



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:25 AM GMT

PDB ID : 2Q4K  
Title : Ensemble refinement of the protein crystal structure of gene product from Homo sapiens Hs.433573  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-31  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

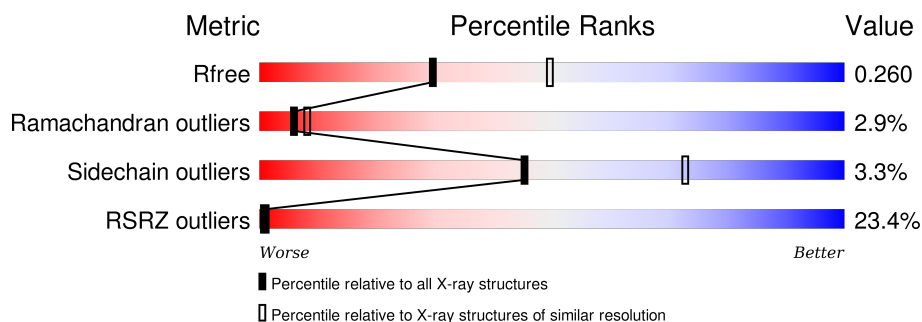
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3553 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	1-A	251	<div> <div>31%</div> <div>84% 6% 9%</div> </div>
1	1-B	251	<div> <div>20%</div> <div>86% 8% 6%</div> </div>
1	1-C	251	<div> <div>12%</div> <div>85% • 12%</div> </div>
1	10-A	251	<div> <div>31%</div> <div>87% • 9%</div> </div>
1	10-B	251	<div> <div>20%</div> <div>90% • 6%</div> </div>
1	10-C	251	<div> <div>12%</div> <div>85% • 12%</div> </div>
1	11-A	251	<div> <div>31%</div> <div>86% • 9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	11-B	251	
1	11-C	251	
1	12-A	251	
1	12-B	251	
1	12-C	251	
1	13-A	251	
1	13-B	251	
1	13-C	251	
1	14-A	251	
1	14-B	251	
1	14-C	251	
1	15-A	251	
1	15-B	251	
1	15-C	251	
1	16-A	251	
1	16-B	251	
1	16-C	251	
1	2-A	251	
1	2-B	251	
1	2-C	251	
1	3-A	251	
1	3-B	251	
1	3-C	251	
1	4-A	251	
1	4-B	251	

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Mol	Chain	Length	Quality of chain
1	4-C	251	
1	5-A	251	
1	5-B	251	
1	5-C	251	
1	6-A	251	
1	6-B	251	
1	6-C	251	
1	7-A	251	
1	7-B	251	
1	7-C	251	
1	8-A	251	
1	8-B	251	
1	8-C	251	
1	9-A	251	
1	9-B	251	
1	9-C	251	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 88208 atoms, of which 0 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 Uncharacterized protein C11orf68.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	2-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	3-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	4-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	5-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	6-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	7-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	8-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	9-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	10-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	11-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	12-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	13-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	14-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	15-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			
1	16-A	228	Total	C	N	O	S	Se	0	0	0
			1769	1123	313	327	3	3			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	2-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	3-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	4-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	5-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	6-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	7-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	8-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	9-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	10-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	11-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	12-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	13-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	14-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	15-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	16-B	235	Total	C	N	O	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	1-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	2-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	3-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	4-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	5-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	6-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	7-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	8-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	9-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	10-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	11-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	12-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	13-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	14-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	15-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			
1	16-C	221	Total	C	N	O	S	Se	0	0	0
			1712	1087	307	312	3	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9H3H3
A	30	MSE	MET	MODIFIED RESIDUE	UNP Q9H3H3
A	34	MSE	MET	MODIFIED RESIDUE	UNP Q9H3H3
A	131	MSE	MET	MODIFIED RESIDUE	UNP Q9H3H3
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9H3H3
B	30	MSE	MET	MODIFIED RESIDUE	UNP Q9H3H3
B	34	MSE	MET	MODIFIED RESIDUE	UNP Q9H3H3
B	131	MSE	MET	MODIFIED RESIDUE	UNP Q9H3H3
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9H3H3
C	30	MSE	MET	MODIFIED RESIDUE	UNP Q9H3H3
C	34	MSE	MET	MODIFIED RESIDUE	UNP Q9H3H3
C	131	MSE	MET	MODIFIED RESIDUE	UNP Q9H3H3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	50	Total 50	O 50	0	0
2	2-A	55	Total 55	O 55	0	0
2	3-A	56	Total 56	O 56	0	0
2	4-A	55	Total 55	O 55	0	0
2	5-A	55	Total 55	O 55	0	0
2	6-A	56	Total 56	O 56	0	0
2	7-A	54	Total 54	O 54	0	0
2	8-A	56	Total 56	O 56	0	0
2	9-A	57	Total 57	O 57	0	0
2	10-A	56	Total 56	O 56	0	0
2	11-A	58	Total 58	O 58	0	0
2	12-A	55	Total 55	O 55	0	0
2	13-A	53	Total 53	O 53	0	0
2	14-A	56	Total 56	O 56	0	0
2	15-A	53	Total 53	O 53	0	0
2	16-A	53	Total 53	O 53	0	0
2	1-B	91	Total 91	O 91	0	0
2	2-B	88	Total 88	O 88	0	0
2	3-B	88	Total 88	O 88	0	0
2	4-B	90	Total 90	O 90	0	0
2	5-B	89	Total 89	O 89	0	0
2	6-B	89	Total 89	O 89	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	7-B	89	Total O 89 89	0	0
2	8-B	88	Total O 88 88	0	0
2	9-B	88	Total O 88 88	0	0
2	10-B	88	Total O 88 88	0	0
2	11-B	87	Total O 87 87	0	0
2	12-B	87	Total O 87 87	0	0
2	13-B	91	Total O 91 91	0	0
2	14-B	87	Total O 87 87	0	0
2	15-B	91	Total O 91 91	0	0
2	16-B	91	Total O 91 91	0	0
2	1-C	76	Total O 76 76	0	0
2	2-C	74	Total O 74 74	0	0
2	3-C	73	Total O 73 73	0	0
2	4-C	72	Total O 72 72	0	0
2	5-C	73	Total O 73 73	0	0
2	6-C	72	Total O 72 72	0	0
2	7-C	74	Total O 74 74	0	0
2	8-C	73	Total O 73 73	0	0
2	9-C	72	Total O 72 72	0	0
2	10-C	73	Total O 73 73	0	0
2	11-C	72	Total O 72 72	0	0

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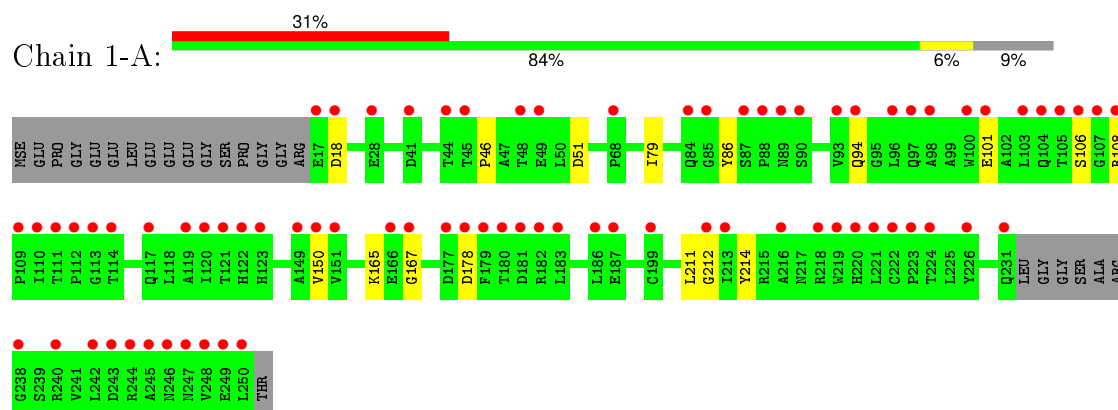
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	12-C	75	Total 75	O 75	0	0
2	13-C	73	Total 73	O 73	0	0
2	14-C	74	Total 74	O 74	0	0
2	15-C	73	Total 73	O 73	0	0
2	16-C	73	Total 73	O 73	0	0

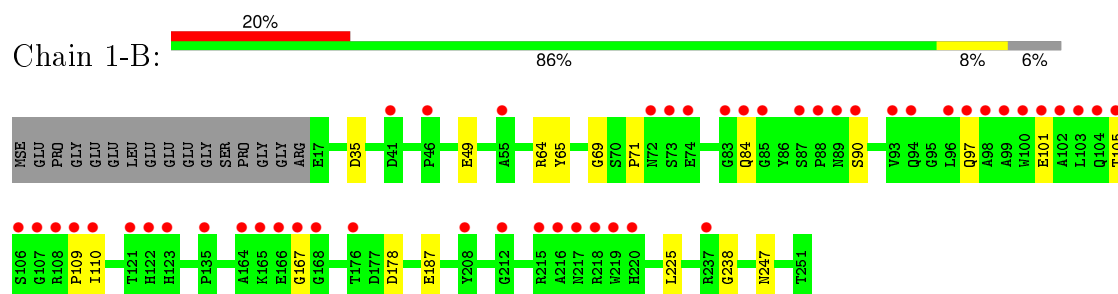
### 3 Residue-property plots [i](#)

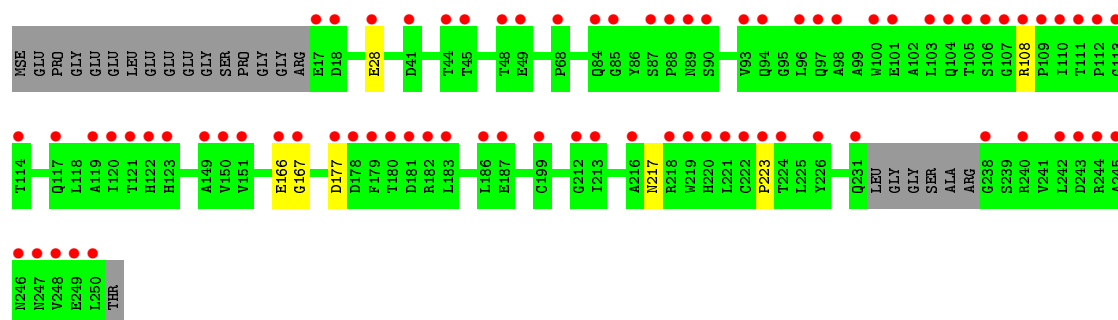
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: Uncharacterized protein C11orf68

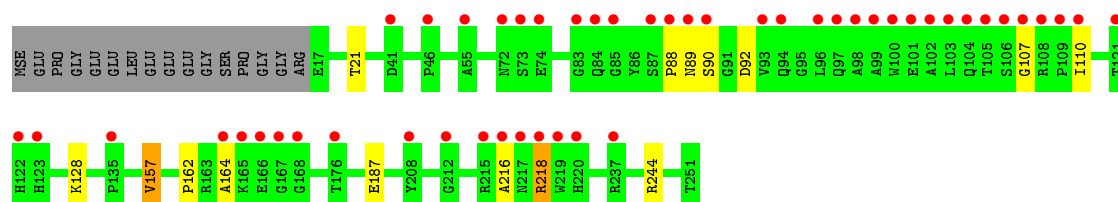
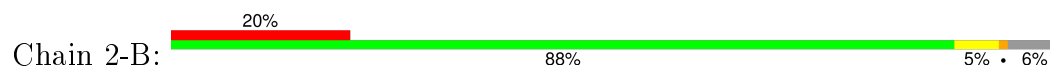


#### • Molecule 1: Uncharacterized protein C11orf68

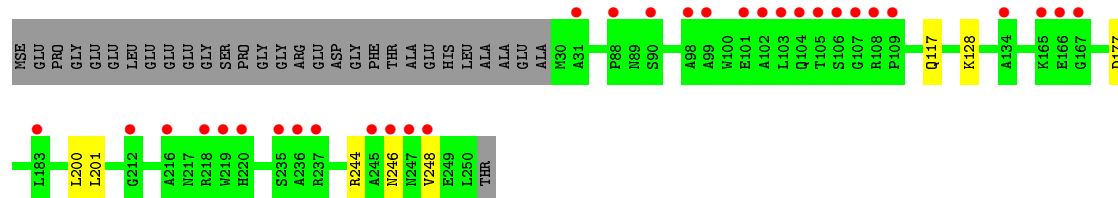
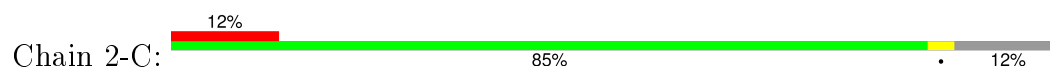




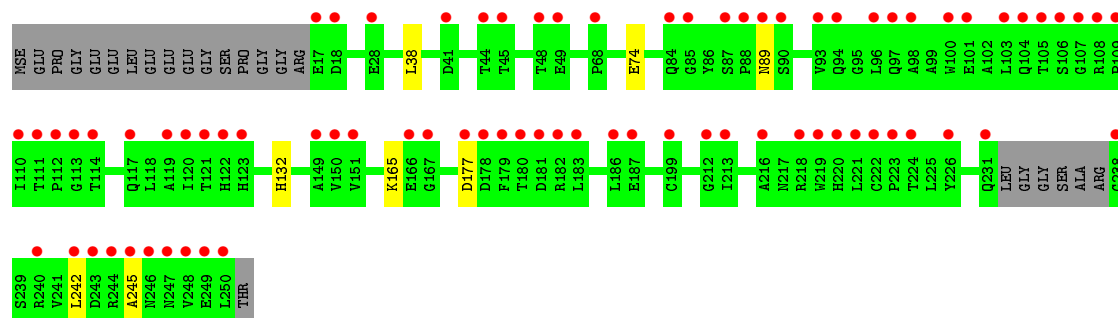
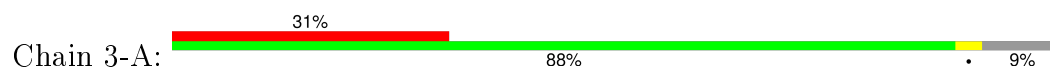
- Molecule 1: Uncharacterized protein C11orf68



- Molecule 1: Uncharacterized protein C11orf68

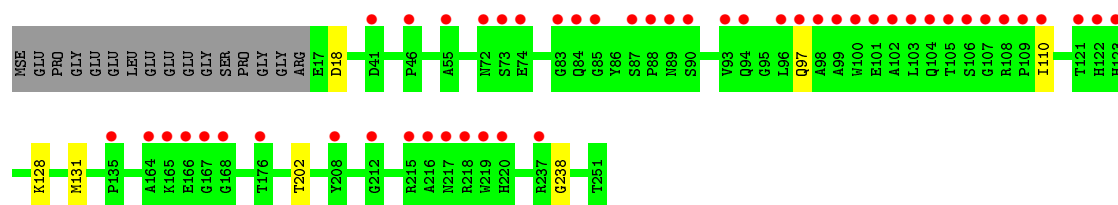


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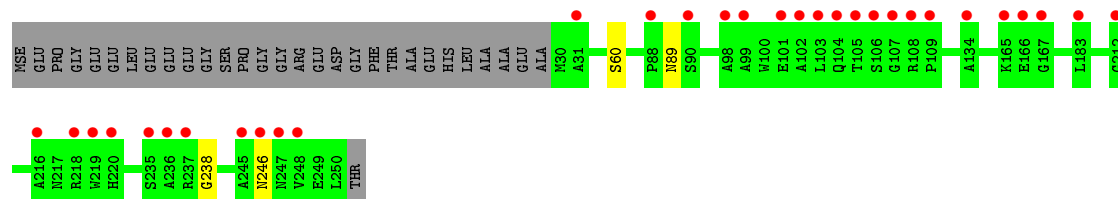
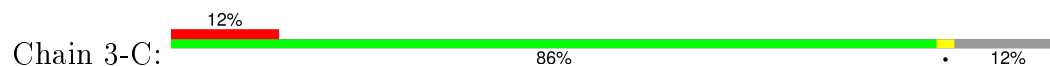


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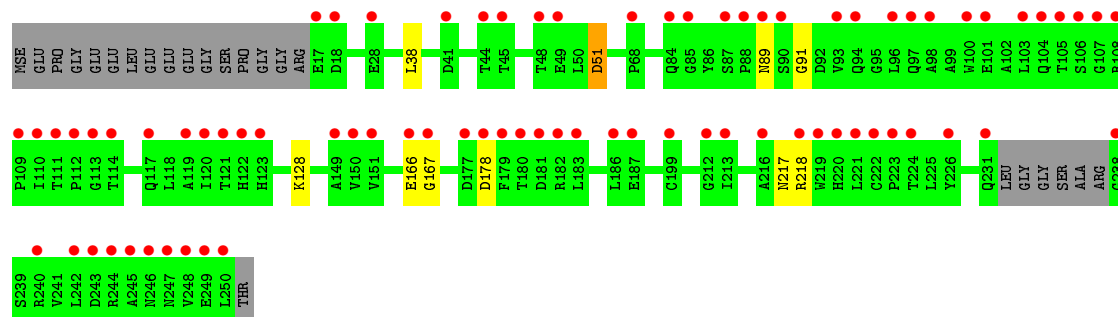
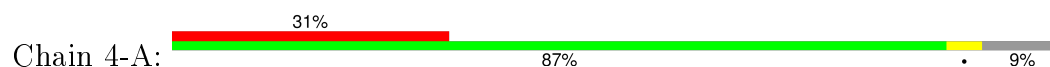




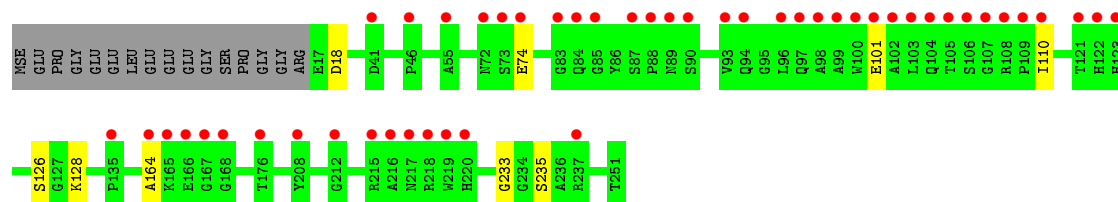
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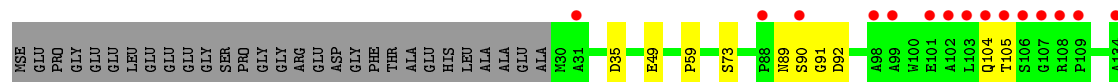
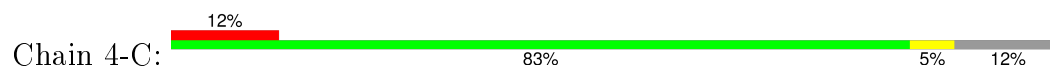
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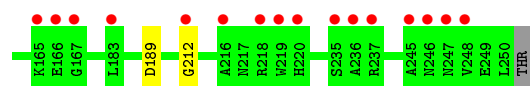


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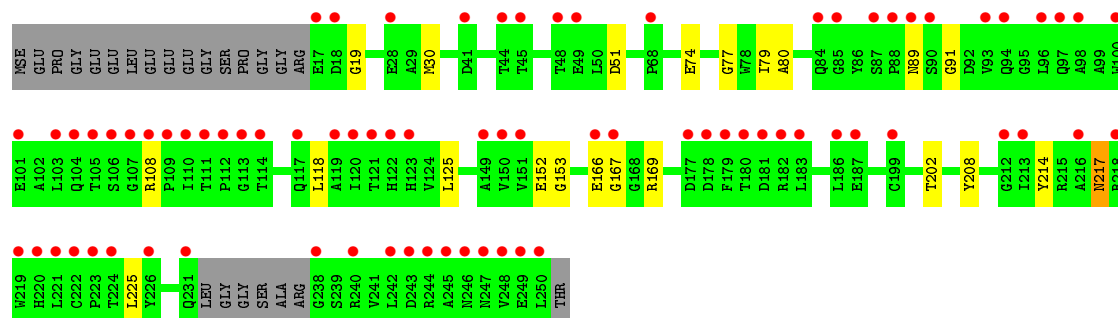
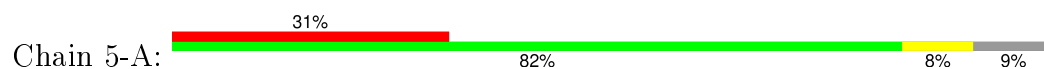


- Molecule 1: Uncharacterized protein C11orf68

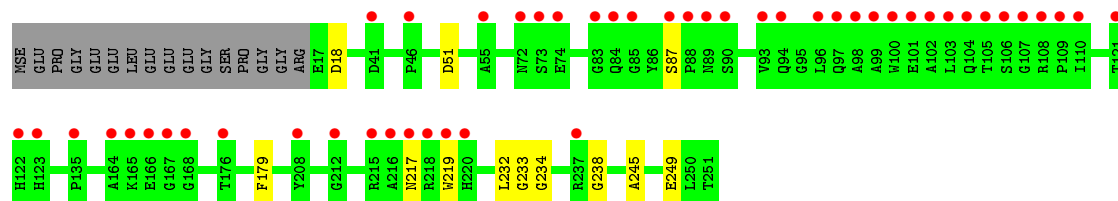
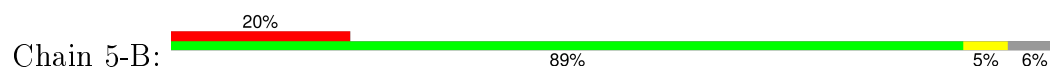




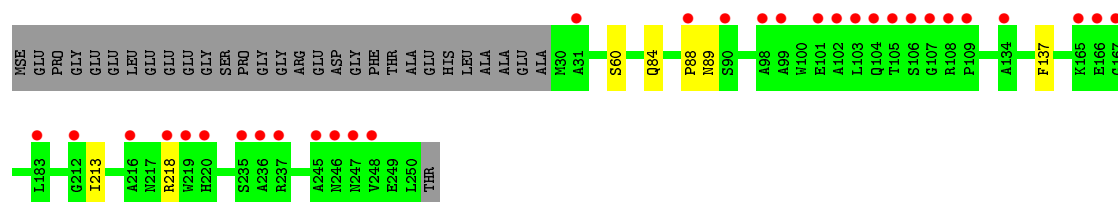
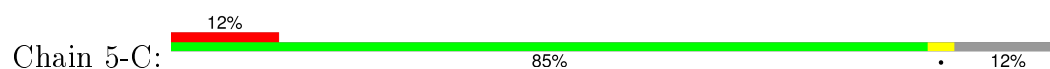
• Molecule 1: Uncharacterized protein C11orf68



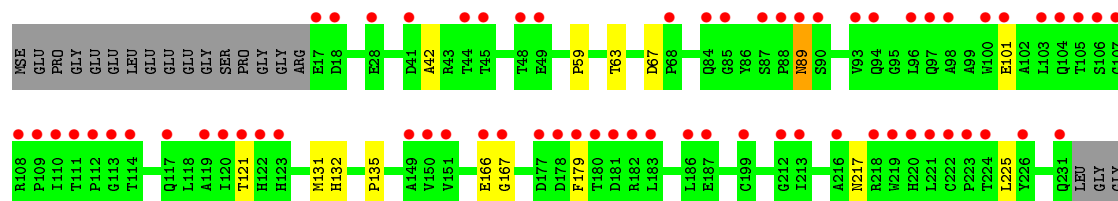
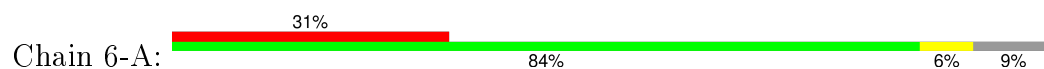
• Molecule 1: Uncharacterized protein C11orf68

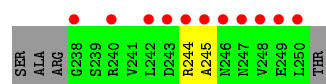


• Molecule 1: Uncharacterized protein C11orf68

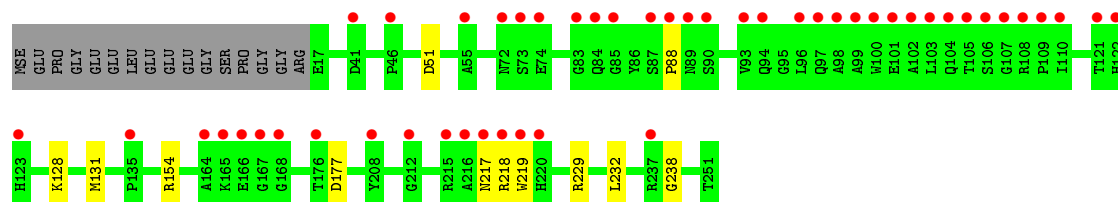
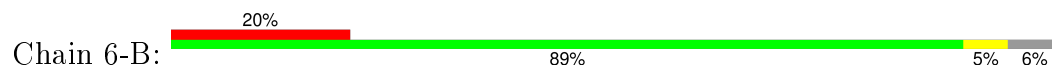


