



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:23 PM UTC

PDB ID : 2ZVM / pdb_00002zvm
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

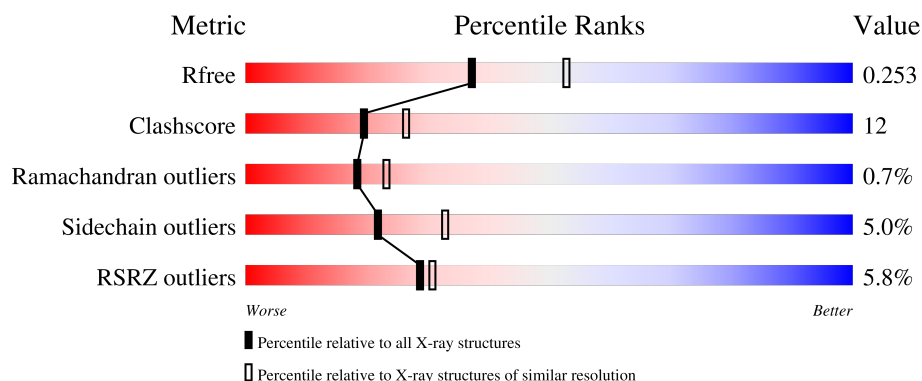
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

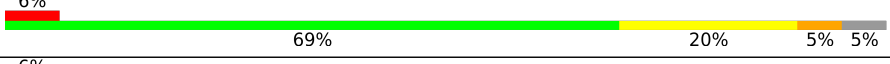
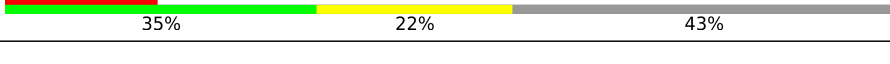
The reported resolution of this entry is 2.30 Å.

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_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	
1	B	261	
1	C	261	
2	U	23	
2	V	23	

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Mol	Chain	Length	Quality of chain
2	W	23	

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			

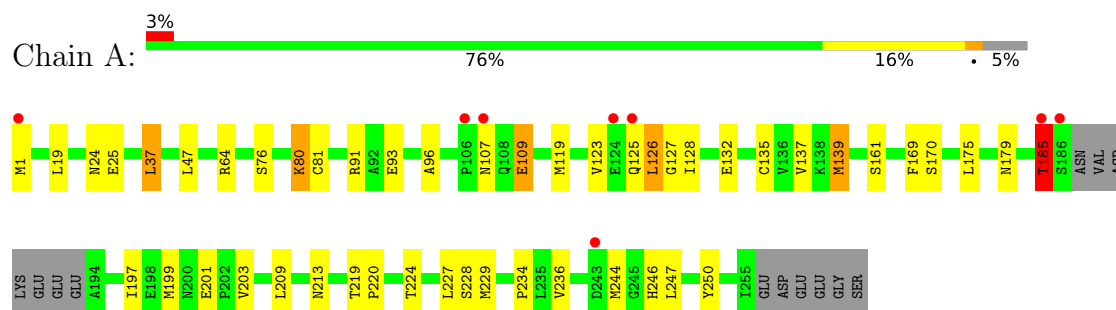
- Molecule 3 is water.

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

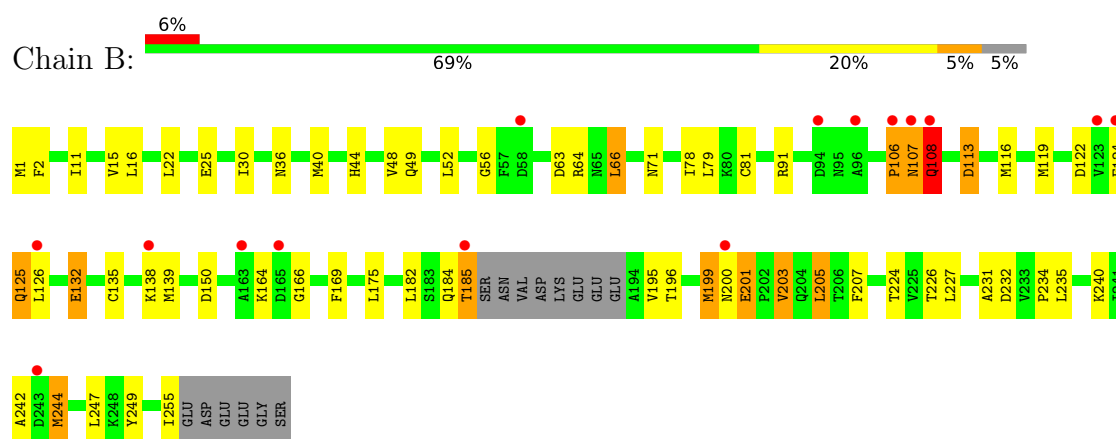
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

