

Full wwPDB X-ray Structure Validation Report (i)

May 31, 2022 – 12:14 PM JST

PDB ID	:	7W82
Title	:	Crystal structure of maize RDR2
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Deposited on	:	2021-12-07
Resolution	:	3.10 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 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	:	2.28.1
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)	:	2.28.1

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 3.10 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	
		1004	2%		
	А	1024	56%	32% • 89	%



7W82

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7492 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a protein called RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	944	Total 7492	C 4758	N 1303	0 1384	S 47	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	104	ALA	-	expression tag	UNP Q19VG2
А	105	MET	-	expression tag	UNP Q19VG2
А	106	GLY	-	expression tag	UNP Q19VG2
А	841	ALA	GLU	engineered mutation	UNP Q19VG2
А	842	ALA	LYS	engineered mutation	UNP Q19VG2
А	962	ALA	GLU	engineered mutation	UNP Q19VG2
А	963	ALA	GLU	engineered mutation	UNP Q19VG2
А	966	ALA	GLU	engineered mutation	UNP Q19VG2



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: RNA-dependent RNA polymerase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants	149.04Å 149.04Å 345.47Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{B}_{\mathrm{ascolution}}\left(\overset{\mathrm{A}}{\mathbf{\lambda}}\right)$	43.02 - 3.10	Depositor
Resolution (A)	43.02 - 3.10	EDS
% Data completeness	99.5(43.02 - 3.10)	Depositor
(in resolution range)	99.7 (43.02 - 3.10)	EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.59 (at 3.12 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
P. P.	0.230 , 0.270	Depositor
n, n_{free}	0.255 , 0.288	DCC
R_{free} test set	1357 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	83.8	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.31 , 43.1	EDS
L-test for $twinning^2$	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
	0.000 for -h, 1/3 *h-1/3 *k-1/3 *l, -4/3 *h-8/3 *k	
	+1/3*l	
Estimated twinning fraction	0.000 for $-1/3*h+1/3*k+1/3*l,-k,8/3*h+4/$	Xtriage
0	$3^{*}k+1/3^{*}l$	
	0.010 IOF -2/3 II-1/3 K-1/3 I,-1/3 H-2/3 K+ 1/2*1 4/2*b + 4/2*1 + 1/2*1	
E E correlation	$\frac{1/3^{-1}-4/3^{-1}+4/3^{-1}+4/3^{-1}}{0.00}$	EDS
Total number of atoms	7409	WWDDB VD
Average \mathbf{P} all storms $\begin{pmatrix} \lambda 2 \end{pmatrix}$	<u> </u>	
Average D, all atoms (A^2)	ð 3 .U	WWFDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.35% 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).

Mol	Chain	Bond	lengths	Bond angles	
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.54	0/7657	0.62	0/10352

There are no bond length outliers.

There are no bond angle outliers.

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	А	7492	0	7444	370	0
All	All	7492	0	7444	370	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (370) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:LEU:HD21	1:A:868:LYS:HD3	1.19	1.17
1:A:189:ARG:CG	1:A:221:ARG:HH12	1.61	1.14
1:A:818:ASN:HA	1:A:823:GLY:HA3	1.24	1.12
1:A:444:TYR:CD2	1:A:875:ILE:HD11	1.90	1.07
1:A:189:ARG:HG3	1:A:221:ARG:NH1	1.70	1.06



	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:189:ARG:HB3	1:A:221:ARG:HH22	1.15	1.05
1:A:189:ARG:HG3	1:A:221:ARG:HH12	0.91	1.05
1:A:223:LEU:H	1:A:223:LEU:HD12	1.24	0.99
1:A:425:ALA:O	1:A:443:LEU:HD12	1.62	0.99
1:A:758:PHE:O	1:A:770:VAL:HG23	1.63	0.98
1:A:489:GLU:HG2	1:A:493:ARG:HH21	1.25	0.98
1:A:760:CYS:SG	1:A:761:ASN:N	2.32	0.95
1:A:187:ALA:HB3	1:A:416:GLU:OE1	1.67	0.95
1:A:121:VAL:HG21	1:A:309:ARG:HH22	1.31	0.94
1:A:760:CYS:HB3	1:A:770:VAL:HG21	1.47	0.94
1:A:448:LEU:HD21	1:A:868:LYS:CD	1.98	0.94
1:A:189:ARG:HB3	1:A:221:ARG:NH2	1.84	0.92
1:A:818:ASN:CA	1:A:823:GLY:HA3	2.00	0.91
1:A:309:ARG:HH11	1:A:309:ARG:HG2	1.36	0.90
1:A:444:TYR:HD2	1:A:875:ILE:HD11	1.37	0.90
1:A:1069:ALA:HA	1:A:1072:VAL:CG2	2.02	0.90
1:A:817:PRO:O	1:A:823:GLY:HA2	1.72	0.89
1:A:121:VAL:CG2	1:A:309:ARG:HH22	1.86	0.88
1:A:1086:ARG:HB2	1:A:1089:LYS:HE2	1.57	0.87
1:A:1004:ARG:HH11	1:A:1004:ARG:HG3	1.40	0.86
1:A:878:THR:O	1:A:882:ILE:HG13	1.76	0.86
1:A:862:THR:HG23	1:A:865:GLU:OE2	1.76	0.86
1:A:192:ILE:HG12	1:A:222:ALA:HB2	1.57	0.86
1:A:174:LEU:HD12	1:A:240:LYS:HD2	1.54	0.86
1:A:1065:LYS:HD3	1:A:1067:ASP:OD2	1.75	0.86
1:A:444:TYR:CE2	1:A:875:ILE:HD11	2.12	0.85
1:A:324:ILE:HD12	1:A:324:ILE:O	1.77	0.84
1:A:1069:ALA:HA	1:A:1072:VAL:HG23	1.58	0.84
1:A:1069:ALA:O	1:A:1072:VAL:HG23	1.77	0.83
1:A:862:THR:O	1:A:866:ILE:HD13	1.79	0.82
1:A:293:VAL:HG22	1:A:327:LEU:HD23	1.60	0.82
1:A:277:VAL:HG11	1:A:384:ILE:HD12	1.62	0.81
1:A:310:HIS:HD2	1:A:344:PRO:HD2	1.46	0.81
1:A:552:LYS:HG3	1:A:598:SER:HB2	1.64	0.80
1:A:1069:ALA:CA	1:A:1072:VAL:HG23	2.12	0.80
1:A:817:PRO:O	1:A:823:GLY:CA	2.30	0.80
1:A:1065:LYS:CB	1:A:1068:ASP:HB2	2.12	0.80
1:A:1065:LYS:HB3	1:A:1068:ASP:HB2	1.63	0.79
1:A:1069:ALA:C	1:A:1072:VAL:HG23	2.02	0.79
1:A:192:ILE:HD11	1:A:222:ALA:HB3	1.65	0.79
1:A:489:GLU:HG3	1:A:493:ARG:HE	1.48	0.78