• Molecule 1: Uncharacterized protein C11orf68

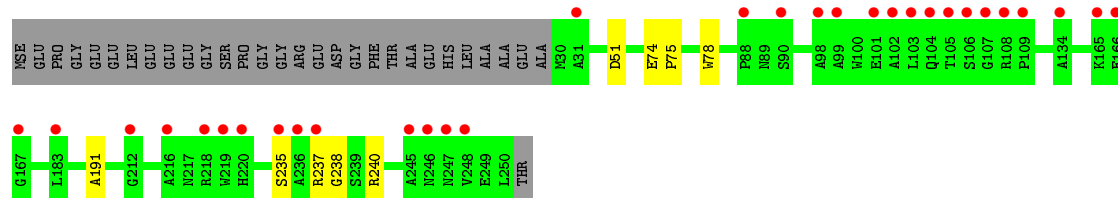
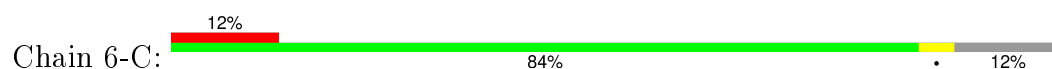




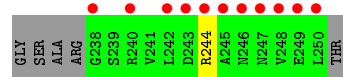
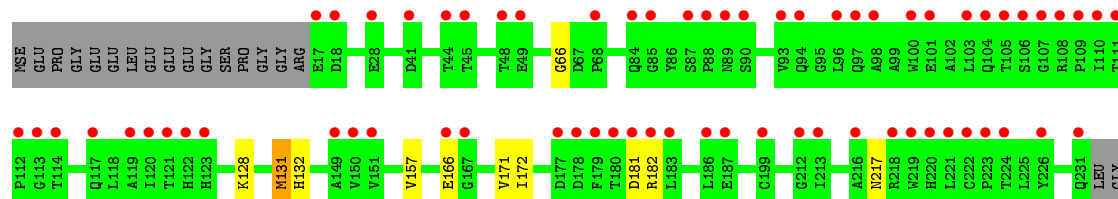
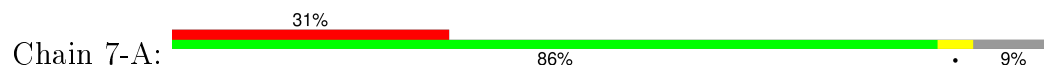
- Molecule 1: Uncharacterized protein C11orf68



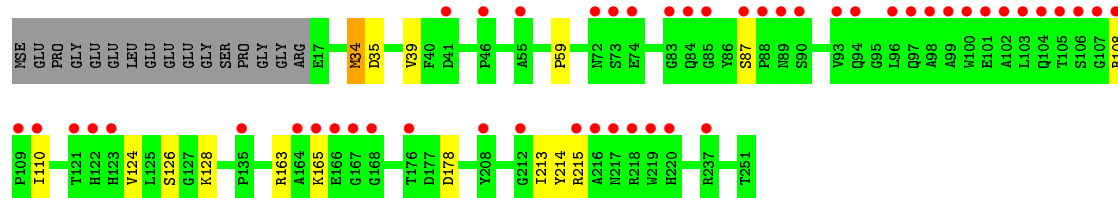
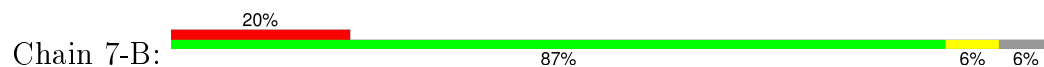
- Molecule 1: Uncharacterized protein C11orf68



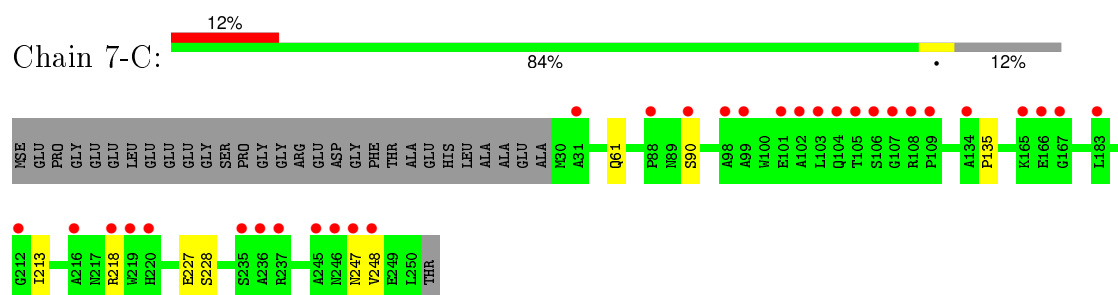
- Molecule 1: Uncharacterized protein C11orf68



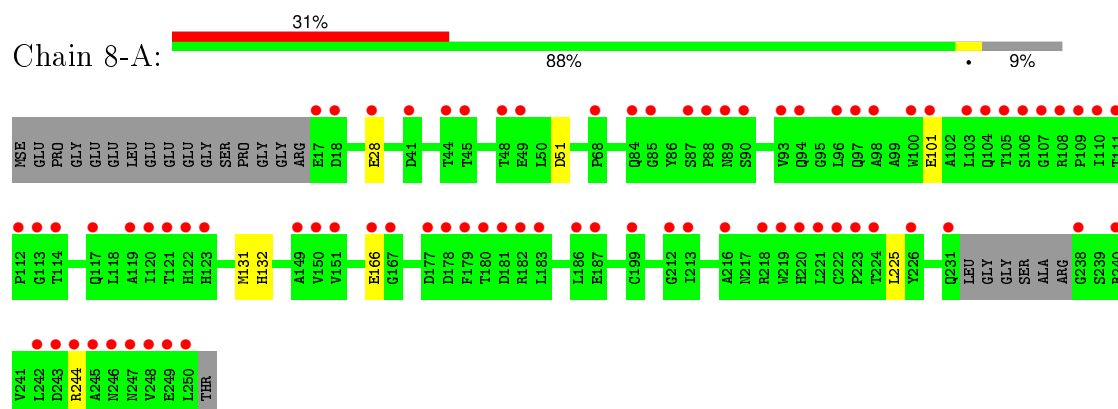
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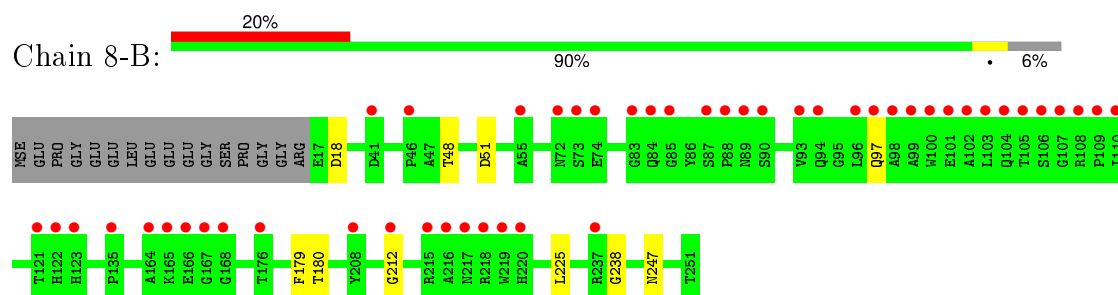
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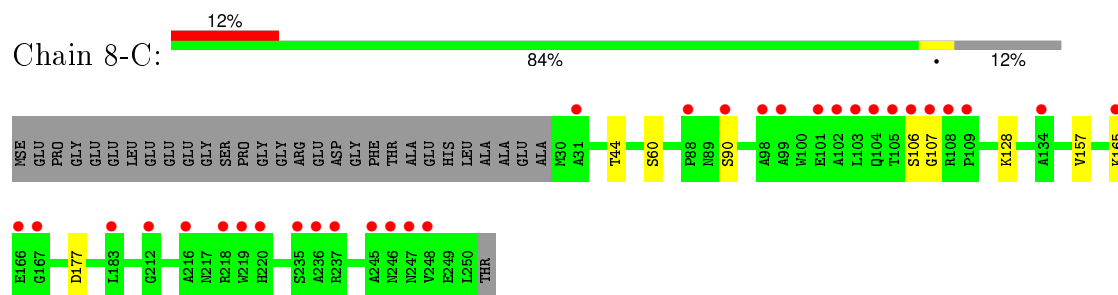
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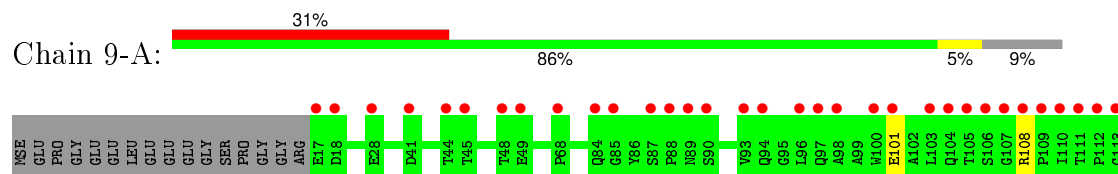
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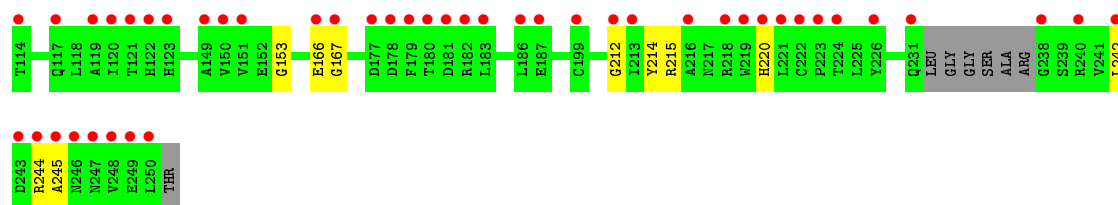
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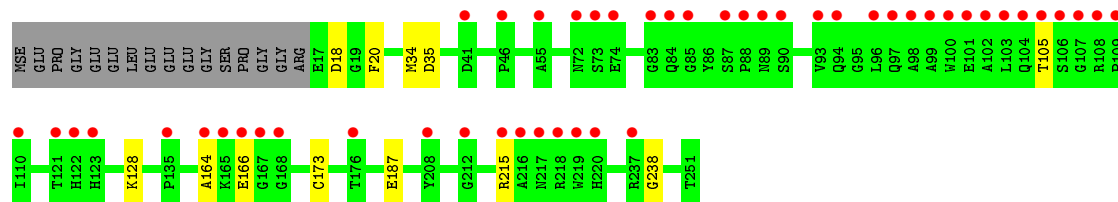
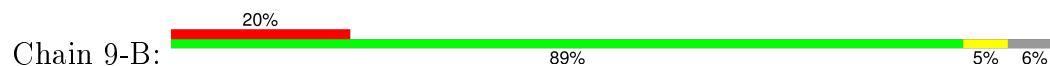
- Molecule 1: Uncharacterized protein C11orf68



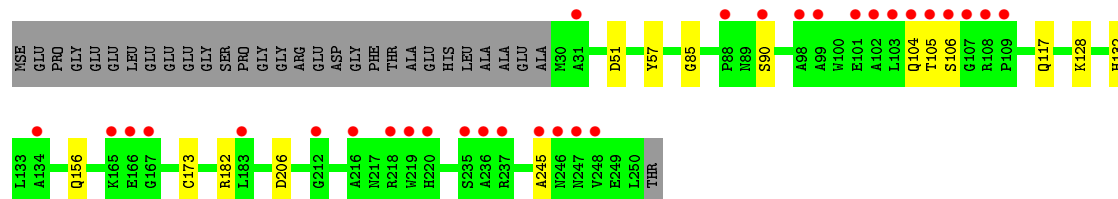
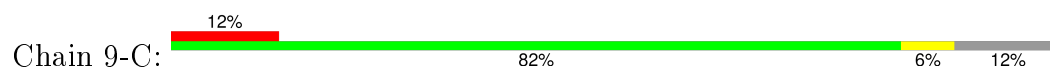




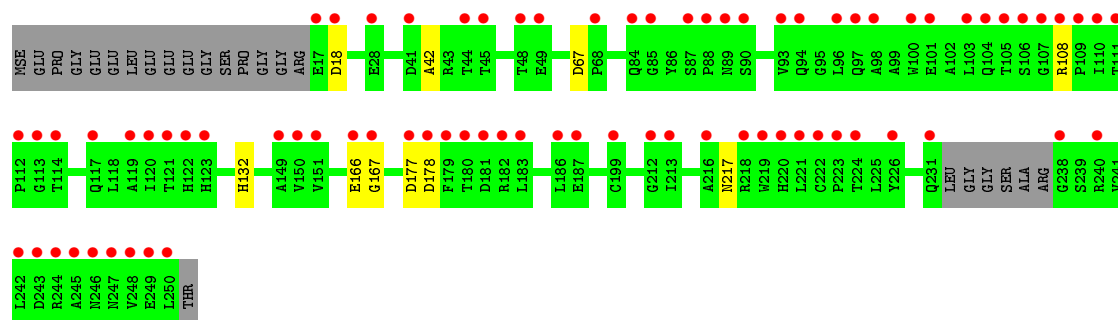
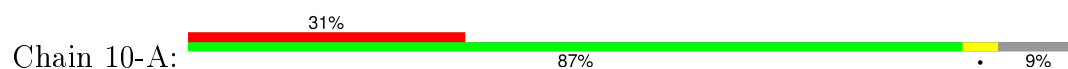
- Molecule 1: Uncharacterized protein C11orf68



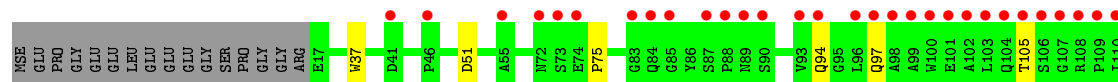
- Molecule 1: Uncharacterized protein C11orf68



- Molecule 1: Uncharacterized protein C11orf68

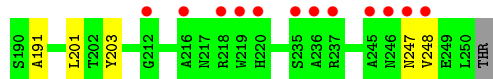
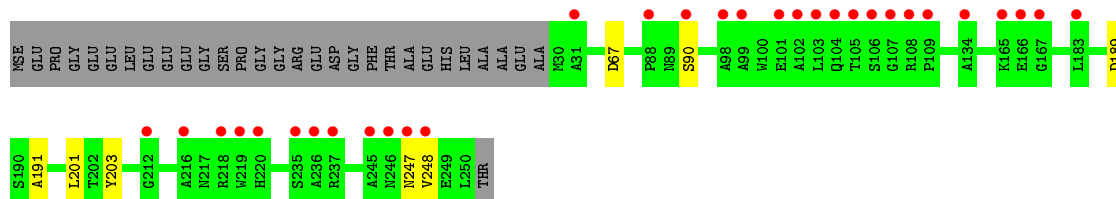
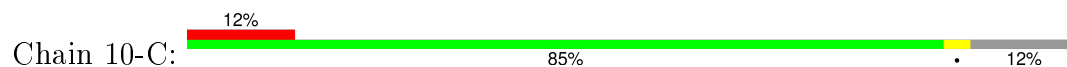


- Molecule 1: Uncharacterized protein C11orf68

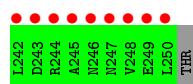
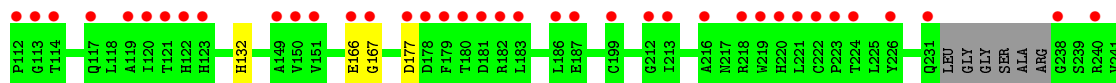
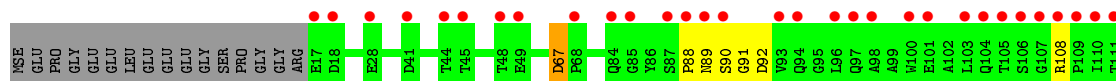
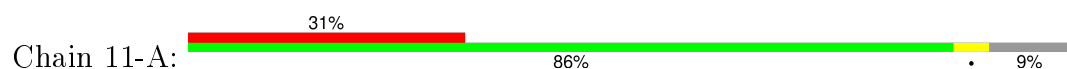




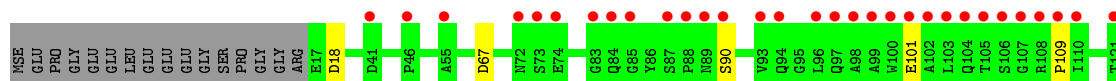
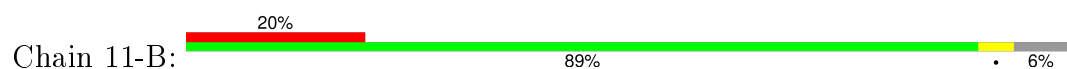
- Molecule 1: Uncharacterized protein C11orf68



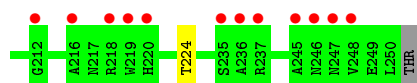
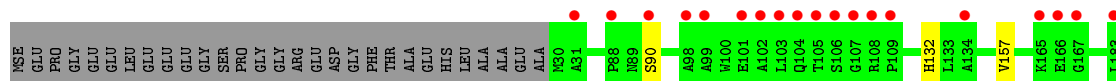
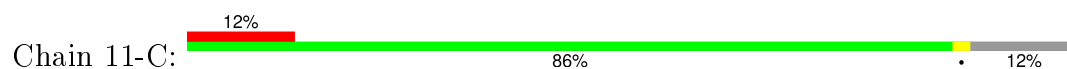
- Molecule 1: Uncharacterized protein C11orf68



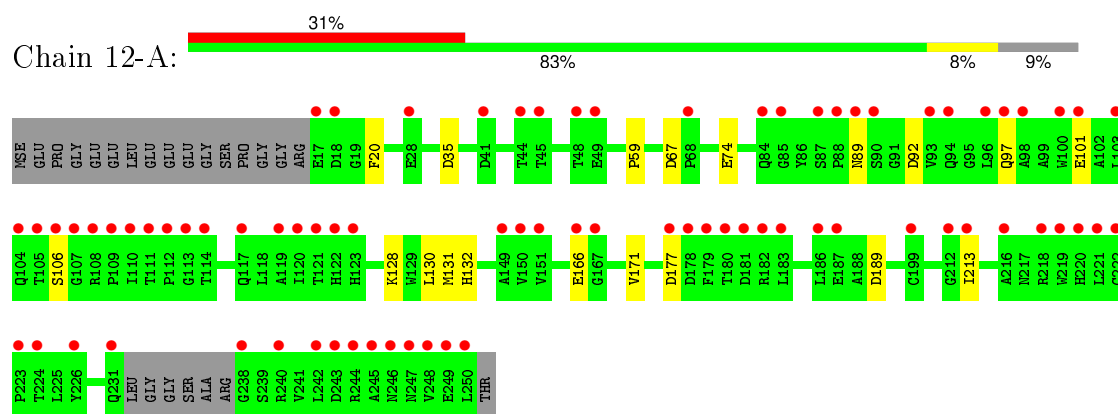
- Molecule 1: Uncharacterized protein C11orf68



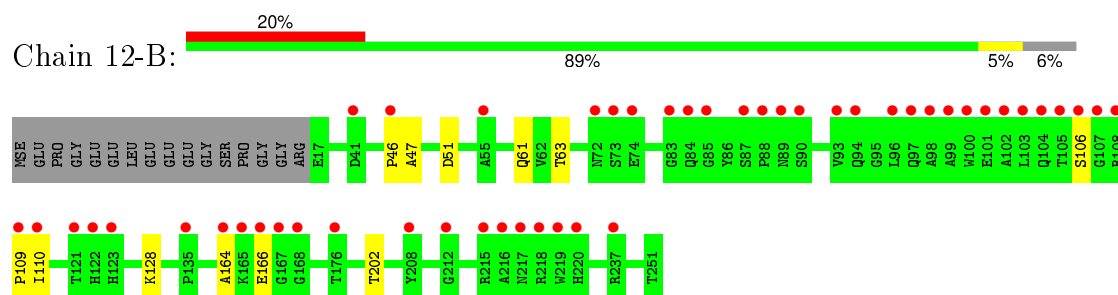
- Molecule 1: Uncharacterized protein C11orf68



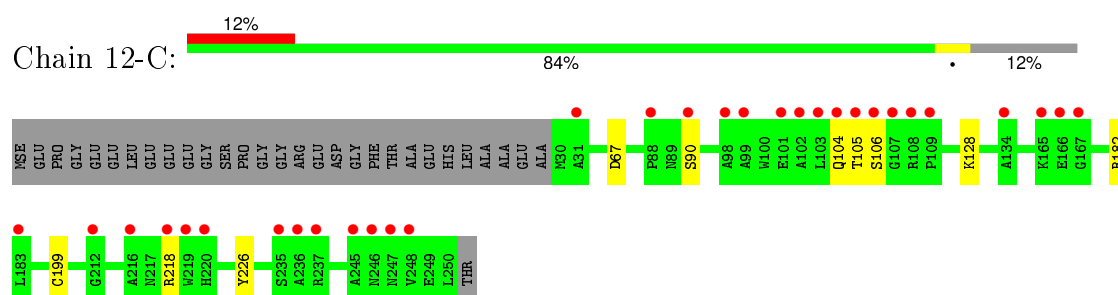
- Molecule 1: Uncharacterized protein C11orf68



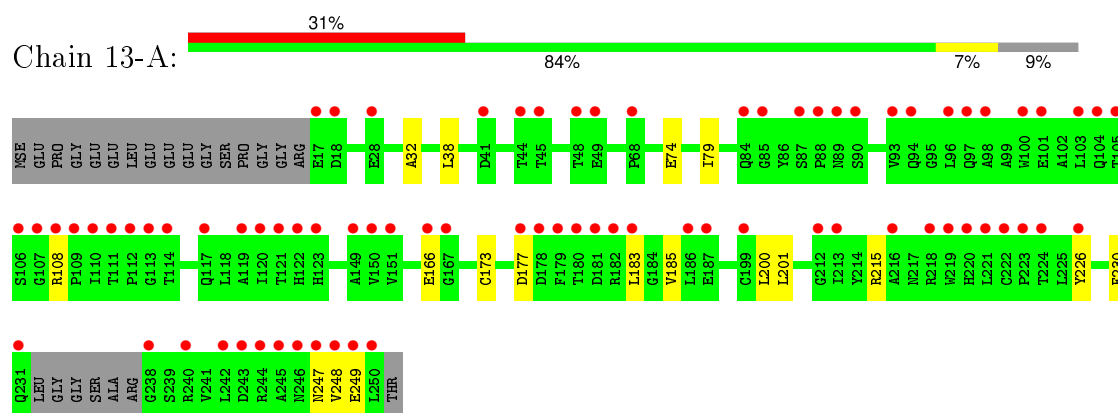
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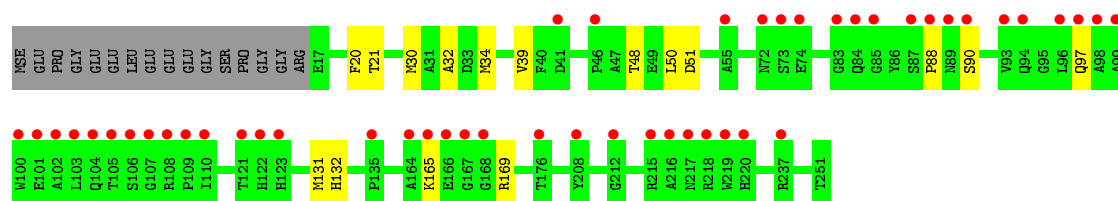


- Molecule 1: Uncharacterized protein C11orf68

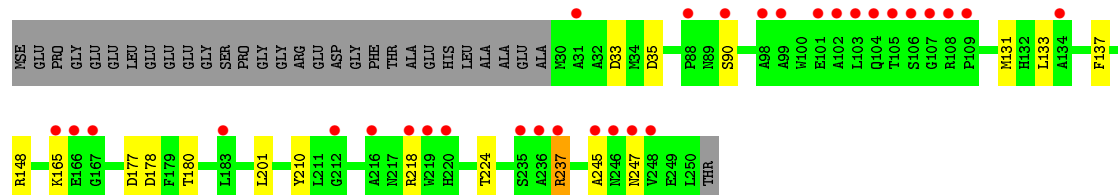
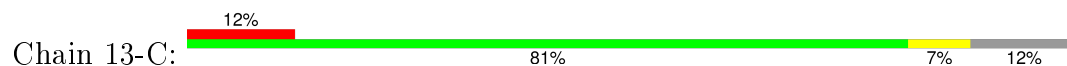


