

Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 - 03:35 AM EDT

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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

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	Similar resolution			
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$			
R _{free}	130704	$4661 \ (2.50-2.50)$			
Ramachandran outliers	138981	$5231 \ (2.50-2.50)$			
Sidechain outliers	138945	$5233 \ (2.50-2.50)$			
RSRZ outliers	127900	4559 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	
			28%	
1	1-A	251	84%	6% 9%
			18%	
1	1-B	251	86%	8% 6%
			12%	
1	1-C	251	85%	• 12%
			28%	
1	10-A	251	87%	• 9%
			18%	
1	10-B	251	90%	• 6%
			12%	
1	10-C	251	85%	• 12%
			28%	
1	11-A	251	86%	• 9%



Chain Length Quality of chain Mol 18% 2511 11**-**B 89% • 6% 12% 1 11-C 25186% 12% 28% 12-A 2511 83% 8% 9% 18% 1 12-B 25189% 5% 6% 12% 12-C 2511 84% 12% • 28% 13-A 2511 9% 84% 7% 18% 13-B 1 25187% 6% 6% 12% 13-C 1 25181% 7% 12% 28% 14-A 2511 82% 8% • 9% 18% 1 14-B 25187% 6% 6% 12% 1 14-C 25184% 12% • 28% 15-A 2511 84% 7% 9% 18% 15-B 2511 85% 8% 6% 12% 1 15-C 25183% 12% 5% 28% 16-A 2511 86% • • 9% 18% 1 16-B 25190% • 6% 12% 16-C 1 25181% 6% 12% 28% 1 2-A 25188% 9% • 18% 2-B 2511 88% 5%•6% 12% 2-C2511 85% 12% • 28% 1 3-A 2519% 88% • 18% 3-B 2511 91% • 6% 12% 3-C 1 25186% 12% • 28% 1 4-A 2519% 87% • 18% 4**-**B 2511 • 6% 90%

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Mol	Chain	Length	Quality of chain	
1	4-C	251	83%	5% 12%
1	5-A	251	82%	8% 9%
1	5-B	251	18%	5% 6%
1	5-C	251	85%	• 12%
1	6-A	251	28%	6% 9%
1	6-B	251	18%	5% 6%
1	6-C	251	84%	• 12%
1	7-A	251	28%	• 9%
1	7-B	251	18%	6% 6%
1	7-C	251	84%	• 12%
1	8-A	251	28%	• 9%
1	8-B	251	18%	• 6%
1	8-C	251	84%	• 12%
1	9-A	251	28%	5% 9%
1	9-B	251	18%	5% 6%
1	9-C	251	82%	6% 12%



2 Entry composition (i)

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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	228	Total	C 1123	N 313	0 327	S 3	Se 3	0	0	0
1	2-A	228	Total 1760	C 1123	N 313	$\frac{021}{0}$	S 3	Se 3	0	0	0
1	3-A	228	Total 1769	C 1123	N 313	$\begin{array}{r} 327 \\ \hline 0 \\ 327 \end{array}$	5 S 3	Se 3	0	0	0
1	4-A	228	Total 1769	C 1123	N 313	0 327	S 3	Se 3	0	0	0
1	5-A	228	Total 1769	C 1123	N 313	0 327	S 3	Se 3	0	0	0
1	6-A	228	Total 1769	C 1123	N 313	0 327	${ m S} { m 3}$	Se 3	0	0	0
1	7-A	228	Total 1769	C 1123	N 313	0 327	${ m S} { m 3}$	Se 3	0	0	0
1	8-A	228	Total 1769	C 1123	N 313	O 327	S 3	Se 3	0	0	0
1	9-A	228	Total 1769	C 1123	N 313	O 327	S 3	Se 3	0	0	0
1	10-A	228	Total 1769	C 1123	N 313	O 327	${ m S} { m 3}$	Se 3	0	0	0
1	11-A	228	Total 1769	C 1123	N 313	O 327	${ m S} { m 3}$	${ m Se} { m 3}$	0	0	0
1	12-A	228	Total 1769	C 1123	N 313	0 327	${ m S} { m 3}$	${ m Se} { m 3}$	0	0	0
1	13-A	228	Total 1769	C 1123	N 313	0 327	${ m S} { m 3}$	${ m Se} { m 3}$	0	0	0
1	14-A	228	Total 1769	C 1123	N 313	O 327	${ m S} { m 3}$	${ m Se} { m 3}$	0	0	0
1	15-A	228	Total 1769	C 1123	N 313	0 327	${ m S} { m 3}$	Se 3	0	0	0
1	16-A	228	Total 1769	C 1123	N 313	0 327	$\frac{S}{3}$	Se 3	0	0	0

• Molecule 1 is a protein called Uncharacterized protein C11orf68.



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Mol	Chain	Residues		A	Atoms	5			ZeroOcc	AltConf	Trace
1	1 D	025	Total	С	Ν	0	S	Se	0	0	0
	1-D	230	1815	1149	323	337	3	3	0	0	0
1	2_B	235	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	Se	0	0	0
	2-D	200	1815	1149	323	337	3	3	0	0	0
1	3-B	235	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	Se	0	0	0
	0.5	200	1815	1149	323	337	3	3	Ŭ	Ŭ	
1	4-B	235	Total	С	Ν	Ο	S	Se	0	0	0
			1815	1149	323	337	3	3		-	
1	5-B	235	Total	C	N	0	S	Se	0	0	0
			1815	1149	323	337	3	3			
1	6-B	235	Total	C	N	0	S	Se	0	0	0
			1815 Tt 1	1149	323	337	3	3			
1	7-B	235		1140	N 202	0	3	Se	0	0	0
			Total	1149 C	$\frac{323}{N}$	337	<u>0</u> C	<u> </u>	_		
1	8-B	235	10tai 1815	1140	1N 202	337	2 2	े उ	0	0	0
			Total	$\frac{1149}{C}$	<u>323</u> N	001	3 C	<u> </u>			
1	9-B	235	1815	11/0	202 1N	337	3 3	3	0	0	0
			Total	<u> </u>	<u>020</u> N	001	$\frac{s}{s}$	Se		0	
1	10-B	235	1815	1149	323	337	3	3	0		0
			Total	<u>C</u>	N	0	$\frac{\mathrm{o}}{\mathrm{S}}$	Se	0		
1	11-B	235	1815	1149	323	337	3	3		0	0
			Total	C	N	0	S	Se	0		
1	12-B	235	1815	1149	323	337	3	3	0	0	
-	10 D	225	Total	С	Ν	0	S	Se	0	0	
	13-B	235	1815	1149	323	337	3	3	0	0	0
1	14 D	0.97	Total	С	Ν	0	S	Se	0	0	0
	14 - B	235	1815	1149	323	337	3	3	0	0	0
1	15 D	025	Total	С	Ν	Ο	S	Se	0	0	0
	19-D	230	1815	1149	323	337	3	3	0	0	0
1	16 B	235	Total	С	Ν	Ο	S	Se	0	0	0
1	10-D	230	1815	1149	323	337	3	3	0	0	0
1	1-C	221	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	Se	0	0	0
	10	221	1712	1087	307	312	3	3	0	0	0
1	2-C	221	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	Se	0	0	0
-	20		1712	1087	307	312	3	3	Ŭ	0	0
1	1 3-C 221	221	Total	С	Ν	0	S	Se	0	0	0
			1712	1087	307	312	3	3		0	
1	4-C	221	Total	С	N	0	S	Se	0	0	0
			1712	1087	307	312	3	3		Ŭ	
1	5-C	221	'Total	С	N	0	S	Se	0	0	0
			1712	1087	307	312	3	3	j ř		, j



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Mol	Chain	Residues		A	Atoms	S			ZeroOcc	AltConf	Trace
1	6-C	221	Total	С	Ν	0	\mathbf{S}	Se	0	0	0
	0.0		1712	1087	307	312	3	3	0	0	0
1	7-C	221	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	Se	0	0	0
1	1-0	221	1712	1087	307	312	3	3	0	0	0
1	8 C	991	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	Se	0	0	0
	0-0		1712	1087	307	312	3	3	0	0	0
1	0 C	221	Total	С	Ν	0	\mathbf{S}	Se	0	0	0
	<i>J</i> -0		1712	1087	307	312	3	3	0	0	U
1	10 C	991	Total	\mathbf{C}	Ν	0	\mathbf{S}	Se	0	0	0
	10-0		1712	1087	307	312	3	3	0	0	0
1	11 C	221	Total	С	Ν	0	S	Se	0	0	0
	11-0		1712	1087	307	312	3	3	0	0	0
1	12 C	991	Total	С	Ν	Ο	\mathbf{S}	Se	0	0	0
	12-0		1712	1087	307	312	3	3	0	0	0
1	13 C	221	Total	С	Ν	0	\mathbf{S}	Se	0	0	0
	10-0		1712	1087	307	312	3	3	0	0	0
1	14 C	991	Total	С	Ν	Ο	\mathbf{S}	Se	0	0	0
L	14-0		1712	1087	307	312	3	3	U	0	0
1	15 C	221	Total	С	Ν	0	S	Se	0	0	0
	10-0		1712	1087	307	312	3	3		U	
1	16 C	221	Total	С	Ν	0	S	Se	0	0	0
	10-0		1712	1087	307	312	3	3	0	U	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	MSE	MET	modified residue	UNP Q9H3H3
А	30	MSE	MET	modified residue	UNP Q9H3H3
А	34	MSE	MET	modified residue	UNP Q9H3H3
А	131	MSE	MET	modified residue	UNP Q9H3H3
В	1	MSE	MET	modified residue	UNP Q9H3H3
В	30	MSE	MET	modified residue	UNP Q9H3H3
В	34	MSE	MET	modified residue	UNP Q9H3H3
В	131	MSE	MET	modified residue	UNP Q9H3H3
С	1	MSE	MET	modified residue	UNP Q9H3H3
С	30	MSE	MET	modified residue	UNP Q9H3H3
Ċ	34	MSE	MET	modified residue	UNP Q9H3H3
C	131	MSE	MET	modified residue	UNP Q9H3H3

• Molecule 2 is water.



n	\cap	Λ	\mathbf{V}
4	Q	4	\mathbf{n}

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	50	Total O	0	0
			50 50		
2	2-A	55	55 55	0	0
	- 1	7 0	Total O		
2	3-A	56	56 56	0	0
2	4- A	55	Total O	0	0
	111		55 55	0	0
2	5-A	55	Total O	0	0
			55 55		
2	6-A	56	Total O	0	0
			00 00 Total O		
2	7-A	54	54 54	0	0
			Total O		
2	8-A	56	56 56	0	0
			Total O		
2	9-A	57	57 57	0	0
	10.1		Total O		
2	10-A	56	56 56	0	0
0	11 1	50	Total O	0	0
2	11-A	58	58 58	0	0
2	19 A	55	Total O	0	0
	12-11		55 55	0	0
2	13-A	53	Total O	0	0
	10 11		53 53		
2	14-A	56	Total O	0	0
			56 56		
2	15-A	53	Total O	0	0
			DO DO DO		
2	16-A	53	53 53	0	0
			Total O		
2	1 - B	91	91 91	0	0
			Total O		-
2	2-B	88	88 88	0	0
0	9 D	00	Total O	0	0
2	<u></u> З-В	88	88 88	0	U
0	ΛD	00	Total O	0	Ο
	4-D	90	90 90	0	U
2	5-B	89	Total O	0	0
		00	89 89		0
2	6-B	89	Total O	0	0
			89 89		-



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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	TotalO7272	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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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	12-C	75	Total O 75 75	0	0
2	13-C	73	Total O 73 73	0	0
2	14-C	74	Total O 74 74	0	0
2	15-C	73	Total O 73 73	0	0
2	16-C	73	Total O 73 73	0	0



3 Residue-property plots (i)

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



• Molecule 1: Uncharacterized protein C11orf68

• Molecule 1: Uncharacterized protein C11orf68





• Molecule 1: Uncharacterized protein C11orf68



















• Molecule 1: Uncharacterized protein C11orf68 18% Chain 10-B: 90% 6% MSE GLU GLV GLV GLU GLU GLU GLU GLU GLV SER PRO GLV GLY SER SER • Molecule 1: Uncharacterized protein C11orf68 12% Chain 10-C: 85% 12% N2 N2 V2 • Molecule 1: Uncharacterized protein C11orf68 28% Chain 11-A: 86% 9% MSE GLU GLU GLU GLU GLU GLU GLU GLV GLY SER R 691 092 092 LEU GLY GLY SER ALA ALA ARG G23 S23 R24(V24: L245 D245 • Molecule 1: Uncharacterized protein C11orf68 18% Chain 11-B: 89% 6% Q94 G95 L96 Q97 Q97 A98 A98 N100 E101 E101 • Molecule 1: Uncharacterized protein C11orf68 12% Chain 11-C: 86% 12%



MSE GLU GLU GLU GLU GLU GLU GLU GLU SER R SER ARG GLY ARG





BANK









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	62.55Å 116.81Å 123.64Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	43.97 - 2.50	Depositor
Resolution (A)	43.97 - 2.50	EDS
% Data completeness	98.0 (43.97-2.50)	Depositor
(in resolution range)	97.8(43.97-2.50)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.79 (at 2.51 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
B B.	0.166 , 0.236	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.189 , 0.260	DCC
R_{free} test set	1607 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.32 , 120.7	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	88208	wwPDB-VP
Average B, all atoms $(Å^2)$	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.

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



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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).

Mal	Chain	Bond lengths		Bond angles		
	Unam	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	



Mal	Chain	Bond lengths		Bond angles		
10101	Unam	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:
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Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
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 (i)

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

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



2	\cap	Λ	\mathbf{K}
4	ખ	T	τ.

