

Full wwPDB X-ray Structure Validation Report (i)

Sep 19, 2023 – 02:08 AM EDT

PDB ID	:	3VON
Title	:	Crystalstructure of the ubiquitin protease
Authors	:	Sato, Y.; Fukai, S.
Deposited on	:	2012-01-30
Resolution	:	3.15 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
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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

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 3.15 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				
Wiethe	$(\# \mathbf{Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$				
R _{free}	130704	1665 (3.20-3.12)				
Ramachandran outliers	138981	1770 (3.20-3.12)				
Sidechain outliers	138945	1769(3.20-3.12)				
RSRZ outliers	127900	1616 (3.20-3.12)				

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		
1	٨	000	%		
	A	228	85%	7%	8%
			7%		
1	H	228	84%	10%	6%
1	Ο	228	88%	7%	5%
			2%		
1	V	228	90%	•	6%
			4%		
1	с	228	87%	8%	5%
			13%		
1	j	228	83%	9%	8%



Chain Length Quality of chain Mol 2В 13895% 5% 2D 1387% • 93% 2F 13892% 7% • Ι 213885% 14% . .% Κ 213894% 6% .% 2М 13891% 9% 2% Р 213891% 9% ... 2 \mathbf{R} 13898% Т 213810% • 89% .% W 213810% • 89% 2Υ 1385%• 94% .% 2138 \mathbf{a} 93% 6% • .% 2d 13893% 7% .% 2f 9% • 13890% .% 2h 1387% 93% 3% 2k 1389% 91% $\mathbf{2}$ 138 \mathbf{m} 96% • • .% 21380 7% 93% С 3 148••• 84% 14% Е 8% •• 3 14891% \mathbf{G} 3 148•• 89% 10% 3 J • 14891% 9% % L 1483 91% 9% • Ν 1483 9% •• 89% 3 Q 1488% •• 90%

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Mol	Chain	Length	Quality of chain	
3	S	148	90%	9% •
3	U	148	91%	7% ••
3	Х	148	89%	11% •
3	Z	148	91%	9%
3	b	148	91%	8% •
3	е	148	88%	9% ••
3	g	148	91%	9%
3	i	148	91%	9%
3	1	148	% 	9% ••
3	n	148	.% 91%	9% •
3	р	148	% 9 0%	9% •



3VON

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 51450 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		At	oms			ZeroOcc	AltConf	Trace
1	Δ	910	Total	С	Ν	0	S	0	0	0
	210	1731	1111	284	330	6	0	0	0	
1	ц	214	Total	С	Ν	0	S	0	0	0
	ГП	214	1767	1133	290	339	5	0	0	0
1	1 0	216	Total	С	Ν	0	S	0	0	0
	0		1786	1148	292	340	6		0	0
1	V	215	Total	С	Ν	0	S	0	0	0
	v		1777	1140	292	339	6	0		U
1	0	217	Total	С	Ν	0	S	0	0	0
		217	1785	1144	293	342	6	0	0	0
1	1 ј	210	Total	С	Ν	0	S	0	0	0
			1730	1112	284	329	5		U	

• Molecule 1 is a protein called Ubiquitin thioesterase OTUB1.

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference	
А	44	SER	-	expression tag	UNP Q96FW1	
Н	44	SER	-	expression tag	UNP Q96FW1	
0	44	SER	-	expression tag	UNP Q96FW1	
V	44	SER	-	expression tag	UNP Q96FW1	
с	44	SER	-	expression tag	UNP Q96FW1	
j	44	SER	-	expression tag	UNP Q96FW1	

• Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 variant 2.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	В	138	Total	С	Ν	0	S	0	0	0
		150	1096	689	191	208	8	0	0	0
0	Л	127	Total	С	Ν	0	S	0	0	0
	2 D	157	1092	687	190	207	8	0	0	0
0	9 F	190	Total	С	Ν	0	S	0	0	0
2 F	199	1096	689	191	208	8	0	0	U	



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
	т	190	Total	С	Ν	0	S	0	0	0
	1	138	1096	689	191	208	8	0	0	0
0	V	190	Total	С	Ν	0	S	0	0	0
	ñ	199	1096	689	191	208	8	0	0	0
2	М	138	Total	С	Ν	0	S	0	0	0
2	111	150	1096	689	191	208	8	0	0	0
2	р	138	Total	С	Ν	Ο	\mathbf{S}	0	0	0
2	I	130	1096	689	191	208	8	0	0	0
2	B	137	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	10	107	1092	687	190	207	8	0	0	0
2	Т	138	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	1	100	1096	689	191	208	8	0	0	0
2	W	137	Total	С	Ν	Ο	\mathbf{S}	0	0	0
			1092	687	190	207	8	Ŭ	0	0
2	Y	137	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	-	101	1092	687	190	207	8	Ŭ		0
2	a	138	Total	С	Ν	Ο	S	0	0	0
		100	1096	689	191	208	8	Ŭ	0	0
2	d	138	Total	С	Ν	Ο	S	0	0	0
			1096	689	191	208	8	Ŭ		
2	f	137	Total	С	Ν	0	S	0	0	0
			1092	687	190	207	8			
2	h	138	Total	С	N	0	S	0	0	0
			1096	689	191	208	8		_	
2	k	138	Total	С	N	0	S	0	0	0
			1096	689	191	208	8		_	
2	2 m	137	Total	C	N	0	S	0	0	0
			1092	687	190	207	8			
2	О	138	Total	C	N	0	S	0	0	0
	~		1096	689	191	208	8	, v	Ŭ	

• Molecule 3 is a protein called Ubiquitin-conjugating enzyme E2 N.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	2 C	1.47	Total	С	Ν	0	S	0	0	0
3	C	147	1175	755	202	214	4	0	0	0
2	3 E	E 147	Total	С	Ν	0	S	0	0	0
J			1175	755	202	214	4		0	
2	С	147	Total	С	Ν	0	S	0	0	0
J	3 G		1175	755	202	214	4			0
2	3 J	147	Total	С	Ν	0	S	0	0	0
J			1175	755	202	214	4		0	U