- Molecule 1: Uncharacterized protein C11orf68

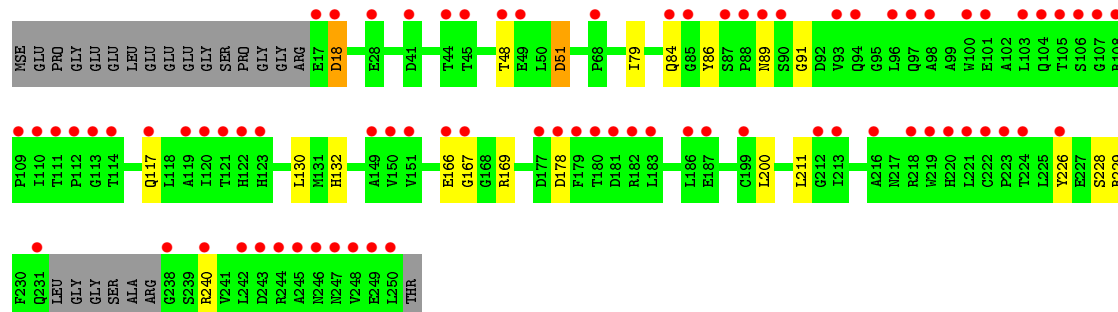
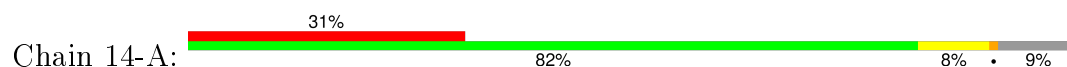




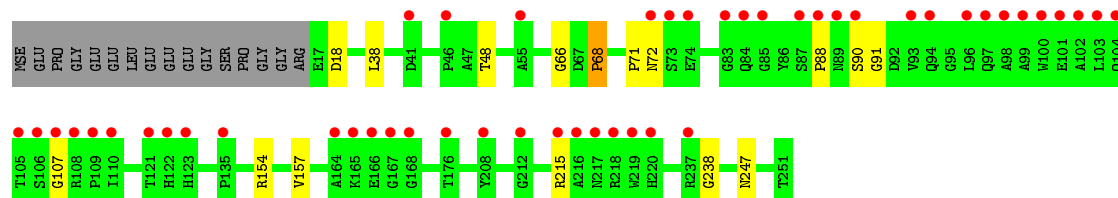
- Molecule 1: Uncharacterized protein C11orf68



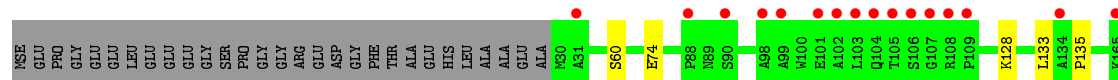
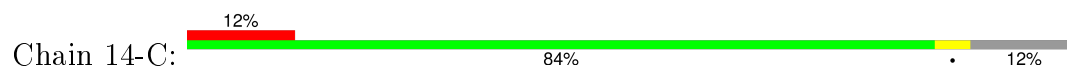
- Molecule 1: Uncharacterized protein C11orf68

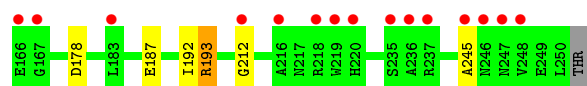


- Molecule 1: Uncharacterized protein C11orf68

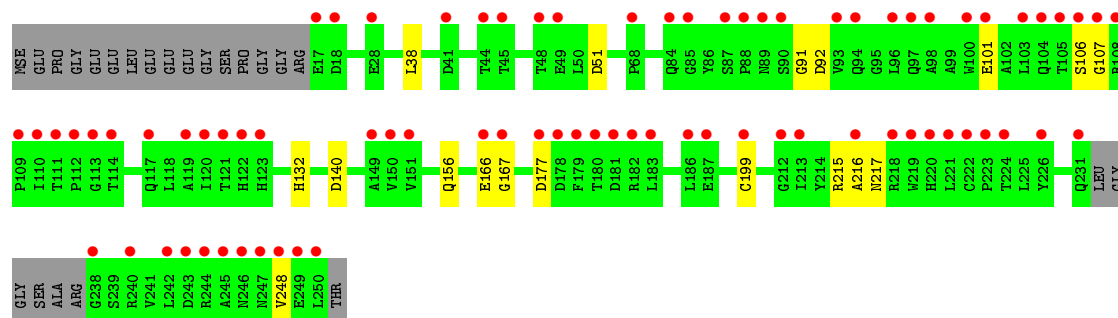
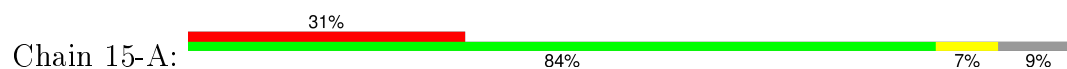


- Molecule 1: Uncharacterized protein C11orf68

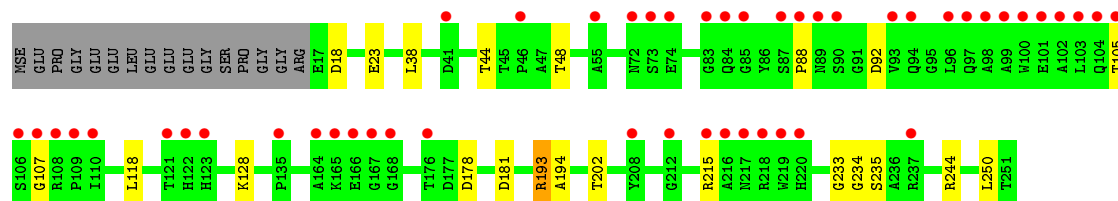
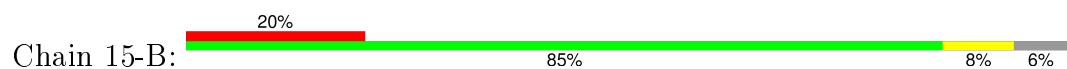




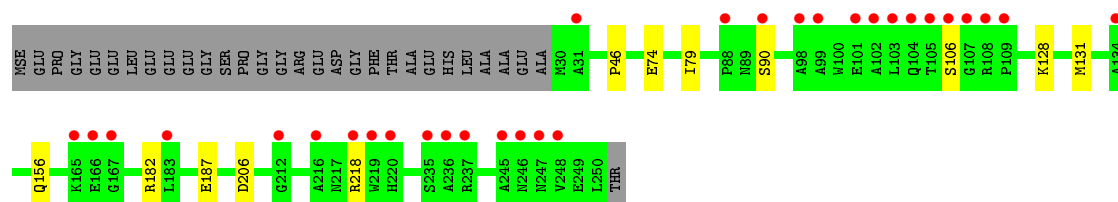
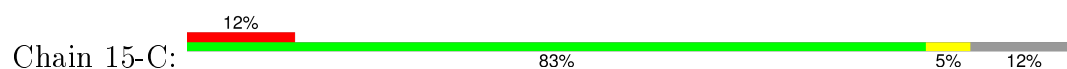
- Molecule 1: Uncharacterized protein C11orf68



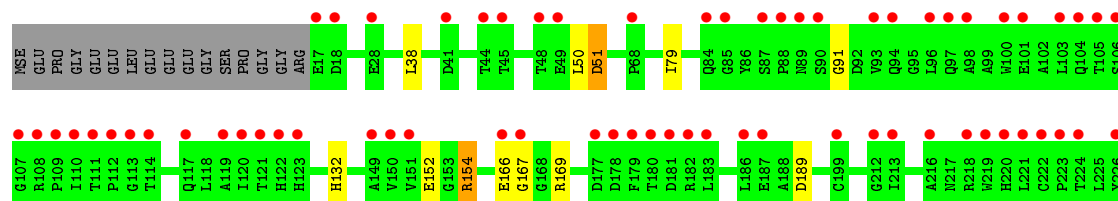
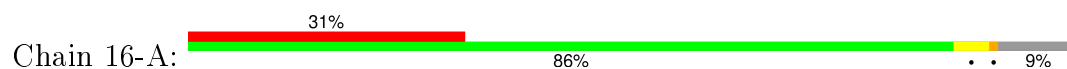
- Molecule 1: Uncharacterized protein C11orf68

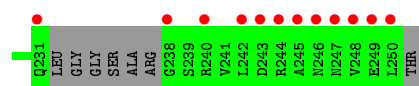


- Molecule 1: Uncharacterized protein C11orf68

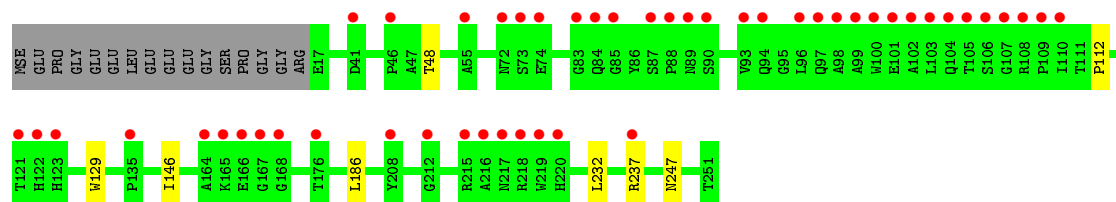


- Molecule 1: Uncharacterized protein C11orf68

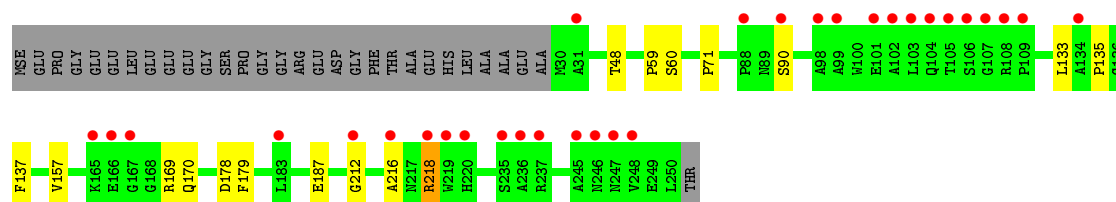
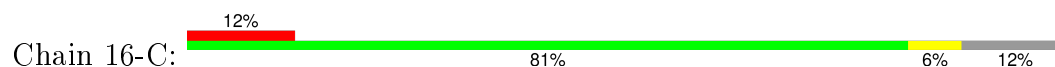




- Molecule 1: Uncharacterized protein C11orf68



- Molecule 1: Uncharacterized protein C11orf68



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.55Å 116.81Å 123.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.97 – 2.50 43.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.97-2.50) 97.8 (43.97-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.166 , 0.236 0.193 , 0.260	Depositor DCC
$R_{free}$ test set	1606 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 120.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 31489 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	88208	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.32	0/1813	0.56	1/2468 (0.0%)
1	1-B	0.35	0/1860	0.58	0/2531
1	1-C	0.35	0/1756	0.57	0/2392
1	2-A	0.31	0/1813	0.56	0/2468
1	2-B	0.34	0/1860	0.58	0/2531
1	2-C	0.35	0/1756	0.58	0/2392
1	3-A	0.31	0/1813	0.55	0/2468
1	3-B	0.35	0/1860	0.57	0/2531
1	3-C	0.34	0/1756	0.58	0/2392
1	4-A	0.32	0/1813	0.56	0/2468
1	4-B	0.34	0/1860	0.59	0/2531
1	4-C	0.36	0/1756	0.59	0/2392
1	5-A	0.32	0/1813	0.55	0/2468
1	5-B	0.34	0/1860	0.58	0/2531
1	5-C	0.35	0/1756	0.58	0/2392
1	6-A	0.32	0/1813	0.59	0/2468
1	6-B	0.34	0/1860	0.59	0/2531
1	6-C	0.35	0/1756	0.57	0/2392
1	7-A	0.32	0/1813	0.56	0/2468
1	7-B	0.34	0/1860	0.58	0/2531
1	7-C	0.36	0/1756	0.61	0/2392
1	8-A	0.32	0/1813	0.56	0/2468
1	8-B	0.34	0/1860	0.56	0/2531
1	8-C	0.35	0/1756	0.58	0/2392
1	9-A	0.32	0/1813	0.57	1/2468 (0.0%)
1	9-B	0.34	0/1860	0.57	0/2531
1	9-C	0.35	0/1756	0.59	0/2392
1	10-A	0.32	0/1813	0.56	0/2468
1	10-B	0.33	0/1860	0.58	0/2531
1	10-C	0.35	0/1756	0.59	0/2392
1	11-A	0.32	0/1813	0.57	0/2468
1	11-B	0.34	0/1860	0.57	0/2531
1	11-C	0.35	0/1756	0.57	0/2392
1	12-A	0.32	0/1813	0.58	0/2468



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	12-B	0.35	0/1860	0.59	0/2531
1	12-C	0.34	0/1756	0.60	0/2392
1	13-A	0.35	0/1813	0.61	1/2468 (0.0%)
1	13-B	0.38	0/1860	0.64	0/2531
1	13-C	0.39	0/1756	0.65	0/2392
1	14-A	0.35	0/1813	0.62	1/2468 (0.0%)
1	14-B	0.38	0/1860	0.65	1/2531 (0.0%)
1	14-C	0.39	0/1756	0.65	0/2392
1	15-A	0.35	0/1813	0.62	0/2468
1	15-B	0.38	0/1860	0.65	1/2531 (0.0%)
1	15-C	0.39	0/1756	0.66	1/2392 (0.0%)
1	16-A	0.35	0/1813	0.60	1/2468 (0.0%)
1	16-B	0.38	0/1860	0.62	0/2531
1	16-C	0.40	0/1756	0.66	0/2392
All	All	0.35	0/86864	0.59	8/118256 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	15-C	79	ILE	N-CA-C	-6.41	93.69	111.00
1	14-B	38	LEU	N-CA-C	-6.04	94.69	111.00
1	9-A	153	GLY	N-CA-C	5.67	127.26	113.10
1	16-A	79	ILE	N-CA-C	-5.44	96.31	111.00
1	14-A	79	ILE	N-CA-C	-5.41	96.41	111.00
1	1-A	79	ILE	N-CA-C	-5.31	96.66	111.00
1	15-B	38	LEU	N-CA-C	-5.29	96.71	111.00
1	13-A	79	ILE	N-CA-C	-5.20	96.97	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	1769	0	1722	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-B	1815	0	1770	0	0
1	1-C	1712	0	1684	0	0
1	2-A	1769	0	1722	0	0
1	2-B	1815	0	1770	0	0
1	2-C	1712	0	1684	0	0
1	3-A	1769	0	1722	0	0
1	3-B	1815	0	1770	0	0
1	3-C	1712	0	1684	0	0
1	4-A	1769	0	1722	0	0
1	4-B	1815	0	1770	0	0
1	4-C	1712	0	1684	0	0
1	5-A	1769	0	1722	0	0
1	5-B	1815	0	1770	0	0
1	5-C	1712	0	1684	0	0
1	6-A	1769	0	1722	0	0
1	6-B	1815	0	1770	0	0
1	6-C	1712	0	1684	0	0
1	7-A	1769	0	1722	0	0
1	7-B	1815	0	1770	0	0
1	7-C	1712	0	1684	0	0
1	8-A	1769	0	1722	0	0
1	8-B	1815	0	1770	0	0
1	8-C	1712	0	1684	0	0
1	9-A	1769	0	1722	0	0
1	9-B	1815	0	1770	0	0
1	9-C	1712	0	1684	0	0
1	10-A	1769	0	1722	0	0
1	10-B	1815	0	1770	0	0
1	10-C	1712	0	1684	0	0
1	11-A	1769	0	1722	0	0
1	11-B	1815	0	1770	0	0
1	11-C	1712	0	1684	0	0
1	12-A	1769	0	1722	0	0
1	12-B	1815	0	1770	0	0
1	12-C	1712	0	1684	0	0
1	13-A	1769	0	1722	0	0
1	13-B	1815	0	1770	0	0
1	13-C	1712	0	1684	0	0
1	14-A	1769	0	1722	0	0
1	14-B	1815	0	1770	0	0
1	14-C	1712	0	1684	0	0
1	15-A	1769	0	1722	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	15-B	1815	0	1770	0	0
1	15-C	1712	0	1684	0	0
1	16-A	1769	0	1722	0	0
1	16-B	1815	0	1770	0	0
1	16-C	1712	0	1684	0	0
2	1-A	50	0	0	0	0
2	1-B	91	0	0	0	0
2	1-C	76	0	0	0	0
2	2-A	55	0	0	0	0
2	2-B	88	0	0	0	0
2	2-C	74	0	0	0	0
2	3-A	56	0	0	0	0
2	3-B	88	0	0	0	0
2	3-C	73	0	0	0	0
2	4-A	55	0	0	0	0
2	4-B	90	0	0	0	0
2	4-C	72	0	0	0	0
2	5-A	55	0	0	0	0
2	5-B	89	0	0	0	0
2	5-C	73	0	0	0	0
2	6-A	56	0	0	0	0
2	6-B	89	0	0	0	0
2	6-C	72	0	0	0	0
2	7-A	54	0	0	0	0
2	7-B	89	0	0	0	0
2	7-C	74	0	0	0	0
2	8-A	56	0	0	0	0
2	8-B	88	0	0	0	0
2	8-C	73	0	0	0	0
2	9-A	57	0	0	0	0
2	9-B	88	0	0	0	0
2	9-C	72	0	0	0	0
2	10-A	56	0	0	0	0
2	10-B	88	0	0	0	0
2	10-C	73	0	0	0	0
2	11-A	58	0	0	0	0
2	11-B	87	0	0	0	0
2	11-C	72	0	0	0	0
2	12-A	55	0	0	0	0
2	12-B	87	0	0	0	0
2	12-C	75	0	0	0	0
2	13-A	53	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	13-B	91	0	0	0	0
2	13-C	73	0	0	0	0
2	14-A	56	0	0	0	0
2	14-B	87	0	0	0	0
2	14-C	74	0	0	0	0
2	15-A	53	0	0	0	0
2	15-B	91	0	0	0	0
2	15-C	73	0	0	0	0
2	16-A	53	0	0	0	0
2	16-B	91	0	0	0	0
2	16-C	73	0	0	0	0
All	All	88208	0	82816	0	0

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

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	224/251 (89%)	185 (83%)	27 (12%)	12 (5%)	2	2
1	1-B	233/251 (93%)	204 (88%)	19 (8%)	10 (4%)	3	4
1	1-C	219/251 (87%)	193 (88%)	20 (9%)	6 (3%)	6	9
1	2-A	224/251 (89%)	192 (86%)	28 (12%)	4 (2%)	11	18
1	2-B	233/251 (93%)	195 (84%)	28 (12%)	10 (4%)	3	4
1	2-C	219/251 (87%)	198 (90%)	18 (8%)	3 (1%)	14	24
1	3-A	224/251 (89%)	196 (88%)	25 (11%)	3 (1%)	15	26
1	3-B	233/251 (93%)	219 (94%)	12 (5%)	2 (1%)	21	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3-C	219/251 (87%)	202 (92%)	15 (7%)	2 (1%)	21	37
1	4-A	224/251 (89%)	197 (88%)	21 (9%)	6 (3%)	6	9
1	4-B	233/251 (93%)	205 (88%)	23 (10%)	5 (2%)	9	14
1	4-C	219/251 (87%)	186 (85%)	24 (11%)	9 (4%)	3	4
1	5-A	224/251 (89%)	178 (80%)	35 (16%)	11 (5%)	3	3
1	5-B	233/251 (93%)	203 (87%)	22 (9%)	8 (3%)	5	6
1	5-C	219/251 (87%)	201 (92%)	13 (6%)	5 (2%)	8	12
1	6-A	224/251 (89%)	189 (84%)	25 (11%)	10 (4%)	3	3
1	6-B	233/251 (93%)	210 (90%)	18 (8%)	5 (2%)	9	14
1	6-C	219/251 (87%)	200 (91%)	13 (6%)	6 (3%)	6	9
1	7-A	224/251 (89%)	185 (83%)	34 (15%)	5 (2%)	8	13
1	7-B	233/251 (93%)	195 (84%)	29 (12%)	9 (4%)	4	5
1	7-C	219/251 (87%)	192 (88%)	21 (10%)	6 (3%)	6	9
1	8-A	224/251 (89%)	202 (90%)	20 (9%)	2 (1%)	21	37
1	8-B	233/251 (93%)	214 (92%)	17 (7%)	2 (1%)	21	37
1	8-C	219/251 (87%)	199 (91%)	14 (6%)	6 (3%)	6	9
1	9-A	224/251 (89%)	200 (89%)	19 (8%)	5 (2%)	8	13
1	9-B	233/251 (93%)	207 (89%)	21 (9%)	5 (2%)	9	14
1	9-C	219/251 (87%)	193 (88%)	16 (7%)	10 (5%)	3	3
1	10-A	224/251 (89%)	202 (90%)	20 (9%)	2 (1%)	21	37
1	10-B	233/251 (93%)	211 (91%)	19 (8%)	3 (1%)	15	26
1	10-C	219/251 (87%)	198 (90%)	15 (7%)	6 (3%)	6	9
1	11-A	224/251 (89%)	199 (89%)	18 (8%)	7 (3%)	5	7
1	11-B	233/251 (93%)	209 (90%)	18 (8%)	6 (3%)	7	10
1	11-C	219/251 (87%)	203 (93%)	15 (7%)	1 (0%)	34	55
1	12-A	224/251 (89%)	188 (84%)	29 (13%)	7 (3%)	5	7
1	12-B	233/251 (93%)	199 (85%)	25 (11%)	9 (4%)	4	5
1	12-C	219/251 (87%)	197 (90%)	16 (7%)	6 (3%)	6	9
1	13-A	224/251 (89%)	193 (86%)	23 (10%)	8 (4%)	4	5
1	13-B	233/251 (93%)	208 (89%)	18 (8%)	7 (3%)	5	7
1	13-C	219/251 (87%)	187 (85%)	25 (11%)	7 (3%)	5	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	14-A	224/251 (89%)	181 (81%)	32 (14%)	11 (5%)	3	3
1	14-B	233/251 (93%)	194 (83%)	27 (12%)	12 (5%)	2	2
1	14-C	219/251 (87%)	184 (84%)	29 (13%)	6 (3%)	6	9
1	15-A	224/251 (89%)	188 (84%)	26 (12%)	10 (4%)	3	3
1	15-B	233/251 (93%)	195 (84%)	24 (10%)	14 (6%)	2	2
1	15-C	219/251 (87%)	189 (86%)	25 (11%)	5 (2%)	8	12
1	16-A	224/251 (89%)	193 (86%)	25 (11%)	6 (3%)	6	9
1	16-B	233/251 (93%)	207 (89%)	24 (10%)	2 (1%)	21	37
1	16-C	219/251 (87%)	196 (90%)	13 (6%)	10 (5%)	3	3
All	All	10816/12048 (90%)	9461 (88%)	1043 (10%)	312 (3%)	6	8

All (312) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	18	ASP
1	1-A	165	LYS
1	1-A	178	ASP
1	1-A	214	TYR
1	1-B	90	SER
1	1-C	90	SER
1	1-C	226	TYR
1	2-A	217	ASN
1	2-B	89	ASN
1	2-B	164	ALA
1	2-C	200	LEU
1	2-C	244	ARG
1	3-A	245	ALA
1	4-C	89	ASN
1	4-C	90	SER
1	5-A	80	ALA
1	5-B	233	GLY
1	6-A	63	THR
1	6-A	131	MSE
1	6-A	217	ASN
1	6-A	244	ARG
1	6-B	154	ARG
1	7-A	131	MSE
1	7-B	87	SER
1	7-B	178	ASP

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Mol	Chain	Res	Type
1	7-C	90	SER
1	7-C	135	PRO
1	8-C	90	SER
1	8-C	177	ASP
1	9-C	104	GLN
1	9-C	105	THR
1	9-C	206	ASP
1	10-C	90	SER
1	11-A	89	ASN
1	11-A	91	GLY
1	11-B	109	PRO
1	11-B	237	ARG
1	12-A	89	ASN
1	12-B	128	LYS
1	12-C	106	SER
1	13-C	90	SER
1	13-C	178	ASP
1	13-C	237	ARG
1	14-A	51	ASP
1	14-A	84	GLN
1	14-B	90	SER
1	14-B	215	ARG
1	14-C	135	PRO
1	15-A	92	ASP
1	15-A	167	GLY
1	15-B	88	PRO
1	15-B	194	ALA
1	15-B	234	GLY
1	15-B	235	SER
1	15-C	90	SER
1	16-A	152	GLU
1	16-B	237	ARG
1	16-C	90	SER
1	16-C	135	PRO
1	16-C	178	ASP
1	1-A	106	SER
1	1-A	167	GLY
1	1-A	212	GLY
1	1-B	64	ARG
1	1-B	65	TYR
1	1-B	69	GLY
1	1-B	71	PRO

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Mol	Chain	Res	Type
1	1-B	238	GLY
1	1-C	246	ASN
1	1-C	247	ASN
1	2-B	157	VAL
1	2-C	246	ASN
1	3-A	165	LYS
1	3-B	238	GLY
1	4-A	89	ASN
1	4-A	178	ASP
1	4-B	164	ALA
1	4-B	233	GLY
1	4-C	91	GLY
1	4-C	105	THR
1	5-A	79	ILE
1	5-A	89	ASN
1	5-A	91	GLY
1	5-A	217	ASN
1	5-B	217	ASN
1	5-B	219	TRP
1	5-B	234	GLY
1	5-B	245	ALA
1	5-C	89	ASN
1	6-A	42	ALA
1	6-A	89	ASN
1	6-A	167	GLY
1	6-A	245	ALA
1	6-B	219	TRP
1	6-C	191	ALA
1	6-C	238	GLY
1	7-A	66	GLY
1	7-A	172	ILE
1	7-A	244	ARG
1	7-B	126	SER
1	7-B	165	LYS
1	8-B	212	GLY
1	8-B	238	GLY
1	8-C	106	SER
1	9-A	215	ARG
1	9-A	220	HIS
1	9-B	238	GLY
1	10-A	167	GLY
1	10-C	189	ASP