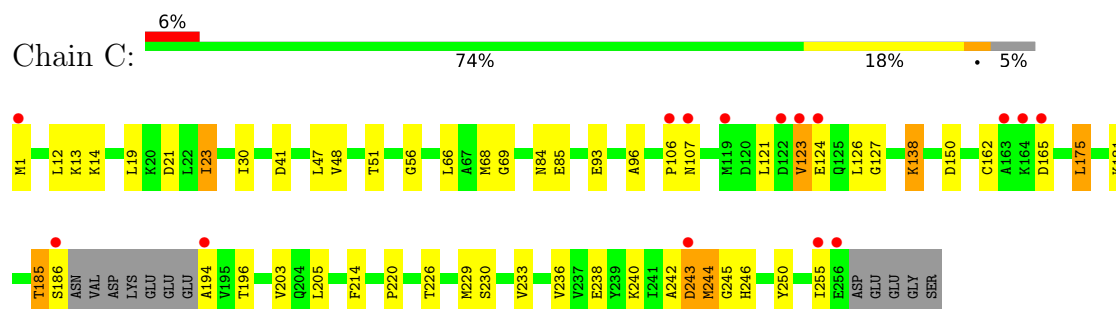
- Molecule 1: Proliferating cell nuclear antigen



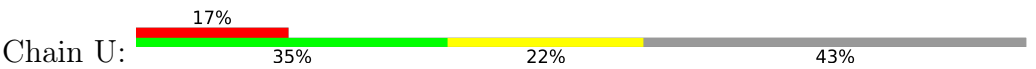
- Molecule 1: Proliferating cell nuclear antigen



- Molecule 1: Proliferating cell nuclear antigen



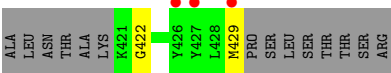
- Molecule 2: DNA polymerase iota



• 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, α , β , γ	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) 98.3 (19.95-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

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.

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	1.18	3/1929 (0.2%)	1.12	4/2605 (0.2%)
1	B	1.15	2/1923 (0.1%)	1.16	8/2597 (0.3%)
1	C	1.14	0/1938	1.08	1/2617 (0.0%)
2	U	0.90	0/109	1.05	0/145
2	V	1.01	0/87	1.13	0/114
2	W	0.75	0/78	0.71	0/103
All	All	1.15	5/6064 (0.1%)	1.11	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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	ASN	CA-C	-8.55	1.42	1.53
1	B	164	LYS	CA-CB	-6.22	1.43	1.53
1	A	109	GLU	CA-CB	5.14	1.60	1.52
1	B	242	ALA	CA-C	-5.09	1.48	1.53
1	A	64	ARG	CB-CG	-5.04	1.37	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	GLN	CA-CB-CG	15.37	144.83	114.10
1	B	132	GLU	CB-CA-C	9.19	127.42	109.33
1	B	132	GLU	N-CA-CB	8.77	126.08	111.08
1	A	125	GLN	CB-CG-CD	8.19	126.52	112.60
1	B	242	ALA	CB-CA-C	-7.06	108.42	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	GLU	CA-CB-CG	6.90	127.89	114.10
1	A	139	MET	N-CA-C	6.41	113.78	108.07
1	C	107	ASN	CB-CA-C	6.03	122.31	111.03
1	A	185	THR	N-CA-C	5.59	118.35	109.24
1	B	166	GLY	N-CA-C	5.59	119.84	110.56
1	B	201	GLU	CA-C-N	5.49	125.44	119.78
1	B	201	GLU	C-N-CA	5.49	125.44	119.78
1	A	80	LYS	CD-CE-NZ	5.09	128.18	111.90

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	40	0
1	B	1898	0	1917	57	0
1	C	1913	0	1928	38	0
2	U	107	0	115	11	0
2	V	86	0	92	6	0
2	W	77	0	79	4	0
3	A	225	0	0	4	0
All	All	6210	0	6053	137	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 12.