Conti Mol	Chain	Non-H	$\frac{page}{\mathbf{H}(\mathbf{model})}$	H(addad)	Clashes	Symm-Clashes
1		1915		1770		0
	1-D 1 C	1010	0	1684	0	0
1	1-0 2 A	1712	0	1084	0	0
1	2-A 2 B	1709	0	1722	0	0
1	2-D	1010	0	1684	0	0
	2-0	1712	0	1004	0	0
1	3-A	1709	0	1720	0	0
	3-B	1810	0	1770	0	0
	3-0	1712	0	1084	0	0
	4-A	1/09	0	1770	0	0
	4-B	1810	0	1770	0	0
	4-C	1/12	0	1084	0	0
	5-A	1/09	0	1722	0	0
	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



2Q4N	2°	Q4K	
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	Chain	Non-H	H(model)	(poppe)H	Clashes	Symm-Clashes
1	15 D	1011-11		1770	Olaslies	Symm-Clashes
	10-D 15 C	1010	0	1770	0	0
	10-0 16 A	1712	0	1084	0	0
1	10-A 16 B	1815	0	1722	0	0
1	10-D	1712	0	1684	0	0
$\frac{1}{2}$	10-0	50	0	0	0	0
$\frac{2}{2}$	1-A 1_R	01 01	0	0	0	0
$\frac{2}{2}$	1-D	76	0	0	0	0
2	2-A	55	0	0	0	0
2	2-R	88	0	0	0	0
2	2-C	74	0	0	0	0
2	<u>-</u> = = = = = = = = = = = = = = = = = = =	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
2	11-B	87	0	0	0	0
2	11-C	72	0	0	0	0
2	12-A	55 07	0	0		0
2	12-B	87	0			0
2	12-C	(5	0	0	0	0
2	13-A	53	U	0	0	U



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	Perce	entiles
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%)	2	3
1	1-C	219/251~(87%)	193 (88%)	20~(9%)	6 (3%)	5	7
1	2-A	224/251~(89%)	192 (86%)	28~(12%)	4 (2%)	8	14
1	2-B	233/251~(93%)	195 (84%)	28~(12%)	10 (4%)	2	3
1	2-C	219/251~(87%)	198 (90%)	18 (8%)	3 (1%)	11	20
1	3-A	224/251 (89%)	196 (88%)	25 (11%)	3 (1%)	12	21
1	3-B	233/251~(93%)	219 (94%)	12 (5%)	2 (1%)	17	31



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	3-C	219/251~(87%)	202~(92%)	15~(7%)	2 (1%)	17	31
1	4-A	224/251~(89%)	197 (88%)	$21 \ (9\%)$	6 (3%)	5	7
1	4-B	233/251~(93%)	205 (88%)	23~(10%)	5 (2%)	7	11
1	4-C	219/251~(87%)	186 (85%)	24 (11%)	9 (4%)	3	3
1	5-A	224/251~(89%)	178 (80%)	35~(16%)	11 (5%)	2	2
1	5-B	233/251~(93%)	203 (87%)	22 (9%)	8 (3%)	3	5
1	5-C	219/251~(87%)	201 (92%)	13 (6%)	5 (2%)	6	10
1	6-A	224/251~(89%)	189 (84%)	25~(11%)	10 (4%)	2	3
1	6-B	233/251~(93%)	210 (90%)	18 (8%)	5 (2%)	7	11
1	6-C	219/251~(87%)	200 (91%)	13 (6%)	6 (3%)	5	7
1	7-A	224/251~(89%)	185 (83%)	34 (15%)	5 (2%)	6	10
1	7-B	233/251~(93%)	195 (84%)	29 (12%)	9 (4%)	3	4
1	7-C	219/251~(87%)	192 (88%)	21 (10%)	6 (3%)	5	7
1	8-A	224/251~(89%)	202 (90%)	20 (9%)	2 (1%)	17	31
1	8-B	233/251~(93%)	214 (92%)	17 (7%)	2 (1%)	17	31
1	8-C	219/251~(87%)	199 (91%)	14 (6%)	6 (3%)	5	7
1	9-A	224/251~(89%)	200 (89%)	19 (8%)	5 (2%)	6	10
1	9-B	233/251~(93%)	207 (89%)	21 (9%)	5 (2%)	7	11
1	9-C	219/251~(87%)	193 (88%)	16 (7%)	10 (5%)	2	2
1	10-A	224/251~(89%)	202 (90%)	20 (9%)	2 (1%)	17	31
1	10-B	233/251~(93%)	211 (91%)	19 (8%)	3 (1%)	12	21
1	10-C	219/251~(87%)	198 (90%)	15 (7%)	6 (3%)	5	7
1	11-A	224/251~(89%)	199 (89%)	18 (8%)	7(3%)	4	5
1	11-B	233/251~(93%)	209 (90%)	18 (8%)	6 (3%)	5	8
1	11-C	219/251~(87%)	203 (93%)	15 (7%)	1 (0%)	29	48
1	12-A	224/251~(89%)	188 (84%)	29~(13%)	7 (3%)	4	5
1	12-B	233/251~(93%)	199 (85%)	25 (11%)	9 (4%)	3	4
1	12-C	219/251~(87%)	197 (90%)	16 (7%)	6 (3%)	5	7
1	13-A	$\overline{224/251}\ (89\%)$	193 (86%)	23 (10%)	8 (4%)	3	4
1	13-B	233/251 (93%)	208 (89%)	18 (8%)	7(3%)	4	6
1	13-C	219/251~(87%)	187 (85%)	25 (11%)	7 (3%)	4	5



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	14-A	224/251~(89%)	181 (81%)	32~(14%)	11 (5%)	2	2
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%)	5	7
1	15-A	224/251~(89%)	188 (84%)	26 (12%)	10 (4%)	2	3
1	15-B	233/251~(93%)	195 (84%)	24~(10%)	14 (6%)	1	1
1	15-C	219/251~(87%)	189 (86%)	25~(11%)	5 (2%)	6	10
1	16-A	224/251~(89%)	193 (86%)	25~(11%)	6 (3%)	5	7
1	16-B	233/251~(93%)	207 (89%)	24 (10%)	2 (1%)	17	31
1	16-C	219/251 (87%)	196 (90%)	13 (6%)	10 (5%)	2	2
All	All	10816/12048~(90%)	9461 (88%)	1043 (10%)	312 (3%)	4	6

Continued from previous page...

All (312) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{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



\mathbf{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



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 3-B 238 GLY 1 4-A 89 ASN 1 4-A 178 ASP 1 4-B 164 ALA 1 4-B 164 ALA 1 4-C 91 GLY 1 4-C 105 THR 1 5-A 79 ILE 1 5-A 91 GLY 1 5-A 91 GLY 1 5-A 91 GLY 1 5-B 217 ASN 1 5-B 217 ASN 1 5-B 245 ALA 1 5-B 245 ALA	Mol	Chain	Res	Type
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-B 233 GLY 1 4-C 91 GLY 1 4-C 105 THR 1 5-A 79 ILE 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-A 89 ASN 1	1	1-B	238	GLY
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 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 91 GLY 1 4-C 105 THR 1 5-A 79 ILE 1 5-A 91 GLY 1 5-A 217 ASN 1 5-B 217 ASN 1 5-B 217 ASN 1 5-B 234 GLY 1 5-B 234 GLY 1 5-C 89 ASN 1 6-A 42 ALA	1	1-C	246	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 91 GLY 1 4-C 91 GLY 1 5-A 79 ILE 1 5-A 91 GLY 1 5-A 91 GLY 1 5-A 91 GLY 1 5-B 217 ASN 1 5-B 234 GLY 1 5-B 234 GLY 1 5-C 89 ASN 1 6-A 42 ALA 1	1	1-C	247	ASN
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-A 178 ASP 1 4-A 178 ASP 1 4-B 233 GLY 1 4-C 91 GLY 1 4-C 105 THR 1 5-A 79 ILE 1 5-A 91 GLY 1 5-A 91 GLY 1 5-A 91 GLY 1 5-B 217 ASN 1 5-B 219 TRP 1 5-B 234 GLY 1 5-C 89 ASN 1 6-A 42 ALA 1 6-A 245 ALA 1	1	2-B	157	VAL
1 3-A 165 LYS 1 3-B 238 GLY 1 4-A 89 ASN 1 4-A 178 ASP 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 91 GLY 1 5-B 217 ASN 1 5-B 234 GLY 1 5-B 234 ALA 1	1	2-C	246	ASN
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-B 233 GLY 1 4-C 91 GLY 1 4-C 105 THR 1 5-A 79 ILE 1 5-A 91 GLY 1 5-B 217 ASN 1 5-B 217 ASN 1 5-B 219 TRP 1 5-B 234 GLY 1 5-C 89 ASN 1 6-A 42 ALA 1 6-A 167 GLY <th>1</th> <th>3-A</th> <th>165</th> <th>LYS</th>	1	3-A	165	LYS
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 91 GLY 1 5-B 217 ASN 1 5-B 219 TRP 1 5-B 234 GLY 1 5-C 89 ASN 1 6-A 42 ALA 1 6-A 245 ALA 1 6-A 245 ALA 1 6-C 191 ALA 1 6-C 191 ALA <th>1</th> <th>3-B</th> <th>238</th> <th>GLY</th>	1	3-B	238	GLY
14-A178ASP14-B164ALA14-B233GLY14-C91GLY14-C105THR15-A79ILE15-A91GLY15-A91GLY15-A91GLY15-A91GLY15-A217ASN15-B217ASN15-B219TRP15-B245ALA15-B245ALA15-C89ASN16-A42ALA16-A167GLY16-A245ALA16-A245ALA16-C191ALA16-C191ALA16-C238GLY17-A66GLY17-A172ILE17-A165LYS18-B212GLY18-B212GLY18-B238GLY19-A215ARG19-A220HIS19-A220HIS19-A220HIS19-A220HIS19-B238GLY	1	4-A	89	ASN
14-B164ALA14-B233GLY14-C91GLY14-C105THR15-A79ILE15-A91GLY15-A91GLY15-A91GLY15-A91GLY15-A217ASN15-B217ASN15-B219TRP15-B234GLY15-B245ALA15-C89ASN16-A42ALA16-A167GLY16-A245ALA16-A245ALA16-C191ALA16-C191ALA16-C191ALA16-C238GLY17-A66GLY17-A126SER17-B126SER17-B165LYS18-B238GLY18-B238GLY19-A215ARG19-A220HIS19-A220HIS19-B238GLY	1	4-A	178	ASP
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 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 5-C 89 ASN 1 6-A 42 ALA 1 6-A 42 ALA 1 6-A 245 ALA 1 6-A 245 ALA 1 6-C 191 ALA 1 6-C 191 ALA 1 6-C 238 GLY 1 7-A 26 SER <th>1</th> <th>4-B</th> <th>164</th> <th>ALA</th>	1	4-B	164	ALA
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 91 GLY 1 5-A 91 GLY 1 5-A 217 ASN 1 5-B 217 ASN 1 5-B 234 GLY 1 5-B 245 ALA 1 5-C 89 ASN 1 5-C 89 ASN 1 6-A 42 ALA 1 6-A 42 ALA 1 6-A 245 ALA 1 6-A 245 ALA 1 6-C 191 ALA 1 6-C 191 ALA 1 6-C 191 ALA 1 7-A 26 GLY 1 7-A 244 ARG <th>1</th> <th>4-B</th> <th>233</th> <th>GLY</th>	1	4-B	233	GLY
14-C105THR15-A79ILE15-A89ASN15-A91GLY15-A217ASN15-B217ASN15-B219TRP15-B234GLY15-B245ALA15-C89ASN16-A42ALA16-A89ASN16-A167GLY16-A245ALA16-A245ALA16-A245ALA16-C191ALA16-C238GLY17-A66GLY17-A172ILE17-A126SER17-B165LYS18-B212GLY18-B238GLY19-A215ARG19-A220HIS19-B238GLY	1	4-C	91	GLY
15-A79ILE15-A89ASN15-A91GLY15-A217ASN15-B219TRP15-B234GLY15-B245ALA15-B245ALA15-C89ASN16-A42ALA16-A89ASN16-A167GLY16-A245ALA16-A167GLY16-A245ALA16-C191ALA16-C238GLY17-A66GLY17-A172ILE17-A244ARG17-B126SER17-B165LYS18-B238GLY18-B238GLY19-A215ARG19-A220HIS19-B238GLY	1	4-C	105	THR
1 5-A 89 ASN 1 5-A 91 GLY 1 5-A 217 ASN 1 5-B 217 ASN 1 5-B 217 ASN 1 5-B 219 TRP 1 5-B 234 GLY 1 5-B 234 GLY 1 5-B 245 ALA 1 5-C 89 ASN 1 6-A 42 ALA 1 6-A 42 ALA 1 6-A 245 ALA 1 6-A 245 ALA 1 6-A 245 ALA 1 6-C 191 TRP 1 6-C 191 ALA 1 6-C 191 ALA 1 7-A 165 GLY 1 7-A 126 SER 1	1	5-A	79	ILE
15-A91 GLY 15-A217ASN15-B219TRP15-B234 GLY 15-B245ALA15-C89ASN16-A42ALA16-A89ASN16-A167GLY16-A167GLY16-A167GLY16-A245ALA16-A167GLY16-C191ALA16-C238GLY17-A66GLY17-A172ILE17-A244ARG17-B165LYS18-B212GLY18-B238GLY18-C106SER19-A215ARG19-A220HIS19-B238GLY	1	5-A	89	ASN
15-A217ASN15-B217ASN15-B219TRP15-B234GLY15-B245ALA15-C89ASN16-A42ALA16-A89ASN16-A245ALA16-A167GLY16-A245ALA16-A245ALA16-C191ALA16-C191ALA16-C238GLY17-A66GLY17-A172ILE17-A126SER17-B165LYS18-B238GLY18-B238GLY19-A215ARG19-A220HIS19-B238GLY	1	5-A	91	GLY
15-B 217 ASN15-B 219 TRP15-B 234 GLY15-B 245 ALA15-C 89 ASN16-A 42 ALA16-A 42 ALA16-A167GLY16-A245ALA16-A245ALA16-A245ALA16-C191ALA16-C238GLY17-A66GLY17-A172ILE17-A244ARG17-B126SER17-B165LYS18-B212GLY18-B238GLY19-A215ARG19-A220HIS19-B238GLY	1	5-A	217	ASN
15-B219TRP15-B234GLY15-B245ALA15-C89ASN16-A42ALA16-A89ASN16-A167GLY16-A245ALA16-A245ALA16-A245ALA16-C191ALA16-C191ALA16-C238GLY17-A66GLY17-A172ILE17-A126SER17-B165LYS18-B238GLY18-B238GLY19-A215ARG19-A220HIS19-B238GLY	1	5-B	217	ASN
1 5-B 234 GLY 1 5-B 245 ALA 1 5-C 89 ASN 1 6-A 42 ALA 1 6-A 42 ALA 1 6-A 42 ALA 1 6-A 42 ALA 1 6-A 245 ALA 1 6-A 245 ALA 1 6-A 245 ALA 1 6-C 191 ALA 1 6-C 191 ALA 1 6-C 238 GLY 1 7-A 66 GLY 1 7-A 172 ILE 1 7-A 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	1	5-B	219	TRP
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	5-B	234	GLY
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	5-B	245	ALA
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	5-C	89	ASN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	6-A	42	ALA
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	6-A	89	ASN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	6-A	167	GLY
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	6-A	245	ALA
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	6-B	219	TRP
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	6-C	191	ALA
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	6-C	238	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	7-A	66	GLY
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	7-A	172	ILE
1 7-B 126 SER 1 7-B 165 LYS 1 8-B 212 GLY 1 8-B 238 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	7-A	244	ARG
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	7-B	126	SER
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	7-B	165	LYS
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	8-B	212	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	8-B	238	GLY
1 9-A 215 ARG 1 9-A 220 HIS 1 9-B 238 GLY 1 10-A 167 GLY	1	8-C	106	SER
1 9-A 220 HIS 1 9-B 238 GLY 1 10 167 GLY	1	9-A	215	ARG
1 9-B 238 GLY	1	9-A	220	HIS
1 10 10 107 0IV	1	9-B	238	GLY
I 10-A 107 GLY	1	10-A	167	GLY
1 10-C 189 ASP	1	10-C	189	ASP



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



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



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	1 5- B	23	GLU
1	15-B	181	ASP
1	15-C	156	GLN
1	1-A	150	VAL



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


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

Continued from previous page...

5.3.2 Protein sidechains (i)

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

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



2Q4K

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles	
1	1-A	180/192 (94%)	177 (98%)	3 (2%)	60	82	
1	1-B	184/192~(96%)	175 (95%)	9(5%)	25	47	
1	1-C	175/192~(91%)	174 (99%)	1 (1%)	86	95	
1	2-A	180/192 (94%)	177 (98%)	3 (2%)	60	82	
1	2-B	184/192~(96%)	177 (96%)	7 (4%)	33	58	
1	2-C	175/192~(91%)	170 (97%)	5 (3%)	42	69	
1	3-A	180/192 (94%)	175 (97%)	5 (3%)	43	70	
1	3-B	184/192~(96%)	179 (97%)	5 (3%)	44	71	
1	3-C	175/192~(91%)	173 (99%)	2 (1%)	73	89	
1	4-A	180/192 (94%)	175 (97%)	5 (3%)	43	70	
1	4-B	184/192~(96%)	180 (98%)	4 (2%)	52	77	
1	4-C	175/192 (91%)	172 (98%)	3 (2%)	60	82	
1	5-A	180/192 (94%)	168 (93%)	12 (7%)	16	31	
1	5-B	184/192~(96%)	180 (98%)	4 (2%)	52	77	
1	5-C	175/192 (91%)	173 (99%)	2 (1%)	73	89	
1	6-A	180/192 (94%)	172 (96%)	8 (4%)	28	52	
1	6-B	184/192~(96%)	177 (96%)	7 (4%)	33	58	
1	6-C	175/192~(91%)	172 (98%)	3 (2%)	60	82	
1	7-A	180/192 (94%)	172 (96%)	8 (4%)	28	52	
1	7-B	184/192~(96%)	176 (96%)	8 (4%)	29	53	
1	7-C	175/192~(91%)	172 (98%)	3 (2%)	60	82	
1	8-A	180/192~(94%)	174 (97%)	6 (3%)	38	64	
1	8-B	184/192~(96%)	176 (96%)	8 (4%)	29	53	
1	8-C	175/192~(91%)	172 (98%)	3 (2%)	60	82	
1	9-A	180/192 (94%)	174 (97%)	6 (3%)	38	64	_
1	9-B	184/192~(96%)	177 (96%)	7 (4%)	33	58	
1	9-C	175/192~(91%)	170 (97%)	5 (3%)	42	69	
1	10-A	180/192~(94%)	172 (96%)	8 (4%)	28	52	
1	10-B	184/192~(96%)	178 (97%)	6(3%)	38	64	
1	10-C	175/192~(91%)	173 (99%)	2 (1%)	73	89	
1	11-A	180/192 (94%)	175 (97%)	5 (3%)	43	70	

analysed, and the total number of residues.



