



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:57 PM GMT

PDB ID : 1VYM  
Title : NATIVE HUMAN PCNA  
Authors : Kontopidis, G.; Wu, S.; Zheleva, D.; Taylor, P.; Mcinnes, C.; Lane, D.; Fischer, P.; Walkinshaw, M.  
Deposited on : 2004-05-03  
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

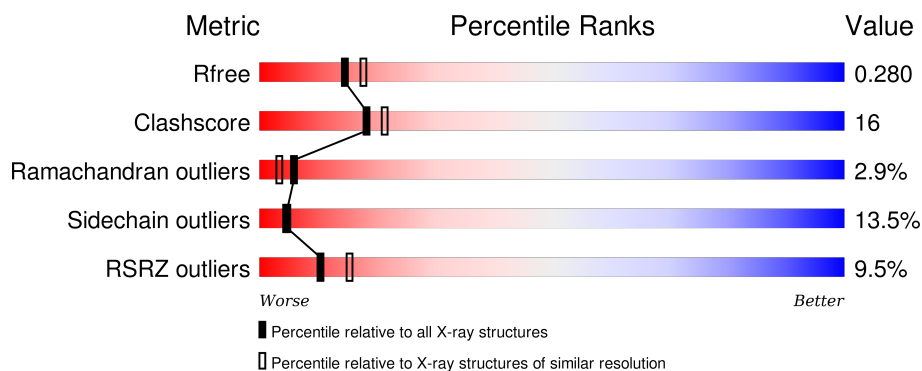
# 1 Overall quality at a glance

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))
$R_{free}$	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>10%</div> <div> <div></div> <div>68%</div> <div>23%</div> <div>6%</div> <div>..</div> </div> </div>
1	B	261	<div> <div>11%</div> <div> <div></div> <div>62%</div> <div>27%</div> <div>8%</div> <div>..</div> </div> </div>
1	C	261	<div> <div>7%</div> <div> <div></div> <div>68%</div> <div>24%</div> <div>5%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6033 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	256	Total	C	N	O	S	0	0	1
			1964	1233	323	392	16			
1	B	256	Total	C	N	O	S	0	0	1
			1964	1233	323	392	16			
1	C	256	Total	C	N	O	S	0	0	1
			1964	1233	323	392	16			

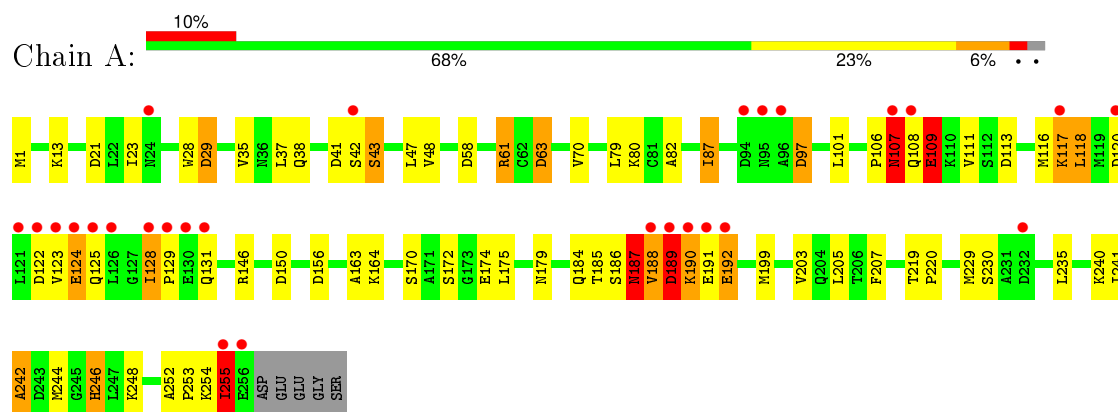
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	39	Total	O	0	0
			39	39		
2	B	44	Total	O	0	0
			44	44		
2	C	58	Total	O	0	0
			58	58		

