0	0
1	44-A	1706	1700	1690	0	0
1	44-B	1706	1700	1690	0	0
1	45-A	1706	1700	1690	0	0
1	45-B	1706	1700	1690	0	0
1	46-A	1706	1700	1690	0	0
1	46-B	1706	1700	1690	0	0
1	47-A	1706	1700	1690	0	0
1	47-B	1706	1700	1690	0	0
1	48-A	1706	1700	1690	0	0
1	48-B	1706	1700	1690	0	0
1	49-A	1706	1700	1690	0	0
1	49-B	1706	1700	1690	0	0
1	50-A	1706	1700	1690	0	0
1	50-B	1706	1700	1690	0	0
1	51-A	1706	1700	1690	0	0
1	51-B	1706	1700	1690	0	0
1	52-A	1706	1700	1690	0	0
1	52-B	1706	1700	1690	0	0
1	53-A	1706	1700	1690	0	0
1	53-B	1706	1700	1690	0	0
1	54-A	1706	1700	1690	0	0
1	54-B	1706	1700	1690	0	0
1	55-A	1706	1700	1690	0	0
1	55-B	1706	1700	1690	0	0
1	56-A	1706	1700	1690	0	0
1	56-B	1706	1700	1690	0	0
1	57-A	1706	1700	1690	0	0
1	57-B	1706	1700	1690	0	0
1	58-A	1706	1700	1690	0	0
1	58-B	1706	1700	1690	0	0
1	59-A	1706	1700	1690	0	0
1	59-B	1706	1700	1690	0	0
1	60-A	1706	1700	1690	0	0
1	60-B	1706	1700	1690	0	0
1	61-A	1706	1700	1690	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	61-B	1706	1700	1690	0	0
1	62-A	1706	1700	1690	0	0
1	62-B	1706	1700	1690	0	0
1	63-A	1706	1700	1690	0	0
1	63-B	1706	1700	1690	0	0
1	64-A	1706	1700	1690	0	0
1	64-B	1706	1700	1690	0	0
1	65-A	1706	1700	1690	0	0
1	65-B	1706	1700	1690	0	0
1	66-A	1706	1700	1690	0	0
1	66-B	1706	1700	1690	0	0
1	67-A	1706	1700	1690	0	0
1	67-B	1706	1700	1690	0	0
1	68-A	1706	1700	1690	0	0
1	68-B	1706	1700	1690	0	0
1	69-A	1706	1700	1690	0	0
1	69-B	1706	1700	1690	0	0
1	70-A	1706	1700	1690	0	0
1	70-B	1706	1700	1690	0	0
1	71-A	1706	1700	1690	0	0
1	71-B	1706	1700	1690	0	0
1	72-A	1706	1700	1690	0	0
1	72-B	1706	1700	1690	0	0
1	73-A	1706	1700	1690	0	0
1	73-B	1706	1700	1690	0	0
1	74-A	1706	1700	1690	0	0
1	74-B	1706	1700	1690	0	0
1	75-A	1706	1700	1690	0	0
1	75-B	1706	1700	1690	0	0
1	76-A	1706	1700	1690	0	0
1	76-B	1706	1700	1690	0	0
1	77-A	1706	1700	1690	0	0
1	77-B	1706	1700	1690	0	0
2	1-A	6	8	8	0	0
2	1-B	6	8	8	0	0
2	2-A	6	8	8	0	0
2	2-B	6	8	8	0	0
2	3-A	6	8	8	0	0
2	3-B	6	8	8	0	0
2	4-A	6	8	8	0	0
2	4-B	6	8	8	0	0
2	5-A	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	5-B	6	8	8	0	0
2	6-A	6	8	8	0	0
2	6-B	6	8	8	0	0
2	7-A	6	8	8	0	0
2	7-B	6	8	8	0	0
2	8-A	6	8	8	0	0
2	8-B	6	8	8	0	0
2	9-A	6	8	8	0	0
2	9-B	6	8	8	0	0
2	10-A	6	8	8	0	0
2	10-B	6	8	8	0	0
2	11-A	6	8	8	0	0
2	11-B	6	8	8	0	0
2	12-A	6	8	8	0	0
2	12-B	6	8	8	0	0
2	13-A	6	8	8	0	0
2	13-B	6	8	8	0	0
2	14-A	6	8	8	0	0
2	14-B	6	8	8	0	0
2	15-A	6	8	8	0	0
2	15-B	6	8	8	0	0
2	16-A	6	8	8	0	0
2	16-B	6	8	8	0	0
2	17-A	6	8	8	0	0
2	17-B	6	8	8	0	0
2	18-A	6	8	8	0	0
2	18-B	6	8	8	0	0
2	19-A	6	8	8	0	0
2	19-B	6	8	8	0	0
2	20-A	6	8	8	0	0
2	20-B	6	8	8	0	0
2	21-A	6	8	8	0	0
2	21-B	6	8	8	0	0
2	22-A	6	8	8	0	0
2	22-B	6	8	8	0	0
2	23-A	6	8	8	0	0
2	23-B	6	8	8	0	0
2	24-A	6	8	8	0	0
2	24-B	6	8	8	0	0
2	25-A	6	8	8	0	0
2	25-B	6	8	8	0	0
2	26-A	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	26-B	6	8	8	0	0
2	27-A	6	8	8	0	0
2	27-B	6	8	8	0	0
2	28-A	6	8	8	0	0
2	28-B	6	8	8	0	0
2	29-A	6	8	8	0	0
2	29-B	6	8	8	0	0
2	30-A	6	8	8	0	0
2	30-B	6	8	8	0	0
2	31-A	6	8	8	0	0
2	31-B	6	8	8	0	0
2	32-A	6	8	8	0	0
2	32-B	6	8	8	0	0
2	33-A	6	8	8	0	0
2	33-B	6	8	8	0	0
2	34-A	6	8	8	0	0
2	34-B	6	8	8	0	0
2	35-A	6	8	8	0	0
2	35-B	6	8	8	0	0
2	36-A	6	8	8	0	0
2	36-B	6	8	8	0	0
2	37-A	6	8	8	0	0
2	37-B	6	8	8	0	0
2	38-A	6	8	8	0	0
2	38-B	6	8	8	0	0
2	39-A	6	8	8	0	0
2	39-B	6	8	8	0	0
2	40-A	6	8	8	0	0
2	40-B	6	8	8	0	0
2	41-A	6	8	8	0	0
2	41-B	6	8	8	0	0
2	42-A	6	8	8	0	0
2	42-B	6	8	8	0	0
2	43-A	6	8	8	0	0
2	43-B	6	8	8	0	0
2	44-A	6	8	8	0	0
2	44-B	6	8	8	0	0
2	45-A	6	8	8	0	0
2	45-B	6	8	8	0	0
2	46-A	6	8	8	0	0
2	46-B	6	8	8	0	0
2	47-A	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	47-B	6	8	8	0	0
2	48-A	6	8	8	0	0
2	48-B	6	8	8	0	0
2	49-A	6	8	8	0	0
2	49-B	6	8	8	0	0
2	50-A	6	8	8	0	0
2	50-B	6	8	8	0	0
2	51-A	6	8	8	0	0
2	51-B	6	8	8	0	0
2	52-A	6	8	8	0	0
2	52-B	6	8	8	0	0
2	53-A	6	8	8	0	0
2	53-B	6	8	8	0	0
2	54-A	6	8	8	0	0
2	54-B	6	8	8	0	0
2	55-A	6	8	8	0	0
2	55-B	6	8	8	0	0
2	56-A	6	8	8	0	0
2	56-B	6	8	8	0	0
2	57-A	6	8	8	0	0
2	57-B	6	8	8	0	0
2	58-A	6	8	8	0	0
2	58-B	6	8	8	0	0
2	59-A	6	8	8	0	0
2	59-B	6	8	8	0	0
2	60-A	6	8	8	0	0
2	60-B	6	8	8	0	0
2	61-A	6	8	8	0	0
2	61-B	6	8	8	0	0
2	62-A	6	8	8	0	0
2	62-B	6	8	8	0	0
2	63-A	6	8	8	0	0
2	63-B	6	8	8	0	0
2	64-A	6	8	8	0	0
2	64-B	6	8	8	0	0
2	65-A	6	8	8	0	0
2	65-B	6	8	8	0	0
2	66-A	6	8	8	0	0
2	66-B	6	8	8	0	0
2	67-A	6	8	8	0	0
2	67-B	6	8	8	0	0
2	68-A	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	68-B	6	8	8	0	0
2	69-A	6	8	8	0	0
2	69-B	6	8	8	0	0
2	70-A	6	8	8	0	0
2	70-B	6	8	8	0	0
2	71-A	6	8	8	0	0
2	71-B	6	8	8	0	0
2	72-A	6	8	8	0	0
2	72-B	6	8	8	0	0
2	73-A	6	8	8	0	0
2	73-B	6	8	8	0	0
2	74-A	6	8	8	0	0
2	74-B	6	8	8	0	0
2	75-A	6	8	8	0	0
2	75-B	6	8	8	0	0
2	76-A	6	8	8	0	0
2	76-B	6	8	8	0	0
2	77-A	6	8	8	0	0
2	77-B	6	8	8	0	0
3	1-A	148	0	0	0	0
3	1-B	113	0	0	0	0
3	2-A	139	0	0	0	0
3	2-B	122	0	0	0	0
3	3-A	142	0	0	0	0
3	3-B	96	0	0	0	0
3	4-A	129	0	0	0	0
3	4-B	108	0	0	0	0
3	5-A	129	0	0	0	0
3	5-B	109	0	0	0	0
3	6-A	136	0	0	0	0
3	6-B	111	0	0	0	0
3	7-A	134	0	0	0	0
3	7-B	111	0	0	0	0
3	8-A	136	0	0	0	0
3	8-B	104	0	0	0	0
3	9-A	138	0	0	0	0
3	9-B	119	0	0	0	0
3	10-A	135	0	0	0	0
3	10-B	117	0	0	0	0
3	11-A	123	0	0	0	0
3	11-B	118	0	0	0	0
3	12-A	145	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	12-B	115	0	0	0	0
3	13-A	165	0	0	0	0
3	13-B	109	0	0	0	0
3	14-A	157	0	0	0	0
3	14-B	115	0	0	0	0
3	15-A	142	0	0	0	0
3	15-B	113	0	0	0	0
3	16-A	135	0	0	0	0
3	16-B	117	0	0	0	0
3	17-A	142	0	0	0	0
3	17-B	122	0	0	0	0
3	18-A	147	0	0	0	0
3	18-B	111	0	0	0	0
3	19-A	127	0	0	0	0
3	19-B	117	0	0	0	0
3	20-A	131	0	0	0	0
3	20-B	123	0	0	0	0
3	21-A	144	0	0	0	0
3	21-B	103	0	0	0	0
3	22-A	143	0	0	0	0
3	22-B	122	0	0	0	0
3	23-A	142	0	0	0	0
3	23-B	113	0	0	0	0
3	24-A	127	0	0	0	0
3	24-B	116	0	0	0	0
3	25-A	137	0	0	0	0
3	25-B	120	0	0	0	0
3	26-A	145	0	0	0	0
3	26-B	114	0	0	0	0
3	27-A	139	0	0	0	0
3	27-B	114	0	0	0	0
3	28-A	137	0	0	0	0
3	28-B	123	0	0	0	0
3	29-A	135	0	0	0	0
3	29-B	132	0	0	0	0
3	30-A	149	0	0	0	0
3	30-B	115	0	0	0	0
3	31-A	146	0	0	0	0
3	31-B	117	0	0	0	0
3	32-A	135	0	0	0	0
3	32-B	127	0	0	0	0
3	33-A	133	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	33-B	119	0	0	0	0
3	34-A	139	0	0	0	0
3	34-B	109	0	0	0	0
3	35-A	125	0	0	0	0
3	35-B	102	0	0	0	0
3	36-A	130	0	0	0	0
3	36-B	120	0	0	0	0
3	37-A	138	0	0	0	0
3	37-B	110	0	0	0	0
3	38-A	134	0	0	0	0
3	38-B	118	0	0	0	0
3	39-A	130	0	0	0	0
3	39-B	112	0	0	0	0
3	40-A	128	0	0	0	0
3	40-B	118	0	0	0	0
3	41-A	139	0	0	0	0
3	41-B	106	0	0	0	0
3	42-A	128	0	0	0	0
3	42-B	124	0	0	0	0
3	43-A	155	0	0	0	0
3	43-B	125	0	0	0	0
3	44-A	143	0	0	0	0
3	44-B	118	0	0	0	0
3	45-A	140	0	0	0	0
3	45-B	108	0	0	0	0
3	46-A	131	0	0	0	0
3	46-B	105	0	0	0	0
3	47-A	127	0	0	0	0
3	47-B	118	0	0	0	0
3	48-A	141	0	0	0	0
3	48-B	129	0	0	0	0
3	49-A	121	0	0	0	0
3	49-B	109	0	0	0	0
3	50-A	139	0	0	0	0
3	50-B	111	0	0	0	0
3	51-A	137	0	0	0	0
3	51-B	131	0	0	0	0
3	52-A	145	0	0	0	0
3	52-B	119	0	0	0	0
3	53-A	141	0	0	0	0
3	53-B	113	0	0	0	0
3	54-A	137	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	54-B	109	0	0	0	0
3	55-A	136	0	0	0	0
3	55-B	120	0	0	0	0
3	56-A	153	0	0	0	0
3	56-B	127	0	0	0	0
3	57-A	124	0	0	0	0
3	57-B	122	0	0	0	0
3	58-A	133	0	0	0	0
3	58-B	122	0	0	0	0
3	59-A	143	0	0	0	0
3	59-B	117	0	0	0	0
3	60-A	132	0	0	0	0
3	60-B	116	0	0	0	0
3	61-A	138	0	0	0	0
3	61-B	119	0	0	0	0
3	62-A	137	0	0	0	0
3	62-B	121	0	0	0	0
3	63-A	151	0	0	0	0
3	63-B	123	0	0	0	0
3	64-A	142	0	0	0	0
3	64-B	121	0	0	0	0
3	65-A	149	0	0	0	0
3	65-B	128	0	0	0	0
3	66-A	135	0	0	0	0
3	66-B	112	0	0	0	0
3	67-A	143	0	0	0	0
3	67-B	125	0	0	0	0
3	68-A	137	0	0	0	0
3	68-B	126	0	0	0	0
3	69-A	131	0	0	0	0
3	69-B	112	0	0	0	0
3	70-A	136	0	0	0	0
3	70-B	123	0	0	0	0
3	71-A	138	0	0	0	0
3	71-B	122	0	0	0	0
3	72-A	135	0	0	0	0
3	72-B	121	0	0	0	0
3	73-A	134	0	0	0	0
3	73-B	132	0	0	0	0
3	74-A	153	0	0	0	0
3	74-B	113	0	0	0	0
3	75-A	147	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	75-B	111	0	0	0	0
3	76-A	145	0	0	0	0
3	76-B	105	0	0	0	0
3	77-A	131	0	0	0	0
3	77-B	119	0	0	0	0
All	All	283267	263032	261492	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.

4.3 Torsion angles [i](#)

4.3.1 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	226/228 (99%)	191 (84%)	19 (8%)	16 (7%)	1	0
1	1-B	226/228 (99%)	203 (90%)	15 (7%)	8 (4%)	3	0
1	2-A	226/228 (99%)	184 (81%)	15 (7%)	27 (12%)	0	0
1	2-B	226/228 (99%)	197 (87%)	18 (8%)	11 (5%)	2	0
1	3-A	226/228 (99%)	184 (81%)	27 (12%)	15 (7%)	1	0
1	3-B	226/228 (99%)	204 (90%)	13 (6%)	9 (4%)	3	0
1	4-A	226/228 (99%)	181 (80%)	23 (10%)	22 (10%)	0	0
1	4-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	3	0
1	5-A	226/228 (99%)	187 (83%)	24 (11%)	15 (7%)	1	0
1	5-B	226/228 (99%)	198 (88%)	24 (11%)	4 (2%)	8	2
1	6-A	226/228 (99%)	185 (82%)	26 (12%)	15 (7%)	1	0
1	6-B	226/228 (99%)	201 (89%)	18 (8%)	7 (3%)	4	0
1	7-A	226/228 (99%)	180 (80%)	21 (9%)	25 (11%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	7-B	226/228 (99%)	204 (90%)	18 (8%)	4 (2%)	8	2
1	8-A	226/228 (99%)	185 (82%)	18 (8%)	23 (10%)	0	0
1	8-B	226/228 (99%)	202 (89%)	16 (7%)	8 (4%)	3	0
1	9-A	226/228 (99%)	186 (82%)	20 (9%)	20 (9%)	1	0
1	9-B	226/228 (99%)	197 (87%)	19 (8%)	10 (4%)	2	0
1	10-A	226/228 (99%)	176 (78%)	28 (12%)	22 (10%)	0	0
1	10-B	226/228 (99%)	203 (90%)	19 (8%)	4 (2%)	8	2
1	11-A	226/228 (99%)	185 (82%)	25 (11%)	16 (7%)	1	0
1	11-B	226/228 (99%)	205 (91%)	15 (7%)	6 (3%)	5	1
1	12-A	226/228 (99%)	182 (80%)	21 (9%)	23 (10%)	0	0
1	12-B	226/228 (99%)	197 (87%)	15 (7%)	14 (6%)	1	0
1	13-A	226/228 (99%)	191 (84%)	17 (8%)	18 (8%)	1	0
1	13-B	226/228 (99%)	199 (88%)	20 (9%)	7 (3%)	4	0
1	14-A	226/228 (99%)	193 (85%)	11 (5%)	22 (10%)	0	0
1	14-B	226/228 (99%)	206 (91%)	14 (6%)	6 (3%)	5	1
1	15-A	226/228 (99%)	181 (80%)	21 (9%)	24 (11%)	0	0
1	15-B	226/228 (99%)	200 (88%)	20 (9%)	6 (3%)	5	1
1	16-A	226/228 (99%)	186 (82%)	20 (9%)	20 (9%)	1	0
1	16-B	226/228 (99%)	198 (88%)	18 (8%)	10 (4%)	2	0
1	17-A	226/228 (99%)	189 (84%)	14 (6%)	23 (10%)	0	0
1	17-B	226/228 (99%)	187 (83%)	26 (12%)	13 (6%)	1	0
1	18-A	226/228 (99%)	184 (81%)	26 (12%)	16 (7%)	1	0
1	18-B	226/228 (99%)	200 (88%)	17 (8%)	9 (4%)	3	0
1	19-A	226/228 (99%)	184 (81%)	26 (12%)	16 (7%)	1	0
1	19-B	226/228 (99%)	198 (88%)	17 (8%)	11 (5%)	2	0
1	20-A	226/228 (99%)	190 (84%)	25 (11%)	11 (5%)	2	0
1	20-B	226/228 (99%)	197 (87%)	19 (8%)	10 (4%)	2	0
1	21-A	226/228 (99%)	189 (84%)	25 (11%)	12 (5%)	2	0
1	21-B	226/228 (99%)	200 (88%)	16 (7%)	10 (4%)	2	0
1	22-A	226/228 (99%)	189 (84%)	20 (9%)	17 (8%)	1	0
1	22-B	226/228 (99%)	198 (88%)	16 (7%)	12 (5%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	23-A	226/228 (99%)	189 (84%)	21 (9%)	16 (7%)	1	0
1	23-B	226/228 (99%)	200 (88%)	16 (7%)	10 (4%)	2	0
1	24-A	226/228 (99%)	183 (81%)	26 (12%)	17 (8%)	1	0
1	24-B	226/228 (99%)	202 (89%)	18 (8%)	6 (3%)	5	1
1	25-A	226/228 (99%)	188 (83%)	25 (11%)	13 (6%)	1	0
1	25-B	226/228 (99%)	202 (89%)	18 (8%)	6 (3%)	5	1
1	26-A	226/228 (99%)	184 (81%)	26 (12%)	16 (7%)	1	0
1	26-B	226/228 (99%)	197 (87%)	19 (8%)	10 (4%)	2	0
1	27-A	226/228 (99%)	184 (81%)	20 (9%)	22 (10%)	0	0
1	27-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	3	0
1	28-A	226/228 (99%)	183 (81%)	24 (11%)	19 (8%)	1	0
1	28-B	226/228 (99%)	198 (88%)	17 (8%)	11 (5%)	2	0
1	29-A	226/228 (99%)	187 (83%)	27 (12%)	12 (5%)	2	0
1	29-B	226/228 (99%)	197 (87%)	22 (10%)	7 (3%)	4	0
1	30-A	226/228 (99%)	195 (86%)	21 (9%)	10 (4%)	2	0
1	30-B	226/228 (99%)	201 (89%)	17 (8%)	8 (4%)	3	0
1	31-A	226/228 (99%)	185 (82%)	22 (10%)	19 (8%)	1	0
1	31-B	226/228 (99%)	207 (92%)	9 (4%)	10 (4%)	2	0
1	32-A	226/228 (99%)	188 (83%)	21 (9%)	17 (8%)	1	0
1	32-B	226/228 (99%)	202 (89%)	15 (7%)	9 (4%)	3	0
1	33-A	226/228 (99%)	193 (85%)	20 (9%)	13 (6%)	1	0
1	33-B	226/228 (99%)	203 (90%)	13 (6%)	10 (4%)	2	0
1	34-A	226/228 (99%)	189 (84%)	23 (10%)	14 (6%)	1	0
1	34-B	226/228 (99%)	198 (88%)	18 (8%)	10 (4%)	2	0
1	35-A	226/228 (99%)	188 (83%)	25 (11%)	13 (6%)	1	0
1	35-B	226/228 (99%)	201 (89%)	15 (7%)	10 (4%)	2	0
1	36-A	226/228 (99%)	186 (82%)	22 (10%)	18 (8%)	1	0
1	36-B	226/228 (99%)	206 (91%)	11 (5%)	9 (4%)	3	0
1	37-A	226/228 (99%)	181 (80%)	23 (10%)	22 (10%)	0	0
1	37-B	226/228 (99%)	205 (91%)	13 (6%)	8 (4%)	3	0
1	38-A	226/228 (99%)	183 (81%)	22 (10%)	21 (9%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	38-B	226/228 (99%)	200 (88%)	17 (8%)	9 (4%)	3	0
1	39-A	226/228 (99%)	190 (84%)	18 (8%)	18 (8%)	1	0
1	39-B	226/228 (99%)	196 (87%)	22 (10%)	8 (4%)	3	0
1	40-A	226/228 (99%)	186 (82%)	28 (12%)	12 (5%)	2	0
1	40-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	3	0
1	41-A	226/228 (99%)	185 (82%)	16 (7%)	25 (11%)	0	0
1	41-B	226/228 (99%)	201 (89%)	19 (8%)	6 (3%)	5	1
1	42-A	226/228 (99%)	186 (82%)	19 (8%)	21 (9%)	0	0
1	42-B	226/228 (99%)	199 (88%)	23 (10%)	4 (2%)	8	2
1	43-A	226/228 (99%)	189 (84%)	20 (9%)	17 (8%)	1	0
1	43-B	226/228 (99%)	197 (87%)	20 (9%)	9 (4%)	3	0
1	44-A	226/228 (99%)	184 (81%)	24 (11%)	18 (8%)	1	0
1	44-B	226/228 (99%)	204 (90%)	13 (6%)	9 (4%)	3	0
1	45-A	226/228 (99%)	183 (81%)	25 (11%)	18 (8%)	1	0
1	45-B	226/228 (99%)	203 (90%)	14 (6%)	9 (4%)	3	0
1	46-A	226/228 (99%)	182 (80%)	27 (12%)	17 (8%)	1	0
1	46-B	226/228 (99%)	198 (88%)	15 (7%)	13 (6%)	1	0
1	47-A	226/228 (99%)	182 (80%)	22 (10%)	22 (10%)	0	0
1	47-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	3	0
1	48-A	226/228 (99%)	184 (81%)	26 (12%)	16 (7%)	1	0
1	48-B	226/228 (99%)	197 (87%)	22 (10%)	7 (3%)	4	0
1	49-A	226/228 (99%)	181 (80%)	25 (11%)	20 (9%)	1	0
1	49-B	226/228 (99%)	201 (89%)	16 (7%)	9 (4%)	3	0
1	50-A	226/228 (99%)	185 (82%)	22 (10%)	19 (8%)	1	0
1	50-B	226/228 (99%)	196 (87%)	22 (10%)	8 (4%)	3	0
1	51-A	226/228 (99%)	190 (84%)	17 (8%)	19 (8%)	1	0
1	51-B	226/228 (99%)	195 (86%)	20 (9%)	11 (5%)	2	0
1	52-A	226/228 (99%)	182 (80%)	26 (12%)	18 (8%)	1	0
1	52-B	226/228 (99%)	206 (91%)	13 (6%)	7 (3%)	4	0
1	53-A	226/228 (99%)	185 (82%)	28 (12%)	13 (6%)	1	0
1	53-B	226/228 (99%)	204 (90%)	14 (6%)	8 (4%)	3	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	54-A	226/228 (99%)	188 (83%)	21 (9%)	17 (8%)	1	0
1	54-B	226/228 (99%)	200 (88%)	19 (8%)	7 (3%)	4	0
1	55-A	226/228 (99%)	183 (81%)	25 (11%)	18 (8%)	1	0
1	55-B	226/228 (99%)	197 (87%)	18 (8%)	11 (5%)	2	0
1	56-A	226/228 (99%)	191 (84%)	23 (10%)	12 (5%)	2	0
1	56-B	226/228 (99%)	199 (88%)	19 (8%)	8 (4%)	3	0
1	57-A	226/228 (99%)	184 (81%)	19 (8%)	23 (10%)	0	0
1	57-B	226/228 (99%)	195 (86%)	23 (10%)	8 (4%)	3	0
1	58-A	226/228 (99%)	189 (84%)	16 (7%)	21 (9%)	0	0
1	58-B	226/228 (99%)	201 (89%)	11 (5%)	14 (6%)	1	0
1	59-A	226/228 (99%)	193 (85%)	14 (6%)	19 (8%)	1	0
1	59-B	226/228 (99%)	199 (88%)	19 (8%)	8 (4%)	3	0
1	60-A	226/228 (99%)	186 (82%)	23 (10%)	17 (8%)	1	0
1	60-B	226/228 (99%)	197 (87%)	16 (7%)	13 (6%)	1	0
1	61-A	226/228 (99%)	177 (78%)	28 (12%)	21 (9%)	0	0
1	61-B	226/228 (99%)	203 (90%)	10 (4%)	13 (6%)	1	0
1	62-A	226/228 (99%)	187 (83%)	22 (10%)	17 (8%)	1	0
1	62-B	226/228 (99%)	202 (89%)	17 (8%)	7 (3%)	4	0
1	63-A	226/228 (99%)	186 (82%)	24 (11%)	16 (7%)	1	0
1	63-B	226/228 (99%)	205 (91%)	13 (6%)	8 (4%)	3	0
1	64-A	226/228 (99%)	183 (81%)	20 (9%)	23 (10%)	0	0
1	64-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	3	0
1	65-A	226/228 (99%)	187 (83%)	22 (10%)	17 (8%)	1	0
1	65-B	226/228 (99%)	198 (88%)	21 (9%)	7 (3%)	4	0
1	66-A	226/228 (99%)	192 (85%)	21 (9%)	13 (6%)	1	0
1	66-B	226/228 (99%)	202 (89%)	16 (7%)	8 (4%)	3	0
1	67-A	226/228 (99%)	185 (82%)	24 (11%)	17 (8%)	1	0
1	67-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	3	0
1	68-A	226/228 (99%)	179 (79%)	23 (10%)	24 (11%)	0	0
1	68-B	226/228 (99%)	202 (89%)	14 (6%)	10 (4%)	2	0
1	69-A	226/228 (99%)	184 (81%)	28 (12%)	14 (6%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	69-B	226/228 (99%)	195 (86%)	18 (8%)	13 (6%)	1	0
1	70-A	226/228 (99%)	186 (82%)	24 (11%)	16 (7%)	1	0
1	70-B	226/228 (99%)	202 (89%)	14 (6%)	10 (4%)	2	0
1	71-A	226/228 (99%)	184 (81%)	27 (12%)	15 (7%)	1	0
1	71-B	226/228 (99%)	197 (87%)	22 (10%)	7 (3%)	4	0
1	72-A	226/228 (99%)	183 (81%)	30 (13%)	13 (6%)	1	0
1	72-B	226/228 (99%)	207 (92%)	14 (6%)	5 (2%)	6	1
1	73-A	226/228 (99%)	185 (82%)	21 (9%)	20 (9%)	1	0
1	73-B	226/228 (99%)	203 (90%)	18 (8%)	5 (2%)	6	1
1	74-A	226/228 (99%)	187 (83%)	20 (9%)	19 (8%)	1	0
1	74-B	226/228 (99%)	205 (91%)	13 (6%)	8 (4%)	3	0
1	75-A	226/228 (99%)	185 (82%)	23 (10%)	18 (8%)	1	0
1	75-B	226/228 (99%)	200 (88%)	23 (10%)	3 (1%)	12	3
1	76-A	226/228 (99%)	190 (84%)	19 (8%)	17 (8%)	1	0
1	76-B	226/228 (99%)	207 (92%)	13 (6%)	6 (3%)	5	1
1	77-A	226/228 (99%)	183 (81%)	25 (11%)	18 (8%)	1	0
1	77-B	226/228 (99%)	197 (87%)	19 (8%)	10 (4%)	2	0
All	All	34804/35112 (99%)	29722 (85%)	3047 (9%)	2035 (6%)	1	0