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Mol	Chain	Res	Type
1	11-B	167	GLY
1	12-A	92	ASP
1	12-B	47	ALA
1	12-B	110	ILE
1	12-B	166	GLU
1	12-C	90	SER
1	12-C	104	GLN
1	12-C	105	THR
1	13-A	226	TYR
1	13-A	248	VAL
1	13-A	249	GLU
1	13-B	21	THR
1	13-B	169	ARG
1	13-C	165	LYS
1	14-A	18	ASP
1	14-A	86	TYR
1	14-A	211	LEU
1	14-B	66	GLY
1	14-B	68	PRO
1	14-B	154	ARG
1	14-B	157	VAL
1	14-B	238	GLY
1	14-C	178	ASP
1	14-C	192	ILE
1	15-A	91	GLY
1	15-A	140	ASP
1	15-A	156	GLN
1	15-A	248	VAL
1	15-B	105	THR
1	15-B	233	GLY
1	15-B	244	ARG
1	16-A	50	LEU
1	16-A	51	ASP
1	16-A	154	ARG
1	16-A	167	GLY
1	1-A	46	PRO
1	1-A	86	TYR
1	1-A	211	LEU
1	2-A	28	GLU
1	2-A	167	GLY
1	2-B	216	ALA
1	2-B	218	ARG

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Mol	Chain	Res	Type
1	3-A	89	ASN
1	3-C	246	ASN
1	4-A	51	ASP
1	4-A	167	GLY
1	4-B	126	SER
1	4-C	73	SER
1	4-C	92	ASP
1	5-A	77	GLY
1	5-A	214	TYR
1	5-B	232	LEU
1	7-B	34	MSE
1	7-C	213	ILE
1	7-C	247	ASN
1	7-C	248	VAL
1	8-A	28	GLU
1	9-A	245	ALA
1	9-B	105	THR
1	9-B	164	ALA
1	9-B	166	GLU
1	9-C	90	SER
1	9-C	245	ALA
1	10-B	216	ALA
1	10-C	191	ALA
1	11-A	167	GLY
1	11-B	90	SER
1	11-B	244	ARG
1	11-C	90	SER
1	12-C	218	ARG
1	13-A	183	LEU
1	13-A	247	ASN
1	13-B	32	ALA
1	13-B	90	SER
1	13-B	165	LYS
1	13-C	247	ASN
1	14-A	48	THR
1	14-A	89	ASN
1	14-A	117	GLN
1	14-B	71	PRO
1	14-B	72	ASN
1	14-B	91	GLY
1	14-C	212	GLY
1	15-A	107	GLY

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Mol	Chain	Res	Type
1	15-B	92	ASP
1	15-B	250	LEU
1	15-C	106	SER
1	16-C	59	PRO
1	16-C	179	PHE
1	16-C	218	ARG
1	1-A	94	GLN
1	1-C	225	LEU
1	2-B	90	SER
1	4-A	38	LEU
1	4-B	235	SER
1	4-C	59	PRO
1	4-C	212	GLY
1	5-A	19	GLY
1	5-B	87	SER
1	5-C	218	ARG
1	6-A	59	PRO
1	6-B	238	GLY
1	6-C	240	ARG
1	7-A	157	VAL
1	7-C	218	ARG
1	8-A	244	ARG
1	8-C	44	THR
1	9-B	215	ARG
1	9-C	106	SER
1	9-C	156	GLN
1	9-C	182	ARG
1	10-B	105	THR
1	11-A	92	ASP
1	12-B	61	GLN
1	12-C	182	ARG
1	13-B	50	LEU
1	13-C	218	ARG
1	13-C	245	ALA
1	14-A	91	GLY
1	14-C	245	ALA
1	15-A	106	SER
1	15-A	215	ARG
1	15-B	23	GLU
1	15-B	181	ASP
1	15-C	156	GLN
1	1-A	150	VAL

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Mol	Chain	Res	Type
1	1-B	105	THR
1	1-B	109	PRO
1	1-B	110	ILE
1	1-C	213	ILE
1	2-B	162	PRO
1	4-A	91	GLY
1	5-B	238	GLY
1	5-C	84	GLN
1	6-B	88	PRO
1	6-B	217	ASN
1	6-C	74	GLU
1	6-C	75	PRO
1	8-C	107	GLY
1	8-C	165	LYS
1	10-A	42	ALA
1	10-C	201	LEU
1	10-C	247	ASN
1	12-A	59	PRO
1	12-A	74	GLU
1	12-B	164	ALA
1	13-A	32	ALA
1	13-A	215	ARG
1	13-B	88	PRO
1	14-A	167	GLY
1	14-A	228	SER
1	14-B	107	GLY
1	15-A	216	ALA
1	15-B	215	ARG
1	16-C	48	THR
1	16-C	216	ALA
1	1-B	167	GLY
1	2-B	107	GLY
1	2-B	110	ILE
1	3-C	238	GLY
1	4-B	110	ILE
1	4-C	104	GLN
1	5-A	152	GLU
1	6-C	235	SER
1	11-A	88	PRO
1	11-A	90	SER
1	12-A	106	SER
1	12-A	131	MSE

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Mol	Chain	Res	Type
1	12-B	106	SER
1	14-C	193	ARG
1	15-B	193	ARG
1	15-C	182	ARG
1	2-A	223	PRO
1	2-B	88	PRO
1	3-B	110	ILE
1	5-A	153	GLY
1	7-B	35	ASP
1	7-B	124	VAL
1	9-C	57	TYR
1	9-C	85	GLY
1	11-A	67	ASP
1	11-B	238	GLY
1	12-B	46	PRO
1	15-C	46	PRO
1	16-C	71	PRO
1	5-A	167	GLY
1	5-C	88	PRO
1	7-B	59	PRO
1	9-A	167	GLY
1	9-A	212	GLY
1	12-A	213	ILE
1	12-B	109	PRO
1	5-C	213	ILE
1	7-B	213	ILE
1	10-C	248	VAL
1	14-B	88	PRO
1	16-B	112	PRO
1	16-C	212	GLY
1	6-A	135	PRO
1	10-B	75	PRO
1	13-A	185	VAL
1	15-B	107	GLY
1	16-A	91	GLY

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	180/192 (94%)	177 (98%)	3 (2%)	68	89
1	1-B	184/192 (96%)	175 (95%)	9 (5%)	31	55
1	1-C	175/192 (91%)	174 (99%)	1 (1%)	90	97
1	2-A	180/192 (94%)	177 (98%)	3 (2%)	68	89
1	2-B	184/192 (96%)	177 (96%)	7 (4%)	40	67
1	2-C	175/192 (91%)	170 (97%)	5 (3%)	50	77
1	3-A	180/192 (94%)	175 (97%)	5 (3%)	51	78
1	3-B	184/192 (96%)	179 (97%)	5 (3%)	52	79
1	3-C	175/192 (91%)	173 (99%)	2 (1%)	80	94
1	4-A	180/192 (94%)	175 (97%)	5 (3%)	51	78
1	4-B	184/192 (96%)	180 (98%)	4 (2%)	60	84
1	4-C	175/192 (91%)	172 (98%)	3 (2%)	68	89
1	5-A	180/192 (94%)	168 (93%)	12 (7%)	20	37
1	5-B	184/192 (96%)	180 (98%)	4 (2%)	60	84
1	5-C	175/192 (91%)	173 (99%)	2 (1%)	80	94
1	6-A	180/192 (94%)	172 (96%)	8 (4%)	35	60
1	6-B	184/192 (96%)	177 (96%)	7 (4%)	40	67
1	6-C	175/192 (91%)	172 (98%)	3 (2%)	68	89
1	7-A	180/192 (94%)	172 (96%)	8 (4%)	35	60
1	7-B	184/192 (96%)	176 (96%)	8 (4%)	35	61
1	7-C	175/192 (91%)	172 (98%)	3 (2%)	68	89
1	8-A	180/192 (94%)	174 (97%)	6 (3%)	45	73
1	8-B	184/192 (96%)	176 (96%)	8 (4%)	35	61
1	8-C	175/192 (91%)	172 (98%)	3 (2%)	68	89
1	9-A	180/192 (94%)	174 (97%)	6 (3%)	45	73
1	9-B	184/192 (96%)	177 (96%)	7 (4%)	40	67
1	9-C	175/192 (91%)	170 (97%)	5 (3%)	50	77
1	10-A	180/192 (94%)	172 (96%)	8 (4%)	35	60
1	10-B	184/192 (96%)	178 (97%)	6 (3%)	45	73
1	10-C	175/192 (91%)	173 (99%)	2 (1%)	80	94
1	11-A	180/192 (94%)	175 (97%)	5 (3%)	51	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	11-B	184/192 (96%)	179 (97%)	5 (3%)	52	79
1	11-C	175/192 (91%)	172 (98%)	3 (2%)	68	89
1	12-A	180/192 (94%)	168 (93%)	12 (7%)	20	37
1	12-B	184/192 (96%)	181 (98%)	3 (2%)	70	90
1	12-C	175/192 (91%)	171 (98%)	4 (2%)	58	83
1	13-A	180/192 (94%)	171 (95%)	9 (5%)	30	53
1	13-B	184/192 (96%)	175 (95%)	9 (5%)	31	55
1	13-C	175/192 (91%)	163 (93%)	12 (7%)	19	35
1	14-A	180/192 (94%)	169 (94%)	11 (6%)	23	42
1	14-B	184/192 (96%)	180 (98%)	4 (2%)	60	84
1	14-C	175/192 (91%)	169 (97%)	6 (3%)	44	72
1	15-A	180/192 (94%)	172 (96%)	8 (4%)	35	60
1	15-B	184/192 (96%)	176 (96%)	8 (4%)	35	61
1	15-C	175/192 (91%)	169 (97%)	6 (3%)	44	72
1	16-A	180/192 (94%)	173 (96%)	7 (4%)	39	66
1	16-B	184/192 (96%)	178 (97%)	6 (3%)	45	73
1	16-C	175/192 (91%)	167 (95%)	8 (5%)	33	57
All	All	8624/9216 (94%)	8340 (97%)	284 (3%)	45	73

All (284) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	51	ASP
1	1-A	101	GLU
1	1-A	108	ARG
1	1-B	35	ASP
1	1-B	49	GLU
1	1-B	84	GLN
1	1-B	97	GLN
1	1-B	101	GLU
1	1-B	178	ASP
1	1-B	187	GLU
1	1-B	225	LEU
1	1-B	247	ASN
1	1-C	179	PHE
1	2-A	108	ARG

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Mol	Chain	Res	Type
1	2-A	166	GLU
1	2-A	177	ASP
1	2-B	21	THR
1	2-B	92	ASP
1	2-B	128	LYS
1	2-B	157	VAL
1	2-B	187	GLU
1	2-B	218	ARG
1	2-B	244	ARG
1	2-C	117	GLN
1	2-C	128	LYS
1	2-C	177	ASP
1	2-C	201	LEU
1	2-C	248	VAL
1	3-A	38	LEU
1	3-A	74	GLU
1	3-A	132	HIS
1	3-A	177	ASP
1	3-A	242	LEU
1	3-B	18	ASP
1	3-B	97	GLN
1	3-B	128	LYS
1	3-B	131	MSE
1	3-B	202	THR
1	3-C	60	SER
1	3-C	89	ASN
1	4-A	51	ASP
1	4-A	128	LYS
1	4-A	166	GLU
1	4-A	217	ASN
1	4-A	218	ARG
1	4-B	18	ASP
1	4-B	74	GLU
1	4-B	101	GLU
1	4-B	128	LYS
1	4-C	35	ASP
1	4-C	49	GLU
1	4-C	189	ASP
1	5-A	30	MSE
1	5-A	51	ASP
1	5-A	74	GLU
1	5-A	108	ARG

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Mol	Chain	Res	Type
1	5-A	118	LEU
1	5-A	125	LEU
1	5-A	166	GLU
1	5-A	169	ARG
1	5-A	202	THR
1	5-A	208	TYR
1	5-A	217	ASN
1	5-A	225	LEU
1	5-B	18	ASP
1	5-B	51	ASP
1	5-B	179	PHE
1	5-B	249	GLU
1	5-C	60	SER
1	5-C	137	PHE
1	6-A	67	ASP
1	6-A	89	ASN
1	6-A	101	GLU
1	6-A	121	THR
1	6-A	132	HIS
1	6-A	166	GLU
1	6-A	179	PHE
1	6-A	225	LEU
1	6-B	51	ASP
1	6-B	128	LYS
1	6-B	131	MSE
1	6-B	177	ASP
1	6-B	218	ARG
1	6-B	229	ARG
1	6-B	232	LEU
1	6-C	51	ASP
1	6-C	78	TRP
1	6-C	237	ARG
1	7-A	128	LYS
1	7-A	131	MSE
1	7-A	132	HIS
1	7-A	166	GLU
1	7-A	171	VAL
1	7-A	181	ASP
1	7-A	182	ARG
1	7-A	217	ASN
1	7-B	34	MSE
1	7-B	39	VAL

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Mol	Chain	Res	Type
1	7-B	108	ARG
1	7-B	110	ILE
1	7-B	128	LYS
1	7-B	163	ARG
1	7-B	214	TYR
1	7-B	215	ARG
1	7-C	61	GLN
1	7-C	227	GLU
1	7-C	228	SER
1	8-A	51	ASP
1	8-A	101	GLU
1	8-A	131	MSE
1	8-A	132	HIS
1	8-A	166	GLU
1	8-A	225	LEU
1	8-B	18	ASP
1	8-B	48	THR
1	8-B	51	ASP
1	8-B	97	GLN
1	8-B	179	PHE
1	8-B	180	THR
1	8-B	225	LEU
1	8-B	247	ASN
1	8-C	60	SER
1	8-C	128	LYS
1	8-C	157	VAL
1	9-A	101	GLU
1	9-A	108	ARG
1	9-A	166	GLU
1	9-A	214	TYR
1	9-A	242	LEU
1	9-A	244	ARG
1	9-B	18	ASP
1	9-B	20	PHE
1	9-B	34	MSE
1	9-B	35	ASP
1	9-B	128	LYS
1	9-B	173	CYS
1	9-B	187	GLU
1	9-C	51	ASP
1	9-C	117	GLN
1	9-C	128	LYS

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Mol	Chain	Res	Type
1	9-C	132	HIS
1	9-C	173	CYS
1	10-A	18	ASP
1	10-A	67	ASP
1	10-A	108	ARG
1	10-A	132	HIS
1	10-A	166	GLU
1	10-A	177	ASP
1	10-A	178	ASP
1	10-A	217	ASN
1	10-B	37	TRP
1	10-B	51	ASP
1	10-B	94	GLN
1	10-B	97	GLN
1	10-B	128	LYS
1	10-B	177	ASP
1	10-C	67	ASP
1	10-C	203	TYR
1	11-A	67	ASP
1	11-A	108	ARG
1	11-A	132	HIS
1	11-A	166	GLU
1	11-A	177	ASP
1	11-B	18	ASP
1	11-B	67	ASP
1	11-B	101	GLU
1	11-B	177	ASP
1	11-B	220	HIS
1	11-C	132	HIS
1	11-C	157	VAL
1	11-C	224	THR
1	12-A	20	PHE
1	12-A	35	ASP
1	12-A	67	ASP
1	12-A	97	GLN
1	12-A	101	GLU
1	12-A	128	LYS
1	12-A	130	LEU
1	12-A	132	HIS
1	12-A	166	GLU
1	12-A	171	VAL
1	12-A	177	ASP

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Mol	Chain	Res	Type
1	12-A	189	ASP
1	12-B	51	ASP
1	12-B	63	THR
1	12-B	202	THR
1	12-C	67	ASP
1	12-C	128	LYS
1	12-C	199	CYS
1	12-C	226	TYR
1	13-A	38	LEU
1	13-A	74	GLU
1	13-A	108	ARG
1	13-A	166	GLU
1	13-A	173	CYS
1	13-A	177	ASP
1	13-A	200	LEU
1	13-A	201	LEU
1	13-A	230	PHE
1	13-B	20	PHE
1	13-B	30	MSE
1	13-B	34	MSE
1	13-B	39	VAL
1	13-B	48	THR
1	13-B	51	ASP
1	13-B	97	GLN
1	13-B	131	MSE
1	13-B	132	HIS
1	13-C	33	ASP
1	13-C	35	ASP
1	13-C	131	MSE
1	13-C	133	LEU
1	13-C	137	PHE
1	13-C	148	ARG
1	13-C	177	ASP
1	13-C	180	THR
1	13-C	201	LEU
1	13-C	210	TYR
1	13-C	224	THR
1	13-C	237	ARG
1	14-A	18	ASP
1	14-A	51	ASP
1	14-A	130	LEU
1	14-A	132	HIS

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Mol	Chain	Res	Type
1	14-A	166	GLU
1	14-A	169	ARG
1	14-A	178	ASP
1	14-A	200	LEU
1	14-A	226	TYR
1	14-A	229	ARG
1	14-A	240	ARG
1	14-B	18	ASP
1	14-B	48	THR
1	14-B	68	PRO
1	14-B	247	ASN
1	14-C	60	SER
1	14-C	74	GLU
1	14-C	128	LYS
1	14-C	133	LEU
1	14-C	187	GLU
1	14-C	193	ARG
1	15-A	38	LEU
1	15-A	51	ASP
1	15-A	101	GLU
1	15-A	132	HIS
1	15-A	166	GLU
1	15-A	177	ASP
1	15-A	199	CYS
1	15-A	217	ASN
1	15-B	18	ASP
1	15-B	44	THR
1	15-B	48	THR
1	15-B	118	LEU
1	15-B	128	LYS
1	15-B	178	ASP
1	15-B	193	ARG
1	15-B	202	THR
1	15-C	74	GLU
1	15-C	128	LYS
1	15-C	131	MSE
1	15-C	187	GLU
1	15-C	206	ASP
1	15-C	218	ARG
1	16-A	38	LEU
1	16-A	51	ASP
1	16-A	132	HIS

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Mol	Chain	Res	Type
1	16-A	154	ARG
1	16-A	166	GLU
1	16-A	169	ARG
1	16-A	189	ASP
1	16-B	48	THR
1	16-B	129	TRP
1	16-B	146	ILE
1	16-B	186	LEU
1	16-B	232	LEU
1	16-B	247	ASN
1	16-C	60	SER
1	16-C	133	LEU
1	16-C	137	PHE
1	16-C	157	VAL
1	16-C	169	ARG
1	16-C	170	GLN
1	16-C	187	GLU
1	16-C	218	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	84	GLN
1	1-A	104	GLN
1	1-A	156	GLN
1	1-A	170	GLN
1	1-A	220	HIS
1	1-B	84	GLN
1	1-B	89	ASN
1	1-B	94	GLN
1	1-B	117	GLN
1	1-B	156	GLN
1	1-B	170	GLN
1	1-B	247	ASN
1	1-C	61	GLN
1	1-C	84	GLN
1	1-C	104	GLN
1	2-A	61	GLN
1	2-A	156	GLN
1	2-A	247	ASN
1	2-B	117	GLN
1	2-B	156	GLN

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Mol	Chain	Res	Type
1	2-B	247	ASN
1	2-C	117	GLN
1	2-C	231	GLN
1	3-A	61	GLN
1	3-B	156	GLN
1	3-B	247	ASN
1	3-C	231	GLN
1	3-C	247	ASN
1	4-A	61	GLN
1	4-A	84	GLN
1	4-A	117	GLN
1	4-B	117	GLN
1	4-B	156	GLN
1	4-B	231	GLN
1	4-C	61	GLN
1	4-C	84	GLN
1	4-C	104	GLN
1	4-C	122	HIS
1	4-C	123	HIS
1	4-C	231	GLN
1	4-C	246	ASN
1	4-C	247	ASN
1	5-A	61	GLN
1	5-A	220	HIS
1	5-A	247	ASN
1	5-B	104	GLN
1	5-B	231	GLN
1	5-B	247	ASN
1	5-C	89	ASN
1	5-C	247	ASN
1	6-A	61	GLN
1	6-A	89	ASN
1	6-A	156	GLN
1	6-A	231	GLN
1	6-A	247	ASN
1	6-C	123	HIS
1	6-C	132	HIS
1	6-C	231	GLN
1	6-C	246	ASN
1	7-A	246	ASN
1	7-A	247	ASN
1	7-B	97	GLN

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Mol	Chain	Res	Type
1	7-B	117	GLN
1	7-B	122	HIS
1	7-B	156	GLN
1	7-C	61	GLN
1	7-C	94	GLN
1	7-C	97	GLN
1	8-A	24	HIS
1	8-A	61	GLN
1	8-A	156	GLN
1	8-A	247	ASN
1	8-B	156	GLN
1	8-B	170	GLN
1	8-B	247	ASN
1	9-A	61	GLN
1	9-A	122	HIS
1	9-A	231	GLN
1	9-B	84	GLN
1	9-B	104	GLN
1	9-B	156	GLN
1	9-B	170	GLN
1	9-C	61	GLN
1	9-C	89	ASN
1	9-C	104	GLN
1	9-C	117	GLN
1	10-A	61	GLN
1	10-A	231	GLN
1	10-B	84	GLN
1	10-B	94	GLN
1	10-B	117	GLN
1	10-B	156	GLN
1	10-C	123	HIS
1	11-A	61	GLN
1	11-A	247	ASN
1	11-C	104	GLN
1	11-C	231	GLN
1	11-C	246	ASN
1	12-A	84	GLN
1	12-A	97	GLN
1	12-A	246	ASN
1	12-B	84	GLN
1	12-B	117	GLN
1	12-B	156	GLN