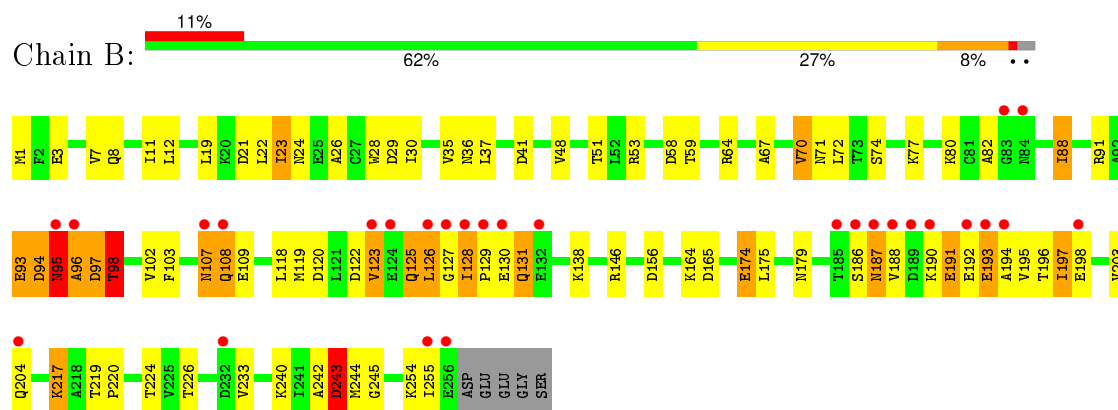
### 3 Residue-property plots

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.

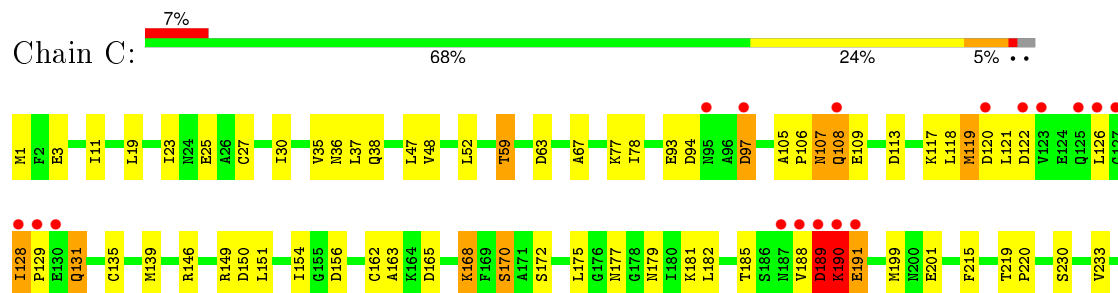
#### • Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN

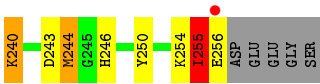


#### • Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN



#### • Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.65Å 83.27Å 71.63Å 90.00° 117.49° 90.00°	Depositor
Resolution (Å)	14.00 – 2.30 13.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (14.00-2.30) 99.4 (13.93-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.187 , 0.279 0.197 , 0.280	Depositor DCC
$R_{free}$ test set	1274 reflections (4.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.1	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 55.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 31413 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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 [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	A	0.57	0/1990	0.95	11/2689 (0.4%)
1	B	0.61	0/1990	1.00	10/2689 (0.4%)
1	C	0.67	0/1990	1.01	11/2689 (0.4%)
All	All	0.62	0/5970	0.99	32/8067 (0.4%)