All (137) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:40:MET:HE3	2:V:424:ILE:HB	1.58	0.83
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:B:139:MET:HE3	1:B:227:LEU:HD11	1.67	0.76
1:A:126:LEU:HD21	2:U:429:MET:O	1.88	0.74
1:C:30:ILE:HG13	1:C:68:MET:HE2	1.71	0.73
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:40:MET:HE2	1:B:44:HIS:HA	1.75	0.68
1:A:199:MET:HE3	1:A:201:GLU:CA	2.26	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:A:228:SER:HB2	1:A:236:VAL:HG12	1.80	0.62
1:C:175:LEU:C	1:C:175:LEU:HD12	2.24	0.62
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:1:MET:HE2	1:B:91:ARG:HD3	1.81	0.60
1:B:52:LEU:HB3	1:B:244:MET:HE2	1.84	0.60
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:A:126:LEU:HD22	2:U:428:LEU:CB	2.33	0.59
1:A:199:MET:HE3	1:A:201:GLU:HA	1.87	0.57
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:C:30:ILE:CG1	1:C:68:MET:HE2	2.33	0.57
1:B:1:MET:HE2	1:B:91:ARG:CD	2.34	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:C:126:LEU:HD22	2:W:429:MET:O	2.06	0.55
1:B:25:GLU:OE2	1:B:119:MET:HE1	2.06	0.55
1:A:137:VAL:HG11	1:A:139:MET:HE2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:113:ASP:OD1	1:C:181:LYS:NZ	2.36	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: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:B:139:MET:HE1	1:B:169:PHE:HZ	1.74	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:B:1:MET:CE	1:B:91:ARG:HG2	2.41	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:A:139:MET:HE1	1:A:169:PHE:HZ	1.76	0.50
1:B:135:CYS:HG	1:B:199:MET:HB2	1.75	0.50
1:B:138:LYS:HE2	1:B:226:THR:HG22	1.93	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:175:LEU:C	1:B:175:LEU:HD12	2.37	0.49
1:B:1:MET:HE3	1:B:91:ARG:HG2	1.95	0.48
1:A:25:GLU:OE2	1:A:119:MET:HE1	2.13	0.48
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:137:VAL:CG1	1:A:139:MET:HE2	2.42	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: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:139:MET:HE3	1:B:227:LEU:CD1	2.39	0.46
1:A:25:GLU:CD	1:A:119:MET:HE1	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:244:MET:HB2	1:A:244:MET:HE2	1.49	0.46
1:B:184:GLN:O	1:B:185:THR:O	2.33	0.45
1:B:1:MET:N	1:B:63:ASP:OD2	2.47	0.45
1:B:231:ALA:O	1:B:232:ASP:HB2	2.15	0.45
1:B:40:MET:HE2	1:B:44:HIS:CA	2.45	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:C:243:ASP:OD1	1:C:243:ASP:C	2.60	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
1:B:139:MET:HE1	1:B:169:PHE:CZ	2.53	0.43
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: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:B:81:CYS:SG	1:C:150:ASP:HB3	2.58	0.43
1:B:255:ILE:HD11	2:V:421:LYS:CB	2.49	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:B:71:ASN:OD1	1:B:71:ASN:C	2.62	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:C:246:HIS:C	1:C:246:HIS:CD2	2.97	0.42
1:A:137:VAL:HG11	1:A:139:MET:CE	2.48	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:37:LEU:C	1:A:37:LEU:HD23	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:199:MET:O	1:B:199:MET:HE3	2.21	0.41
1:C:127:GLY:C	2:W:429:MET:HE2	2.46	0.41
1:B:107:ASN:O	1:B:108:GLN:HB2	2.22	0.40
1:A:175:LEU:C	1:A:175:LEU:HD12	2.47	0.40
1:A:236:VAL:HG13	1:A:236:VAL:O	2.21	0.40
1:A:139:MET:HE3	1:A:227:LEU:CD1	2.51	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 ⓘ