			5	• •						_
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
9	т	1.47	Total	С	Ν	0	\mathbf{S}	0	0	0
9	L	141	1175	755	202	214	4	0	0	0
9	N	147	Total	С	Ν	0	S	0	0	0
3	IN		1175	755	202	214	4	0	0	0
9	0	1.47	Total	С	Ν	0	S	0	0	0
3	Q	147	1175	755	202	214	4	0	0	0
9	C	140	Total	С	Ν	0	S	0	0	0
9	S	148	1179	757	203	215	4	0	0	0
9	TT	1.47	Total	С	Ν	0	S	0	0	0
3	U	147	1175	755	202	214	4	0	0	0
9	v	1.47	Total	С	Ν	0	S	0	0	0
3	Λ	147	1175	755	202	214	4	0	0	0
9	7	148	Total	С	Ν	0	S	0	0	0
9	L		1179	757	203	215	4	0	0	0
2	h	147	Total	С	Ν	0	S	0	0	0
ა	U	141	1175	755	202	214	4	0	0	0
2	0	1.47	Total	С	Ν	0	S	0	0	0
ა	е	141	1175	755	202	214	4	0	0	0
9	ar.	149	Total	С	Ν	0	S	0	0	0
9	g	140	1179	757	203	215	4	0	0	0
9	;	149	Total	С	Ν	0	S	0	0	0
9	1	140	1179	757	203	215	4	0	0	0
9	1	1.47	Total	С	Ν	0	S	0	0	0
3	3 I	147	1175	755	202	214	4	0	0	0
9	2	1.47	Total	С	Ν	0	S	0	0	0
o n	147	1175	755	202	214	4		U	U	
2	n	1/12	Total	С	Ν	0	S	0	0	0
3	p p	140	1179	757	203	215	4	0	0	U



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: Ubiquitin thioesterase OTUB1





• Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2

Chain B:	95%	5%



• Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2

Chain D:	93%	7%
GLY V7 E21 E21 821 821 821 849 849 849 8181 8181 8108 81008	4110 K133	
• Molecule 2: Ubiquitin	n-conjugating enzyme E2 variant 2	
Chain F:	92%	7% •
G6 E33 M60 M60 M60 K72 E75 M92 M92 M93	V106 K116 K133 Y143	
• Molecule 2: Ubiquitin	n-conjugating enzyme E2 variant 2	
Chain I:	85%	14% •
06 V7 K8 K14 V26 V26 M35 M36 M49 N57 N57	R61 K72 F75 F75 F82 F82 F82 F82 F82 F106 M106 M106 M106 M100 M110 M110 M110 M	
• Molecule 2: Ubiquitin	1-conjugating enzyme E2 variant 2	
Chain K:	94%	6%
	WORLDWIDE	

DB



• Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2



C6 K8 K14 C27 C27 C27 C27 C27 C35 K45 N92 N92 N92 N92 N92 N92 K143

• Molecule 2: Ubiquitin-conjugating enzyme E2 variant 2



• Molecule 3: Ubiquitin-conjugating enzyme E2 N



Chain C:	84%	14% ••
GLY L4 K10 K10 R14 R14 K24 K24 K24 E26 E26 E29 E29	D44 P44 R70 R92 R102 L106 S107 S107 S107 P117 P117 P118 P118 P118 P118 P119 P118 P119 P119 P120 P128 U128	
• Molecule 3: Ubiquitin	n-conjugating enzyme E2 N	
Chain E:	91%	8% ••
GLY 14 14 14 14 14 14 14 17 36 193 293 296	1106 1106 1111 1111 1111 1111 1111 1111	
• Molecule 3: Ubiquiti:	n-conjugating enzyme E2 N	
Chain G:	89%	10% ••
GLY 14 R6 R6 R6 R2 R2 R10 1100 L100 L100 L100 N116 N116	D119 P120 1221 A122 A122 D124 Q126 A141 N150	
• Molecule 3: Ubiquiti:	n-conjugating enzyme E2 N	
Chain J:	91%	9% •
GLY L4 R5 R1 R1 R1 R1 R1 R1 R1 R1 R1 R1 R5 R1 R1 R1 R1 R1 R1 R1 R1 R1 R1 R1 R1 R1	R70 F71 M72 K82 K92 B89 C100 F100 N150	
• Molecule 3: Ubiquiti:	n-conjugating enzyme E2 N	
Chain L:	91%	9% •
GLY L4 K10 R14 B18 Y34 Y34 Y73 K74 D89 K22	1105 L106 D118 D118 D124 N150	
• Molecule 3: Ubiquitin	n-conjugating enzyme E2 N	
Chain N:	89%	9% ••
GLY L4 230 830 846 846 846 846 846 846 710 010 8113	P120 P124 E127 Q128 R145 L146 L146 N150	
• Molecule 3: Ubiquitin	n-conjugating enzyme E2 N	
Chain Q:	90%	8% ••
GLY L4 L4 K24 R70 R70 R70 R70 R70	R102 L106 L121 N123 N123 R145 R145 N150	
• Molecule 3: Ubiquitiz	n-conjugating enzyme E2 N	



Chain S:	90%	9% •
G3 L4 E18 E29 E29 E61 T173 E61 E61 D93 D93 D93 C105	N116 N123 D124 Q128 (128 N150 N150	
• Molecule 3: Ubiquitin-	conjugating enzyme E2 N	
Chain U:	91%	7% ••
GLY L4 R14 L15 L16 L16 R12 B93 D93 C105 L105 D93 D93 C124 V124	4129 4135 1137 1137 N150	
• Molecule 3: Ubiquitin-	conjugating enzyme E2 N	
Chain X:	89%	11% •
6LY 14 76 76 76 76 76 76 76 76 76 76 76 76 76	K82 K92 L105 L105 L105 A122 A122 A122 A122 A126 A135	
• Molecule 3: Ubiquitin-	conjugating enzyme E2 N	
Chain Z:	91%	9%
G3 V20 E29 E61 K74 K74 K74 D89 D89 D83 D83 L105 L105	9128 9135 1137 1137 1137 1137 1137 1137 1136	
• Molecule 3: Ubiquitin-	conjugating enzyme E2 N	
Chain b:	91%	8% •
GLY L4 V20 B81 B89 B89 B89 B89 B89 B89 B89 B89 B89 B89	1137 1141 1141 1150 1150	
• Molecule 3: Ubiquitin-	conjugating enzyme E2 N	
Chain e:	88%	9% ••
GLY L4 19 K10 K10 K10 M64 M72 M72 L106 L106	1111 1119 1119 1119 1119 1119 1128 1128	
• Molecule 3: Ubiquitin-	conjugating enzyme E2 N	
Chain g:	91%	9%
G3 F6 F6 M72 M72 C37 173 C37 173 C37 C37 C37 C37 C37 C37 C37 C37 C37 C	8113 113 113 113 113 113 113 113 113 113	
• Molecule 3: Ubiquitin-	conjugating enzyme E2 N	