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	A	0	3
1	B	0	2
All	All	0	5

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	ASP	CB-CG-OD2	8.27	125.74	118.30
1	B	243	ASP	CB-CG-OD2	7.22	124.80	118.30
1	C	150	ASP	CB-CG-OD2	7.20	124.78	118.30
1	C	156	ASP	CB-CG-OD2	6.93	124.53	118.30
1	B	156	ASP	CB-CG-OD2	6.72	124.34	118.30
1	C	97	ASP	CB-CG-OD2	6.54	124.18	118.30
1	A	41	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	63	ASP	CB-CG-OD2	6.42	124.07	118.30
1	A	29	ASP	CB-CG-OD2	6.39	124.05	118.30
1	B	97	ASP	CB-CG-OD2	6.36	124.02	118.30
1	B	120	ASP	CB-CG-OD2	6.29	123.96	118.30
1	C	94	ASP	CB-CG-OD2	6.05	123.75	118.30
1	C	139	MET	CG-SD-CE	-6.03	90.56	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	122	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	150	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	21	ASP	CB-CG-OD2	5.53	123.28	118.30
1	C	120	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	113	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	58	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	217	LYS	CG-CD-CE	5.39	128.07	111.90
1	B	217	LYS	CD-CE-NZ	5.36	124.03	111.70
1	B	122	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	189	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	189	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	165	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	97	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	156	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	122	ASP	CB-CG-OD2	5.06	122.86	118.30
1	C	243	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	70	VAL	CB-CA-C	-5.05	101.80	111.40
1	A	113	ASP	CB-CG-OD2	5.03	122.82	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ASN	Peptide
1	A	109	GLU	Peptide
1	A	192	GLU	Peptide
1	B	95	ASN	Mainchain
1	B	98	THR	Peptide

## 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	1964	0	1973	58	0
1	B	1964	0	1973	68	1
1	C	1964	0	1973	63	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	39	0	0	4	0
2	B	44	0	0	11	0
2	C	58	0	0	7	0
All	All	6033	0	5919	183	1

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 16.

