



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:11 AM GMT

PDB ID : 2ZVM  
Title : Crystal structure of PCNA in complex with DNA polymerase iota fragment  
Authors : Hishiki, A.; Hashimoto, H.; Hanafusa, T.; Kamei, K.; Ohashi, E.; Shimizu, T.; Ohmori, H.; Sato, M.  
Deposited on : 2008-11-11  
Resolution : 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

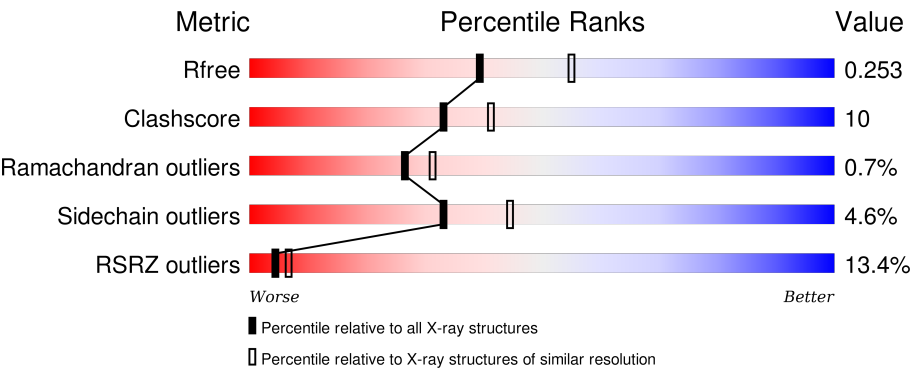
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	261	<div><div>12%</div><div><div></div><div></div><div></div><div></div></div><div>79%</div><div><div></div><div></div><div></div><div></div></div><div>14%</div><div>• 5%</div></div>
1	B	261	<div><div>12%</div><div><div></div><div></div><div></div><div></div></div><div>72%</div><div><div></div><div></div><div></div><div></div></div><div>18%</div><div>• • 5%</div></div>
1	C	261	<div><div>13%</div><div><div></div><div></div><div></div><div></div></div><div>74%</div><div><div></div><div></div><div></div><div></div></div><div>19%</div><div>• 5%</div></div>
2	U	23	<div><div>9%</div><div><div></div><div></div><div></div><div></div></div><div>35%</div><div><div></div><div></div><div></div><div></div></div><div>22%</div><div>43%</div></div>
2	V	23	<div><div>9%</div><div><div></div><div></div><div></div><div></div></div><div>26%</div><div><div></div><div></div><div></div><div></div></div><div>17%</div><div>57%</div></div>

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Mol	Chain	Length	Quality of chain
2	W	23	 A horizontal bar chart showing the quality of chain W. The bar is divided into four segments: red (17%), green (30%), yellow (9%), and grey (61%). The percentages are labeled below the bar.

## 2 Entry composition

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.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	30	0	0
			1904	1199	313	376	16			
1	B	247	Total	C	N	O	S	44	0	0
			1898	1196	312	374	16			
1	C	249	Total	C	N	O	S	38	0	0
			1913	1204	314	379	16			

- Molecule 2 is a protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	13	Total	C	N	O	S	0	0	0
			107	73	15	18	1			
2	V	10	Total	C	N	O	S	2	0	0
			86	59	12	14	1			
2	W	9	Total	C	N	O	S	0	0	0
			77	53	10	13	1			

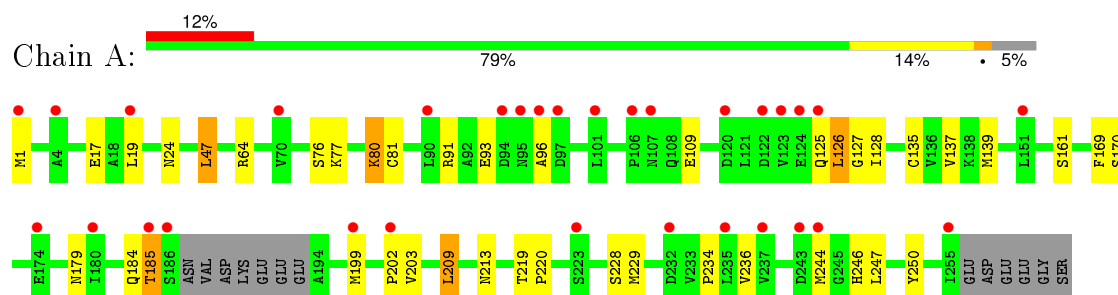
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	225	Total	O	0	0
			225	225		