	A construction of the cons	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:121:VAL:HG21	1:A:309:ARG:NH2	1.98	0.78
1:A:504:VAL:HG23	1:A:866:ILE:HD12	1.64	0.78
1:A:998:TYR:CE2	1:A:1089:LYS:HD2	2.19	0.77
1:A:282:ASP:OD2	1:A:283:CYS:N	2.18	0.77
1:A:656:ASP:OD2	1:A:961:HIS:CE1	2.37	0.77
1:A:135:VAL:HG22	1:A:150:LEU:HD13	1.67	0.77
1:A:113:ALA:HB2	1:A:241:LEU:HD23	1.69	0.74
1:A:121:VAL:CG1	1:A:309:ARG:HH12	1.99	0.74
1:A:223:LEU:HD12	1:A:223:LEU:N	2.02	0.74
1:A:733:CYS:HB2	1:A:810:GLN:OE1	1.87	0.74
1:A:817:PRO:C	1:A:823:GLY:HA2	2.07	0.74
1:A:628:ARG:NH1	1:A:713:THR:O	2.21	0.73
1:A:309:ARG:HG2	1:A:309:ARG:NH1	2.03	0.73
1:A:1004:ARG:HG3	1:A:1004:ARG:NH1	2.01	0.73
1:A:600:ARG:NH2	1:A:731:GLU:OE2	2.22	0.72
1:A:192:ILE:HG12	1:A:222:ALA:CB	2.20	0.72
1:A:174:LEU:HD13	1:A:175:ASP:OD2	1.89	0.72
1:A:761:ASN:ND2	1:A:793:TYR:CZ	2.58	0.71
1:A:1065:LYS:O	1:A:1068:ASP:N	2.24	0.71
1:A:987:PHE:O	1:A:988:ASP:HB2	1.91	0.71
1:A:109:ARG:NH2	1:A:252:GLU:OE1	2.22	0.70
1:A:690:PRO:HG3	1:A:700:LEU:HD12	1.72	0.70
1:A:121:VAL:HG13	1:A:309:ARG:HH12	1.56	0.70
1:A:192:ILE:N	1:A:220:VAL:O	2.21	0.70
1:A:336:LYS:HE2	1:A:1010:THR:HG21	1.72	0.70
1:A:344:PRO:O	1:A:348:ILE:HD12	1.92	0.70
1:A:319:LEU:O	1:A:322:LEU:CB	2.39	0.69
1:A:506:LYS:HD3	1:A:917:LYS:HE3	1.74	0.69
1:A:817:PRO:C	1:A:823:GLY:CA	2.60	0.69
1:A:760:CYS:HB3	1:A:770:VAL:CG2	2.20	0.69
1:A:1079:VAL:O	1:A:1089:LYS:NZ	2.25	0.69
1:A:285:ASN:HD22	1:A:285:ASN:N	1.91	0.69
1:A:323:SER:O	1:A:326:THR:HG22	1.92	0.69
1:A:1069:ALA:HA	1:A:1072:VAL:HG21	1.74	0.67
1:A:189:ARG:CB	1:A:221:ARG:HH22	2.02	0.67
1:A:1015:GLU:HG2	1:A:1016:ARG:HG3	1.75	0.67
1:A:469:ALA:O	1:A:473:ARG:NH1	2.27	0.67
1:A:1069:ALA:O	1:A:1072:VAL:N	2.27	0.67
1:A:293:VAL:HG22	1:A:327:LEU:CD2	2.25	0.66
1:A:997:ARG:HG3	1:A:1060:TRP:CE3	2.31	0.66
1:A:323:SER:OG	1:A:326:THR:HG22	1.95	0.66