All (183) 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:C:254:LYS:O	1:C:255:ILE:HB	1.28	1.09
1:C:128:ILE:HD13	1:C:129:PRO:HD2	1.36	1.07
1:B:187:ASN:ND2	1:B:188:VAL:HG23	1.75	0.99
1:A:37:LEU:HD23	1:A:38:GLN:N	1.80	0.96
1:A:187:ASN:HB3	1:A:190:LYS:NZ	1.81	0.95
1:B:187:ASN:HD22	1:B:188:VAL:HG23	1.28	0.94
1:A:188:VAL:O	1:A:189:ASP:HB2	1.70	0.92
1:C:128:ILE:CD1	1:C:129:PRO:HD2	2.00	0.92
1:A:254:LYS:O	1:A:255:ILE:O	1.88	0.91
1:C:254:LYS:O	1:C:255:ILE:CB	2.19	0.88
1:B:226:THR:HB	2:B:2039:HOH:O	1.72	0.88
1:A:37:LEU:C	1:A:37:LEU:HD23	1.95	0.87
1:A:107:ASN:O	1:A:109:GLU:HG3	1.73	0.87
1:C:185:THR:HB	1:C:188:VAL:HG22	1.62	0.82
1:B:29:ASP:OD1	1:B:123:VAL:HG22	1.79	0.82
1:C:189:ASP:OD2	1:C:189:ASP:O	1.99	0.81
1:B:29:ASP:OD1	1:B:123:VAL:CG2	2.30	0.79
1:A:174:GLU:HG2	2:A:2029:HOH:O	1.82	0.79
1:A:187:ASN:HB3	1:A:190:LYS:HZ1	1.52	0.74
1:C:117:LYS:HA	2:C:2030:HOH:O	1.86	0.74
1:C:52:LEU:HD22	1:C:244:MET:HE3	1.68	0.74
1:B:125:GLN:O	1:B:126:LEU:HB2	1.86	0.74
1:A:106:PRO:HA	2:A:2017:HOH:O	1.87	0.73
1:B:36:ASN:HB3	2:B:2008:HOH:O	1.87	0.72
1:C:128:ILE:CG1	1:C:129:PRO:HD2	2.19	0.72
1:A:117:LYS:O	1:A:118:LEU:HB2	1.88	0.72
1:C:25:GLU:HG2	1:C:119:MET:SD	2.31	0.70
1:C:106:PRO:HD2	2:C:2024:HOH:O	1.92	0.69
1:C:126:LEU:HG	1:C:128:ILE:H	1.57	0.69
1:B:97:ASP:OD2	1:B:98:THR:HG23	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:THR:HG22	2:C:2001:HOH:O	1.95	0.67
1:B:188:VAL:HG12	1:B:188:VAL:O	1.94	0.67
1:A:246:HIS:CE1	1:A:248:LYS:HE3	2.30	0.66
1:C:190:LYS:O	1:C:191:GLU:HB3	1.96	0.65
1:B:174:GLU:CD	1:B:174:GLU:H	1.99	0.65
1:A:123:VAL:HG13	1:A:124:GLU:N	2.11	0.65
1:B:226:THR:CB	2:B:2039:HOH:O	2.38	0.64
1:A:186:SER:O	1:A:188:VAL:HG23	1.96	0.64
1:C:255:ILE:HG23	1:C:256:GLU:N	2.12	0.64
1:A:187:ASN:HB3	1:A:190:LYS:HZ2	1.63	0.64
1:B:67:ALA:HB1	1:B:123:VAL:HG23	1.79	0.63
1:C:59:THR:CG2	2:C:2001:HOH:O	2.46	0.62
1:B:93:GLU:O	1:B:94:ASP:CB	2.47	0.62
1:C:154:ILE:HD13	1:C:175:LEU:HD11	1.82	0.62
1:C:107:ASN:HD22	1:C:107:ASN:C	2.04	0.62
1:B:59:THR:HG22	2:B:2001:HOH:O	1.99	0.61
1:B:23:ILE:HD11	1:B:26:ALA:HB2	1.82	0.61
1:A:1:MET:SD	1:A:61:ARG:NH1	2.73	0.61
1:A:117:LYS:O	1:A:118:LEU:CB	2.49	0.61
1:B:107:ASN:C	1:B:108:GLN:HG2	2.20	0.61
1:A:203:VAL:HG11	1:A:205:LEU:HD11	1.83	0.61
1:C:128:ILE:HD13	1:C:129:PRO:CD	2.20	0.60
1:C:255:ILE:CG2	1:C:256:GLU:N	2.64	0.59
1:B:94:ASP:O	1:B:95:ASN:HB2	2.02	0.59
1:B:242:ALA:O	1:B:244:MET:N	2.34	0.59
1:B:191:GLU:HG2	1:B:191:GLU:O	2.03	0.58
1:C:189:ASP:O	1:C:189:ASP:CG	2.42	0.58
1:B:21:ASP:OD2	1:B:217:LYS:CE	2.51	0.58
1:B:21:ASP:OD2	1:B:217:LYS:NZ	2.37	0.58
1:B:71:ASN:HB3	1:B:74:SER:OG	2.03	0.58
1:A:87:ILE:HD13	1:A:87:ILE:N	2.20	0.57