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Mol	Chain	Res	Type
1	12-B	231	GLN
1	12-B	247	ASN
1	12-C	89	ASN
1	12-C	104	GLN
1	12-C	141	HIS
1	12-C	156	GLN
1	12-C	246	ASN
1	13-A	156	GLN
1	13-B	156	GLN
1	13-B	247	ASN
1	13-C	123	HIS
1	13-C	231	GLN
1	14-A	117	GLN
1	14-A	217	ASN
1	14-A	231	GLN
1	14-A	247	ASN
1	14-B	122	HIS
1	14-B	231	GLN
1	14-B	247	ASN
1	14-C	61	GLN
1	14-C	246	ASN
1	15-A	170	GLN
1	15-B	141	HIS
1	15-C	156	GLN
1	15-C	246	ASN
1	15-C	247	ASN
1	16-A	117	GLN
1	16-B	89	ASN
1	16-B	104	GLN
1	16-B	117	GLN
1	16-B	170	GLN
1	16-B	247	ASN
1	16-C	61	GLN
1	16-C	141	HIS
1	16-C	156	GLN
1	16-C	170	GLN
1	16-C	231	GLN
1	16-C	246	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1-A	225/251 (89%)	1.60	78 (34%) 0 0	17, 40, 75, 91	225 (100%)
1	1-B	232/251 (92%)	1.12	49 (21%) 1 1	17, 33, 68, 85	232 (100%)
1	1-C	218/251 (86%)	0.85	31 (14%) 4 3	8, 29, 65, 84	218 (100%)
1	2-A	225/251 (89%)	1.60	78 (34%) 0 0	17, 40, 75, 91	225 (100%)
1	2-B	232/251 (92%)	1.12	49 (21%) 1 1	17, 33, 68, 85	232 (100%)
1	2-C	218/251 (86%)	0.85	31 (14%) 4 3	8, 29, 65, 84	218 (100%)
1	3-A	225/251 (89%)	1.60	78 (34%) 0 0	17, 40, 75, 91	225 (100%)
1	3-B	232/251 (92%)	1.12	49 (21%) 1 1	17, 33, 68, 85	232 (100%)
1	3-C	218/251 (86%)	0.85	31 (14%) 4 3	8, 29, 65, 84	218 (100%)
1	4-A	225/251 (89%)	1.60	78 (34%) 0 0	17, 40, 75, 91	225 (100%)
1	4-B	232/251 (92%)	1.12	49 (21%) 1 1	17, 33, 68, 85	232 (100%)
1	4-C	218/251 (86%)	0.85	31 (14%) 4 3	8, 29, 65, 84	218 (100%)
1	5-A	225/251 (89%)	1.60	78 (34%) 0 0	17, 40, 75, 91	225 (100%)
1	5-B	232/251 (92%)	1.12	49 (21%) 1 1	17, 33, 68, 85	232 (100%)
1	5-C	218/251 (86%)	0.85	31 (14%) 4 3	8, 29, 65, 84	218 (100%)
1	6-A	225/251 (89%)	1.60	78 (34%) 0 0	17, 40, 75, 91	225 (100%)
1	6-B	232/251 (92%)	1.12	49 (21%) 1 1	17, 33, 68, 85	232 (100%)
1	6-C	218/251 (86%)	0.85	31 (14%) 4 3	8, 29, 65, 84	218 (100%)
1	7-A	225/251 (89%)	1.60	78 (34%) 0 0	17, 40, 75, 91	225 (100%)
1	7-B	232/251 (92%)	1.12	49 (21%) 1 1	17, 33, 68, 85	232 (100%)
1	7-C	218/251 (86%)	0.85	31 (14%) 4 3	8, 29, 65, 84	218 (100%)
1	8-A	225/251 (89%)	1.60	78 (34%) 0 0	17, 40, 75, 91	225 (100%)
1	8-B	232/251 (92%)	1.12	49 (21%) 1 1	17, 33, 68, 85	232 (100%)
1	8-C	218/251 (86%)	0.85	31 (14%) 4 3	8, 29, 65, 84	218 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9	
1	9-A	225/251 (89%)	1.60	78 (34%)	0 0	17, 40, 75, 91	225 (100%)
1	9-B	232/251 (92%)	1.12	49 (21%)	1 1	17, 33, 68, 85	232 (100%)
1	9-C	218/251 (86%)	0.85	31 (14%)	4 3	8, 29, 65, 84	218 (100%)
1	10-A	225/251 (89%)	1.60	78 (34%)	0 0	17, 40, 75, 91	225 (100%)
1	10-B	232/251 (92%)	1.12	49 (21%)	1 1	17, 33, 68, 85	232 (100%)
1	10-C	218/251 (86%)	0.85	31 (14%)	4 3	8, 29, 65, 84	218 (100%)
1	11-A	225/251 (89%)	1.60	78 (34%)	0 0	17, 40, 75, 91	225 (100%)
1	11-B	232/251 (92%)	1.12	49 (21%)	1 1	17, 33, 68, 85	232 (100%)
1	11-C	218/251 (86%)	0.85	31 (14%)	4 3	8, 29, 65, 84	218 (100%)
1	12-A	225/251 (89%)	1.60	78 (34%)	0 0	17, 40, 75, 91	225 (100%)
1	12-B	232/251 (92%)	1.12	49 (21%)	1 1	17, 33, 68, 85	232 (100%)
1	12-C	218/251 (86%)	0.85	31 (14%)	4 3	8, 29, 65, 84	218 (100%)
1	13-A	225/251 (89%)	1.60	78 (34%)	0 0	17, 40, 75, 91	225 (100%)
1	13-B	232/251 (92%)	1.12	49 (21%)	1 1	17, 33, 68, 85	232 (100%)
1	13-C	218/251 (86%)	0.85	31 (14%)	4 3	8, 29, 65, 84	218 (100%)
1	14-A	225/251 (89%)	1.60	78 (34%)	0 0	17, 40, 75, 91	225 (100%)
1	14-B	232/251 (92%)	1.12	49 (21%)	1 1	17, 33, 68, 85	232 (100%)
1	14-C	218/251 (86%)	0.85	31 (14%)	4 3	8, 29, 65, 84	218 (100%)
1	15-A	225/251 (89%)	1.60	78 (34%)	0 0	17, 40, 75, 91	225 (100%)
1	15-B	232/251 (92%)	1.12	49 (21%)	1 1	17, 33, 68, 85	232 (100%)
1	15-C	218/251 (86%)	0.85	31 (14%)	4 3	8, 29, 65, 84	218 (100%)
1	16-A	225/251 (89%)	1.60	78 (34%)	0 0	17, 40, 75, 91	225 (100%)
1	16-B	232/251 (92%)	1.12	49 (21%)	1 1	17, 33, 68, 85	232 (100%)
1	16-C	218/251 (86%)	0.85	31 (14%)	4 3	8, 29, 65, 84	218 (100%)
All	All	10800/12048 (89%)	1.19	2528 (23%)	1 1	8, 34, 72, 91	10800 (100%)

All (2528) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-C	105	THR	11.6
1	2-C	105	THR	11.6
1	3-C	105	THR	11.6
1	4-C	105	THR	11.6
1	5-C	105	THR	11.6

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Mol	Chain	Res	Type	RSRZ
1	6-C	105	THR	11.6
1	7-C	105	THR	11.6
1	8-C	105	THR	11.6
1	9-C	105	THR	11.6
1	10-C	105	THR	11.6
1	11-C	105	THR	11.6
1	12-C	105	THR	11.6
1	13-C	105	THR	11.6
1	14-C	105	THR	11.6
1	15-C	105	THR	11.6
1	16-C	105	THR	11.6
1	1-A	248	VAL	10.5
1	2-A	248	VAL	10.5
1	3-A	248	VAL	10.5
1	4-A	248	VAL	10.5
1	5-A	248	VAL	10.5
1	6-A	248	VAL	10.5
1	7-A	248	VAL	10.5
1	8-A	248	VAL	10.5
1	9-A	248	VAL	10.5
1	10-A	248	VAL	10.5
1	11-A	248	VAL	10.5
1	12-A	248	VAL	10.5
1	13-A	248	VAL	10.5
1	14-A	248	VAL	10.5
1	15-A	248	VAL	10.5
1	16-A	248	VAL	10.5
1	1-B	89	ASN	10.1
1	2-B	89	ASN	10.1
1	3-B	89	ASN	10.1
1	4-B	89	ASN	10.1
1	5-B	89	ASN	10.1
1	6-B	89	ASN	10.1
1	7-B	89	ASN	10.1
1	8-B	89	ASN	10.1
1	9-B	89	ASN	10.1
1	10-B	89	ASN	10.1
1	11-B	89	ASN	10.1
1	12-B	89	ASN	10.1
1	13-B	89	ASN	10.1
1	14-B	89	ASN	10.1
1	15-B	89	ASN	10.1

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Mol	Chain	Res	Type	RSRZ
1	16-B	89	ASN	10.1
1	1-B	105	THR	9.4
1	2-B	105	THR	9.4
1	3-B	105	THR	9.4
1	4-B	105	THR	9.4
1	5-B	105	THR	9.4
1	6-B	105	THR	9.4
1	7-B	105	THR	9.4
1	8-B	105	THR	9.4
1	9-B	105	THR	9.4
1	10-B	105	THR	9.4
1	11-B	105	THR	9.4
1	12-B	105	THR	9.4
1	13-B	105	THR	9.4
1	14-B	105	THR	9.4
1	15-B	105	THR	9.4
1	16-B	105	THR	9.4
1	1-A	105	THR	9.4
1	2-A	105	THR	9.4
1	3-A	105	THR	9.4
1	4-A	105	THR	9.4
1	5-A	105	THR	9.4
1	6-A	105	THR	9.4
1	7-A	105	THR	9.4
1	8-A	105	THR	9.4
1	9-A	105	THR	9.4
1	10-A	105	THR	9.4
1	11-A	105	THR	9.4
1	12-A	105	THR	9.4
1	13-A	105	THR	9.4
1	14-A	105	THR	9.4
1	15-A	105	THR	9.4
1	16-A	105	THR	9.4
1	1-C	107	GLY	8.5
1	2-C	107	GLY	8.5
1	3-C	107	GLY	8.5
1	4-C	107	GLY	8.5
1	5-C	107	GLY	8.5
1	6-C	107	GLY	8.5
1	7-C	107	GLY	8.5
1	8-C	107	GLY	8.5
1	9-C	107	GLY	8.5

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Mol	Chain	Res	Type	RSRZ
1	10-C	107	GLY	8.5
1	11-C	107	GLY	8.5
1	12-C	107	GLY	8.5
1	13-C	107	GLY	8.5
1	14-C	107	GLY	8.5
1	15-C	107	GLY	8.5
1	16-C	107	GLY	8.5
1	1-C	245	ALA	8.1
1	2-C	245	ALA	8.1
1	3-C	245	ALA	8.1
1	4-C	245	ALA	8.1
1	5-C	245	ALA	8.1
1	6-C	245	ALA	8.1
1	7-C	245	ALA	8.1
1	8-C	245	ALA	8.1
1	9-C	245	ALA	8.1
1	10-C	245	ALA	8.1
1	11-C	245	ALA	8.1
1	12-C	245	ALA	8.1
1	13-C	245	ALA	8.1
1	14-C	245	ALA	8.1
1	15-C	245	ALA	8.1
1	16-C	245	ALA	8.1
1	1-A	114	THR	8.1
1	2-A	114	THR	8.1
1	3-A	114	THR	8.1
1	4-A	114	THR	8.1
1	5-A	114	THR	8.1
1	6-A	114	THR	8.1
1	7-A	114	THR	8.1
1	8-A	114	THR	8.1
1	9-A	114	THR	8.1
1	10-A	114	THR	8.1
1	11-A	114	THR	8.1
1	12-A	114	THR	8.1
1	13-A	114	THR	8.1
1	14-A	114	THR	8.1
1	15-A	114	THR	8.1
1	16-A	114	THR	8.1
1	1-C	108	ARG	7.8
1	2-C	108	ARG	7.8
1	3-C	108	ARG	7.8

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Mol	Chain	Res	Type	RSRZ
1	4-C	108	ARG	7.8
1	5-C	108	ARG	7.8
1	6-C	108	ARG	7.8
1	7-C	108	ARG	7.8
1	8-C	108	ARG	7.8
1	9-C	108	ARG	7.8
1	10-C	108	ARG	7.8
1	11-C	108	ARG	7.8
1	12-C	108	ARG	7.8
1	13-C	108	ARG	7.8
1	14-C	108	ARG	7.8
1	15-C	108	ARG	7.8
1	16-C	108	ARG	7.8
1	1-A	245	ALA	7.0
1	2-A	245	ALA	7.0
1	3-A	245	ALA	7.0
1	4-A	245	ALA	7.0
1	5-A	245	ALA	7.0
1	6-A	245	ALA	7.0
1	7-A	245	ALA	7.0
1	8-A	245	ALA	7.0
1	9-A	245	ALA	7.0
1	10-A	245	ALA	7.0
1	11-A	245	ALA	7.0
1	12-A	245	ALA	7.0
1	13-A	245	ALA	7.0
1	14-A	245	ALA	7.0
1	15-A	245	ALA	7.0
1	16-A	245	ALA	7.0
1	1-B	106	SER	6.9
1	2-B	106	SER	6.9
1	3-B	106	SER	6.9
1	4-B	106	SER	6.9
1	5-B	106	SER	6.9
1	6-B	106	SER	6.9
1	7-B	106	SER	6.9
1	8-B	106	SER	6.9
1	9-B	106	SER	6.9
1	10-B	106	SER	6.9
1	11-B	106	SER	6.9
1	12-B	106	SER	6.9
1	13-B	106	SER	6.9

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Mol	Chain	Res	Type	RSRZ
1	14-B	106	SER	6.9
1	15-B	106	SER	6.9
1	16-B	106	SER	6.9
1	1-B	88	PRO	6.8
1	2-B	88	PRO	6.8
1	3-B	88	PRO	6.8
1	4-B	88	PRO	6.8
1	5-B	88	PRO	6.8
1	6-B	88	PRO	6.8
1	7-B	88	PRO	6.8
1	8-B	88	PRO	6.8
1	9-B	88	PRO	6.8
1	10-B	88	PRO	6.8
1	11-B	88	PRO	6.8
1	12-B	88	PRO	6.8
1	13-B	88	PRO	6.8
1	14-B	88	PRO	6.8
1	15-B	88	PRO	6.8
1	16-B	88	PRO	6.8
1	1-B	90	SER	6.8
1	2-B	90	SER	6.8
1	3-B	90	SER	6.8
1	4-B	90	SER	6.8
1	5-B	90	SER	6.8
1	6-B	90	SER	6.8
1	7-B	90	SER	6.8
1	8-B	90	SER	6.8
1	9-B	90	SER	6.8
1	10-B	90	SER	6.8
1	11-B	90	SER	6.8
1	12-B	90	SER	6.8
1	13-B	90	SER	6.8
1	14-B	90	SER	6.8
1	15-B	90	SER	6.8
1	16-B	90	SER	6.8
1	1-B	216	ALA	6.7
1	2-B	216	ALA	6.7
1	3-B	216	ALA	6.7
1	4-B	216	ALA	6.7
1	5-B	216	ALA	6.7
1	6-B	216	ALA	6.7
1	7-B	216	ALA	6.7

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Mol	Chain	Res	Type	RSRZ
1	8-B	216	ALA	6.7
1	9-B	216	ALA	6.7
1	10-B	216	ALA	6.7
1	11-B	216	ALA	6.7
1	12-B	216	ALA	6.7
1	13-B	216	ALA	6.7
1	14-B	216	ALA	6.7
1	15-B	216	ALA	6.7
1	16-B	216	ALA	6.7
1	1-A	246	ASN	6.6
1	2-A	246	ASN	6.6
1	3-A	246	ASN	6.6
1	4-A	246	ASN	6.6
1	5-A	246	ASN	6.6
1	6-A	246	ASN	6.6
1	7-A	246	ASN	6.6
1	8-A	246	ASN	6.6
1	9-A	246	ASN	6.6
1	10-A	246	ASN	6.6
1	11-A	246	ASN	6.6
1	12-A	246	ASN	6.6
1	13-A	246	ASN	6.6
1	14-A	246	ASN	6.6
1	15-A	246	ASN	6.6
1	16-A	246	ASN	6.6
1	1-A	90	SER	6.4
1	2-A	90	SER	6.4
1	3-A	90	SER	6.4
1	4-A	90	SER	6.4
1	5-A	90	SER	6.4
1	6-A	90	SER	6.4
1	7-A	90	SER	6.4
1	8-A	90	SER	6.4
1	9-A	90	SER	6.4
1	10-A	90	SER	6.4
1	11-A	90	SER	6.4
1	12-A	90	SER	6.4
1	13-A	90	SER	6.4
1	14-A	90	SER	6.4
1	15-A	90	SER	6.4
1	16-A	90	SER	6.4
1	1-C	237	ARG	6.3

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Mol	Chain	Res	Type	RSRZ
1	2-C	237	ARG	6.3
1	3-C	237	ARG	6.3
1	4-C	237	ARG	6.3
1	5-C	237	ARG	6.3
1	6-C	237	ARG	6.3
1	7-C	237	ARG	6.3
1	8-C	237	ARG	6.3
1	9-C	237	ARG	6.3
1	10-C	237	ARG	6.3
1	11-C	237	ARG	6.3
1	12-C	237	ARG	6.3
1	13-C	237	ARG	6.3
1	14-C	237	ARG	6.3
1	15-C	237	ARG	6.3
1	16-C	237	ARG	6.3
1	1-B	87	SER	6.2
1	2-B	87	SER	6.2
1	3-B	87	SER	6.2
1	4-B	87	SER	6.2
1	5-B	87	SER	6.2
1	6-B	87	SER	6.2
1	7-B	87	SER	6.2
1	8-B	87	SER	6.2
1	9-B	87	SER	6.2
1	10-B	87	SER	6.2
1	11-B	87	SER	6.2
1	12-B	87	SER	6.2
1	13-B	87	SER	6.2
1	14-B	87	SER	6.2
1	15-B	87	SER	6.2
1	16-B	87	SER	6.2
1	1-A	121	THR	6.2
1	2-A	121	THR	6.2
1	3-A	121	THR	6.2
1	4-A	121	THR	6.2
1	5-A	121	THR	6.2
1	6-A	121	THR	6.2
1	7-A	121	THR	6.2
1	8-A	121	THR	6.2
1	9-A	121	THR	6.2
1	10-A	121	THR	6.2
1	11-A	121	THR	6.2

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Mol	Chain	Res	Type	RSRZ
1	12-A	121	THR	6.2
1	13-A	121	THR	6.2
1	14-A	121	THR	6.2
1	15-A	121	THR	6.2
1	16-A	121	THR	6.2
1	1-B	107	GLY	6.2
1	2-B	107	GLY	6.2
1	3-B	107	GLY	6.2
1	4-B	107	GLY	6.2
1	5-B	107	GLY	6.2
1	6-B	107	GLY	6.2
1	7-B	107	GLY	6.2
1	8-B	107	GLY	6.2
1	9-B	107	GLY	6.2
1	10-B	107	GLY	6.2
1	11-B	107	GLY	6.2
1	12-B	107	GLY	6.2
1	13-B	107	GLY	6.2
1	14-B	107	GLY	6.2
1	15-B	107	GLY	6.2
1	16-B	107	GLY	6.2
1	1-B	85	GLY	6.1
1	2-B	85	GLY	6.1
1	3-B	85	GLY	6.1
1	4-B	85	GLY	6.1
1	5-B	85	GLY	6.1
1	6-B	85	GLY	6.1
1	7-B	85	GLY	6.1
1	8-B	85	GLY	6.1
1	9-B	85	GLY	6.1
1	10-B	85	GLY	6.1
1	11-B	85	GLY	6.1
1	12-B	85	GLY	6.1
1	13-B	85	GLY	6.1
1	14-B	85	GLY	6.1
1	15-B	85	GLY	6.1
1	16-B	85	GLY	6.1
1	1-B	166	GLU	5.9
1	2-B	166	GLU	5.9
1	3-B	166	GLU	5.9
1	4-B	166	GLU	5.9
1	5-B	166	GLU	5.9

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Mol	Chain	Res	Type	RSRZ
1	6-B	166	GLU	5.9
1	7-B	166	GLU	5.9
1	8-B	166	GLU	5.9
1	9-B	166	GLU	5.9
1	10-B	166	GLU	5.9
1	11-B	166	GLU	5.9
1	12-B	166	GLU	5.9
1	13-B	166	GLU	5.9
1	14-B	166	GLU	5.9
1	15-B	166	GLU	5.9
1	16-B	166	GLU	5.9
1	1-A	120	ILE	5.7
1	2-A	120	ILE	5.7
1	3-A	120	ILE	5.7
1	4-A	120	ILE	5.7
1	5-A	120	ILE	5.7
1	6-A	120	ILE	5.7
1	7-A	120	ILE	5.7
1	8-A	120	ILE	5.7
1	9-A	120	ILE	5.7
1	10-A	120	ILE	5.7
1	11-A	120	ILE	5.7
1	12-A	120	ILE	5.7
1	13-A	120	ILE	5.7
1	14-A	120	ILE	5.7
1	15-A	120	ILE	5.7
1	16-A	120	ILE	5.7
1	1-A	88	PRO	5.5
1	2-A	88	PRO	5.5
1	3-A	88	PRO	5.5
1	4-A	88	PRO	5.5
1	5-A	88	PRO	5.5
1	6-A	88	PRO	5.5
1	7-A	88	PRO	5.5
1	8-A	88	PRO	5.5
1	9-A	88	PRO	5.5
1	10-A	88	PRO	5.5
1	11-A	88	PRO	5.5
1	12-A	88	PRO	5.5
1	13-A	88	PRO	5.5
1	14-A	88	PRO	5.5
1	15-A	88	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
1	16-A	88	PRO	5.5
1	1-A	110	ILE	5.5
1	2-A	110	ILE	5.5
1	3-A	110	ILE	5.5
1	4-A	110	ILE	5.5
1	5-A	110	ILE	5.5
1	6-A	110	ILE	5.5
1	7-A	110	ILE	5.5
1	8-A	110	ILE	5.5
1	9-A	110	ILE	5.5
1	10-A	110	ILE	5.5
1	11-A	110	ILE	5.5
1	12-A	110	ILE	5.5
1	13-A	110	ILE	5.5
1	14-A	110	ILE	5.5
1	15-A	110	ILE	5.5
1	16-A	110	ILE	5.5
1	1-A	89	ASN	5.4
1	2-A	89	ASN	5.4
1	3-A	89	ASN	5.4
1	4-A	89	ASN	5.4
1	5-A	89	ASN	5.4
1	6-A	89	ASN	5.4
1	7-A	89	ASN	5.4
1	8-A	89	ASN	5.4
1	9-A	89	ASN	5.4
1	10-A	89	ASN	5.4
1	11-A	89	ASN	5.4
1	12-A	89	ASN	5.4
1	13-A	89	ASN	5.4
1	14-A	89	ASN	5.4
1	15-A	89	ASN	5.4
1	16-A	89	ASN	5.4
1	1-A	106	SER	5.3
1	2-A	106	SER	5.3
1	3-A	106	SER	5.3
1	4-A	106	SER	5.3
1	5-A	106	SER	5.3
1	6-A	106	SER	5.3
1	7-A	106	SER	5.3
1	8-A	106	SER	5.3
1	9-A	106	SER	5.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	10-A	106	SER	5.3
1	11-A	106	SER	5.3
1	12-A	106	SER	5.3
1	13-A	106	SER	5.3
1	14-A	106	SER	5.3
1	15-A	106	SER	5.3
1	16-A	106	SER	5.3
1	1-B	84	GLN	5.1
1	2-B	84	GLN	5.1
1	3-B	84	GLN	5.1
1	4-B	84	GLN	5.1
1	5-B	84	GLN	5.1
1	6-B	84	GLN	5.1
1	7-B	84	GLN	5.1
1	8-B	84	GLN	5.1
1	9-B	84	GLN	5.1
1	10-B	84	GLN	5.1
1	11-B	84	GLN	5.1
1	12-B	84	GLN	5.1
1	13-B	84	GLN	5.1
1	14-B	84	GLN	5.1
1	15-B	84	GLN	5.1
1	16-B	84	GLN	5.1
1	1-A	177	ASP	4.9
1	2-A	177	ASP	4.9
1	3-A	177	ASP	4.9
1	4-A	177	ASP	4.9
1	5-A	177	ASP	4.9
1	6-A	177	ASP	4.9
1	7-A	177	ASP	4.9
1	8-A	177	ASP	4.9
1	9-A	177	ASP	4.9
1	10-A	177	ASP	4.9
1	11-A	177	ASP	4.9
1	12-A	177	ASP	4.9
1	13-A	177	ASP	4.9
1	14-A	177	ASP	4.9
1	15-A	177	ASP	4.9
1	16-A	177	ASP	4.9
1	1-C	167	GLY	4.9
1	2-C	167	GLY	4.9
1	3-C	167	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	4-C	167	GLY	4.9
1	5-C	167	GLY	4.9
1	6-C	167	GLY	4.9
1	7-C	167	GLY	4.9
1	8-C	167	GLY	4.9
1	9-C	167	GLY	4.9
1	10-C	167	GLY	4.9
1	11-C	167	GLY	4.9
1	12-C	167	GLY	4.9
1	13-C	167	GLY	4.9
1	14-C	167	GLY	4.9
1	15-C	167	GLY	4.9
1	16-C	167	GLY	4.9
1	1-A	17	GLU	4.9
1	2-A	17	GLU	4.9
1	3-A	17	GLU	4.9
1	4-A	17	GLU	4.9
1	5-A	17	GLU	4.9
1	6-A	17	GLU	4.9
1	7-A	17	GLU	4.9
1	8-A	17	GLU	4.9
1	9-A	17	GLU	4.9
1	10-A	17	GLU	4.9
1	11-A	17	GLU	4.9
1	12-A	17	GLU	4.9
1	13-A	17	GLU	4.9
1	14-A	17	GLU	4.9
1	15-A	17	GLU	4.9
1	16-A	17	GLU	4.9
1	1-C	109	PRO	4.9
1	2-C	109	PRO	4.9
1	3-C	109	PRO	4.9
1	4-C	109	PRO	4.9
1	5-C	109	PRO	4.9
1	6-C	109	PRO	4.9
1	7-C	109	PRO	4.9
1	8-C	109	PRO	4.9
1	9-C	109	PRO	4.9
1	10-C	109	PRO	4.9
1	11-C	109	PRO	4.9
1	12-C	109	PRO	4.9
1	13-C	109	PRO	4.9