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:165:ASP:OD2	1:A:189:ARG:NH1	2.29	0.65
1:A:444:TYR:CE2	1:A:875:ILE:CD1	2.79	0.65
1:A:1098:ILE:HG22	1:A:1101:THR:HB	1.78	0.65
1:A:446:ARG:O	1:A:450:ILE:HG12	1.97	0.65
1:A:157:TYR:CD1	1:A:192:ILE:HD12	2.32	0.65
1:A:426:LEU:HA	1:A:441:THR:CG2	2.27	0.65
1:A:1086:ARG:HB2	1:A:1089:LYS:CE	2.25	0.65
1:A:426:LEU:HA	1:A:441:THR:HG21	1.79	0.65
1:A:761:ASN:ND2	1:A:793:TYR:CE2	2.65	0.65
1:A:1021:LEU:HD11	1:A:1093:SER:OG	1.97	0.64
1:A:307:VAL:HG21	1:A:310:HIS:ND1	2.12	0.64
1:A:510:ARG:HD2	1:A:605:LYS:HB3	1.80	0.64
1:A:732:THR:HG22	1:A:800:ARG:HH11	1.62	0.64
1:A:941:GLU:HG2	1:A:942:ARG:HG2	1.78	0.64
1:A:648:GLN:O	1:A:652:MET:HG3	1.97	0.64
1:A:174:LEU:CD1	1:A:240:LYS:HD2	2.27	0.64
1:A:192:ILE:CD1	1:A:222:ALA:HB3	2.28	0.64
1:A:489:GLU:CG	1:A:493:ARG:HE	2.10	0.63
1:A:489:GLU:HG2	1:A:493:ARG:NH2	2.06	0.63
1:A:302:HIS:HD1	1:A:385:TYR:HA	1.65	0.62
1:A:1102:LEU:O	1:A:1105:ILE:HG12	1.98	0.62
1:A:743:ARG:HG2	1:A:803:ILE:HG13	1.80	0.62
1:A:1086:ARG:HD2	1:A:1089:LYS:HE3	1.82	0.61
1:A:628:ARG:NH2	1:A:936:PHE:HB2	2.16	0.61
1:A:862:THR:CG2	1:A:865:GLU:OE2	2.47	0.61
1:A:861:VAL:HG12	1:A:866:ILE:CD1	2.30	0.61
1:A:862:THR:OG1	1:A:865:GLU:N	2.21	0.61
1:A:993:ALA:O	1:A:996:GLU:HB2	2.00	0.61
1:A:121:VAL:CG2	1:A:309:ARG:NH2	2.58	0.61
1:A:285:ASN:ND2	1:A:286:GLY:H	1.99	0.61
1:A:448:LEU:HD22	1:A:871:VAL:HG21	1.83	0.61
1:A:310:HIS:CD2	1:A:344:PRO:HD2	2.33	0.60
1:A:563:LYS:HB2	1:A:569:PRO:HG3	1.82	0.60
1:A:183:GLN:C	1:A:184:LEU:HD12	2.20	0.60
1:A:189:ARG:CB	1:A:221:ARG:HH12	2.14	0.60
1:A:997:ARG:HG3	1:A:1060:TRP:CZ3	2.36	0.60
1:A:659:LEU:HD21	1:A:701:LYS:HG2	1.82	0.60
1:A:861:VAL:CG1	1:A:866:ILE:HD11	2.32	0.59
1:A:1086:ARG:CB	1:A:1089:LYS:HE2	2.31	0.59
1:A:285:ASN:HD22	1:A:285:ASN:H	1.50	0.59
1:A:344:PRO:C	1:A:348:ILE:HD12	2.22	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:319:LEU:O	1:A:322:LEU:HB2	2.02	0.59
1:A:425:ALA:HB1	1:A:443:LEU:CD1	2.33	0.58
1:A:590:ASP:OD2	1:A:800:ARG:NH2	2.36	0.58
1:A:319:LEU:HA	1:A:322:LEU:HB2	1.84	0.58
1:A:157:TYR:HE1	1:A:192:ILE:HG23	1.66	0.58
1:A:324:ILE:HD12	1:A:324:ILE:C	2.22	0.58
1:A:425:ALA:O	1:A:443:LEU:CD1	2.45	0.58
1:A:189:ARG:HH21	1:A:417:ASP:CG	2.07	0.58
1:A:489:GLU:HG3	1:A:493:ARG:NE	2.17	0.58
1:A:1075:ALA:O	1:A:1079:VAL:HG13	2.04	0.57
1:A:192:ILE:CG1	1:A:222:ALA:CB	2.81	0.57
1:A:658:MET:HE2	1:A:700:LEU:HD22	1.87	0.57
1:A:287:PHE:N	1:A:287:PHE:CD1	2.72	0.57
1:A:1069:ALA:O	1:A:1072:VAL:CG2	2.51	0.57
1:A:296:ARG:HE	1:A:389:PRO:HD2	1.69	0.57
1:A:743:ARG:NH2	1:A:798:ASP:O	2.38	0.56
1:A:307:VAL:HG21	1:A:310:HIS:CE1	2.41	0.56
1:A:223:LEU:H	1:A:223:LEU:CD1	2.06	0.56
1:A:1073:ALA:O	1:A:1076:TRP:HB2	2.05	0.56
1:A:497:HIS:ND1	1:A:499:GLU:OE2	2.39	0.56
1:A:249:TYR:CD1	1:A:250:ILE:CD1	2.89	0.55
1:A:1101:THR:O	1:A:1105:ILE:HG23	2.06	0.55
1:A:762:ASP:OD1	1:A:764:GLY:N	2.37	0.55
1:A:988:ASP:HA	1:A:991:LEU:HD13	1.89	0.55
1:A:818:ASN:N	1:A:823:GLY:HA3	2.22	0.54
1:A:293:VAL:CG2	1:A:327:LEU:CD2	2.85	0.54
1:A:1065:LYS:CB	1:A:1068:ASP:CB	2.85	0.54
1:A:1065:LYS:HB2	1:A:1068:ASP:HB2	1.89	0.54
1:A:163:PHE:CD2	1:A:255:PRO:HD3	2.43	0.54
1:A:994:ALA:HB3	1:A:1079:VAL:HG11	1.90	0.54
1:A:861:VAL:CG1	1:A:866:ILE:CD1	2.85	0.54
1:A:157:TYR:CE1	1:A:192:ILE:HG23	2.42	0.54
1:A:506:LYS:O	1:A:510:ARG:HG2	2.07	0.54
1:A:991:LEU:HD22	1:A:1085:ARG:NH1	2.23	0.54
1:A:132:CYS:SG	1:A:150:LEU:HD11	2.48	0.54
1:A:189:ARG:N	1:A:189:ARG:CD	2.71	0.54
1:A:521:THR:OG1	1:A:613:LEU:O	2.22	0.54
1:A:182:LEU:HB3	1:A:184:LEU:HD11	1.90	0.53
1:A:655:SER:O	1:A:658:MET:HG3	2.09	0.53
1:A:686:GLN:HG3	1:A:1103:LEU:HD22	1.90	0.53
1:A:159:LEU:HD21	1:A:231:PHE:CZ	2.43	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:773:VAL:HG12	1:A:834:TRP:HB3	1.89	0.53
1:A:709:THR:O	1:A:713:THR:OG1	2.23	0.53
1:A:554:SER:HB3	1:A:596:ASN:HA	1.90	0.53
1:A:882:ILE:HD13	1:A:908:LEU:HB3	1.90	0.53
1:A:1076:TRP:O	1:A:1079:VAL:HG22	2.09	0.53
1:A:448:LEU:CD2	1:A:868:LYS:HD3	2.13	0.53
1:A:425:ALA:O	1:A:441:THR:HG21	2.09	0.52
1:A:861:VAL:HG12	1:A:866:ILE:HD11	1.92	0.52
1:A:294:LEU:HA	1:A:297:LEU:HD12	1.92	0.52
1:A:120:ARG:HD3	1:A:181:LEU:HD21	1.92	0.52
1:A:157:TYR:CE1	1:A:192:ILE:HD12	2.44	0.52
1:A:998:TYR:HA	1:A:1094:PHE:CE1	2.44	0.52
1:A:413:PHE:CG	1:A:447:ILE:CG2	2.93	0.52
1:A:656:ASP:OD2	1:A:961:HIS:NE2	2.41	0.52
1:A:290:PRO:HG2	1:A:293:VAL:HG23	1.92	0.52
1:A:866:ILE:CD1	1:A:866:ILE:N	2.73	0.52
1:A:1032:LEU:HD13	1:A:1039:TYR:HD1	1.74	0.52
1:A:121:VAL:HG11	1:A:309:ARG:HH12	1.75	0.52
1:A:307:VAL:CG2	1:A:310:HIS:ND1	2.73	0.52
1:A:504:VAL:O	1:A:507:CYS:HB3	2.10	0.51
1:A:292:GLU:HG3	1:A:389:PRO:HG2	1.91	0.51
1:A:817:PRO:C	1:A:823:GLY:HA3	2.28	0.51
1:A:319:LEU:CA	1:A:322:LEU:HB2	2.40	0.51
1:A:161:VAL:HG22	1:A:188:PRO:HB3	1.92	0.51
1:A:174:LEU:HD13	1:A:175:ASP:CG	2.31	0.51
1:A:997:ARG:CG	1:A:1060:TRP:CE3	2.93	0.51
1:A:444:TYR:HE2	1:A:875:ILE:CD1	2.23	0.51
1:A:116:ILE:HB	1:A:238:VAL:HB	1.93	0.51
1:A:283:CYS:SG	1:A:284:PRO:HD2	2.51	0.51
1:A:732:THR:CG2	1:A:800:ARG:HH11	2.24	0.51
1:A:464:PHE:HA	1:A:479:MET:HG2	1.92	0.50
1:A:489:GLU:HA	1:A:492:ARG:HG3	1.92	0.50
1:A:899:SER:O	1:A:902:CYS:N	2.43	0.50
1:A:467:PHE:CZ	1:A:508:ALA:HB1	2.46	0.50
1:A:844:ASP:OD1	1:A:898:ARG:NH1	2.45	0.50
1:A:285:ASN:ND2	1:A:286:GLY:N	2.60	0.50
1:A:318:VAL:O	1:A:322:LEU:HB2	2.12	0.49
1:A:413:PHE:CD1	1:A:447:ILE:HG23	2.47	0.49
1:A:668:VAL:HA	1:A:671:LYS:HE3	1.95	0.49
1:A:521:THR:HG21	1:A:561:VAL:HG13	1.95	0.49
1:A:995:GLU:OE2	1:A:1079:VAL:HB	2.13	0.49