1:B:21:ASP:OD2	1:B:217:LYS:HE2	2.05	0.57
1:B:93:GLU:O	1:B:94:ASP:HB2	2.06	0.56
1:A:123:VAL:HG22	1:A:124:GLU:H	1.71	0.56
1:C:190:LYS:O	1:C:191:GLU:CB	2.54	0.55
1:B:77:LYS:O	1:B:80:LYS:HB2	2.06	0.55
1:B:97:ASP:HA	1:B:118:LEU:H	1.71	0.55
1:B:67:ALA:CB	1:B:123:VAL:HG23	2.35	0.55
1:A:175:LEU:CD1	1:C:78:ILE:HD11	2.37	0.54
1:A:175:LEU:HD13	1:C:78:ILE:HD11	1.90	0.54
1:C:240:LYS:NZ	2:C:2056:HOH:O	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ALA:HB1	1:C:106:PRO:CD	2.38	0.53
1:B:187:ASN:HD22	1:B:188:VAL:CG2	2.12	0.53
1:A:23:ILE:HD11	1:A:48:VAL:CG2	2.38	0.53
1:C:189:ASP:O	1:C:190:LYS:HB2	2.08	0.53
1:B:26:ALA:HB1	1:B:37:LEU:HD11	1.91	0.53
1:A:61:ARG:NE	1:A:63:ASP:OD1	2.42	0.53
1:C:27:CYS:SG	1:C:67:ALA:HB1	2.49	0.53
1:A:13:LYS:NZ	1:A:82:ALA:O	2.38	0.53
1:B:226:THR:CG2	2:B:2038:HOH:O	2.58	0.52
1:B:197:ILE:HD12	1:B:198:GLU:N	2.25	0.51
1:C:11:ILE:HG21	1:C:244:MET:HE2	1.92	0.51
1:C:185:THR:HB	1:C:188:VAL:CG2	2.38	0.51
1:C:154:ILE:HG21	1:C:177:ASN:HA	1.92	0.51
1:B:59:THR:CG2	2:B:2001:HOH:O	2.57	0.51
1:B:29:ASP:OD1	1:B:123:VAL:HG21	2.11	0.51
1:B:108:GLN:HA	2:B:2018:HOH:O	2.10	0.51
1:A:187:ASN:CB	1:A:190:LYS:HZ2	2.23	0.51
1:C:185:THR:CB	1:C:188:VAL:HG22	2.37	0.50
1:C:240:LYS:HE2	1:C:246:HIS:HB3	1.92	0.50
1:A:37:LEU:CD2	1:A:37:LEU:C	2.68	0.50
1:B:30:ILE:HD13	1:B:35:VAL:HG22	1.94	0.50
1:C:118:LEU:HD23	2:C:2028:HOH:O	2.12	0.50
1:B:123:VAL:HG12	1:B:123:VAL:O	2.13	0.49
1:A:185:THR:HG21	1:C:109:GLU:HG2	1.93	0.49
1:B:41:ASP:C	1:B:41:ASP:OD1	2.49	0.49
1:B:174:GLU:N	1:B:174:GLU:CD	2.65	0.49
1:C:219:THR:N	1:C:220:PRO:CD	2.74	0.49
1:B:226:THR:C	2:B:2039:HOH:O	2.51	0.49
1:B:88:ILE:HD13	1:B:103:PHE:CE1	2.48	0.48
1:A:87:ILE:N	1:A:87:ILE:CD1	2.76	0.48
1:B:82:ALA:HB2	1:B:103:PHE:CG	2.49	0.48
1:A:109:GLU:OE1	1:B:193:GLU:OE2	2.32	0.47
1:A:241:ILE:HG22	1:A:241:ILE:O	2.14	0.47
1:C:19:LEU:HD21	1:C:48:VAL:HG11	1.96	0.47
1:A:254:LYS:O	1:A:255:ILE:C	2.53	0.47
1:C:107:ASN:O	1:C:108:GLN:HG2	2.14	0.47
1:A:175:LEU:HD12	1:A:175:LEU:C	2.35	0.47
1:A:37:LEU:HD23	1:A:38:GLN:CA	2.45	0.46
1:A:255:ILE:HG22	1:A:255:ILE:O	2.16	0.46
1:C:185:THR:CB	1:C:188:VAL:CG2	2.94	0.46
1:C:25:GLU:OE2	1:C:119:MET:SD	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:THR:HB	1:C:220:PRO:HD3	1.98	0.46
1:B:82:ALA:HB2	1:B:103:PHE:CD2	2.51	0.46
1:A:101:LEU:HD12	1:A:101:LEU:N	2.30	0.46
1:B:8:GLN:HA	2:B:2002:HOH:O	2.16	0.46
1:A:205:LEU:HB2	1:A:207:PHE:CE2	2.50	0.46
1:B:226:THR:HG23	2:B:2038:HOH:O	2.17	0.45
1:B:11:ILE:HD13	1:B:244:MET:CE	2.46	0.45
1:A:246:HIS:CD2	1:A:246:HIS:C	2.90	0.45
1:B:125:GLN:O	1:B:126:LEU:CB	2.58	0.45
1:A:229:MET:HG3	1:A:235:LEU:HD13	1.98	0.45