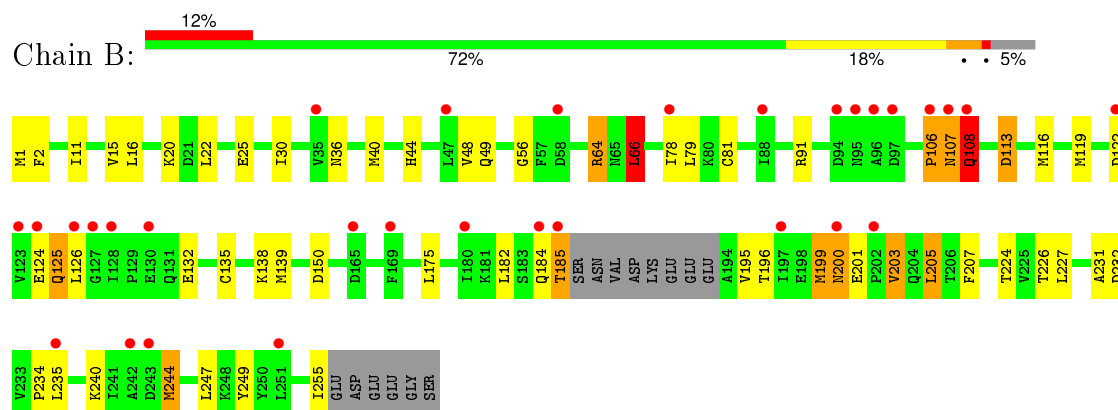
### 3 Residue-property plots [i](#)

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

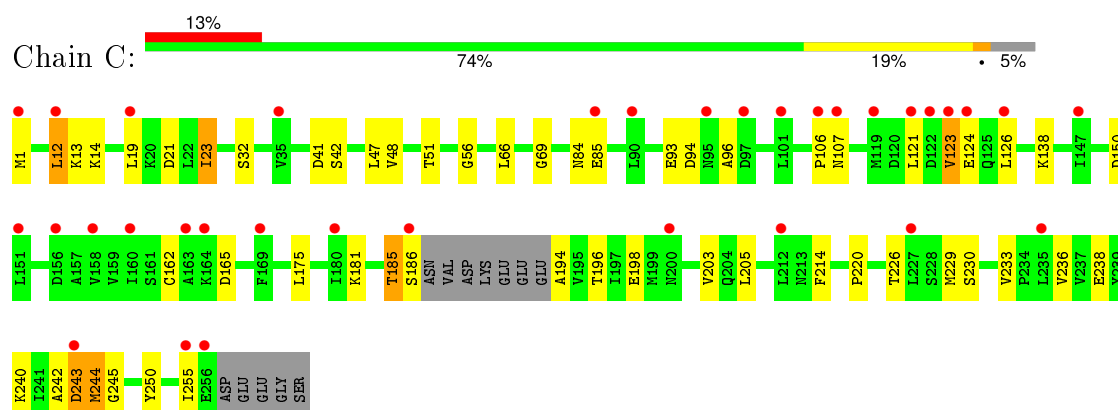
- Molecule 1: Proliferating cell nuclear antigen



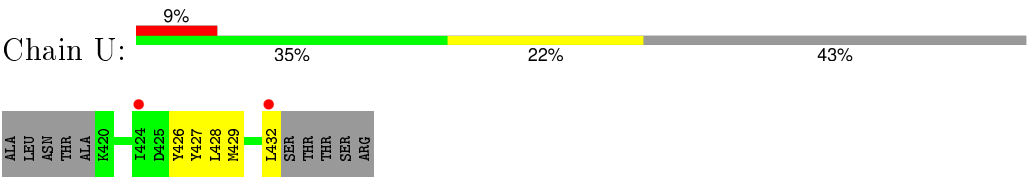
- Molecule 1: Proliferating cell nuclear antigen



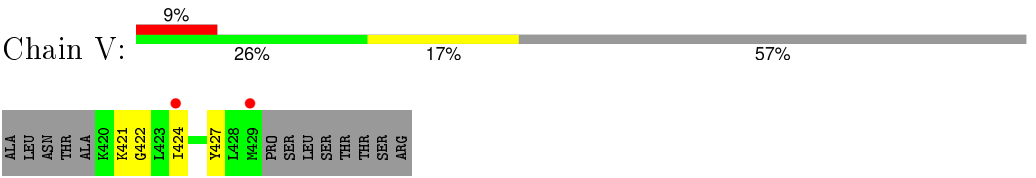
- Molecule 1: Proliferating cell nuclear antigen