A + a 1	1 J	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:310:HIS:HD2	1:A:344:PRO:CD	2.20	0.49
1:A:376:ARG:HB2	1:A:387:LEU:HB2	1.94	0.49
1:A:584:LYS:HE3	1:A:605:LYS:HE3	1.95	0.49
1:A:939:ARG:HB3	1:A:942:ARG:HG3	1.95	0.49
1:A:293:VAL:CG2	1:A:327:LEU:HD23	2.38	0.49
1:A:425:ALA:HB1	1:A:443:LEU:HD13	1.94	0.49
1:A:464:PHE:C	1:A:464:PHE:CD2	2.86	0.49
1:A:796:GLY:O	1:A:800:ARG:HG3	2.13	0.49
1:A:189:ARG:NH2	1:A:417:ASP:CG	2.66	0.49
1:A:322:LEU:HB3	1:A:327:LEU:HD13	1.94	0.48
1:A:542:THR:HG21	1:A:849:TYR:CD2	2.48	0.48
1:A:1109:ARG:O	1:A:1111:CYS:N	2.45	0.48
1:A:223:LEU:O	1:A:224:ASP:C	2.51	0.48
1:A:298:ASN:O	1:A:302:HIS:HD2	1.96	0.48
1:A:444:TYR:C	1:A:444:TYR:CD1	2.86	0.48
1:A:862:THR:OG1	1:A:865:GLU:OE2	2.28	0.48
1:A:302:HIS:HE1	1:A:384:ILE:HG23	1.79	0.48
1:A:417:ASP:OD1	1:A:419:SER:OG	2.24	0.48
1:A:998:TYR:HD1	1:A:1094:PHE:CD1	2.32	0.48
1:A:189:ARG:CG	1:A:221:ARG:NH1	2.45	0.47
1:A:374:CYS:O	1:A:389:PRO:HA	2.14	0.47
1:A:590:ASP:HB3	1:A:593:SER:HB2	1.95	0.47
1:A:191:HIS:HA	1:A:221:ARG:HA	1.96	0.47
1:A:319:LEU:C	1:A:322:LEU:HB2	2.35	0.47
1:A:640:LYS:O	1:A:643:VAL:HG22	2.14	0.47
1:A:1015:GLU:HG2	1:A:1016:ARG:CG	2.43	0.47
1:A:189:ARG:HB3	1:A:221:ARG:CZ	2.42	0.47
1:A:861:VAL:HG11	1:A:866:ILE:HD11	1.96	0.47
1:A:287:PHE:HE2	1:A:317:LYS:HB2	1.78	0.47
1:A:307:VAL:HG23	1:A:310:HIS:CG	2.50	0.47
1:A:732:THR:O	1:A:733:CYS:HB3	2.14	0.47
1:A:1059:GLY:O	1:A:1060:TRP:C	2.49	0.47
1:A:302:HIS:ND1	1:A:385:TYR:HA	2.30	0.47
1:A:173:HIS:H	1:A:261:GLY:HA2	1.79	0.47
1:A:530:GLU:HB2	1:A:595:PHE:CG	2.49	0.47
1:A:284:PRO:HD3	1:A:316:PHE:CD2	2.49	0.47
1:A:172:CYS:HG	1:A:179:ALA:C	2.19	0.46
1:A:172:CYS:N	1:A:179:ALA:O	2.46	0.46
1:A:732:THR:HG22	1:A:800:ARG:NH1	2.30	0.46
1:A:181:LEU:HD11	1:A:236:THR:HG22	1.97	0.46
1:A:322:LEU:HG	1:A:327:LEU:CD1	2.45	0.46



	A L O	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:765:LYS:O	1:A:766:THR:HG22	2.15	0.46	
1:A:877:ASP:OD1	1:A:878:THR:N	2.49	0.46	
1:A:1018:ASP:O	1:A:1022:THR:OG1	2.31	0.46	
1:A:136:ARG:HE	1:A:149:TYR:HB2	1.81	0.46	
1:A:782:HIS:ND1	1:A:783:PRO:O	2.48	0.46	
1:A:223:LEU:CD2	1:A:446:ARG:HB2	2.45	0.46	
1:A:578:ILE:HG22	1:A:615:ILE:HD13	1.98	0.46	
1:A:584:LYS:NZ	1:A:826:ASP:OD1	2.45	0.46	
1:A:143:MET:HG3	1:A:145:ARG:HH21	1.81	0.46	
1:A:287:PHE:N	1:A:287:PHE:HD1	2.14	0.46	
1:A:381:PRO:HD3	1:A:414:VAL:O	2.16	0.46	
1:A:191:HIS:C	1:A:192:ILE:HD13	2.36	0.45	
1:A:248:SER:O	1:A:252:GLU:HG3	2.16	0.45	
1:A:285:ASN:N	1:A:285:ASN:ND2	2.60	0.45	
1:A:495:MET:HE1	1:A:511:MET:O	2.17	0.45	
1:A:862:THR:HG1	1:A:865:GLU:HB2	1.81	0.45	
1:A:172:CYS:SG	1:A:179:ALA:HB3	2.57	0.45	
1:A:307:VAL:HG23	1:A:310:HIS:HB2	1.97	0.45	
1:A:323:SER:O	1:A:327:LEU:N	2.45	0.45	
1:A:1072:VAL:O	1:A:1075:ALA:HB3	2.17	0.45	
1:A:241:LEU:HD13	1:A:245:ALA:HB1	1.99	0.45	
1:A:510:ARG:CD	1:A:605:LYS:HB3	2.45	0.45	
1:A:249:TYR:CD1	1:A:250:ILE:HD12	2.52	0.45	
1:A:284:PRO:HD3	1:A:316:PHE:CE2	2.51	0.45	
1:A:309:ARG:NH1	1:A:309:ARG:CG	2.73	0.45	
1:A:441:THR:HG23	1:A:443:LEU:N	2.31	0.45	
1:A:1109:ARG:NH1	1:A:1111:CYS:O	2.50	0.45	
1:A:487:THR:O	1:A:490:ASN:HB2	2.17	0.45	
1:A:504:VAL:HG21	1:A:865:GLU:HB3	1.97	0.45	
1:A:184:LEU:N	1:A:184:LEU:CD1	2.80	0.44	
1:A:588:THR:HG21	1:A:728:CYS:HB3	1.98	0.44	
1:A:127:GLU:HA	1:A:265:ILE:O	2.17	0.44	
1:A:817:PRO:O	1:A:823:GLY:HA3	2.17	0.44	
1:A:1029:LEU:HD23	1:A:1031:TYR:HE1	1.83	0.44	
1:A:1004:ARG:NH1	1:A:1004:ARG:CG	2.73	0.44	
1:A:501:ILE:O	1:A:501:ILE:HD12	2.18	0.44	
1:A:624:CYS:HB3	1:A:719:VAL:O	2.17	0.44	
1:A:319:LEU:O	1:A:322:LEU:HB3	2.16	0.44	
1:A:395:ASN:O	1:A:399:LYS:HB2	2.18	0.44	
1:A:510:ARG:HA	1:A:513:GLN:HG3	2.00	0.44	
1:A:223:LEU:HD21	1:A:446:ARG:HB2	1.99	0.44	