1:C:37:LEU:HD23	1:C:38:GLN:N	2.32	0.45
1:B:53:ARG:NH1	1:B:243:ASP:O	2.49	0.45
1:B:11:ILE:HD13	1:B:244:MET:HE3	1.99	0.45
1:B:19:LEU:CD2	1:B:48:VAL:HG11	2.46	0.45
1:A:70:VAL:HG13	1:A:116:MET:CE	2.47	0.45
1:A:219:THR:HB	1:A:220:PRO:HD3	1.97	0.45
1:B:244:MET:N	2:B:2044:HOH:O	2.50	0.45
1:A:246:HIS:HD2	1:A:246:HIS:O	1.98	0.45
1:A:203:VAL:HG12	1:A:205:LEU:HG	1.98	0.45
1:C:37:LEU:HD23	1:C:37:LEU:C	2.38	0.45
1:A:241:ILE:O	1:A:242:ALA:C	2.55	0.44
1:C:215:PHE:N	1:C:215:PHE:CD1	2.83	0.44
1:C:19:LEU:CD2	1:C:48:VAL:HG11	2.48	0.44
1:C:135:CYS:SG	1:C:162:CYS:HB2	2.58	0.44
1:A:174:GLU:O	1:C:117:LYS:HD2	2.17	0.44
1:A:128:ILE:HG13	1:A:129:PRO:HD2	1.99	0.44
1:C:131:GLN:HE22	1:C:233:VAL:HG21	1.83	0.44
1:C:47:LEU:HB3	1:C:250:TYR:HB2	2.00	0.44
1:A:111:VAL:HG22	2:A:2018:HOH:O	2.16	0.44
1:C:107:ASN:ND2	1:C:109:GLU:H	2.15	0.44
1:A:203:VAL:CG1	1:A:205:LEU:HD11	2.46	0.44
1:C:105:ALA:HB1	1:C:106:PRO:HD2	2.01	0.43
1:A:123:VAL:HG13	1:A:124:GLU:H	1.79	0.43
1:A:61:ARG:NH2	1:A:63:ASP:OD2	2.51	0.43
1:B:219:THR:HB	1:B:220:PRO:HD3	2.01	0.43
1:B:3:GLU:OE2	1:B:91:ARG:NH1	2.51	0.43
1:A:187:ASN:CG	1:A:190:LYS:HZ2	2.20	0.43
1:C:25:GLU:CG	1:C:119:MET:SD	3.04	0.43
1:A:185:THR:CG2	1:C:109:GLU:HG2	2.48	0.43
1:B:88:ILE:HD13	1:B:103:PHE:CD1	2.53	0.43
1:A:255:ILE:CG2	1:A:255:ILE:O	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ALA:HA	1:A:199:MET:HE2	2.00	0.43
1:B:51:THR:O	1:B:245:GLY:HA3	2.18	0.43
1:A:97:ASP:O	1:A:117:LYS:O	2.37	0.43
1:A:252:ALA:HA	1:A:253:PRO:HD3	1.92	0.42
1:B:95:ASN:O	1:B:96:ALA:C	2.57	0.42
1:B:128:ILE:HA	1:B:129:PRO:HD3	1.80	0.42
1:B:23:ILE:HG13	1:B:24:ASN:N	2.35	0.42
1:A:28:TRP:CZ3	1:A:35:VAL:HG11	2.55	0.42
1:B:12:LEU:HA	1:B:12:LEU:HD12	1.84	0.42
1:C:126:LEU:HG	1:C:128:ILE:N	2.30	0.42
1:C:11:ILE:HG21	1:C:244:MET:CE	2.49	0.42
1:B:127:GLY:O	1:B:128:ILE:C	2.58	0.42
1:C:30:ILE:HD13	1:C:35:VAL:HG13	2.02	0.42
1:C:1:MET:SD	1:C:3:GLU:HB2	2.60	0.42
1:B:23:ILE:HG12	1:B:72:LEU:HD12	2.02	0.41
1:B:88:ILE:HA	1:B:102:VAL:O	2.19	0.41
1:B:130:GLU:C	1:B:131:GLN:HG2	2.41	0.41
1:C:168:LYS:CE	1:C:170:SER:OG	2.69	0.41
1:C:128:ILE:HG12	1:C:129:PRO:HD2	1.98	0.41
1:C:52:LEU:HD22	1:C:244:MET:CE	2.45	0.41
1:A:106:PRO:CA	2:A:2017:HOH:O	2.60	0.41
1:B:93:GLU:O	1:B:94:ASP:OD2	2.39	0.41
1:C:151:LEU:HA	1:C:151:LEU:HD23	1.93	0.41
1:B:194:ALA:O	1:B:196:THR:CG2	2.68	0.41
1:B:28:TRP:CD1	1:B:70:VAL:HG23	2.56	0.41
1:C:131:GLN:HE22	1:C:233:VAL:HG11	1.85	0.40
1:A:37:LEU:CD2	1:A:38:GLN:N	2.67	0.40
1:B:53:ARG:NH2	1:B:243:ASP:O	2.54	0.40
1:C:163:ALA:HB3	2:C:2039:HOH:O	2.22	0.40
1:B:93:GLU:O	1:B:94:ASP:CG	2.59	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLN:NE2	1:C:93:GLU:OE1[1_545]	1.89	0.31