All (2035) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	45	ASP
1	1-A	131	VAL
1	1-A	134	ALA
1	1-A	180	LYS
1	1-A	206	ASN
1	1-A	207	ARG
1	1-B	47	ALA
1	1-B	227	LEU
1	2-A	2	LEU
1	2-A	42	CYS
1	2-A	43	LEU
1	2-A	45	ASP
1	2-A	46	ALA
1	2-A	50	LYS

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Mol	Chain	Res	Type
1	2-A	137	ARG
1	2-A	175	ARG
1	2-A	176	ARG
1	2-A	178	SER
1	2-A	179	CYS
1	2-A	182	ASP
1	2-A	183	SER
1	2-A	202	ALA
1	2-A	203	VAL
1	2-A	207	ARG
1	2-A	210	PRO
1	2-B	199	SER
1	2-B	203	VAL
1	2-B	225	SER
1	3-A	45	ASP
1	3-A	46	ALA
1	3-A	47	ALA
1	3-A	131	VAL
1	3-A	137	ARG
1	3-A	199	SER
1	3-A	227	LEU
1	3-B	44	GLU
1	3-B	202	ALA
1	3-B	204	CYS
1	3-B	207	ARG
1	3-B	227	LEU
1	4-A	2	LEU
1	4-A	4	GLY
1	4-A	46	ALA
1	4-A	50	LYS
1	4-A	137	ARG
1	4-A	198	THR
1	4-A	202	ALA
1	4-A	203	VAL
1	4-A	208	LYS
1	5-A	47	ALA
1	5-A	50	LYS
1	5-A	137	ARG
1	5-A	174	ASN
1	5-A	176	ARG
1	5-A	183	SER
1	5-A	198	THR

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Mol	Chain	Res	Type
1	5-A	208	LYS
1	5-B	207	ARG
1	6-A	46	ALA
1	6-A	48	ASP
1	6-A	137	ARG
1	6-A	176	ARG
1	6-A	180	LYS
1	6-A	202	ALA
1	6-A	204	CYS
1	6-A	207	ARG
1	6-B	44	GLU
1	6-B	202	ALA
1	7-A	2	LEU
1	7-A	45	ASP
1	7-A	48	ASP
1	7-A	50	LYS
1	7-A	139	ASP
1	7-A	173	SER
1	7-A	176	ARG
1	7-A	182	ASP
1	7-A	202	ALA
1	7-A	208	LYS
1	7-A	210	PRO
1	7-B	84	ASP
1	7-B	199	SER
1	8-A	5	ARG
1	8-A	42	CYS
1	8-A	44	GLU
1	8-A	50	LYS
1	8-A	131	VAL
1	8-A	132	ASN
1	8-A	135	GLY
1	8-A	199	SER
1	8-A	204	CYS
1	8-A	208	LYS
1	8-B	42	CYS
1	8-B	46	ALA
1	9-A	2	LEU
1	9-A	45	ASP
1	9-A	130	ILE
1	9-A	174	ASN
1	9-A	175	ARG

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Mol	Chain	Res	Type
1	9-A	176	ARG
1	9-A	178	SER
1	9-A	180	LYS
1	9-B	42	CYS
1	9-B	225	SER
1	10-A	5	ARG
1	10-A	45	ASP
1	10-A	130	ILE
1	10-A	137	ARG
1	10-A	177	ASP
1	10-A	178	SER
1	10-A	199	SER
1	10-A	208	LYS
1	10-B	225	SER
1	11-A	50	LYS
1	11-A	130	ILE
1	11-A	134	ALA
1	11-A	137	ARG
1	11-A	174	ASN
1	11-A	202	ALA
1	11-A	207	ARG
1	11-A	209	LYS
1	11-B	43	LEU
1	11-B	199	SER
1	11-B	204	CYS
1	11-B	207	ARG
1	12-A	2	LEU
1	12-A	3	GLY
1	12-A	134	ALA
1	12-A	137	ARG
1	12-A	174	ASN
1	12-A	182	ASP
1	12-A	210	PRO
1	12-B	45	ASP
1	12-B	175	ARG
1	12-B	202	ALA
1	12-B	206	ASN
1	12-B	225	SER
1	12-B	226	VAL
1	13-A	2	LEU
1	13-A	46	ALA
1	13-A	132	ASN

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Mol	Chain	Res	Type
1	13-A	133	HIS
1	13-A	157	ARG
1	13-A	207	ARG
1	13-B	43	LEU
1	13-B	45	ASP
1	13-B	224	ASP
1	14-A	2	LEU
1	14-A	46	ALA
1	14-A	47	ALA
1	14-A	131	VAL
1	14-A	159	HIS
1	14-A	173	SER
1	14-A	179	CYS
1	14-A	203	VAL
1	14-A	207	ARG
1	14-B	45	ASP
1	14-B	203	VAL
1	15-A	2	LEU
1	15-A	21	ASN
1	15-A	46	ALA
1	15-A	47	ALA
1	15-A	129	GLY
1	15-A	130	ILE
1	15-A	138	PRO
1	15-A	174	ASN
1	15-A	176	ARG
1	15-A	179	CYS
1	15-A	180	LYS
1	15-A	199	SER
1	15-A	204	CYS
1	15-A	208	LYS
1	15-B	43	LEU
1	15-B	227	LEU
1	16-A	46	ALA
1	16-A	48	ASP
1	16-A	174	ASN
1	16-A	176	ARG
1	16-A	180	LYS
1	16-A	185	GLY
1	16-A	210	PRO
1	16-B	43	LEU
1	16-B	47	ALA

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Mol	Chain	Res	Type
1	16-B	176	ARG
1	16-B	203	VAL
1	16-B	206	ASN
1	17-A	42	CYS
1	17-A	48	ASP
1	17-A	136	ARG
1	17-A	157	ARG
1	17-A	174	ASN
1	17-A	175	ARG
1	17-A	176	ARG
1	17-A	179	CYS
1	17-A	203	VAL
1	17-A	208	LYS
1	17-B	33	GLU
1	17-B	43	LEU
1	17-B	46	ALA
1	17-B	199	SER
1	17-B	200	GLY
1	17-B	203	VAL
1	18-A	46	ALA
1	18-A	48	ASP
1	18-A	173	SER
1	18-A	176	ARG
1	18-A	179	CYS
1	18-A	199	SER
1	18-A	200	GLY
1	18-A	203	VAL
1	18-B	44	GLU
1	18-B	45	ASP
1	18-B	225	SER
1	19-A	2	LEU
1	19-A	46	ALA
1	19-A	132	ASN
1	19-A	133	HIS
1	19-A	180	LYS
1	19-A	207	ARG
1	19-B	47	ALA
1	19-B	224	ASP
1	19-B	225	SER
1	20-A	46	ALA
1	20-A	136	ARG
1	20-A	180	LYS

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Mol	Chain	Res	Type
1	20-A	203	VAL
1	20-B	50	LYS
1	20-B	202	ALA
1	20-B	225	SER
1	21-A	138	PRO
1	21-A	179	CYS
1	21-A	203	VAL
1	21-B	42	CYS
1	21-B	47	ALA
1	21-B	175	ARG
1	21-B	202	ALA
1	22-A	2	LEU
1	22-A	44	GLU
1	22-A	131	VAL
1	22-A	174	ASN
1	22-A	178	SER
1	22-A	179	CYS
1	22-A	182	ASP
1	22-A	198	THR
1	22-A	207	ARG
1	22-B	161	ASP
1	22-B	199	SER
1	23-A	44	GLU
1	23-A	45	ASP
1	23-A	48	ASP
1	23-A	134	ALA
1	23-A	174	ASN
1	23-A	176	ARG
1	23-A	178	SER
1	23-A	208	LYS
1	23-B	45	ASP
1	23-B	47	ALA
1	23-B	206	ASN
1	23-B	225	SER
1	24-A	84	ASP
1	24-A	130	ILE
1	24-A	138	PRO
1	24-A	179	CYS
1	24-A	198	THR
1	24-A	203	VAL
1	24-A	207	ARG
1	24-B	48	ASP

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Mol	Chain	Res	Type
1	24-B	133	HIS
1	25-A	44	GLU
1	25-A	45	ASP
1	25-A	137	ARG
1	25-A	173	SER
1	25-A	175	ARG
1	25-A	180	LYS
1	25-B	47	ALA
1	25-B	226	VAL
1	26-A	45	ASP
1	26-A	46	ALA
1	26-A	130	ILE
1	26-A	132	ASN
1	26-A	137	ARG
1	26-A	203	VAL
1	26-A	204	CYS
1	26-A	208	LYS
1	26-B	201	SER
1	26-B	203	VAL
1	26-B	206	ASN
1	26-B	225	SER
1	27-A	2	LEU
1	27-A	132	ASN
1	27-A	133	HIS
1	27-A	139	ASP
1	27-A	174	ASN
1	27-A	175	ARG
1	27-B	199	SER
1	27-B	203	VAL
1	27-B	226	VAL
1	28-A	48	ASP
1	28-A	177	ASP
1	28-A	182	ASP
1	28-A	199	SER
1	28-A	209	LYS
1	28-B	21	ASN
1	28-B	46	ALA
1	28-B	226	VAL
1	29-A	48	ASP
1	29-A	203	VAL
1	29-A	204	CYS
1	29-A	210	PRO

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Mol	Chain	Res	Type
1	29-B	43	LEU
1	29-B	50	LYS
1	29-B	225	SER
1	30-A	44	GLU
1	30-A	48	ASP
1	30-A	130	ILE
1	30-A	177	ASP
1	30-A	203	VAL
1	30-A	204	CYS
1	30-B	21	ASN
1	30-B	42	CYS
1	30-B	201	SER
1	30-B	202	ALA
1	30-B	203	VAL
1	31-A	2	LEU
1	31-A	45	ASP
1	31-A	173	SER
1	31-A	177	ASP
1	31-A	180	LYS
1	31-A	182	ASP
1	31-A	203	VAL
1	31-A	206	ASN
1	31-A	226	VAL
1	31-B	134	ALA
1	31-B	174	ASN
1	31-B	175	ARG
1	31-B	204	CYS
1	32-A	44	GLU
1	32-A	131	VAL
1	32-A	134	ALA
1	32-B	47	ALA
1	32-B	204	CYS
1	32-B	227	LEU
1	33-A	130	ILE
1	33-A	173	SER
1	33-A	176	ARG
1	33-A	180	LYS
1	33-A	226	VAL
1	33-B	203	VAL
1	33-B	206	ASN
1	33-B	224	ASP
1	33-B	226	VAL

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Mol	Chain	Res	Type
1	33-B	227	LEU
1	34-A	2	LEU
1	34-A	131	VAL
1	34-A	182	ASP
1	34-A	202	ALA
1	34-A	227	LEU
1	34-B	199	SER
1	34-B	226	VAL
1	34-B	227	LEU
1	35-A	44	GLU
1	35-A	134	ALA
1	35-A	157	ARG
1	35-A	176	ARG
1	35-A	182	ASP
1	35-A	204	CYS
1	35-A	206	ASN
1	35-A	208	LYS
1	35-B	47	ALA
1	35-B	199	SER
1	35-B	203	VAL
1	35-B	206	ASN
1	35-B	226	VAL
1	36-A	43	LEU
1	36-A	130	ILE
1	36-A	180	LYS
1	36-A	182	ASP
1	36-A	204	CYS
1	36-B	201	SER
1	36-B	203	VAL
1	36-B	206	ASN
1	36-B	207	ARG
1	36-B	225	SER
1	36-B	226	VAL
1	36-B	227	LEU
1	37-A	21	ASN
1	37-A	43	LEU
1	37-A	85	THR
1	37-A	173	SER
1	37-A	176	ARG
1	37-A	178	SER
1	37-A	182	ASP
1	37-A	202	ALA

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Mol	Chain	Res	Type
1	37-A	203	VAL
1	37-A	204	CYS
1	37-A	206	ASN
1	37-A	227	LEU
1	37-B	47	ALA
1	37-B	202	ALA
1	37-B	224	ASP
1	38-A	2	LEU
1	38-A	43	LEU
1	38-A	46	ALA
1	38-A	136	ARG
1	38-A	138	PRO
1	38-A	174	ASN
1	38-A	175	ARG
1	38-A	203	VAL
1	38-B	199	SER
1	39-A	2	LEU
1	39-A	44	GLU
1	39-A	46	ALA
1	39-A	130	ILE
1	39-A	132	ASN
1	39-A	173	SER
1	39-A	177	ASP
1	39-A	199	SER
1	39-A	202	ALA
1	39-A	226	VAL
1	39-A	227	LEU
1	39-B	42	CYS
1	39-B	203	VAL
1	39-B	225	SER
1	39-B	227	LEU
1	40-A	130	ILE
1	40-A	161	ASP
1	40-A	174	ASN
1	40-A	183	SER
1	40-A	204	CYS
1	40-A	225	SER
1	40-A	226	VAL
1	40-B	199	SER
1	40-B	202	ALA
1	40-B	207	ARG
1	40-B	225	SER

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Mol	Chain	Res	Type
1	41-A	45	ASP
1	41-A	85	THR
1	41-A	130	ILE
1	41-A	132	ASN
1	41-A	137	ARG
1	41-A	183	SER
1	41-A	206	ASN
1	41-A	226	VAL
1	41-A	227	LEU
1	41-B	45	ASP
1	41-B	199	SER
1	42-A	3	GLY
1	42-A	45	ASP
1	42-A	130	ILE
1	42-A	139	ASP
1	42-A	176	ARG
1	42-A	179	CYS
1	42-A	180	LYS
1	42-A	199	SER
1	42-A	202	ALA
1	42-A	203	VAL
1	42-A	207	ARG
1	42-A	225	SER
1	42-A	227	LEU
1	42-B	45	ASP
1	42-B	203	VAL
1	42-B	224	ASP
1	43-A	131	VAL
1	43-A	174	ASN
1	43-A	178	SER
1	43-A	180	LYS
1	43-A	202	ALA
1	43-A	205	GLY
1	43-B	45	ASP
1	43-B	133	HIS
1	43-B	203	VAL
1	43-B	204	CYS
1	43-B	225	SER
1	43-B	227	LEU
1	44-A	2	LEU
1	44-A	45	ASP
1	44-A	130	ILE

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Mol	Chain	Res	Type
1	44-A	131	VAL
1	44-A	132	ASN
1	44-A	133	HIS
1	44-A	175	ARG
1	44-A	176	ARG
1	44-A	178	SER
1	44-A	182	ASP
1	44-A	199	SER
1	44-A	202	ALA
1	44-A	207	ARG
1	44-A	227	LEU
1	44-B	46	ALA
1	44-B	85	THR
1	44-B	175	ARG
1	44-B	202	ALA
1	44-B	204	CYS
1	45-A	2	LEU
1	45-A	131	VAL
1	45-A	132	ASN
1	45-A	133	HIS
1	45-A	178	SER
1	45-A	198	THR
1	45-B	85	THR
1	45-B	134	ALA
1	45-B	206	ASN
1	45-B	225	SER
1	45-B	226	VAL
1	46-A	45	ASP
1	46-A	46	ALA
1	46-A	85	THR
1	46-A	130	ILE
1	46-A	132	ASN
1	46-A	178	SER
1	46-A	183	SER
1	46-A	198	THR
1	46-A	199	SER
1	46-A	204	CYS
1	46-A	208	LYS
1	46-B	46	ALA
1	46-B	47	ALA
1	46-B	134	ALA
1	46-B	199	SER

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Mol	Chain	Res	Type
1	46-B	204	CYS
1	46-B	225	SER
1	46-B	226	VAL
1	47-A	43	LEU
1	47-A	44	GLU
1	47-A	45	ASP
1	47-A	132	ASN
1	47-A	178	SER
1	47-A	183	SER
1	47-A	199	SER
1	47-A	204	CYS
1	47-B	201	SER
1	47-B	206	ASN
1	48-A	2	LEU
1	48-A	44	GLU
1	48-A	48	ASP
1	48-A	130	ILE
1	48-A	131	VAL
1	48-A	173	SER
1	48-A	178	SER
1	48-A	181	GLY
1	48-A	182	ASP
1	48-A	206	ASN
1	48-A	208	LYS
1	48-B	203	VAL
1	48-B	226	VAL
1	49-A	43	LEU
1	49-A	47	ALA
1	49-A	130	ILE
1	49-A	133	HIS
1	49-A	134	ALA
1	49-A	138	PRO
1	49-A	173	SER
1	49-A	174	ASN
1	49-A	177	ASP
1	49-A	178	SER
1	49-A	183	SER
1	49-A	204	CYS
1	49-A	208	LYS
1	49-B	161	ASP
1	49-B	226	VAL
1	50-A	43	LEU

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Mol	Chain	Res	Type
1	50-A	48	ASP
1	50-A	132	ASN
1	50-A	138	PRO
1	50-A	139	ASP
1	50-A	174	ASN
1	50-A	204	CYS
1	50-A	207	ARG
1	50-A	208	LYS
1	50-B	199	SER
1	50-B	203	VAL
1	50-B	226	VAL
1	51-A	45	ASP
1	51-A	47	ALA
1	51-A	129	GLY
1	51-A	133	HIS
1	51-A	157	ARG
1	51-A	177	ASP
1	51-A	179	CYS
1	51-A	201	SER
1	51-A	207	ARG
1	51-B	174	ASN
1	51-B	175	ARG
1	51-B	199	SER
1	52-A	43	LEU
1	52-A	46	ALA
1	52-A	47	ALA
1	52-A	174	ASN
1	52-A	176	ARG
1	52-A	177	ASP
1	52-A	178	SER
1	52-A	179	CYS
1	52-A	180	LYS
1	52-A	182	ASP
1	52-B	203	VAL
1	53-A	46	ALA
1	53-A	131	VAL
1	53-A	132	ASN
1	53-A	173	SER
1	53-A	184	GLY
1	53-A	201	SER
1	53-A	202	ALA
1	53-A	203	VAL

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Mol	Chain	Res	Type
1	53-A	207	ARG
1	53-B	49	GLY
1	53-B	50	LYS
1	53-B	204	CYS
1	53-B	226	VAL
1	54-A	48	ASP
1	54-A	132	ASN
1	54-A	174	ASN
1	54-A	178	SER
1	54-A	183	SER
1	54-A	199	SER
1	54-A	201	SER
1	54-A	202	ALA
1	54-A	204	CYS
1	54-B	46	ALA
1	54-B	49	GLY
1	54-B	175	ARG
1	54-B	202	ALA
1	54-B	204	CYS
1	54-B	227	LEU
1	55-A	46	ALA
1	55-A	83	PRO
1	55-A	161	ASP
1	55-A	176	ARG
1	55-A	179	CYS
1	55-A	207	ARG
1	55-B	46	ALA
1	55-B	199	SER
1	55-B	227	LEU
1	56-A	43	LEU
1	56-A	46	ALA
1	56-A	134	ALA
1	56-A	138	PRO
1	56-A	179	CYS
1	56-A	201	SER
1	56-A	204	CYS
1	56-A	205	GLY
1	56-A	206	ASN
1	56-A	207	ARG
1	56-B	199	SER
1	56-B	204	CYS
1	57-A	48	ASP

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Mol	Chain	Res	Type
1	57-A	134	ALA
1	57-A	136	ARG
1	57-A	137	ARG
1	57-A	179	CYS
1	57-A	199	SER
1	57-A	201	SER
1	57-A	203	VAL
1	57-A	207	ARG
1	57-A	209	LYS
1	57-B	86	ILE
1	57-B	87	ASP
1	57-B	199	SER
1	57-B	204	CYS
1	57-B	227	LEU
1	58-A	45	ASP
1	58-A	132	ASN
1	58-A	137	ARG
1	58-A	174	ASN
1	58-A	183	SER
1	58-A	184	GLY
1	58-A	207	ARG
1	58-B	44	GLU
1	58-B	47	ALA
1	58-B	86	ILE
1	58-B	207	ARG
1	58-B	226	VAL
1	59-A	45	ASP
1	59-A	46	ALA
1	59-A	129	GLY
1	59-A	134	ALA
1	59-A	137	ARG
1	59-A	138	PRO
1	59-A	139	ASP
1	59-A	174	ASN
1	59-A	178	SER
1	59-A	182	ASP
1	59-A	183	SER
1	59-B	46	ALA
1	59-B	199	SER
1	60-A	47	ALA
1	60-A	130	ILE
1	60-A	132	ASN

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Mol	Chain	Res	Type
1	60-A	134	ALA
1	60-A	136	ARG
1	60-A	137	ARG
1	60-A	138	PRO
1	60-A	139	ASP
1	60-A	178	SER
1	60-A	183	SER
1	60-A	201	SER
1	60-B	47	ALA
1	60-B	165	THR
1	60-B	204	CYS
1	60-B	207	ARG
1	60-B	227	LEU
1	61-A	3	GLY
1	61-A	46	ALA
1	61-A	47	ALA
1	61-A	130	ILE
1	61-A	137	ARG
1	61-A	174	ASN
1	61-A	178	SER
1	61-A	179	CYS
1	61-A	180	LYS
1	61-A	182	ASP
1	61-B	45	ASP
1	61-B	47	ALA
1	61-B	202	ALA
1	61-B	227	LEU
1	62-A	130	ILE
1	62-A	132	ASN
1	62-A	134	ALA
1	62-A	137	ARG
1	62-A	139	ASP
1	62-A	174	ASN
1	62-A	176	ARG
1	62-A	179	CYS
1	62-A	203	VAL
1	62-B	46	ALA
1	62-B	199	SER
1	62-B	203	VAL
1	62-B	227	LEU
1	63-A	2	LEU
1	63-A	43	LEU

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Mol	Chain	Res	Type
1	63-A	130	ILE
1	63-A	137	ARG
1	63-A	180	LYS
1	63-A	183	SER
1	63-A	201	SER
1	63-A	204	CYS
1	63-B	46	ALA
1	63-B	203	VAL
1	63-B	204	CYS
1	63-B	226	VAL
1	64-A	2	LEU
1	64-A	42	CYS
1	64-A	47	ALA
1	64-A	131	VAL
1	64-A	137	ARG
1	64-A	139	ASP
1	64-A	175	ARG
1	64-A	176	ARG
1	64-A	180	LYS
1	64-A	183	SER
1	64-A	202	ALA
1	64-A	204	CYS
1	64-B	45	ASP
1	64-B	48	ASP
1	64-B	203	VAL
1	64-B	227	LEU
1	65-A	45	ASP
1	65-A	137	ARG
1	65-A	173	SER
1	65-A	180	LYS
1	65-A	183	SER
1	65-A	207	ARG
1	65-B	47	ALA
1	65-B	174	ASN
1	65-B	202	ALA
1	66-A	173	SER
1	66-A	178	SER
1	66-A	182	ASP
1	66-A	183	SER
1	66-B	174	ASN
1	66-B	203	VAL
1	67-A	45	ASP

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Mol	Chain	Res	Type
1	67-A	130	ILE
1	67-A	131	VAL
1	67-A	137	ARG
1	67-A	199	SER
1	67-A	202	ALA
1	67-B	33	GLU
1	67-B	47	ALA
1	67-B	134	ALA
1	67-B	203	VAL
1	67-B	204	CYS
1	67-B	226	VAL
1	68-A	3	GLY
1	68-A	44	GLU
1	68-A	45	ASP
1	68-A	46	ALA
1	68-A	131	VAL
1	68-A	137	ARG
1	68-A	139	ASP
1	68-A	177	ASP
1	68-A	179	CYS
1	68-A	182	ASP
1	68-A	199	SER
1	68-A	201	SER
1	68-A	203	VAL
1	68-A	207	ARG
1	68-B	207	ARG
1	69-A	46	ALA
1	69-A	137	ARG
1	69-A	175	ARG
1	69-A	199	SER
1	69-A	205	GLY
1	69-A	208	LYS
1	69-B	134	ALA
1	69-B	199	SER
1	69-B	200	GLY
1	69-B	201	SER
1	69-B	202	ALA
1	69-B	203	VAL
1	69-B	207	ARG
1	70-A	45	ASP
1	70-A	131	VAL
1	70-A	134	ALA

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Mol	Chain	Res	Type
1	70-A	137	ARG
1	70-A	199	SER
1	70-A	210	PRO
1	70-B	201	SER
1	70-B	203	VAL
1	70-B	226	VAL
1	70-B	227	LEU
1	71-A	21	ASN
1	71-A	130	ILE
1	71-A	136	ARG
1	71-A	161	ASP
1	71-A	182	ASP
1	71-A	210	PRO
1	71-B	174	ASN
1	71-B	175	ARG
1	71-B	199	SER
1	71-B	202	ALA
1	71-B	226	VAL
1	72-A	46	ALA
1	72-A	47	ALA
1	72-A	130	ILE
1	72-A	132	ASN
1	72-A	133	HIS
1	72-A	134	ALA
1	72-A	137	ARG
1	72-A	208	LYS
1	72-B	46	ALA
1	72-B	47	ALA
1	72-B	73	LEU
1	72-B	202	ALA
1	73-A	46	ALA
1	73-A	130	ILE
1	73-A	136	ARG
1	73-A	177	ASP
1	73-A	206	ASN
1	73-A	208	LYS
1	73-B	46	ALA
1	73-B	199	SER
1	73-B	200	GLY
1	74-A	3	GLY
1	74-A	132	ASN
1	74-A	133	HIS

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Mol	Chain	Res	Type
1	74-A	176	ARG
1	74-A	179	CYS
1	74-A	182	ASP
1	74-A	206	ASN
1	74-A	226	VAL
1	74-B	134	ALA
1	74-B	203	VAL
1	75-A	133	HIS
1	75-A	157	ARG
1	75-A	175	ARG
1	75-A	177	ASP
1	75-A	201	SER
1	75-A	206	ASN
1	75-B	225	SER
1	76-A	45	ASP
1	76-A	46	ALA
1	76-A	131	VAL
1	76-A	198	THR
1	76-A	201	SER
1	76-A	202	ALA
1	76-A	204	CYS
1	76-A	227	LEU
1	76-B	47	ALA
1	76-B	203	VAL
1	76-B	225	SER
1	76-B	226	VAL
1	77-A	46	ALA
1	77-A	130	ILE
1	77-A	177	ASP
1	77-A	179	CYS
1	77-A	180	LYS
1	77-A	182	ASP
1	77-A	198	THR
1	77-A	207	ARG
1	77-B	44	GLU
1	77-B	84	ASP
1	77-B	174	ASN
1	77-B	226	VAL
1	77-B	227	LEU
1	1-A	137	ARG
1	1-A	159	HIS
1	1-B	42	CYS