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:555:THR:O	1:A:559:ARG:HG3	2.17	0.44
1:A:1069:ALA:O	1:A:1072:VAL:CB	2.66	0.44
1:A:1080:THR:O	1:A:1086:ARG:HD3	2.18	0.44
1:A:192:ILE:CG1	1:A:222:ALA:HB2	2.35	0.44
1:A:404:TYR:HE1	1:A:485:SER:HB2	1.82	0.44
1:A:735:LEU:O	1:A:811:ARG:HG3	2.18	0.44
1:A:223:LEU:HD11	1:A:442:GLY:HA3	1.99	0.43
1:A:530:GLU:HG2	1:A:532:ILE:HG23	1.99	0.43
1:A:520:GLN:OE1	1:A:520:GLN:N	2.49	0.43
1:A:380:THR:HG23	1:A:416:GLU:HA	1.99	0.43
1:A:867:GLN:O	1:A:871:VAL:HG23	2.19	0.43
1:A:729:LEU:HD12	1:A:730:ASP:H	1.83	0.43
1:A:1073:ALA:O	1:A:1076:TRP:N	2.52	0.43
1:A:190:ILE:O	1:A:221:ARG:HA	2.19	0.43
1:A:380:THR:HB	1:A:383:LYS:HB2	2.01	0.43
1:A:415:ASP:OD1	1:A:416:GLU:N	2.40	0.43
1:A:476:SER:OG	1:A:477:VAL:N	2.52	0.43
1:A:559:ARG:NH2	1:A:570:ALA:O	2.51	0.43
1:A:871:VAL:O	1:A:874:MET:HB2	2.18	0.43
1:A:448:LEU:HD21	1:A:868:LYS:CE	2.49	0.43
1:A:765:LYS:C	1:A:766:THR:CG2	2.87	0.43
1:A:905:LEU:HD23	1:A:905:LEU:HA	1.79	0.43
1:A:1109:ARG:C	1:A:1109:ARG:HD3	2.40	0.43
1:A:181:LEU:HD13	1:A:238:VAL:HG22	2.00	0.42
1:A:775:ILE:HG12	1:A:832:ILE:HG23	2.00	0.42
1:A:836:ASP:OD2	1:A:837:LYS:NZ	2.52	0.42
1:A:390:GLU:OE2	1:A:1045:ARG:NH1	2.52	0.42
1:A:917:LYS:O	1:A:917:LYS:HG3	2.19	0.42
1:A:249:TYR:HD1	1:A:250:ILE:CD1	2.33	0.42
1:A:510:ARG:HH22	1:A:917:LYS:HZ1	1.66	0.42
1:A:532:ILE:HB	1:A:533:PRO:HD2	2.00	0.42
1:A:307:VAL:CG2	1:A:310:HIS:CG	3.02	0.42
1:A:637:LEU:HD23	1:A:840:PRO:HG2	2.01	0.42
1:A:376:ARG:NE	1:A:392:GLU:OE2	2.49	0.42
1:A:519:ARG:HE	1:A:519:ARG:HB2	1.57	0.42
1:A:736:GLU:H	1:A:739:GLN:NE2	2.18	0.42
1:A:441:THR:HG23	1:A:444:TYR:H	1.85	0.42
1:A:542:THR:HG21	1:A:849:TYR:CE2	2.54	0.42
1:A:994:ALA:CB	1:A:1079:VAL:HG11	2.50	0.42
1:A:1017:GLU:HG2	1:A:1021:LEU:CD1	2.50	0.42
1:A:150:LEU:HD12	1:A:151:LYS:H	1.84	0.42



A 4 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:521:THR:HB	1:A:522:PHE:H	1.66	0.42
1:A:905:LEU:HD22	1:A:924:MET:HE1	2.02	0.42
1:A:980:PRO:O	1:A:981:ASP:C	2.58	0.41
1:A:1057:VAL:O	1:A:1060:TRP:N	2.53	0.41
1:A:310:HIS:CD2	1:A:344:PRO:CD	3.01	0.41
1:A:466:ALA:O	1:A:478:TRP:HB2	2.21	0.41
1:A:863:LEU:HD23	1:A:863:LEU:HA	1.71	0.41
1:A:248:SER:HA	1:A:251:LEU:HB2	2.02	0.41
1:A:302:HIS:HE1	1:A:384:ILE:CG2	2.33	0.41
1:A:322:LEU:HD13	1:A:322:LEU:HA	1.88	0.41
1:A:524:VAL:O	1:A:611:THR:HB	2.20	0.41
1:A:189:ARG:HD2	1:A:416:GLU:HG3	2.02	0.41
1:A:1053:LEU:O	1:A:1057:VAL:HG23	2.21	0.41
1:A:1078:HIS:CD2	1:A:1082:HIS:HB2	2.56	0.41
1:A:155:GLN:OE1	1:A:156:SER:N	2.52	0.41
1:A:501:ILE:HD12	1:A:501:ILE:C	2.41	0.41
1:A:577:GLN:O	1:A:616:THR:N	2.48	0.41
1:A:925:PRO:HG2	1:A:928:LEU:HB2	2.02	0.41
1:A:947:SER:O	1:A:956:ARG:NH2	2.50	0.41
1:A:982:LEU:HD12	1:A:982:LEU:HA	1.72	0.41
1:A:639:ILE:HD13	1:A:639:ILE:HA	1.76	0.41
1:A:298:ASN:O	1:A:301:VAL:N	2.54	0.41
1:A:487:THR:O	1:A:491:ILE:HD12	2.21	0.41
1:A:181:LEU:HD11	1:A:236:THR:CG2	2.51	0.41
1:A:466:ALA:HB3	1:A:515:PHE:CE2	2.56	0.41
1:A:952:GLY:O	1:A:956:ARG:HG3	2.21	0.41
1:A:170:PHE:HB2	1:A:181:LEU:HB3	2.03	0.40
1:A:440:LYS:HD3	1:A:440:LYS:HA	1.53	0.40
1:A:543:LYS:HB3	1:A:543:LYS:HE2	1.89	0.40
1:A:1059:GLY:O	1:A:1062:ARG:N	2.48	0.40
1:A:564:LEU:HD12	1:A:564:LEU:HA	1.90	0.40
1:A:726:ILE:O	1:A:805:CYS:HB2	2.21	0.40
1:A:733:CYS:O	1:A:733:CYS:SG	2.78	0.40
1:A:814:ARG:NH1	1:A:846:PRO:HB2	2.36	0.40
1:A:250:ILE:CD1	1:A:250:ILE:N	2.84	0.40
1:A:396:TYR:HA	1:A:520:GLN:HE21	1.86	0.40
1:A:413:PHE:HB2	1:A:874:MET:HE1	2.03	0.40