## 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	254/261 (97%)	223 (88%)	20 (8%)	11 (4%)	3	1
1	B	254/261 (97%)	229 (90%)	17 (7%)	8 (3%)	5	3
1	C	254/261 (97%)	238 (94%)	13 (5%)	3 (1%)	16	16
All	All	762/783 (97%)	690 (91%)	50 (7%)	22 (3%)	6	3

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	A	108	GLN
1	A	187	ASN
1	A	188	VAL
1	A	189	ASP
1	A	255	ILE
1	B	94	ASP
1	B	95	ASN
1	B	98	THR
1	B	243	ASP
1	C	190	LYS
1	C	255	ILE
1	A	118	LEU
1	B	126	LEU
1	B	186	SER
1	B	195	VAL
1	C	191	GLU
1	A	128	ILE
1	A	242	ALA
1	A	125	GLN
1	B	96	ALA
1	A	117	LYS

### 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	223/228 (98%)	195 (87%)	28 (13%)	5	5
1	B	223/228 (98%)	189 (85%)	34 (15%)	3	3
1	C	223/228 (98%)	195 (87%)	28 (13%)	5	5
All	All	669/684 (98%)	579 (86%)	90 (14%)	5	4

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	42	SER
1	A	43	SER
1	A	47	LEU
1	A	58	ASP
1	A	61	ARG
1	A	79	LEU
1	A	80	LYS
1	A	87	ILE
1	A	107	ASN
1	A	109	GLU
1	A	124	GLU
1	A	131	GLN
1	A	146	ARG
1	A	164	LYS
1	A	170	SER
1	A	172	SER
1	A	179	ASN
1	A	184	GLN
1	A	187	ASN
1	A	190	LYS
1	A	191	GLU
1	A	192	GLU
1	A	230	SER
1	A	240	LYS
1	A	244	MET

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Mol	Chain	Res	Type
1	A	246	HIS
1	A	255	ILE
1	B	1	MET
1	B	7	VAL
1	B	22	LEU
1	B	23	ILE
1	B	64	ARG
1	B	88	ILE
1	B	93	GLU
1	B	107	ASN
1	B	108	GLN
1	B	109	GLU
1	B	119	MET
1	B	123	VAL
1	B	125	GLN
1	B	128	ILE
1	B	131	GLN
1	B	138	LYS
1	B	146	ARG
1	B	164	LYS
1	B	174	GLU
1	B	175	LEU
1	B	179	ASN
1	B	187	ASN
1	B	190	LYS
1	B	191	GLU
1	B	192	GLU
1	B	193	GLU
1	B	197	ILE
1	B	203	VAL
1	B	204	GLN
1	B	224	THR
1	B	233	VAL
1	B	240	LYS
1	B	254	LYS
1	B	255	ILE
1	C	23	ILE
1	C	36	ASN
1	C	59	THR
1	C	77	LYS
1	C	97	ASP
1	C	107	ASN