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Mol	Chain	Res	Type
1	1-B	201	SER
1	1-B	202	ALA
1	1-B	225	SER
1	2-A	131	VAL
1	2-A	135	GLY
1	2-A	157	ARG
1	2-A	180	LYS
1	2-A	206	ASN
1	2-B	46	ALA
1	2-B	47	ALA
1	3-A	85	THR
1	3-A	177	ASP
1	3-A	206	ASN
1	3-B	115	ARG
1	3-B	205	GLY
1	4-A	47	ALA
1	4-A	157	ARG
1	4-A	175	ARG
1	4-A	178	SER
1	4-B	207	ARG
1	4-B	225	SER
1	4-B	227	LEU
1	5-A	46	ALA
1	5-A	136	ARG
1	5-A	178	SER
1	6-A	47	ALA
1	6-A	174	ASN
1	6-A	183	SER
1	6-A	208	LYS
1	6-B	47	ALA
1	7-A	42	CYS
1	7-A	131	VAL
1	7-A	135	GLY
1	7-A	175	ARG
1	7-A	179	CYS
1	7-A	180	LYS
1	7-A	185	GLY
1	7-A	203	VAL
1	7-A	209	LYS
1	7-B	225	SER
1	8-A	2	LEU
1	8-A	43	LEU

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Mol	Chain	Res	Type
1	8-A	138	PRO
1	8-A	157	ARG
1	8-A	177	ASP
1	8-A	206	ASN
1	8-B	134	ALA
1	8-B	175	ARG
1	9-A	42	CYS
1	9-A	50	LYS
1	9-A	131	VAL
1	9-A	132	ASN
1	9-A	134	ALA
1	9-A	207	ARG
1	9-B	46	ALA
1	9-B	84	ASP
1	9-B	199	SER
1	10-A	46	ALA
1	10-A	50	LYS
1	10-A	182	ASP
1	10-A	202	ALA
1	10-A	205	GLY
1	10-A	206	ASN
1	10-B	44	GLU
1	11-A	3	GLY
1	11-A	44	GLU
1	12-A	4	GLY
1	12-A	177	ASP
1	12-A	179	CYS
1	12-A	200	GLY
1	12-A	201	SER
1	12-B	42	CYS
1	12-B	43	LEU
1	12-B	199	SER
1	13-A	47	ALA
1	13-A	178	SER
1	13-B	227	LEU
1	14-A	129	GLY
1	14-A	136	ARG
1	14-A	181	GLY
1	14-A	182	ASP
1	14-A	199	SER
1	14-A	202	ALA
1	14-B	43	LEU

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Mol	Chain	Res	Type
1	14-B	50	LYS
1	14-B	159	HIS
1	14-B	227	LEU
1	15-A	137	ARG
1	15-A	157	ARG
1	15-A	181	GLY
1	15-B	201	SER
1	15-B	226	VAL
1	16-A	42	CYS
1	16-A	175	ARG
1	16-A	178	SER
1	16-B	174	ASN
1	16-B	226	VAL
1	16-B	227	LEU
1	17-A	46	ALA
1	17-A	47	ALA
1	17-A	50	LYS
1	17-A	132	ASN
1	18-A	132	ASN
1	18-A	181	GLY
1	18-B	199	SER
1	18-B	202	ALA
1	18-B	227	LEU
1	19-A	48	ASP
1	19-A	199	SER
1	19-A	203	VAL
1	19-B	50	LYS
1	19-B	199	SER
1	19-B	201	SER
1	19-B	227	LEU
1	20-A	172	GLU
1	20-A	179	CYS
1	20-A	181	GLY
1	20-B	84	ASP
1	21-A	3	GLY
1	21-A	134	ALA
1	21-A	139	ASP
1	21-A	180	LYS
1	21-A	207	ARG
1	21-B	50	LYS
1	21-B	165	THR
1	21-B	225	SER

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Mol	Chain	Res	Type
1	21-B	226	VAL
1	21-B	227	LEU
1	22-A	135	GLY
1	22-A	175	ARG
1	22-A	203	VAL
1	22-B	47	ALA
1	22-B	50	LYS
1	23-A	22	GLY
1	23-A	226	VAL
1	23-B	84	ASP
1	23-B	199	SER
1	23-B	226	VAL
1	23-B	227	LEU
1	24-A	2	LEU
1	24-A	46	ALA
1	24-A	133	HIS
1	24-A	174	ASN
1	24-A	176	ARG
1	24-B	134	ALA
1	24-B	199	SER
1	24-B	206	ASN
1	25-B	200	GLY
1	25-B	206	ASN
1	25-B	227	LEU
1	26-A	174	ASN
1	26-B	85	THR
1	26-B	198	THR
1	26-B	226	VAL
1	27-A	46	ALA
1	27-A	47	ALA
1	27-A	135	GLY
1	27-A	157	ARG
1	27-A	177	ASP
1	27-A	178	SER
1	27-A	201	SER
1	27-A	202	ALA
1	27-A	204	CYS
1	27-A	208	LYS
1	27-B	21	ASN
1	28-A	46	ALA
1	28-A	130	ILE
1	28-A	131	VAL

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Mol	Chain	Res	Type
1	28-A	135	GLY
1	28-A	139	ASP
1	28-A	204	CYS
1	28-A	210	PRO
1	28-B	199	SER
1	28-B	200	GLY
1	28-B	201	SER
1	28-B	227	LEU
1	29-A	177	ASP
1	29-A	200	GLY
1	29-A	201	SER
1	29-B	49	GLY
1	30-A	202	ALA
1	30-B	199	SER
1	31-A	42	CYS
1	31-A	48	ASP
1	31-A	129	GLY
1	31-A	131	VAL
1	31-A	136	ARG
1	31-A	201	SER
1	31-B	133	HIS
1	32-A	45	ASP
1	32-A	203	VAL
1	32-A	207	ARG
1	32-B	199	SER
1	32-B	206	ASN
1	32-B	226	VAL
1	33-A	201	SER
1	33-B	161	ASP
1	33-B	199	SER
1	34-A	46	ALA
1	34-A	130	ILE
1	34-A	177	ASP
1	34-A	181	GLY
1	34-A	208	LYS
1	34-B	203	VAL
1	35-A	130	ILE
1	35-A	133	HIS
1	35-B	174	ASN
1	35-B	200	GLY
1	35-B	224	ASP
1	35-B	225	SER

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Mol	Chain	Res	Type
1	36-A	44	GLU
1	36-A	131	VAL
1	36-A	133	HIS
1	36-A	138	PRO
1	36-A	176	ARG
1	36-A	227	LEU
1	37-A	157	ARG
1	37-A	177	ASP
1	37-B	161	ASP
1	37-B	204	CYS
1	37-B	227	LEU
1	38-A	134	ALA
1	38-A	225	SER
1	38-B	45	ASP
1	38-B	202	ALA
1	38-B	203	VAL
1	39-B	44	GLU
1	40-A	85	THR
1	40-A	129	GLY
1	40-A	157	ARG
1	40-B	45	ASP
1	40-B	161	ASP
1	40-B	204	CYS
1	41-A	131	VAL
1	41-A	133	HIS
1	41-A	134	ALA
1	41-A	139	ASP
1	41-A	174	ASN
1	41-A	176	ARG
1	41-A	198	THR
1	41-A	200	GLY
1	41-A	204	CYS
1	41-B	225	SER
1	42-A	134	ALA
1	42-A	135	GLY
1	42-A	138	PRO
1	42-A	200	GLY
1	42-A	204	CYS
1	43-A	3	GLY
1	43-A	46	ALA
1	43-A	130	ILE
1	43-A	133	HIS

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Mol	Chain	Res	Type
1	43-A	134	ALA
1	43-A	137	ARG
1	43-A	225	SER
1	43-B	44	GLU
1	44-B	203	VAL
1	45-A	3	GLY
1	45-A	45	ASP
1	45-A	85	THR
1	45-A	139	ASP
1	45-A	203	VAL
1	45-B	46	ALA
1	45-B	204	CYS
1	46-A	182	ASP
1	46-B	161	ASP
1	46-B	201	SER
1	47-A	2	LEU
1	47-A	139	ASP
1	47-A	208	LYS
1	47-B	47	ALA
1	47-B	199	SER
1	47-B	227	LEU
1	48-A	45	ASP
1	48-B	47	ALA
1	48-B	225	SER
1	49-A	44	GLU
1	49-A	46	ALA
1	49-A	182	ASP
1	49-A	207	ARG
1	49-B	47	ALA
1	49-B	134	ALA
1	49-B	159	HIS
1	49-B	224	ASP
1	50-A	130	ILE
1	50-A	201	SER
1	50-B	204	CYS
1	51-A	42	CYS
1	51-A	134	ALA
1	51-A	159	HIS
1	51-A	204	CYS
1	51-A	206	ASN
1	51-B	47	ALA
1	51-B	203	VAL

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Mol	Chain	Res	Type
1	51-B	224	ASP
1	52-A	3	GLY
1	52-A	42	CYS
1	52-A	129	GLY
1	52-B	21	ASN
1	52-B	48	ASP
1	52-B	49	GLY
1	52-B	50	LYS
1	53-A	42	CYS
1	53-B	45	ASP
1	53-B	47	ALA
1	54-A	45	ASP
1	54-A	134	ALA
1	54-A	177	ASP
1	54-A	200	GLY
1	55-A	177	ASP
1	55-A	178	SER
1	55-A	200	GLY
1	55-A	201	SER
1	55-B	48	ASP
1	55-B	204	CYS
1	56-A	176	ARG
1	56-B	46	ALA
1	56-B	47	ALA
1	57-A	43	LEU
1	57-A	46	ALA
1	57-A	182	ASP
1	57-A	206	ASN
1	57-B	44	GLU
1	57-B	202	ALA
1	58-A	2	LEU
1	58-A	22	GLY
1	58-A	46	ALA
1	58-A	47	ALA
1	58-A	133	HIS
1	58-A	139	ASP
1	58-A	176	ARG
1	58-A	203	VAL
1	58-B	175	ARG
1	58-B	227	LEU
1	59-A	48	ASP
1	59-A	130	ILE

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Mol	Chain	Res	Type
1	59-A	136	ARG
1	59-A	176	ARG
1	59-A	199	SER
1	59-B	134	ALA
1	59-B	202	ALA
1	59-B	203	VAL
1	59-B	207	ARG
1	59-B	227	LEU
1	60-A	180	LYS
1	60-B	45	ASP
1	60-B	200	GLY
1	60-B	203	VAL
1	61-A	133	HIS
1	61-A	176	ARG
1	61-B	174	ASN
1	61-B	203	VAL
1	62-A	45	ASP
1	62-A	178	SER
1	62-A	180	LYS
1	62-A	199	SER
1	62-B	48	ASP
1	62-B	175	ARG
1	63-A	46	ALA
1	63-A	132	ASN
1	63-A	138	PRO
1	63-B	227	LEU
1	64-A	134	ALA
1	64-A	138	PRO
1	64-A	185	GLY
1	64-B	202	ALA
1	65-A	2	LEU
1	65-A	133	HIS
1	65-A	177	ASP
1	65-A	199	SER
1	65-A	202	ALA
1	66-A	135	GLY
1	66-A	184	GLY
1	66-B	45	ASP
1	66-B	199	SER
1	66-B	226	VAL
1	67-A	177	ASP
1	67-A	183	SER

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Mol	Chain	Res	Type
1	67-A	203	VAL
1	68-A	48	ASP
1	68-A	134	ALA
1	68-A	174	ASN
1	68-A	183	SER
1	68-A	202	ALA
1	68-B	134	ALA
1	68-B	199	SER
1	68-B	201	SER
1	68-B	203	VAL
1	68-B	227	LEU
1	69-A	47	ALA
1	69-A	129	GLY
1	69-A	182	ASP
1	69-A	183	SER
1	70-A	46	ALA
1	70-A	136	ARG
1	70-A	158	THR
1	70-A	173	SER
1	70-A	205	GLY
1	70-A	207	ARG
1	70-B	50	LYS
1	70-B	159	HIS
1	70-B	200	GLY
1	71-A	133	HIS
1	71-A	173	SER
1	71-A	175	ARG
1	71-A	177	ASP
1	71-A	183	SER
1	71-B	161	ASP
1	72-A	177	ASP
1	72-A	203	VAL
1	72-B	199	SER
1	73-A	47	ALA
1	73-A	138	PRO
1	73-A	210	PRO
1	73-B	47	ALA
1	74-A	48	ASP
1	74-A	175	ARG
1	74-B	199	SER
1	74-B	204	CYS
1	74-B	227	LEU

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Mol	Chain	Res	Type
1	75-A	46	ALA
1	75-A	131	VAL
1	75-A	139	ASP
1	75-A	182	ASP
1	75-A	203	VAL
1	75-A	204	CYS
1	75-A	227	LEU
1	76-A	2	LEU
1	76-A	42	CYS
1	76-A	132	ASN
1	76-A	139	ASP
1	76-A	184	GLY
1	76-B	202	ALA
1	77-A	43	LEU
1	77-A	139	ASP
1	77-A	204	CYS
1	77-B	48	ASP
1	77-B	199	SER
1	1-A	174	ASN
1	2-A	198	THR
1	2-A	204	CYS
1	2-B	165	THR
1	3-A	186	PRO
1	3-A	202	ALA
1	4-A	48	ASP
1	4-A	85	THR
1	4-A	173	SER
1	4-A	183	SER
1	4-B	198	THR
1	4-B	200	GLY
1	5-A	175	ARG
1	5-B	21	ASN
1	5-B	202	ALA
1	6-A	134	ALA
1	6-A	186	PRO
1	6-B	45	ASP
1	6-B	85	THR
1	6-B	175	ARG
1	7-A	157	ARG
1	8-A	45	ASP
1	8-A	130	ILE
1	8-B	45	ASP

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Mol	Chain	Res	Type
1	8-B	199	SER
1	9-A	138	PRO
1	9-A	177	ASP
1	9-B	33	GLU
1	9-B	159	HIS
1	9-B	165	THR
1	10-A	4	GLY
1	10-B	43	LEU
1	10-B	203	VAL
1	11-A	133	HIS
1	11-A	205	GLY
1	12-A	130	ILE
1	12-A	133	HIS
1	12-A	138	PRO
1	12-A	139	ASP
1	12-A	199	SER
1	12-B	21	ASN
1	13-A	159	HIS
1	13-A	202	ALA
1	13-B	226	VAL
1	14-A	48	ASP
1	14-A	138	PRO
1	14-A	157	ARG
1	14-A	176	ARG
1	15-A	178	SER
1	15-A	183	SER
1	15-A	186	PRO
1	15-A	200	GLY
1	15-B	45	ASP
1	15-B	48	ASP
1	16-A	2	LEU
1	16-A	50	LYS
1	16-A	131	VAL
1	16-A	199	SER
1	16-A	200	GLY
1	16-A	206	ASN
1	16-B	175	ARG
1	17-A	44	GLU
1	17-A	133	HIS
1	17-A	178	SER
1	17-A	207	ARG
1	17-B	44	GLU

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Mol	Chain	Res	Type
1	17-B	48	ASP
1	17-B	50	LYS
1	17-B	190	GLY
1	18-A	3	GLY
1	18-A	47	ALA
1	18-A	133	HIS
1	18-B	50	LYS
1	19-B	45	ASP
1	19-B	49	GLY
1	20-A	182	ASP
1	20-B	47	ALA
1	20-B	204	CYS
1	20-B	227	LEU
1	21-B	116	ASP
1	22-A	46	ALA
1	22-B	191	GLY
1	22-B	227	LEU
1	23-A	2	LEU
1	23-A	157	ARG
1	23-A	225	SER
1	24-A	182	ASP
1	25-A	179	CYS
1	25-A	181	GLY
1	25-A	201	SER
1	26-A	134	ALA
1	26-A	139	ASP
1	26-A	177	ASP
1	26-A	179	CYS
1	26-A	182	ASP
1	26-A	207	ARG
1	27-A	48	ASP
1	27-A	137	ARG
1	27-B	175	ARG
1	28-A	133	HIS
1	28-A	208	LYS
1	28-B	47	ALA
1	28-B	202	ALA
1	29-A	207	ARG
1	29-A	209	LYS
1	31-A	204	CYS
1	31-B	159	HIS
1	32-A	46	ALA

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Mol	Chain	Res	Type
1	32-A	174	ASN
1	32-A	177	ASP
1	32-B	46	ALA
1	33-A	49	GLY
1	33-A	203	VAL
1	33-B	198	THR
1	33-B	210	PRO
1	34-B	45	ASP
1	34-B	47	ALA
1	34-B	161	ASP
1	34-B	202	ALA
1	35-B	204	CYS
1	36-A	134	ALA
1	36-A	135	GLY
1	36-A	174	ASN
1	36-A	199	SER
1	36-B	205	GLY
1	37-A	44	GLU
1	37-A	207	ARG
1	38-A	132	ASN
1	38-A	202	ALA
1	38-A	208	LYS
1	38-B	159	HIS
1	38-B	204	CYS
1	39-A	133	HIS
1	39-A	175	ARG
1	39-A	225	SER
1	39-B	83	PRO
1	41-A	46	ALA
1	41-A	177	ASP
1	41-A	210	PRO
1	43-A	181	GLY
1	43-B	85	THR
1	44-A	134	ALA
1	44-B	225	SER
1	46-A	138	PRO
1	46-A	176	ARG
1	46-A	177	ASP
1	46-B	206	ASN
1	47-A	47	ALA
1	47-A	48	ASP
1	47-A	182	ASP

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Mol	Chain	Res	Type
1	47-A	201	SER
1	47-B	44	GLU
1	48-A	139	ASP
1	49-B	133	HIS
1	50-B	47	ALA
1	50-B	116	ASP
1	51-A	173	SER
1	51-B	48	ASP
1	51-B	225	SER
1	52-B	202	ALA
1	53-A	136	ARG
1	53-B	46	ALA
1	54-A	130	ILE
1	54-A	207	ARG
1	55-A	48	ASP
1	55-A	173	SER
1	55-A	182	ASP
1	55-A	210	PRO
1	55-B	47	ALA
1	55-B	159	HIS
1	55-B	201	SER
1	56-B	226	VAL
1	56-B	227	LEU
1	57-A	198	THR
1	58-A	178	SER
1	58-A	182	ASP
1	58-A	204	CYS
1	58-B	21	ASN
1	58-B	87	ASP
1	60-A	157	ARG
1	60-A	186	PRO
1	60-B	46	ALA
1	61-A	132	ASN
1	61-B	200	GLY
1	61-B	204	CYS
1	62-A	201	SER
1	62-A	204	CYS
1	63-A	157	ARG
1	63-A	159	HIS
1	63-A	174	ASN
1	63-B	47	ALA
1	63-B	202	ALA

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Mol	Chain	Res	Type
1	64-A	45	ASP
1	64-A	46	ALA
1	64-A	173	SER
1	64-A	174	ASN
1	64-B	47	ALA
1	64-B	74	ARG
1	64-B	226	VAL
1	65-A	139	ASP
1	65-A	157	ARG
1	65-A	185	GLY
1	65-B	175	ARG
1	66-A	136	ARG
1	66-A	202	ALA
1	66-A	207	ARG
1	66-B	201	SER
1	67-A	134	ALA
1	67-A	178	SER
1	67-A	180	LYS
1	67-B	44	GLU
1	68-A	175	ARG
1	68-B	47	ALA
1	68-B	133	HIS
1	68-B	204	CYS
1	69-A	44	GLU
1	69-A	202	ALA
1	69-B	45	ASP
1	70-A	132	ASN
1	70-B	43	LEU
1	70-B	199	SER
1	71-A	22	GLY
1	71-B	47	ALA
1	73-A	132	ASN
1	73-A	133	HIS
1	73-A	134	ALA
1	73-A	182	ASP
1	73-B	226	VAL
1	74-A	41	HIS
1	74-A	157	ARG
1	74-A	178	SER
1	74-A	204	CYS
1	74-B	226	VAL
1	75-A	48	ASP

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Mol	Chain	Res	Type
1	75-A	138	PRO
1	76-A	138	PRO
1	76-A	210	PRO
1	77-A	132	ASN
1	77-A	201	SER
1	77-B	47	ALA
1	77-B	161	ASP
1	1-A	177	ASP
1	1-A	183	SER
1	2-A	174	ASN
1	2-B	45	ASP
1	2-B	159	HIS
1	3-B	199	SER
1	4-A	176	ARG
1	4-A	179	CYS
1	4-A	199	SER
1	4-B	204	CYS
1	5-B	44	GLU
1	7-A	85	THR
1	7-A	130	ILE
1	7-A	177	ASP
1	7-B	200	GLY
1	8-A	174	ASN
1	8-A	175	ARG
1	8-A	178	SER
1	8-A	202	ALA
1	8-B	202	ALA
1	10-A	204	CYS
1	12-A	172	GLU
1	12-A	178	SER
1	12-A	204	CYS
1	12-B	198	THR
1	12-B	201	SER
1	13-A	172	GLU
1	13-B	225	SER
1	14-A	21	ASN
1	14-A	137	ARG
1	15-A	202	ALA
1	15-A	203	VAL
1	16-A	158	THR
1	16-B	48	ASP
1	17-B	21	ASN

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Mol	Chain	Res	Type
1	18-A	2	LEU
1	18-A	49	GLY
1	19-A	47	ALA
1	19-A	129	GLY
1	19-A	177	ASP
1	19-A	182	ASP
1	19-B	200	GLY
1	19-B	203	VAL
1	20-A	173	SER
1	20-B	203	VAL
1	21-A	46	ALA
1	21-A	173	SER
1	21-A	174	ASN
1	21-A	206	ASN
1	22-A	130	ILE
1	22-A	138	PRO
1	22-B	43	LEU
1	22-B	116	ASP
1	22-B	190	GLY
1	24-A	137	ARG
1	26-B	204	CYS
1	26-B	227	LEU
1	28-A	47	ALA
1	28-B	48	ASP
1	29-B	47	ALA
1	30-A	46	ALA
1	30-A	173	SER
1	30-B	226	VAL
1	31-A	207	ARG
1	31-B	206	ASN
1	32-A	43	LEU
1	32-A	49	GLY
1	32-A	129	GLY
1	32-A	130	ILE
1	32-A	201	SER
1	33-A	175	ARG
1	33-A	178	SER
1	33-A	202	ALA
1	34-A	157	ARG
1	34-A	203	VAL
1	36-A	83	PRO
1	37-A	138	PRO

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Mol	Chain	Res	Type
1	37-A	174	ASN
1	38-A	22	GLY
1	38-A	157	ARG
1	38-A	177	ASP
1	38-A	179	CYS
1	39-A	47	ALA
1	39-B	46	ALA
1	41-A	129	GLY
1	41-A	159	HIS
1	41-A	178	SER
1	41-B	166	GLU
1	41-B	203	VAL
1	42-A	174	ASN
1	43-B	220	ALA
1	44-A	206	ASN
1	45-A	137	ARG
1	45-A	202	ALA
1	45-B	161	ASP
1	47-A	134	ALA
1	47-A	186	PRO
1	48-A	134	ALA
1	48-A	184	GLY
1	48-B	165	THR
1	48-B	206	ASN
1	50-A	47	ALA
1	50-A	133	HIS
1	50-A	182	ASP
1	50-A	227	LEU
1	50-B	45	ASP
1	50-B	198	THR
1	51-A	139	ASP
1	51-B	46	ALA
1	52-A	2	LEU
1	53-A	47	ALA
1	54-A	2	LEU
1	55-A	133	HIS
1	55-A	202	ALA
1	55-A	204	CYS
1	55-B	174	ASN
1	55-B	226	VAL
1	56-B	49	GLY
1	56-B	202	ALA

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Mol	Chain	Res	Type
1	57-A	200	GLY
1	58-A	206	ASN
1	58-B	161	ASP
1	59-A	3	GLY
1	60-A	129	GLY
1	60-A	199	SER
1	60-B	159	HIS
1	60-B	175	ARG
1	61-A	129	GLY
1	61-A	134	ALA
1	61-B	48	ASP
1	61-B	198	THR
1	61-B	226	VAL
1	62-A	46	ALA
1	64-A	136	ARG
1	65-A	49	GLY
1	65-A	129	GLY
1	65-B	159	HIS
1	66-A	44	GLU
1	66-A	159	HIS
1	66-A	210	PRO
1	66-B	175	ARG
1	67-A	173	SER
1	67-A	175	ARG
1	67-A	227	LEU
1	68-A	176	ARG
1	69-A	45	ASP
1	69-B	227	LEU
1	70-A	47	ALA
1	70-A	176	ARG
1	71-A	205	GLY
1	72-A	182	ASP
1	73-A	174	ASN
1	73-A	181	GLY
1	73-A	201	SER
1	73-A	207	ARG
1	74-B	165	THR
1	75-A	179	CYS
1	76-B	200	GLY
1	77-A	3	GLY
1	77-A	203	VAL
1	1-A	130	ILE

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Mol	Chain	Res	Type
1	1-A	199	SER
1	2-B	43	LEU
1	3-A	182	ASP
1	3-B	46	ALA
1	4-B	161	ASP
1	5-A	186	PRO
1	6-B	33	GLU
1	8-A	21	ASN
1	9-A	5	ARG
1	9-A	181	GLY
1	9-B	201	SER
1	10-A	85	THR
1	10-A	131	VAL
1	10-A	138	PRO
1	10-A	173	SER
1	11-A	206	ASN
1	11-B	45	ASP
1	11-B	224	ASP
1	12-A	47	ALA
1	12-A	181	GLY
1	12-A	206	ASN
1	13-A	83	PRO
1	13-A	134	ALA
1	13-A	137	ARG
1	13-A	177	ASP
1	13-A	179	CYS
1	13-A	201	SER
1	15-A	131	VAL
1	16-A	137	ARG
1	16-A	204	CYS
1	17-A	131	VAL
1	18-A	183	SER
1	18-B	159	HIS
1	18-B	210	PRO
1	19-A	208	LYS
1	20-B	164	ILE
1	22-A	180	LYS
1	22-B	44	GLU
1	23-A	46	ALA
1	23-B	83	PRO
1	23-B	85	THR
1	24-A	139	ASP

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Mol	Chain	Res	Type
1	25-A	139	ASP
1	25-A	178	SER
1	25-B	220	ALA
1	26-A	133	HIS
1	26-B	202	ALA
1	27-A	50	LYS
1	27-A	136	ARG
1	27-B	47	ALA
1	27-B	190	GLY
1	28-A	134	ALA
1	28-A	138	PRO
1	28-A	202	ALA
1	29-A	96	SER
1	30-A	201	SER
1	30-B	44	GLU
1	31-A	130	ILE
1	31-A	178	SER
1	31-B	226	VAL
1	32-A	180	LYS
1	33-A	206	ASN
1	33-B	202	ALA
1	34-B	79	PRO
1	35-A	131	VAL
1	36-A	47	ALA
1	36-A	208	LYS
1	37-A	180	LYS
1	38-B	158	THR
1	38-B	224	ASP
1	38-B	226	VAL
1	39-A	136	ARG
1	39-A	138	PRO
1	39-B	41	HIS
1	41-B	202	ALA
1	42-A	132	ASN
1	42-A	210	PRO
1	42-B	210	PRO
1	43-A	199	SER
1	44-A	137	ARG
1	45-A	130	ILE
1	45-A	207	ARG
1	47-A	133	HIS
1	47-A	184	GLY

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Mol	Chain	Res	Type
1	48-B	135	GLY
1	49-A	131	VAL
1	49-A	175	ARG
1	49-B	199	SER
1	50-A	49	GLY
1	51-A	182	ASP
1	51-A	198	THR
1	52-A	138	PRO
1	52-A	201	SER
1	52-B	161	ASP
1	54-B	47	ALA
1	57-A	21	ASN
1	57-A	176	ARG
1	57-A	183	SER
1	57-A	204	CYS
1	58-B	135	GLY
1	58-B	203	VAL
1	59-A	133	HIS
1	60-B	198	THR
1	61-A	157	ARG
1	61-A	183	SER
1	61-A	200	GLY
1	61-A	203	VAL
1	61-B	199	SER
1	62-B	47	ALA
1	63-A	139	ASP
1	63-B	159	HIS
1	64-A	44	GLU
1	65-B	203	VAL
1	66-A	176	ARG
1	67-A	132	ASN
1	67-B	201	SER
1	68-A	204	CYS
1	69-A	157	ARG
1	69-B	226	VAL
1	70-B	49	GLY
1	71-A	159	HIS
1	71-A	208	LYS
1	72-A	131	VAL
1	74-A	181	GLY
1	74-A	210	PRO
1	75-A	137	ARG