There are no symmetry-related clashes.



5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	932/1024~(91%)	889~(95%)	42 (4%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	988	ASP

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 analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	812/875~(93%)	734 (90%)	78 (10%)	8 31

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	117	LEU
1	А	185	THR
1	А	221	ARG
1	А	223	LEU
1	А	246	SER
1	А	250	ILE
1	А	257	SER
1	А	262	GLU
1	А	263	LEU
1	А	265	ILE



1 A 278 VAL 1 A 281 VAL 1 A 285 ASN 1 A 287 PHE 1 A 306 LEU 1 A 307 VAL 1 A 307 VAL 1 A 309 ARG 1 A 322 LEU 1 A 322 LEU 1 A 324 ILE 1 A 324 ILE 1 A 345 LEU 1 A 346 GLN 1 A 346 GLN 1 A 402 SER 1 A 402 SER 1 A 402 SER 1 A 440 LYS 1 A 440 LYS 1 A 444 TYR 1 A 519 ARG <th>Mol</th> <th>Chain</th> <th>Res</th> <th>Type</th>	Mol	Chain	Res	Type
1 A 281 VAL 1 A 285 ASN 1 A 287 PHE 1 A 306 LEU 1 A 307 VAL 1 A 309 ARG 1 A 320 GLU 1 A 322 LEU 1 A 322 LEU 1 A 322 LEU 1 A 322 LEU 1 A 324 ILE 1 A 345 LEU 1 A 345 LEU 1 A 402 SER 1 A 402 SER 1 A 443 LEU 1 A 443 LEU 1 A 444 TYR 1 A 444 TYR 1 A 444 TYR 1 A 519 ARG 1	1	А	278	VAL
1 A 285 ASN 1 A 287 PHE 1 A 306 LEU 1 A 307 VAL 1 A 309 ARG 1 A 320 GLU 1 A 322 LEU 1 A 324 ILE 1 A 328 ARG 1 A 345 LEU 1 A 345 LEU 1 A 346 GLN 1 A 345 LEU 1 A 402 SER 1 A 403 LEU 1 A 439 LEU 1 A 440 LYS 1 A 444 TYR 1 A 444 TYR 1 A 519 ARG 1 A 521<	1	А	281	VAL
1 A 287 PHE 1 A 306 LEU 1 A 307 VAL 1 A 309 ARG 1 A 320 GLU 1 A 322 LEU 1 A 322 LEU 1 A 324 ILE 1 A 328 ARG 1 A 345 LEU 1 A 346 GLN 1 A 347 LYS 1 A 402 SER 1 A 437 LYS 1 A 439 LEU 1 A 440 LYS 1 A 440 LYS 1 A 444 TYR 1 A 444 TYR 1 A 444 TYR 1 A 519 ARG 1 A 554 SER 1	1	А	285	ASN
1 A 306 LEU 1 A 307 VAL 1 A 309 ARG 1 A 320 GLU 1 A 322 LEU 1 A 322 LEU 1 A 324 ILE 1 A 328 ARG 1 A 345 LEU 1 A 346 GLN 1 A 346 GLN 1 A 346 GLN 1 A 402 SER 1 A 402 SER 1 A 439 LEU 1 A 440 LYS 1 A 443 LEU 1 A 444 TYR 1 A 444 TYR 1 A 519 ARG 1 A 519 ARG 1 A 640 LYS <td>1</td> <td>А</td> <td>287</td> <td>PHE</td>	1	А	287	PHE
1 A 307 VAL 1 A 309 ARG 1 A 320 GLU 1 A 322 LEU 1 A 324 ILE 1 A 324 ILE 1 A 324 ILE 1 A 345 LEU 1 A 346 GLN 1 A 346 GLN 1 A 346 GLN 1 A 402 SER 1 A 402 SER 1 A 437 LYS 1 A 439 LEU 1 A 440 LYS 1 A 444 TYR 1 A 444 TYR 1 A 444 TYR 1 A 506 LYS 1 A 519 ARG 1 A 640 LYS <td>1</td> <td>А</td> <td>306</td> <td>LEU</td>	1	А	306	LEU
1 A 309 ARG 1 A 320 GLU 1 A 322 LEU 1 A 324 ILE 1 A 328 ARG 1 A 345 LEU 1 A 345 LEU 1 A 346 GLN 1 A 346 GLN 1 A 370 LYS 1 A 402 SER 1 A 439 LEU 1 A 439 LEU 1 A 440 LYS 1 A 444 TYR 1 A 444 TYR 1 A 444 TYR 1 A 444 TYR 1 A 519 ARG 1 A 521 THR 1 A 554 SER 1 A 640 LYS <td>1</td> <td>А</td> <td>307</td> <td>VAL</td>	1	А	307	VAL
1 A 320 GLU 1 A 322 LEU 1 A 324 ILE 1 A 328 ARG 1 A 345 LEU 1 A 346 GLN 1 A 346 GLN 1 A 347 LYS 1 A 402 SER 1 A 437 LYS 1 A 439 LEU 1 A 443 LEU 1 A 443 LEU 1 A 444 TYR 1 A 444 TYR 1 A 444 TYR 1 A 444 PHE 1 A 506 LYS 1 A 519 ARG 1 A 554 SER 1 A 640 LYS 1 A 656 ASP 1	1	А	309	ARG
1 A 322 LEU 1 A 324 ILE 1 A 328 ARG 1 A 345 LEU 1 A 345 LEU 1 A 346 GLN 1 A 370 LYS 1 A 402 SER 1 A 437 LYS 1 A 437 LYS 1 A 442 SER 1 A 443 LEU 1 A 444 TYR 1 A 444 TYR 1 A 444 TYR 1 A 444 TYR 1 A 464 PHE 1 A 519 ARG 1 A 521 THR 1 A 640 LYS 1 A 640 LYS 1 A 656 ASP <td>1</td> <td>А</td> <td>320</td> <td>GLU</td>	1	А	320	GLU
1 A 324 ILE 1 A 328 ARG 1 A 345 LEU 1 A 346 GLN 1 A 370 LYS 1 A 402 SER 1 A 402 SER 1 A 437 LYS 1 A 439 LEU 1 A 443 LEU 1 A 444 TYR 1 A 506 LYS 1 A 519 ARG 1 A 554 SER 1 A 641 ASP 1 A 656 ASP 1 A 728 CYS <td>1</td> <td>А</td> <td>322</td> <td>LEU</td>	1	А	322	LEU
1 A 328 ARG 1 A 345 LEU 1 A 346 GLN 1 A 370 LYS 1 A 402 SER 1 A 437 LYS 1 A 439 LEU 1 A 443 LEU 1 A 443 LEU 1 A 443 LEU 1 A 444 TYR 1 A 444 LEU 1 A 444 LEU 1 A 444 LEU 1 A 444 PHE 1 A 464 PHE 1 A 506 LYS 1 A 519 ARG 1 A 554 SER 1 A 640 LYS 1 A 656 ASP 1 A 723 ARG 1	1	А	324	ILE
1 A 345 LEU 1 A 346 GLN 1 A 370 LYS 1 A 402 SER 1 A 437 LYS 1 A 439 LEU 1 A 439 LEU 1 A 440 LYS 1 A 444 TYR 1 A 444 THR 1 A 506 LYS 1 A 519 ARG 1 A 554 SER 1 A 641 ASP 1 A 656 ASP 1 A 723 ARG <td>1</td> <td>А</td> <td>328</td> <td>ARG</td>	1	А	328	ARG
1 A 346 GLN 1 A 370 LYS 1 A 402 SER 1 A 437 LYS 1 A 437 LYS 1 A 439 LEU 1 A 440 LYS 1 A 443 LEU 1 A 444 TYR 1 A 464 PHE 1 A 506 LYS 1 A 554 SER 1 A 640 LYS 1 A 656 ASP 1 A 671 LYS 1 A 723 ARG 1	1	А	345	LEU
1 A 370 LYS 1 A 402 SER 1 A 437 LYS 1 A 439 LEU 1 A 440 LYS 1 A 440 LYS 1 A 440 LYS 1 A 444 TYR 1 A 444 THR 1 A 506 LYS 1 A 519 ARG 1 A 54 SER 1 A 641 ASP 1 A 641 ASP 1 A 656 ASP 1 A 723 ARG <td>1</td> <td>А</td> <td>346</td> <td>GLN</td>	1	А	346	GLN