2Q4K

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	11-B	184/192~(96%)	179 (97%)	5 (3%)	44	71
1	11-C	175/192~(91%)	172 (98%)	3 (2%)	60	82
1	12-A	180/192~(94%)	168 (93%)	12 (7%)	16	31
1	12-B	184/192~(96%)	181 (98%)	3 (2%)	62	84
1	12-C	175/192~(91%)	171 (98%)	4 (2%)	50	76
1	13-A	180/192~(94%)	171 (95%)	9(5%)	24	46
1	13-B	184/192~(96%)	175~(95%)	9(5%)	25	47
1	13-C	175/192~(91%)	163~(93%)	12 (7%)	15	30
1	14-A	180/192~(94%)	169 (94%)	11 (6%)	18	36
1	14-B	184/192~(96%)	180 (98%)	4 (2%)	52	77
1	14-C	175/192~(91%)	169~(97%)	6 (3%)	37	63
1	15-A	180/192~(94%)	172 (96%)	8 (4%)	28	52
1	15-B	184/192~(96%)	176~(96%)	8 (4%)	29	53
1	15-C	175/192~(91%)	169 (97%)	6 (3%)	37	63
1	16-A	180/192~(94%)	173~(96%)	7 (4%)	32	57
1	16-B	184/192~(96%)	178 (97%)	6 (3%)	38	64
1	16-C	$17\overline{5}/192~(91\%)$	$1\overline{67}\ (95\%)$	8 (5%)	27	50
All	All	$862\overline{4/9216}\ (94\%)$	8340 (97%)	$2\overline{84} (3\%)$	38	64

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



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



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



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



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



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



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



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

Sometimes 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



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



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



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 (i)

There are no RNA molecules in this entry.



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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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	$\langle RSRZ \rangle$	#RSR	\mathbf{Z}	2	$OWAB(Å^2)$	Q<0.9
1	1-A	225/251~(89%)	1.51	71 (31%)	0	0	17, 40, 75, 91	225~(100%)
1	1-B	232/251~(92%)	1.04	45~(19%)	1	1	17, 33, 68, 85	232~(100%)
1	1-C	218/251~(86%)	0.77	31 (14%)	2	2	8, 29, 65, 84	218 (100%)
1	2-A	225/251~(89%)	1.51	71 (31%)	0	0	17, 40, 75, 91	225 (100%)
1	2-B	232/251~(92%)	1.04	45~(19%)	1	1	17, 33, 68, 85	232 (100%)
1	2-C	218/251~(86%)	0.77	31 (14%)	2	2	8, 29, 65, 84	218 (100%)
1	3-A	225/251~(89%)	1.51	71 (31%)	0	0	17, 40, 75, 91	225 (100%)
1	3-B	232/251~(92%)	1.04	45 (19%)	1	1	17, 33, 68, 85	232 (100%)
1	3-C	218/251~(86%)	0.77	31~(14%)	2	2	8, 29, 65, 84	218 (100%)
1	4-A	225/251~(89%)	1.51	71 (31%)	0	0	17, 40, 75, 91	225 (100%)
1	4-B	232/251~(92%)	1.04	45~(19%)	1	1	17, 33, 68, 85	232 (100%)
1	4-C	218/251~(86%)	0.77	31~(14%)	2	2	8, 29, 65, 84	218 (100%)
1	5-A	225/251~(89%)	1.51	71 (31%)	0	0	17, 40, 75, 91	225 (100%)
1	5-B	232/251~(92%)	1.04	45~(19%)	1	1	17, 33, 68, 85	232 (100%)
1	5-C	218/251~(86%)	0.77	31 (14%)	2	2	8, 29, 65, 84	218 (100%)
1	6-A	225/251~(89%)	1.51	71 (31%)	0	0	17, 40, 75, 91	225 (100%)
1	6-B	232/251~(92%)	1.04	45~(19%)	1	1	17, 33, 68, 85	232 (100%)
1	6-C	218/251~(86%)	0.77	31~(14%)	2	2	8, 29, 65, 84	218 (100%)
1	7-A	225/251~(89%)	1.51	71 (31%)	0	0	17, 40, 75, 91	225 (100%)
1	7-B	232/251~(92%)	1.04	45~(19%)	1	1	17, 33, 68, 85	232 (100%)
1	7-C	218/251~(86%)	0.77	31~(14%)	2	2	8, 29, 65, 84	218 (100%)
1	8-A	225/251~(89%)	1.51	71 (31%)	0	0	17, 40, 75, 91	225 (100%)
1	8-B	232/251~(92%)	1.04	45 (19%)	1	1	17, 33, 68, 85	232 (100%)
1	8-C	218/251~(86%)	0.77	31 (14%)	2	2	8, 29, 65, 84	218 (100%)



Mol	Chain	Analysed	<RSRZ $>$	#RSR	Z>2	2	$OWAB(Å^2)$	$\mathbf{Q}{<}0.9$
1	9-A	225/251~(89%)	1.51	71 (31%)	0	0	17, 40, 75, 91	225~(100%)
1	9-B	232/251~(92%)	1.04	45 (19%)	1	1	17, 33, 68, 85	232~(100%)
1	9-C	218/251~(86%)	0.77	31 (14%)	2	2	8, 29, 65, 84	218 (100%)
1	10-A	225/251~(89%)	1.51	71 (31%)	0	0	17, 40, 75, 91	225 (100%)
1	10-B	232/251~(92%)	1.04	45 (19%)	1	1	17, 33, 68, 85	232 (100%)
1	10-C	218/251~(86%)	0.77	31 (14%)	2	2	8, 29, 65, 84	218 (100%)
1	11-A	225/251~(89%)	1.51	71 (31%)	0	0	17, 40, 75, 91	225 (100%)
1	11-B	232/251~(92%)	1.04	45 (19%)	1	1	17, 33, 68, 85	232 (100%)
1	11-C	218/251~(86%)	0.77	31 (14%)	2	2	8, 29, 65, 84	218 (100%)
1	12-A	225/251~(89%)	1.51	71 (31%)	0	0	17, 40, 75, 91	225 (100%)
1	12-B	232/251~(92%)	1.04	45 (19%)	1	1	17, 33, 68, 85	232 (100%)
1	12-C	218/251~(86%)	0.77	31 (14%)	2	2	8, 29, 65, 84	218 (100%)
1	13-A	225/251~(89%)	1.51	71 (31%)	0	0	17, 40, 75, 91	225 (100%)
1	13-B	232/251~(92%)	1.04	45 (19%)	1	1	17, 33, 68, 85	232 (100%)
1	13-C	218/251~(86%)	0.77	31 (14%)	2	2	8, 29, 65, 84	218 (100%)
1	14-A	225/251 (89%)	1.51	71 (31%)	0	0	17, 40, 75, 91	225 (100%)
1	14-B	232/251~(92%)	1.04	45 (19%)	1	1	17, 33, 68, 85	232 (100%)
1	14-C	218/251~(86%)	0.77	31 (14%)	2	2	8, 29, 65, 84	218 (100%)
1	15-A	225/251~(89%)	1.51	71 (31%)	0	0	17, 40, 75, 91	225 (100%)
1	15-B	232/251~(92%)	1.04	45 (19%)	1	1	17, 33, 68, 85	232 (100%)
1	15-C	218/251~(86%)	0.77	31 (14%)	2	2	8, 29, 65, 84	218 (100%)
1	16-A	$\overline{225/251}\ (89\%)$	1.51	71 (31%)	0	0	17, 40, 75, 91	225 (100%)
1	16-B	$\overline{232/251}\ (92\%)$	1.04	45 (19%)	1	1	17, 33, 68, 85	232 (100%)
1	16-C	218/251~(86%)	0.77	31 (14%)	2	2	8, 29, 65, 84	218 (100%)
All	All	10800/12048~(89%)	1.11	2352 (21%)	0	C	8, 34, 72, 91	10800 (100%)

All (2352) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-C	105	THR	11.3
1	2-C	105	THR	11.3
1	3-C	105	THR	11.3
1	4-C	105	THR	11.3
1	5-C	105	THR	11.3



2Q4K

Mol	Chain	Res	Type	RSRZ
1	6-C	105	THR	11.3
1	7-C	105	THR	11.3
1	8-C	105	THR	11.3
1	9-C	105	THR	11.3
1	10-C	105	THR	11.3
1	11-C	105	THR	11.3
1	12-C	105	THR	11.3
1	13-C	105	THR	11.3
1	14-C	105	THR	11.3
1	15-C	105	THR	11.3
1	16-C	105	THR	11.3
1	1-A	248	VAL	10.0
1	2-A	248	VAL	10.0
1	3-A	248	VAL	10.0
1	4-A	248	VAL	10.0
1	5-A	248	VAL	10.0
1	6-A	248	VAL	10.0
1	7-A	248	VAL	10.0
1	8-A	248	VAL	10.0
1	9-A	248	VAL	10.0
1	10-A	248	VAL	10.0
1	11-A	248	VAL	10.0
1	12-A	248	VAL	10.0
1	13-A	248	VAL	10.0
1	14-A	248	VAL	10.0
1	15-A	248	VAL	10.0
1	16-A	248	VAL	10.0
1	1-B	89	ASN	9.8
1	2-B	89	ASN	9.8
1	3-B	89	ASN	9.8
1	4-B	89	ASN	9.8
1	5-B	89	ASN	9.8
1	6-B	89	ASN	9.8
1	7-B	89	ASN	9.8
1	8-B	89	ASN	9.8
1	9-B	89	ASN	9.8
1	10-B	89	ASN	9.8
1	11-B	89	ASN	9.8
1	12-B	89	ASN	9.8
1	13-B	89	ASN	9.8
1	14-B	89	ASN	9.8
1	15-B	89	ASN	9.8



Mol	Chain	Res	Type	RSRZ
1	16-B	89	ASN	9.8
1	1-B	105	THR	9.0
1	2-B	105	THR	9.0
1	3-B	105	THR	9.0
1	4-B	105	THR	9.0
1	5-B	105	THR	9.0
1	6-B	105	THR	9.0
1	7-B	105	THR	9.0
1	8-B	105	THR	9.0
1	9-B	105	THR	9.0
1	10-B	105	THR	9.0
1	11-B	105	THR	9.0
1	12-B	105	THR	9.0
1	13-B	105	THR	9.0
1	14 - B	105	THR	9.0
1	15-B	105	THR	9.0
1	16-B	105	THR	9.0
1	1-A	105	THR	8.9
1	2-A	105	THR	8.9
1	3-A	105	THR	8.9
1	4-A	105	THR	8.9
1	5-A	105	THR	8.9
1	6-A	105	THR	8.9
1	7-A	105	THR	8.9
1	8-A	105	THR	8.9
1	9-A	105	THR	8.9
1	10-A	105	THR	8.9
1	11-A	105	THR	8.9
1	12-A	105	THR	8.9
1	13-A	105	THR	8.9
1	14-A	105	THR	8.9
1	15-A	105	THR	8.9
1	16-A	105	THR	8.9
1	1-C	107	GLY	8.2
1	2-C	107	GLY	8.2
1	3-C	107	GLY	8.2
1	4-C	107	GLY	8.2
1	5-C	107	GLY	8.2
1	6-C	107	GLY	8.2
1	7-C	107	GLY	8.2
1	8-C	107	GLY	8.2
1	9-C	107	GLY	8.2



2Q4K

Mol	Chain	Res	Type	RSRZ
1	10-C	107	GLY	8.2
1	11-C	107	GLY	8.2
1	12-C	107	GLY	8.2
1	13-C	107	GLY	8.2
1	14-C	107	GLY	8.2
1	15-C	107	GLY	8.2
1	16-C	107	GLY	8.2
1	1-A	114	THR	7.8
1	2-A	114	THR	7.8
1	3-A	114	THR	7.8
1	4-A	114	THR	7.8
1	5-A	114	THR	7.8
1	6-A	114	THR	7.8
1	7-A	114	THR	7.8
1	8-A	114	THR	7.8
1	9-A	114	THR	7.8
1	10-A	114	THR	7.8
1	11-A	114	THR	7.8
1	12-A	114	THR	7.8
1	13-A	114	THR	7.8
1	14-A	114	THR	7.8
1	15-A	114	THR	7.8
1	16-A	114	THR	7.8
1	1-C	108	ARG	7.6
1	2-C	108	ARG	7.6
1	3-C	108	ARG	7.6
1	4-C	108	ARG	7.6
1	5-C	108	ARG	7.6
1	6-C	108	ARG	7.6
1	7-C	108	ARG	7.6
1	8-C	108	ARG	7.6
1	9-C	108	ARG	7.6
1	10-C	108	ARG	7.6
1	11-C	108	ARG	7.6
1	12-C	108	ARG	7.6
1	13-C	108	ARG	7.6
1	14-C	108	ARG	7.6
1	15-C	108	ARG	7.6
1	16-C	108	ARG	7.6
1	1-C	245	ALA	7.6
1	2-C	245	ALA	7.6
1	3-C	245	ALA	7.6



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Mol	Chain	Res	Type	RSRZ
1	4-C	245	ALA	7.6
1	5-C	245	ALA	7.6
1	6-C	245	ALA	7.6
1	7-C	245	ALA	7.6
1	8-C	245	ALA	7.6
1	9-C	245	ALA	7.6
1	10-C	245	ALA	7.6
1	11-C	245	ALA	7.6
1	12-C	245	ALA	7.6
1	13-C	245	ALA	7.6
1	14-C	245	ALA	7.6
1	15-C	245	ALA	7.6
1	16-C	245	ALA	7.6
1	1-A	245	ALA	6.9
1	2-A	245	ALA	6.9
1	3-A	245	ALA	6.9
1	4-A	245	ALA	6.9
1	5-A	245	ALA	6.9
1	6-A	245	ALA	6.9
1	7-A	245	ALA	6.9
1	8-A	245	ALA	6.9
1	9-A	245	ALA	6.9
1	10-A	245	ALA	6.9
1	11-A	245	ALA	6.9
1	12-A	245	ALA	6.9
1	13-A	245	ALA	6.9
1	14-A	245	ALA	6.9
1	15-A	245	ALA	6.9
1	16-A	245	ALA	6.9
1	1-B	90	SER	6.7
1	1-B	106	SER	6.7
1	2-B	90	SER	6.7
1	2-B	106	SER	6.7
1	3-B	90	SER	6.7
1	3-B	106	SER	6.7
1	4-B	90	SER	6.7
1	4-B	106	SER	6.7
1	5-B	90	SER	6.7
1	5-B	106	SER	6.7
1	6-B	90	SER	6.7
1	6-B	106	SER	6.7
1	7-B	90	SER	6.7