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Mol	Chain	Res	Type	RSRZ
1	14-C	109	PRO	4.9
1	15-C	109	PRO	4.9
1	16-C	109	PRO	4.9
1	1-B	165	LYS	4.8
1	2-B	165	LYS	4.8
1	3-B	165	LYS	4.8
1	4-B	165	LYS	4.8
1	5-B	165	LYS	4.8
1	6-B	165	LYS	4.8
1	7-B	165	LYS	4.8
1	8-B	165	LYS	4.8
1	9-B	165	LYS	4.8
1	10-B	165	LYS	4.8
1	11-B	165	LYS	4.8
1	12-B	165	LYS	4.8
1	13-B	165	LYS	4.8
1	14-B	165	LYS	4.8
1	15-B	165	LYS	4.8
1	16-B	165	LYS	4.8
1	1-A	216	ALA	4.8
1	2-A	216	ALA	4.8
1	3-A	216	ALA	4.8
1	4-A	216	ALA	4.8
1	5-A	216	ALA	4.8
1	6-A	216	ALA	4.8
1	7-A	216	ALA	4.8
1	8-A	216	ALA	4.8
1	9-A	216	ALA	4.8
1	10-A	216	ALA	4.8
1	11-A	216	ALA	4.8
1	12-A	216	ALA	4.8
1	13-A	216	ALA	4.8
1	14-A	216	ALA	4.8
1	15-A	216	ALA	4.8
1	16-A	216	ALA	4.8
1	1-C	101	GLU	4.8
1	2-C	101	GLU	4.8
1	3-C	101	GLU	4.8
1	4-C	101	GLU	4.8
1	5-C	101	GLU	4.8
1	6-C	101	GLU	4.8
1	7-C	101	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	8-C	101	GLU	4.8
1	9-C	101	GLU	4.8
1	10-C	101	GLU	4.8
1	11-C	101	GLU	4.8
1	12-C	101	GLU	4.8
1	13-C	101	GLU	4.8
1	14-C	101	GLU	4.8
1	15-C	101	GLU	4.8
1	16-C	101	GLU	4.8
1	1-A	247	ASN	4.7
1	2-A	247	ASN	4.7
1	3-A	247	ASN	4.7
1	4-A	247	ASN	4.7
1	5-A	247	ASN	4.7
1	6-A	247	ASN	4.7
1	7-A	247	ASN	4.7
1	8-A	247	ASN	4.7
1	9-A	247	ASN	4.7
1	10-A	247	ASN	4.7
1	11-A	247	ASN	4.7
1	12-A	247	ASN	4.7
1	13-A	247	ASN	4.7
1	14-A	247	ASN	4.7
1	15-A	247	ASN	4.7
1	16-A	247	ASN	4.7
1	1-B	218	ARG	4.7
1	2-B	218	ARG	4.7
1	3-B	218	ARG	4.7
1	4-B	218	ARG	4.7
1	5-B	218	ARG	4.7
1	6-B	218	ARG	4.7
1	7-B	218	ARG	4.7
1	8-B	218	ARG	4.7
1	9-B	218	ARG	4.7
1	10-B	218	ARG	4.7
1	11-B	218	ARG	4.7
1	12-B	218	ARG	4.7
1	13-B	218	ARG	4.7
1	14-B	218	ARG	4.7
1	15-B	218	ARG	4.7
1	16-B	218	ARG	4.7
1	1-B	168	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	2-B	168	GLY	4.6
1	3-B	168	GLY	4.6
1	4-B	168	GLY	4.6
1	5-B	168	GLY	4.6
1	6-B	168	GLY	4.6
1	7-B	168	GLY	4.6
1	8-B	168	GLY	4.6
1	9-B	168	GLY	4.6
1	10-B	168	GLY	4.6
1	11-B	168	GLY	4.6
1	12-B	168	GLY	4.6
1	13-B	168	GLY	4.6
1	14-B	168	GLY	4.6
1	15-B	168	GLY	4.6
1	16-B	168	GLY	4.6
1	1-C	106	SER	4.6
1	2-C	106	SER	4.6
1	3-C	106	SER	4.6
1	4-C	106	SER	4.6
1	5-C	106	SER	4.6
1	6-C	106	SER	4.6
1	7-C	106	SER	4.6
1	8-C	106	SER	4.6
1	9-C	106	SER	4.6
1	10-C	106	SER	4.6
1	11-C	106	SER	4.6
1	12-C	106	SER	4.6
1	13-C	106	SER	4.6
1	14-C	106	SER	4.6
1	15-C	106	SER	4.6
1	16-C	106	SER	4.6
1	1-A	111	THR	4.5
1	2-A	111	THR	4.5
1	3-A	111	THR	4.5
1	4-A	111	THR	4.5
1	5-A	111	THR	4.5
1	6-A	111	THR	4.5
1	7-A	111	THR	4.5
1	8-A	111	THR	4.5
1	9-A	111	THR	4.5
1	10-A	111	THR	4.5
1	11-A	111	THR	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	12-A	111	THR	4.5
1	13-A	111	THR	4.5
1	14-A	111	THR	4.5
1	15-A	111	THR	4.5
1	16-A	111	THR	4.5
1	1-A	222	CYS	4.5
1	2-A	222	CYS	4.5
1	3-A	222	CYS	4.5
1	4-A	222	CYS	4.5
1	5-A	222	CYS	4.5
1	6-A	222	CYS	4.5
1	7-A	222	CYS	4.5
1	8-A	222	CYS	4.5
1	9-A	222	CYS	4.5
1	10-A	222	CYS	4.5
1	11-A	222	CYS	4.5
1	12-A	222	CYS	4.5
1	13-A	222	CYS	4.5
1	14-A	222	CYS	4.5
1	15-A	222	CYS	4.5
1	16-A	222	CYS	4.5
1	1-B	215	ARG	4.5
1	2-B	215	ARG	4.5
1	3-B	215	ARG	4.5
1	4-B	215	ARG	4.5
1	5-B	215	ARG	4.5
1	6-B	215	ARG	4.5
1	7-B	215	ARG	4.5
1	8-B	215	ARG	4.5
1	9-B	215	ARG	4.5
1	10-B	215	ARG	4.5
1	11-B	215	ARG	4.5
1	12-B	215	ARG	4.5
1	13-B	215	ARG	4.5
1	14-B	215	ARG	4.5
1	15-B	215	ARG	4.5
1	16-B	215	ARG	4.5
1	1-C	102	ALA	4.5
1	2-C	102	ALA	4.5
1	3-C	102	ALA	4.5
1	4-C	102	ALA	4.5
1	5-C	102	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	6-C	102	ALA	4.5
1	7-C	102	ALA	4.5
1	8-C	102	ALA	4.5
1	9-C	102	ALA	4.5
1	10-C	102	ALA	4.5
1	11-C	102	ALA	4.5
1	12-C	102	ALA	4.5
1	13-C	102	ALA	4.5
1	14-C	102	ALA	4.5
1	15-C	102	ALA	4.5
1	16-C	102	ALA	4.5
1	1-C	166	GLU	4.5
1	2-C	166	GLU	4.5
1	3-C	166	GLU	4.5
1	4-C	166	GLU	4.5
1	5-C	166	GLU	4.5
1	6-C	166	GLU	4.5
1	7-C	166	GLU	4.5
1	8-C	166	GLU	4.5
1	9-C	166	GLU	4.5
1	10-C	166	GLU	4.5
1	11-C	166	GLU	4.5
1	12-C	166	GLU	4.5
1	13-C	166	GLU	4.5
1	14-C	166	GLU	4.5
1	15-C	166	GLU	4.5
1	16-C	166	GLU	4.5
1	1-A	98	ALA	4.4
1	2-A	98	ALA	4.4
1	3-A	98	ALA	4.4
1	4-A	98	ALA	4.4
1	5-A	98	ALA	4.4
1	6-A	98	ALA	4.4
1	7-A	98	ALA	4.4
1	8-A	98	ALA	4.4
1	9-A	98	ALA	4.4
1	10-A	98	ALA	4.4
1	11-A	98	ALA	4.4
1	12-A	98	ALA	4.4
1	13-A	98	ALA	4.4
1	14-A	98	ALA	4.4
1	15-A	98	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	16-A	98	ALA	4.4
1	1-A	109	PRO	4.4
1	2-A	109	PRO	4.4
1	3-A	109	PRO	4.4
1	4-A	109	PRO	4.4
1	5-A	109	PRO	4.4
1	6-A	109	PRO	4.4
1	7-A	109	PRO	4.4
1	8-A	109	PRO	4.4
1	9-A	109	PRO	4.4
1	10-A	109	PRO	4.4
1	11-A	109	PRO	4.4
1	12-A	109	PRO	4.4
1	13-A	109	PRO	4.4
1	14-A	109	PRO	4.4
1	15-A	109	PRO	4.4
1	16-A	109	PRO	4.4
1	1-A	180	THR	4.3
1	2-A	180	THR	4.3
1	3-A	180	THR	4.3
1	4-A	180	THR	4.3
1	5-A	180	THR	4.3
1	6-A	180	THR	4.3
1	7-A	180	THR	4.3
1	8-A	180	THR	4.3
1	9-A	180	THR	4.3
1	10-A	180	THR	4.3
1	11-A	180	THR	4.3
1	12-A	180	THR	4.3
1	13-A	180	THR	4.3
1	14-A	180	THR	4.3
1	15-A	180	THR	4.3
1	16-A	180	THR	4.3
1	1-A	107	GLY	4.3
1	2-A	107	GLY	4.3
1	3-A	107	GLY	4.3
1	4-A	107	GLY	4.3
1	5-A	107	GLY	4.3
1	6-A	107	GLY	4.3
1	7-A	107	GLY	4.3
1	8-A	107	GLY	4.3
1	9-A	107	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	10-A	107	GLY	4.3
1	11-A	107	GLY	4.3
1	12-A	107	GLY	4.3
1	13-A	107	GLY	4.3
1	14-A	107	GLY	4.3
1	15-A	107	GLY	4.3
1	16-A	107	GLY	4.3
1	1-B	104	GLN	4.2
1	2-B	104	GLN	4.2
1	3-B	104	GLN	4.2
1	4-B	104	GLN	4.2
1	5-B	104	GLN	4.2
1	6-B	104	GLN	4.2
1	7-B	104	GLN	4.2
1	8-B	104	GLN	4.2
1	9-B	104	GLN	4.2
1	10-B	104	GLN	4.2
1	11-B	104	GLN	4.2
1	12-B	104	GLN	4.2
1	13-B	104	GLN	4.2
1	14-B	104	GLN	4.2
1	15-B	104	GLN	4.2
1	16-B	104	GLN	4.2
1	1-A	231	GLN	4.2
1	2-A	231	GLN	4.2
1	3-A	231	GLN	4.2
1	4-A	231	GLN	4.2
1	5-A	231	GLN	4.2
1	6-A	231	GLN	4.2
1	7-A	231	GLN	4.2
1	8-A	231	GLN	4.2
1	9-A	231	GLN	4.2
1	10-A	231	GLN	4.2
1	11-A	231	GLN	4.2
1	12-A	231	GLN	4.2
1	13-A	231	GLN	4.2
1	14-A	231	GLN	4.2
1	15-A	231	GLN	4.2
1	16-A	231	GLN	4.2
1	1-A	44	THR	4.2
1	2-A	44	THR	4.2
1	3-A	44	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	4-A	44	THR	4.2
1	5-A	44	THR	4.2
1	6-A	44	THR	4.2
1	7-A	44	THR	4.2
1	8-A	44	THR	4.2
1	9-A	44	THR	4.2
1	10-A	44	THR	4.2
1	11-A	44	THR	4.2
1	12-A	44	THR	4.2
1	13-A	44	THR	4.2
1	14-A	44	THR	4.2
1	15-A	44	THR	4.2
1	16-A	44	THR	4.2
1	1-B	219	TRP	4.2
1	2-B	219	TRP	4.2
1	3-B	219	TRP	4.2
1	4-B	219	TRP	4.2
1	5-B	219	TRP	4.2
1	6-B	219	TRP	4.2
1	7-B	219	TRP	4.2
1	8-B	219	TRP	4.2
1	9-B	219	TRP	4.2
1	10-B	219	TRP	4.2
1	11-B	219	TRP	4.2
1	12-B	219	TRP	4.2
1	13-B	219	TRP	4.2
1	14-B	219	TRP	4.2
1	15-B	219	TRP	4.2
1	16-B	219	TRP	4.2
1	1-C	248	VAL	4.1
1	2-C	248	VAL	4.1
1	3-C	248	VAL	4.1
1	4-C	248	VAL	4.1
1	5-C	248	VAL	4.1
1	6-C	248	VAL	4.1
1	7-C	248	VAL	4.1
1	8-C	248	VAL	4.1
1	9-C	248	VAL	4.1
1	10-C	248	VAL	4.1
1	11-C	248	VAL	4.1
1	12-C	248	VAL	4.1
1	13-C	248	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	14-C	248	VAL	4.1
1	15-C	248	VAL	4.1
1	16-C	248	VAL	4.1
1	1-C	218	ARG	4.1
1	2-C	218	ARG	4.1
1	3-C	218	ARG	4.1
1	4-C	218	ARG	4.1
1	5-C	218	ARG	4.1
1	6-C	218	ARG	4.1
1	7-C	218	ARG	4.1
1	8-C	218	ARG	4.1
1	9-C	218	ARG	4.1
1	10-C	218	ARG	4.1
1	11-C	218	ARG	4.1
1	12-C	218	ARG	4.1
1	13-C	218	ARG	4.1
1	14-C	218	ARG	4.1
1	15-C	218	ARG	4.1
1	16-C	218	ARG	4.1
1	1-A	103	LEU	4.1
1	2-A	103	LEU	4.1
1	3-A	103	LEU	4.1
1	4-A	103	LEU	4.1
1	5-A	103	LEU	4.1
1	6-A	103	LEU	4.1
1	7-A	103	LEU	4.1
1	8-A	103	LEU	4.1
1	9-A	103	LEU	4.1
1	10-A	103	LEU	4.1
1	11-A	103	LEU	4.1
1	12-A	103	LEU	4.1
1	13-A	103	LEU	4.1
1	14-A	103	LEU	4.1
1	15-A	103	LEU	4.1
1	16-A	103	LEU	4.1
1	1-A	179	PHE	4.1
1	2-A	179	PHE	4.1
1	3-A	179	PHE	4.1
1	4-A	179	PHE	4.1
1	5-A	179	PHE	4.1
1	6-A	179	PHE	4.1
1	7-A	179	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	8-A	179	PHE	4.1
1	9-A	179	PHE	4.1
1	10-A	179	PHE	4.1
1	11-A	179	PHE	4.1
1	12-A	179	PHE	4.1
1	13-A	179	PHE	4.1
1	14-A	179	PHE	4.1
1	15-A	179	PHE	4.1
1	16-A	179	PHE	4.1
1	1-A	226	TYR	4.1
1	2-A	226	TYR	4.1
1	3-A	226	TYR	4.1
1	4-A	226	TYR	4.1
1	5-A	226	TYR	4.1
1	6-A	226	TYR	4.1
1	7-A	226	TYR	4.1
1	8-A	226	TYR	4.1
1	9-A	226	TYR	4.1
1	10-A	226	TYR	4.1
1	11-A	226	TYR	4.1
1	12-A	226	TYR	4.1
1	13-A	226	TYR	4.1
1	14-A	226	TYR	4.1
1	15-A	226	TYR	4.1
1	16-A	226	TYR	4.1
1	1-B	98	ALA	4.0
1	2-B	98	ALA	4.0
1	3-B	98	ALA	4.0
1	4-B	98	ALA	4.0
1	5-B	98	ALA	4.0
1	6-B	98	ALA	4.0
1	7-B	98	ALA	4.0
1	8-B	98	ALA	4.0
1	9-B	98	ALA	4.0
1	10-B	98	ALA	4.0
1	11-B	98	ALA	4.0
1	12-B	98	ALA	4.0
1	13-B	98	ALA	4.0
1	14-B	98	ALA	4.0
1	15-B	98	ALA	4.0
1	16-B	98	ALA	4.0
1	1-A	167	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	2-A	167	GLY	4.0
1	3-A	167	GLY	4.0
1	4-A	167	GLY	4.0
1	5-A	167	GLY	4.0
1	6-A	167	GLY	4.0
1	7-A	167	GLY	4.0
1	8-A	167	GLY	4.0
1	9-A	167	GLY	4.0
1	10-A	167	GLY	4.0
1	11-A	167	GLY	4.0
1	12-A	167	GLY	4.0
1	13-A	167	GLY	4.0
1	14-A	167	GLY	4.0
1	15-A	167	GLY	4.0
1	16-A	167	GLY	4.0
1	1-B	74	GLU	4.0
1	2-B	74	GLU	4.0
1	3-B	74	GLU	4.0
1	4-B	74	GLU	4.0
1	5-B	74	GLU	4.0
1	6-B	74	GLU	4.0
1	7-B	74	GLU	4.0
1	8-B	74	GLU	4.0
1	9-B	74	GLU	4.0
1	10-B	74	GLU	4.0
1	11-B	74	GLU	4.0
1	12-B	74	GLU	4.0
1	13-B	74	GLU	4.0
1	14-B	74	GLU	4.0
1	15-B	74	GLU	4.0
1	16-B	74	GLU	4.0
1	1-A	104	GLN	3.9
1	2-A	104	GLN	3.9
1	3-A	104	GLN	3.9
1	4-A	104	GLN	3.9
1	5-A	104	GLN	3.9
1	6-A	104	GLN	3.9
1	7-A	104	GLN	3.9
1	8-A	104	GLN	3.9
1	9-A	104	GLN	3.9
1	10-A	104	GLN	3.9
1	11-A	104	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	12-A	104	GLN	3.9
1	13-A	104	GLN	3.9
1	14-A	104	GLN	3.9
1	15-A	104	GLN	3.9
1	16-A	104	GLN	3.9
1	1-A	250	LEU	3.9
1	2-A	250	LEU	3.9
1	3-A	250	LEU	3.9
1	4-A	250	LEU	3.9
1	5-A	250	LEU	3.9
1	6-A	250	LEU	3.9
1	7-A	250	LEU	3.9
1	8-A	250	LEU	3.9
1	9-A	250	LEU	3.9
1	10-A	250	LEU	3.9
1	11-A	250	LEU	3.9
1	12-A	250	LEU	3.9
1	13-A	250	LEU	3.9
1	14-A	250	LEU	3.9
1	15-A	250	LEU	3.9
1	16-A	250	LEU	3.9
1	1-A	238	GLY	3.9
1	2-A	238	GLY	3.9
1	3-A	238	GLY	3.9
1	4-A	238	GLY	3.9
1	5-A	238	GLY	3.9
1	6-A	238	GLY	3.9
1	7-A	238	GLY	3.9
1	8-A	238	GLY	3.9
1	9-A	238	GLY	3.9
1	10-A	238	GLY	3.9
1	11-A	238	GLY	3.9
1	12-A	238	GLY	3.9
1	13-A	238	GLY	3.9
1	14-A	238	GLY	3.9
1	15-A	238	GLY	3.9
1	16-A	238	GLY	3.9
1	1-A	18	ASP	3.8
1	2-A	18	ASP	3.8
1	3-A	18	ASP	3.8
1	4-A	18	ASP	3.8
1	5-A	18	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	6-A	18	ASP	3.8
1	7-A	18	ASP	3.8
1	8-A	18	ASP	3.8
1	9-A	18	ASP	3.8
1	10-A	18	ASP	3.8
1	11-A	18	ASP	3.8
1	12-A	18	ASP	3.8
1	13-A	18	ASP	3.8
1	14-A	18	ASP	3.8
1	15-A	18	ASP	3.8
1	16-A	18	ASP	3.8
1	1-B	110	ILE	3.8
1	2-B	110	ILE	3.8
1	3-B	110	ILE	3.8
1	4-B	110	ILE	3.8
1	5-B	110	ILE	3.8
1	6-B	110	ILE	3.8
1	7-B	110	ILE	3.8
1	8-B	110	ILE	3.8
1	9-B	110	ILE	3.8
1	10-B	110	ILE	3.8
1	11-B	110	ILE	3.8
1	12-B	110	ILE	3.8
1	13-B	110	ILE	3.8
1	14-B	110	ILE	3.8
1	15-B	110	ILE	3.8
1	16-B	110	ILE	3.8
1	1-A	48	THR	3.7
1	2-A	48	THR	3.7
1	3-A	48	THR	3.7
1	4-A	48	THR	3.7
1	5-A	48	THR	3.7
1	6-A	48	THR	3.7
1	7-A	48	THR	3.7
1	8-A	48	THR	3.7
1	9-A	48	THR	3.7
1	10-A	48	THR	3.7
1	11-A	48	THR	3.7
1	12-A	48	THR	3.7
1	13-A	48	THR	3.7
1	14-A	48	THR	3.7
1	15-A	48	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	16-A	48	THR	3.7
1	1-B	103	LEU	3.7
1	2-B	103	LEU	3.7
1	3-B	103	LEU	3.7
1	4-B	103	LEU	3.7
1	5-B	103	LEU	3.7
1	6-B	103	LEU	3.7
1	7-B	103	LEU	3.7
1	8-B	103	LEU	3.7
1	9-B	103	LEU	3.7
1	10-B	103	LEU	3.7
1	11-B	103	LEU	3.7
1	12-B	103	LEU	3.7
1	13-B	103	LEU	3.7
1	14-B	103	LEU	3.7
1	15-B	103	LEU	3.7
1	16-B	103	LEU	3.7
1	1-C	220	HIS	3.7
1	2-C	220	HIS	3.7
1	3-C	220	HIS	3.7
1	4-C	220	HIS	3.7
1	5-C	220	HIS	3.7
1	6-C	220	HIS	3.7
1	7-C	220	HIS	3.7
1	8-C	220	HIS	3.7
1	9-C	220	HIS	3.7
1	10-C	220	HIS	3.7
1	11-C	220	HIS	3.7
1	12-C	220	HIS	3.7
1	13-C	220	HIS	3.7
1	14-C	220	HIS	3.7
1	15-C	220	HIS	3.7
1	16-C	220	HIS	3.7
1	1-A	150	VAL	3.6
1	2-A	150	VAL	3.6
1	3-A	150	VAL	3.6
1	4-A	150	VAL	3.6
1	5-A	150	VAL	3.6
1	6-A	150	VAL	3.6
1	7-A	150	VAL	3.6
1	8-A	150	VAL	3.6
1	9-A	150	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	10-A	150	VAL	3.6
1	11-A	150	VAL	3.6
1	12-A	150	VAL	3.6
1	13-A	150	VAL	3.6
1	14-A	150	VAL	3.6
1	15-A	150	VAL	3.6
1	16-A	150	VAL	3.6
1	1-B	108	ARG	3.6
1	2-B	108	ARG	3.6
1	3-B	108	ARG	3.6
1	4-B	108	ARG	3.6
1	5-B	108	ARG	3.6
1	6-B	108	ARG	3.6
1	7-B	108	ARG	3.6
1	8-B	108	ARG	3.6
1	9-B	108	ARG	3.6
1	10-B	108	ARG	3.6
1	11-B	108	ARG	3.6
1	12-B	108	ARG	3.6
1	13-B	108	ARG	3.6
1	14-B	108	ARG	3.6
1	15-B	108	ARG	3.6
1	16-B	108	ARG	3.6
1	1-C	235	SER	3.6
1	2-C	235	SER	3.6
1	3-C	235	SER	3.6
1	4-C	235	SER	3.6
1	5-C	235	SER	3.6
1	6-C	235	SER	3.6
1	7-C	235	SER	3.6
1	8-C	235	SER	3.6
1	9-C	235	SER	3.6
1	10-C	235	SER	3.6
1	11-C	235	SER	3.6
1	12-C	235	SER	3.6
1	13-C	235	SER	3.6
1	14-C	235	SER	3.6
1	15-C	235	SER	3.6
1	16-C	235	SER	3.6
1	1-C	246	ASN	3.6
1	2-C	246	ASN	3.6
1	3-C	246	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	4-C	246	ASN	3.6
1	5-C	246	ASN	3.6
1	6-C	246	ASN	3.6
1	7-C	246	ASN	3.6
1	8-C	246	ASN	3.6
1	9-C	246	ASN	3.6
1	10-C	246	ASN	3.6
1	11-C	246	ASN	3.6
1	12-C	246	ASN	3.6
1	13-C	246	ASN	3.6
1	14-C	246	ASN	3.6
1	15-C	246	ASN	3.6
1	16-C	246	ASN	3.6
1	1-A	220	HIS	3.5
1	2-A	220	HIS	3.5
1	3-A	220	HIS	3.5
1	4-A	220	HIS	3.5
1	5-A	220	HIS	3.5
1	6-A	220	HIS	3.5
1	7-A	220	HIS	3.5
1	8-A	220	HIS	3.5
1	9-A	220	HIS	3.5
1	10-A	220	HIS	3.5
1	11-A	220	HIS	3.5
1	12-A	220	HIS	3.5
1	13-A	220	HIS	3.5
1	14-A	220	HIS	3.5
1	15-A	220	HIS	3.5
1	16-A	220	HIS	3.5
1	1-C	219	TRP	3.5
1	2-C	219	TRP	3.5
1	3-C	219	TRP	3.5
1	4-C	219	TRP	3.5
1	5-C	219	TRP	3.5
1	6-C	219	TRP	3.5
1	7-C	219	TRP	3.5
1	8-C	219	TRP	3.5
1	9-C	219	TRP	3.5
1	10-C	219	TRP	3.5