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Mol	Chain	Res	Type
1	75-B	226	VAL
1	76-A	137	ARG
1	77-A	22	GLY
1	77-B	46	ALA
1	1-B	165	THR
1	2-B	205	GLY
1	3-A	159	HIS
1	4-A	129	GLY
1	4-A	181	GLY
1	4-B	50	LYS
1	5-A	185	GLY
1	6-A	182	ASP
1	7-A	3	GLY
1	8-B	83	PRO
1	9-A	46	ALA
1	9-A	179	CYS
1	10-A	47	ALA
1	12-B	203	VAL
1	16-A	203	VAL
1	17-B	201	SER
1	19-A	159	HIS
1	20-A	137	ARG
1	20-A	138	PRO
1	22-A	176	ARG
1	22-B	206	ASN
1	23-A	203	VAL
1	24-A	83	PRO
1	24-B	159	HIS
1	25-A	130	ILE
1	27-B	174	ASN
1	29-A	2	LEU
1	29-A	181	GLY
1	31-B	203	VAL
1	32-B	190	GLY
1	32-B	203	VAL
1	34-A	44	GLU
1	34-B	206	ASN
1	35-A	203	VAL
1	35-A	226	VAL
1	37-A	131	VAL
1	37-A	186	PRO
1	37-B	203	VAL

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Mol	Chain	Res	Type
1	38-A	226	VAL
1	40-A	201	SER
1	40-A	203	VAL
1	40-B	79	PRO
1	43-A	129	GLY
1	43-A	200	GLY
1	44-A	49	GLY
1	44-B	79	PRO
1	44-B	210	PRO
1	45-A	46	ALA
1	46-B	83	PRO
1	47-A	203	VAL
1	47-B	161	ASP
1	48-A	136	ARG
1	49-B	204	CYS
1	50-A	184	GLY
1	53-A	200	GLY
1	56-A	130	ILE
1	58-A	135	GLY
1	58-A	179	CYS
1	58-B	45	ASP
1	58-B	134	ALA
1	59-B	210	PRO
1	61-A	138	PRO
1	61-A	201	SER
1	61-B	46	ALA
1	65-A	175	ARG
1	65-B	226	VAL
1	67-A	207	ARG
1	68-A	2	LEU
1	68-A	197	VAL
1	69-B	44	GLU
1	74-A	135	GLY
1	74-A	138	PRO
1	75-A	200	GLY
1	77-A	4	GLY
1	1-A	129	GLY
1	1-A	210	PRO
1	1-B	83	PRO
1	2-A	49	GLY
1	2-B	200	GLY
1	9-B	200	GLY

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Mol	Chain	Res	Type
1	13-B	223	ILE
1	17-A	210	PRO
1	19-A	210	PRO
1	24-A	181	GLY
1	28-B	203	VAL
1	32-A	181	GLY
1	38-A	131	VAL
1	38-A	135	GLY
1	39-A	181	GLY
1	45-B	203	VAL
1	47-A	138	PRO
1	50-A	137	ARG
1	55-A	3	GLY
1	55-B	200	GLY
1	57-A	135	GLY
1	57-A	205	GLY
1	57-A	210	PRO
1	59-A	203	VAL
1	63-A	210	PRO
1	68-B	226	VAL
1	73-A	3	GLY
1	73-A	131	VAL
1	1-A	181	GLY
1	11-A	83	PRO
1	14-A	200	GLY
1	20-B	210	PRO
1	25-A	131	VAL
1	38-A	137	ARG
1	49-A	129	GLY
1	57-B	226	VAL
1	60-A	22	GLY
1	73-A	203	VAL
1	76-A	203	VAL
1	5-A	130	ILE
1	11-A	200	GLY
1	17-A	186	PRO
1	22-B	210	PRO
1	23-A	138	PRO
1	27-A	203	VAL
1	34-A	138	PRO
1	37-A	209	LYS
1	46-B	210	PRO

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Mol	Chain	Res	Type
1	47-A	205	GLY
1	47-B	210	PRO
1	52-A	135	GLY
1	52-A	181	GLY
1	60-B	210	PRO
1	62-A	83	PRO
1	70-A	129	GLY
1	74-A	131	VAL
1	74-B	210	PRO
1	75-B	223	ILE
1	77-A	210	PRO
1	2-A	3	GLY
1	3-A	181	GLY
1	10-A	209	LYS
1	11-A	138	PRO
1	12-B	200	GLY
1	13-A	135	GLY
1	17-A	130	ILE
1	17-A	205	GLY
1	27-A	130	ILE
1	28-A	200	GLY
1	29-B	79	PRO
1	31-B	210	PRO
1	33-A	135	GLY
1	37-B	226	VAL
1	41-A	135	GLY
1	45-A	83	PRO
1	45-A	129	GLY
1	46-B	203	VAL
1	50-A	203	VAL
1	51-B	205	GLY
1	54-A	135	GLY
1	64-A	129	GLY
1	66-B	83	PRO
1	69-B	83	PRO
1	72-A	138	PRO
1	17-B	83	PRO
1	29-B	210	PRO
1	32-A	138	PRO
1	36-B	200	GLY
1	46-A	131	VAL
1	46-A	137	ARG

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Mol	Chain	Res	Type
1	51-A	135	GLY
1	51-B	226	VAL
1	53-B	83	PRO
1	64-A	130	ILE
1	69-B	190	GLY

4.3.2 Protein sidechains [i](#)

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	181/181 (100%)	156 (86%)	25 (14%)	3 1
1	1-B	181/181 (100%)	166 (92%)	15 (8%)	11 3
1	2-A	181/181 (100%)	156 (86%)	25 (14%)	3 1
1	2-B	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	3-A	181/181 (100%)	153 (84%)	28 (16%)	2 0
1	3-B	181/181 (100%)	163 (90%)	18 (10%)	8 2
1	4-A	181/181 (100%)	159 (88%)	22 (12%)	5 1
1	4-B	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	5-A	181/181 (100%)	155 (86%)	26 (14%)	3 0
1	5-B	181/181 (100%)	160 (88%)	21 (12%)	5 1
1	6-A	181/181 (100%)	152 (84%)	29 (16%)	2 0
1	6-B	181/181 (100%)	165 (91%)	16 (9%)	10 3
1	7-A	181/181 (100%)	154 (85%)	27 (15%)	3 0
1	7-B	181/181 (100%)	164 (91%)	17 (9%)	8 2
1	8-A	181/181 (100%)	157 (87%)	24 (13%)	4 1
1	8-B	181/181 (100%)	166 (92%)	15 (8%)	11 3
1	9-A	181/181 (100%)	158 (87%)	23 (13%)	4 1
1	9-B	181/181 (100%)	161 (89%)	20 (11%)	6 1
1	10-A	181/181 (100%)	156 (86%)	25 (14%)	3 1
1	10-B	181/181 (100%)	158 (87%)	23 (13%)	4 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	11-A	181/181 (100%)	156 (86%)	25 (14%)	3	1
1	11-B	181/181 (100%)	160 (88%)	21 (12%)	5	1
1	12-A	181/181 (100%)	162 (90%)	19 (10%)	7	1
1	12-B	181/181 (100%)	164 (91%)	17 (9%)	8	2
1	13-A	181/181 (100%)	155 (86%)	26 (14%)	3	0
1	13-B	181/181 (100%)	167 (92%)	14 (8%)	13	4
1	14-A	181/181 (100%)	157 (87%)	24 (13%)	4	1
1	14-B	181/181 (100%)	163 (90%)	18 (10%)	8	2
1	15-A	181/181 (100%)	158 (87%)	23 (13%)	4	1
1	15-B	181/181 (100%)	160 (88%)	21 (12%)	5	1
1	16-A	181/181 (100%)	163 (90%)	18 (10%)	8	2
1	16-B	181/181 (100%)	155 (86%)	26 (14%)	3	0
1	17-A	181/181 (100%)	150 (83%)	31 (17%)	2	0
1	17-B	181/181 (100%)	159 (88%)	22 (12%)	5	1
1	18-A	181/181 (100%)	163 (90%)	18 (10%)	8	2
1	18-B	181/181 (100%)	162 (90%)	19 (10%)	7	1
1	19-A	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	19-B	181/181 (100%)	162 (90%)	19 (10%)	7	1
1	20-A	181/181 (100%)	154 (85%)	27 (15%)	3	0
1	20-B	181/181 (100%)	154 (85%)	27 (15%)	3	0
1	21-A	181/181 (100%)	163 (90%)	18 (10%)	8	2
1	21-B	181/181 (100%)	154 (85%)	27 (15%)	3	0
1	22-A	181/181 (100%)	159 (88%)	22 (12%)	5	1
1	22-B	181/181 (100%)	162 (90%)	19 (10%)	7	1
1	23-A	181/181 (100%)	159 (88%)	22 (12%)	5	1
1	23-B	181/181 (100%)	157 (87%)	24 (13%)	4	1
1	24-A	181/181 (100%)	149 (82%)	32 (18%)	2	0
1	24-B	181/181 (100%)	163 (90%)	18 (10%)	8	2
1	25-A	181/181 (100%)	150 (83%)	31 (17%)	2	0
1	25-B	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	26-A	181/181 (100%)	163 (90%)	18 (10%)	8	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	26-B	181/181 (100%)	159 (88%)	22 (12%)	5	1
1	27-A	181/181 (100%)	155 (86%)	26 (14%)	3	0
1	27-B	181/181 (100%)	160 (88%)	21 (12%)	5	1
1	28-A	181/181 (100%)	163 (90%)	18 (10%)	8	2
1	28-B	181/181 (100%)	157 (87%)	24 (13%)	4	1
1	29-A	181/181 (100%)	159 (88%)	22 (12%)	5	1
1	29-B	181/181 (100%)	155 (86%)	26 (14%)	3	0
1	30-A	181/181 (100%)	152 (84%)	29 (16%)	2	0
1	30-B	181/181 (100%)	164 (91%)	17 (9%)	8	2
1	31-A	181/181 (100%)	156 (86%)	25 (14%)	3	1
1	31-B	181/181 (100%)	167 (92%)	14 (8%)	13	4
1	32-A	181/181 (100%)	151 (83%)	30 (17%)	2	0
1	32-B	181/181 (100%)	160 (88%)	21 (12%)	5	1
1	33-A	181/181 (100%)	160 (88%)	21 (12%)	5	1
1	33-B	181/181 (100%)	160 (88%)	21 (12%)	5	1
1	34-A	181/181 (100%)	156 (86%)	25 (14%)	3	1
1	34-B	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	35-A	181/181 (100%)	159 (88%)	22 (12%)	5	1
1	35-B	181/181 (100%)	163 (90%)	18 (10%)	8	2
1	36-A	181/181 (100%)	154 (85%)	27 (15%)	3	0
1	36-B	181/181 (100%)	164 (91%)	17 (9%)	8	2
1	37-A	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	37-B	181/181 (100%)	162 (90%)	19 (10%)	7	1
1	38-A	181/181 (100%)	160 (88%)	21 (12%)	5	1
1	38-B	181/181 (100%)	165 (91%)	16 (9%)	10	3
1	39-A	181/181 (100%)	156 (86%)	25 (14%)	3	1
1	39-B	181/181 (100%)	166 (92%)	15 (8%)	11	3
1	40-A	181/181 (100%)	163 (90%)	18 (10%)	8	2
1	40-B	181/181 (100%)	167 (92%)	14 (8%)	13	4
1	41-A	181/181 (100%)	155 (86%)	26 (14%)	3	0
1	41-B	181/181 (100%)	161 (89%)	20 (11%)	6	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	42-A	181/181 (100%)	153 (84%)	28 (16%)	2	0
1	42-B	181/181 (100%)	165 (91%)	16 (9%)	10	3
1	43-A	181/181 (100%)	155 (86%)	26 (14%)	3	0
1	43-B	181/181 (100%)	163 (90%)	18 (10%)	8	2
1	44-A	181/181 (100%)	147 (81%)	34 (19%)	1	0
1	44-B	181/181 (100%)	164 (91%)	17 (9%)	8	2
1	45-A	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	45-B	181/181 (100%)	164 (91%)	17 (9%)	8	2
1	46-A	181/181 (100%)	146 (81%)	35 (19%)	1	0
1	46-B	181/181 (100%)	166 (92%)	15 (8%)	11	3
1	47-A	181/181 (100%)	153 (84%)	28 (16%)	2	0
1	47-B	181/181 (100%)	160 (88%)	21 (12%)	5	1
1	48-A	181/181 (100%)	154 (85%)	27 (15%)	3	0
1	48-B	181/181 (100%)	157 (87%)	24 (13%)	4	1
1	49-A	181/181 (100%)	153 (84%)	28 (16%)	2	0
1	49-B	181/181 (100%)	162 (90%)	19 (10%)	7	1
1	50-A	181/181 (100%)	157 (87%)	24 (13%)	4	1
1	50-B	181/181 (100%)	158 (87%)	23 (13%)	4	1
1	51-A	181/181 (100%)	159 (88%)	22 (12%)	5	1
1	51-B	181/181 (100%)	165 (91%)	16 (9%)	10	3
1	52-A	181/181 (100%)	159 (88%)	22 (12%)	5	1
1	52-B	181/181 (100%)	160 (88%)	21 (12%)	5	1
1	53-A	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	53-B	181/181 (100%)	159 (88%)	22 (12%)	5	1
1	54-A	181/181 (100%)	158 (87%)	23 (13%)	4	1
1	54-B	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	55-A	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	55-B	181/181 (100%)	162 (90%)	19 (10%)	7	1
1	56-A	181/181 (100%)	151 (83%)	30 (17%)	2	0
1	56-B	181/181 (100%)	166 (92%)	15 (8%)	11	3
1	57-A	181/181 (100%)	154 (85%)	27 (15%)	3	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	57-B	181/181 (100%)	166 (92%)	15 (8%)	11	3
1	58-A	181/181 (100%)	155 (86%)	26 (14%)	3	0
1	58-B	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	59-A	181/181 (100%)	155 (86%)	26 (14%)	3	0
1	59-B	181/181 (100%)	160 (88%)	21 (12%)	5	1
1	60-A	181/181 (100%)	155 (86%)	26 (14%)	3	0
1	60-B	181/181 (100%)	165 (91%)	16 (9%)	10	3
1	61-A	181/181 (100%)	157 (87%)	24 (13%)	4	1
1	61-B	181/181 (100%)	153 (84%)	28 (16%)	2	0
1	62-A	181/181 (100%)	159 (88%)	22 (12%)	5	1
1	62-B	181/181 (100%)	160 (88%)	21 (12%)	5	1
1	63-A	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	63-B	181/181 (100%)	168 (93%)	13 (7%)	14	4
1	64-A	181/181 (100%)	162 (90%)	19 (10%)	7	1
1	64-B	181/181 (100%)	157 (87%)	24 (13%)	4	1
1	65-A	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	65-B	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	66-A	181/181 (100%)	150 (83%)	31 (17%)	2	0
1	66-B	181/181 (100%)	156 (86%)	25 (14%)	3	1
1	67-A	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	67-B	181/181 (100%)	169 (93%)	12 (7%)	16	5
1	68-A	181/181 (100%)	152 (84%)	29 (16%)	2	0
1	68-B	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	69-A	181/181 (100%)	162 (90%)	19 (10%)	7	1
1	69-B	181/181 (100%)	163 (90%)	18 (10%)	8	2
1	70-A	181/181 (100%)	158 (87%)	23 (13%)	4	1
1	70-B	181/181 (100%)	165 (91%)	16 (9%)	10	3
1	71-A	181/181 (100%)	154 (85%)	27 (15%)	3	0
1	71-B	181/181 (100%)	162 (90%)	19 (10%)	7	1
1	72-A	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	72-B	181/181 (100%)	162 (90%)	19 (10%)	7	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	73-A	181/181 (100%)	155 (86%)	26 (14%)	3	0
1	73-B	181/181 (100%)	162 (90%)	19 (10%)	7	1
1	74-A	181/181 (100%)	164 (91%)	17 (9%)	8	2
1	74-B	181/181 (100%)	165 (91%)	16 (9%)	10	3
1	75-A	181/181 (100%)	160 (88%)	21 (12%)	5	1
1	75-B	181/181 (100%)	159 (88%)	22 (12%)	5	1
1	76-A	181/181 (100%)	156 (86%)	25 (14%)	3	1
1	76-B	181/181 (100%)	161 (89%)	20 (11%)	6	1
1	77-A	181/181 (100%)	162 (90%)	19 (10%)	7	1
1	77-B	181/181 (100%)	166 (92%)	15 (8%)	11	3
All	All	27874/27874 (100%)	24533 (88%)	3341 (12%)	5	1

All (3341) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	1	ILE
1	1-A	2	LEU
1	1-A	5	ARG
1	1-A	30	LEU
1	1-A	44	GLU
1	1-A	45	ASP
1	1-A	48	ASP
1	1-A	69	LEU
1	1-A	73	LEU
1	1-A	82	GLN
1	1-A	131	VAL
1	1-A	132	ASN
1	1-A	136	ARG
1	1-A	137	ARG
1	1-A	145	LEU
1	1-A	172	GLU
1	1-A	180	LYS
1	1-A	182	ASP
1	1-A	187	LEU
1	1-A	198	THR
1	1-A	206	ASN
1	1-A	207	ARG
1	1-A	208	LYS

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Mol	Chain	Res	Type
1	1-A	209	LYS
1	1-A	227	LEU
1	1-B	21	ASN
1	1-B	43	LEU
1	1-B	45	ASP
1	1-B	62	GLN
1	1-B	71	ASP
1	1-B	74	ARG
1	1-B	96	SER
1	1-B	115	ARG
1	1-B	136	ARG
1	1-B	150	ASP
1	1-B	174	ASN
1	1-B	176	ARG
1	1-B	198	THR
1	1-B	206	ASN
1	1-B	227	LEU
1	2-A	1	ILE
1	2-A	5	ARG
1	2-A	8	GLU
1	2-A	25	LEU
1	2-A	30	LEU
1	2-A	68	ARG
1	2-A	74	ARG
1	2-A	84	ASP
1	2-A	97	GLU
1	2-A	98	LYS
1	2-A	133	HIS
1	2-A	136	ARG
1	2-A	137	ARG
1	2-A	156	ARG
1	2-A	157	ARG
1	2-A	174	ASN
1	2-A	177	ASP
1	2-A	178	SER
1	2-A	180	LYS
1	2-A	207	ARG
1	2-A	208	LYS
1	2-A	210	PRO
1	2-A	215	ARG
1	2-A	224	ASP
1	2-A	227	LEU

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Mol	Chain	Res	Type
1	2-B	5	ARG
1	2-B	8	GLU
1	2-B	29	VAL
1	2-B	43	LEU
1	2-B	45	ASP
1	2-B	48	ASP
1	2-B	50	LYS
1	2-B	68	ARG
1	2-B	85	THR
1	2-B	98	LYS
1	2-B	149	LEU
1	2-B	150	ASP
1	2-B	174	ASN
1	2-B	175	ARG
1	2-B	176	ARG
1	2-B	179	CYS
1	2-B	203	VAL
1	2-B	206	ASN
1	2-B	207	ARG
1	2-B	227	LEU
1	3-A	2	LEU
1	3-A	20	LEU
1	3-A	30	LEU
1	3-A	44	GLU
1	3-A	48	ASP
1	3-A	50	LYS
1	3-A	53	VAL
1	3-A	68	ARG
1	3-A	71	ASP
1	3-A	73	LEU
1	3-A	74	ARG
1	3-A	82	GLN
1	3-A	84	ASP
1	3-A	85	THR
1	3-A	98	LYS
1	3-A	106	ARG
1	3-A	115	ARG
1	3-A	137	ARG
1	3-A	175	ARG
1	3-A	178	SER
1	3-A	179	CYS
1	3-A	180	LYS

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Mol	Chain	Res	Type
1	3-A	182	ASP
1	3-A	187	LEU
1	3-A	198	THR
1	3-A	203	VAL
1	3-A	209	LYS
1	3-A	227	LEU
1	3-B	21	ASN
1	3-B	43	LEU
1	3-B	45	ASP
1	3-B	50	LYS
1	3-B	74	ARG
1	3-B	85	THR
1	3-B	98	LYS
1	3-B	133	HIS
1	3-B	136	ARG
1	3-B	149	LEU
1	3-B	187	LEU
1	3-B	201	SER
1	3-B	204	CYS
1	3-B	207	ARG
1	3-B	216	VAL
1	3-B	218	SER
1	3-B	225	SER
1	3-B	227	LEU
1	4-A	1	ILE
1	4-A	2	LEU
1	4-A	8	GLU
1	4-A	20	LEU
1	4-A	33	GLU
1	4-A	45	ASP
1	4-A	48	ASP
1	4-A	68	ARG
1	4-A	73	LEU
1	4-A	82	GLN
1	4-A	115	ARG
1	4-A	130	ILE
1	4-A	131	VAL
1	4-A	133	HIS
1	4-A	137	ARG
1	4-A	156	ARG
1	4-A	172	GLU
1	4-A	175	ARG

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Mol	Chain	Res	Type
1	4-A	178	SER
1	4-A	180	LYS
1	4-A	199	SER
1	4-A	215	ARG
1	4-B	2	LEU
1	4-B	8	GLU
1	4-B	29	VAL
1	4-B	41	HIS
1	4-B	45	ASP
1	4-B	73	LEU
1	4-B	74	ARG
1	4-B	84	ASP
1	4-B	96	SER
1	4-B	97	GLU
1	4-B	115	ARG
1	4-B	154	CYS
1	4-B	158	THR
1	4-B	166	GLU
1	4-B	167	ARG
1	4-B	207	ARG
1	4-B	216	VAL
1	4-B	225	SER
1	4-B	226	VAL
1	4-B	227	LEU
1	5-A	1	ILE
1	5-A	2	LEU
1	5-A	43	LEU
1	5-A	44	GLU
1	5-A	45	ASP
1	5-A	48	ASP
1	5-A	50	LYS
1	5-A	68	ARG
1	5-A	73	LEU
1	5-A	98	LYS
1	5-A	115	ARG
1	5-A	130	ILE
1	5-A	136	ARG
1	5-A	137	ARG
1	5-A	140	SER
1	5-A	166	GLU
1	5-A	172	GLU
1	5-A	173	SER

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Mol	Chain	Res	Type
1	5-A	177	ASP
1	5-A	180	LYS
1	5-A	182	ASP
1	5-A	187	LEU
1	5-A	198	THR
1	5-A	199	SER
1	5-A	203	VAL
1	5-A	209	LYS
1	5-B	5	ARG
1	5-B	41	HIS
1	5-B	43	LEU
1	5-B	44	GLU
1	5-B	73	LEU
1	5-B	82	GLN
1	5-B	97	GLU
1	5-B	98	LYS
1	5-B	136	ARG
1	5-B	137	ARG
1	5-B	143	HIS
1	5-B	154	CYS
1	5-B	174	ASN
1	5-B	176	ARG
1	5-B	198	THR
1	5-B	199	SER
1	5-B	203	VAL
1	5-B	204	CYS
1	5-B	206	ASN
1	5-B	207	ARG
1	5-B	227	LEU
1	6-A	1	ILE
1	6-A	5	ARG
1	6-A	25	LEU
1	6-A	30	LEU
1	6-A	41	HIS
1	6-A	43	LEU
1	6-A	50	LYS
1	6-A	51	VAL
1	6-A	73	LEU
1	6-A	96	SER
1	6-A	97	GLU
1	6-A	115	ARG
1	6-A	125	VAL

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Mol	Chain	Res	Type
1	6-A	130	ILE
1	6-A	136	ARG
1	6-A	137	ARG
1	6-A	156	ARG
1	6-A	157	ARG
1	6-A	166	GLU
1	6-A	172	GLU
1	6-A	174	ASN
1	6-A	175	ARG
1	6-A	176	ARG
1	6-A	177	ASP
1	6-A	183	SER
1	6-A	201	SER
1	6-A	204	CYS
1	6-A	209	LYS
1	6-A	227	LEU
1	6-B	5	ARG
1	6-B	43	LEU
1	6-B	52	GLN
1	6-B	73	LEU
1	6-B	74	ARG
1	6-B	97	GLU
1	6-B	98	LYS
1	6-B	133	HIS
1	6-B	174	ASN
1	6-B	176	ARG
1	6-B	201	SER
1	6-B	204	CYS
1	6-B	206	ASN
1	6-B	224	ASP
1	6-B	225	SER
1	6-B	227	LEU
1	7-A	5	ARG
1	7-A	30	LEU
1	7-A	48	ASP
1	7-A	50	LYS
1	7-A	68	ARG
1	7-A	73	LEU
1	7-A	74	ARG
1	7-A	82	GLN
1	7-A	84	ASP
1	7-A	85	THR

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Mol	Chain	Res	Type
1	7-A	100	THR
1	7-A	106	ARG
1	7-A	107	PRO
1	7-A	115	ARG
1	7-A	133	HIS
1	7-A	136	ARG
1	7-A	137	ARG
1	7-A	156	ARG
1	7-A	158	THR
1	7-A	173	SER
1	7-A	174	ASN
1	7-A	179	CYS
1	7-A	182	ASP
1	7-A	183	SER
1	7-A	204	CYS
1	7-A	209	LYS
1	7-A	210	PRO
1	7-B	8	GLU
1	7-B	43	LEU
1	7-B	44	GLU
1	7-B	45	ASP
1	7-B	50	LYS
1	7-B	68	ARG
1	7-B	82	GLN
1	7-B	84	ASP
1	7-B	115	ARG
1	7-B	136	ARG
1	7-B	166	GLU
1	7-B	167	ARG
1	7-B	174	ASN
1	7-B	198	THR
1	7-B	199	SER
1	7-B	201	SER
1	7-B	226	VAL
1	8-A	5	ARG
1	8-A	29	VAL
1	8-A	44	GLU
1	8-A	50	LYS
1	8-A	68	ARG
1	8-A	73	LEU
1	8-A	74	ARG
1	8-A	82	GLN

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Mol	Chain	Res	Type
1	8-A	84	ASP
1	8-A	98	LYS
1	8-A	136	ARG
1	8-A	137	ARG
1	8-A	156	ARG
1	8-A	175	ARG
1	8-A	176	ARG
1	8-A	179	CYS
1	8-A	180	LYS
1	8-A	182	ASP
1	8-A	203	VAL
1	8-A	204	CYS
1	8-A	207	ARG
1	8-A	208	LYS
1	8-A	209	LYS
1	8-A	224	ASP
1	8-B	29	VAL
1	8-B	43	LEU
1	8-B	44	GLU
1	8-B	68	ARG
1	8-B	73	LEU
1	8-B	82	GLN
1	8-B	84	ASP
1	8-B	96	SER
1	8-B	108	LEU
1	8-B	133	HIS
1	8-B	136	ARG
1	8-B	158	THR
1	8-B	172	GLU
1	8-B	174	ASN
1	8-B	207	ARG
1	9-A	1	ILE
1	9-A	5	ARG
1	9-A	30	LEU
1	9-A	34	GLN
1	9-A	41	HIS
1	9-A	44	GLU
1	9-A	53	VAL
1	9-A	68	ARG
1	9-A	74	ARG
1	9-A	98	LYS
1	9-A	115	ARG

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Mol	Chain	Res	Type
1	9-A	132	ASN
1	9-A	136	ARG
1	9-A	137	ARG
1	9-A	145	LEU
1	9-A	174	ASN
1	9-A	176	ARG
1	9-A	179	CYS
1	9-A	183	SER
1	9-A	198	THR
1	9-A	204	CYS
1	9-A	207	ARG
1	9-A	227	LEU
1	9-B	2	LEU
1	9-B	21	ASN
1	9-B	31	VAL
1	9-B	41	HIS
1	9-B	44	GLU
1	9-B	45	ASP
1	9-B	50	LYS
1	9-B	71	ASP
1	9-B	84	ASP
1	9-B	96	SER
1	9-B	115	ARG
1	9-B	116	ASP
1	9-B	133	HIS
1	9-B	150	ASP
1	9-B	154	CYS
1	9-B	167	ARG
1	9-B	174	ASN
1	9-B	178	SER
1	9-B	201	SER
1	9-B	207	ARG
1	10-A	2	LEU
1	10-A	20	LEU
1	10-A	30	LEU
1	10-A	43	LEU
1	10-A	45	ASP
1	10-A	48	ASP
1	10-A	68	ARG
1	10-A	74	ARG
1	10-A	82	GLN
1	10-A	83	PRO