2Q4K

Mol	Chain	Res	Type	RSRZ
1	7-B	106	SER	6.7
1	8-B	90	SER	6.7
1	8-B	106	SER	6.7
1	9-B	90	SER	6.7
1	9-B	106	SER	6.7
1	10-B	90	SER	6.7
1	10-B	106	SER	6.7
1	11-B	90	SER	6.7
1	11 - B	106	SER	6.7
1	12-B	90	SER	6.7
1	12-B	106	SER	6.7
1	13-B	90	SER	6.7
1	13-B	106	SER	6.7
1	14-B	90	SER	6.7
1	14-B	106	SER	6.7
1	15-B	90	SER	6.7
1	15-B	106	SER	6.7
1	16-B	90	SER	6.7
1	16-B	106	SER	6.7
1	1-B	88	PRO	6.4
1	2-B	88	PRO	6.4
1	3-B	88	PRO	6.4
1	4-B	88	PRO	6.4
1	5-B	88	PRO	6.4
1	6-B	88	PRO	6.4
1	7-B	88	PRO	6.4
1	8-B	88	PRO	6.4
1	9-B	88	PRO	6.4
1	10-B	88	PRO	6.4
1	11-B	88	PRO	6.4
1	12-B	88	PRO	6.4
1	13-B	88	PRO	6.4
1	14-B	88	PRO	6.4
1	15-B	88	PRO	6.4
1	16-B	88	PRO	6.4
1	1-A	$24\overline{6}$	ASN	6.4
1	2-A	246	ASN	6.4
1	3-A	246	ASN	6.4
1	4-A	246	ASN	6.4
1	5-A	246	ASN	6.4
1	6-A	246	ASN	6.4
1	7-A	246	ASN	6.4



2Q4K

Mol	Chain	Res	Type	RSRZ
1	8-A	246	ASN	6.4
1	9-A	246	ASN	6.4
1	10-A	246	ASN	6.4
1	11-A	246	ASN	6.4
1	12-A	246	ASN	6.4
1	13-A	246	ASN	6.4
1	14-A	246	ASN	6.4
1	15-A	246	ASN	6.4
1	16-A	246	ASN	6.4
1	1-B	216	ALA	6.4
1	2-B	216	ALA	6.4
1	3-B	216	ALA	6.4
1	4-B	216	ALA	6.4
1	5-B	216	ALA	6.4
1	6-B	216	ALA	6.4
1	7-B	216	ALA	6.4
1	8-B	216	ALA	6.4
1	9-B	216	ALA	6.4
1	10-B	216	ALA	6.4
1	11-B	216	ALA	6.4
1	12-B	216	ALA	6.4
1	13-B	216	ALA	6.4
1	14-B	216	ALA	6.4
1	15-B	216	ALA	6.4
1	16-B	216	ALA	6.4
1	1-A	90	SER	6.1
1	2-A	90	SER	6.1
1	3-A	90	SER	6.1
1	4-A	90	SER	6.1
1	5-A	90	SER	6.1
1	6-A	90	SER	6.1
1	7-A	90	SER	6.1
1	8-A	90	SER	6.1
1	9-A	90	SER	6.1
1	10-A	90	SER	6.1
1	11-A	90	SER	6.1
1	12-A	90	SER	6.1
1	13-A	90	SER	6.1
1	14-A	90	SER	6.1
1	15-A	90	SER	6.1
1	16-A	90	SER	6.1
1	1-A	121	THR	6.1



0 0		Proces	F = J	
Mol	Chain	Res	Type	RSRZ
1	2-A	121	THR	6.1
1	3-A	121	THR	6.1
1	4-A	121	THR	6.1
1	5-A	121	THR	6.1
1	6-A	121	THR	6.1
1	7-A	121	THR	6.1
1	8-A	121	THR	6.1
1	9-A	121	THR	6.1
1	10-A	121	THR	6.1
1	11-A	121	THR	6.1
1	12-A	121	THR	6.1
1	13-A	121	THR	6.1
1	14-A	121	THR	6.1
1	15-A	121	THR	6.1
1	16-A	121	THR	6.1
1	1-B	87	SER	6.0
1	2-B	87	SER	6.0
1	3-B	87	SER	6.0
1	4-B	87	SER	6.0
1	5-B	87	SER	6.0
1	6-B	87	SER	6.0
1	7-B	87	SER	6.0
1	8-B	87	SER	6.0
1	9-B	87	SER	6.0
1	10-B	87	SER	6.0
1	11-B	87	SER	6.0
1	12-B	87	SER	6.0
1	13-B	87	SER	6.0
1	14-B	87	SER	6.0
1	15-B	87	SER	6.0
1	16-B	87	SER	6.0
1	1-C	237	ARG	6.0
1	2-C	237	ARG	6.0
1	3-C	237	ARG	6.0
1	4-C	237	ARG	6.0
1	5-C	237	ARG	6.0
1	6-C	237	ARG	6.0
1	7-C	237	ARG	6.0
1	8-C	237	ARG	6.0
1	9-C	237	ARG	6.0
1	10-C	237	ARG	6.0
1	11-C	237	ARG	6.0



2Q	4]	K

Mol	Chain	Res	Type	RSRZ
1	12-C	237	ARG	6.0
1	13-C	237	ARG	6.0
1	14-C	237	ARG	6.0
1	15-C	237	ARG	6.0
1	16-C	237	ARG	6.0
1	1-B	107	GLY	5.8
1	2-B	107	GLY	5.8
1	3-B	107	GLY	5.8
1	4-B	107	GLY	5.8
1	5-B	107	GLY	5.8
1	6-B	107	GLY	5.8
1	7-B	107	GLY	5.8
1	8-B	107	GLY	5.8
1	9-B	107	GLY	5.8
1	10-B	107	GLY	5.8
1	11-B	107	GLY	5.8
1	12-B	107	GLY	5.8
1	13-B	107	GLY	5.8
1	14-B	107	GLY	5.8
1	15-B	107	GLY	5.8
1	16-B	107	GLY	5.8
1	1-B	85	GLY	5.8
1	2-B	85	GLY	5.8
1	3-B	85	GLY	5.8
1	4-B	85	GLY	5.8
1	5-B	85	GLY	5.8
1	6-B	85	GLY	5.8
1	7-B	85	GLY	5.8
1	8-B	85	GLY	5.8
1	9-B	85	GLY	5.8
1	10-B	85	GLY	5.8
1	11-B	85	GLY	5.8
1	12-B	85	GLY	5.8
1	13-B	85	GLY	5.8
1	14-B	85	GLY	5.8
1	15-B	85	GLY	5.8
1	16-B	85	GLY	5.8
1	1-B	166	GLU	5.7
1	2-B	166	GLU	5.7
1	3-B	166	GLU	5.7
1	4-B	166	$GL\overline{U}$	5.7
1	5-B	166	GLU	5.7



2Q4K

Mol	Chain	Res	Type	RSRZ
1	6-B	166	GLU	5.7
1	7-B	166	GLU	5.7
1	8-B	166	GLU	5.7
1	9-B	166	GLU	5.7
1	10-B	166	GLU	5.7
1	11-B	166	GLU	5.7
1	12-B	166	GLU	5.7
1	13-B	166	GLU	5.7
1	14-B	166	GLU	5.7
1	15-B	166	GLU	5.7
1	16-B	166	GLU	5.7
1	1-A	120	ILE	5.4
1	2-A	120	ILE	5.4
1	3-A	120	ILE	5.4
1	4-A	120	ILE	5.4
1	5-A	120	ILE	5.4
1	6-A	120	ILE	5.4
1	7-A	120	ILE	5.4
1	8-A	120	ILE	5.4
1	9-A	120	ILE	5.4
1	10-A	120	ILE	5.4
1	11-A	120	ILE	5.4
1	12-A	120	ILE	5.4
1	13-A	120	ILE	5.4
1	14-A	120	ILE	5.4
1	15-A	120	ILE	5.4
1	16-A	120	ILE	5.4
1	1-A	110	ILE	5.3
1	2-A	110	ILE	5.3
1	3-A	110	ILE	5.3
1	4-A	110	ILE	5.3
1	5-A	110	ILE	5.3
1	6-A	110	ILE	5.3
1	7-A	110	ILE	5.3
1	8-A	110	ILE	5.3
1	9-A	110	ILE	5.3
1	10-A	110	ILE	5.3
1	11-A	110	ILE	5.3
1	12-A	110	ILE	5.3
1	13-A	110	ILE	5.3
1	14-A	110	ILE	5.3
1	15-A	110	ILE	5.3



Mol	Chain	Res	Type	RSRZ
1	16-A	110	ILE	5.3
1	1-A	88	PRO	5.3
1	2-A	88	PRO	5.3
1	3-A	88	PRO	5.3
1	4-A	88	PRO	5.3
1	5-A	88	PRO	5.3
1	6-A	88	PRO	5.3
1	7-A	88	PRO	5.3
1	8-A	88	PRO	5.3
1	9-A	88	PRO	5.3
1	10-A	88	PRO	5.3
1	11-A	88	PRO	5.3
1	12-A	88	PRO	5.3
1	13-A	88	PRO	5.3
1	14-A	88	PRO	5.3
1	15-A	88	PRO	5.3
1	16-A	88	PRO	5.3
1	1-A	89	ASN	5.2
1	2-A	89	ASN	5.2
1	3-A	89	ASN	5.2
1	4-A	89	ASN	5.2
1	5-A	89	ASN	5.2
1	6-A	89	ASN	5.2
1	7-A	89	ASN	5.2
1	8-A	89	ASN	5.2
1	9-A	89	ASN	5.2
1	10-A	89	ASN	5.2
1	11-A	89	ASN	5.2
1	12-A	89	ASN	5.2
1	13-A	89	ASN	5.2
1	14-A	89	ASN	5.2
1	15-A	89	ASN	5.2
1	16-A	89	ASN	5.2
1	1-A	106	SER	5.1
1	2-A	106	SER	5.1
1	3-A	106	SER	5.1
1	4-A	106	SER	5.1
1	5-A	106	SER	5.1
1	6-A	106	SER	5.1
1	7-A	106	SER	5.1
1	8-A	106	SER	5.1
1	9-A	106	SER	5.1



2Q4K

Mol	Chain	Res	Type	RSRZ
1	10-A	106	SER	5.1
1	11-A	106	SER	5.1
1	12-A	106	SER	5.1
1	13-A	106	SER	5.1
1	14-A	106	SER	5.1
1	15-A	106	SER	5.1
1	16-A	106	SER	5.1
1	1-B	84	GLN	4.8
1	2-B	84	GLN	4.8
1	3-B	84	GLN	4.8
1	4-B	84	GLN	4.8
1	5-B	84	GLN	4.8
1	6-B	84	GLN	4.8
1	7-B	84	GLN	4.8
1	8-B	84	GLN	4.8
1	9-B	84	GLN	4.8
1	10-B	84	GLN	4.8
1	11-B	84	GLN	4.8
1	12-B	84	GLN	4.8
1	13-B	84	GLN	4.8
1	14-B	84	GLN	4.8
1	15-B	84	GLN	4.8
1	16-B	84	GLN	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-A	17	GLU	4.7
1	2-A	17	GLU	4.7
1	3-A	17	GLU	4.7



Mol	Chain	Res	Type	RSRZ
1	4-A	17	GLU	4.7
1	5-A	17	GLU	4.7
1	6-A	17	GLU	4.7
1	7-A	17	GLU	4.7
1	8-A	17	GLU	4.7
1	9-A	17	GLU	4.7
1	10-A	17	GLU	4.7
1	11-A	17	GLU	4.7
1	12-A	17	GLU	4.7
1	13-A	17	GLU	4.7
1	14-A	17	GLU	4.7
1	15-A	17	GLU	4.7
1	16-A	17	GLU	4.7
1	1-C	167	GLY	4.7
1	2-C	167	GLY	4.7
1	3-C	167	GLY	4.7
1	4-C	167	GLY	4.7
1	5-C	167	GLY	4.7
1	6-C	167	GLY	4.7
1	7-C	167	GLY	4.7
1	8-C	167	GLY	4.7
1	9-C	167	GLY	4.7
1	10-C	167	GLY	4.7
1	11-C	167	GLY	4.7
1	12-C	167	GLY	4.7
1	13-C	167	GLY	4.7
1	14-C	167	GLY	4.7
1	15-C	167	GLY	4.7
1	16-C	167	GLY	4.7
1	1-B	165	LYS	4.7
1	2-B	165	LYS	4.7
1	3-B	165	LYS	4.7
1	4-B	165	LYS	4.7
1	5-B	165	LYS	4.7
1	6-B	165	LYS	4.7
1	7-B	165	LYS	4.7
1	8-B	165	LYS	4.7
1	9-B	165	LYS	4.7
1	10-B	165	LYS	4.7
1	11-B	165	LYS	4.7
1	12-B	165	LYS	4.7
1	13-B	165	LYS	4.7



2Q4K

Mol	Chain	Res	Type	RSRZ
1	14-B	165	LYS	4.7
1	15-B	165	LYS	4.7
1	16-B	165	LYS	4.7
1	1-C	101	GLU	4.6
1	2-C	101	GLU	4.6
1	3-C	101	GLU	4.6
1	4-C	101	GLU	4.6
1	5-C	101	GLU	4.6
1	6-C	101	GLU	4.6
1	7-C	101	GLU	4.6
1	8-C	101	GLU	4.6
1	9-C	101	GLU	4.6
1	10-C	101	GLU	4.6
1	11-C	101	GLU	4.6
1	12-C	101	GLU	4.6
1	13-C	101	GLU	4.6
1	14-C	101	GLU	4.6
1	15-C	101	GLU	4.6
1	16-C	101	GLU	4.6
1	1-A	177	ASP	4.6
1	2-A	177	ASP	4.6
1	3-A	177	ASP	4.6
1	4-A	177	ASP	4.6
1	5-A	177	ASP	4.6
1	6-A	177	ASP	4.6
1	7-A	177	ASP	4.6
1	8-A	177	ASP	4.6
1	9-A	177	ASP	4.6
1	10-A	177	ASP	4.6
1	11-A	177	ASP	4.6
1	12-A	177	ASP	4.6
1	13-A	177	ASP	4.6
1	14-A	177	ASP	4.6
1	15-A	177	ASP	4.6
1	16-A	177	ASP	4.6
1	1-C	109	PRO	4.6
1	2-C	109	PRO	4.6
1	3-C	109	PRO	4.6
1	4-C	109	PRO	4.6
1	5-C	109	PRO	4.6
1	6-C	109	PRO	4.6
1	7-C	109	PRO	4.6



2	Q	4	K	

Mol	Chain	Res	Type	RSRZ
1	8-C	109	PRO	4.6
1	9-C	109	PRO	4.6
1	10-C	109	PRO	4.6
1	11-C	109	PRO	4.6
1	12-C	109	PRO	4.6
1	13-C	109	PRO	4.6
1	14-C	109	PRO	4.6
1	15-C	109	PRO	4.6
1	16-C	109	PRO	4.6
1	1-A	247	ASN	4.6
1	2-A	247	ASN	4.6
1	3-A	247	ASN	4.6
1	4-A	247	ASN	4.6
1	5-A	247	ASN	4.6
1	6-A	247	ASN	4.6
1	7-A	247	ASN	4.6
1	8-A	247	ASN	4.6
1	9-A	247	ASN	4.6
1	10-A	247	ASN	4.6
1	11-A	247	ASN	4.6
1	12-A	247	ASN	4.6
1	13-A	247	ASN	4.6
1	14-A	247	ASN	4.6
1	15-A	247	ASN	4.6
1	16-A	247	ASN	4.6
1	1-B	218	ARG	4.6
1	2-B	218	ARG	4.6
1	3-B	218	ARG	4.6
1	4-B	218	ARG	4.6
1	5-B	218	ARG	4.6
1	6-B	218	ARG	4.6
1	7-B	218	ARG	4.6
1	8-B	218	ARG	4.6
1	9-B	218	ARG	4.6
1	10-B	218	ARG	4.6
1	11-B	218	ARG	4.6
1	12-B	218	ARG	4.6
1	13-B	218	ARG	4.6
1	14-B	218	ARG	4.6
1	15-B	218	ARG	4.6
1	16-B	218	ARG	4.6
1	1-B	168	GLY	4.6