1	11-C	219	TRP	3.5
1	12-C	219	TRP	3.5
1	13-C	219	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	14-C	219	TRP	3.5
1	15-C	219	TRP	3.5
1	16-C	219	TRP	3.5
1	1-A	249	GLU	3.5
1	2-A	249	GLU	3.5
1	3-A	249	GLU	3.5
1	4-A	249	GLU	3.5
1	5-A	249	GLU	3.5
1	6-A	249	GLU	3.5
1	7-A	249	GLU	3.5
1	8-A	249	GLU	3.5
1	9-A	249	GLU	3.5
1	10-A	249	GLU	3.5
1	11-A	249	GLU	3.5
1	12-A	249	GLU	3.5
1	13-A	249	GLU	3.5
1	14-A	249	GLU	3.5
1	15-A	249	GLU	3.5
1	16-A	249	GLU	3.5
1	1-A	123	HIS	3.5
1	2-A	123	HIS	3.5
1	3-A	123	HIS	3.5
1	4-A	123	HIS	3.5
1	5-A	123	HIS	3.5
1	6-A	123	HIS	3.5
1	7-A	123	HIS	3.5
1	8-A	123	HIS	3.5
1	9-A	123	HIS	3.5
1	10-A	123	HIS	3.5
1	11-A	123	HIS	3.5
1	12-A	123	HIS	3.5
1	13-A	123	HIS	3.5
1	14-A	123	HIS	3.5
1	15-A	123	HIS	3.5
1	16-A	123	HIS	3.5
1	1-B	94	GLN	3.4
1	2-B	94	GLN	3.4
1	3-B	94	GLN	3.4
1	4-B	94	GLN	3.4
1	5-B	94	GLN	3.4
1	6-B	94	GLN	3.4
1	7-B	94	GLN	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	8-B	94	GLN	3.4
1	9-B	94	GLN	3.4
1	10-B	94	GLN	3.4
1	11-B	94	GLN	3.4
1	12-B	94	GLN	3.4
1	13-B	94	GLN	3.4
1	14-B	94	GLN	3.4
1	15-B	94	GLN	3.4
1	16-B	94	GLN	3.4
1	1-A	242	LEU	3.4
1	2-A	242	LEU	3.4
1	3-A	242	LEU	3.4
1	4-A	242	LEU	3.4
1	5-A	242	LEU	3.4
1	6-A	242	LEU	3.4
1	7-A	242	LEU	3.4
1	8-A	242	LEU	3.4
1	9-A	242	LEU	3.4
1	10-A	242	LEU	3.4
1	11-A	242	LEU	3.4
1	12-A	242	LEU	3.4
1	13-A	242	LEU	3.4
1	14-A	242	LEU	3.4
1	15-A	242	LEU	3.4
1	16-A	242	LEU	3.4
1	1-B	99	ALA	3.4
1	1-B	102	ALA	3.4
1	2-B	99	ALA	3.4
1	2-B	102	ALA	3.4
1	3-B	99	ALA	3.4
1	3-B	102	ALA	3.4
1	4-B	99	ALA	3.4
1	4-B	102	ALA	3.4
1	5-B	99	ALA	3.4
1	5-B	102	ALA	3.4
1	6-B	99	ALA	3.4
1	6-B	102	ALA	3.4
1	7-B	99	ALA	3.4
1	7-B	102	ALA	3.4
1	8-B	99	ALA	3.4
1	8-B	102	ALA	3.4
1	9-B	99	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	9-B	102	ALA	3.4
1	10-B	99	ALA	3.4
1	10-B	102	ALA	3.4
1	11-B	99	ALA	3.4
1	11-B	102	ALA	3.4
1	12-B	99	ALA	3.4
1	12-B	102	ALA	3.4
1	13-B	99	ALA	3.4
1	13-B	102	ALA	3.4
1	14-B	99	ALA	3.4
1	14-B	102	ALA	3.4
1	15-B	99	ALA	3.4
1	15-B	102	ALA	3.4
1	16-B	99	ALA	3.4
1	16-B	102	ALA	3.4
1	1-A	97	GLN	3.3
1	2-A	97	GLN	3.3
1	3-A	97	GLN	3.3
1	4-A	97	GLN	3.3
1	5-A	97	GLN	3.3
1	6-A	97	GLN	3.3
1	7-A	97	GLN	3.3
1	8-A	97	GLN	3.3
1	9-A	97	GLN	3.3
1	10-A	97	GLN	3.3
1	11-A	97	GLN	3.3
1	12-A	97	GLN	3.3
1	13-A	97	GLN	3.3
1	14-A	97	GLN	3.3
1	15-A	97	GLN	3.3
1	16-A	97	GLN	3.3
1	1-C	236	ALA	3.3
1	2-C	236	ALA	3.3
1	3-C	236	ALA	3.3
1	4-C	236	ALA	3.3
1	5-C	236	ALA	3.3
1	6-C	236	ALA	3.3
1	7-C	236	ALA	3.3
1	8-C	236	ALA	3.3
1	9-C	236	ALA	3.3
1	10-C	236	ALA	3.3
1	11-C	236	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	12-C	236	ALA	3.3
1	13-C	236	ALA	3.3
1	14-C	236	ALA	3.3
1	15-C	236	ALA	3.3
1	16-C	236	ALA	3.3
1	1-C	134	ALA	3.2
1	1-C	216	ALA	3.2
1	2-C	134	ALA	3.2
1	2-C	216	ALA	3.2
1	3-C	134	ALA	3.2
1	3-C	216	ALA	3.2
1	4-C	134	ALA	3.2
1	4-C	216	ALA	3.2
1	5-C	134	ALA	3.2
1	5-C	216	ALA	3.2
1	6-C	134	ALA	3.2
1	6-C	216	ALA	3.2
1	7-C	134	ALA	3.2
1	7-C	216	ALA	3.2
1	8-C	134	ALA	3.2
1	8-C	216	ALA	3.2
1	9-C	134	ALA	3.2
1	9-C	216	ALA	3.2
1	10-C	134	ALA	3.2
1	10-C	216	ALA	3.2
1	11-C	134	ALA	3.2
1	11-C	216	ALA	3.2
1	12-C	134	ALA	3.2
1	12-C	216	ALA	3.2
1	13-C	134	ALA	3.2
1	13-C	216	ALA	3.2
1	14-C	134	ALA	3.2
1	14-C	216	ALA	3.2
1	15-C	134	ALA	3.2
1	15-C	216	ALA	3.2
1	16-C	134	ALA	3.2
1	16-C	216	ALA	3.2
1	1-A	178	ASP	3.2
1	2-A	178	ASP	3.2
1	3-A	178	ASP	3.2
1	4-A	178	ASP	3.2
1	5-A	178	ASP	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	6-A	178	ASP	3.2
1	7-A	178	ASP	3.2
1	8-A	178	ASP	3.2
1	9-A	178	ASP	3.2
1	10-A	178	ASP	3.2
1	11-A	178	ASP	3.2
1	12-A	178	ASP	3.2
1	13-A	178	ASP	3.2
1	14-A	178	ASP	3.2
1	15-A	178	ASP	3.2
1	16-A	178	ASP	3.2
1	1-B	109	PRO	3.2
1	2-B	109	PRO	3.2
1	3-B	109	PRO	3.2
1	4-B	109	PRO	3.2
1	5-B	109	PRO	3.2
1	6-B	109	PRO	3.2
1	7-B	109	PRO	3.2
1	8-B	109	PRO	3.2
1	9-B	109	PRO	3.2
1	10-B	109	PRO	3.2
1	11-B	109	PRO	3.2
1	12-B	109	PRO	3.2
1	13-B	109	PRO	3.2
1	14-B	109	PRO	3.2
1	15-B	109	PRO	3.2
1	16-B	109	PRO	3.2
1	1-A	243	ASP	3.2
1	2-A	243	ASP	3.2
1	3-A	243	ASP	3.2
1	4-A	243	ASP	3.2
1	5-A	243	ASP	3.2
1	6-A	243	ASP	3.2
1	7-A	243	ASP	3.2
1	8-A	243	ASP	3.2
1	9-A	243	ASP	3.2
1	10-A	243	ASP	3.2
1	11-A	243	ASP	3.2
1	12-A	243	ASP	3.2
1	13-A	243	ASP	3.2
1	14-A	243	ASP	3.2
1	15-A	243	ASP	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	16-A	243	ASP	3.2
1	1-A	219	TRP	3.2
1	2-A	219	TRP	3.2
1	3-A	219	TRP	3.2
1	4-A	219	TRP	3.2
1	5-A	219	TRP	3.2
1	6-A	219	TRP	3.2
1	7-A	219	TRP	3.2
1	8-A	219	TRP	3.2
1	9-A	219	TRP	3.2
1	10-A	219	TRP	3.2
1	11-A	219	TRP	3.2
1	12-A	219	TRP	3.2
1	13-A	219	TRP	3.2
1	14-A	219	TRP	3.2
1	15-A	219	TRP	3.2
1	16-A	219	TRP	3.2
1	1-B	208	TYR	3.1
1	2-B	208	TYR	3.1
1	3-B	208	TYR	3.1
1	4-B	208	TYR	3.1
1	5-B	208	TYR	3.1
1	6-B	208	TYR	3.1
1	7-B	208	TYR	3.1
1	8-B	208	TYR	3.1
1	9-B	208	TYR	3.1
1	10-B	208	TYR	3.1
1	11-B	208	TYR	3.1
1	12-B	208	TYR	3.1
1	13-B	208	TYR	3.1
1	14-B	208	TYR	3.1
1	15-B	208	TYR	3.1
1	16-B	208	TYR	3.1
1	1-B	212	GLY	3.1
1	2-B	212	GLY	3.1
1	3-B	212	GLY	3.1
1	4-B	212	GLY	3.1
1	5-B	212	GLY	3.1
1	6-B	212	GLY	3.1
1	7-B	212	GLY	3.1
1	8-B	212	GLY	3.1
1	9-B	212	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	10-B	212	GLY	3.1
1	11-B	212	GLY	3.1
1	12-B	212	GLY	3.1
1	13-B	212	GLY	3.1
1	14-B	212	GLY	3.1
1	15-B	212	GLY	3.1
1	16-B	212	GLY	3.1
1	1-C	183	LEU	3.1
1	2-C	183	LEU	3.1
1	3-C	183	LEU	3.1
1	4-C	183	LEU	3.1
1	5-C	183	LEU	3.1
1	6-C	183	LEU	3.1
1	7-C	183	LEU	3.1
1	8-C	183	LEU	3.1
1	9-C	183	LEU	3.1
1	10-C	183	LEU	3.1
1	11-C	183	LEU	3.1
1	12-C	183	LEU	3.1
1	13-C	183	LEU	3.1
1	14-C	183	LEU	3.1
1	15-C	183	LEU	3.1
1	16-C	183	LEU	3.1
1	1-A	45	THR	3.1
1	1-B	176	THR	3.1
1	2-A	45	THR	3.1
1	2-B	176	THR	3.1
1	3-A	45	THR	3.1
1	3-B	176	THR	3.1
1	4-A	45	THR	3.1
1	4-B	176	THR	3.1
1	5-A	45	THR	3.1
1	5-B	176	THR	3.1
1	6-A	45	THR	3.1
1	6-B	176	THR	3.1
1	7-A	45	THR	3.1
1	7-B	176	THR	3.1
1	8-A	45	THR	3.1
1	8-B	176	THR	3.1
1	9-A	45	THR	3.1
1	9-B	176	THR	3.1
1	10-A	45	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	10-B	176	THR	3.1
1	11-A	45	THR	3.1
1	11-B	176	THR	3.1
1	12-A	45	THR	3.1
1	12-B	176	THR	3.1
1	13-A	45	THR	3.1
1	13-B	176	THR	3.1
1	14-A	45	THR	3.1
1	14-B	176	THR	3.1
1	15-A	45	THR	3.1
1	15-B	176	THR	3.1
1	16-A	45	THR	3.1
1	16-B	176	THR	3.1
1	1-C	165	LYS	3.1
1	2-C	165	LYS	3.1
1	3-C	165	LYS	3.1
1	4-C	165	LYS	3.1
1	5-C	165	LYS	3.1
1	6-C	165	LYS	3.1
1	7-C	165	LYS	3.1
1	8-C	165	LYS	3.1
1	9-C	165	LYS	3.1
1	10-C	165	LYS	3.1
1	11-C	165	LYS	3.1
1	12-C	165	LYS	3.1
1	13-C	165	LYS	3.1
1	14-C	165	LYS	3.1
1	15-C	165	LYS	3.1
1	16-C	165	LYS	3.1
1	1-B	100	TRP	3.1
1	2-B	100	TRP	3.1
1	3-B	100	TRP	3.1
1	4-B	100	TRP	3.1
1	5-B	100	TRP	3.1
1	6-B	100	TRP	3.1
1	7-B	100	TRP	3.1
1	8-B	100	TRP	3.1
1	9-B	100	TRP	3.1
1	10-B	100	TRP	3.1
1	11-B	100	TRP	3.1
1	12-B	100	TRP	3.1
1	13-B	100	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	14-B	100	TRP	3.1
1	15-B	100	TRP	3.1
1	16-B	100	TRP	3.1
1	1-A	212	GLY	3.0
1	2-A	212	GLY	3.0
1	3-A	212	GLY	3.0
1	4-A	212	GLY	3.0
1	5-A	212	GLY	3.0
1	6-A	212	GLY	3.0
1	7-A	212	GLY	3.0
1	8-A	212	GLY	3.0
1	9-A	212	GLY	3.0
1	10-A	212	GLY	3.0
1	11-A	212	GLY	3.0
1	12-A	212	GLY	3.0
1	13-A	212	GLY	3.0
1	14-A	212	GLY	3.0
1	15-A	212	GLY	3.0
1	16-A	212	GLY	3.0
1	1-B	164	ALA	3.0
1	2-B	164	ALA	3.0
1	3-B	164	ALA	3.0
1	4-B	164	ALA	3.0
1	5-B	164	ALA	3.0
1	6-B	164	ALA	3.0
1	7-B	164	ALA	3.0
1	8-B	164	ALA	3.0
1	9-B	164	ALA	3.0
1	10-B	164	ALA	3.0
1	11-B	164	ALA	3.0
1	12-B	164	ALA	3.0
1	13-B	164	ALA	3.0
1	14-B	164	ALA	3.0
1	15-B	164	ALA	3.0
1	16-B	164	ALA	3.0
1	1-A	166	GLU	3.0
1	2-A	166	GLU	3.0
1	3-A	166	GLU	3.0
1	4-A	166	GLU	3.0
1	5-A	166	GLU	3.0
1	6-A	166	GLU	3.0
1	7-A	166	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	8-A	166	GLU	3.0
1	9-A	166	GLU	3.0
1	10-A	166	GLU	3.0
1	11-A	166	GLU	3.0
1	12-A	166	GLU	3.0
1	13-A	166	GLU	3.0
1	14-A	166	GLU	3.0
1	15-A	166	GLU	3.0
1	16-A	166	GLU	3.0
1	1-B	96	LEU	3.0
1	2-B	96	LEU	3.0
1	3-B	96	LEU	3.0
1	4-B	96	LEU	3.0
1	5-B	96	LEU	3.0
1	6-B	96	LEU	3.0
1	7-B	96	LEU	3.0
1	8-B	96	LEU	3.0
1	9-B	96	LEU	3.0
1	10-B	96	LEU	3.0
1	11-B	96	LEU	3.0
1	12-B	96	LEU	3.0
1	13-B	96	LEU	3.0
1	14-B	96	LEU	3.0
1	15-B	96	LEU	3.0
1	16-B	96	LEU	3.0
1	1-C	103	LEU	2.9
1	2-C	103	LEU	2.9
1	3-C	103	LEU	2.9
1	4-C	103	LEU	2.9
1	5-C	103	LEU	2.9
1	6-C	103	LEU	2.9
1	7-C	103	LEU	2.9
1	8-C	103	LEU	2.9
1	9-C	103	LEU	2.9
1	10-C	103	LEU	2.9
1	11-C	103	LEU	2.9
1	12-C	103	LEU	2.9
1	13-C	103	LEU	2.9
1	14-C	103	LEU	2.9
1	15-C	103	LEU	2.9
1	16-C	103	LEU	2.9
1	1-A	240	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	2-A	240	ARG	2.9
1	3-A	240	ARG	2.9
1	4-A	240	ARG	2.9
1	5-A	240	ARG	2.9
1	6-A	240	ARG	2.9
1	7-A	240	ARG	2.9
1	8-A	240	ARG	2.9
1	9-A	240	ARG	2.9
1	10-A	240	ARG	2.9
1	11-A	240	ARG	2.9
1	12-A	240	ARG	2.9
1	13-A	240	ARG	2.9
1	14-A	240	ARG	2.9
1	15-A	240	ARG	2.9
1	16-A	240	ARG	2.9
1	1-A	151	VAL	2.8
1	2-A	151	VAL	2.8
1	3-A	151	VAL	2.8
1	4-A	151	VAL	2.8
1	5-A	151	VAL	2.8
1	6-A	151	VAL	2.8
1	7-A	151	VAL	2.8
1	8-A	151	VAL	2.8
1	9-A	151	VAL	2.8
1	10-A	151	VAL	2.8
1	11-A	151	VAL	2.8
1	12-A	151	VAL	2.8
1	13-A	151	VAL	2.8
1	14-A	151	VAL	2.8
1	15-A	151	VAL	2.8
1	16-A	151	VAL	2.8
1	1-A	224	THR	2.8
1	2-A	224	THR	2.8
1	3-A	224	THR	2.8
1	4-A	224	THR	2.8
1	5-A	224	THR	2.8
1	6-A	224	THR	2.8
1	7-A	224	THR	2.8
1	8-A	224	THR	2.8
1	9-A	224	THR	2.8
1	10-A	224	THR	2.8
1	11-A	224	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	12-A	224	THR	2.8
1	13-A	224	THR	2.8
1	14-A	224	THR	2.8
1	15-A	224	THR	2.8
1	16-A	224	THR	2.8
1	1-B	73	SER	2.8
1	2-B	73	SER	2.8
1	3-B	73	SER	2.8
1	4-B	73	SER	2.8
1	5-B	73	SER	2.8
1	6-B	73	SER	2.8
1	7-B	73	SER	2.8
1	8-B	73	SER	2.8
1	9-B	73	SER	2.8
1	10-B	73	SER	2.8
1	11-B	73	SER	2.8
1	12-B	73	SER	2.8
1	13-B	73	SER	2.8
1	14-B	73	SER	2.8
1	15-B	73	SER	2.8
1	16-B	73	SER	2.8
1	1-B	121	THR	2.8
1	2-B	121	THR	2.8
1	3-B	121	THR	2.8
1	4-B	121	THR	2.8
1	5-B	121	THR	2.8
1	6-B	121	THR	2.8
1	7-B	121	THR	2.8
1	8-B	121	THR	2.8
1	9-B	121	THR	2.8
1	10-B	121	THR	2.8
1	11-B	121	THR	2.8
1	12-B	121	THR	2.8
1	13-B	121	THR	2.8
1	14-B	121	THR	2.8
1	15-B	121	THR	2.8
1	16-B	121	THR	2.8
1	1-A	87	SER	2.7
1	2-A	87	SER	2.7
1	3-A	87	SER	2.7
1	4-A	87	SER	2.7
1	5-A	87	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	6-A	87	SER	2.7
1	7-A	87	SER	2.7
1	8-A	87	SER	2.7
1	9-A	87	SER	2.7
1	10-A	87	SER	2.7
1	11-A	87	SER	2.7
1	12-A	87	SER	2.7
1	13-A	87	SER	2.7
1	14-A	87	SER	2.7
1	15-A	87	SER	2.7
1	16-A	87	SER	2.7
1	1-A	199	CYS	2.7
1	2-A	199	CYS	2.7
1	3-A	199	CYS	2.7
1	4-A	199	CYS	2.7
1	5-A	199	CYS	2.7
1	6-A	199	CYS	2.7
1	7-A	199	CYS	2.7
1	8-A	199	CYS	2.7
1	9-A	199	CYS	2.7
1	10-A	199	CYS	2.7
1	11-A	199	CYS	2.7
1	12-A	199	CYS	2.7
1	13-A	199	CYS	2.7
1	14-A	199	CYS	2.7
1	15-A	199	CYS	2.7
1	16-A	199	CYS	2.7
1	1-C	31	ALA	2.7
1	2-C	31	ALA	2.7
1	3-C	31	ALA	2.7
1	4-C	31	ALA	2.7
1	5-C	31	ALA	2.7
1	6-C	31	ALA	2.7
1	7-C	31	ALA	2.7
1	8-C	31	ALA	2.7
1	9-C	31	ALA	2.7
1	10-C	31	ALA	2.7
1	11-C	31	ALA	2.7
1	12-C	31	ALA	2.7
1	13-C	31	ALA	2.7
1	14-C	31	ALA	2.7
1	15-C	31	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	16-C	31	ALA	2.7
1	1-A	213	ILE	2.7
1	2-A	213	ILE	2.7
1	3-A	213	ILE	2.7
1	4-A	213	ILE	2.7
1	5-A	213	ILE	2.7
1	6-A	213	ILE	2.7
1	7-A	213	ILE	2.7
1	8-A	213	ILE	2.7
1	9-A	213	ILE	2.7
1	10-A	213	ILE	2.7
1	11-A	213	ILE	2.7
1	12-A	213	ILE	2.7
1	13-A	213	ILE	2.7
1	14-A	213	ILE	2.7
1	15-A	213	ILE	2.7
1	16-A	213	ILE	2.7
1	1-A	84	GLN	2.7
1	2-A	84	GLN	2.7
1	3-A	84	GLN	2.7
1	4-A	84	GLN	2.7
1	5-A	84	GLN	2.7
1	6-A	84	GLN	2.7
1	7-A	84	GLN	2.7
1	8-A	84	GLN	2.7
1	9-A	84	GLN	2.7
1	10-A	84	GLN	2.7
1	11-A	84	GLN	2.7
1	12-A	84	GLN	2.7
1	13-A	84	GLN	2.7
1	14-A	84	GLN	2.7
1	15-A	84	GLN	2.7
1	16-A	84	GLN	2.7
1	1-C	98	ALA	2.6
1	2-C	98	ALA	2.6
1	3-C	98	ALA	2.6
1	4-C	98	ALA	2.6
1	5-C	98	ALA	2.6
1	6-C	98	ALA	2.6
1	7-C	98	ALA	2.6
1	8-C	98	ALA	2.6
1	9-C	98	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	10-C	98	ALA	2.6
1	11-C	98	ALA	2.6
1	12-C	98	ALA	2.6
1	13-C	98	ALA	2.6
1	14-C	98	ALA	2.6
1	15-C	98	ALA	2.6
1	16-C	98	ALA	2.6
1	1-A	94	GLN	2.6
1	2-A	94	GLN	2.6
1	3-A	94	GLN	2.6
1	4-A	94	GLN	2.6
1	5-A	94	GLN	2.6
1	6-A	94	GLN	2.6
1	7-A	94	GLN	2.6
1	8-A	94	GLN	2.6
1	9-A	94	GLN	2.6
1	10-A	94	GLN	2.6
1	11-A	94	GLN	2.6
1	12-A	94	GLN	2.6
1	13-A	94	GLN	2.6
1	14-A	94	GLN	2.6
1	15-A	94	GLN	2.6
1	16-A	94	GLN	2.6
1	1-B	101	GLU	2.6
1	2-B	101	GLU	2.6
1	3-B	101	GLU	2.6
1	4-B	101	GLU	2.6
1	5-B	101	GLU	2.6
1	6-B	101	GLU	2.6
1	7-B	101	GLU	2.6
1	8-B	101	GLU	2.6
1	9-B	101	GLU	2.6
1	10-B	101	GLU	2.6
1	11-B	101	GLU	2.6
1	12-B	101	GLU	2.6
1	13-B	101	GLU	2.6
1	14-B	101	GLU	2.6
1	15-B	101	GLU	2.6
1	16-B	101	GLU	2.6
1	1-B	220	HIS	2.6
1	2-B	220	HIS	2.6
1	3-B	220	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	4-B	220	HIS	2.6
1	5-B	220	HIS	2.6
1	6-B	220	HIS	2.6
1	7-B	220	HIS	2.6
1	8-B	220	HIS	2.6
1	9-B	220	HIS	2.6
1	10-B	220	HIS	2.6
1	11-B	220	HIS	2.6
1	12-B	220	HIS	2.6
1	13-B	220	HIS	2.6
1	14-B	220	HIS	2.6
1	15-B	220	HIS	2.6
1	16-B	220	HIS	2.6
1	1-A	113	GLY	2.6
1	2-A	113	GLY	2.6
1	3-A	113	GLY	2.6
1	4-A	113	GLY	2.6
1	5-A	113	GLY	2.6
1	6-A	113	GLY	2.6
1	7-A	113	GLY	2.6
1	8-A	113	GLY	2.6
1	9-A	113	GLY	2.6
1	10-A	113	GLY	2.6
1	11-A	113	GLY	2.6
1	12-A	113	GLY	2.6
1	13-A	113	GLY	2.6
1	14-A	113	GLY	2.6
1	15-A	113	GLY	2.6
1	16-A	113	GLY	2.6
1	1-B	72	ASN	2.6
1	2-B	72	ASN	2.6
1	3-B	72	ASN	2.6
1	4-B	72	ASN	2.6
1	5-B	72	ASN	2.6
1	6-B	72	ASN	2.6
1	7-B	72	ASN	2.6
1	8-B	72	ASN	2.6
1	9-B	72	ASN	2.6
1	10-B	72	ASN	2.6
1	11-B	72	ASN	2.6
1	12-B	72	ASN	2.6
