

Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 08:39 AM EDT

:	2ZVM
:	Crystal structure of PCNA in complex with DNA polymerase iota fragment
:	Hishiki, A.; Hashimoto, H.; Hanafusa, T.; Kamei, K.; Ohashi, E.; Shimizu, T.;
	Ohmori, H.; Sato, M.
:	2008-11-11
:	2.30 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	:	2.36
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)	:	2.36

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575(2.30-2.30)
Sidechain outliers	138945	5575(2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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			Q	uality of	chain		
			10%						
1	A	261			799	6		14%	• 5%
			11%						
1	В	261			72%			18%	• • 5%
			11%						
1	С	261			74%			19%	• 5%
			9%						
2	U	23		35%		22%		43%	
			9%						
2	V	23	2	:6%	17%		57%	Ď	



Mol	Chain	Length		Quality of chain					
			17%						
2	W	23	30%	9%	61%				



2ZVM

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6210 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	A 948	Total	С	Ν	0	\mathbf{S}	20	0	0	
1	A	248	1904	1199	313	376	16	30	0	
1	В	247	Total	С	Ν	0	S	4.4	0	0
1	D	241	1898	1196	312	374	16	44	0	0
1	С	240	Total	С	Ν	0	S	20	0	0
	1 0 249	249	1913	1204	314	379	16	30	0	0

• Molecule 1 is a protein called Proliferating cell nuclear antigen.

• Molecule 2 is a protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	II	12	Total	С	Ν	0	O S O	0	0	
	U	15	107	73	15	18	1	0	0	0
0	V	10	Total	С	Ν	0	S	2	0	0
	v	10	86	59	12	14	1	2	0	0
0	W/	0	Total	С	Ν	0	S	0	0	0
	vv	9	77	53	10	13	1	0	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	225	Total O 225 225	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: Proliferating cell nuclear antigen







4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	167.62Å 68.82Å 90.18Å	Deperitor
a, b, c, α , β , γ	90.00° 95.05° 90.00°	Depositor
Bosolution(A)	19.95 - 2.30	Depositor
Resolution (A)	19.95 - 2.30	EDS
% Data completeness	100.0 (19.95-2.30)	Depositor
(in resolution range)	98.5(19.95-2.30)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.60 (at 2.30 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
B B.	0.193 , 0.251	Depositor
Λ, Λ_{free}	0.201 , 0.253	DCC
R_{free} test set	2249 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	35.3	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.31 , 48.3	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6210	wwPDB-VP
Average B, all atoms $(Å^2)$	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.99% 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	Bo	nd lengths	Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.97	2/1929~(0.1%)	0.93	4/2605~(0.2%)	
1	В	0.94	0/1923	0.97	5/2597~(0.2%)	
1	С	0.93	1/1938~(0.1%)	0.91	4/2617~(0.2%)	
2	U	0.75	0/109	0.89	0/145	
2	V	0.88	0/87	0.93	0/114	
2	W	0.67	0/78	0.65	0/103	
All	All	0.94	3/6064~(0.0%)	0.93	13/8181~(0.2%)	

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	В	1	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	64	ARG	CB-CG	-5.64	1.37	1.52
1	А	17	GLU	CB-CG	-5.50	1.41	1.52
1	С	32	SER	CB-OG	-5.35	1.35	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	125	GLN	CA-CB-CG	14.29	144.83	113.40
1	В	132	GLU	N-CA-CB	8.60	126.08	110.60
1	В	132	GLU	CB-CA-C	8.51	127.42	110.40
1	В	66	LEU	CA-CB-CG	7.35	132.20	115.30
1	А	80	LYS	CD-CE-NZ	7.17	128.18	111.70
1	В	132	GLU	CA-CB-CG	6.59	127.89	113.40
1	А	77	LYS	CD-CE-NZ	-6.00	97.91	111.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	107	ASN	CB-CA-C	5.96	122.31	110.40
1	А	125	GLN	CB-CG-CD	5.74	126.52	111.60
1	С	12	LEU	CB-CG-CD2	-5.66	101.38	111.00
1	С	94	ASP	CB-CG-OD1	5.62	123.36	118.30
1	А	209	LEU	CB-CG-CD1	5.19	119.83	111.00
1	С	198	GLU	CG-CD-OE1	5.05	128.40	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	В	132	GLU	CA

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	1904	0	1922	33	0
1	В	1898	0	1917	53	0
1	С	1913	0	1928	34	0
2	U	107	0	115	11	0
2	V	86	0	92	7	0
2	W	77	0	79	3	0
3	А	225	0	0	4	0
All	All	6210	0	6053	122	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 10.