2Q4K

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	4.4
1	2-C	106	SER	4.4
1	3-C	106	SER	4.4
1	4-C	106	SER	4.4
1	5-C	106	SER	4.4
1	6-C	106	SER	4.4
1	7-C	106	SER	4.4
1	8-C	106	SER	4.4
1	9-C	106	SER	4.4
1	10-C	106	SER	4.4
1	11-C	106	SER	4.4
1	12-C	106	SER	4.4
1	13-C	106	SER	4.4
1	14-C	106	SER	4.4
1	15-C	106	SER	4.4
1	16-C	106	SER	4.4
1	1-C	102	ALA	4.4
1	2-C	102	ALA	4.4
1	3-C	102	ALA	4.4
1	4-C	102	ALA	4.4
1	5-C	102	ALA	4.4
1	6-C	102	ALA	4.4
1	7-C	102	ALA	4.4
1	8-C	102	ALA	4.4
1	9-C	102	ALA	4.4
1	10-C	102	ALA	4.4
1	11-C	102	ALA	4.4



2Q4K

Mol	Chain	Res	Type	RSRZ
1	12-C	102	ALA	4.4
1	13-C	102	ALA	4.4
1	14-C	102	ALA	4.4
1	15-C	102	ALA	4.4
1	16-C	102	ALA	4.4
1	1-C	166	GLU	4.4
1	2-C	166	GLU	4.4
1	3-C	166	GLU	4.4
1	4-C	166	GLU	4.4
1	5-C	166	GLU	4.4
1	6-C	166	GLU	4.4
1	7-C	166	GLU	4.4
1	8-C	166	GLU	4.4
1	9-C	166	GLU	4.4
1	10-C	166	GLU	4.4
1	11-C	166	GLU	4.4
1	12-C	166	GLU	4.4
1	13-C	166	GLU	4.4
1	14-C	166	GLU	4.4
1	15-C	166	GLU	4.4
1	16-C	166	GLU	4.4
1	1-A	111	THR	4.4
1	2-A	111	THR	4.4
1	3-A	111	THR	4.4
1	4-A	111	THR	4.4
1	5-A	111	THR	4.4
1	6-A	111	THR	4.4
1	7-A	111	THR	4.4
1	8-A	111	THR	4.4
1	9-A	111	THR	4.4
1	10-A	111	THR	4.4
1	11-A	111	THR	4.4
1	12-A	111	THR	4.4
1	13-A	111	THR	4.4
1	14-A	111	THR	4.4
1	15-A	111	THR	4.4
1	16-A	111	THR	4.4
1	1-B	215	ARG	4.3
1	2-B	215	ARG	4.3
1	3-B	215	ARG	4.3
1	4-B	215	ARG	4.3
1	5-B	215	ARG	4.3



Mol	Chain	Res	Type	RSRZ
1	6-B	215	ARG	4.3
1	7-B	215	ARG	4.3
1	8-B	215	ARG	4.3
1	9-B	215	ARG	4.3
1	10-B	215	ARG	4.3
1	11-B	215	ARG	4.3
1	12-B	215	ARG	4.3
1	13-B	215	ARG	4.3
1	14-B	215	ARG	4.3
1	15-B	215	ARG	4.3
1	16-B	215	ARG	4.3
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	98	ALA	4.2
1	2-A	98	ALA	4.2
1	3-A	98	ALA	4.2
1	4-A	98	ALA	4.2
1	5-A	98	ALA	4.2
1	6-A	98	ALA	4.2
1	7-A	98	ALA	4.2
1	8-A	98	ALA	4.2
1	9-A	98	ALA	4.2
1	10-A	98	ALA	4.2
1	11-A	98	ALA	4.2
1	12-A	98	ALA	4.2
1	13-A	98	ALA	4.2
1	14-A	98	ALA	4.2
1	15-A	98	ALA	4.2



2Q4K

Mol	Chain	Res	Type	RSRZ
1	16-A	98	ALA	4.2
1	1-A	222	CYS	4.2
1	2-A	222	CYS	4.2
1	3-A	222	CYS	4.2
1	4-A	222	CYS	4.2
1	5-A	222	CYS	4.2
1	6-A	222	CYS	4.2
1	7-A	222	CYS	4.2
1	8-A	222	CYS	4.2
1	9-A	222	CYS	4.2
1	10-A	222	CYS	4.2
1	11-A	222	CYS	4.2
1	12-A	222	CYS	4.2
1	13-A	222	CYS	4.2
1	14-A	222	CYS	4.2
1	15-A	222	CYS	4.2
1	16-A	222	CYS	4.2
1	1-A	109	PRO	4.1
1	2-A	109	PRO	4.1
1	3-A	109	PRO	4.1
1	4-A	109	PRO	4.1
1	5-A	109	PRO	4.1
1	6-A	109	PRO	4.1
1	7-A	109	PRO	4.1
1	8-A	109	PRO	4.1
1	9-A	109	PRO	4.1
1	10-A	109	PRO	4.1
1	11-A	109	PRO	4.1
1	12-A	109	PRO	4.1
1	13-A	109	PRO	4.1
1	14-A	109	PRO	4.1
1	15-A	109	PRO	4.1
1	16-A	109	PRO	4.1
1	1-A	44	THR	4.1
1	2-A	44	THR	4.1
1	3-A	44	THR	4.1
1	4-A	44	THR	4.1
1	5-A	44	THR	4.1
1	6-A	44	THR	4.1
1	7-A	44	THR	4.1
1	8-A	44	THR	4.1
1	9-A	44	THR	4.1



2Q4K

Mol	Chain	Res	Type	RSRZ
1	10-A	44	THR	4.1
1	11-A	44	THR	4.1
1	12-A	44	THR	4.1
1	13-A	44	THR	4.1
1	14-A	44	THR	4.1
1	15-A	44	THR	4.1
1	16-A	44	THR	4.1
1	1-B	104	GLN	4.0
1	2-B	104	GLN	4.0
1	3-B	104	GLN	4.0
1	4-B	104	GLN	4.0
1	5-B	104	GLN	4.0
1	6-B	104	GLN	4.0
1	7-B	104	GLN	4.0
1	8-B	104	GLN	4.0
1	9-B	104	GLN	4.0
1	10-B	104	GLN	4.0
1	11-B	104	GLN	4.0
1	12-B	104	GLN	4.0
1	13-B	104	GLN	4.0
1	14-B	104	GLN	4.0
1	15-B	104	GLN	4.0
1	16-B	104	GLN	4.0
1	1-A	107	GLY	4.0
1	2-A	107	GLY	4.0
1	3-A	107	GLY	4.0
1	4-A	107	GLY	4.0
1	5-A	107	GLY	4.0
1	6-A	107	GLY	4.0
1	7-A	107	GLY	4.0
1	8-A	107	GLY	4.0
1	9-A	107	GLY	4.0
1	10-A	107	GLY	4.0
1	11-A	107	GLY	4.0
1	12-A	107	GLY	4.0
1	13-A	107	GLY	4.0
1	14-A	107	GLY	4.0
1	15-A	107	GLY	4.0
1	16-A	107	GLY	4.0
1	1-B	219	TRP	4.0
1	2-B	219	TRP	4.0
1	3-B	219	TRP	4.0

Continued from previous page...



2	Q	4	K

Mol	Chain	Res	Type	RSRZ
1	4-B	219	TRP	4.0
1	5-B	219	TRP	4.0
1	6-B	219	TRP	4.0
1	7-B	219	TRP	4.0
1	8-B	219	TRP	4.0
1	9-B	219	TRP	4.0
1	10-B	219	TRP	4.0
1	11-B	219	TRP	4.0
1	12-B	219	TRP	4.0
1	13-B	219	TRP	4.0
1	14-B	219	TRP	4.0
1	15-B	219	TRP	4.0
1	16-B	219	TRP	4.0
1	1-C	218	ARG	4.0
1	2-C	218	ARG	4.0
1	3-C	218	ARG	4.0
1	4-C	218	ARG	4.0
1	5-C	218	ARG	4.0
1	6-C	218	ARG	4.0
1	7-C	218	ARG	4.0
1	8-C	218	ARG	4.0
1	9-C	218	ARG	4.0
1	10-C	218	ARG	4.0
1	11-C	218	ARG	4.0
1	12-C	218	ARG	4.0
1	13-C	218	ARG	4.0
1	14-C	218	ARG	4.0
1	15-C	218	ARG	4.0
1	16-C	218	ARG	4.0
1	1-A	103	LEU	4.0
1	1-A	167	GLY	4.0
1	1-A	179	PHE	4.0
1	2-A	103	LEU	4.0
1	2-A	167	GLY	4.0
1	2-A	179	PHE	4.0
1	3-A	103	LEU	4.0
1	3-A	167	GLY	4.0
1	3-A	179	PHE	4.0
1	4-A	103	LEU	4.0
1	4-A	167	GLY	4.0
1	4-A	179	PHE	4.0
1	5-A	103	LEU	4.0


2Q4K

Mol	Chain	Res	Type	RSRZ
1	5-A	167	GLY	4.0
1	5-A	179	PHE	4.0
1	6-A	103	LEU	4.0
1	6-A	167	GLY	4.0
1	6-A	179	PHE	4.0
1	7-A	103	LEU	4.0
1	7-A	167	GLY	4.0
1	7-A	179	PHE	4.0
1	8-A	103	LEU	4.0
1	8-A	167	GLY	4.0
1	8-A	179	PHE	4.0
1	9-A	103	LEU	4.0
1	9-A	167	GLY	4.0
1	9-A	179	PHE	4.0
1	10-A	103	LEU	4.0
1	10-A	167	GLY	4.0
1	10-A	179	PHE	4.0
1	11-A	103	LEU	4.0
1	11-A	167	GLY	4.0
1	11-A	179	PHE	4.0
1	12-A	103	LEU	4.0
1	12-A	167	GLY	4.0
1	12-A	179	PHE	4.0
1	13-A	103	LEU	4.0
1	13-A	167	GLY	4.0
1	13-A	179	PHE	4.0
1	14-A	103	LEU	4.0
1	14-A	167	GLY	4.0
1	14-A	179	PHE	4.0
1	15-A	103	LEU	4.0
1	15-A	167	GLY	4.0
1	15-A	179	PHE	4.0
1	16-A	103	LEU	4.0
1	16-A	167	GLY	4.0
1	16-A	179	PHE	4.0
1	1-A	231	GLN	4.0
1	2-A	231	GLN	4.0
1	3-A	231	GLN	4.0
1	4-A	231	GLN	4.0
1	5-A	231	GLN	4.0
1	6-A	231	GLN	4.0
1	7-A	231	GLN	4.0



2Q	94K	

Mol	Chain	Res	Type	RSRZ
1	8-A	231	GLN	4.0
1	9-A	231	GLN	4.0
1	10-A	231	GLN	4.0
1	11-A	231	GLN	4.0
1	12-A	231	GLN	4.0
1	13-A	231	GLN	4.0
1	14-A	231	GLN	4.0
1	15-A	231	GLN	4.0
1	16-A	231	GLN	4.0
1	1-A	226	TYR	3.9
1	2-A	226	TYR	3.9
1	3-A	226	TYR	3.9
1	4-A	226	TYR	3.9
1	5-A	226	TYR	3.9
1	6-A	226	TYR	3.9
1	7-A	226	TYR	3.9
1	8-A	226	TYR	3.9
1	9-A	226	TYR	3.9
1	10-A	226	TYR	3.9
1	11-A	226	TYR	3.9
1	12-A	226	TYR	3.9
1	13-A	226	TYR	3.9
1	14-A	226	TYR	3.9
1	15-A	226	TYR	3.9
1	16-A	226	TYR	3.9
1	1-B	74	GLU	3.9
1	2-B	74	GLU	3.9
1	3-B	74	GLU	3.9
1	4-B	74	GLU	3.9
1	5-B	74	GLU	3.9
1	6-B	74	GLU	3.9
1	7-B	74	GLU	3.9
1	8-B	74	GLU	3.9
1	9-B	74	GLU	3.9
1	10-B	74	GLU	3.9
1	11-B	74	GLU	3.9
1	12-B	74	GLU	3.9
1	13-B	74	GLU	3.9
1	14-B	74	GLU	3.9
1	15-B	74	GLU	3.9
1	16-B	74	GLU	3.9
1	1-C	248	VAL	3.9



2Q4K

Mol	Chain	Res	Type	RSRZ
1	2-C	248	VAL	3.9
1	3-C	248	VAL	3.9
1	4-C	248	VAL	3.9
1	5-C	248	VAL	3.9
1	6-C	248	VAL	3.9
1	7-C	248	VAL	3.9
1	8-C	248	VAL	3.9
1	9-C	248	VAL	3.9
1	10-C	248	VAL	3.9
1	11-C	248	VAL	3.9
1	12-C	248	VAL	3.9
1	13-C	248	VAL	3.9
1	14-C	248	VAL	3.9
1	15-C	248	VAL	3.9
1	16-C	248	VAL	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-B	98	ALA	3.8
1	2-B	98	ALA	3.8
1	3-B	98	ALA	3.8
1	4-B	98	ALA	3.8
1	5-B	98	ALA	3.8
1	6-B	98	ALA	3.8
1	7-B	98	ALA	3.8
1	8-B	98	ALA	3.8
1	9-B	98	ALA	3.8
1	10-B	98	ALA	3.8
1	11-B	98	ALA	3.8



Mol	Chain	Res	Type	RSRZ
1	12-B	98	ALA	3.8
1	13-B	98	ALA	3.8
1	14-B	98	ALA	3.8
1	15-B	98	ALA	3.8
1	16-B	98	ALA	3.8
1	1-A	104	GLN	3.7
1	2-A	104	GLN	3.7
1	3-A	104	GLN	3.7
1	4-A	104	GLN	3.7
1	5-A	104	GLN	3.7
1	6-A	104	GLN	3.7
1	7-A	104	GLN	3.7
1	8-A	104	GLN	3.7
1	9-A	104	GLN	3.7
1	10-A	104	GLN	3.7
1	11-A	104	GLN	3.7
1	12-A	104	GLN	3.7
1	13-A	104	GLN	3.7
1	14-A	104	GLN	3.7
1	15-A	104	GLN	3.7
1	16-A	104	GLN	3.7
1	1-B	110	ILE	3.7
1	2-B	110	ILE	3.7
1	3-B	110	ILE	3.7
1	4-B	110	ILE	3.7
1	5-B	110	ILE	3.7
1	6-B	110	ILE	3.7
1	7-B	110	ILE	3.7
1	8-B	110	ILE	3.7
1	9-B	110	ILE	3.7
1	10-B	110	ILE	3.7
1	11 - B	110	ILE	3.7
1	12-B	110	ILE	3.7
1	13-B	110	ILE	3.7
1	14-B	110	ILE	3.7
1	15-B	110	ILE	3.7
1	16-B	110	ILE	3.7
1	1-A	48	THR	3.6
1	2-A	48	THR	3.6
1	3-A	48	THR	3.6
1	4-A	48	THR	3.6
1	5-A	48	THR	3.6