1 A 402 SER 1 A 437 LYS 1 A 439 LEU 1 A 440 LYS 1 A 440 LYS 1 A 443 LEU 1 A 444 TYR 1 A 444 EU 1 A 444 TYR 1 A 506 LYS 1 A 506 LYS 1 A 554 SER 1 A 640 LYS 1 A 641 ASP 1 A 656 ASP 1 A 723 ARG 1 A 728 CYS 1 A 770 VAL 1	1	А	370	LYS
1A437LYS1A439LEU1A440LYS1A443LEU1A444TYR1A444TYR1A444TYR1A444TYR1A444LEU1A444PHE1A464PHE1A506LYS1A519ARG1A521THR1A640LYS1A641ASP1A656ASP1A671LYS1A723ARG1A758PHE1A770VAL1A802LEU1A825LEU1A844ASP1A848ASP1A848ASP1A848ASP1A848ASP	1	А	402	SER
1 A 439 LEU 1 A 440 LYS 1 A 443 LEU 1 A 444 TYR 1 A 444 LEU 1 A 444 PHE 1 A 444 PHE 1 A 506 LYS 1 A 506 LYS 1 A 521 THR 1 A 554 SER 1 A 640 LYS 1 A 641 ASP 1 A 656 ASP 1 A 723 ARG 1 A 728 CYS 1 A 770 VAL 1 A 802 LEU 1	1	А	437	LYS
1A440LYS1A443LEU1A444TYR1A447ILE1A447ILE1A448LEU1A464PHE1A506LYS1A519ARG1A521THR1A554SER1A640LYS1A641ASP1A656ASP1A671LYS1A723ARG1A758PHE1A770VAL1A802LEU1A825LEU1A844ASP1A848ASP1A848ASP1A848ASP	1	А	439	LEU
1A443LEU1A444TYR1A447ILE1A448LEU1A464PHE1A506LYS1A519ARG1A521THR1A554SER1A640LYS1A641ASP1A656ASP1A656ASP1A723ARG1A758PHE1A770VAL1A802LEU1A825LEU1A844ASP1A847MET1A848ASP1A848ASP	1	А	440	LYS
1A444TYR1A447ILE1A448LEU1A464PHE1A506LYS1A519ARG1A521THR1A554SER1A640LYS1A641ASP1A666ASP1A671LYS1A723ARG1A758PHE1A770VAL1A802LEU1A825LEU1A844ASP1A847MET1A848ASP1A848ASP1A848ASP	1	А	443	LEU
1 A 447 ILE 1 A 448 LEU 1 A 464 PHE 1 A 506 LYS 1 A 519 ARG 1 A 519 ARG 1 A 521 THR 1 A 554 SER 1 A 640 LYS 1 A 641 ASP 1 A 641 ASP 1 A 641 ASP 1 A 671 LYS 1 A 723 ARG 1 A 728 CYS 1 A 770 VAL 1 A 802 LEU 1 A 825 LEU 1 A 844 ASP 1 A 847 MET 1 A 848 ASP 1 A 848 ASP <td>1</td> <td>А</td> <td>444</td> <td>TYR</td>	1	А	444	TYR
1 A 448 LEU 1 A 464 PHE 1 A 506 LYS 1 A 519 ARG 1 A 521 THR 1 A 554 SER 1 A 640 LYS 1 A 641 ASP 1 A 666 ASP 1 A 671 LYS 1 A 671 LYS 1 A 723 ARG 1 A 758 PHE 1 A 770 VAL 1 A 802 LEU 1 A 825 LEU 1 A 844 ASP 1 A 844 ASP 1 A 848 ASP 1 A 848 ASP 1 A 848 ASP	1	А	447	ILE
1 A 464 PHE 1 A 506 LYS 1 A 519 ARG 1 A 521 THR 1 A 521 THR 1 A 554 SER 1 A 640 LYS 1 A 641 ASP 1 A 656 ASP 1 A 671 LYS 1 A 671 LYS 1 A 723 ARG 1 A 728 CYS 1 A 758 PHE 1 A 770 VAL 1 A 802 LEU 1 A 825 LEU 1 A 844 ASP 1 A 847 MET 1 A 848 ASP 1 A 848 ASP 1 A 849 TYB	1	А	448	LEU
1 A 506 LYS 1 A 519 ARG 1 A 521 THR 1 A 554 SER 1 A 640 LYS 1 A 641 ASP 1 A 666 ASP 1 A 6671 LYS 1 A 6723 ARG 1 A 723 ARG 1 A 728 CYS 1 A 758 PHE 1 A 770 VAL 1 A 802 LEU 1 A 825 LEU 1 A 844 ASP 1 A 847 MET 1 A 848 ASP 1 A 848 ASP 1 A 849 TYB	1	А	464	PHE
1 A 519 ARG 1 A 521 THR 1 A 554 SER 1 A 640 LYS 1 A 641 ASP 1 A 641 ASP 1 A 656 ASP 1 A 671 LYS 1 A 6723 ARG 1 A 723 ARG 1 A 728 CYS 1 A 758 PHE 1 A 802 LEU 1 A 802 LEU 1 A 825 LEU 1 A 844 ASP 1 A 847 MET 1 A 848 ASP 1 A 848 ASP 1 A 849 TYB	1	А	506	LYS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	519	ARG
1 A 554 SER 1 A 640 LYS 1 A 641 ASP 1 A 656 ASP 1 A 671 LYS 1 A 671 LYS 1 A 671 LYS 1 A 723 ARG 1 A 728 CYS 1 A 758 PHE 1 A 770 VAL 1 A 802 LEU 1 A 841 ARG 1 A 844 ASP 1 A 844 ASP 1 A 847 MET 1 A 848 ASP 1 A 848 ASP 1 A 849 TYB	1	А	521	THR
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	554	SER
1 A 641 ASP 1 A 656 ASP 1 A 671 LYS 1 A 723 ARG 1 A 723 CYS 1 A 728 CYS 1 A 758 PHE 1 A 770 VAL 1 A 802 LEU 1 A 825 LEU 1 A 844 ASP 1 A 847 MET 1 A 848 ASP 1 A 848 ASP 1 A 849 TYB	1	А	640	LYS
1 A 656 ASP 1 A 671 LYS 1 A 723 ARG 1 A 728 CYS 1 A 758 PHE 1 A 770 VAL 1 A 802 LEU 1 A 811 ARG 1 A 825 LEU 1 A 844 ASP 1 A 847 MET 1 A 848 ASP 1 A 848 ASP	1	А	641	ASP
1 A 671 LYS 1 A 723 ARG 1 A 728 CYS 1 A 758 PHE 1 A 770 VAL 1 A 802 LEU 1 A 811 ARG 1 A 825 LEU 1 A 844 ASP 1 A 847 MET 1 A 848 ASP 1 A 848 ASP 1 A 849 TYB	1	А	656	ASP
1 A 723 ARG 1 A 728 CYS 1 A 758 PHE 1 A 758 PHE 1 A 770 VAL 1 A 802 LEU 1 A 811 ARG 1 A 825 LEU 1 A 844 ASP 1 A 847 MET 1 A 848 ASP 1 A 848 ASP 1 A 849 TYB	1	А	671	LYS
1 A 728 CYS 1 A 758 PHE 1 A 770 VAL 1 A 802 LEU 1 A 802 LEU 1 A 811 ARG 1 A 825 LEU 1 A 844 ASP 1 A 847 MET 1 A 848 ASP 1 A 848 ASP 1 A 849 TYB	1	А	723	ARG
1 A 758 PHE 1 A 770 VAL 1 A 802 LEU 1 A 811 ARG 1 A 825 LEU 1 A 844 ASP 1 A 847 MET 1 A 848 ASP 1 A 848 TYB	1	А	728	CYS
1 A 770 VAL 1 A 802 LEU 1 A 811 ARG 1 A 825 LEU 1 A 825 LEU 1 A 844 ASP 1 A 847 MET 1 A 848 ASP 1 A 848 TYB	1	А	758	PHE
1 A 802 LEU 1 A 811 ARG 1 A 825 LEU 1 A 825 LEU 1 A 844 ASP 1 A 847 MET 1 A 848 ASP 1 A 848 TYB	1	А	770	VAL
1 A 811 ARG 1 A 825 LEU 1 A 844 ASP 1 A 847 MET 1 A 848 ASP 1 A 848 TYB	1	А	802	LEU
1 A 825 LEU 1 A 844 ASP 1 A 847 MET 1 A 848 ASP 1 A 848 TYB	1	А	811	ARG
1 A 844 ASP 1 A 847 MET 1 A 848 ASP 1 A 848 TYB	1	А	825	LEU
1 A 847 MET 1 A 848 ASP 1 A 849 TYB	1	А	844	ASP
1 A 848 ASP 1 A 849 TVB	1	А	847	MET
1 A 849 TVR	1	А	848	ASP
	1	А	849	TYR