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	102.06Å 137.28Å 257.11Å	Deperitor
a, b, c, α , β , γ	90.00° 90.03° 90.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	50.00 - 3.15	Depositor
Resolution (A)	46.92 - 3.15	EDS
% Data completeness	96.8 (50.00-3.15)	Depositor
(in resolution range)	96.6~(46.92 - 3.15)	EDS
R_{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.22 (at 3.12 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
D D.	0.223 , 0.281	Depositor
Π, Π_{free}	0.223 , 0.280	DCC
R_{free} test set	5967 reflections (5.02%)	wwPDB-VP
Wilson B-factor $(Å^2)$	63.3	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.28, 5.5	EDS
L-test for $twinning^2$	$< L >=0.46, < L^2>=0.29$	Xtriage
Estimated twinning fraction	0.427 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	51450	wwPDB-VP
Average B, all atoms $(Å^2)$	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 51.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4409e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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	$\mathbf{lengths}$	Bo	ond angles
	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.36	0/1769	0.48	0/2381
1	Н	0.35	0/1806	0.49	0/2434
1	0	0.36	0/1826	0.47	0/2457
1	V	0.36	0/1816	0.48	0/2444
1	с	0.36	0/1824	0.49	0/2458
1	j	0.35	0/1768	0.47	0/2381
2	В	0.34	0/1119	0.50	0/1512
2	D	0.32	0/1115	0.51	0/1507
2	F	0.37	0/1119	0.54	0/1512
2	Ι	0.35	0/1119	0.54	0/1512
2	Κ	0.34	0/1119	0.53	0/1512
2	М	0.34	0/1119	0.52	0/1512
2	Р	0.35	0/1119	0.53	0/1512
2	R	0.34	0/1115	0.52	0/1507
2	Т	0.34	0/1119	0.51	0/1512
2	W	0.36	0/1115	0.52	0/1507
2	Y	0.33	0/1115	0.52	0/1507
2	a	0.34	0/1119	0.53	0/1512
2	d	0.34	0/1119	0.51	0/1512
2	f	0.32	0/1115	0.53	0/1507
2	h	0.38	0/1119	0.52	0/1512
2	k	0.35	0/1119	0.54	0/1512
2	m	0.34	0/1115	0.52	0/1507
2	0	0.34	0/1119	0.50	0/1512
3	С	0.35	0/1205	0.57	1/1640~(0.1%)
3	Ε	0.33	0/1205	0.55	1/1640~(0.1%)
3	G	0.36	0/1205	0.59	1/1640~(0.1%)
3	J	0.34	0/1205	0.54	0/1640
3	L	0.34	0/1205	0.53	$0/1\overline{640}$
3	Ν	0.36	0/1205	0.55	0/1640
3	Q	0.34	0/1205	0.59	$1/1640~(0.1\overline{\%})$
3	S	0.34	0/1209	$\overline{0.50}$	0/1645
3	U	0.35	0/1205	0.55	1/1640~(0.1%)
3	X	0.34	$0/1\overline{205}$	0.55	$0/1\overline{640}$



Mal	Chain	Bond	lengths	Bo	ond angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
3	Ζ	0.35	0/1209	0.54	0/1645
3	b	0.35	0/1205	0.52	0/1640
3	е	0.34	0/1205	0.58	2/1640~(0.1%)
3	g	0.34	0/1209	0.50	0/1645
3	i	0.36	0/1209	0.54	0/1645
3	1	0.33	0/1205	0.55	1/1640~(0.1%)
3	n	0.32	0/1205	0.51	0/1640
3	р	0.35	0/1209	0.55	1/1645~(0.1%)
All	All	0.35	0/52637	0.52	9/71286~(0.0%)

There are no bond length outliers.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	G	121	LEU	CA-CB-CG	7.25	131.98	115.30
3	С	106	LEU	CA-CB-CG	6.32	129.83	115.30
3	1	106	LEU	CA-CB-CG	6.17	129.50	115.30
3	е	106	LEU	CA-CB-CG	6.05	129.21	115.30
3	е	146	LEU	CA-CB-CG	5.66	128.33	115.30
3	Е	54	LEU	CA-CB-CG	5.48	127.91	115.30
3	р	4	LEU	CA-CB-CG	5.39	127.70	115.30
3	U	4	LEU	CA-CB-CG	5.13	127.09	115.30
3	Q	106	LEU	CA-CB-CG	5.10	127.02	115.30

All (9) bond angle outliers are listed below:

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	ntiles
1	А	204/228~(90%)	195 (96%)	8 (4%)	1 (0%)	29	65
1	Н	208/228~(91%)	199 (96%)	7 (3%)	2(1%)	15	51
1	Ο	210/228~(92%)	202 (96%)	7 (3%)	1 (0%)	29	65
1	V	209/228~(92%)	201 (96%)	7 (3%)	1 (0%)	29	65
1	с	211/228~(92%)	200 (95%)	9 (4%)	2 (1%)	17	53
1	j	204/228~(90%)	190 (93%)	11 (5%)	3(2%)	10	41
2	В	136/138~(99%)	134 (98%)	2 (2%)	0	100	100
2	D	135/138~(98%)	129 (96%)	5 (4%)	1 (1%)	22	59
2	F	136/138~(99%)	130 (96%)	4 (3%)	2 (2%)	10	41
2	Ι	136/138~(99%)	122 (90%)	11 (8%)	3 (2%)	6	32
2	K	136/138~(99%)	132 (97%)	4 (3%)	0	100	100
2	М	136/138~(99%)	133 (98%)	2 (2%)	1 (1%)	22	59
2	Р	136/138~(99%)	128 (94%)	6 (4%)	2(2%)	10	41
2	R	135/138~(98%)	129 (96%)	6 (4%)	0	100	100
2	Т	136/138~(99%)	128 (94%)	5 (4%)	3 (2%)	6	32
2	W	135/138~(98%)	129 (96%)	5 (4%)	1 (1%)	22	59
2	Y	135/138~(98%)	130 (96%)	4 (3%)	1 (1%)	22	59
2	a	136/138~(99%)	128 (94%)	5 (4%)	3(2%)	6	32
2	d	136/138~(99%)	133 (98%)	2 (2%)	1 (1%)	22	59
2	f	135/138~(98%)	129 (96%)	5 (4%)	1 (1%)	22	59
2	h	136/138~(99%)	132 (97%)	3 (2%)	1 (1%)	22	59
2	k	136/138~(99%)	127 (93%)	9 (7%)	0	100	100
2	m	135/138~(98%)	130 (96%)	5 (4%)	0	100	100
2	О	136/138~(99%)	131 (96%)	3 (2%)	2(2%)	10	41
3	С	145/148 (98%)	135 (93%)	7 (5%)	3 (2%)	7	33
3	Е	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
3	G	145/148 (98%)	134 (92%)	9 (6%)	2 (1%)	11	43
3	J	145/148~(98%)	136 (94%)	9 (6%)	0	100	100
3	L	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
3	N	145/148 (98%)	136 (94%)	7 (5%)	2 (1%)	11	43
3	Q	$\overline{145/148} \ (98\%)$	135 (93%)	8 (6%)	2 (1%)	11	43
3	S	146/148 (99%)	142 (97%)	3 (2%)	1 (1%)	22	59



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
3	U	145/148~(98%)	136 (94%)	9 (6%)	0	100	100
3	Х	145/148~(98%)	135~(93%)	8 (6%)	2(1%)	11	43
3	Z	146/148~(99%)	142 (97%)	4 (3%)	0	100	100
3	b	145/148~(98%)	135~(93%)	10 (7%)	0	100	100
3	е	145/148 (98%)	136 (94%)	7 (5%)	2(1%)	11	43
3	g	146/148~(99%)	140 (96%)	6 (4%)	0	100	100
3	i	146/148~(99%)	135~(92%)	11 (8%)	0	100	100
3	1	145/148~(98%)	134 (92%)	11 (8%)	0	100	100
3	n	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
3	р	146/148~(99%)	136 (93%)	10 (7%)	0	100	100
All	All	6303/6516~(97%)	5983 (95%)	274 (4%)	46 (1%)	22	59

Continued from previous page...

All (46) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
2	F	93	ASN
1	Н	152	GLN
2	Ι	107	ALA
2	Т	93	ASN
1	V	152	GLN
1	j	152	GLN
2	Ι	26	VAL
2	а	27	GLY
2	а	93	ASN
1	с	152	GLN
1	j	263	PRO
2	0	27	GLY
3	G	119	ASP
3	Ν	120	PRO
2	Р	27	GLY
3	Q	121	LEU
2	Т	92	ASN
3	Х	120	PRO
3	Х	122	ALA
2	f	57	ASN
2	0	40	ASP
3	С	119	ASP
1	Н	263	PRO



Mol	Chain	Res	Type
2	М	27	GLY
3	N	44	ASP
1	0	152	GLN
2	Y	40	ASP
1	с	263	PRO
3	е	123	ASN
2	h	27	GLY
1	A	263	PRO
3	С	116	ASN
2	D	57	ASN
3	G	122	ALA
3	S	123	ASN
2	F	92	ASN
2	Ι	105	VAL
2	Р	54	PRO
3	Q	123	ASN
2	Т	27	GLY
2	a	92	ASN
3	е	120	PRO
1	j	88	ASP
3	С	117	PRO
2	W	29	GLY
2	d	29	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	193/207~(93%)	178 (92%)	15 (8%)	12 40
1	Н	197/207~(95%)	177 (90%)	20 (10%)	7 27
1	Ο	198/207~(96%)	182 (92%)	16 (8%)	11 39
1	V	198/207~(96%)	190 (96%)	8 (4%)	31 64
1	с	199/207~(96%)	183 (92%)	16 (8%)	12 39
1	j	193/207~(93%)	176 (91%)	17 (9%)	10 34



α \cdot \cdot \cdot	C		
I 'ontimuod	trom	mromonie	naao
Commutate	11011	pretious	puye
	9	1	1 0

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
2	В	123/123~(100%)	116 (94%)	7~(6%)	20	53
2	D	123/123~(100%)	115 (94%)	8 (6%)	17	48
2	F	123/123~(100%)	113~(92%)	10 (8%)	11	39
2	Ι	123/123~(100%)	104 (85%)	19 (15%)	2	12
2	Κ	123/123~(100%)	115 (94%)	8 (6%)	17	48
2	М	123/123~(100%)	112 (91%)	11 (9%)	9	33
2	Р	123/123~(100%)	112 (91%)	11 (9%)	9	33
2	R	123/123~(100%)	121 (98%)	2 (2%)	62	83
2	Т	123/123~(100%)	110 (89%)	13 (11%)	6	25
2	W	123/123~(100%)	110 (89%)	13 (11%)	6	25
2	Y	123/123~(100%)	117 (95%)	6 (5%)	25	59
2	a	123/123~(100%)	116 (94%)	7 (6%)	20	53
2	d	123/123~(100%)	115 (94%)	8 (6%)	17	48
2	f	123/123~(100%)	111 (90%)	12 (10%)	8	28
2	h	123/123~(100%)	115 (94%)	8 (6%)	17	48
2	k	123/123~(100%)	110 (89%)	13 (11%)	6	25
2	m	123/123~(100%)	118 (96%)	5 (4%)	30	63
2	0	123/123~(100%)	115 (94%)	8 (6%)	17	48
3	С	126/126~(100%)	105 (83%)	21 (17%)	2	9
3	Е	126/126~(100%)	113 (90%)	13 (10%)	7	26
3	G	126/126~(100%)	112 (89%)	14 (11%)	6	24
3	J	126/126~(100%)	113 (90%)	13 (10%)	7	26
3	L	126/126~(100%)	113 (90%)	13 (10%)	7	26
3	Ν	126/126~(100%)	112 (89%)	14 (11%)	6	24
3	Q	126/126~(100%)	113 (90%)	13 (10%)	7	26
3	S	126/126~(100%)	111 (88%)	15 (12%)	5	21
3	U	126/126~(100%)	114 (90%)	12 (10%)	8	30
3	Х	126/126~(100%)	112 (89%)	14 (11%)	6	24
3	Ζ	126/126 (100%)	113 (90%)	13 (10%)	7	26
3	b	126/126~(100%)	114 (90%)	12 (10%)	8	30
3	е	126/126~(100%)	110 (87%)	16 (13%)	4	19