Mol	Chain	Res	Type	RSRZ
1	6-A	48	THR	3.6
1	7-A	48	THR	3.6
1	8-A	48	THR	3.6
1	9-A	48	THR	3.6
1	10-A	48	THR	3.6
1	11-A	48	THR	3.6
1	12-A	48	THR	3.6
1	13-A	48	THR	3.6
1	14-A	48	THR	3.6
1	15-A	48	THR	3.6
1	16-A	48	THR	3.6
1	1-A	150	VAL	3.6
1	1-A	238	GLY	3.6
1	2-A	150	VAL	3.6
1	2-A	238	GLY	3.6
1	3-A	150	VAL	3.6
1	3-A	238	GLY	3.6
1	4-A	150	VAL	3.6
1	4-A	238	GLY	3.6
1	5-A	150	VAL	3.6
1	5-A	238	GLY	3.6
1	6-A	150	VAL	3.6
1	6-A	238	GLY	3.6
1	7-A	150	VAL	3.6
1	7-A	238	GLY	3.6
1	8-A	150	VAL	3.6
1	8-A	238	GLY	3.6
1	9-A	150	VAL	3.6
1	9-A	238	GLY	3.6
1	10-A	150	VAL	3.6
1	10-A	238	GLY	3.6
1	11-A	150	VAL	3.6
1	11-A	238	GLY	3.6
1	12-A	150	VAL	3.6
1	12-A	238	GLY	3.6
1	13-A	150	VAL	3.6
1	13-A	238	GLY	3.6
1	14-A	150	VAL	3.6
1	14-A	238	GLY	3.6
1	15-A	150	VAL	3.6
1	15-A	238	GLY	3.6
1	16-A	150	VAL	3.6



2	Q	4	K

Mol	Chain	Res	Type	RSRZ
1	16-A	238	GLY	3.6
1	1-C	220	HIS	3.6
1	2-C	220	HIS	3.6
1	3-C	220	HIS	3.6
1	4-C	220	HIS	3.6
1	5-C	220	HIS	3.6
1	6-C	220	HIS	3.6
1	7-C	220	HIS	3.6
1	8-C	220	HIS	3.6
1	9-C	220	HIS	3.6
1	10-C	220	HIS	3.6
1	11-C	220	HIS	3.6
1	12-C	220	HIS	3.6
1	13-C	220	HIS	3.6
1	14-C	220	HIS	3.6
1	15-C	220	HIS	3.6
1	16-C	220	HIS	3.6
1	1-B	103	LEU	3.6
1	2-B	103	LEU	3.6
1	3-B	103	LEU	3.6
1	4-B	103	LEU	3.6
1	5-B	103	LEU	3.6
1	6-B	103	LEU	3.6
1	7-B	103	LEU	3.6
1	8-B	103	LEU	3.6
1	9-B	103	LEU	3.6
1	10-B	103	LEU	3.6
1	11-B	103	LEU	3.6
1	12-B	103	LEU	3.6
1	13-B	103	LEU	3.6
1	14-B	103	LEU	3.6
1	15-B	103	LEU	3.6
1	16-B	103	LEU	3.6
1	1-A	18	ASP	3.6
1	2-A	18	ASP	3.6
1	3-A	18	ASP	3.6
1	4-A	18	ASP	3.6
1	5-A	18	ASP	3.6
1	6-A	18	ASP	3.6
1	7-A	18	ASP	3.6
1	8-A	18	ASP	3.6
1	9-A	18	ASP	3.6



2Q4K	

Mol	Chain	Res	Type	RSRZ
1	10-A	18	ASP	3.6
1	11-A	18	ASP	3.6
1	12-A	18	ASP	3.6
1	13-A	18	ASP	3.6
1	14-A	18	ASP	3.6
1	15-A	18	ASP	3.6
1	16-A	18	ASP	3.6
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
1	14-C	219	TRP	3.5
1	15-C	219	TRP	3.5
1	16-C	219	TRP	3.5
1	1-C	235	SER	3.4
1	2-C	235	SER	3.4
1	3-C	235	SER	3.4
1	4-C	235	SER	3.4
1	5-C	235	SER	3.4
1	6-C	235	SER	3.4
1	7-C	235	SER	3.4
1	8-C	235	SER	3.4
1	9-C	235	SER	3.4
1	10-C	235	SER	3.4
1	11-C	235	SER	3.4
1	12-C	235	SER	3.4
1	13-C	235	SER	3.4
1	14-C	235	SER	3.4
1	15-C	235	SER	3.4
1	16-C	235	SER	3.4
1	1-A	123	HIS	3.4
1	2-A	123	HIS	3.4
1	3-A	123	HIS	3.4



2Q4K

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



2Q4K

Mol	Chain	Res	Type	RSRZ
1	14-A	249	GLU	3.4
1	15-A	249	GLU	3.4
1	16-A	249	GLU	3.4
1	1-B	108	ARG	3.4
1	1-C	246	ASN	3.4
1	2-B	108	ARG	3.4
1	2-C	246	ASN	3.4
1	3-B	108	ARG	3.4
1	3-C	246	ASN	3.4
1	4-B	108	ARG	3.4
1	4-C	246	ASN	3.4
1	5-B	108	ARG	3.4
1	5-C	246	ASN	3.4
1	6-B	108	ARG	3.4
1	6-C	246	ASN	3.4
1	7-B	108	ARG	3.4
1	7-C	246	ASN	3.4
1	8-B	108	ARG	3.4
1	8-C	246	ASN	3.4
1	9-B	108	ARG	3.4
1	9-C	246	ASN	3.4
1	10-B	108	ARG	3.4
1	10-C	246	ASN	3.4
1	11 - B	108	ARG	3.4
1	11-C	246	ASN	3.4
1	12-B	108	ARG	3.4
1	12-C	246	ASN	3.4
1	13-B	108	ARG	3.4
1	13-C	246	ASN	3.4
1	14-B	108	ARG	3.4
1	14-C	246	ASN	3.4
1	15-B	108	ARG	3.4
1	15-C	246	ASN	3.4
1	16-B	108	ARG	3.4
1	16-C	246	ASN	3.4
1	1-A	220	HIS	3.4
1	2-A	220	HIS	3.4
1	3-A	220	HIS	3.4
1	4-A	220	HIS	3.4
1	5-A	220	HIS	3.4
1	6-A	220	HIS	3.4
1	7-A	220	HIS	3.4



2Q4K

Mol	Chain	Res	Type	RSRZ
1	8-A	220	HIS	3.4
1	9-A	220	HIS	3.4
1	10-A	220	HIS	3.4
1	11-A	220	HIS	3.4
1	12-A	220	HIS	3.4
1	13-A	220	HIS	3.4
1	14-A	220	HIS	3.4
1	15-A	220	HIS	3.4
1	16-A	220	HIS	3.4
1	1-B	102	ALA	3.3
1	2-B	102	ALA	3.3
1	3-B	102	ALA	3.3
1	4-B	102	ALA	3.3
1	5-B	102	ALA	3.3
1	6-B	102	ALA	3.3
1	7-B	102	ALA	3.3
1	8-B	102	ALA	3.3
1	9-B	102	ALA	3.3
1	10-B	102	ALA	3.3
1	11-B	102	ALA	3.3
1	12-B	102	ALA	3.3
1	13-B	102	ALA	3.3
1	14-B	102	ALA	3.3
1	15-B	102	ALA	3.3
1	16-B	102	ALA	3.3
1	1-B	99	ALA	3.3
1	2-B	99	ALA	3.3
1	3-B	99	ALA	3.3
1	4-B	99	ALA	3.3
1	5-B	99	ALA	3.3
1	6-B	99	ALA	3.3
1	7-B	99	ALA	3.3
1	8-B	99	ALA	3.3
1	9-B	99	ALA	3.3
1	10-B	99	ALA	3.3
1	11-B	99	ALA	3.3
1	12-B	99	ALA	3.3
1	13-B	99	ALA	3.3
1	14-B	99	ALA	3.3
1	15-B	99	ALA	3.3
1	16-B	99	ALA	3.3
1	1-A	97	GLN	3.3



2Q	4K

Mol	Chain	Res	Type	RSRZ
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	3.2
1	2-C	236	ALA	3.2
1	3-C	236	ALA	3.2
1	4-C	236	ALA	3.2
1	5-C	236	ALA	3.2
1	6-C	236	ALA	3.2
1	7-C	236	ALA	3.2
1	8-C	236	ALA	3.2
1	9-C	236	ALA	3.2
1	10-C	236	ALA	3.2
1	11-C	236	ALA	3.2
1	12-C	236	ALA	3.2
1	13-C	236	ALA	3.2
1	14-C	236	ALA	3.2
1	15-C	236	ALA	3.2
1	16-C	236	ALA	3.2
1	1-A	242	LEU	3.2
1	2-A	242	LEU	3.2
1	3-A	242	LEU	3.2
1	4-A	242	LEU	3.2
1	5-A	242	LEU	3.2
1	6-A	242	LEU	3.2
1	7-A	242	LEU	3.2
1	8-A	242	LEU	3.2
1	9-A	242	LEU	3.2
1	10-A	242	LEU	3.2
1	11-A	242	LEU	3.2



III	2Q4K
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Mol	Chain	Res	Type	RSRZ
1	12-A	242	LEU	3.2
1	13-A	242	LEU	3.2
1	14-A	242	LEU	3.2
1	15-A	242	LEU	3.2
1	16-A	242	LEU	3.2
1	1-C	134	ALA	3.1
1	2-C	134	ALA	3.1
1	3-C	134	ALA	3.1
1	4-C	134	ALA	3.1
1	5-C	134	ALA	3.1
1	6-C	134	ALA	3.1
1	7-C	134	ALA	3.1
1	8-C	134	ALA	3.1
1	9-C	134	ALA	3.1
1	10-C	134	ALA	3.1
1	11-C	134	ALA	3.1
1	12-C	134	ALA	3.1
1	13-C	134	ALA	3.1
1	14-C	134	ALA	3.1
1	15-C	134	ALA	3.1
1	16-C	134	ALA	3.1
1	1-A	219	TRP	3.1
1	2-A	219	TRP	3.1
1	3-A	219	TRP	3.1
1	4-A	219	TRP	3.1
1	5-A	219	TRP	3.1
1	6-A	219	TRP	3.1
1	7-A	219	TRP	3.1
1	8-A	219	TRP	3.1
1	9-A	219	TRP	3.1
1	10-A	219	TRP	3.1
1	11-A	219	TRP	3.1
1	12-A	219	TRP	3.1
1	13-A	219	TRP	3.1
1	14-A	219	TRP	3.1
1	15-A	219	TRP	3.1
1	16-A	219	TRP	3.1
1	1-A	178	ASP	3.1
1	2-A	178	ASP	3.1
1	3-A	178	ASP	3.1
1	4-A	178	ASP	3.1
1	5-A	178	ASP	3.1



2Q4K

Mol	Chain	Res	Type	RSRZ
1	6-A	178	ASP	3.1
1	7-A	178	ASP	3.1
1	8-A	178	ASP	3.1
1	9-A	178	ASP	3.1
1	10-A	178	ASP	3.1
1	11-A	178	ASP	3.1
1	12-A	178	ASP	3.1
1	13-A	178	ASP	3.1
1	14-A	178	ASP	3.1
1	15-A	178	ASP	3.1
1	16-A	178	ASP	3.1
1	1-C	216	ALA	3.1
1	2-C	216	ALA	3.1
1	3-C	216	ALA	3.1
1	4-C	216	ALA	3.1
1	5-C	216	ALA	3.1
1	6-C	216	ALA	3.1
1	7-C	216	ALA	3.1
1	8-C	216	ALA	3.1
1	9-C	216	ALA	3.1
1	10-C	216	ALA	3.1
1	11-C	216	ALA	3.1
1	12-C	216	ALA	3.1
1	13-C	216	ALA	3.1
1	14-C	216	ALA	3.1
1	15-C	216	ALA	3.1
1	16-C	216	ALA	3.1
1	1-B	208	TYR	3.0
1	2-B	208	TYR	3.0
1	3-B	208	TYR	3.0
1	4-B	208	TYR	3.0
1	5-B	208	TYR	3.0
1	6-B	208	TYR	3.0
1	7-B	208	TYR	3.0
1	8-B	208	TYR	3.0
1	9-B	208	TYR	3.0
1	10-B	208	TYR	3.0
1	11-B	208	TYR	3.0
1	12-B	208	TYR	3.0
1	13-B	208	TYR	3.0
1	14-B	208	TYR	3.0
1	15-B	208	TYR	3.0



III	2Q4K
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Mol	Chain	Res	Type	RSRZ
1	16-B	208	TYR	3.0
1	1-C	183	LEU	3.0
1	2-C	183	LEU	3.0
1	3-C	183	LEU	3.0
1	4-C	183	LEU	3.0
1	5-C	183	LEU	3.0
1	6-C	183	LEU	3.0
1	7-C	183	LEU	3.0
1	8-C	183	LEU	3.0
1	9-C	183	LEU	3.0
1	10-C	183	LEU	3.0
1	11-C	183	LEU	3.0
1	12-C	183	LEU	3.0
1	13-C	183	LEU	3.0
1	14-C	183	LEU	3.0
1	15-C	183	LEU	3.0
1	16-C	183	LEU	3.0
1	1-A	243	ASP	3.0
1	2-A	243	ASP	3.0
1	3-A	243	ASP	3.0
1	4-A	243	ASP	3.0
1	5-A	243	ASP	3.0
1	6-A	243	ASP	3.0
1	7-A	243	ASP	3.0
1	8-A	243	ASP	3.0
1	9-A	243	ASP	3.0
1	10-A	243	ASP	3.0
1	11-A	243	ASP	3.0
1	12-A	243	ASP	3.0
1	13-A	243	ASP	3.0
1	14-A	243	ASP	3.0
1	15-A	243	ASP	3.0
1	16-A	243	ASP	3.0
1	1-A	45	THR	3.0
1	2-A	45	THR	3.0
1	3-A	45	THR	3.0
1	4-A	45	THR	3.0
1	5-A	45	THR	3.0
1	6-A	45	THR	3.0
1	7-A	45	THR	3.0
1	8-A	45	THR	3.0
1	9-A	45	THR	3.0



Mol	Chain	Res	Type	RSRZ
1	10-A	45	THR	3.0
1	11-A	45	THR	3.0
1	12-A	45	THR	3.0
1	13-A	45	THR	3.0
1	14-A	45	THR	3.0
1	15-A	45	THR	3.0
1	16-A	45	THR	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
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	109	PRO	3.0
1	2-B	109	PRO	3.0
1	3-B	109	PRO	3.0
1	4-B	109	PRO	3.0
1	5-B	109	PRO	3.0
1	6-B	109	PRO	3.0
1	7-B	109	PRO	3.0
1	8-B	109	PRO	3.0
1	9-B	109	PRO	3.0
1	10-B	109	PRO	3.0
1	11-B	109	PRO	3.0
1	12-B	109	PRO	3.0
1	13-B	109	PRO	3.0
1	14-B	109	PRO	3.0
1	15-B	109	PRO	3.0
1	16-B	109	PRO	3.0
1	1-C	165	LYS	2.9
1	2-C	165	LYS	2.9
1	3-C	165	LYS	2.9