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Mol	Chain	Res	Type
1	10-A	97	GLU
1	10-A	106	ARG
1	10-A	115	ARG
1	10-A	130	ILE
1	10-A	132	ASN
1	10-A	136	ARG
1	10-A	137	ARG
1	10-A	158	THR
1	10-A	166	GLU
1	10-A	176	ARG
1	10-A	179	CYS
1	10-A	182	ASP
1	10-A	204	CYS
1	10-A	208	LYS
1	10-A	227	LEU
1	10-B	8	GLU
1	10-B	29	VAL
1	10-B	41	HIS
1	10-B	45	ASP
1	10-B	71	ASP
1	10-B	73	LEU
1	10-B	82	GLN
1	10-B	84	ASP
1	10-B	96	SER
1	10-B	133	HIS
1	10-B	158	THR
1	10-B	166	GLU
1	10-B	167	ARG
1	10-B	174	ASN
1	10-B	175	ARG
1	10-B	178	SER
1	10-B	198	THR
1	10-B	199	SER
1	10-B	201	SER
1	10-B	203	VAL
1	10-B	204	CYS
1	10-B	206	ASN
1	10-B	207	ARG
1	11-A	2	LEU
1	11-A	29	VAL
1	11-A	43	LEU
1	11-A	44	GLU

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Mol	Chain	Res	Type
1	11-A	45	ASP
1	11-A	53	VAL
1	11-A	68	ARG
1	11-A	84	ASP
1	11-A	103	PRO
1	11-A	106	ARG
1	11-A	115	ARG
1	11-A	130	ILE
1	11-A	137	ARG
1	11-A	145	LEU
1	11-A	158	THR
1	11-A	174	ASN
1	11-A	176	ARG
1	11-A	179	CYS
1	11-A	180	LYS
1	11-A	182	ASP
1	11-A	183	SER
1	11-A	198	THR
1	11-A	199	SER
1	11-A	206	ASN
1	11-A	224	ASP
1	11-B	44	GLU
1	11-B	48	ASP
1	11-B	62	GLN
1	11-B	63	PRO
1	11-B	73	LEU
1	11-B	84	ASP
1	11-B	108	LEU
1	11-B	132	ASN
1	11-B	133	HIS
1	11-B	136	ARG
1	11-B	140	SER
1	11-B	158	THR
1	11-B	170	CYS
1	11-B	175	ARG
1	11-B	176	ARG
1	11-B	180	LYS
1	11-B	204	CYS
1	11-B	206	ASN
1	11-B	207	ARG
1	11-B	224	ASP
1	11-B	227	LEU

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Mol	Chain	Res	Type
1	12-A	2	LEU
1	12-A	20	LEU
1	12-A	25	LEU
1	12-A	43	LEU
1	12-A	68	ARG
1	12-A	73	LEU
1	12-A	115	ARG
1	12-A	130	ILE
1	12-A	136	ARG
1	12-A	137	ARG
1	12-A	158	THR
1	12-A	174	ASN
1	12-A	176	ARG
1	12-A	177	ASP
1	12-A	180	LYS
1	12-A	201	SER
1	12-A	204	CYS
1	12-A	208	LYS
1	12-A	215	ARG
1	12-B	2	LEU
1	12-B	43	LEU
1	12-B	44	GLU
1	12-B	48	ASP
1	12-B	50	LYS
1	12-B	68	ARG
1	12-B	73	LEU
1	12-B	84	ASP
1	12-B	112	ARG
1	12-B	137	ARG
1	12-B	158	THR
1	12-B	180	LYS
1	12-B	198	THR
1	12-B	204	CYS
1	12-B	207	ARG
1	12-B	225	SER
1	12-B	227	LEU
1	13-A	5	ARG
1	13-A	8	GLU
1	13-A	25	LEU
1	13-A	30	LEU
1	13-A	43	LEU
1	13-A	44	GLU

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Mol	Chain	Res	Type
1	13-A	45	ASP
1	13-A	48	ASP
1	13-A	50	LYS
1	13-A	53	VAL
1	13-A	68	ARG
1	13-A	84	ASP
1	13-A	85	THR
1	13-A	112	ARG
1	13-A	115	ARG
1	13-A	130	ILE
1	13-A	133	HIS
1	13-A	136	ARG
1	13-A	142	GLN
1	13-A	174	ASN
1	13-A	175	ARG
1	13-A	180	LYS
1	13-A	182	ASP
1	13-A	198	THR
1	13-A	201	SER
1	13-A	203	VAL
1	13-B	29	VAL
1	13-B	68	ARG
1	13-B	82	GLN
1	13-B	112	ARG
1	13-B	133	HIS
1	13-B	154	CYS
1	13-B	158	THR
1	13-B	175	ARG
1	13-B	199	SER
1	13-B	201	SER
1	13-B	204	CYS
1	13-B	207	ARG
1	13-B	208	LYS
1	13-B	226	VAL
1	14-A	1	ILE
1	14-A	5	ARG
1	14-A	30	LEU
1	14-A	44	GLU
1	14-A	45	ASP
1	14-A	50	LYS
1	14-A	62	GLN
1	14-A	68	ARG

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Mol	Chain	Res	Type
1	14-A	74	ARG
1	14-A	84	ASP
1	14-A	115	ARG
1	14-A	132	ASN
1	14-A	136	ARG
1	14-A	137	ARG
1	14-A	158	THR
1	14-A	173	SER
1	14-A	175	ARG
1	14-A	176	ARG
1	14-A	178	SER
1	14-A	180	LYS
1	14-A	198	THR
1	14-A	204	CYS
1	14-A	206	ASN
1	14-A	215	ARG
1	14-B	5	ARG
1	14-B	29	VAL
1	14-B	62	GLN
1	14-B	68	ARG
1	14-B	73	LEU
1	14-B	85	THR
1	14-B	97	GLU
1	14-B	112	ARG
1	14-B	115	ARG
1	14-B	136	ARG
1	14-B	150	ASP
1	14-B	175	ARG
1	14-B	183	SER
1	14-B	199	SER
1	14-B	203	VAL
1	14-B	207	ARG
1	14-B	225	SER
1	14-B	227	LEU
1	15-A	1	ILE
1	15-A	2	LEU
1	15-A	20	LEU
1	15-A	43	LEU
1	15-A	44	GLU
1	15-A	50	LYS
1	15-A	68	ARG
1	15-A	73	LEU

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Mol	Chain	Res	Type
1	15-A	84	ASP
1	15-A	112	ARG
1	15-A	115	ARG
1	15-A	131	VAL
1	15-A	136	ARG
1	15-A	142	GLN
1	15-A	143	HIS
1	15-A	166	GLU
1	15-A	172	GLU
1	15-A	175	ARG
1	15-A	178	SER
1	15-A	180	LYS
1	15-A	182	ASP
1	15-A	203	VAL
1	15-A	204	CYS
1	15-B	5	ARG
1	15-B	25	LEU
1	15-B	33	GLU
1	15-B	44	GLU
1	15-B	48	ASP
1	15-B	68	ARG
1	15-B	73	LEU
1	15-B	112	ARG
1	15-B	115	ARG
1	15-B	133	HIS
1	15-B	136	ARG
1	15-B	137	ARG
1	15-B	149	LEU
1	15-B	172	GLU
1	15-B	174	ASN
1	15-B	175	ARG
1	15-B	183	SER
1	15-B	199	SER
1	15-B	201	SER
1	15-B	225	SER
1	15-B	227	LEU
1	16-A	2	LEU
1	16-A	44	GLU
1	16-A	50	LYS
1	16-A	74	ARG
1	16-A	115	ARG
1	16-A	131	VAL

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Mol	Chain	Res	Type
1	16-A	132	ASN
1	16-A	136	ARG
1	16-A	140	SER
1	16-A	158	THR
1	16-A	174	ASN
1	16-A	176	ARG
1	16-A	180	LYS
1	16-A	182	ASP
1	16-A	183	SER
1	16-A	204	CYS
1	16-A	215	ARG
1	16-A	227	LEU
1	16-B	25	LEU
1	16-B	31	VAL
1	16-B	48	ASP
1	16-B	51	VAL
1	16-B	62	GLN
1	16-B	68	ARG
1	16-B	74	ARG
1	16-B	84	ASP
1	16-B	85	THR
1	16-B	112	ARG
1	16-B	115	ARG
1	16-B	133	HIS
1	16-B	136	ARG
1	16-B	137	ARG
1	16-B	150	ASP
1	16-B	156	ARG
1	16-B	161	ASP
1	16-B	172	GLU
1	16-B	174	ASN
1	16-B	199	SER
1	16-B	201	SER
1	16-B	203	VAL
1	16-B	206	ASN
1	16-B	208	LYS
1	16-B	218	SER
1	16-B	226	VAL
1	17-A	5	ARG
1	17-A	20	LEU
1	17-A	25	LEU
1	17-A	29	VAL

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Mol	Chain	Res	Type
1	17-A	30	LEU
1	17-A	43	LEU
1	17-A	45	ASP
1	17-A	48	ASP
1	17-A	50	LYS
1	17-A	68	ARG
1	17-A	74	ARG
1	17-A	96	SER
1	17-A	106	ARG
1	17-A	112	ARG
1	17-A	115	ARG
1	17-A	125	VAL
1	17-A	130	ILE
1	17-A	131	VAL
1	17-A	133	HIS
1	17-A	137	ARG
1	17-A	143	HIS
1	17-A	157	ARG
1	17-A	159	HIS
1	17-A	175	ARG
1	17-A	180	LYS
1	17-A	182	ASP
1	17-A	187	LEU
1	17-A	198	THR
1	17-A	201	SER
1	17-A	204	CYS
1	17-A	224	ASP
1	17-B	25	LEU
1	17-B	33	GLU
1	17-B	62	GLN
1	17-B	73	LEU
1	17-B	81	SER
1	17-B	84	ASP
1	17-B	85	THR
1	17-B	98	LYS
1	17-B	112	ARG
1	17-B	115	ARG
1	17-B	136	ARG
1	17-B	137	ARG
1	17-B	143	HIS
1	17-B	154	CYS
1	17-B	156	ARG

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Mol	Chain	Res	Type
1	17-B	158	THR
1	17-B	176	ARG
1	17-B	178	SER
1	17-B	199	SER
1	17-B	203	VAL
1	17-B	218	SER
1	17-B	226	VAL
1	18-A	2	LEU
1	18-A	21	ASN
1	18-A	30	LEU
1	18-A	48	ASP
1	18-A	50	LYS
1	18-A	71	ASP
1	18-A	97	GLU
1	18-A	131	VAL
1	18-A	136	ARG
1	18-A	173	SER
1	18-A	175	ARG
1	18-A	176	ARG
1	18-A	177	ASP
1	18-A	179	CYS
1	18-A	180	LYS
1	18-A	201	SER
1	18-A	224	ASP
1	18-A	227	LEU
1	18-B	2	LEU
1	18-B	5	ARG
1	18-B	25	LEU
1	18-B	29	VAL
1	18-B	33	GLU
1	18-B	43	LEU
1	18-B	45	ASP
1	18-B	62	GLN
1	18-B	74	ARG
1	18-B	115	ARG
1	18-B	136	ARG
1	18-B	137	ARG
1	18-B	156	ARG
1	18-B	158	THR
1	18-B	166	GLU
1	18-B	175	ARG
1	18-B	176	ARG

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Mol	Chain	Res	Type
1	18-B	199	SER
1	18-B	226	VAL
1	19-A	1	ILE
1	19-A	2	LEU
1	19-A	25	LEU
1	19-A	44	GLU
1	19-A	45	ASP
1	19-A	68	ARG
1	19-A	82	GLN
1	19-A	97	GLU
1	19-A	112	ARG
1	19-A	131	VAL
1	19-A	133	HIS
1	19-A	136	ARG
1	19-A	157	ARG
1	19-A	174	ASN
1	19-A	175	ARG
1	19-A	179	CYS
1	19-A	182	ASP
1	19-A	199	SER
1	19-A	201	SER
1	19-A	204	CYS
1	19-B	29	VAL
1	19-B	31	VAL
1	19-B	33	GLU
1	19-B	43	LEU
1	19-B	52	GLN
1	19-B	62	GLN
1	19-B	73	LEU
1	19-B	74	ARG
1	19-B	115	ARG
1	19-B	136	ARG
1	19-B	137	ARG
1	19-B	154	CYS
1	19-B	156	ARG
1	19-B	166	GLU
1	19-B	170	CYS
1	19-B	175	ARG
1	19-B	204	CYS
1	19-B	207	ARG
1	19-B	218	SER
1	20-A	1	ILE

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Mol	Chain	Res	Type
1	20-A	2	LEU
1	20-A	5	ARG
1	20-A	15	MET
1	20-A	30	LEU
1	20-A	43	LEU
1	20-A	48	ASP
1	20-A	53	VAL
1	20-A	68	ARG
1	20-A	73	LEU
1	20-A	74	ARG
1	20-A	84	ASP
1	20-A	106	ARG
1	20-A	112	ARG
1	20-A	136	ARG
1	20-A	142	GLN
1	20-A	156	ARG
1	20-A	172	GLU
1	20-A	173	SER
1	20-A	176	ARG
1	20-A	177	ASP
1	20-A	179	CYS
1	20-A	182	ASP
1	20-A	201	SER
1	20-A	203	VAL
1	20-A	215	ARG
1	20-A	227	LEU
1	20-B	20	LEU
1	20-B	25	LEU
1	20-B	33	GLU
1	20-B	41	HIS
1	20-B	45	ASP
1	20-B	48	ASP
1	20-B	62	GLN
1	20-B	66	SER
1	20-B	68	ARG
1	20-B	71	ASP
1	20-B	85	THR
1	20-B	96	SER
1	20-B	115	ARG
1	20-B	133	HIS
1	20-B	136	ARG
1	20-B	137	ARG

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Mol	Chain	Res	Type
1	20-B	158	THR
1	20-B	167	ARG
1	20-B	172	GLU
1	20-B	175	ARG
1	20-B	176	ARG
1	20-B	180	LYS
1	20-B	199	SER
1	20-B	201	SER
1	20-B	218	SER
1	20-B	226	VAL
1	20-B	227	LEU
1	21-A	2	LEU
1	21-A	5	ARG
1	21-A	30	LEU
1	21-A	43	LEU
1	21-A	45	ASP
1	21-A	50	LYS
1	21-A	62	GLN
1	21-A	68	ARG
1	21-A	115	ARG
1	21-A	133	HIS
1	21-A	136	ARG
1	21-A	158	THR
1	21-A	172	GLU
1	21-A	174	ASN
1	21-A	175	ARG
1	21-A	177	ASP
1	21-A	182	ASP
1	21-A	183	SER
1	21-B	5	ARG
1	21-B	21	ASN
1	21-B	25	LEU
1	21-B	41	HIS
1	21-B	43	LEU
1	21-B	62	GLN
1	21-B	73	LEU
1	21-B	74	ARG
1	21-B	81	SER
1	21-B	82	GLN
1	21-B	85	THR
1	21-B	86	ILE
1	21-B	115	ARG

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Mol	Chain	Res	Type
1	21-B	136	ARG
1	21-B	150	ASP
1	21-B	156	ARG
1	21-B	166	GLU
1	21-B	167	ARG
1	21-B	172	GLU
1	21-B	176	ARG
1	21-B	183	SER
1	21-B	198	THR
1	21-B	204	CYS
1	21-B	206	ASN
1	21-B	207	ARG
1	21-B	226	VAL
1	21-B	227	LEU
1	22-A	1	ILE
1	22-A	2	LEU
1	22-A	43	LEU
1	22-A	68	ARG
1	22-A	82	GLN
1	22-A	96	SER
1	22-A	98	LYS
1	22-A	112	ARG
1	22-A	115	ARG
1	22-A	136	ARG
1	22-A	156	ARG
1	22-A	157	ARG
1	22-A	158	THR
1	22-A	166	GLU
1	22-A	172	GLU
1	22-A	175	ARG
1	22-A	176	ARG
1	22-A	179	CYS
1	22-A	180	LYS
1	22-A	182	ASP
1	22-A	201	SER
1	22-A	204	CYS
1	22-B	5	ARG
1	22-B	25	LEU
1	22-B	33	GLU
1	22-B	44	GLU
1	22-B	50	LYS
1	22-B	51	VAL

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Mol	Chain	Res	Type
1	22-B	68	ARG
1	22-B	74	ARG
1	22-B	112	ARG
1	22-B	115	ARG
1	22-B	136	ARG
1	22-B	150	ASP
1	22-B	156	ARG
1	22-B	158	THR
1	22-B	166	GLU
1	22-B	167	ARG
1	22-B	201	SER
1	22-B	206	ASN
1	22-B	218	SER
1	23-A	1	ILE
1	23-A	2	LEU
1	23-A	25	LEU
1	23-A	43	LEU
1	23-A	44	GLU
1	23-A	45	ASP
1	23-A	68	ARG
1	23-A	74	ARG
1	23-A	115	ARG
1	23-A	136	ARG
1	23-A	137	ARG
1	23-A	156	ARG
1	23-A	158	THR
1	23-A	166	GLU
1	23-A	174	ASN
1	23-A	175	ARG
1	23-A	176	ARG
1	23-A	178	SER
1	23-A	180	LYS
1	23-A	183	SER
1	23-A	207	ARG
1	23-A	227	LEU
1	23-B	2	LEU
1	23-B	5	ARG
1	23-B	20	LEU
1	23-B	25	LEU
1	23-B	29	VAL
1	23-B	33	GLU
1	23-B	41	HIS

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Mol	Chain	Res	Type
1	23-B	43	LEU
1	23-B	50	LYS
1	23-B	68	ARG
1	23-B	73	LEU
1	23-B	82	GLN
1	23-B	97	GLU
1	23-B	112	ARG
1	23-B	136	ARG
1	23-B	176	ARG
1	23-B	179	CYS
1	23-B	180	LYS
1	23-B	198	THR
1	23-B	203	VAL
1	23-B	206	ASN
1	23-B	224	ASP
1	23-B	226	VAL
1	23-B	227	LEU
1	24-A	1	ILE
1	24-A	2	LEU
1	24-A	30	LEU
1	24-A	41	HIS
1	24-A	43	LEU
1	24-A	44	GLU
1	24-A	45	ASP
1	24-A	48	ASP
1	24-A	65	PRO
1	24-A	68	ARG
1	24-A	74	ARG
1	24-A	82	GLN
1	24-A	115	ARG
1	24-A	130	ILE
1	24-A	133	HIS
1	24-A	136	ARG
1	24-A	137	ARG
1	24-A	142	GLN
1	24-A	143	HIS
1	24-A	145	LEU
1	24-A	156	ARG
1	24-A	157	ARG
1	24-A	174	ASN
1	24-A	177	ASP
1	24-A	178	SER

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Mol	Chain	Res	Type
1	24-A	180	LYS
1	24-A	199	SER
1	24-A	204	CYS
1	24-A	206	ASN
1	24-A	207	ARG
1	24-A	208	LYS
1	24-A	227	LEU
1	24-B	5	ARG
1	24-B	20	LEU
1	24-B	29	VAL
1	24-B	33	GLU
1	24-B	51	VAL
1	24-B	68	ARG
1	24-B	74	ARG
1	24-B	85	THR
1	24-B	88	HIS
1	24-B	112	ARG
1	24-B	133	HIS
1	24-B	145	LEU
1	24-B	172	GLU
1	24-B	175	ARG
1	24-B	176	ARG
1	24-B	207	ARG
1	24-B	218	SER
1	24-B	227	LEU
1	25-A	2	LEU
1	25-A	5	ARG
1	25-A	30	LEU
1	25-A	41	HIS
1	25-A	43	LEU
1	25-A	44	GLU
1	25-A	45	ASP
1	25-A	48	ASP
1	25-A	68	ARG
1	25-A	74	ARG
1	25-A	82	GLN
1	25-A	86	ILE
1	25-A	96	SER
1	25-A	115	ARG
1	25-A	130	ILE
1	25-A	131	VAL
1	25-A	137	ARG

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Mol	Chain	Res	Type
1	25-A	156	ARG
1	25-A	157	ARG
1	25-A	158	THR
1	25-A	174	ASN
1	25-A	175	ARG
1	25-A	179	CYS
1	25-A	180	LYS
1	25-A	182	ASP
1	25-A	183	SER
1	25-A	206	ASN
1	25-A	207	ARG
1	25-A	208	LYS
1	25-A	224	ASP
1	25-A	227	LEU
1	25-B	2	LEU
1	25-B	33	GLU
1	25-B	45	ASP
1	25-B	50	LYS
1	25-B	51	VAL
1	25-B	62	GLN
1	25-B	74	ARG
1	25-B	85	THR
1	25-B	97	GLU
1	25-B	112	ARG
1	25-B	133	HIS
1	25-B	136	ARG
1	25-B	137	ARG
1	25-B	149	LEU
1	25-B	154	CYS
1	25-B	166	GLU
1	25-B	175	ARG
1	25-B	180	LYS
1	25-B	204	CYS
1	25-B	207	ARG
1	26-A	2	LEU
1	26-A	5	ARG
1	26-A	43	LEU
1	26-A	44	GLU
1	26-A	68	ARG
1	26-A	82	GLN
1	26-A	84	ASP
1	26-A	115	ARG

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Mol	Chain	Res	Type
1	26-A	136	ARG
1	26-A	137	ARG
1	26-A	145	LEU
1	26-A	166	GLU
1	26-A	175	ARG
1	26-A	177	ASP
1	26-A	178	SER
1	26-A	180	LYS
1	26-A	206	ASN
1	26-A	208	LYS
1	26-B	44	GLU
1	26-B	48	ASP
1	26-B	50	LYS
1	26-B	68	ARG
1	26-B	69	LEU
1	26-B	73	LEU
1	26-B	96	SER
1	26-B	97	GLU
1	26-B	112	ARG
1	26-B	115	ARG
1	26-B	133	HIS
1	26-B	137	ARG
1	26-B	149	LEU
1	26-B	150	ASP
1	26-B	154	CYS
1	26-B	156	ARG
1	26-B	175	ARG
1	26-B	198	THR
1	26-B	199	SER
1	26-B	201	SER
1	26-B	224	ASP
1	26-B	225	SER
1	27-A	2	LEU
1	27-A	5	ARG
1	27-A	20	LEU
1	27-A	25	LEU
1	27-A	30	LEU
1	27-A	43	LEU
1	27-A	50	LYS
1	27-A	82	GLN
1	27-A	97	GLU
1	27-A	115	ARG

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Mol	Chain	Res	Type
1	27-A	132	ASN
1	27-A	137	ARG
1	27-A	156	ARG
1	27-A	157	ARG
1	27-A	158	THR
1	27-A	166	GLU
1	27-A	173	SER
1	27-A	175	ARG
1	27-A	177	ASP
1	27-A	178	SER
1	27-A	180	LYS
1	27-A	182	ASP
1	27-A	199	SER
1	27-A	203	VAL
1	27-A	208	LYS
1	27-A	224	ASP
1	27-B	5	ARG
1	27-B	8	GLU
1	27-B	41	HIS
1	27-B	48	ASP
1	27-B	50	LYS
1	27-B	71	ASP
1	27-B	73	LEU
1	27-B	82	GLN
1	27-B	97	GLU
1	27-B	112	ARG
1	27-B	133	HIS
1	27-B	137	ARG
1	27-B	150	ASP
1	27-B	156	ARG
1	27-B	166	GLU
1	27-B	174	ASN
1	27-B	175	ARG
1	27-B	176	ARG
1	27-B	201	SER
1	27-B	204	CYS
1	27-B	227	LEU
1	28-A	2	LEU
1	28-A	5	ARG
1	28-A	41	HIS
1	28-A	43	LEU
1	28-A	44	GLU

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Mol	Chain	Res	Type
1	28-A	50	LYS
1	28-A	74	ARG
1	28-A	82	GLN
1	28-A	115	ARG
1	28-A	136	ARG
1	28-A	145	LEU
1	28-A	157	ARG
1	28-A	158	THR
1	28-A	174	ASN
1	28-A	175	ARG
1	28-A	180	LYS
1	28-A	183	SER
1	28-A	208	LYS
1	28-B	2	LEU
1	28-B	21	ASN
1	28-B	45	ASP
1	28-B	48	ASP
1	28-B	50	LYS
1	28-B	51	VAL
1	28-B	62	GLN
1	28-B	67	LYS
1	28-B	73	LEU
1	28-B	96	SER
1	28-B	133	HIS
1	28-B	136	ARG
1	28-B	137	ARG
1	28-B	140	SER
1	28-B	156	ARG
1	28-B	174	ASN
1	28-B	176	ARG
1	28-B	199	SER
1	28-B	204	CYS
1	28-B	206	ASN
1	28-B	207	ARG
1	28-B	225	SER
1	28-B	226	VAL
1	28-B	227	LEU
1	29-A	2	LEU
1	29-A	25	LEU
1	29-A	43	LEU
1	29-A	48	ASP
1	29-A	74	ARG

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Mol	Chain	Res	Type
1	29-A	82	GLN
1	29-A	84	ASP
1	29-A	106	ARG
1	29-A	115	ARG
1	29-A	124	ASP
1	29-A	130	ILE
1	29-A	131	VAL
1	29-A	133	HIS
1	29-A	136	ARG
1	29-A	137	ARG
1	29-A	166	GLU
1	29-A	178	SER
1	29-A	180	LYS
1	29-A	183	SER
1	29-A	198	THR
1	29-A	210	PRO
1	29-A	227	LEU
1	29-B	5	ARG
1	29-B	8	GLU
1	29-B	21	ASN
1	29-B	43	LEU
1	29-B	44	GLU
1	29-B	45	ASP
1	29-B	48	ASP
1	29-B	50	LYS
1	29-B	68	ARG
1	29-B	82	GLN
1	29-B	84	ASP
1	29-B	97	GLU
1	29-B	137	ARG
1	29-B	156	ARG
1	29-B	166	GLU
1	29-B	174	ASN
1	29-B	175	ARG
1	29-B	176	ARG
1	29-B	198	THR
1	29-B	199	SER
1	29-B	206	ASN
1	29-B	207	ARG
1	29-B	223	ILE
1	29-B	224	ASP
1	29-B	225	SER

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Mol	Chain	Res	Type
1	29-B	226	VAL
1	30-A	2	LEU
1	30-A	5	ARG
1	30-A	8	GLU
1	30-A	30	LEU
1	30-A	33	GLU
1	30-A	43	LEU
1	30-A	50	LYS
1	30-A	65	PRO
1	30-A	82	GLN
1	30-A	86	ILE
1	30-A	97	GLU
1	30-A	106	ARG
1	30-A	115	ARG
1	30-A	131	VAL
1	30-A	133	HIS
1	30-A	136	ARG
1	30-A	137	ARG
1	30-A	145	LEU
1	30-A	156	ARG
1	30-A	158	THR
1	30-A	159	HIS
1	30-A	166	GLU
1	30-A	175	ARG
1	30-A	180	LYS
1	30-A	182	ASP
1	30-A	183	SER
1	30-A	203	VAL
1	30-A	206	ASN
1	30-A	227	LEU
1	30-B	2	LEU
1	30-B	5	ARG
1	30-B	21	ASN
1	30-B	43	LEU
1	30-B	62	GLN
1	30-B	68	ARG
1	30-B	82	GLN
1	30-B	136	ARG
1	30-B	137	ARG
1	30-B	140	SER
1	30-B	156	ARG
1	30-B	175	ARG

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Mol	Chain	Res	Type
1	30-B	206	ASN
1	30-B	207	ARG
1	30-B	218	SER
1	30-B	226	VAL
1	30-B	227	LEU
1	31-A	1	ILE
1	31-A	2	LEU
1	31-A	20	LEU
1	31-A	25	LEU
1	31-A	74	ARG
1	31-A	84	ASP
1	31-A	85	THR
1	31-A	97	GLU
1	31-A	106	ARG
1	31-A	115	ARG
1	31-A	130	ILE
1	31-A	132	ASN
1	31-A	136	ARG
1	31-A	156	ARG
1	31-A	173	SER
1	31-A	175	ARG
1	31-A	176	ARG
1	31-A	178	SER
1	31-A	180	LYS
1	31-A	182	ASP
1	31-A	187	LEU
1	31-A	198	THR
1	31-A	208	LYS
1	31-A	215	ARG
1	31-A	227	LEU
1	31-B	21	ASN
1	31-B	33	GLU
1	31-B	44	GLU
1	31-B	96	SER
1	31-B	133	HIS
1	31-B	136	ARG
1	31-B	137	ARG
1	31-B	166	GLU
1	31-B	167	ARG
1	31-B	199	SER
1	31-B	206	ASN
1	31-B	207	ARG