Mol	Chain	Analysed	Rotameric	Outliers	Per	centiles
3	g	126/126~(100%)	113 (90%)	13 (10%)	7	26
3	i	126/126~(100%)	112 (89%)	14 (11%)	6	24
3	1	126/126~(100%)	111 (88%)	15 (12%)	5	21
3	n	126/126~(100%)	113 (90%)	13 (10%)	7	26
3	р	126/126~(100%)	111 (88%)	15 (12%)	5	21
All	All	5660/5724~(99%)	5146 (91%)	514 (9%)	9	32

Continued from previous page...

All (514) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	70	GLN
1	А	91	CYS
1	А	113	ARG
1	А	124	ASP
1	А	131	THR
1	А	133	PHE
1	А	135	ILE
1	А	144	ASP
1	А	171	LEU
1	А	188	LYS
1	А	195	GLU
1	А	198	ARG
1	А	217	HIS
1	А	248	ILE
1	А	256	LYS
2	В	32	SER
2	В	49	MET
2	В	50	ILE
2	В	93	ASN
2	В	101	ARG
2	В	129	LYS
2	В	133	LYS
3	С	10	LYS
3	С	13	GLN
3	С	14	ARG
3	С	18	GLU
3	С	24	LYS
3	С	26	GLU
3	С	29	GLU
3	С	43	GLN



Mol	Chain	Res	Type
3	С	44	ASP
3	С	70	ARG
3	С	92	LYS
3	С	102	ARG
3	С	106	LEU
3	С	107	SER
3	С	108	ILE
3	С	116	ASN
3	С	121	LEU
3	С	127	GLU
3	С	128	GLN
3	С	129	TRP
3	С	146	LEU
2	D	21	GLU
2	D	31	VAL
2	D	35	LEU
2	D	49	MET
2	D	81	ARG
2	D	108	LYS
2	D	110	GLN
2	D	133	LYS
3	Е	6	ARG
3	Е	14	ARG
3	Е	54	LEU
3	Е	73	THR
3	Е	87	CYS
3	E	92	LYS
3	E	93	ASP
3	Е	96	SER
3	Е	106	LEU
3	Е	107	SER
3	Е	111	LEU
3	E	124	ASP
3	E	138	GLU
2	F	39	GLU
2	F	55	ARG
2	F	60	ASN
2	F	62	ILE
2	F	72	LYS
2	F	75	GLU
2	F	93	ASN
2	F	105	VAL



Mol	Chain	Res	Type
2	F	116	LYS
2	F	133	LYS
3	G	4	LEU
3	G	6	ARG
3	G	24	LYS
3	G	64	MET
3	G	103	THR
3	G	105	LEU
3	G	107	SER
3	G	116	ASN
3	G	121	LEU
3	G	123	ASN
3	G	124	ASP
3	G	128	GLN
3	G	141	ARG
3	G	150	ASN
1	Н	53	GLU
1	Н	65	ASP
1	Н	70	GLN
1	Н	77	LYS
1	Н	83	ARG
1	Н	105	LEU
1	Н	106	ASP
1	Н	109	LYS
1	Н	120	LYS
1	Н	125	LEU
1	Н	132	GLU
1	Н	144	ASP
1	Н	148	GLN
1	Н	163	ASN
1	Н	171	LEU
1	Н	194	ILE
1	Н	199	THR
1	Н	215	SER
1	Н	256	LYS
1	Н	260	LEU
2	Ι	8	LYS
2	Ι	14	ARG
2	Ι	30	THR
2	Ι	35	LEU
2	Ι	49	MET
2	Ι	56	THR



Mol	Chain	Res	Type
2	Ι	57	ASN
2	Ι	61	ARG
2	Ι	72	LYS
2	Ι	75	GLU
2	Ι	82	PHE
2	Ι	91	ILE
2	Ι	101	ARG
2	Ι	105	VAL
2	Ι	109	TRP
2	Ι	110	GLN
2	Ι	111	ASN
2	Ι	120	GLN
2	Ι	125	LEU
3	J	6	ARG
3	J	13	GLN
3	J	15	LEU
3	J	43	GLN
3	J	53	LYS
3	J	64	MET
3	J	70	ARG
3	J	72	MET
3	J	82	LYS
3	J	89	ASP
3	J	92	LYS
3	J	102	ARG
3	J	105	LEU
2	К	8	LYS
2	K	16	LEU
2	K	35	LEU
2	K	64	SER
2	K	68	GLU
2	K	97	MET
2	K	101	ARG
2	K	110	GLN
3	L	10	LYS
3	L	14	ARG
3	L	18	GLU
3	L	34	TYR
3	L	73	THR
3	L	74	LYS
3	L	89	ASP
3	L	92	LYS



Mol	Chain	Res	Type
3	L	105	LEU
3	L	106	LEU
3	L	118	ASP
3	L	121	LEU
3	L	124	ASP
2	М	39	GLU
2	М	49	MET
2	М	55	ARG
2	М	59	GLU
2	М	62	ILE
2	М	64	SER
2	М	81	ARG
2	М	84	THR
2	Μ	93	ASN
2	М	101	ARG
2	М	105	VAL
3	Ν	30	SER
3	Ν	44	ASP
3	Ν	45	SER
3	Ν	51	THR
3	N	53	LYS
3	N	105	LEU
3	N	109	GLN
3	N	113	SER
3	N	124	ASP
3	N	127	GLU
3	N	128	GLN
3	N	141	ARG
3	Ν	145	ARG
3	N	146	LEU
1	0	51	ARG
1	0	69	GLN
1	0	70	GLN
1	0	73	LYS
1	0	109	LYS
1	0	134	THR
1	0	144	ASP
1	0	152	GLN
1	0	166	SER
1	0	171	LEU
1	0	186	GLU
1	0	192	HIS