2Q4K

Mol	Chain	Res	Type	RSRZ
1	4-C	165	LYS	2.9
1	5-C	165	LYS	2.9
1	6-C	165	LYS	2.9
1	7-C	165	LYS	2.9
1	8-C	165	LYS	2.9
1	9-C	165	LYS	2.9
1	10-C	165	LYS	2.9
1	11-C	165	LYS	2.9
1	12-C	165	LYS	2.9
1	13-C	165	LYS	2.9
1	14-C	165	LYS	2.9
1	15-C	165	LYS	2.9
1	16-C	165	LYS	2.9
1	1-B	212	GLY	2.9
1	2-B	212	GLY	2.9
1	3-B	212	GLY	2.9
1	4-B	212	GLY	2.9
1	5-B	212	GLY	2.9
1	6-B	212	GLY	2.9
1	7-B	212	GLY	2.9
1	8-B	212	GLY	2.9
1	9-B	212	GLY	2.9
1	10-B	212	GLY	2.9
1	11-B	212	GLY	2.9
1	12-B	212	GLY	2.9
1	13-B	212	GLY	2.9
1	14-B	212	GLY	2.9
1	15-B	212	GLY	2.9
1	16-B	212	GLY	2.9
1	1-B	100	TRP	2.9
1	2-B	100	TRP	2.9
1	3-B	100	TRP	2.9
1	4-B	100	TRP	2.9
1	5-B	100	TRP	2.9
1	6-B	100	TRP	2.9
1	7-B	100	TRP	2.9
1	8-B	100	TRP	2.9
1	9-B	100	TRP	2.9
1	10-B	100	TRP	2.9
1	11-B	100	TRP	2.9
1	12-B	100	TRP	2.9
1	13-B	100	TRP	2.9



Mol	Chain	Res	Type	RSRZ
1	14-B	100	TRP	2.9
1	15-B	100	TRP	2.9
1	16-B	100	TRP	2.9
1	1-B	176	THR	2.9
1	2-B	176	THR	2.9
1	3-B	176	THR	2.9
1	4-B	176	THR	2.9
1	5-B	176	THR	2.9
1	6-B	176	THR	2.9
1	7-B	176	THR	2.9
1	8-B	176	THR	2.9
1	9-B	176	THR	2.9
1	10-B	176	THR	2.9
1	11-B	176	THR	2.9
1	12-B	176	THR	2.9
1	13-B	176	THR	2.9
1	14 - B	176	THR	2.9
1	15-B	176	THR	2.9
1	16-B	176	THR	2.9
1	1-B	96	LEU	2.9
1	2-B	96	LEU	2.9
1	3-B	96	LEU	2.9
1	4-B	96	LEU	2.9
1	5-B	96	LEU	2.9
1	6-B	96	LEU	2.9
1	7-B	96	LEU	2.9
1	8-B	96	LEU	2.9
1	9-B	96	LEU	2.9
1	10-B	96	LEU	2.9
1	11-B	96	LEU	2.9
1	12-B	96	LEU	2.9
1	13-B	96	LEU	2.9
1	14-B	96	LEU	2.9
1	15-B	96	LEU	2.9
1	16-B	96	LEU	2.9
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



2Q4K	

Mol	Chain	Res	Type	RSRZ
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-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	164	ALA	2.8
1	2-B	164	ALA	2.8
1	3-B	164	ALA	2.8
1	4-B	164	ALA	2.8
1	5-B	164	ALA	2.8
1	6-B	164	ALA	2.8
1	7-B	164	ALA	2.8
1	8-B	164	ALA	2.8
1	9-B	164	ALA	2.8
1	10-B	164	ALA	2.8
1	11-B	164	ALA	2.8
1	12-B	164	ALA	2.8
1	13-B	164	ALA	2.8
1	14-B	164	ALA	2.8
1	15-B	164	ALA	2.8
1	16-B	164	ALA	2.8
1	1-A	212	GLY	2.8



2Q4K

Mol	Chain	Res	Type	RSRZ	
1	2-A	212	GLY	2.8	
1	3-A	212	GLY	2.8	
1	4-A	212	GLY	2.8	
1	5-A	212	GLY	2.8	
1	6-A	212	GLY	2.8	
1	7-A	212	GLY	2.8	
1	8-A	212	GLY	2.8	
1	9-A	212	GLY	2.8	
1	10-A	212	GLY	2.8	
1	11-A	212	GLY	2.8	
1	12-A	212	GLY	2.8	
1	13-A	212	GLY	2.8	
1	14-A	212	GLY	2.8	
1	15-A	212	GLY	2.8	
1	16-A	212	GLY	2.8	
1	1-A	240	ARG	2.8	
1	2-A	240	ARG	2.8	
1	3-A	240	ARG	2.8	
1	4-A	240	ARG	2.8	
1	5-A	240	ARG	2.8	
1	6-A	240	ARG	2.8	
1	7-A	240	ARG	2.8	
1	8-A	240	ARG	2.8	
1	9-A	240	ARG	2.8	
1	10-A	240	ARG	2.8	
1	11-A	240	ARG	2.8	
1	12-A	240	ARG	2.8	
1	13-A	240	ARG	2.8	
1	14-A	240	ARG	2.8	
1	15-A	240	ARG	2.8	
1	16-A	240	ARG	2.8	
1	1-A	224	THR	2.7	
1	2-A	224	THR	2.7	
1	3-A	224	THR	2.7	
1	4-A	224	THR	2.7	
1	5-A	224	THR	2.7	
1	6-A	224	THR	2.7	
1	7-A	224	THR	2.7	
1	8-A	224	THR	2.7	
1	9-A	224	THR	2.7	
1	10-A	224	THR	2.7	
1	11-A	224	THR	2.7	



Mol	Chain	Res	Type	RSRZ	
1	12-A	224	THR	2.7	
1	13-A	224	THR	2.7	
1	14-A	224	THR	2.7	
1	15-A	224	THR	2.7	
1	16-A	224	THR	2.7	
1	1-A	151	VAL	2.6	
1	2-A	151	VAL	2.6	
1	3-A	151	VAL	2.6	
1	4-A	151	VAL	2.6	
1	5-A	151	VAL	2.6	
1	6-A	151	VAL	2.6	
1	7-A	151	VAL	2.6	
1	8-A	151	VAL	2.6	
1	9-A	151	VAL	2.6	
1	10-A	151	VAL	2.6	
1	11-A	151	VAL	2.6	
1	12-A	151	VAL	2.6	
1	13-A	151	VAL	2.6	
1	14-A	151	VAL	2.6	
1	15-A	151	VAL	2.6	
1	16-A	151	VAL	2.6	
1	1-B	121	THR	2.6	
1	2-B	121	THR	2.6	
1	3-B	121	THR	2.6	
1	4-B	121	THR	2.6	
1	5-B	121	THR	2.6	
1	6-B	121	THR	2.6	
1	7-B	121	THR	2.6	
1	8-B	121	THR	2.6	
1	9-B	121	THR	2.6	
1	10-B	121	THR	2.6	
1	11-B	121	THR	2.6	
1	12-B	121	THR	2.6	
1	13-B	121	THR	2.6	
1	14-B	121	THR	2.6	
1	15-B	121	THR	2.6	
1	16-B	121	THR	2.6	
1	1-A	87	SER	2.6	
1	2-A	87	SER	2.6	
1	3-A	87	SER	2.6	
1	4-A	87	SER	2.6	
1	5-A	87	SER	2.6	



Mol	Chain	Res	Type	RSRZ	
1	6-A	87	SER	2.6	
1	7-A	87	SER	2.6	
1	8-A	87	SER	2.6	
1	9-A	87	SER	2.6	
1	10-A	87	SER	2.6	
1	11-A	87	SER	2.6	
1	12-A	87	SER	2.6	
1	13-A	87	SER	2.6	
1	14-A	87	SER	2.6	
1	15-A	87	SER	2.6	
1	16-A	87	SER	2.6	
1	1-A	213	ILE	2.6	
1	2-A	213	ILE	2.6	
1	3-A	213	ILE	2.6	
1	4-A	213	ILE	2.6	
1	5-A	213	ILE	2.6	
1	6-A	213	ILE	2.6	
1	7-A	213	ILE	2.6	
1	8-A	213	ILE	2.6	
1	9-A	213	ILE	2.6	
1	10-A	213	ILE	2.6	
1	11-A	213	ILE	2.6	
1	12-A	213	ILE	2.6	
1	13-A	213	ILE	2.6	
1	14-A	213	ILE	2.6	
1	15-A	213	ILE	2.6	
1	16-A	213	ILE	2.6	
1	1-A	199	CYS	2.6	
1	2-A	199	CYS	2.6	
1	3-A	199	CYS	2.6	
1	4-A	199	CYS	2.6	
1	5-A	199	CYS	2.6	
1	6-A	199	CYS	2.6	
1	7-A	199	CYS	2.6	
1	8-A	199	CYS	2.6	
1	9-A	199	CYS	2.6	
1	10-A	199	CYS	2.6	
1	11-A	199	CYS	2.6	
1	12-A	199	CYS	2.6	
1	13-A	199	CYS	2.6	
1	14-A	199	CYS	2.6	
1	15-A	199	CYS	2.6	



2Q4K

Mol	Chain	Res	Type	RSRZ	
1	16-A	199	CYS	2.6	
1	1-C	31	ALA	2.5	
1	2-C	31	ALA	2.5	
1	3-C	31	ALA	2.5	
1	4-C	31	ALA	2.5	
1	5-C	31	ALA	2.5	
1	6-C	31	ALA	2.5	
1	7-C	31	ALA	2.5	
1	8-C	31	ALA	2.5	
1	9-C	31	ALA	2.5	
1	10-C	31	ALA	2.5	
1	11-C	31	ALA	2.5	
1	12-C	31	ALA	2.5	
1	13-C	31	ALA	2.5	
1	14-C	31	ALA	2.5	
1	15-C	31	ALA	2.5	
1	16-C	31	ALA	2.5	
1	1-A	113	GLY	2.5	
1	2-A	113	GLY	2.5	
1	3-A	113	GLY	2.5	
1	4-A	113	GLY	2.5	
1	5-A	113	GLY	2.5	
1	6-A	113	GLY	2.5	
1	7-A	113	GLY	2.5	
1	8-A	113	GLY	2.5	
1	9-A	113	GLY	2.5	
1	10-A	113	GLY	2.5	
1	11-A	113	GLY	2.5	
1	12-A	113	GLY	2.5	
1	13-A	113	GLY	2.5	
1	14-A	113	GLY	2.5	
1	15-A	113	GLY	2.5	
1	16-A	113	GLY	2.5	
1	1-A	84	GLN	2.5	
1	2-A	84	GLN	2.5	
1	3-A	84	GLN	2.5	
1	4-A	84	GLN	2.5	
1	5-A	84	GLN	2.5	
1	6-A	84	GLN	2.5	
1	7-A	84	GLN	2.5	
1	8-A	84	GLN	2.5	
1	9-A	84	GLN	2.5	



2Q	4K

Mol	Chain	Res	Type	RSRZ	
1	10-A	84	GLN	2.5	
1	11-A	84	GLN	2.5	
1	12-A	84	GLN	2.5	
1	13-A	84	GLN	2.5	
1	14-A	84	GLN	2.5	
1	15-A	84	GLN	2.5	
1	16-A	84	GLN	2.5	
1	1-A	94	GLN	2.5	
1	1-B	101	GLU	2.5	
1	2-A	94	GLN	2.5	
1	2-B	101	GLU	2.5	
1	3-A	94	GLN	2.5	
1	3-B	101	GLU	2.5	
1	4-A	94	GLN	2.5	
1	4-B	101	GLU	2.5	
1	5-A	94	GLN	2.5	
1	5-B	101	GLU	2.5	
1	6-A	94	GLN	2.5	
1	6-B	101	GLU	2.5	
1	7-A	94	GLN	2.5	
1	7-B	101	GLU	2.5	
1	8-A	94	GLN	2.5	
1	8-B	101	GLU	2.5	
1	9-A	94	GLN	2.5	
1	9-B	101	GLU	2.5	
1	10-A	94	GLN	2.5	
1	10-B	101	GLU	2.5	
1	11-A	94	GLN	2.5	
1	11 - B	101	GLU	2.5	
1	12-A	94	GLN	2.5	
1	12-B	101	GLU	2.5	
1	13-A	94	GLN	2.5	
1	13-B	101	GLU	2.5	
1	14-A	94	GLN	2.5	
1	14-B	101	GLU	2.5	
1	15-A	94	GLN	2.5	
1	15-B	101	GLU	2.5	
1	16-A	94	GLN	2.5	
1	16-B	101	GLU	2.5	
1	1-B	220	HIS	2.5	
1	2-B	220	HIS	2.5	
1	3-B	220	HIS	2.5	



Mol	Chain	Res	Type	RSRZ	
1	4-B	220	HIS	2.5	
1	5-B	220	HIS	2.5	
1	6-B	220	HIS	2.5	
1	7-B	220	HIS	2.5	
1	8-B	220	HIS	2.5	
1	9-B	220	HIS	2.5	
1	10-B	220	HIS	2.5	
1	11-B	220	HIS	2.5	
1	12-B	220	HIS	2.5	
1	13-B	220	HIS	2.5	
1	14-B	220	HIS	2.5	
1	15-B	220	HIS	2.5	
1	16-B	220	HIS	2.5	
1	1-A	41	ASP	2.4	
1	2-A	41	ASP	2.4	
1	3-A	41	ASP	2.4	
1	4-A	41	ASP	2.4	
1	5-A	41	ASP	2.4	
1	6-A	41	ASP	2.4	
1	7-A	41	ASP	2.4	
1	8-A	41	ASP	2.4	
1	9-A	41	ASP	2.4	
1	10-A	41	ASP	2.4	
1	11-A	41	ASP	2.4	
1	12-A	41	ASP	2.4	
1	13-A	41	ASP	2.4	
1	14-A	41	ASP	2.4	
1	15-A	41	ASP	2.4	
1	16-A	41	ASP	2.4	
1	1-C	98	ALA	2.4	
1	2-C	98	ALA	2.4	
1	3-C	98	ALA	2.4	
1	4-C	98	ALA	2.4	
1	5-C	98	ALA	2.4	
1	6-C	98	ALA	2.4	
1	7-C	98	ALA	2.4	
1	8-C	98	ALA	2.4	
1	9-C	98	ALA	2.4	
1	10-C	98	ALA	2.4	
1	11-C	98	ALA	2.4	
1	12-C	98	ALA	2.4	
1	13-C	98	ALA	2.4	



2Q4K

Mol	Chain	Res	Type	RSRZ
1	14-C	98	ALA	2.4
1	15-C	98	ALA	2.4
1	16-C	98	ALA	2.4
1	1-B	123	HIS	2.4
1	2-B	123	HIS	2.4
1	3-B	123	HIS	2.4
1	4-B	123	HIS	2.4
1	5-B	123	HIS	2.4
1	6-B	123	HIS	2.4
1	7-B	123	HIS	2.4
1	8-B	123	HIS	2.4
1	9-B	123	HIS	2.4
1	10-B	123	HIS	2.4
1	11-B	123	HIS	2.4
1	12-B	123	HIS	2.4
1	13-B	123	HIS	2.4
1	14-B	123	HIS	2.4
1	15-B	123	HIS	2.4
1	16-B	123	HIS	2.4
1	1-C	90	SER	2.4
1	2-C	90	SER	2.4
1	3-C	90	SER	2.4
1	4-C	90	SER	2.4
1	5-C	90	SER	2.4
1	6-C	90	SER	2.4
1	7-C	90	SER	2.4
1	8-C	90	SER	2.4
1	9-C	90	SER	2.4
1	10-C	90	SER	2.4
1	11-C	90	SER	2.4
1	12-C	90	SER	2.4
1	13-C	90	SER	2.4
1	14-C	90	SER	2.4
1	15-C	90	SER	2.4
1	16-C	90	SER	2.4
1	1-A	93	VAL	2.4
1	2-A	93	VAL	2.4
1	3-A	93	VAL	2.4
1	4-A	93	VAL	2.4
1	5-A	93	VAL	2.4
1	6-A	93	VAL	2.4
1	7-A	93	VAL	2.4