All (122) 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)
2:U:426:TYR:CE1	2:U:432:LEU:HD22	1.94	1.02
1:C:138:LYS:HB3	1:C:196:THR:HG22	1.44	0.99
1:B:135:CYS:SG	1:B:199:MET:HB2	2.18	0.84



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:139:MET:CE	1:B:227:LEU:HD11	2.09	0.82
1:B:124:GLU:OE1	1:B:126:LEU:HD11	1.80	0.82
1:A:1:MET:HG2	1:A:91:ARG:NH2	1.96	0.80
1:C:185:THR:HG21	1:C:194:ALA:HA	1.64	0.80
2:U:426:TYR:CE1	2:U:432:LEU:CD2	2.65	0.79
1:A:126:LEU:HD22	2:U:428:LEU:HB3	1.66	0.78
1:C:123:VAL:HG12	1:C:124:GLU:N	2.00	0.76
1:A:126:LEU:HD21	2:U:429:MET:O	1.88	0.74
1:C:138:LYS:HB3	1:C:196:THR:CG2	2.19	0.72
1:B:139:MET:CE	1:B:227:LEU:CD1	2.68	0.71
1:B:25:GLU:OE2	1:B:119:MET:HE1	1.95	0.66
1:B:203:VAL:HG13	1:B:205:LEU:HD22	1.76	0.66
1:C:185:THR:HG23	1:C:186:SER:N	2.11	0.66
1:B:255:ILE:CD1	2:V:421:LYS:HB2	2.27	0.64
1:B:1:MET:HE2	1:B:91:ARG:HG2	1.79	0.64
1:A:228:SER:HB2	1:A:236:VAL:HG12	1.80	0.62
1:B:139:MET:HE1	1:B:227:LEU:HD11	1.81	0.61
1:B:22:LEU:HD23	1:B:48:VAL:CG2	2.30	0.61
1:B:124:GLU:OE1	1:B:126:LEU:CD1	2.49	0.61
1:B:139:MET:HE3	1:B:227:LEU:HD11	1.83	0.61
1:A:170:SER:HB3	1:A:179:ASN:HB3	1.84	0.59
1:B:64:ARG:O	1:B:66:LEU:HD12	2.02	0.59
1:B:16:LEU:HG	1:B:79:LEU:HD12	1.85	0.59
1:B:113:ASP:OD1	1:C:181:LYS:NZ	2.36	0.59
1:A:126:LEU:HD22	2:U:428:LEU:CB	2.33	0.59
1:C:175:LEU:C	1:C:175:LEU:HD12	2.24	0.58
1:C:255:ILE:HD11	2:W:422:GLY:N	2.19	0.57
1:A:19:LEU:HD21	1:A:247:LEU:HD21	1.86	0.57
1:B:40:MET:HE2	1:B:44:HIS:CB	2.35	0.57
2:U:426:TYR:HE1	2:U:432:LEU:HD22	1.60	0.56
1:C:238:GLU:OE2	1:C:240:LYS:HE2	2.04	0.56
2:U:426:TYR:CD1	2:U:432:LEU:HD22	2.38	0.56
1:B:40:MET:HE1	2:V:424:ILE:HB	1.89	0.55
1:C:126:LEU:HD22	2:W:429:MET:O	2.06	0.55
1:C:138:LYS:HG3	1:C:226:THR:HG22	1.88	0.54
1:C:21:ASP:HB3	1:C:214:PHE:HE1	1.73	0.54
1:B:2:PHE:CD2	1:B:30:ILE:HG21	2.42	0.53
1:A:213:ASN:ND2	3:A:264:HOH:O	2.42	0.53
1:A:126:LEU:CD2	2:U:428:LEU:HB3	2.37	0.53
1:A:185:THR:HG22	1:A:185:THR:O	2.08	0.53
1:B:40:MET:HE2	1:B:44:HIS:CA	2.39	0.53