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Mol	Chain	Res	Type
1	31-B	226	VAL
1	31-B	227	LEU
1	32-A	21	ASN
1	32-A	25	LEU
1	32-A	29	VAL
1	32-A	30	LEU
1	32-A	44	GLU
1	32-A	48	ASP
1	32-A	50	LYS
1	32-A	74	ARG
1	32-A	96	SER
1	32-A	98	LYS
1	32-A	106	ARG
1	32-A	115	ARG
1	32-A	130	ILE
1	32-A	131	VAL
1	32-A	133	HIS
1	32-A	137	ARG
1	32-A	156	ARG
1	32-A	157	ARG
1	32-A	176	ARG
1	32-A	177	ASP
1	32-A	178	SER
1	32-A	182	ASP
1	32-A	183	SER
1	32-A	201	SER
1	32-A	203	VAL
1	32-A	206	ASN
1	32-A	207	ARG
1	32-A	208	LYS
1	32-A	224	ASP
1	32-A	227	LEU
1	32-B	2	LEU
1	32-B	5	ARG
1	32-B	29	VAL
1	32-B	33	GLU
1	32-B	48	ASP
1	32-B	51	VAL
1	32-B	68	ARG
1	32-B	74	ARG
1	32-B	85	THR
1	32-B	88	HIS

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Mol	Chain	Res	Type
1	32-B	133	HIS
1	32-B	136	ARG
1	32-B	137	ARG
1	32-B	158	THR
1	32-B	175	ARG
1	32-B	198	THR
1	32-B	199	SER
1	32-B	207	ARG
1	32-B	224	ASP
1	32-B	226	VAL
1	32-B	227	LEU
1	33-A	2	LEU
1	33-A	20	LEU
1	33-A	41	HIS
1	33-A	43	LEU
1	33-A	44	GLU
1	33-A	45	ASP
1	33-A	96	SER
1	33-A	106	ARG
1	33-A	115	ARG
1	33-A	131	VAL
1	33-A	137	ARG
1	33-A	156	ARG
1	33-A	158	THR
1	33-A	175	ARG
1	33-A	182	ASP
1	33-A	187	LEU
1	33-A	198	THR
1	33-A	201	SER
1	33-A	206	ASN
1	33-A	209	LYS
1	33-A	227	LEU
1	33-B	5	ARG
1	33-B	33	GLU
1	33-B	43	LEU
1	33-B	48	ASP
1	33-B	50	LYS
1	33-B	73	LEU
1	33-B	82	GLN
1	33-B	84	ASP
1	33-B	86	ILE
1	33-B	97	GLU

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Mol	Chain	Res	Type
1	33-B	112	ARG
1	33-B	136	ARG
1	33-B	137	ARG
1	33-B	149	LEU
1	33-B	166	GLU
1	33-B	170	CYS
1	33-B	174	ASN
1	33-B	175	ARG
1	33-B	176	ARG
1	33-B	204	CYS
1	33-B	225	SER
1	34-A	1	ILE
1	34-A	5	ARG
1	34-A	20	LEU
1	34-A	33	GLU
1	34-A	43	LEU
1	34-A	44	GLU
1	34-A	53	VAL
1	34-A	82	GLN
1	34-A	84	ASP
1	34-A	85	THR
1	34-A	115	ARG
1	34-A	131	VAL
1	34-A	137	ARG
1	34-A	140	SER
1	34-A	145	LEU
1	34-A	157	ARG
1	34-A	159	HIS
1	34-A	166	GLU
1	34-A	172	GLU
1	34-A	175	ARG
1	34-A	177	ASP
1	34-A	180	LYS
1	34-A	204	CYS
1	34-A	209	LYS
1	34-A	227	LEU
1	34-B	33	GLU
1	34-B	43	LEU
1	34-B	50	LYS
1	34-B	51	VAL
1	34-B	73	LEU
1	34-B	82	GLN

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Mol	Chain	Res	Type
1	34-B	86	ILE
1	34-B	97	GLU
1	34-B	108	LEU
1	34-B	133	HIS
1	34-B	136	ARG
1	34-B	137	ARG
1	34-B	174	ASN
1	34-B	175	ARG
1	34-B	176	ARG
1	34-B	178	SER
1	34-B	198	THR
1	34-B	204	CYS
1	34-B	218	SER
1	34-B	226	VAL
1	35-A	2	LEU
1	35-A	25	LEU
1	35-A	43	LEU
1	35-A	45	ASP
1	35-A	48	ASP
1	35-A	68	ARG
1	35-A	74	ARG
1	35-A	84	ASP
1	35-A	86	ILE
1	35-A	98	LYS
1	35-A	112	ARG
1	35-A	115	ARG
1	35-A	136	ARG
1	35-A	156	ARG
1	35-A	166	GLU
1	35-A	174	ASN
1	35-A	175	ARG
1	35-A	176	ARG
1	35-A	180	LYS
1	35-A	182	ASP
1	35-A	201	SER
1	35-A	227	LEU
1	35-B	43	LEU
1	35-B	44	GLU
1	35-B	48	ASP
1	35-B	115	ARG
1	35-B	136	ARG
1	35-B	137	ARG

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Mol	Chain	Res	Type
1	35-B	150	ASP
1	35-B	170	CYS
1	35-B	172	GLU
1	35-B	175	ARG
1	35-B	176	ARG
1	35-B	179	CYS
1	35-B	198	THR
1	35-B	201	SER
1	35-B	204	CYS
1	35-B	216	VAL
1	35-B	224	ASP
1	35-B	227	LEU
1	36-A	1	ILE
1	36-A	2	LEU
1	36-A	5	ARG
1	36-A	8	GLU
1	36-A	25	LEU
1	36-A	43	LEU
1	36-A	48	ASP
1	36-A	50	LYS
1	36-A	85	THR
1	36-A	96	SER
1	36-A	98	LYS
1	36-A	106	ARG
1	36-A	115	ARG
1	36-A	130	ILE
1	36-A	136	ARG
1	36-A	137	ARG
1	36-A	143	HIS
1	36-A	166	GLU
1	36-A	173	SER
1	36-A	175	ARG
1	36-A	176	ARG
1	36-A	180	LYS
1	36-A	182	ASP
1	36-A	206	ASN
1	36-A	209	LYS
1	36-A	224	ASP
1	36-A	227	LEU
1	36-B	43	LEU
1	36-B	44	GLU
1	36-B	45	ASP

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Mol	Chain	Res	Type
1	36-B	68	ARG
1	36-B	71	ASP
1	36-B	73	LEU
1	36-B	97	GLU
1	36-B	115	ARG
1	36-B	137	ARG
1	36-B	145	LEU
1	36-B	150	ASP
1	36-B	154	CYS
1	36-B	174	ASN
1	36-B	175	ARG
1	36-B	176	ARG
1	36-B	206	ASN
1	36-B	226	VAL
1	37-A	2	LEU
1	37-A	5	ARG
1	37-A	20	LEU
1	37-A	48	ASP
1	37-A	50	LYS
1	37-A	74	ARG
1	37-A	85	THR
1	37-A	106	ARG
1	37-A	112	ARG
1	37-A	115	ARG
1	37-A	131	VAL
1	37-A	136	ARG
1	37-A	137	ARG
1	37-A	145	LEU
1	37-A	158	THR
1	37-A	177	ASP
1	37-A	180	LYS
1	37-A	209	LYS
1	37-A	215	ARG
1	37-A	227	LEU
1	37-B	2	LEU
1	37-B	43	LEU
1	37-B	48	ASP
1	37-B	68	ARG
1	37-B	73	LEU
1	37-B	88	HIS
1	37-B	96	SER
1	37-B	115	ARG

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Mol	Chain	Res	Type
1	37-B	116	ASP
1	37-B	133	HIS
1	37-B	136	ARG
1	37-B	137	ARG
1	37-B	145	LEU
1	37-B	174	ASN
1	37-B	203	VAL
1	37-B	204	CYS
1	37-B	206	ASN
1	37-B	225	SER
1	37-B	226	VAL
1	38-A	25	LEU
1	38-A	30	LEU
1	38-A	41	HIS
1	38-A	44	GLU
1	38-A	50	LYS
1	38-A	82	GLN
1	38-A	84	ASP
1	38-A	106	ARG
1	38-A	133	HIS
1	38-A	136	ARG
1	38-A	158	THR
1	38-A	173	SER
1	38-A	176	ARG
1	38-A	179	CYS
1	38-A	180	LYS
1	38-A	182	ASP
1	38-A	183	SER
1	38-A	199	SER
1	38-A	203	VAL
1	38-A	206	ASN
1	38-A	208	LYS
1	38-B	5	ARG
1	38-B	29	VAL
1	38-B	33	GLU
1	38-B	44	GLU
1	38-B	87	ASP
1	38-B	98	LYS
1	38-B	115	ARG
1	38-B	137	ARG
1	38-B	149	LEU
1	38-B	150	ASP

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Mol	Chain	Res	Type
1	38-B	167	ARG
1	38-B	175	ARG
1	38-B	180	LYS
1	38-B	201	SER
1	38-B	206	ASN
1	38-B	218	SER
1	39-A	1	ILE
1	39-A	2	LEU
1	39-A	25	LEU
1	39-A	43	LEU
1	39-A	68	ARG
1	39-A	82	GLN
1	39-A	84	ASP
1	39-A	98	LYS
1	39-A	106	ARG
1	39-A	108	LEU
1	39-A	112	ARG
1	39-A	132	ASN
1	39-A	136	ARG
1	39-A	140	SER
1	39-A	145	LEU
1	39-A	166	GLU
1	39-A	173	SER
1	39-A	178	SER
1	39-A	179	CYS
1	39-A	180	LYS
1	39-A	183	SER
1	39-A	198	THR
1	39-A	204	CYS
1	39-A	207	ARG
1	39-A	208	LYS
1	39-B	2	LEU
1	39-B	5	ARG
1	39-B	41	HIS
1	39-B	43	LEU
1	39-B	44	GLU
1	39-B	62	GLN
1	39-B	68	ARG
1	39-B	96	SER
1	39-B	115	ARG
1	39-B	137	ARG
1	39-B	149	LEU

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Mol	Chain	Res	Type
1	39-B	154	CYS
1	39-B	166	GLU
1	39-B	203	VAL
1	39-B	206	ASN
1	40-A	1	ILE
1	40-A	2	LEU
1	40-A	41	HIS
1	40-A	43	LEU
1	40-A	48	ASP
1	40-A	85	THR
1	40-A	97	GLU
1	40-A	100	THR
1	40-A	103	PRO
1	40-A	115	ARG
1	40-A	176	ARG
1	40-A	178	SER
1	40-A	180	LYS
1	40-A	182	ASP
1	40-A	198	THR
1	40-A	199	SER
1	40-A	207	ARG
1	40-A	208	LYS
1	40-B	5	ARG
1	40-B	43	LEU
1	40-B	50	LYS
1	40-B	62	GLN
1	40-B	96	SER
1	40-B	115	ARG
1	40-B	136	ARG
1	40-B	137	ARG
1	40-B	166	GLU
1	40-B	174	ASN
1	40-B	175	ARG
1	40-B	176	ARG
1	40-B	206	ASN
1	40-B	218	SER
1	41-A	1	ILE
1	41-A	2	LEU
1	41-A	20	LEU
1	41-A	25	LEU
1	41-A	50	LYS
1	41-A	53	VAL

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Mol	Chain	Res	Type
1	41-A	68	ARG
1	41-A	73	LEU
1	41-A	74	ARG
1	41-A	97	GLU
1	41-A	98	LYS
1	41-A	106	ARG
1	41-A	115	ARG
1	41-A	132	ASN
1	41-A	136	ARG
1	41-A	137	ARG
1	41-A	157	ARG
1	41-A	158	THR
1	41-A	166	GLU
1	41-A	174	ASN
1	41-A	180	LYS
1	41-A	182	ASP
1	41-A	201	SER
1	41-A	203	VAL
1	41-A	207	ARG
1	41-A	227	LEU
1	41-B	2	LEU
1	41-B	5	ARG
1	41-B	21	ASN
1	41-B	48	ASP
1	41-B	51	VAL
1	41-B	68	ARG
1	41-B	74	ARG
1	41-B	82	GLN
1	41-B	86	ILE
1	41-B	98	LYS
1	41-B	136	ARG
1	41-B	137	ARG
1	41-B	166	GLU
1	41-B	176	ARG
1	41-B	180	LYS
1	41-B	183	SER
1	41-B	198	THR
1	41-B	199	SER
1	41-B	204	CYS
1	41-B	206	ASN
1	42-A	2	LEU
1	42-A	5	ARG

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Mol	Chain	Res	Type
1	42-A	15	MET
1	42-A	20	LEU
1	42-A	21	ASN
1	42-A	25	LEU
1	42-A	43	LEU
1	42-A	98	LYS
1	42-A	106	ARG
1	42-A	112	ARG
1	42-A	115	ARG
1	42-A	133	HIS
1	42-A	136	ARG
1	42-A	139	ASP
1	42-A	140	SER
1	42-A	173	SER
1	42-A	174	ASN
1	42-A	175	ARG
1	42-A	180	LYS
1	42-A	182	ASP
1	42-A	183	SER
1	42-A	187	LEU
1	42-A	198	THR
1	42-A	201	SER
1	42-A	204	CYS
1	42-A	215	ARG
1	42-A	226	VAL
1	42-A	227	LEU
1	42-B	29	VAL
1	42-B	62	GLN
1	42-B	68	ARG
1	42-B	73	LEU
1	42-B	85	THR
1	42-B	96	SER
1	42-B	106	ARG
1	42-B	108	LEU
1	42-B	112	ARG
1	42-B	133	HIS
1	42-B	136	ARG
1	42-B	137	ARG
1	42-B	150	ASP
1	42-B	175	ARG
1	42-B	203	VAL
1	42-B	226	VAL

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Mol	Chain	Res	Type
1	43-A	1	ILE
1	43-A	2	LEU
1	43-A	20	LEU
1	43-A	21	ASN
1	43-A	33	GLU
1	43-A	53	VAL
1	43-A	68	ARG
1	43-A	73	LEU
1	43-A	84	ASP
1	43-A	85	THR
1	43-A	98	LYS
1	43-A	106	ARG
1	43-A	112	ARG
1	43-A	115	ARG
1	43-A	124	ASP
1	43-A	131	VAL
1	43-A	136	ARG
1	43-A	156	ARG
1	43-A	172	GLU
1	43-A	175	ARG
1	43-A	178	SER
1	43-A	180	LYS
1	43-A	183	SER
1	43-A	199	SER
1	43-A	204	CYS
1	43-A	224	ASP
1	43-B	33	GLU
1	43-B	43	LEU
1	43-B	51	VAL
1	43-B	73	LEU
1	43-B	82	GLN
1	43-B	84	ASP
1	43-B	86	ILE
1	43-B	106	ARG
1	43-B	115	ARG
1	43-B	133	HIS
1	43-B	136	ARG
1	43-B	137	ARG
1	43-B	150	ASP
1	43-B	154	CYS
1	43-B	172	GLU
1	43-B	175	ARG

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Mol	Chain	Res	Type
1	43-B	204	CYS
1	43-B	224	ASP
1	44-A	2	LEU
1	44-A	5	ARG
1	44-A	20	LEU
1	44-A	25	LEU
1	44-A	29	VAL
1	44-A	43	LEU
1	44-A	44	GLU
1	44-A	45	ASP
1	44-A	48	ASP
1	44-A	50	LYS
1	44-A	73	LEU
1	44-A	74	ARG
1	44-A	84	ASP
1	44-A	86	ILE
1	44-A	97	GLU
1	44-A	98	LYS
1	44-A	106	ARG
1	44-A	115	ARG
1	44-A	125	VAL
1	44-A	133	HIS
1	44-A	156	ARG
1	44-A	173	SER
1	44-A	178	SER
1	44-A	179	CYS
1	44-A	180	LYS
1	44-A	182	ASP
1	44-A	183	SER
1	44-A	199	SER
1	44-A	203	VAL
1	44-A	204	CYS
1	44-A	206	ASN
1	44-A	208	LYS
1	44-A	224	ASP
1	44-A	226	VAL
1	44-B	29	VAL
1	44-B	41	HIS
1	44-B	43	LEU
1	44-B	44	GLU
1	44-B	48	ASP
1	44-B	50	LYS

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Mol	Chain	Res	Type
1	44-B	73	LEU
1	44-B	96	SER
1	44-B	112	ARG
1	44-B	115	ARG
1	44-B	137	ARG
1	44-B	166	GLU
1	44-B	170	CYS
1	44-B	174	ASN
1	44-B	175	ARG
1	44-B	199	SER
1	44-B	227	LEU
1	45-A	25	LEU
1	45-A	48	ASP
1	45-A	82	GLN
1	45-A	98	LYS
1	45-A	115	ARG
1	45-A	131	VAL
1	45-A	133	HIS
1	45-A	145	LEU
1	45-A	156	ARG
1	45-A	157	ARG
1	45-A	173	SER
1	45-A	175	ARG
1	45-A	178	SER
1	45-A	180	LYS
1	45-A	182	ASP
1	45-A	203	VAL
1	45-A	204	CYS
1	45-A	209	LYS
1	45-A	226	VAL
1	45-A	227	LEU
1	45-B	8	GLU
1	45-B	33	GLU
1	45-B	44	GLU
1	45-B	50	LYS
1	45-B	51	VAL
1	45-B	85	THR
1	45-B	87	ASP
1	45-B	137	ARG
1	45-B	149	LEU
1	45-B	150	ASP
1	45-B	154	CYS

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Mol	Chain	Res	Type
1	45-B	175	ARG
1	45-B	176	ARG
1	45-B	178	SER
1	45-B	203	VAL
1	45-B	204	CYS
1	45-B	224	ASP
1	46-A	1	ILE
1	46-A	2	LEU
1	46-A	5	ARG
1	46-A	21	ASN
1	46-A	25	LEU
1	46-A	33	GLU
1	46-A	41	HIS
1	46-A	43	LEU
1	46-A	48	ASP
1	46-A	50	LYS
1	46-A	51	VAL
1	46-A	73	LEU
1	46-A	74	ARG
1	46-A	82	GLN
1	46-A	84	ASP
1	46-A	86	ILE
1	46-A	98	LYS
1	46-A	106	ARG
1	46-A	112	ARG
1	46-A	115	ARG
1	46-A	133	HIS
1	46-A	136	ARG
1	46-A	140	SER
1	46-A	156	ARG
1	46-A	173	SER
1	46-A	175	ARG
1	46-A	176	ARG
1	46-A	180	LYS
1	46-A	187	LEU
1	46-A	201	SER
1	46-A	203	VAL
1	46-A	206	ASN
1	46-A	207	ARG
1	46-A	208	LYS
1	46-A	209	LYS
1	46-B	29	VAL

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Mol	Chain	Res	Type
1	46-B	43	LEU
1	46-B	45	ASP
1	46-B	74	ARG
1	46-B	86	ILE
1	46-B	97	GLU
1	46-B	136	ARG
1	46-B	137	ARG
1	46-B	174	ASN
1	46-B	176	ARG
1	46-B	207	ARG
1	46-B	208	LYS
1	46-B	223	ILE
1	46-B	226	VAL
1	46-B	227	LEU
1	47-A	2	LEU
1	47-A	5	ARG
1	47-A	20	LEU
1	47-A	25	LEU
1	47-A	43	LEU
1	47-A	50	LYS
1	47-A	51	VAL
1	47-A	73	LEU
1	47-A	84	ASP
1	47-A	85	THR
1	47-A	97	GLU
1	47-A	98	LYS
1	47-A	112	ARG
1	47-A	115	ARG
1	47-A	130	ILE
1	47-A	131	VAL
1	47-A	136	ARG
1	47-A	156	ARG
1	47-A	166	GLU
1	47-A	175	ARG
1	47-A	177	ASP
1	47-A	178	SER
1	47-A	179	CYS
1	47-A	182	ASP
1	47-A	207	ARG
1	47-A	208	LYS
1	47-A	209	LYS
1	47-A	226	VAL

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Mol	Chain	Res	Type
1	47-B	29	VAL
1	47-B	41	HIS
1	47-B	43	LEU
1	47-B	44	GLU
1	47-B	50	LYS
1	47-B	68	ARG
1	47-B	71	ASP
1	47-B	73	LEU
1	47-B	84	ASP
1	47-B	133	HIS
1	47-B	137	ARG
1	47-B	149	LEU
1	47-B	150	ASP
1	47-B	154	CYS
1	47-B	158	THR
1	47-B	175	ARG
1	47-B	176	ARG
1	47-B	187	LEU
1	47-B	203	VAL
1	47-B	208	LYS
1	47-B	226	VAL
1	48-A	2	LEU
1	48-A	5	ARG
1	48-A	33	GLU
1	48-A	43	LEU
1	48-A	50	LYS
1	48-A	68	ARG
1	48-A	84	ASP
1	48-A	98	LYS
1	48-A	112	ARG
1	48-A	115	ARG
1	48-A	130	ILE
1	48-A	133	HIS
1	48-A	136	ARG
1	48-A	137	ARG
1	48-A	139	ASP
1	48-A	156	ARG
1	48-A	158	THR
1	48-A	159	HIS
1	48-A	173	SER
1	48-A	175	ARG
1	48-A	177	ASP

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Mol	Chain	Res	Type
1	48-A	178	SER
1	48-A	179	CYS
1	48-A	182	ASP
1	48-A	203	VAL
1	48-A	206	ASN
1	48-A	209	LYS
1	48-B	33	GLU
1	48-B	41	HIS
1	48-B	43	LEU
1	48-B	48	ASP
1	48-B	50	LYS
1	48-B	51	VAL
1	48-B	67	LYS
1	48-B	73	LEU
1	48-B	74	ARG
1	48-B	86	ILE
1	48-B	97	GLU
1	48-B	108	LEU
1	48-B	136	ARG
1	48-B	137	ARG
1	48-B	174	ASN
1	48-B	176	ARG
1	48-B	180	LYS
1	48-B	203	VAL
1	48-B	204	CYS
1	48-B	208	LYS
1	48-B	216	VAL
1	48-B	218	SER
1	48-B	226	VAL
1	48-B	227	LEU
1	49-A	2	LEU
1	49-A	5	ARG
1	49-A	8	GLU
1	49-A	25	LEU
1	49-A	41	HIS
1	49-A	43	LEU
1	49-A	45	ASP
1	49-A	68	ARG
1	49-A	73	LEU
1	49-A	82	GLN
1	49-A	98	LYS
1	49-A	112	ARG

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Mol	Chain	Res	Type
1	49-A	115	ARG
1	49-A	133	HIS
1	49-A	136	ARG
1	49-A	137	ARG
1	49-A	139	ASP
1	49-A	145	LEU
1	49-A	156	ARG
1	49-A	175	ARG
1	49-A	177	ASP
1	49-A	182	ASP
1	49-A	198	THR
1	49-A	199	SER
1	49-A	201	SER
1	49-A	206	ASN
1	49-A	207	ARG
1	49-A	209	LYS
1	49-B	2	LEU
1	49-B	29	VAL
1	49-B	33	GLU
1	49-B	45	ASP
1	49-B	50	LYS
1	49-B	66	SER
1	49-B	67	LYS
1	49-B	74	ARG
1	49-B	84	ASP
1	49-B	86	ILE
1	49-B	112	ARG
1	49-B	115	ARG
1	49-B	137	ARG
1	49-B	169	MET
1	49-B	174	ASN
1	49-B	175	ARG
1	49-B	180	LYS
1	49-B	206	ASN
1	49-B	225	SER
1	50-A	2	LEU
1	50-A	8	GLU
1	50-A	43	LEU
1	50-A	44	GLU
1	50-A	50	LYS
1	50-A	68	ARG
1	50-A	73	LEU

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Mol	Chain	Res	Type
1	50-A	74	ARG
1	50-A	82	GLN
1	50-A	84	ASP
1	50-A	86	ILE
1	50-A	115	ARG
1	50-A	133	HIS
1	50-A	136	ARG
1	50-A	137	ARG
1	50-A	156	ARG
1	50-A	172	GLU
1	50-A	177	ASP
1	50-A	182	ASP
1	50-A	183	SER
1	50-A	198	THR
1	50-A	201	SER
1	50-A	204	CYS
1	50-A	209	LYS
1	50-B	41	HIS
1	50-B	44	GLU
1	50-B	45	ASP
1	50-B	50	LYS
1	50-B	62	GLN
1	50-B	68	ARG
1	50-B	73	LEU
1	50-B	82	GLN
1	50-B	96	SER
1	50-B	113	VAL
1	50-B	115	ARG
1	50-B	133	HIS
1	50-B	137	ARG
1	50-B	172	GLU
1	50-B	174	ASN
1	50-B	179	CYS
1	50-B	180	LYS
1	50-B	187	LEU
1	50-B	201	SER
1	50-B	203	VAL
1	50-B	204	CYS
1	50-B	206	ASN
1	50-B	218	SER
1	51-A	2	LEU
1	51-A	5	ARG

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Mol	Chain	Res	Type
1	51-A	8	GLU
1	51-A	33	GLU
1	51-A	43	LEU
1	51-A	74	ARG
1	51-A	82	GLN
1	51-A	84	ASP
1	51-A	85	THR
1	51-A	115	ARG
1	51-A	130	ILE
1	51-A	131	VAL
1	51-A	136	ARG
1	51-A	140	SER
1	51-A	157	ARG
1	51-A	175	ARG
1	51-A	177	ASP
1	51-A	178	SER
1	51-A	182	ASP
1	51-A	201	SER
1	51-A	209	LYS
1	51-A	227	LEU
1	51-B	2	LEU
1	51-B	21	ASN
1	51-B	41	HIS
1	51-B	43	LEU
1	51-B	45	ASP
1	51-B	50	LYS
1	51-B	62	GLN
1	51-B	73	LEU
1	51-B	85	THR
1	51-B	87	ASP
1	51-B	97	GLU
1	51-B	136	ARG
1	51-B	167	ARG
1	51-B	175	ARG
1	51-B	176	ARG
1	51-B	204	CYS
1	52-A	2	LEU
1	52-A	5	ARG
1	52-A	29	VAL
1	52-A	33	GLU
1	52-A	45	ASP
1	52-A	73	LEU

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Mol	Chain	Res	Type
1	52-A	97	GLU
1	52-A	115	ARG
1	52-A	130	ILE
1	52-A	131	VAL
1	52-A	137	ARG
1	52-A	145	LEU
1	52-A	157	ARG
1	52-A	166	GLU
1	52-A	173	SER
1	52-A	175	ARG
1	52-A	176	ARG
1	52-A	177	ASP
1	52-A	198	THR
1	52-A	204	CYS
1	52-A	206	ASN
1	52-A	224	ASP
1	52-B	21	ASN
1	52-B	43	LEU
1	52-B	48	ASP
1	52-B	51	VAL
1	52-B	67	LYS
1	52-B	68	ARG
1	52-B	74	ARG
1	52-B	81	SER
1	52-B	96	SER
1	52-B	133	HIS
1	52-B	136	ARG
1	52-B	137	ARG
1	52-B	154	CYS
1	52-B	176	ARG
1	52-B	180	LYS
1	52-B	198	THR
1	52-B	199	SER
1	52-B	201	SER
1	52-B	209	LYS
1	52-B	225	SER
1	52-B	227	LEU
1	53-A	1	ILE
1	53-A	5	ARG
1	53-A	25	LEU
1	53-A	33	GLU
1	53-A	96	SER

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Mol	Chain	Res	Type
1	53-A	97	GLU
1	53-A	115	ARG
1	53-A	124	ASP
1	53-A	130	ILE
1	53-A	136	ARG
1	53-A	145	LEU
1	53-A	156	ARG
1	53-A	175	ARG
1	53-A	176	ARG
1	53-A	177	ASP
1	53-A	182	ASP
1	53-A	201	SER
1	53-A	203	VAL
1	53-A	206	ASN
1	53-A	207	ARG
1	53-B	2	LEU
1	53-B	5	ARG
1	53-B	33	GLU
1	53-B	41	HIS
1	53-B	62	GLN
1	53-B	67	LYS
1	53-B	71	ASP
1	53-B	86	ILE
1	53-B	87	ASP
1	53-B	108	LEU
1	53-B	133	HIS
1	53-B	136	ARG
1	53-B	137	ARG
1	53-B	143	HIS
1	53-B	154	CYS
1	53-B	174	ASN
1	53-B	176	ARG
1	53-B	198	THR
1	53-B	199	SER
1	53-B	201	SER
1	53-B	203	VAL
1	53-B	224	ASP
1	54-A	1	ILE
1	54-A	25	LEU
1	54-A	43	LEU
1	54-A	44	GLU
1	54-A	48	ASP