Mol	Chain	Res	Type	RSRZ
1	8-A	93	VAL	2.4
1	9-A	93	VAL	2.4
1	10-A	93	VAL	2.4
1	11-A	93	VAL	2.4
1	12-A	93	VAL	2.4
1	13-A	93	VAL	2.4
1	14-A	93	VAL	2.4
1	15-A	93	VAL	2.4
1	16-A	93	VAL	2.4
1	1-C	212	GLY	2.4
1	2-C	212	GLY	2.4
1	3-C	212	GLY	2.4
1	4-C	212	GLY	2.4
1	5-C	212	GLY	2.4
1	6-C	212	GLY	2.4
1	7-C	212	GLY	2.4
1	8-C	212	GLY	2.4
1	9-C	212	GLY	2.4
1	10-C	212	GLY	2.4
1	11-C	212	GLY	2.4
1	12-C	212	GLY	2.4
1	13-C	212	GLY	2.4
1	14-C	212	GLY	2.4
1	15-C	212	GLY	2.4
1	16-C	212	GLY	2.4
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-A	85	GLY	2.4



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Mol	Chain	Res	Type	RSRZ
1	1-B	72	ASN	2.4
1	2-A	85	GLY	2.4
1	2-B	72	ASN	2.4
1	3-A	85	GLY	2.4
1	3-B	72	ASN	2.4
1	4-A	85	GLY	2.4
1	4-B	72	ASN	2.4
1	5-A	85	GLY	2.4
1	5-B	72	ASN	2.4
1	6-A	85	GLY	2.4
1	6-B	72	ASN	2.4
1	7-A	85	GLY	2.4
1	7-B	72	ASN	2.4
1	8-A	85	GLY	2.4
1	8-B	72	ASN	2.4
1	9-A	85	GLY	2.4
1	9-B	72	ASN	2.4
1	10-A	85	GLY	2.4
1	10-B	72	ASN	2.4
1	11-A	85	GLY	2.4
1	11 - B	72	ASN	2.4
1	12-A	85	GLY	2.4
1	12-B	72	ASN	2.4
1	13-A	85	GLY	2.4
1	13-B	72	ASN	2.4
1	14-A	85	GLY	2.4
1	14-B	72	ASN	2.4
1	15-A	85	GLY	2.4
1	15-B	72	ASN	2.4
1	16-A	85	GLY	2.4
1	16-B	72	ASN	2.4
1	1-C	104	GLN	2.4
1	2-C	104	GLN	2.4
1	3-C	104	GLN	2.4
1	4-C	104	GLN	2.4
1	5-C	104	GLN	2.4
1	6-C	104	GLN	2.4
1	7-C	104	GLN	2.4
1	8-C	104	GLN	2.4
1	9-C	104	GLN	2.4
1	10-C	104	GLN	2.4
1	11-C	104	GLN	2.4



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Mol	Chain	Res	Type	RSRZ
1	12-C	104	GLN	2.4
1	13-C	104	GLN	2.4
1	14-C	104	GLN	2.4
1	15-C	104	GLN	2.4
1	16-C	104	GLN	2.4
1	1-B	41	ASP	2.3
1	2-B	41	ASP	2.3
1	3-B	41	ASP	2.3
1	4-B	41	ASP	2.3
1	5-B	41	ASP	2.3
1	6-B	41	ASP	2.3
1	7-B	41	ASP	2.3
1	8-B	41	ASP	2.3
1	9-B	41	ASP	2.3
1	10-B	41	ASP	2.3
1	11-B	41	ASP	2.3
1	12-B	41	ASP	2.3
1	13-B	41	ASP	2.3
1	14-B	41	ASP	2.3
1	15-B	41	ASP	2.3
1	16-B	41	ASP	2.3
1	1-A	183	LEU	2.3
1	2-A	183	LEU	2.3
1	3-A	183	LEU	2.3
1	4-A	183	LEU	2.3
1	5-A	183	LEU	2.3
1	6-A	183	LEU	2.3
1	7-A	183	LEU	2.3
1	8-A	183	LEU	2.3
1	9-A	183	LEU	2.3
1	10-A	183	LEU	2.3
1	11-A	183	LEU	2.3
1	12-A	183	LEU	2.3
1	13-A	183	LEU	2.3
1	14-A	183	LEU	2.3
1	15-A	183	LEU	2.3
1	16-A	183	LEU	2.3
1	1-A	100	TRP	2.3
1	2-A	100	TRP	2.3
1	3-A	100	TRP	2.3
1	4-A	100	TRP	2.3
1	5-A	100	TRP	2.3



Mol	Chain	Res	Type	RSRZ
1	6-A	100	TRP	2.3
1	7-A	100	TRP	2.3
1	8-A	100	TRP	2.3
1	9-A	100	TRP	2.3
1	10-A	100	TRP	2.3
1	11-A	100	TRP	2.3
1	12-A	100	TRP	2.3
1	13-A	100	TRP	2.3
1	14-A	100	TRP	2.3
1	15-A	100	TRP	2.3
1	16-A	100	TRP	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-C	88	PRO	2.2
1	2-C	88	PRO	2.2
1	3-C	88	PRO	2.2
1	4-C	88	PRO	2.2
1	5-C	88	PRO	2.2
1	6-C	88	PRO	2.2
1	7-C	88	PRO	2.2
1	8-C	88	PRO	2.2
1	9-C	88	PRO	2.2
1	10-C	88	PRO	2.2
1	11-C	88	PRO	2.2
1	12-C	88	PRO	2.2
1	13-C	88	PRO	2.2
1	14-C	88	PRO	2.2
1	15-C	88	PRO	2.2



Mol	Chain	Res	Type	RSRZ
1	16-C	88	PRO	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-A	108	ARG	2.2
1	1-A	182	ARG	2.2
1	2-A	108	ARG	2.2
1	2-A	182	ARG	2.2
1	3-A	108	ARG	2.2
1	3-A	182	ARG	2.2
1	4-A	108	ARG	2.2
1	4-A	182	ARG	2.2
1	5-A	108	ARG	2.2
1	5-A	182	ARG	2.2
1	6-A	108	ARG	2.2
1	6-A	182	ARG	2.2
1	7-A	108	ARG	2.2
1	7-A	182	ARG	2.2
1	8-A	108	ARG	2.2
1	8-A	182	ARG	2.2
1	9-A	108	ARG	2.2
1	9-A	182	ARG	2.2
1	10-A	108	ARG	2.2
1	10-A	182	ARG	2.2
1	11-A	108	ARG	2.2
1	11-A	182	ARG	2.2
1	12-A	108	ARG	2.2
1	12-A	182	ARG	2.2
1	13-A	108	ARG	2.2



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Mol	Chain	Res	Type	RSRZ
1	13-A	182	ARG	2.2
1	14-A	108	ARG	2.2
1	14-A	182	ARG	2.2
1	15-A	108	ARG	2.2
1	15-A	182	ARG	2.2
1	16-A	108	ARG	2.2
1	16-A	182	ARG	2.2
1	1-A	28	GLU	2.2
1	1-C	247	ASN	2.2
1	2-A	28	GLU	2.2
1	2-C	247	ASN	2.2
1	3-A	28	GLU	2.2
1	3-C	247	ASN	2.2
1	4-A	28	GLU	2.2
1	4-C	247	ASN	2.2
1	5-A	28	GLU	2.2
1	5-C	247	ASN	2.2
1	6-A	28	GLU	2.2
1	6-C	247	ASN	2.2
1	7-A	28	GLU	2.2
1	7-C	247	ASN	2.2
1	8-A	28	GLU	2.2
1	8-C	247	ASN	2.2
1	9-A	28	GLU	2.2
1	9-C	247	ASN	2.2
1	10-A	28	GLU	2.2
1	10-C	247	ASN	2.2
1	11-A	28	GLU	2.2
1	11-C	247	ASN	2.2
1	12-A	28	GLU	2.2
1	12-C	247	ASN	2.2
1	13-A	28	GLU	2.2
1	13-C	247	ASN	2.2
1	14-A	28	GLU	2.2
1	14-C	247	ASN	2.2
1	15-A	28	GLU	2.2
1	15-C	247	ASN	2.2
1	16-A	28	GLU	2.2
1	16-C	247	ASN	2.2
1	1-B	55	ALA	2.2
1	2-B	55	ALA	2.2
1	3-B	55	ALA	2.2



2Q4k	`

Mol	Chain	Res	Type	RSRZ
1	4-B	55	ALA	2.2
1	5-B	55	ALA	2.2
1	6-B	55	ALA	2.2
1	7-B	55	ALA	2.2
1	8-B	55	ALA	2.2
1	9-B	55	ALA	2.2
1	10-B	55	ALA	2.2
1	11-B	55	ALA	2.2
1	12-B	55	ALA	2.2
1	13-B	55	ALA	2.2
1	14-B	55	ALA	2.2
1	15-B	55	ALA	2.2
1	16-B	55	ALA	2.2
1	1-B	237	ARG	2.2
1	2-B	237	ARG	2.2
1	3-B	237	ARG	2.2
1	4-B	237	ARG	2.2
1	5-B	237	ARG	2.2
1	6-B	237	ARG	2.2
1	7-B	237	ARG	2.2
1	8-B	237	ARG	2.2
1	9-B	237	ARG	2.2
1	10-B	237	ARG	2.2
1	11-B	237	ARG	2.2
1	12-B	237	ARG	2.2
1	13-B	237	ARG	2.2
1	14-B	237	ARG	2.2
1	15-B	237	ARG	2.2
1	16-B	237	ARG	2.2
1	1-A	186	LEU	2.2
1	2-A	186	LEU	2.2
1	3-A	186	LEU	2.2
1	4-A	186	LEU	2.2
1	5-A	186	LEU	2.2
1	6-A	186	LEU	2.2
1	7-A	186	LEU	2.2
1	8-A	186	LEU	2.2
1	9-A	186	LEU	2.2
1	10-A	186	LEU	2.2
1	11-A	186	LEU	2.2
1	12-A	186	LEU	2.2
1	13-A	186	LEU	2.2



Mol	Chain	Res	Type	RSRZ
1	14-A	186	LEU	2.2
1	15-A	186	LEU	2.2
1	16-A	186	LEU	2.2
1	1-A	187	GLU	2.1
1	2-A	187	GLU	2.1
1	3-A	187	GLU	2.1
1	4-A	187	GLU	2.1
1	5-A	187	GLU	2.1
1	6-A	187	GLU	2.1
1	7-A	187	GLU	2.1
1	8-A	187	GLU	2.1
1	9-A	187	GLU	2.1
1	10-A	187	GLU	2.1
1	11-A	187	GLU	2.1
1	12-A	187	GLU	2.1
1	13-A	187	GLU	2.1
1	14-A	187	GLU	2.1
1	15-A	187	GLU	2.1
1	16-A	187	GLU	2.1
1	1-B	217	ASN	2.1
1	2-B	217	ASN	2.1
1	3-B	217	ASN	2.1
1	4-B	217	ASN	2.1
1	5-B	217	ASN	2.1
1	6-B	217	ASN	2.1
1	7-B	217	ASN	2.1
1	8-B	217	ASN	2.1
1	9-B	217	ASN	2.1
1	10-B	217	ASN	2.1
1	11-B	217	ASN	2.1
1	12-B	217	ASN	2.1
1	13-B	217	ASN	2.1
1	14-B	217	ASN	2.1
1	15-B	217	ASN	2.1
1	16-B	217	ASN	2.1
1	1-B	122	HIS	2.1
1	2-B	122	HIS	2.1
1	3-B	122	HIS	2.1
1	4-B	122	HIS	2.1
1	5-B	122	HIS	2.1
1	6-B	122	HIS	2.1
1	7-B	122	HIS	2.1



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Mol	Chain	Res	Type	RSRZ
1	8-B	122	HIS	2.1
1	9-B	122	HIS	2.1
1	10-B	122	HIS	2.1
1	11-B	122	HIS	2.1
1	12-B	122	HIS	2.1
1	13-B	122	HIS	2.1
1	14-B	122	HIS	2.1
1	15-B	122	HIS	2.1
1	16-B	122	HIS	2.1
1	1-A	181	ASP	2.1
1	2-A	181	ASP	2.1
1	3-A	181	ASP	2.1
1	4-A	181	ASP	2.1
1	5-A	181	ASP	2.1
1	6-A	181	ASP	2.1
1	7-A	181	ASP	2.1
1	8-A	181	ASP	2.1
1	9-A	181	ASP	2.1
1	10-A	181	ASP	2.1
1	11-A	181	ASP	2.1
1	12-A	181	ASP	2.1
1	13-A	181	ASP	2.1
1	14-A	181	ASP	2.1
1	15-A	181	ASP	2.1
1	16-A	181	ASP	2.1
1	1-A	149	ALA	2.1
1	2-A	149	ALA	2.1
1	3-A	149	ALA	2.1
1	4-A	149	ALA	2.1
1	5-A	149	ALA	2.1
1	6-A	149	ALA	2.1
1	7-A	149	ALA	2.1
1	8-A	149	ALA	2.1
1	9-A	149	ALA	2.1
1	10-A	149	ALA	2.1
1	11-A	149	ALA	2.1
1	12-A	149	ALA	2.1
1	13-A	149	ALA	2.1
1	14-A	149	ALA	2.1
1	15-A	149	ALA	2.1
1	16-A	149	ALA	2.1
1	1-A	122	HIS	2.1



2Q4k	`

Mol	Chain	Res	Type	RSRZ
1	2-A	122	HIS	2.1
1	3-A	122	HIS	2.1
1	4-A	122	HIS	2.1
1	5-A	122	HIS	2.1
1	6-A	122	HIS	2.1
1	7-A	122	HIS	2.1
1	8-A	122	HIS	2.1
1	9-A	122	HIS	2.1
1	10-A	122	HIS	2.1
1	11-A	122	HIS	2.1
1	12-A	122	HIS	2.1
1	13-A	122	HIS	2.1
1	14-A	122	HIS	2.1
1	15-A	122	HIS	2.1
1	16-A	122	HIS	2.1
1	1-A	119	ALA	2.1
1	1-C	99	ALA	2.1
1	2-A	119	ALA	2.1
1	2-C	99	ALA	2.1
1	3-A	119	ALA	2.1
1	3-C	99	ALA	2.1
1	4-A	119	ALA	2.1
1	4-C	99	ALA	2.1
1	5-A	119	ALA	2.1
1	5-C	99	ALA	2.1
1	6-A	119	ALA	2.1
1	6-C	99	ALA	2.1
1	7-A	119	ALA	2.1
1	7-C	99	ALA	2.1
1	8-A	119	ALA	2.1
1	8-C	99	ALA	2.1
1	9-A	119	ALA	2.1
1	9-C	99	ALA	2.1
1	10-A	119	ALA	2.1
1	10-C	99	ALA	2.1
1	11-A	119	ALA	2.1
1	11-C	99	ALA	2.1
1	12-A	119	ALA	2.1
1	12-C	99	ALA	2.1
1	13-A	119	ALA	2.1
1	13-C	99	ALA	2.1
1	14-A	119	ALA	2.1



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Mol	Chain	Res	Type	RSRZ
1	14-C	99	ALA	2.1
1	15-A	119	ALA	2.1
1	15-C	99	ALA	2.1
1	16-A	119	ALA	2.1
1	16-C	99	ALA	2.1
1	1-A	101	GLU	2.1
1	2-A	101	GLU	2.1
1	3-A	101	GLU	2.1
1	4-A	101	GLU	2.1
1	5-A	101	GLU	2.1
1	6-A	101	GLU	2.1
1	7-A	101	GLU	2.1
1	8-A	101	GLU	2.1
1	9-A	101	GLU	2.1
1	10-A	101	GLU	2.1
1	11-A	101	GLU	2.1
1	12-A	101	GLU	2.1
1	13-A	101	GLU	2.1
1	14-A	101	GLU	2.1
1	15-A	101	GLU	2.1
1	16-A	101	GLU	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
1	16-A	244	ARG	2.1

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 monosaccharides 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.