1	13-B	72	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	14-B	72	ASN	2.6
1	15-B	72	ASN	2.6
1	16-B	72	ASN	2.6
1	1-B	123	HIS	2.6
1	2-B	123	HIS	2.6
1	3-B	123	HIS	2.6
1	4-B	123	HIS	2.6
1	5-B	123	HIS	2.6
1	6-B	123	HIS	2.6
1	7-B	123	HIS	2.6
1	8-B	123	HIS	2.6
1	9-B	123	HIS	2.6
1	10-B	123	HIS	2.6
1	11-B	123	HIS	2.6
1	12-B	123	HIS	2.6
1	13-B	123	HIS	2.6
1	14-B	123	HIS	2.6
1	15-B	123	HIS	2.6
1	16-B	123	HIS	2.6
1	1-A	41	ASP	2.5
1	2-A	41	ASP	2.5
1	3-A	41	ASP	2.5
1	4-A	41	ASP	2.5
1	5-A	41	ASP	2.5
1	6-A	41	ASP	2.5
1	7-A	41	ASP	2.5
1	8-A	41	ASP	2.5
1	9-A	41	ASP	2.5
1	10-A	41	ASP	2.5
1	11-A	41	ASP	2.5
1	12-A	41	ASP	2.5
1	13-A	41	ASP	2.5
1	14-A	41	ASP	2.5
1	15-A	41	ASP	2.5
1	16-A	41	ASP	2.5
1	1-C	90	SER	2.5
1	1-C	212	GLY	2.5
1	2-C	90	SER	2.5
1	2-C	212	GLY	2.5
1	3-C	90	SER	2.5
1	3-C	212	GLY	2.5
1	4-C	90	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	4-C	212	GLY	2.5
1	5-C	90	SER	2.5
1	5-C	212	GLY	2.5
1	6-C	90	SER	2.5
1	6-C	212	GLY	2.5
1	7-C	90	SER	2.5
1	7-C	212	GLY	2.5
1	8-C	90	SER	2.5
1	8-C	212	GLY	2.5
1	9-C	90	SER	2.5
1	9-C	212	GLY	2.5
1	10-C	90	SER	2.5
1	10-C	212	GLY	2.5
1	11-C	90	SER	2.5
1	11-C	212	GLY	2.5
1	12-C	90	SER	2.5
1	12-C	212	GLY	2.5
1	13-C	90	SER	2.5
1	13-C	212	GLY	2.5
1	14-C	90	SER	2.5
1	14-C	212	GLY	2.5
1	15-C	90	SER	2.5
1	15-C	212	GLY	2.5
1	16-C	90	SER	2.5
1	16-C	212	GLY	2.5
1	1-A	93	VAL	2.5
1	2-A	93	VAL	2.5
1	3-A	93	VAL	2.5
1	4-A	93	VAL	2.5
1	5-A	93	VAL	2.5
1	6-A	93	VAL	2.5
1	7-A	93	VAL	2.5
1	8-A	93	VAL	2.5
1	9-A	93	VAL	2.5
1	10-A	93	VAL	2.5
1	11-A	93	VAL	2.5
1	12-A	93	VAL	2.5
1	13-A	93	VAL	2.5
1	14-A	93	VAL	2.5
1	15-A	93	VAL	2.5
1	16-A	93	VAL	2.5
1	1-A	85	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	2-A	85	GLY	2.5
1	3-A	85	GLY	2.5
1	4-A	85	GLY	2.5
1	5-A	85	GLY	2.5
1	6-A	85	GLY	2.5
1	7-A	85	GLY	2.5
1	8-A	85	GLY	2.5
1	9-A	85	GLY	2.5
1	10-A	85	GLY	2.5
1	11-A	85	GLY	2.5
1	12-A	85	GLY	2.5
1	13-A	85	GLY	2.5
1	14-A	85	GLY	2.5
1	15-A	85	GLY	2.5
1	16-A	85	GLY	2.5
1	1-C	104	GLN	2.5
1	2-C	104	GLN	2.5
1	3-C	104	GLN	2.5
1	4-C	104	GLN	2.5
1	5-C	104	GLN	2.5
1	6-C	104	GLN	2.5
1	7-C	104	GLN	2.5
1	8-C	104	GLN	2.5
1	9-C	104	GLN	2.5
1	10-C	104	GLN	2.5
1	11-C	104	GLN	2.5
1	12-C	104	GLN	2.5
1	13-C	104	GLN	2.5
1	14-C	104	GLN	2.5
1	15-C	104	GLN	2.5
1	16-C	104	GLN	2.5
1	1-A	183	LEU	2.5
1	2-A	183	LEU	2.5
1	3-A	183	LEU	2.5
1	4-A	183	LEU	2.5
1	5-A	183	LEU	2.5
1	6-A	183	LEU	2.5
1	7-A	183	LEU	2.5
1	8-A	183	LEU	2.5
1	9-A	183	LEU	2.5
1	10-A	183	LEU	2.5
1	11-A	183	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	12-A	183	LEU	2.5
1	13-A	183	LEU	2.5
1	14-A	183	LEU	2.5
1	15-A	183	LEU	2.5
1	16-A	183	LEU	2.5
1	1-B	93	VAL	2.4
1	2-B	93	VAL	2.4
1	3-B	93	VAL	2.4
1	4-B	93	VAL	2.4
1	5-B	93	VAL	2.4
1	6-B	93	VAL	2.4
1	7-B	93	VAL	2.4
1	8-B	93	VAL	2.4
1	9-B	93	VAL	2.4
1	10-B	93	VAL	2.4
1	11-B	93	VAL	2.4
1	12-B	93	VAL	2.4
1	13-B	93	VAL	2.4
1	14-B	93	VAL	2.4
1	15-B	93	VAL	2.4
1	16-B	93	VAL	2.4
1	1-C	88	PRO	2.4
1	2-C	88	PRO	2.4
1	3-C	88	PRO	2.4
1	4-C	88	PRO	2.4
1	5-C	88	PRO	2.4
1	6-C	88	PRO	2.4
1	7-C	88	PRO	2.4
1	8-C	88	PRO	2.4
1	9-C	88	PRO	2.4
1	10-C	88	PRO	2.4
1	11-C	88	PRO	2.4
1	12-C	88	PRO	2.4
1	13-C	88	PRO	2.4
1	14-C	88	PRO	2.4
1	15-C	88	PRO	2.4
1	16-C	88	PRO	2.4
1	1-A	100	TRP	2.4
1	2-A	100	TRP	2.4
1	3-A	100	TRP	2.4
1	4-A	100	TRP	2.4
1	5-A	100	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	6-A	100	TRP	2.4
1	7-A	100	TRP	2.4
1	8-A	100	TRP	2.4
1	9-A	100	TRP	2.4
1	10-A	100	TRP	2.4
1	11-A	100	TRP	2.4
1	12-A	100	TRP	2.4
1	13-A	100	TRP	2.4
1	14-A	100	TRP	2.4
1	15-A	100	TRP	2.4
1	16-A	100	TRP	2.4
1	1-A	119	ALA	2.4
1	2-A	119	ALA	2.4
1	3-A	119	ALA	2.4
1	4-A	119	ALA	2.4
1	5-A	119	ALA	2.4
1	6-A	119	ALA	2.4
1	7-A	119	ALA	2.4
1	8-A	119	ALA	2.4
1	9-A	119	ALA	2.4
1	10-A	119	ALA	2.4
1	11-A	119	ALA	2.4
1	12-A	119	ALA	2.4
1	13-A	119	ALA	2.4
1	14-A	119	ALA	2.4
1	15-A	119	ALA	2.4
1	16-A	119	ALA	2.4
1	1-B	41	ASP	2.4
1	2-B	41	ASP	2.4
1	3-B	41	ASP	2.4
1	4-B	41	ASP	2.4
1	5-B	41	ASP	2.4
1	6-B	41	ASP	2.4
1	7-B	41	ASP	2.4
1	8-B	41	ASP	2.4
1	9-B	41	ASP	2.4
1	10-B	41	ASP	2.4
1	11-B	41	ASP	2.4
1	12-B	41	ASP	2.4
1	13-B	41	ASP	2.4
1	14-B	41	ASP	2.4
1	15-B	41	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	16-B	41	ASP	2.4
1	1-A	28	GLU	2.4
1	2-A	28	GLU	2.4
1	3-A	28	GLU	2.4
1	4-A	28	GLU	2.4
1	5-A	28	GLU	2.4
1	6-A	28	GLU	2.4
1	7-A	28	GLU	2.4
1	8-A	28	GLU	2.4
1	9-A	28	GLU	2.4
1	10-A	28	GLU	2.4
1	11-A	28	GLU	2.4
1	12-A	28	GLU	2.4
1	13-A	28	GLU	2.4
1	14-A	28	GLU	2.4
1	15-A	28	GLU	2.4
1	16-A	28	GLU	2.4
1	1-B	55	ALA	2.3
1	2-B	55	ALA	2.3
1	3-B	55	ALA	2.3
1	4-B	55	ALA	2.3
1	5-B	55	ALA	2.3
1	6-B	55	ALA	2.3
1	7-B	55	ALA	2.3
1	8-B	55	ALA	2.3
1	9-B	55	ALA	2.3
1	10-B	55	ALA	2.3
1	11-B	55	ALA	2.3
1	12-B	55	ALA	2.3
1	13-B	55	ALA	2.3
1	14-B	55	ALA	2.3
1	15-B	55	ALA	2.3
1	16-B	55	ALA	2.3
1	1-A	108	ARG	2.3
1	2-A	108	ARG	2.3
1	3-A	108	ARG	2.3
1	4-A	108	ARG	2.3
1	5-A	108	ARG	2.3
1	6-A	108	ARG	2.3
1	7-A	108	ARG	2.3
1	8-A	108	ARG	2.3
1	9-A	108	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	10-A	108	ARG	2.3
1	11-A	108	ARG	2.3
1	12-A	108	ARG	2.3
1	13-A	108	ARG	2.3
1	14-A	108	ARG	2.3
1	15-A	108	ARG	2.3
1	16-A	108	ARG	2.3
1	1-B	46	PRO	2.3
1	2-B	46	PRO	2.3
1	3-B	46	PRO	2.3
1	4-B	46	PRO	2.3
1	5-B	46	PRO	2.3
1	6-B	46	PRO	2.3
1	7-B	46	PRO	2.3
1	8-B	46	PRO	2.3
1	9-B	46	PRO	2.3
1	10-B	46	PRO	2.3
1	11-B	46	PRO	2.3
1	12-B	46	PRO	2.3
1	13-B	46	PRO	2.3
1	14-B	46	PRO	2.3
1	15-B	46	PRO	2.3
1	16-B	46	PRO	2.3
1	1-B	237	ARG	2.3
1	2-B	237	ARG	2.3
1	3-B	237	ARG	2.3
1	4-B	237	ARG	2.3
1	5-B	237	ARG	2.3
1	6-B	237	ARG	2.3
1	7-B	237	ARG	2.3
1	8-B	237	ARG	2.3
1	9-B	237	ARG	2.3
1	10-B	237	ARG	2.3
1	11-B	237	ARG	2.3
1	12-B	237	ARG	2.3
1	13-B	237	ARG	2.3
1	14-B	237	ARG	2.3
1	15-B	237	ARG	2.3
1	16-B	237	ARG	2.3
1	1-C	247	ASN	2.3
1	2-C	247	ASN	2.3
1	3-C	247	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	4-C	247	ASN	2.3
1	5-C	247	ASN	2.3
1	6-C	247	ASN	2.3
1	7-C	247	ASN	2.3
1	8-C	247	ASN	2.3
1	9-C	247	ASN	2.3
1	10-C	247	ASN	2.3
1	11-C	247	ASN	2.3
1	12-C	247	ASN	2.3
1	13-C	247	ASN	2.3
1	14-C	247	ASN	2.3
1	15-C	247	ASN	2.3
1	16-C	247	ASN	2.3
1	1-A	186	LEU	2.3
1	2-A	186	LEU	2.3
1	3-A	186	LEU	2.3
1	4-A	186	LEU	2.3
1	5-A	186	LEU	2.3
1	6-A	186	LEU	2.3
1	7-A	186	LEU	2.3
1	8-A	186	LEU	2.3
1	9-A	186	LEU	2.3
1	10-A	186	LEU	2.3
1	11-A	186	LEU	2.3
1	12-A	186	LEU	2.3
1	13-A	186	LEU	2.3
1	14-A	186	LEU	2.3
1	15-A	186	LEU	2.3
1	16-A	186	LEU	2.3
1	1-C	99	ALA	2.2
1	2-C	99	ALA	2.2
1	3-C	99	ALA	2.2
1	4-C	99	ALA	2.2
1	5-C	99	ALA	2.2
1	6-C	99	ALA	2.2
1	7-C	99	ALA	2.2
1	8-C	99	ALA	2.2
1	9-C	99	ALA	2.2
1	10-C	99	ALA	2.2
1	11-C	99	ALA	2.2
1	12-C	99	ALA	2.2
1	13-C	99	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	14-C	99	ALA	2.2
1	15-C	99	ALA	2.2
1	16-C	99	ALA	2.2
1	1-A	117	GLN	2.2
1	2-A	117	GLN	2.2
1	3-A	117	GLN	2.2
1	4-A	117	GLN	2.2
1	5-A	117	GLN	2.2
1	6-A	117	GLN	2.2
1	7-A	117	GLN	2.2
1	8-A	117	GLN	2.2
1	9-A	117	GLN	2.2
1	10-A	117	GLN	2.2
1	11-A	117	GLN	2.2
1	12-A	117	GLN	2.2
1	13-A	117	GLN	2.2
1	14-A	117	GLN	2.2
1	15-A	117	GLN	2.2
1	16-A	117	GLN	2.2
1	1-B	217	ASN	2.2
1	2-B	217	ASN	2.2
1	3-B	217	ASN	2.2
1	4-B	217	ASN	2.2
1	5-B	217	ASN	2.2
1	6-B	217	ASN	2.2
1	7-B	217	ASN	2.2
1	8-B	217	ASN	2.2
1	9-B	217	ASN	2.2
1	10-B	217	ASN	2.2
1	11-B	217	ASN	2.2
1	12-B	217	ASN	2.2
1	13-B	217	ASN	2.2
1	14-B	217	ASN	2.2
1	15-B	217	ASN	2.2
1	16-B	217	ASN	2.2
1	1-A	182	ARG	2.2
1	2-A	182	ARG	2.2
1	3-A	182	ARG	2.2
1	4-A	182	ARG	2.2
1	5-A	182	ARG	2.2
1	6-A	182	ARG	2.2
1	7-A	182	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	8-A	182	ARG	2.2
1	9-A	182	ARG	2.2
1	10-A	182	ARG	2.2
1	11-A	182	ARG	2.2
1	12-A	182	ARG	2.2
1	13-A	182	ARG	2.2
1	14-A	182	ARG	2.2
1	15-A	182	ARG	2.2
1	16-A	182	ARG	2.2
1	1-A	181	ASP	2.2
1	2-A	181	ASP	2.2
1	3-A	181	ASP	2.2
1	4-A	181	ASP	2.2
1	5-A	181	ASP	2.2
1	6-A	181	ASP	2.2
1	7-A	181	ASP	2.2
1	8-A	181	ASP	2.2
1	9-A	181	ASP	2.2
1	10-A	181	ASP	2.2
1	11-A	181	ASP	2.2
1	12-A	181	ASP	2.2
1	13-A	181	ASP	2.2
1	14-A	181	ASP	2.2
1	15-A	181	ASP	2.2
1	16-A	181	ASP	2.2
1	1-A	101	GLU	2.2
1	2-A	101	GLU	2.2
1	3-A	101	GLU	2.2
1	4-A	101	GLU	2.2
1	5-A	101	GLU	2.2
1	6-A	101	GLU	2.2
1	7-A	101	GLU	2.2
1	8-A	101	GLU	2.2
1	9-A	101	GLU	2.2
1	10-A	101	GLU	2.2
1	11-A	101	GLU	2.2
1	12-A	101	GLU	2.2
1	13-A	101	GLU	2.2
1	14-A	101	GLU	2.2
1	15-A	101	GLU	2.2
1	16-A	101	GLU	2.2
1	1-A	149	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	2-A	149	ALA	2.2
1	3-A	149	ALA	2.2
1	4-A	149	ALA	2.2
1	5-A	149	ALA	2.2
1	6-A	149	ALA	2.2
1	7-A	149	ALA	2.2
1	8-A	149	ALA	2.2
1	9-A	149	ALA	2.2
1	10-A	149	ALA	2.2
1	11-A	149	ALA	2.2
1	12-A	149	ALA	2.2
1	13-A	149	ALA	2.2
1	14-A	149	ALA	2.2
1	15-A	149	ALA	2.2
1	16-A	149	ALA	2.2
1	1-A	122	HIS	2.2
1	2-A	122	HIS	2.2
1	3-A	122	HIS	2.2
1	4-A	122	HIS	2.2
1	5-A	122	HIS	2.2
1	6-A	122	HIS	2.2
1	7-A	122	HIS	2.2
1	8-A	122	HIS	2.2
1	9-A	122	HIS	2.2
1	10-A	122	HIS	2.2
1	11-A	122	HIS	2.2
1	12-A	122	HIS	2.2
1	13-A	122	HIS	2.2
1	14-A	122	HIS	2.2
1	15-A	122	HIS	2.2
1	16-A	122	HIS	2.2
1	1-B	122	HIS	2.2
1	2-B	122	HIS	2.2
1	3-B	122	HIS	2.2
1	4-B	122	HIS	2.2
1	5-B	122	HIS	2.2
1	6-B	122	HIS	2.2
1	7-B	122	HIS	2.2
1	8-B	122	HIS	2.2
1	9-B	122	HIS	2.2
1	10-B	122	HIS	2.2
1	11-B	122	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	12-B	122	HIS	2.2
1	13-B	122	HIS	2.2
1	14-B	122	HIS	2.2
1	15-B	122	HIS	2.2
1	16-B	122	HIS	2.2
1	1-B	167	GLY	2.1
1	2-B	167	GLY	2.1
1	3-B	167	GLY	2.1
1	4-B	167	GLY	2.1
1	5-B	167	GLY	2.1
1	6-B	167	GLY	2.1
1	7-B	167	GLY	2.1
1	8-B	167	GLY	2.1
1	9-B	167	GLY	2.1
1	10-B	167	GLY	2.1
1	11-B	167	GLY	2.1
1	12-B	167	GLY	2.1
1	13-B	167	GLY	2.1
1	14-B	167	GLY	2.1
1	15-B	167	GLY	2.1
1	16-B	167	GLY	2.1
1	1-A	221	LEU	2.1
1	2-A	221	LEU	2.1
1	3-A	221	LEU	2.1
1	4-A	221	LEU	2.1
1	5-A	221	LEU	2.1
1	6-A	221	LEU	2.1
1	7-A	221	LEU	2.1
1	8-A	221	LEU	2.1
1	9-A	221	LEU	2.1
1	10-A	221	LEU	2.1
1	11-A	221	LEU	2.1
1	12-A	221	LEU	2.1
1	13-A	221	LEU	2.1
1	14-A	221	LEU	2.1
1	15-A	221	LEU	2.1
1	16-A	221	LEU	2.1
1	1-A	187	GLU	2.1
1	1-A	223	PRO	2.1
1	2-A	187	GLU	2.1
1	2-A	223	PRO	2.1
1	3-A	187	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	3-A	223	PRO	2.1
1	4-A	187	GLU	2.1
1	4-A	223	PRO	2.1
1	5-A	187	GLU	2.1
1	5-A	223	PRO	2.1
1	6-A	187	GLU	2.1
1	6-A	223	PRO	2.1
1	7-A	187	GLU	2.1
1	7-A	223	PRO	2.1
1	8-A	187	GLU	2.1
1	8-A	223	PRO	2.1
1	9-A	187	GLU	2.1
1	9-A	223	PRO	2.1
1	10-A	187	GLU	2.1
1	10-A	223	PRO	2.1
1	11-A	187	GLU	2.1
1	11-A	223	PRO	2.1
1	12-A	187	GLU	2.1
1	12-A	223	PRO	2.1
1	13-A	187	GLU	2.1
1	13-A	223	PRO	2.1
1	14-A	187	GLU	2.1
1	14-A	223	PRO	2.1
1	15-A	187	GLU	2.1
1	15-A	223	PRO	2.1
1	16-A	187	GLU	2.1
1	16-A	223	PRO	2.1
1	1-A	244	ARG	2.1
1	2-A	244	ARG	2.1
1	3-A	244	ARG	2.1
1	4-A	244	ARG	2.1
1	5-A	244	ARG	2.1
1	6-A	244	ARG	2.1
1	7-A	244	ARG	2.1
1	8-A	244	ARG	2.1
1	9-A	244	ARG	2.1
1	10-A	244	ARG	2.1
1	11-A	244	ARG	2.1
1	12-A	244	ARG	2.1
1	13-A	244	ARG	2.1
1	14-A	244	ARG	2.1
1	15-A	244	ARG	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	16-A	244	ARG	2.1
1	1-A	96	LEU	2.1
1	2-A	96	LEU	2.1
1	3-A	96	LEU	2.1
1	4-A	96	LEU	2.1
1	5-A	96	LEU	2.1
1	6-A	96	LEU	2.1
1	7-A	96	LEU	2.1
1	8-A	96	LEU	2.1
1	9-A	96	LEU	2.1
1	10-A	96	LEU	2.1
1	11-A	96	LEU	2.1
1	12-A	96	LEU	2.1
1	13-A	96	LEU	2.1
1	14-A	96	LEU	2.1
1	15-A	96	LEU	2.1
1	16-A	96	LEU	2.1
1	1-A	218	ARG	2.0
1	2-A	218	ARG	2.0
1	3-A	218	ARG	2.0
1	4-A	218	ARG	2.0
1	5-A	218	ARG	2.0
1	6-A	218	ARG	2.0
1	7-A	218	ARG	2.0
1	8-A	218	ARG	2.0
1	9-A	218	ARG	2.0
1	10-A	218	ARG	2.0
1	11-A	218	ARG	2.0
1	12-A	218	ARG	2.0
1	13-A	218	ARG	2.0
1	14-A	218	ARG	2.0
1	15-A	218	ARG	2.0
1	16-A	218	ARG	2.0
1	1-A	112	PRO	2.0
1	1-B	135	PRO	2.0
1	2-A	112	PRO	2.0
1	2-B	135	PRO	2.0
1	3-A	112	PRO	2.0
1	3-B	135	PRO	2.0
1	4-A	112	PRO	2.0
1	4-B	135	PRO	2.0
1	5-A	112	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	5-B	135	PRO	2.0
1	6-A	112	PRO	2.0
1	6-B	135	PRO	2.0
1	7-A	112	PRO	2.0
1	7-B	135	PRO	2.0
1	8-A	112	PRO	2.0
1	8-B	135	PRO	2.0
1	9-A	112	PRO	2.0
1	9-B	135	PRO	2.0
1	10-A	112	PRO	2.0
1	10-B	135	PRO	2.0
1	11-A	112	PRO	2.0
1	11-B	135	PRO	2.0
1	12-A	112	PRO	2.0
1	12-B	135	PRO	2.0
1	13-A	112	PRO	2.0
1	13-B	135	PRO	2.0
1	14-A	112	PRO	2.0
1	14-B	135	PRO	2.0
1	15-A	112	PRO	2.0
1	15-B	135	PRO	2.0
1	16-A	112	PRO	2.0
1	16-B	135	PRO	2.0
1	1-B	83	GLY	2.0
1	2-B	83	GLY	2.0
1	3-B	83	GLY	2.0
1	4-B	83	GLY	2.0
1	5-B	83	GLY	2.0
1	6-B	83	GLY	2.0
1	7-B	83	GLY	2.0
1	8-B	83	GLY	2.0
1	9-B	83	GLY	2.0
1	10-B	83	GLY	2.0
1	11-B	83	GLY	2.0
1	12-B	83	GLY	2.0
1	13-B	83	GLY	2.0
1	14-B	83	GLY	2.0
1	15-B	83	GLY	2.0
1	16-B	83	GLY	2.0
1	1-B	97	GLN	2.0
1	2-B	97	GLN	2.0
1	3-B	97	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	4-B	97	GLN	2.0
1	5-B	97	GLN	2.0
1	6-B	97	GLN	2.0
1	7-B	97	GLN	2.0
1	8-B	97	GLN	2.0
1	9-B	97	GLN	2.0
1	10-B	97	GLN	2.0
1	11-B	97	GLN	2.0
1	12-B	97	GLN	2.0
1	13-B	97	GLN	2.0
1	14-B	97	GLN	2.0
1	15-B	97	GLN	2.0
1	16-B	97	GLN	2.0
1	1-A	49	GLU	2.0
1	2-A	49	GLU	2.0
1	3-A	49	GLU	2.0
1	4-A	49	GLU	2.0
1	5-A	49	GLU	2.0
1	6-A	49	GLU	2.0
1	7-A	49	GLU	2.0
1	8-A	49	GLU	2.0
1	9-A	49	GLU	2.0
1	10-A	49	GLU	2.0
1	11-A	49	GLU	2.0
1	12-A	49	GLU	2.0
1	13-A	49	GLU	2.0
1	14-A	49	GLU	2.0
1	15-A	49	GLU	2.0
1	16-A	49	GLU	2.0
1	1-A	68	PRO	2.0
1	2-A	68	PRO	2.0
1	3-A	68	PRO	2.0
1	4-A	68	PRO	2.0
1	5-A	68	PRO	2.0
1	6-A	68	PRO	2.0
1	7-A	68	PRO	2.0
1	8-A	68	PRO	2.0
1	9-A	68	PRO	2.0
1	10-A	68	PRO	2.0
1	11-A	68	PRO	2.0
1	12-A	68	PRO	2.0
1	13-A	68	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	14-A	68	PRO	2.0
1	15-A	68	PRO	2.0
1	16-A	68	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.