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:23:ILE:HG22	1:C:41:ASP:HA	1.91	0.53	
1:B:135:CYS:SG	1:B:199:MET:CB	2.94	0.52	
1:A:47:LEU:HD23	1:A:250:TYR:CD2	2.44	0.52	
1:C:19:LEU:CD2	1:C:48:VAL:HG11	2.41	0.51	
1:B:138:LYS:NZ	1:B:224:THR:OG1	2.31	0.51	
1:B:184:GLN:O	1:B:195:VAL:O	2.29	0.51	
1:A:139:MET:HE1	1:A:169:PHE:HZ	1.76	0.51	
1:B:255:ILE:HD12	2:V:422:GLY:N	2.26	0.51	
1:B:138:LYS:HE2	1:B:226:THR:CG2	2.41	0.51	
1:B:234:PRO:HD3	2:V:427:TYR:CD1	2.46	0.51	
1:C:138:LYS:CB	1:C:196:THR:HG22	2.31	0.50	
1:B:139:MET:HE3	1:B:227:LEU:CD1	2.38	0.50	
1:A:199:MET:HE3	1:A:202:PRO:HD3	1.93	0.50	
1:B:138:LYS:HE2	1:B:226:THR:HG22	1.93	0.50	
1:B:1:MET:CE	1:B:91:ARG:HG2	2.41	0.50	
1:B:40:MET:CE	2:V:424:ILE:HB	2.41	0.50	
1:C:205:LEU:CD1	1:C:229:MET:HB2	2.42	0.50	
1:C:14:LYS:HD3	1:C:220:PRO:HB2	1.93	0.49	
1:C:255:ILE:HD11	2:W:422:GLY:H	1.77	0.49	
1:B:11:ILE:O	1:B:15:VAL:HG23	2.14	0.48	
1:A:93:GLU:O	1:A:96:ALA:HB2	2.12	0.48	
1:A:170:SER:CB	1:A:179:ASN:HB3	2.43	0.48	
1:A:126:LEU:CD2	2:U:429:MET:O	2.58	0.48	
1:B:48:VAL:CG1	1:B:247:LEU:HD22	2.44	0.48	
1:B:255:ILE:HD11	2:V:421:LYS:HB2	1.95	0.47	
1:A:47:LEU:HD21	1:A:128:ILE:HD11	1.97	0.47	
1:B:40:MET:HE2	1:B:44:HIS:HA	1.96	0.47	
1:C:242:ALA:O	1:C:243:ASP:OD1	2.31	0.47	
1:A:228:SER:HB2	1:A:236:VAL:CG1	2.44	0.47	
1:B:56:GLY:HA3	1:B:244:MET:HB2	1.97	0.46	
1:B:231:ALA:O	1:B:232:ASP:HB2	2.15	0.46	
1:C:51:THR:O	1:C:245:GLY:HA3	2.16	0.46	
1:A:24:ASN:ND2	3:A:303:HOH:O	2.49	0.46	
1:B:184:GLN:O	1:B:185:THR:O	2.33	0.45	
1:C:205:LEU:HD12	1:C:229:MET:HB2	1.98	0.44	
1:A:135:CYS:SG	1:A:199:MET:HG3	2.57	0.44	
1:A:234:PRO:HD3	2:U:427:TYR:CD1	2.52	0.44	
1:B:175:LEU:C	1:B:175:LEU:HD12	2.37	0.44	
1:C:230:SER:HB2	1:C:233:VAL:HG22	1.98	0.44	
1:A:126:LEU:HD23	1:A:127:GLY:N	2.33	0.44	
2:U:426:TYR:HE1	2:U:432:LEU:CD2	2.23	0.44	