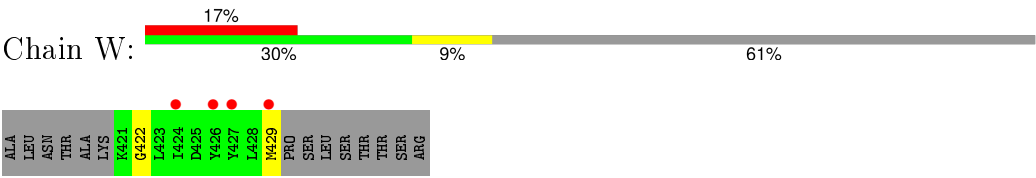
● Molecule 2: DNA polymerase iota



● Molecule 2: DNA polymerase iota



● Molecule 2: DNA polymerase iota



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.62Å 68.82Å 90.18Å 90.00° 95.05° 90.00°	Depositor
Resolution (Å)	19.95 – 2.30 19.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.95-2.30) 98.5 (19.95-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.193 , 0.251 0.201 , 0.253	Depositor DCC
$R_{free}$ test set	2249 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 44964 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

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

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.97	2/1929 (0.1%)	0.93	4/2605 (0.2%)
1	B	0.94	0/1923	0.97	5/2597 (0.2%)
1	C	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	B	1	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	ARG	CB-CG	-5.64	1.37	1.52
1	A	17	GLU	CB-CG	-5.50	1.41	1.52
1	C	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(°)	Ideal(°)
1	B	125	GLN	CA-CB-CG	14.29	144.83	113.40
1	B	132	GLU	N-CA-CB	8.60	126.08	110.60
1	B	132	GLU	CB-CA-C	8.51	127.42	110.40
1	B	66	LEU	CA-CB-CG	7.35	132.20	115.30
1	A	80	LYS	CD-CE-NZ	7.17	128.18	111.70
1	B	132	GLU	CA-CB-CG	6.59	127.89	113.40
1	A	77	LYS	CD-CE-NZ	-6.00	97.91	111.70

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

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	132	GLU	CA

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1904	0	1922	33	0
1	B	1898	0	1917	53	0
1	C	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	A	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:139:MET:HE3	1:B:227:LEU:HD11	1.83	0.61
1:B:124:GLU:OE1	1:B:126:LEU:CD1	2.49	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:HD12	1:C:175:LEU:C	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:B:40:MET:HE2	1:B:44:HIS:CA	2.39	0.53
1:A:185:THR:O	1:A:185:THR:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:B:138:LYS:HE2	1:B:226:THR:HG22	1.93	0.50
1:A:199:MET:HE3	1:A:202:PRO:HD3	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:B:40:MET:HE2	1:B:44:HIS:HA	1.96	0.47
1:A:47:LEU:HD21	1:A:128:ILE:HD11	1.97	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:HD12	1:B:175:LEU:C	2.37	0.44
1:C:230:SER:HB2	1:C:233:VAL:HG22	1.98	0.44
2:U:426:TYR:HE1	2:U:432:LEU:CD2	2.23	0.44
1:A:126:LEU:HD23	1:A:127:GLY:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:C:56:GLY:HA3	1:C:244:MET:HB2	2.01	0.42
1:B:207:PHE:CZ	1:B:235:LEU:HB2	2.55	0.42
1:B:40:MET:HE2	1:B:44:HIS:HB3	2.00	0.42
1:C:138:LYS:CB	1:C:196:THR:CG2	2.94	0.41
1:B:2:PHE:CE2	1:B:30:ILE:HG21	2.55	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:139:MET:CE	1:B:227:LEU:HD12	2.48	0.41
1:B:138:LYS:CE	1:B:226:THR:HG22	2.50	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: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:203:VAL:HG21	1:A:229:MET:HG3	2.02	0.41
1:A:126:LEU:HD23	1:A:127:GLY:H	1.85	0.41
1:B:48:VAL:HG12	1:B:49:GLN:N	2.36	0.41
1:A:76:SER:O	1:A:80:LYS:HG2	2.20	0.41
1:A:246:HIS:ND1	3:A:371:HOH:O	2.37	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:O	1:C:243:ASP:OD1	2.40	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	A	244/261 (94%)	238 (98%)	6 (2%)	0	100	100
1	B	243/261 (93%)	232 (96%)	8 (3%)	3 (1%)	16	16
1	C	245/261 (94%)	236 (96%)	7 (3%)	2 (1%)	24	27
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%)	26	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	123	VAL
1	B	244	MET
1	B	108	GLN
1	C	244	MET
1	B	106	PRO

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/228 (95%)	209 (97%)	7 (3%)	46	62
1	B	215/228 (94%)	199 (93%)	16 (7%)	17	21
1	C	217/228 (95%)	209 (96%)	8 (4%)	41	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	33	44