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Mol	Chain	Res	Type
1	54-A	73	LEU
1	54-A	74	ARG
1	54-A	84	ASP
1	54-A	106	ARG
1	54-A	112	ARG
1	54-A	130	ILE
1	54-A	137	ARG
1	54-A	157	ARG
1	54-A	175	ARG
1	54-A	176	ARG
1	54-A	180	LYS
1	54-A	182	ASP
1	54-A	183	SER
1	54-A	201	SER
1	54-A	203	VAL
1	54-A	204	CYS
1	54-A	206	ASN
1	54-A	207	ARG
1	54-B	41	HIS
1	54-B	43	LEU
1	54-B	51	VAL
1	54-B	67	LYS
1	54-B	71	ASP
1	54-B	73	LEU
1	54-B	87	ASP
1	54-B	112	ARG
1	54-B	113	VAL
1	54-B	136	ARG
1	54-B	150	ASP
1	54-B	157	ARG
1	54-B	170	CYS
1	54-B	172	GLU
1	54-B	174	ASN
1	54-B	176	ARG
1	54-B	179	CYS
1	54-B	198	THR
1	54-B	204	CYS
1	54-B	216	VAL
1	55-A	1	ILE
1	55-A	21	ASN
1	55-A	43	LEU
1	55-A	50	LYS

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Mol	Chain	Res	Type
1	55-A	68	ARG
1	55-A	73	LEU
1	55-A	82	GLN
1	55-A	84	ASP
1	55-A	97	GLU
1	55-A	115	ARG
1	55-A	137	ARG
1	55-A	139	ASP
1	55-A	156	ARG
1	55-A	174	ASN
1	55-A	175	ARG
1	55-A	176	ARG
1	55-A	178	SER
1	55-A	182	ASP
1	55-A	207	ARG
1	55-A	226	VAL
1	55-B	2	LEU
1	55-B	33	GLU
1	55-B	43	LEU
1	55-B	48	ASP
1	55-B	62	GLN
1	55-B	67	LYS
1	55-B	82	GLN
1	55-B	85	THR
1	55-B	112	ARG
1	55-B	136	ARG
1	55-B	143	HIS
1	55-B	149	LEU
1	55-B	156	ARG
1	55-B	166	GLU
1	55-B	167	ARG
1	55-B	175	ARG
1	55-B	203	VAL
1	55-B	204	CYS
1	55-B	207	ARG
1	56-A	1	ILE
1	56-A	2	LEU
1	56-A	5	ARG
1	56-A	43	LEU
1	56-A	45	ASP
1	56-A	74	ARG
1	56-A	83	PRO

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Mol	Chain	Res	Type
1	56-A	86	ILE
1	56-A	97	GLU
1	56-A	98	LYS
1	56-A	106	ARG
1	56-A	131	VAL
1	56-A	132	ASN
1	56-A	136	ARG
1	56-A	137	ARG
1	56-A	138	PRO
1	56-A	157	ARG
1	56-A	158	THR
1	56-A	166	GLU
1	56-A	175	ARG
1	56-A	177	ASP
1	56-A	179	CYS
1	56-A	182	ASP
1	56-A	183	SER
1	56-A	199	SER
1	56-A	203	VAL
1	56-A	207	ARG
1	56-A	209	LYS
1	56-A	215	ARG
1	56-A	226	VAL
1	56-B	33	GLU
1	56-B	45	ASP
1	56-B	62	GLN
1	56-B	67	LYS
1	56-B	80	ASP
1	56-B	82	GLN
1	56-B	112	ARG
1	56-B	136	ARG
1	56-B	157	ARG
1	56-B	158	THR
1	56-B	166	GLU
1	56-B	201	SER
1	56-B	206	ASN
1	56-B	216	VAL
1	56-B	224	ASP
1	57-A	1	ILE
1	57-A	5	ARG
1	57-A	20	LEU
1	57-A	41	HIS

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Mol	Chain	Res	Type
1	57-A	68	ARG
1	57-A	73	LEU
1	57-A	82	GLN
1	57-A	84	ASP
1	57-A	97	GLU
1	57-A	106	ARG
1	57-A	130	ILE
1	57-A	132	ASN
1	57-A	133	HIS
1	57-A	137	ARG
1	57-A	139	ASP
1	57-A	145	LEU
1	57-A	156	ARG
1	57-A	158	THR
1	57-A	159	HIS
1	57-A	172	GLU
1	57-A	173	SER
1	57-A	174	ASN
1	57-A	176	ARG
1	57-A	178	SER
1	57-A	182	ASP
1	57-A	206	ASN
1	57-A	207	ARG
1	57-B	2	LEU
1	57-B	50	LYS
1	57-B	67	LYS
1	57-B	73	LEU
1	57-B	85	THR
1	57-B	96	SER
1	57-B	113	VAL
1	57-B	115	ARG
1	57-B	136	ARG
1	57-B	137	ARG
1	57-B	143	HIS
1	57-B	176	ARG
1	57-B	198	THR
1	57-B	203	VAL
1	57-B	206	ASN
1	58-A	2	LEU
1	58-A	5	ARG
1	58-A	20	LEU
1	58-A	43	LEU

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Mol	Chain	Res	Type
1	58-A	50	LYS
1	58-A	68	ARG
1	58-A	73	LEU
1	58-A	74	ARG
1	58-A	82	GLN
1	58-A	96	SER
1	58-A	106	ARG
1	58-A	115	ARG
1	58-A	131	VAL
1	58-A	157	ARG
1	58-A	166	GLU
1	58-A	172	GLU
1	58-A	176	ARG
1	58-A	177	ASP
1	58-A	179	CYS
1	58-A	182	ASP
1	58-A	198	THR
1	58-A	201	SER
1	58-A	206	ASN
1	58-A	207	ARG
1	58-A	224	ASP
1	58-A	227	LEU
1	58-B	2	LEU
1	58-B	5	ARG
1	58-B	29	VAL
1	58-B	41	HIS
1	58-B	43	LEU
1	58-B	67	LYS
1	58-B	73	LEU
1	58-B	74	ARG
1	58-B	82	GLN
1	58-B	112	ARG
1	58-B	115	ARG
1	58-B	137	ARG
1	58-B	170	CYS
1	58-B	174	ASN
1	58-B	198	THR
1	58-B	199	SER
1	58-B	201	SER
1	58-B	203	VAL
1	58-B	218	SER
1	58-B	227	LEU

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Mol	Chain	Res	Type
1	59-A	2	LEU
1	59-A	8	GLU
1	59-A	33	GLU
1	59-A	43	LEU
1	59-A	82	GLN
1	59-A	84	ASP
1	59-A	97	GLU
1	59-A	115	ARG
1	59-A	130	ILE
1	59-A	137	ARG
1	59-A	139	ASP
1	59-A	140	SER
1	59-A	145	LEU
1	59-A	156	ARG
1	59-A	166	GLU
1	59-A	172	GLU
1	59-A	174	ASN
1	59-A	176	ARG
1	59-A	180	LYS
1	59-A	182	ASP
1	59-A	198	THR
1	59-A	199	SER
1	59-A	201	SER
1	59-A	204	CYS
1	59-A	207	ARG
1	59-A	227	LEU
1	59-B	5	ARG
1	59-B	29	VAL
1	59-B	43	LEU
1	59-B	50	LYS
1	59-B	51	VAL
1	59-B	62	GLN
1	59-B	67	LYS
1	59-B	68	ARG
1	59-B	80	ASP
1	59-B	96	SER
1	59-B	115	ARG
1	59-B	133	HIS
1	59-B	137	ARG
1	59-B	143	HIS
1	59-B	174	ASN
1	59-B	176	ARG

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Mol	Chain	Res	Type
1	59-B	180	LYS
1	59-B	198	THR
1	59-B	199	SER
1	59-B	204	CYS
1	59-B	207	ARG
1	60-A	2	LEU
1	60-A	5	ARG
1	60-A	25	LEU
1	60-A	29	VAL
1	60-A	41	HIS
1	60-A	43	LEU
1	60-A	68	ARG
1	60-A	96	SER
1	60-A	106	ARG
1	60-A	115	ARG
1	60-A	131	VAL
1	60-A	132	ASN
1	60-A	136	ARG
1	60-A	139	ASP
1	60-A	156	ARG
1	60-A	157	ARG
1	60-A	172	GLU
1	60-A	176	ARG
1	60-A	179	CYS
1	60-A	182	ASP
1	60-A	198	THR
1	60-A	199	SER
1	60-A	204	CYS
1	60-A	206	ASN
1	60-A	215	ARG
1	60-A	227	LEU
1	60-B	5	ARG
1	60-B	29	VAL
1	60-B	33	GLU
1	60-B	43	LEU
1	60-B	44	GLU
1	60-B	62	GLN
1	60-B	68	ARG
1	60-B	73	LEU
1	60-B	80	ASP
1	60-B	85	THR
1	60-B	96	SER

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Mol	Chain	Res	Type
1	60-B	174	ASN
1	60-B	176	ARG
1	60-B	203	VAL
1	60-B	207	ARG
1	60-B	227	LEU
1	61-A	1	ILE
1	61-A	2	LEU
1	61-A	20	LEU
1	61-A	43	LEU
1	61-A	44	GLU
1	61-A	45	ASP
1	61-A	48	ASP
1	61-A	50	LYS
1	61-A	68	ARG
1	61-A	82	GLN
1	61-A	84	ASP
1	61-A	97	GLU
1	61-A	133	HIS
1	61-A	139	ASP
1	61-A	158	THR
1	61-A	174	ASN
1	61-A	178	SER
1	61-A	180	LYS
1	61-A	182	ASP
1	61-A	183	SER
1	61-A	198	THR
1	61-A	204	CYS
1	61-A	207	ARG
1	61-A	210	PRO
1	61-B	29	VAL
1	61-B	33	GLU
1	61-B	41	HIS
1	61-B	43	LEU
1	61-B	44	GLU
1	61-B	51	VAL
1	61-B	62	GLN
1	61-B	66	SER
1	61-B	67	LYS
1	61-B	82	GLN
1	61-B	113	VAL
1	61-B	115	ARG
1	61-B	133	HIS

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Mol	Chain	Res	Type
1	61-B	149	LEU
1	61-B	154	CYS
1	61-B	157	ARG
1	61-B	158	THR
1	61-B	166	GLU
1	61-B	170	CYS
1	61-B	174	ASN
1	61-B	175	ARG
1	61-B	176	ARG
1	61-B	179	CYS
1	61-B	180	LYS
1	61-B	198	THR
1	61-B	199	SER
1	61-B	207	ARG
1	61-B	227	LEU
1	62-A	1	ILE
1	62-A	2	LEU
1	62-A	15	MET
1	62-A	43	LEU
1	62-A	50	LYS
1	62-A	68	ARG
1	62-A	73	LEU
1	62-A	82	GLN
1	62-A	97	GLU
1	62-A	106	ARG
1	62-A	130	ILE
1	62-A	131	VAL
1	62-A	133	HIS
1	62-A	137	ARG
1	62-A	139	ASP
1	62-A	145	LEU
1	62-A	156	ARG
1	62-A	174	ASN
1	62-A	176	ARG
1	62-A	177	ASP
1	62-A	198	THR
1	62-A	226	VAL
1	62-B	2	LEU
1	62-B	8	GLU
1	62-B	29	VAL
1	62-B	33	GLU
1	62-B	44	GLU

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Mol	Chain	Res	Type
1	62-B	62	GLN
1	62-B	67	LYS
1	62-B	81	SER
1	62-B	115	ARG
1	62-B	133	HIS
1	62-B	136	ARG
1	62-B	137	ARG
1	62-B	149	LEU
1	62-B	150	ASP
1	62-B	176	ARG
1	62-B	179	CYS
1	62-B	180	LYS
1	62-B	206	ASN
1	62-B	207	ARG
1	62-B	224	ASP
1	62-B	226	VAL
1	63-A	20	LEU
1	63-A	21	ASN
1	63-A	68	ARG
1	63-A	73	LEU
1	63-A	82	GLN
1	63-A	84	ASP
1	63-A	115	ARG
1	63-A	130	ILE
1	63-A	131	VAL
1	63-A	136	ARG
1	63-A	140	SER
1	63-A	158	THR
1	63-A	174	ASN
1	63-A	175	ARG
1	63-A	177	ASP
1	63-A	180	LYS
1	63-A	201	SER
1	63-A	203	VAL
1	63-A	207	ARG
1	63-A	224	ASP
1	63-B	5	ARG
1	63-B	25	LEU
1	63-B	51	VAL
1	63-B	74	ARG
1	63-B	82	GLN
1	63-B	86	ILE

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Mol	Chain	Res	Type
1	63-B	115	ARG
1	63-B	137	ARG
1	63-B	166	GLU
1	63-B	170	CYS
1	63-B	206	ASN
1	63-B	207	ARG
1	63-B	227	LEU
1	64-A	25	LEU
1	64-A	45	ASP
1	64-A	48	ASP
1	64-A	96	SER
1	64-A	106	ARG
1	64-A	115	ARG
1	64-A	130	ILE
1	64-A	132	ASN
1	64-A	133	HIS
1	64-A	137	ARG
1	64-A	145	LEU
1	64-A	166	GLU
1	64-A	174	ASN
1	64-A	175	ARG
1	64-A	180	LYS
1	64-A	198	THR
1	64-A	203	VAL
1	64-A	207	ARG
1	64-A	226	VAL
1	64-B	5	ARG
1	64-B	25	LEU
1	64-B	33	GLU
1	64-B	43	LEU
1	64-B	45	ASP
1	64-B	74	ARG
1	64-B	86	ILE
1	64-B	96	SER
1	64-B	98	LYS
1	64-B	112	ARG
1	64-B	115	ARG
1	64-B	149	LEU
1	64-B	166	GLU
1	64-B	174	ASN
1	64-B	175	ARG
1	64-B	176	ARG

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Mol	Chain	Res	Type
1	64-B	179	CYS
1	64-B	180	LYS
1	64-B	198	THR
1	64-B	199	SER
1	64-B	201	SER
1	64-B	206	ASN
1	64-B	224	ASP
1	64-B	226	VAL
1	65-A	5	ARG
1	65-A	8	GLU
1	65-A	20	LEU
1	65-A	44	GLU
1	65-A	48	ASP
1	65-A	68	ARG
1	65-A	97	GLU
1	65-A	106	ARG
1	65-A	112	ARG
1	65-A	115	ARG
1	65-A	130	ILE
1	65-A	136	ARG
1	65-A	137	ARG
1	65-A	156	ARG
1	65-A	158	THR
1	65-A	166	GLU
1	65-A	177	ASP
1	65-A	179	CYS
1	65-A	182	ASP
1	65-A	204	CYS
1	65-B	2	LEU
1	65-B	5	ARG
1	65-B	48	ASP
1	65-B	62	GLN
1	65-B	73	LEU
1	65-B	74	ARG
1	65-B	85	THR
1	65-B	86	ILE
1	65-B	115	ARG
1	65-B	137	ARG
1	65-B	154	CYS
1	65-B	156	ARG
1	65-B	166	GLU
1	65-B	174	ASN

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Mol	Chain	Res	Type
1	65-B	175	ARG
1	65-B	179	CYS
1	65-B	203	VAL
1	65-B	207	ARG
1	65-B	225	SER
1	65-B	227	LEU
1	66-A	1	ILE
1	66-A	2	LEU
1	66-A	8	GLU
1	66-A	25	LEU
1	66-A	41	HIS
1	66-A	45	ASP
1	66-A	48	ASP
1	66-A	50	LYS
1	66-A	51	VAL
1	66-A	68	ARG
1	66-A	82	GLN
1	66-A	86	ILE
1	66-A	136	ARG
1	66-A	137	ARG
1	66-A	158	THR
1	66-A	174	ASN
1	66-A	176	ARG
1	66-A	177	ASP
1	66-A	179	CYS
1	66-A	180	LYS
1	66-A	182	ASP
1	66-A	199	SER
1	66-A	201	SER
1	66-A	203	VAL
1	66-A	204	CYS
1	66-A	207	ARG
1	66-A	208	LYS
1	66-A	210	PRO
1	66-A	224	ASP
1	66-A	226	VAL
1	66-A	227	LEU
1	66-B	5	ARG
1	66-B	29	VAL
1	66-B	33	GLU
1	66-B	43	LEU
1	66-B	44	GLU

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Mol	Chain	Res	Type
1	66-B	45	ASP
1	66-B	48	ASP
1	66-B	50	LYS
1	66-B	73	LEU
1	66-B	82	GLN
1	66-B	83	PRO
1	66-B	85	THR
1	66-B	87	ASP
1	66-B	97	GLU
1	66-B	115	ARG
1	66-B	133	HIS
1	66-B	143	HIS
1	66-B	149	LEU
1	66-B	156	ARG
1	66-B	167	ARG
1	66-B	175	ARG
1	66-B	179	CYS
1	66-B	198	THR
1	66-B	226	VAL
1	66-B	227	LEU
1	67-A	2	LEU
1	67-A	15	MET
1	67-A	43	LEU
1	67-A	44	GLU
1	67-A	50	LYS
1	67-A	68	ARG
1	67-A	74	ARG
1	67-A	82	GLN
1	67-A	98	LYS
1	67-A	100	THR
1	67-A	106	ARG
1	67-A	132	ASN
1	67-A	137	ARG
1	67-A	166	GLU
1	67-A	178	SER
1	67-A	179	CYS
1	67-A	180	LYS
1	67-A	182	ASP
1	67-A	201	SER
1	67-A	206	ASN
1	67-B	25	LEU
1	67-B	43	LEU

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Mol	Chain	Res	Type
1	67-B	51	VAL
1	67-B	82	GLN
1	67-B	85	THR
1	67-B	96	SER
1	67-B	137	ARG
1	67-B	176	ARG
1	67-B	206	ASN
1	67-B	207	ARG
1	67-B	224	ASP
1	67-B	227	LEU
1	68-A	1	ILE
1	68-A	2	LEU
1	68-A	34	GLN
1	68-A	43	LEU
1	68-A	44	GLU
1	68-A	45	ASP
1	68-A	68	ARG
1	68-A	84	ASP
1	68-A	98	LYS
1	68-A	115	ARG
1	68-A	130	ILE
1	68-A	133	HIS
1	68-A	136	ARG
1	68-A	137	ARG
1	68-A	139	ASP
1	68-A	166	GLU
1	68-A	172	GLU
1	68-A	174	ASN
1	68-A	176	ARG
1	68-A	180	LYS
1	68-A	183	SER
1	68-A	198	THR
1	68-A	201	SER
1	68-A	203	VAL
1	68-A	204	CYS
1	68-A	206	ASN
1	68-A	208	LYS
1	68-A	215	ARG
1	68-A	226	VAL
1	68-B	2	LEU
1	68-B	25	LEU
1	68-B	33	GLU

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Mol	Chain	Res	Type
1	68-B	43	LEU
1	68-B	45	ASP
1	68-B	48	ASP
1	68-B	51	VAL
1	68-B	59	SER
1	68-B	62	GLN
1	68-B	73	LEU
1	68-B	82	GLN
1	68-B	137	ARG
1	68-B	149	LEU
1	68-B	167	ARG
1	68-B	175	ARG
1	68-B	201	SER
1	68-B	204	CYS
1	68-B	206	ASN
1	68-B	225	SER
1	68-B	226	VAL
1	69-A	1	ILE
1	69-A	2	LEU
1	69-A	43	LEU
1	69-A	45	ASP
1	69-A	48	ASP
1	69-A	50	LYS
1	69-A	51	VAL
1	69-A	68	ARG
1	69-A	139	ASP
1	69-A	156	ARG
1	69-A	158	THR
1	69-A	174	ASN
1	69-A	176	ARG
1	69-A	178	SER
1	69-A	180	LYS
1	69-A	206	ASN
1	69-A	208	LYS
1	69-A	224	ASP
1	69-A	227	LEU
1	69-B	43	LEU
1	69-B	62	GLN
1	69-B	68	ARG
1	69-B	71	ASP
1	69-B	74	ARG
1	69-B	85	THR

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Mol	Chain	Res	Type
1	69-B	86	ILE
1	69-B	133	HIS
1	69-B	154	CYS
1	69-B	157	ARG
1	69-B	175	ARG
1	69-B	176	ARG
1	69-B	201	SER
1	69-B	206	ASN
1	69-B	207	ARG
1	69-B	218	SER
1	69-B	226	VAL
1	69-B	227	LEU
1	70-A	1	ILE
1	70-A	2	LEU
1	70-A	20	LEU
1	70-A	34	GLN
1	70-A	48	ASP
1	70-A	68	ARG
1	70-A	84	ASP
1	70-A	97	GLU
1	70-A	106	ARG
1	70-A	136	ARG
1	70-A	145	LEU
1	70-A	146	LEU
1	70-A	158	THR
1	70-A	166	GLU
1	70-A	173	SER
1	70-A	174	ASN
1	70-A	176	ARG
1	70-A	180	LYS
1	70-A	183	SER
1	70-A	204	CYS
1	70-A	207	ARG
1	70-A	209	LYS
1	70-A	227	LEU
1	70-B	5	ARG
1	70-B	21	ASN
1	70-B	41	HIS
1	70-B	43	LEU
1	70-B	48	ASP
1	70-B	62	GLN
1	70-B	68	ARG

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Mol	Chain	Res	Type
1	70-B	132	ASN
1	70-B	156	ARG
1	70-B	170	CYS
1	70-B	174	ASN
1	70-B	175	ARG
1	70-B	176	ARG
1	70-B	206	ASN
1	70-B	207	ARG
1	70-B	227	LEU
1	71-A	1	ILE
1	71-A	2	LEU
1	71-A	45	ASP
1	71-A	48	ASP
1	71-A	68	ARG
1	71-A	74	ARG
1	71-A	98	LYS
1	71-A	115	ARG
1	71-A	130	ILE
1	71-A	131	VAL
1	71-A	133	HIS
1	71-A	137	ARG
1	71-A	157	ARG
1	71-A	158	THR
1	71-A	166	GLU
1	71-A	172	GLU
1	71-A	175	ARG
1	71-A	176	ARG
1	71-A	177	ASP
1	71-A	179	CYS
1	71-A	180	LYS
1	71-A	183	SER
1	71-A	187	LEU
1	71-A	201	SER
1	71-A	208	LYS
1	71-A	209	LYS
1	71-A	227	LEU
1	71-B	2	LEU
1	71-B	21	ASN
1	71-B	43	LEU
1	71-B	45	ASP
1	71-B	48	ASP
1	71-B	62	GLN

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Mol	Chain	Res	Type
1	71-B	87	ASP
1	71-B	96	SER
1	71-B	112	ARG
1	71-B	137	ARG
1	71-B	166	GLU
1	71-B	174	ASN
1	71-B	179	CYS
1	71-B	183	SER
1	71-B	187	LEU
1	71-B	203	VAL
1	71-B	206	ASN
1	71-B	225	SER
1	71-B	227	LEU
1	72-A	2	LEU
1	72-A	43	LEU
1	72-A	48	ASP
1	72-A	84	ASP
1	72-A	112	ARG
1	72-A	130	ILE
1	72-A	136	ARG
1	72-A	157	ARG
1	72-A	166	GLU
1	72-A	173	SER
1	72-A	174	ASN
1	72-A	175	ARG
1	72-A	176	ARG
1	72-A	178	SER
1	72-A	180	LYS
1	72-A	182	ASP
1	72-A	201	SER
1	72-A	207	ARG
1	72-A	226	VAL
1	72-A	227	LEU
1	72-B	5	ARG
1	72-B	21	ASN
1	72-B	43	LEU
1	72-B	45	ASP
1	72-B	48	ASP
1	72-B	62	GLN
1	72-B	73	LEU
1	72-B	74	ARG
1	72-B	81	SER

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Mol	Chain	Res	Type
1	72-B	85	THR
1	72-B	96	SER
1	72-B	112	ARG
1	72-B	136	ARG
1	72-B	149	LEU
1	72-B	198	THR
1	72-B	201	SER
1	72-B	204	CYS
1	72-B	206	ASN
1	72-B	218	SER
1	73-A	1	ILE
1	73-A	2	LEU
1	73-A	6	GLU
1	73-A	25	LEU
1	73-A	29	VAL
1	73-A	43	LEU
1	73-A	45	ASP
1	73-A	68	ARG
1	73-A	85	THR
1	73-A	86	ILE
1	73-A	106	ARG
1	73-A	115	ARG
1	73-A	130	ILE
1	73-A	137	ARG
1	73-A	138	PRO
1	73-A	145	LEU
1	73-A	157	ARG
1	73-A	158	THR
1	73-A	166	GLU
1	73-A	175	ARG
1	73-A	176	ARG
1	73-A	198	THR
1	73-A	210	PRO
1	73-A	224	ASP
1	73-A	226	VAL
1	73-A	227	LEU
1	73-B	43	LEU
1	73-B	44	GLU
1	73-B	62	GLN
1	73-B	68	ARG
1	73-B	73	LEU
1	73-B	82	GLN

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Mol	Chain	Res	Type
1	73-B	84	ASP
1	73-B	88	HIS
1	73-B	132	ASN
1	73-B	133	HIS
1	73-B	149	LEU
1	73-B	172	GLU
1	73-B	174	ASN
1	73-B	175	ARG
1	73-B	180	LYS
1	73-B	207	ARG
1	73-B	218	SER
1	73-B	224	ASP
1	73-B	227	LEU
1	74-A	1	ILE
1	74-A	25	LEU
1	74-A	45	ASP
1	74-A	50	LYS
1	74-A	73	LEU
1	74-A	82	GLN
1	74-A	84	ASP
1	74-A	85	THR
1	74-A	106	ARG
1	74-A	158	THR
1	74-A	166	GLU
1	74-A	176	ARG
1	74-A	180	LYS
1	74-A	183	SER
1	74-A	199	SER
1	74-A	204	CYS
1	74-A	207	ARG
1	74-B	2	LEU
1	74-B	5	ARG
1	74-B	43	LEU
1	74-B	62	GLN
1	74-B	68	ARG
1	74-B	82	GLN
1	74-B	85	THR
1	74-B	86	ILE
1	74-B	132	ASN
1	74-B	133	HIS
1	74-B	136	ARG
1	74-B	149	LEU

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Mol	Chain	Res	Type
1	74-B	154	CYS
1	74-B	174	ASN
1	74-B	201	SER
1	74-B	207	ARG
1	75-A	2	LEU
1	75-A	21	ASN
1	75-A	43	LEU
1	75-A	44	GLU
1	75-A	68	ARG
1	75-A	73	LEU
1	75-A	115	ARG
1	75-A	130	ILE
1	75-A	136	ARG
1	75-A	137	ARG
1	75-A	156	ARG
1	75-A	158	THR
1	75-A	172	GLU
1	75-A	175	ARG
1	75-A	176	ARG
1	75-A	180	LYS
1	75-A	182	ASP
1	75-A	187	LEU
1	75-A	215	ARG
1	75-A	226	VAL
1	75-A	227	LEU
1	75-B	5	ARG
1	75-B	29	VAL
1	75-B	43	LEU
1	75-B	62	GLN
1	75-B	73	LEU
1	75-B	97	GLU
1	75-B	115	ARG
1	75-B	149	LEU
1	75-B	150	ASP
1	75-B	174	ASN
1	75-B	176	ARG
1	75-B	179	CYS
1	75-B	180	LYS
1	75-B	198	THR
1	75-B	199	SER
1	75-B	201	SER
1	75-B	204	CYS