Mol	Chain	Res	Type
1	0	195	GLU
1	0	217	HIS
1	0	248	ILE
1	0	254	GLU
2	Р	8	LYS
2	Р	43	LEU
2	Р	44	THR
2	Р	47	THR
2	Р	60	ASN
2	Р	72	LYS
2	Р	101	ARG
2	Р	102	SER
2	Р	118	VAL
2	Р	120	GLN
2	Р	133	LYS
3	Q	16	LEU
3	Q	24	LYS
3	Q	43	GLN
3	Q	64	MET
3	Q	70	ARG
3	Q	89	ASP
3	Q	92	LYS
3	Q	102	ARG
3	Q	106	LEU
3	Q	123	ASN
3	Q	129	TRP
3	Q	135	GLN
3	Q	145	ARG
2	R	66	LYS
2	R	133	LYS
3	S	4	LEU
3	S	18	GLU
3	S	29	GLU
3	S	61	GLU
3	S	73	THR
3	S	89	ASP
3	S	92	LYS
3	S	93	ASP
3	S	105	LEU
3	S	116	ASN
3	S	123	ASN
3	S	124	ASP



Mol	Chain	Res	Type
3	S	128	GLN
3	S	146	LEU
3	S	150	ASN
2	Т	20	GLU
2	Т	23	GLN
2	Т	26	VAL
2	Т	35	LEU
2	Т	39	GLU
2	Т	49	MET
2	Т	55	ARG
2	Т	62	ILE
2	Т	93	ASN
2	Т	97	MET
2	Т	105	VAL
2	Т	129	LYS
2	Т	133	LYS
3	U	4	LEU
3	U	14	ARG
3	U	16	LEU
3	U	20	VAL
3	U	43	GLN
3	U	93	ASP
3	U	105	LEU
3	U	123	ASN
3	U	125	VAL
3	U	129	TRP
3	U	135	GLN
3	U	137	ILE
1	V	59	LYS
1	V	70	GLN
1	V	71	LYS
1	V	90	ASN
1	V	147	GLU
1	V	151	LYS
1	V	171	LEU
1	V	248	ILE
2	W	23	GLN
2	W	58	TYR
2	W	80	VAL
2	W	86	ILE
2	W	99	ASP
2	W	108	LYS



Mol	Chain	Res	Type
2	W	110	GLN
2	W	118	VAL
2	W	120	GLN
2	W	123	ARG
2	W	124	ARG
2	W	133	LYS
2	W	142	THR
3	Х	6	ARG
3	Х	13	GLN
3	Х	15	LEU
3	Х	24	LYS
3	Х	43	GLN
3	Х	48	GLU
3	Х	55	GLU
3	Х	61	GLU
3	Х	82	LYS
3	Х	92	LYS
3	Х	102	ARG
3	Х	105	LEU
3	Х	121	LEU
3	Х	135	GLN
2	Y	35	LEU
2	Y	61	ARG
2	Y	68	GLU
2	Y	101	ARG
2	Y	112	SER
2	Y	133	LYS
3	Ζ	20	VAL
3	Ζ	29	GLU
3	Ζ	61	GLU
3	Z	73	THR
3	Ζ	74	LYS
3	Ζ	89	ASP
3	Ζ	93	ASP
3	Ζ	105	LEU
3	Ζ	121	LEU
3	Ζ	128	GLN
3	Ζ	135	GLN
3	Ζ	137	ILE
3	Z	145	ARG
2	a	8	LYS
2	a	14	ARG



Mol	Chain	Res	Type
2	a	35	LEU
2	a	45	ARG
2	a	93	ASN
2	a	105	VAL
2	a	127	MET
3	b	20	VAL
3	b	81	ASP
3	b	89	ASP
3	b	93	ASP
3	b	105	LEU
3	b	106	LEU
3	b	123	ASN
3	b	128	GLN
3	b	129	TRP
3	b	137	ILE
3	b	141	ARG
3	b	149	MET
1	с	47	LEU
1	с	70	GLN
1	с	76	HIS
1	с	106	ASP
1	с	120	LYS
1	с	131	THR
1	с	134	THR
1	с	143	MET
1	с	144	ASP
1	с	157	ASP
1	с	171	LEU
1	с	188	LYS
1	с	195	GLU
1	с	217	HIS
1	с	248	ILE
1	с	254	GLU
2	d	31	VAL
2	d	44	THR
2	d	64	SER
2	d	75	GLU
2	d	79	SER
2	d	101	ARG
2	d	123	ARG
2	d	133	LYS
3	е	9	ILE



Mol	Chain	Res	Type
3	е	10	LYS
3	е	11	GLU
3	е	14	ARG
3	е	26	GLU
3	е	64	MET
3	е	70	ARG
3	е	72	MET
3	е	106	LEU
3	е	111	LEU
3	е	118	ASP
3	е	119	ASP
3	е	123	ASN
3	е	128	GLN
3	е	129	TRP
3	е	146	LEU
2	f	8	LYS
2	f	28	ASP
2	f	35	LEU
2	f	49	MET
2	f	59	GLU
2	f	68	GLU
2	f	72	LYS
2	f	93	ASN
2	f	101	ARG
2	f	110	GLN
2	f	117	VAL
2	f	125	LEU
3	g	4	LEU
3	g	6	ARG
3	g	72	MET
3	g	73	THR
3	g	87	CYS
3	g	89	ASP
3	g	92	LYS
3	g	94	LYS
3	g	106	LEU
3	g	107	SER
3	g	113	SER
3	g	121	LEU
3	g	128	GLN
2	h	24	LYS
2	h	47	THR