	A i a	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:47:LEU:HD12	1:C:250:TYR:CD2	2.53	0.43	
1:A:236:VAL:HG13	3:A:268:HOH:O	2.19	0.43	
1:B:36:ASN:HD22	1:B:49:GLN:HE21	1.66	0.43	
1:B:1:MET:HE2	1:B:91:ARG:CG	2.47	0.43	
1:C:69:GLY:HA2	1:C:121:LEU:HD12	1.99	0.43	
1:B:106:PRO:HG2	1:B:107:ASN:H	1.84	0.43	
1:A:137:VAL:HG11	1:A:139:MET:CE	2.48	0.43	
1:B:81:CYS:SG	1:C:150:ASP:HB3	2.58	0.43	
1:C:123:VAL:CG1	1:C:124:GLU:N	2.72	0.42	
1:B:255:ILE:HD11	2:V:421:LYS:CB	2.49	0.42	
1:A:244:MET:HE2	1:A:244:MET:HB2	1.81	0.42	
1:B:78:ILE:CD1	1:B:116:MET:HB2	2.49	0.42	
1:B:200:ASN:HD22	1:B:201:GLU:HG3	1.84	0.42	
1:C:85:GLU:O	1:C:106:PRO:HG2	2.20	0.42	
1:C:93:GLU:O	1:C:96:ALA:HB2	2.19	0.42	
1:B:207:PHE:CZ	1:B:235:LEU:HB2	2.55	0.42	
1:C:56:GLY:HA3	1:C:244:MET:HB2	2.01	0.42	
1:B:40:MET:HE2	1:B:44:HIS:HB3	2.00	0.42	
1:B:2:PHE:CE2	1:B:30:ILE:HG21	2.55	0.41	
1:C:138:LYS:CB	1:C:196:THR:CG2	2.94	0.41	
1:C:236:VAL:HG22	1:C:250:TYR:CD1	2.55	0.41	
1:A:219:THR:N	1:A:220:PRO:CD	2.84	0.41	
1:B:138:LYS:CE	1:B:226:THR:HG22	2.50	0.41	
1:B:139:MET:CE	1:B:227:LEU:HD12	2.48	0.41	
1:A:137:VAL:HG11	1:A:139:MET:HE2	2.03	0.41	
1:C:162:CYS:HB3	1:C:203:VAL:HG22	2.03	0.41	
1:A:203:VAL:HG21	1:A:229:MET:HG3	2.02	0.41	
1:B:48:VAL:HG22	1:B:249:TYR:CD2	2.56	0.41	
1:C:13:LYS:HE2	1:C:84:ASN:ND2	2.36	0.41	
1:A:76:SER:O	1:A:80:LYS:HG2	2.20	0.41	
1:A:126:LEU:HD23	1:A:127:GLY:H	1.85	0.41	
1:A:246:HIS:ND1	3:A:371:HOH:O	2.37	0.41	
1:B:48:VAL:HG12	1:B:49:GLN:N	2.36	0.41	
1:A:81:CYS:SG	1:B:150:ASP:HB3	2.60	0.41	
1:B:107:ASN:O	1:B:108:GLN:HB2	2.22	0.40	
1:A:236:VAL:HG13	1:A:236:VAL:O	2.21	0.40	
1:C:243:ASP:OD1	1:C:243:ASP:O	2.40	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	Perce	ntiles
1	А	244/261~(94%)	238~(98%)	6(2%)	0	100	100
1	В	243/261~(93%)	232~(96%)	8(3%)	3~(1%)	13	14
1	С	245/261~(94%)	236 (96%)	7 (3%)	2(1%)	19	23
2	U	11/23~(48%)	10 (91%)	1 (9%)	0	100	100
2	V	8/23~(35%)	8 (100%)	0	0	100	100
2	W	7/23~(30%)	7 (100%)	0	0	100	100
All	All	758/852~(89%)	731 (96%)	22 (3%)	5 (1%)	22	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	123	VAL
1	В	244	MET
1	В	108	GLN
1	С	244	MET
1	В	106	PRO

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	216/228~(95%)	209~(97%)	7 (3%)	39 54
1	В	215/228~(94%)	199~(93%)	16 (7%)	13 17
1	С	217/228~(95%)	209 (96%)	8 (4%)	34 48



Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
2	U	12/20~(60%)	12~(100%)	0	100	100
2	V	9/20~(45%)	9~(100%)	0	100	100
2	W	8/20 (40%)	8 (100%)	0	100	100
All	All	677/744 (91%)	646 (95%)	31 (5%)	27	38

Continued from previous page...

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	47	LEU
1	А	109	GLU
1	А	126	LEU
1	А	161	SER
1	А	184	GLN
1	А	185	THR
1	А	209	LEU
1	В	20	LYS
1	В	64	ARG
1	В	66	LEU
1	В	107	ASN
1	В	108	GLN
1	В	113	ASP
1	В	122	ASP
1	В	125	GLN
1	В	182	LEU
1	В	185	THR
1	В	196	THR
1	В	199	MET
1	В	200	ASN
1	В	203	VAL
1	В	205	LEU
1	В	240	LYS
1	С	1	MET
1	С	12	LEU
1	С	23	ILE
1	С	42	SER
1	С	66	LEU
1	С	165	ASP
1	С	185	THR
1	С	243	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)



Mol	Chain	Res	Type
1	А	36	ASN
1	А	65	ASN
1	А	84	ASN
1	А	108	GLN
1	А	213	ASN
1	В	36	ASN
1	В	65	ASN
1	В	200	ASN
1	В	213	ASN
1	С	8	GLN
1	С	24	ASN
1	С	36	ASN
1	С	65	ASN
1	С	84	ASN
1	С	213	ASN

such sidechains are listed below:

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 $>$	#RSR	\mathbf{z}	2	$OWAB(Å^2)$	Q<0.9
1	А	248/261~(95%)	0.78	27 (10%)	5	8	33, 51, 67, 80	8 (3%)
1	В	247/261~(94%)	0.88	29 (11%)	4	6	42, 52, 70, 84	10 (4%)
1	С	249/261~(95%)	0.88	28 (11%)	5	7	43, 52, 69, 74	11 (4%)
2	U	13/23~(56%)	1.28	2(15%)	2	3	47, 51, 59, 63	0
2	V	10/23~(43%)	0.71	2(20%)	1	1	53, 56, 64, 65	1 (10%)
2	W	9/23~(39%)	1.53	4 (44%)	0	0	64, 67, 72, 75	0
All	All	776/852 (91%)	0.86	92 (11%)	4	6	33, 52, 69, 84	30 (3%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	106	PRO	8.3
1	С	106	PRO	7.7
1	В	123	VAL	6.8
1	В	96	ALA	6.3
1	С	123	VAL	6.0
1	В	107	ASN	5.7
1	В	126	LEU	5.6
2	U	432	LEU	5.6
1	А	106	PRO	5.6
1	В	243	ASP	5.3
1	В	122	ASP	5.2
1	С	255	ILE	5.1
1	С	107	ASN	5.0
1	В	108	GLN	4.9
1	С	243	ASP	4.7
1	A	124	GLU	4.6
1	А	243	ASP	4.6
1	С	256	GLU	4.2
1	А	95	ASN	4.2



Mol	Chain	Res	Type	RSRZ
1	А	186	SER	4.2
1	В	124	GLU	4.2
1	А	122	ASP	4.1
1	В	185	THR	4.0
1	А	1	MET	3.9
1	А	97	ASP	3.9
1	А	185	THR	3.8
1	А	107	ASN	3.7
2	W	429	MET	3.7
1	В	95	ASN	3.6
1	С	124	GLU	3.6
1	С	151	LEU	3.6
1	С	95	ASN	3.5
1	С	156	ASP	3.4
1	В	165	ASP	3.4
1	С	122	ASP	3.3
1	С	147	ILE	3.2
2	V	424	ILE	3.2
1	В	242	ALA	3.2
1	А	151	LEU	3.1
1	А	235	LEU	3.0
1	С	101	LEU	3.0
1	А	123	VAL	3.0
1	А	202	PRO	3.0
1	С	186	SER	2.9
1	А	96	ALA	2.9
1	С	163	ALA	2.9
1	В	88	ILE	2.8
1	А	125	GLN	2.8
1	В	97	ASP	2.8
1	В	130	GLU	2.8
1	А	101	LEU	2.7
1	A	120	ASP	2.7
1	В	128	ILE	2.7
1	С	164	LYS	2.7
1	С	160	ILE	2.7
1	В	184	GLN	2.6
1	В	58	ASP	2.6
1	С	126	LEU	2.6
1	A	94	ASP	2.6
1	В	200	ASN	2.5
1	А	255	ILE	2.5



|--|

Mol	Chain	Res	Type	RSRZ
2	W	424	ILE	2.5
1	А	90	LEU	2.5
1	В	47	LEU	2.5
1	А	232	ASP	2.4
1	С	97	ASP	2.4
2	U	424	ILE	2.4
1	В	94	ASP	2.4
1	А	4	ALA	2.4
1	А	199	MET	2.3
1	С	158	VAL	2.3
1	В	180	ILE	2.3
2	W	426	TYR	2.3
1	С	119	MET	2.3
1	В	197	ILE	2.3
1	С	180	ILE	2.2
1	С	35	VAL	2.2
1	С	212	LEU	2.2
2	W	427	TYR	2.2
1	В	78	ILE	2.2
1	В	235	LEU	2.2
1	С	121	LEU	2.2
1	В	35	VAL	2.2
1	В	202	PRO	2.2
1	С	19	LEU	2.1
2	V	429	MET	2.1
1	А	174	GLU	2.1
1	А	180	ILE	2.1
1	С	169	PHE	2.1
1	С	85	GLU	2.1
1	А	70	VAL	2.1
1	В	109	GLU	2.1

Continued from previous page...

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.