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Mol	Chain	Res	Type
1	C	108	GLN
1	C	119	MET
1	C	121	LEU
1	C	128	ILE
1	C	131	GLN
1	C	146	ARG
1	C	149	ARG
1	C	165	ASP
1	C	168	LYS
1	C	170	SER
1	C	172	SER
1	C	179	ASN
1	C	181	LYS
1	C	182	LEU
1	C	189	ASP
1	C	190	LYS
1	C	199	MET
1	C	201	GLU
1	C	230	SER
1	C	240	LYS
1	C	244	MET
1	C	255	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	246	HIS
1	B	65	ASN
1	B	108	GLN
1	B	187	ASN
1	C	49	GLN
1	C	107	ASN
1	C	108	GLN
1	C	131	GLN

### 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 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 [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, 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	256/261 (98%)	0.44	27 (10%)	8 12	20, 46, 110, 134	0
1	B	256/261 (98%)	0.43	28 (10%)	7 11	20, 44, 114, 137	0
1	C	256/261 (98%)	0.25	18 (7%)	19 27	20, 40, 93, 120	0
All	All	768/783 (98%)	0.37	73 (9%)	10 15	20, 44, 108, 137	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	ILE	8.7
1	C	123	VAL	8.1
1	A	121	LEU	8.0
1	B	188	VAL	7.3
1	B	95	ASN	7.2
1	B	123	VAL	7.1
1	B	256	GLU	6.6
1	C	190	LYS	6.6
1	A	256	GLU	6.5
1	B	255	ILE	6.2
1	B	129	PRO	6.1
1	C	189	ASP	6.1
1	A	120	ASP	6.0
1	B	190	LYS	5.6
1	A	96	ALA	5.4
1	C	122	ASP	5.4
1	A	189	ASP	5.2
1	B	186	SER	5.2
1	A	123	VAL	5.0
1	A	125	GLN	5.0
1	C	127	GLY	4.7
1	B	130	GLU	4.6
1	A	188	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	129	PRO	4.5
1	A	107	ASN	4.5
1	A	128	ILE	4.4
1	A	126	LEU	4.3
1	C	256	GLU	4.2
1	C	129	PRO	4.2
1	B	189	ASP	4.2
1	B	187	ASN	4.0
1	A	190	LYS	4.0
1	B	128	ILE	4.0
1	C	130	GLU	3.9
1	A	124	GLU	3.9
1	C	125	GLN	3.8
1	A	108	GLN	3.8
1	C	120	ASP	3.8
1	A	232	ASP	3.6
1	C	188	VAL	3.6
1	B	127	GLY	3.6
1	A	122	ASP	3.5
1	A	95	ASN	3.5
1	B	194	ALA	3.5
1	B	107	ASN	3.4
1	A	191	GLU	3.4
1	C	126	LEU	3.4
1	B	96	ALA	3.2
1	A	130	GLU	3.2
1	A	117	LYS	3.2
1	B	132	GLU	3.1
1	B	84	ASN	2.9
1	A	94	ASP	2.9
1	C	108	GLN	2.8
1	C	191	GLU	2.8
1	B	126	LEU	2.7
1	A	42	SER	2.7
1	B	193	GLU	2.7
1	B	192	GLU	2.6
1	C	95	ASN	2.6
1	B	185	THR	2.5
1	B	124	GLU	2.5
1	C	187	ASN	2.5
1	A	192	GLU	2.5
1	A	131	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	198	GLU	2.3
1	C	128	ILE	2.3
1	A	24	ASN	2.2
1	B	83	GLY	2.2
1	B	204	GLN	2.2
1	B	232	ASP	2.1
1	B	108	GLN	2.0
1	C	97	ASP	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.