Mol	Chain	Res	Type
2	h	49	MET
2	h	55	ARG
2	h	62	ILE
2	h	101	ARG
2	h	105	VAL
2	h	130	GLU
3	i	4	LEU
3	i	6	ARG
3	i	14	ARG
3	i	18	GLU
3	i	23	ILE
3	i	26	GLU
3	i	103	THR
3	i	105	LEU
3	i	106	LEU
3	i	118	ASP
3	i	121	LEU
3	i	128	GLN
3	i	129	TRP
3	i	135	GLN
1	j	48	VAL
1	j	70	GLN
1	j	73	LYS
1	j	90	ASN
1	j	100	HIS
1	j	115	LYS
1	j	122	LYS
1	j	131	THR
1	j	143	MET
1	j	144	ASP
1	j	147	GLU
1	j	163	ASN
1	j	171	LEU
1	j	179	THR
1	j	199	THR
1	j	206	GLN
1	j	213	LYS
2	k	14	ARG
2	k	24	LYS
2	k	38	ASP
2	k	49	MET
2	k	57	ASN



Mol	Chain	Res	Type
2	k	82	PHE
2	k	89	ASN
2	k	101	ARG
2	k	102	SER
2	k	109	TRP
2	k	111	ASN
2	k	125	LEU
2	k	127	MET
3	1	6	ARG
3	1	15	LEU
3	1	18	GLU
3	1	24	LYS
3	1	26	GLU
3	1	72	MET
3	1	82	LYS
3	1	89	ASP
3	l	105	LEU
3	1	106	LEU
3	1	107	SER
3	1	116	ASN
3	1	132	ASN
3	1	141	ARG
3	1	149	MET
2	m	12	ASN
2	m	30	THR
2	m	31	VAL
2	m	35	LEU
2	m	68	GLU
3	n	13	GLN
3	n	14	ARG
3	n	73	THR
3	n	87	CYS
3	n	89	ASP
3	n	92	LYS
3	n	94	LYS
3	n	102	ARG
3	n	105	LEU
3	n	106	LEU
3	n	121	LEU
3	n	128	GLN
3	n	150	ASN
2	0	55	ARG



Mol	Chain	Res	Type
2	0	60	ASN
2	0	93	ASN
2	0	101	ARG
2	0	105	VAL
2	0	106	LEU
2	0	130	GLU
2	0	133	LYS
3	р	4	LEU
3	р	9	ILE
3	р	14	ARG
3	р	51	THR
3	р	72	MET
3	р	89	ASP
3	р	90	ILE
3	р	105	LEU
3	р	111	LEU
3	р	116	ASN
3	р	127	GLU
3	р	130	LYS
3	р	139	THR
3	р	141	ARG
3	р	146	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	70	GLN
1	А	76	HIS
1	А	219	HIS
2	В	60	ASN
2	В	89	ASN
2	В	93	ASN
2	В	120	GLN
3	С	43	GLN
3	С	109	GLN
3	С	135	GLN
2	D	12	ASN
2	D	23	GLN
2	D	110	GLN
2	D	120	GLN
2	F	12	ASN
2	F	60	ASN



Mol	Chain	Res	Type
2	F	89	ASN
3	G	79	ASN
3	G	116	ASN
3	G	123	ASN
3	G	135	GLN
1	Н	70	GLN
1	Н	112	GLN
1	Н	148	GLN
2	Ι	60	ASN
2	Ι	110	GLN
2	Ι	111	ASN
3	J	109	GLN
3	J	116	ASN
2	K	23	GLN
2	Κ	92	ASN
3	L	13	GLN
3	L	116	ASN
2	М	60	ASN
2	М	110	GLN
2	М	120	GLN
3	Ν	100	GLN
1	0	45	ASN
1	0	70	GLN
2	Р	60	ASN
2	Р	87	ASN
3	Q	100	GLN
3	Q	123	ASN
3	Q	128	GLN
2	R	120	GLN
3	S	13	GLN
3	S	116	ASN
2	Т	12	ASN
2	Т	60	ASN
2	Т	120	GLN
3	U	13	GLN
3	U	43	GLN
3	U	123	ASN
3	U	135	GLN
1	V	70	GLN
1	V	90	ASN
1	V	219	HIS
1	V	225	GLN



Mol	Chain	Res	Type
2	W	87	ASN
2	W	93	ASN
2	W	110	GLN
2	W	120	GLN
3	Х	109	GLN
3	Х	123	ASN
3	Х	128	GLN
2	Y	110	GLN
2	Y	120	GLN
3	Ζ	116	ASN
2	a	120	GLN
3	b	123	ASN
1	с	66	ASN
1	с	219	HIS
1	с	245	ASN
2	d	89	ASN
2	d	93	ASN
2	d	120	GLN
3	е	79	ASN
3	е	123	ASN
2	f	23	GLN
3	g	43	GLN
3	g	116	ASN
2	h	12	ASN
2	h	23	GLN
2	h	110	GLN
3	i	109	GLN
1	j	219	HIS
2	k	60	ASN
2	k	92	ASN
2	k	111	ASN
2	k	120	GLN
3	1	109	GLN
3	1	116	ASN
3	1	123	ASN
2	m	23	GLN
3	n	13	GLN
2	0	60	ASN
2	0	120	GLN
3	р	43	GLN

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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	<RSRZ $>$	#RSRZ>2	$OWAB(A^2)$	Q<0.9
1	А	210/228~(92%)	0.12	3 (1%) 75 63	58, 87, 128, 158	0
1	Н	214/228~(93%)	0.64	17 (7%) 12 6	95, 128, 181, 205	0
1	Ο	216/228~(94%)	-0.01	1 (0%) 91 86	59, 78, 110, 142	0
1	V	215/228~(94%)	0.10	5 (2%) 60 46	57, 78, 113, 153	0
1	с	217/228~(95%)	0.19	9 (4%) 37 22	58, 87, 133, 174	0
1	j	210/228~(92%)	0.85	30 (14%) 2 1	97, 131, 177, 194	0
2	В	138/138~(100%)	-0.29	0 100 100	47, 62, 80, 106	0
2	D	137/138~(99%)	-0.15	0 100 100	59, 84, 113, 138	0
2	F	138/138~(100%)	-0.26	0 100 100	42, 57, 83, 102	0
2	Ι	138/138~(100%)	-0.01	0 100 100	61, 88, 118, 152	0
2	K	138/138~(100%)	-0.21	1 (0%) 87 81	53, 67, 82, 99	0
2	М	138/138~(100%)	-0.23	1 (0%) 87 81	51, 66, 86, 113	0
2	Р	138/138~(100%)	0.07	3 (2%) 62 47	71, 98, 131, 153	0
2	R	137/138~(99%)	-0.28	0 100 100	53, 67, 84, 94	0
2	Т	138/138~(100%)	-0.17	0 100 100	56, 73, 103, 132	0
2	W	137/138~(99%)	0.01	1 (0%) 87 81	69, 94, 122, 138	0
2	Y	137/138~(99%)	-0.18	0 100 100	54, 70, 87, 97	0
2	a	138/138~(100%)	-0.19	1 (0%) 87 81	53, 71, 103, 127	0
2	d	138/138~(100%)	-0.26	1 (0%) 87 81	48, 62, 81, 105	0
2	f	137/138~(99%)	-0.02	1 (0%) 87 81	61, 83, 109, 131	0
2	h	138/138~(100%)	-0.24	1 (0%) 87 81	42, 57, 81, 100	0
2	k	138/138~(100%)	0.08	4 (2%) 51 35	64, 89, 117, 155	0
2	m	137/138~(99%)	-0.17	0 100 100	54, 69, 84, 98	0
2	О	138/138~(100%)	-0.25	1 (0%) 87 81	50, 65, 87, 107	0



Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(A^2)$	Q<0.9
3	С	147/148~(99%)	-0.14	0 100 100	40, 63, 95, 119	0
3	Е	147/148~(99%)	-0.15	0 100 100	51, 81, 135, 155	0
3	G	147/148~(99%)	-0.21	0 100 100	39, 56, 92, 104	0
3	J	147/148~(99%)	-0.01	2 (1%) 75 63	57, 78, 116, 136	0
3	L	147/148~(99%)	-0.13	1 (0%) 87 81	54, 83, 138, 167	0
3	N	147/148~(99%)	-0.17	0 100 100	54, 68, 97, 106	0
3	Q	147/148~(99%)	-0.21	0 100 100	49, 65, 95, 109	0
3	S	148/148 (100%)	-0.18	0 100 100	49, 75, 103, 115	0
3	U	147/148~(99%)	-0.15	0 100 100	50, 66, 98, 114	0
3	Х	147/148~(99%)	-0.24	0 100 100	50, 67, 98, 110	0
3	Z	148/148~(100%)	-0.21	0 100 100	49, 75, 105, 116	0
3	b	147/148~(99%)	-0.23	0 100 100	49, 66, 96, 113	0
3	е	147/148~(99%)	-0.23	0 100 100	40, 63, 96, 108	0
3	g	148/148~(100%)	-0.13	0 100 100	48, 81, 136, 158	0
3	i	148/148~(100%)	-0.21	0 100 100	39, 57, 93, 111	0
3	1	147/148~(99%)	-0.05	2 (1%) 75 63	57, 82, 121, 145	0
3	n	147/148~(99%)	-0.12	1 (0%) 87 81	58, 86, 140, 166	0
3	р	$1\overline{48/148}\ (100\%)$	-0.13	1 (0%) 87 81	55, 70, 101, 115	0
All	All	6411/6516 (98%)	-0.06	87 (1%) 75 63	39, 74, 129, 205	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	j	96	PHE	5.6
1	Н	68	TYR	5.5
1	с	45	ASN	5.0
1	j	82	ILE	4.8
1	Н	81	TYR	4.4
1	j	95	ALA	4.3
2	Κ	6	GLY	4.2
1	j	269	LEU	4.2
1	j	145	LEU	4.0
1	Н	57	LEU	3.9
1	j	57	LEU	3.8
1	j	83	ARG	3.8
1	j	264	GLY	3.8



Mol	Chain	Res	Type	RSRZ
1	с	242	GLY	3.5
1	Н	156	ALA	3.4
1	Н	106	ASP	3.4
1	j	155	VAL	3.4
1	Н	60	GLU	3.3
1	j	159	LEU	3.3
2	W	26	VAL	3.3
1	Н	82	ILE	3.2
1	j	67	ILE	3.2
1	j	252	GLY	3.2
1	Н	96	PHE	3.2
1	Н	95	ALA	3.2
1	j	154	SER	3.1
1	С	57	LEU	2.9
1	с	97	GLY	2.9
1	j	267	ASP	2.9
2	Р	6	GLY	2.9
1	Н	145	LEU	2.8
1	j	55	SER	2.8
1	j	191	GLU	2.8
1	С	49	SER	2.8
2	Р	63	TYR	2.8
1	с	267	ASP	2.7
1	j	50	GLU	2.7
1	j	107	ASP	2.7
2	k	139	GLU	2.7
1	V	107	ASP	2.7
2	a	6	GLY	2.6
2	h	38	ASP	2.6
1	j	49	SER	2.6
1	j	84	LYS	2.6
3	p	117	PRO	2.6
2	d	6	GLY	2.6
1	Н	161	SER	2.5
1	Ο	68	TYR	2.5
1	V	74	ASP	2.5
2	0	38	ASP	2.5
3	L	150	ASN	2.5
1	j	52	LEU	2.4
1	j	75	LEU	2.4
1	c	243	THR	2.4
1	j	251	GLU	2.4



3VON

Mol	Chain	Res	Type	RSRZ
3	1	116	ASN	2.4
1	j	99	SER	2.4
1	Н	191	GLU	2.4
1	Н	64	ASP	2.3
2	М	27	GLY	2.3
3	1	150	ASN	2.3
2	k	6	GLY	2.3
3	J	120	PRO	2.3
1	j	100	HIS	2.3
1	j	74	ASP	2.3
3	n	150	ASN	2.3
1	Н	66	ASN	2.2
2	k	28	ASP	2.2
2	f	78	PRO	2.2
1	j	263	PRO	2.2
1	Н	269	LEU	2.2
1	Н	69	GLN	2.2
1	А	132	GLU	2.2
1	j	162	PHE	2.2
1	V	263	PRO	2.1
1	Н	135	ILE	2.1
2	Р	26	VAL	2.1
2	k	27	GLY	2.1
1	А	85	THR	2.1
1	V	264	GLY	2.1
1	V	45	ASN	2.1
3	J	29	GLU	2.1
1	с	96	PHE	2.1
1	j	68	TYR	2.1
1	А	60	GLU	2.0
1	с	244	THR	2.0
1	j	54	LEU	2.0

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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.