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Mol	Chain	Res	Type
1	75-B	207	ARG
1	75-B	208	LYS
1	75-B	216	VAL
1	75-B	225	SER
1	75-B	227	LEU
1	76-A	5	ARG
1	76-A	43	LEU
1	76-A	44	GLU
1	76-A	48	ASP
1	76-A	73	LEU
1	76-A	84	ASP
1	76-A	97	GLU
1	76-A	98	LYS
1	76-A	115	ARG
1	76-A	132	ASN
1	76-A	133	HIS
1	76-A	136	ARG
1	76-A	137	ARG
1	76-A	139	ASP
1	76-A	145	LEU
1	76-A	173	SER
1	76-A	174	ASN
1	76-A	175	ARG
1	76-A	180	LYS
1	76-A	183	SER
1	76-A	187	LEU
1	76-A	201	SER
1	76-A	208	LYS
1	76-A	226	VAL
1	76-A	227	LEU
1	76-B	21	ASN
1	76-B	48	ASP
1	76-B	50	LYS
1	76-B	73	LEU
1	76-B	74	ARG
1	76-B	96	SER
1	76-B	97	GLU
1	76-B	98	LYS
1	76-B	132	ASN
1	76-B	133	HIS
1	76-B	150	ASP
1	76-B	167	ARG

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Mol	Chain	Res	Type
1	76-B	172	GLU
1	76-B	176	ARG
1	76-B	178	SER
1	76-B	199	SER
1	76-B	201	SER
1	76-B	204	CYS
1	76-B	225	SER
1	76-B	227	LEU
1	77-A	2	LEU
1	77-A	20	LEU
1	77-A	43	LEU
1	77-A	45	ASP
1	77-A	50	LYS
1	77-A	82	GLN
1	77-A	96	SER
1	77-A	115	ARG
1	77-A	132	ASN
1	77-A	136	ARG
1	77-A	175	ARG
1	77-A	176	ARG
1	77-A	178	SER
1	77-A	183	SER
1	77-A	198	THR
1	77-A	199	SER
1	77-A	201	SER
1	77-A	207	ARG
1	77-A	227	LEU
1	77-B	5	ARG
1	77-B	29	VAL
1	77-B	41	HIS
1	77-B	45	ASP
1	77-B	51	VAL
1	77-B	68	ARG
1	77-B	85	THR
1	77-B	86	ILE
1	77-B	96	SER
1	77-B	115	ARG
1	77-B	149	LEU
1	77-B	158	THR
1	77-B	176	ARG
1	77-B	198	THR
1	77-B	227	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

154 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	GOL	58-B	1000	-	5,5,5	0.22	0	5,5,5	0.53	0
2	GOL	18-B	1000	-	5,5,5	0.25	0	5,5,5	0.38	0
2	GOL	1-B	1000	-	5,5,5	0.24	0	5,5,5	0.25	0
2	GOL	18-A	1000	-	5,5,5	0.54	0	5,5,5	1.56	0
2	GOL	43-A	1000	-	5,5,5	0.34	0	5,5,5	1.25	0
2	GOL	42-A	1000	-	5,5,5	0.69	0	5,5,5	1.19	0
2	GOL	13-A	1000	-	5,5,5	0.81	0	5,5,5	1.03	0
2	GOL	44-B	1000	-	5,5,5	0.28	0	5,5,5	0.45	0
2	GOL	22-A	1000	-	5,5,5	0.39	0	5,5,5	1.60	2 (40%)
2	GOL	63-B	1000	-	5,5,5	0.21	0	5,5,5	0.41	0
2	GOL	2-B	1000	-	5,5,5	0.29	0	5,5,5	0.34	0
2	GOL	23-B	1000	-	5,5,5	0.26	0	5,5,5	0.33	0
2	GOL	33-B	1000	-	5,5,5	0.22	0	5,5,5	0.30	0
2	GOL	4-A	1000	-	5,5,5	0.45	0	5,5,5	1.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	59-A	1000	-	5,5,5	0.36	0	5,5,5	1.37	0
2	GOL	16-B	1000	-	5,5,5	0.21	0	5,5,5	0.42	0
2	GOL	9-A	1000	-	5,5,5	0.38	0	5,5,5	0.51	0
2	GOL	47-A	1000	-	5,5,5	0.67	0	5,5,5	0.66	0
2	GOL	40-B	1000	-	5,5,5	0.22	0	5,5,5	0.37	0
2	GOL	6-B	1000	-	5,5,5	0.20	0	5,5,5	0.26	0
2	GOL	42-B	1000	-	5,5,5	0.29	0	5,5,5	0.30	0
2	GOL	5-A	1000	-	5,5,5	0.41	0	5,5,5	1.45	0
2	GOL	53-A	1000	-	5,5,5	0.41	0	5,5,5	1.49	0
2	GOL	7-B	1000	-	5,5,5	0.23	0	5,5,5	0.27	0
2	GOL	11-B	1000	-	5,5,5	0.21	0	5,5,5	0.34	0
2	GOL	25-B	1000	-	5,5,5	0.24	0	5,5,5	0.37	0
2	GOL	38-B	1000	-	5,5,5	0.26	0	5,5,5	0.54	0
2	GOL	19-A	1000	-	5,5,5	0.45	0	5,5,5	1.56	1 (20%)
2	GOL	4-B	1000	-	5,5,5	0.22	0	5,5,5	0.35	0
2	GOL	39-B	1000	-	5,5,5	0.27	0	5,5,5	0.32	0
2	GOL	27-B	1000	-	5,5,5	0.25	0	5,5,5	0.35	0
2	GOL	54-A	1000	-	5,5,5	0.45	0	5,5,5	1.61	1 (20%)
2	GOL	16-A	1000	-	5,5,5	0.31	0	5,5,5	1.53	1 (20%)
2	GOL	8-B	1000	-	5,5,5	0.23	0	5,5,5	0.39	0
2	GOL	24-B	1000	-	5,5,5	0.23	0	5,5,5	0.33	0
2	GOL	1-A	1000	-	5,5,5	0.40	0	5,5,5	0.40	0
2	GOL	14-B	1000	-	5,5,5	0.25	0	5,5,5	0.47	0
2	GOL	30-B	1000	-	5,5,5	0.35	0	5,5,5	0.35	0
2	GOL	10-B	1000	-	5,5,5	0.23	0	5,5,5	0.38	0
2	GOL	3-B	1000	-	5,5,5	0.23	0	5,5,5	0.29	0
2	GOL	57-A	1000	-	5,5,5	0.38	0	5,5,5	1.17	0
2	GOL	35-B	1000	-	5,5,5	0.21	0	5,5,5	0.33	0
2	GOL	44-A	1000	-	5,5,5	0.45	0	5,5,5	0.49	0
2	GOL	60-B	1000	-	5,5,5	0.24	0	5,5,5	0.45	0
2	GOL	37-A	1000	-	5,5,5	0.59	0	5,5,5	1.53	0
2	GOL	19-B	1000	-	5,5,5	0.26	0	5,5,5	0.38	0
2	GOL	15-B	1000	-	5,5,5	0.20	0	5,5,5	0.39	0
2	GOL	28-A	1000	-	5,5,5	0.53	0	5,5,5	1.66	1 (20%)
2	GOL	8-A	1000	-	5,5,5	0.34	0	5,5,5	1.34	0
2	GOL	9-B	1000	-	5,5,5	0.23	0	5,5,5	0.34	0
2	GOL	52-A	1000	-	5,5,5	0.61	0	5,5,5	1.55	0
2	GOL	50-B	1000	-	5,5,5	0.25	0	5,5,5	0.48	0
2	GOL	2-A	1000	-	5,5,5	0.34	0	5,5,5	1.44	1 (20%)
2	GOL	3-A	1000	-	5,5,5	0.49	0	5,5,5	1.31	0
2	GOL	22-B	1000	-	5,5,5	0.23	0	5,5,5	0.39	0
2	GOL	55-B	1000	-	5,5,5	0.25	0	5,5,5	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	59-B	1000	-	5,5,5	0.20	0	5,5,5	0.49	0
2	GOL	37-B	1000	-	5,5,5	0.25	0	5,5,5	0.33	0
2	GOL	49-B	1000	-	5,5,5	0.22	0	5,5,5	0.56	0
2	GOL	17-B	1000	-	5,5,5	0.22	0	5,5,5	0.42	0
2	GOL	28-B	1000	-	5,5,5	0.24	0	5,5,5	0.41	0
2	GOL	23-A	1000	-	5,5,5	0.56	0	5,5,5	0.97	0
2	GOL	20-A	1000	-	5,5,5	0.36	0	5,5,5	1.48	1 (20%)
2	GOL	34-A	1000	-	5,5,5	0.61	0	5,5,5	1.40	0
2	GOL	52-B	1000	-	5,5,5	0.25	0	5,5,5	0.53	0
2	GOL	13-B	1000	-	5,5,5	0.19	0	5,5,5	0.37	0
2	GOL	32-B	1000	-	5,5,5	0.27	0	5,5,5	0.34	0
2	GOL	14-A	1000	-	5,5,5	0.29	0	5,5,5	1.57	1 (20%)
2	GOL	39-A	1000	-	5,5,5	0.80	0	5,5,5	0.50	0
2	GOL	58-A	1000	-	5,5,5	0.48	0	5,5,5	1.51	1 (20%)
2	GOL	12-A	1000	-	5,5,5	0.44	0	5,5,5	1.53	1 (20%)
2	GOL	6-A	1000	-	5,5,5	0.40	0	5,5,5	1.35	0
2	GOL	38-A	1000	-	5,5,5	0.39	0	5,5,5	1.02	0
2	GOL	7-A	1000	-	5,5,5	0.40	0	5,5,5	1.51	0
2	GOL	24-A	1000	-	5,5,5	0.48	0	5,5,5	0.51	0
2	GOL	48-A	1000	-	5,5,5	0.43	0	5,5,5	1.62	1 (20%)
2	GOL	29-A	1000	-	5,5,5	0.47	0	5,5,5	1.80	2 (40%)
2	GOL	54-B	1000	-	5,5,5	0.23	0	5,5,5	0.50	0
2	GOL	11-A	1000	-	5,5,5	0.38	0	5,5,5	0.62	0
2	GOL	47-B	1000	-	5,5,5	0.18	0	5,5,5	0.35	0
2	GOL	10-A	1000	-	5,5,5	0.33	0	5,5,5	1.28	1 (20%)
2	GOL	12-B	1000	-	5,5,5	0.19	0	5,5,5	0.33	0
2	GOL	27-A	1000	-	5,5,5	0.50	0	5,5,5	1.53	0
2	GOL	57-B	1000	-	5,5,5	0.26	0	5,5,5	0.45	0
2	GOL	29-B	1000	-	5,5,5	0.23	0	5,5,5	0.51	0
2	GOL	34-B	1000	-	5,5,5	0.28	0	5,5,5	0.28	0
2	GOL	15-A	1000	-	5,5,5	0.49	0	5,5,5	0.69	0
2	GOL	17-A	1000	-	5,5,5	0.63	0	5,5,5	1.71	2 (40%)
2	GOL	5-B	1000	-	5,5,5	0.23	0	5,5,5	0.27	0
2	GOL	48-B	1000	-	5,5,5	0.22	0	5,5,5	0.50	0
2	GOL	49-A	1000	-	5,5,5	0.47	0	5,5,5	1.79	2 (40%)
2	GOL	33-A	1000	-	5,5,5	0.60	0	5,5,5	0.90	0
2	GOL	53-B	1000	-	5,5,5	0.25	0	5,5,5	0.55	0
2	GOL	32-A	1000	-	5,5,5	0.34	0	5,5,5	0.27	0
2	GOL	45-B	1000	-	5,5,5	0.24	0	5,5,5	0.37	0
2	GOL	43-B	1000	-	5,5,5	0.24	0	5,5,5	0.29	0
2	GOL	20-B	1000	-	5,5,5	0.27	0	5,5,5	0.35	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	GOL	58-B	1000	-	-	0/4/4/4	-
2	GOL	18-B	1000	-	-	0/4/4/4	-
2	GOL	1-B	1000	-	-	0/4/4/4	-
2	GOL	18-A	1000	-	-	4/4/4/4	-
2	GOL	43-A	1000	-	-	2/4/4/4	-
2	GOL	42-A	1000	-	-	0/4/4/4	-
2	GOL	13-A	1000	-	-	0/4/4/4	-
2	GOL	44-B	1000	-	-	2/4/4/4	-
2	GOL	22-A	1000	-	-	3/4/4/4	-
2	GOL	63-B	1000	-	-	2/4/4/4	-
2	GOL	2-B	1000	-	-	2/4/4/4	-
2	GOL	23-B	1000	-	-	0/4/4/4	-
2	GOL	33-B	1000	-	-	0/4/4/4	-
2	GOL	4-A	1000	-	-	4/4/4/4	-
2	GOL	59-A	1000	-	-	3/4/4/4	-
2	GOL	16-B	1000	-	-	2/4/4/4	-
2	GOL	9-A	1000	-	-	0/4/4/4	-
2	GOL	47-A	1000	-	-	0/4/4/4	-
2	GOL	40-B	1000	-	-	0/4/4/4	-
2	GOL	6-B	1000	-	-	1/4/4/4	-
2	GOL	42-B	1000	-	-	1/4/4/4	-
2	GOL	5-A	1000	-	-	4/4/4/4	-
2	GOL	53-A	1000	-	-	4/4/4/4	-
2	GOL	7-B	1000	-	-	0/4/4/4	-
2	GOL	11-B	1000	-	-	0/4/4/4	-
2	GOL	25-B	1000	-	-	2/4/4/4	-
2	GOL	38-B	1000	-	-	2/4/4/4	-
2	GOL	19-A	1000	-	-	3/4/4/4	-
2	GOL	4-B	1000	-	-	2/4/4/4	-
2	GOL	39-B	1000	-	-	0/4/4/4	-
2	GOL	27-B	1000	-	-	2/4/4/4	-
2	GOL	54-A	1000	-	-	4/4/4/4	-
2	GOL	16-A	1000	-	-	0/4/4/4	-
2	GOL	8-B	1000	-	-	1/4/4/4	-
2	GOL	24-B	1000	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	1-A	1000	-	-	0/4/4/4	-
2	GOL	14-B	1000	-	-	2/4/4/4	-
2	GOL	30-B	1000	-	-	2/4/4/4	-
2	GOL	10-B	1000	-	-	2/4/4/4	-
2	GOL	3-B	1000	-	-	2/4/4/4	-
2	GOL	57-A	1000	-	-	0/4/4/4	-
2	GOL	35-B	1000	-	-	2/4/4/4	-
2	GOL	44-A	1000	-	-	0/4/4/4	-
2	GOL	60-B	1000	-	-	2/4/4/4	-
2	GOL	37-A	1000	-	-	4/4/4/4	-
2	GOL	19-B	1000	-	-	2/4/4/4	-
2	GOL	15-B	1000	-	-	0/4/4/4	-
2	GOL	28-A	1000	-	-	4/4/4/4	-
2	GOL	8-A	1000	-	-	3/4/4/4	-
2	GOL	9-B	1000	-	-	0/4/4/4	-
2	GOL	52-A	1000	-	-	4/4/4/4	-
2	GOL	50-B	1000	-	-	0/4/4/4	-
2	GOL	2-A	1000	-	-	1/4/4/4	-
2	GOL	3-A	1000	-	-	4/4/4/4	-
2	GOL	22-B	1000	-	-	0/4/4/4	-
2	GOL	55-B	1000	-	-	0/4/4/4	-
2	GOL	59-B	1000	-	-	2/4/4/4	-
2	GOL	37-B	1000	-	-	0/4/4/4	-
2	GOL	49-B	1000	-	-	0/4/4/4	-
2	GOL	17-B	1000	-	-	0/4/4/4	-
2	GOL	28-B	1000	-	-	2/4/4/4	-
2	GOL	23-A	1000	-	-	2/4/4/4	-
2	GOL	20-A	1000	-	-	3/4/4/4	-
2	GOL	34-A	1000	-	-	4/4/4/4	-
2	GOL	52-B	1000	-	-	0/4/4/4	-
2	GOL	13-B	1000	-	-	0/4/4/4	-
2	GOL	32-B	1000	-	-	0/4/4/4	-
2	GOL	14-A	1000	-	-	2/4/4/4	-
2	GOL	39-A	1000	-	-	3/4/4/4	-
2	GOL	58-A	1000	-	-	4/4/4/4	-
2	GOL	12-A	1000	-	-	2/4/4/4	-
2	GOL	6-A	1000	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	38-A	1000	-	-	1/4/4/4	-
2	GOL	7-A	1000	-	-	4/4/4/4	-
2	GOL	24-A	1000	-	-	0/4/4/4	-
2	GOL	48-A	1000	-	-	0/4/4/4	-
2	GOL	29-A	1000	-	-	4/4/4/4	-
2	GOL	54-B	1000	-	-	0/4/4/4	-
2	GOL	11-A	1000	-	-	2/4/4/4	-
2	GOL	47-B	1000	-	-	2/4/4/4	-
2	GOL	10-A	1000	-	-	2/4/4/4	-
2	GOL	12-B	1000	-	-	0/4/4/4	-
2	GOL	27-A	1000	-	-	3/4/4/4	-
2	GOL	57-B	1000	-	-	0/4/4/4	-
2	GOL	29-B	1000	-	-	2/4/4/4	-
2	GOL	34-B	1000	-	-	0/4/4/4	-
2	GOL	15-A	1000	-	-	0/4/4/4	-
2	GOL	17-A	1000	-	-	4/4/4/4	-
2	GOL	5-B	1000	-	-	0/4/4/4	-
2	GOL	48-B	1000	-	-	1/4/4/4	-
2	GOL	49-A	1000	-	-	3/4/4/4	-
2	GOL	33-A	1000	-	-	2/4/4/4	-
2	GOL	53-B	1000	-	-	2/4/4/4	-
2	GOL	32-A	1000	-	-	0/4/4/4	-
2	GOL	45-B	1000	-	-	2/4/4/4	-
2	GOL	43-B	1000	-	-	0/4/4/4	-
2	GOL	20-B	1000	-	-	2/4/4/4	-

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	49-A	1000	GOL	O2-C2-C1	2.85	121.66	109.12
2	48-A	1000	GOL	O2-C2-C1	-2.83	96.67	109.12
2	16-A	1000	GOL	O2-C2-C1	-2.76	96.95	109.12
2	12-A	1000	GOL	O2-C2-C1	-2.76	96.98	109.12
2	2-A	1000	GOL	O2-C2-C1	-2.41	98.53	109.12
2	29-A	1000	GOL	O2-C2-C1	2.34	119.44	109.12
2	17-A	1000	GOL	O2-C2-C1	2.25	119.02	109.12
2	17-A	1000	GOL	O1-C1-C2	2.20	120.76	110.20
2	10-A	1000	GOL	O2-C2-C1	-2.17	99.55	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	49-A	1000	GOL	O1-C1-C2	2.15	120.49	110.20
2	14-A	1000	GOL	O2-C2-C1	-2.14	99.68	109.12
2	19-A	1000	GOL	O2-C2-C1	2.13	118.51	109.12
2	54-A	1000	GOL	O2-C2-C1	2.09	118.33	109.12
2	20-A	1000	GOL	O2-C2-C1	2.09	118.31	109.12
2	22-A	1000	GOL	O2-C2-C1	2.05	118.15	109.12
2	29-A	1000	GOL	C3-C2-C1	2.04	119.63	111.70
2	58-A	1000	GOL	O2-C2-C1	2.03	118.08	109.12
2	28-A	1000	GOL	O2-C2-C1	2.03	118.08	109.12
2	22-A	1000	GOL	C3-C2-C1	2.01	119.52	111.70

There are no chirality outliers.

All (150) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	3-A	1000	GOL	O1-C1-C2-O2
2	3-A	1000	GOL	O1-C1-C2-C3
2	3-A	1000	GOL	C1-C2-C3-O3
2	4-A	1000	GOL	O1-C1-C2-C3
2	4-A	1000	GOL	C1-C2-C3-O3
2	5-A	1000	GOL	O1-C1-C2-C3
2	5-A	1000	GOL	C1-C2-C3-O3
2	5-A	1000	GOL	O2-C2-C3-O3
2	6-A	1000	GOL	O1-C1-C2-C3
2	7-A	1000	GOL	O1-C1-C2-C3
2	7-A	1000	GOL	C1-C2-C3-O3
2	8-A	1000	GOL	O1-C1-C2-C3
2	17-A	1000	GOL	O1-C1-C2-C3
2	17-A	1000	GOL	C1-C2-C3-O3
2	18-A	1000	GOL	O1-C1-C2-C3
2	18-A	1000	GOL	C1-C2-C3-O3
2	19-A	1000	GOL	O1-C1-C2-C3
2	19-A	1000	GOL	C1-C2-C3-O3
2	20-A	1000	GOL	O1-C1-C2-C3
2	22-A	1000	GOL	O1-C1-C2-C3
2	22-A	1000	GOL	C1-C2-C3-O3
2	23-A	1000	GOL	C1-C2-C3-O3
2	27-A	1000	GOL	C1-C2-C3-O3
2	28-A	1000	GOL	O1-C1-C2-C3
2	29-A	1000	GOL	O1-C1-C2-C3
2	29-A	1000	GOL	C1-C2-C3-O3
2	34-A	1000	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	34-A	1000	GOL	C1-C2-C3-O3
2	37-A	1000	GOL	O1-C1-C2-C3
2	37-A	1000	GOL	O2-C2-C3-O3
2	49-A	1000	GOL	O1-C1-C2-C3
2	52-A	1000	GOL	O1-C1-C2-C3
2	53-A	1000	GOL	O1-C1-C2-C3
2	53-A	1000	GOL	C1-C2-C3-O3
2	54-A	1000	GOL	O1-C1-C2-C3
2	54-A	1000	GOL	C1-C2-C3-O3
2	58-A	1000	GOL	O1-C1-C2-C3
2	58-A	1000	GOL	C1-C2-C3-O3
2	59-A	1000	GOL	O1-C1-C2-C3
2	14-B	1000	GOL	O1-C1-C2-O2
2	44-B	1000	GOL	O1-C1-C2-C3
2	4-A	1000	GOL	O1-C1-C2-O2
2	4-A	1000	GOL	O2-C2-C3-O3
2	5-A	1000	GOL	O1-C1-C2-O2
2	6-A	1000	GOL	O2-C2-C3-O3
2	7-A	1000	GOL	O1-C1-C2-O2
2	18-A	1000	GOL	O1-C1-C2-O2
2	19-A	1000	GOL	O1-C1-C2-O2
2	28-A	1000	GOL	O1-C1-C2-O2
2	34-A	1000	GOL	O1-C1-C2-O2
2	37-A	1000	GOL	O1-C1-C2-O2
2	52-A	1000	GOL	O1-C1-C2-O2
2	53-A	1000	GOL	O1-C1-C2-O2
2	54-A	1000	GOL	O2-C2-C3-O3
2	58-A	1000	GOL	O1-C1-C2-O2
2	2-B	1000	GOL	O1-C1-C2-O2
2	38-B	1000	GOL	O1-C1-C2-O2
2	6-A	1000	GOL	C1-C2-C3-O3
2	8-A	1000	GOL	C1-C2-C3-O3
2	10-A	1000	GOL	C1-C2-C3-O3
2	12-A	1000	GOL	C1-C2-C3-O3
2	20-A	1000	GOL	C1-C2-C3-O3
2	28-A	1000	GOL	C1-C2-C3-O3
2	33-A	1000	GOL	C1-C2-C3-O3
2	37-A	1000	GOL	C1-C2-C3-O3
2	38-A	1000	GOL	C1-C2-C3-O3
2	39-A	1000	GOL	C1-C2-C3-O3
2	43-A	1000	GOL	C1-C2-C3-O3
2	49-A	1000	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	52-A	1000	GOL	C1-C2-C3-O3
2	2-B	1000	GOL	O1-C1-C2-C3
2	4-B	1000	GOL	O1-C1-C2-C3
2	10-B	1000	GOL	O1-C1-C2-C3
2	14-B	1000	GOL	O1-C1-C2-C3
2	16-B	1000	GOL	O1-C1-C2-C3
2	19-B	1000	GOL	O1-C1-C2-C3
2	20-B	1000	GOL	O1-C1-C2-C3
2	25-B	1000	GOL	O1-C1-C2-C3
2	27-B	1000	GOL	O1-C1-C2-C3
2	28-B	1000	GOL	O1-C1-C2-C3
2	29-B	1000	GOL	O1-C1-C2-C3
2	30-B	1000	GOL	O1-C1-C2-C3
2	38-B	1000	GOL	O1-C1-C2-C3
2	45-B	1000	GOL	O1-C1-C2-C3
2	53-B	1000	GOL	O1-C1-C2-C3
2	59-B	1000	GOL	O1-C1-C2-C3
2	60-B	1000	GOL	O1-C1-C2-C3
2	3-A	1000	GOL	O2-C2-C3-O3
2	6-A	1000	GOL	O1-C1-C2-O2
2	7-A	1000	GOL	O2-C2-C3-O3
2	8-A	1000	GOL	O1-C1-C2-O2
2	12-A	1000	GOL	O2-C2-C3-O3
2	17-A	1000	GOL	O1-C1-C2-O2
2	20-A	1000	GOL	O1-C1-C2-O2
2	23-A	1000	GOL	O2-C2-C3-O3
2	27-A	1000	GOL	O2-C2-C3-O3
2	28-A	1000	GOL	O2-C2-C3-O3
2	29-A	1000	GOL	O1-C1-C2-O2
2	29-A	1000	GOL	O2-C2-C3-O3
2	49-A	1000	GOL	O1-C1-C2-O2
2	52-A	1000	GOL	O2-C2-C3-O3
2	53-A	1000	GOL	O2-C2-C3-O3
2	54-A	1000	GOL	O1-C1-C2-O2
2	29-B	1000	GOL	O1-C1-C2-O2
2	30-B	1000	GOL	O1-C1-C2-O2
2	10-A	1000	GOL	O2-C2-C3-O3
2	22-A	1000	GOL	O1-C1-C2-O2
2	27-A	1000	GOL	O1-C1-C2-O2
2	33-A	1000	GOL	O2-C2-C3-O3
2	58-A	1000	GOL	O2-C2-C3-O3
2	59-A	1000	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	28-B	1000	GOL	O1-C1-C2-O2
2	60-B	1000	GOL	O1-C1-C2-O2
2	59-A	1000	GOL	C1-C2-C3-O3
2	43-A	1000	GOL	O2-C2-C3-O3
2	44-B	1000	GOL	O1-C1-C2-O2
2	39-A	1000	GOL	O2-C2-C3-O3
2	3-B	1000	GOL	O1-C1-C2-C3
2	63-B	1000	GOL	O1-C1-C2-C3
2	18-A	1000	GOL	O2-C2-C3-O3
2	39-A	1000	GOL	O1-C1-C2-O2
2	11-A	1000	GOL	C1-C2-C3-O3
2	14-A	1000	GOL	C1-C2-C3-O3
2	24-B	1000	GOL	O1-C1-C2-C3
2	35-B	1000	GOL	O1-C1-C2-C3
2	2-A	1000	GOL	O1-C1-C2-O2
2	17-A	1000	GOL	O2-C2-C3-O3
2	10-B	1000	GOL	O1-C1-C2-O2
2	19-B	1000	GOL	O1-C1-C2-O2
2	25-B	1000	GOL	O1-C1-C2-O2
2	45-B	1000	GOL	O1-C1-C2-O2
2	42-B	1000	GOL	O1-C1-C2-C3
2	47-B	1000	GOL	O1-C1-C2-C3
2	4-B	1000	GOL	O1-C1-C2-O2
2	20-B	1000	GOL	O1-C1-C2-O2
2	27-B	1000	GOL	O1-C1-C2-O2
2	53-B	1000	GOL	O1-C1-C2-O2
2	59-B	1000	GOL	O1-C1-C2-O2
2	63-B	1000	GOL	O1-C1-C2-O2
2	11-A	1000	GOL	O2-C2-C3-O3
2	34-A	1000	GOL	O2-C2-C3-O3
2	3-B	1000	GOL	O1-C1-C2-O2
2	16-B	1000	GOL	O1-C1-C2-O2
2	24-B	1000	GOL	O1-C1-C2-O2
2	35-B	1000	GOL	O1-C1-C2-O2
2	47-B	1000	GOL	O1-C1-C2-O2
2	6-B	1000	GOL	O1-C1-C2-C3
2	8-B	1000	GOL	O1-C1-C2-C3
2	48-B	1000	GOL	O1-C1-C2-C3
2	14-A	1000	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.