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

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

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

sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	65	ASN
1	A	84	ASN
1	A	108	GLN
1	A	213	ASN
1	B	36	ASN
1	B	65	ASN
1	B	200	ASN
1	B	213	ASN
1	C	8	GLN
1	C	24	ASN
1	C	36	ASN
1	C	65	ASN
1	C	84	ASN
1	C	213	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	248/261 (95%)	0.81	31 (12%) 5 8	33, 51, 67, 81	8 (3%)
1	B	247/261 (94%)	0.92	31 (12%) 5 8	42, 52, 70, 84	10 (4%)
1	C	249/261 (95%)	0.94	34 (13%) 4 6	43, 52, 69, 74	11 (4%)
2	U	13/23 (56%)	1.36	2 (15%) 3 4	47, 51, 59, 63	0
2	V	10/23 (43%)	0.74	2 (20%) 1 2	53, 56, 64, 65	1 (10%)
2	W	9/23 (39%)	1.57	4 (44%) 0 0	64, 67, 72, 75	0
All	All	776/852 (91%)	0.90	104 (13%) 4 7	33, 52, 69, 84	30 (3%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	106	PRO	8.8
1	C	106	PRO	8.0
1	B	123	VAL	6.9
1	B	96	ALA	6.7
1	C	123	VAL	6.2
2	U	432	LEU	6.1
1	B	126	LEU	5.8
1	B	243	ASP	5.7
1	A	106	PRO	5.6
1	B	107	ASN	5.6
1	B	122	ASP	5.4
1	C	255	ILE	5.2
1	C	107	ASN	5.1
1	B	108	GLN	4.7
1	B	124	GLU	4.5
1	C	243	ASP	4.4
1	A	122	ASP	4.4
1	A	124	GLU	4.4
1	A	95	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	185	THR	4.3
1	A	243	ASP	4.3
1	C	256	GLU	4.2
1	A	186	SER	4.1
1	A	1	MET	4.0
1	A	97	ASP	3.9
1	A	185	THR	3.8
1	C	124	GLU	3.7
1	C	151	LEU	3.7
1	C	122	ASP	3.6
2	W	429	MET	3.6
1	A	107	ASN	3.5
1	A	235	LEU	3.4
2	V	424	ILE	3.4
1	C	95	ASN	3.3
1	B	95	ASN	3.3
1	C	156	ASP	3.3
1	A	202	PRO	3.2
1	B	165	ASP	3.2
1	C	147	ILE	3.1
1	B	128	ILE	3.1
1	C	101	LEU	3.1
1	C	163	ALA	3.0
1	C	186	SER	3.0
1	C	164	LYS	2.9
1	A	101	LEU	2.9
1	C	126	LEU	2.9
1	B	242	ALA	2.9
1	A	120	ASP	2.9
1	B	88	ILE	2.9
1	B	97	ASP	2.8
1	A	151	LEU	2.8
1	C	160	ILE	2.8
1	B	58	ASP	2.8
1	B	184	GLN	2.8
1	A	90	LEU	2.7
1	A	96	ALA	2.6
1	C	121	LEU	2.6
1	A	94	ASP	2.6
2	W	424	ILE	2.6
1	B	130	GLU	2.6
2	W	426	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	97	ASP	2.6
1	A	4	ALA	2.6
1	A	123	VAL	2.5
2	U	424	ILE	2.5
1	A	125	GLN	2.5
1	B	200	ASN	2.4
1	B	47	LEU	2.4
1	B	35	VAL	2.4
1	A	199	MET	2.4
1	B	202	PRO	2.4
1	B	180	ILE	2.3
1	C	12	LEU	2.3
1	C	119	MET	2.3
1	C	212	LEU	2.3
1	C	35	VAL	2.3
1	C	158	VAL	2.3
1	B	94	ASP	2.3
1	A	70	VAL	2.3
1	A	255	ILE	2.3
1	C	19	LEU	2.3
1	A	232	ASP	2.2
1	B	197	ILE	2.2
1	C	169	PHE	2.2
1	A	174	GLU	2.2
2	W	427	TYR	2.2
1	B	235	LEU	2.2
1	B	251	LEU	2.2
1	C	180	ILE	2.1
1	B	127	GLY	2.1
1	C	85	GLU	2.1
1	B	169	PHE	2.1
1	B	78	ILE	2.1
1	C	90	LEU	2.1
2	V	429	MET	2.1
1	A	19	LEU	2.1
1	C	235	LEU	2.1
1	A	223	SER	2.1
1	C	1	MET	2.0
1	A	180	ILE	2.0
1	C	200	ASN	2.0
1	A	237	VAL	2.0
1	A	244	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	227	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.