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%)	10	12
1	C	245/261 (94%)	236 (96%)	7 (3%)	2 (1%)	16	20
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%)	18	23

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%)	206 (95%)	10 (5%)	24	36
1	B	215/228 (94%)	201 (94%)	14 (6%)	15	22
1	C	217/228 (95%)	208 (96%)	9 (4%)	27	41
2	U	12/20 (60%)	12 (100%)	0	100	100
2	V	9/20 (45%)	8 (89%)	1 (11%)	6	7
2	W	8/20 (40%)	8 (100%)	0	100	100
All	All	677/744 (91%)	643 (95%)	34 (5%)	22	33

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	109	GLU
1	A	123	VAL
1	A	126	LEU
1	A	132	GLU
1	A	161	SER
1	A	185	THR
1	A	197	ILE
1	A	209	LEU
1	A	224	THR
1	B	66	LEU
1	B	107	ASN
1	B	108	GLN
1	B	113	ASP

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Mol	Chain	Res	Type
1	B	122	ASP
1	B	125	GLN
1	B	132	GLU
1	B	182	LEU
1	B	185	THR
1	B	196	THR
1	B	199	MET
1	B	203	VAL
1	B	205	LEU
1	B	240	LYS
2	V	429	MET
1	C	1	MET
1	C	12	LEU
1	C	23	ILE
1	C	66	LEU
1	C	138	LYS
1	C	165	ASP
1	C	175	LEU
1	C	185	THR
1	C	243	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
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	95	ASN
1	C	213	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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 ⓘ

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, 95th 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	A	248/261 (95%)	0.34	8 (3%)	50 52	26, 50, 64, 80	8 (3%)
1	B	247/261 (94%)	0.41	15 (6%)	27 29	24, 52, 68, 84	10 (4%)
1	C	249/261 (95%)	0.39	15 (6%)	27 29	30, 52, 67, 74	11 (4%)
2	U	13/23 (56%)	1.63	4 (30%)	1 1	47, 51, 59, 63	0
2	V	10/23 (43%)	0.95	0	100 100	47, 56, 64, 65	1 (10%)
2	W	9/23 (39%)	1.39	3 (33%)	1 1	64, 67, 72, 75	0
All	All	776/852 (91%)	0.42	45 (5%)	29 31	24, 52, 67, 84	30 (3%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	5.3
1	B	185	THR	4.4
2	U	432	LEU	4.3
1	B	107	ASN	4.1
1	C	106	PRO	3.8
1	A	125	GLN	3.8
1	B	165	ASP	3.7
1	C	164	LYS	3.6
1	B	123	VAL	3.5
1	A	186	SER	3.3
1	C	163	ALA	3.3
1	B	243	ASP	3.2
1	B	94	ASP	3.2
1	C	186	SER	3.0
1	B	108	GLN	2.9
1	B	106	PRO	2.9
2	U	423	LEU	2.8
1	B	163	ALA	2.8
1	C	256	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	U	431	SER	2.8
1	C	255	ILE	2.7
1	C	107	ASN	2.6
1	A	106	PRO	2.5
1	C	123	VAL	2.5
2	U	424	ILE	2.5
1	C	119	MET	2.5
1	C	243	ASP	2.5
1	A	124	GLU	2.5
1	B	124	GLU	2.5
1	B	200	ASN	2.5
1	B	138	LYS	2.5
1	C	165	ASP	2.4
1	B	126	LEU	2.4
1	C	122	ASP	2.3
1	A	185	THR	2.3
1	C	124	GLU	2.3
1	A	243	ASP	2.2
1	C	1	MET	2.1
2	W	426	TYR	2.1
2	W	427	TYR	2.1
2	W	429	MET	2.1
1	A	107	ASN	2.1
1	B	96	ALA	2.0
1	C	194	ALA	2.0
1	B	58	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.