Mol	Chain	Res	Type
1	А	850	THR
1	А	852	THR
1	А	853	ARG
1	А	855	ARG
1	А	856	ILE
1	А	858	ASP
1	А	859	HIS
1	А	864	GLU
1	А	866	ILE
1	А	878	THR
1	А	879	LEU
1	А	895	LEU
1	А	896	LYS
1	А	924	MET
1	А	926	LEU
1	А	931	ARG
1	А	942	ARG
1	А	944	MET
1	А	981	ASP
1	А	987	PHE
1	A	988	ASP
1	А	1015	GLU
1	A	1018	ASP
1	А	1088	GLU
1	А	1090	ARG
1	A	1110	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	285	ASN
1	А	302	HIS
1	А	756	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

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

5.5 Carbohydrates (i)

There are no 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		$OWAB(Å^2)$	Q<0.9	
1	А	944/1024~(92%)	0.09	19 (2%)	65	44	24, 80, 127, 181	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	849	TYR	3.2
1	А	984	VAL	3.2
1	А	992	ASP	3.1
1	А	855	ARG	2.9
1	А	854	PRO	2.9
1	А	439	LEU	2.8
1	А	1064	CYS	2.7
1	А	985	ALA	2.6
1	А	728	CYS	2.6
1	А	265	ILE	2.5
1	А	1110	ARG	2.5
1	А	1108	ALA	2.5
1	А	1094	PHE	2.3
1	А	991	LEU	2.3
1	А	1076	TRP	2.2
1	А	1061	LEU	2.2
1	А	1111	CYS	2.2
1	А	1077	TYR	2.1
1	А	404	TYR	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.

