



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:31 AM UTC

PDB ID : 1VYM / pdb_00001vym
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

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

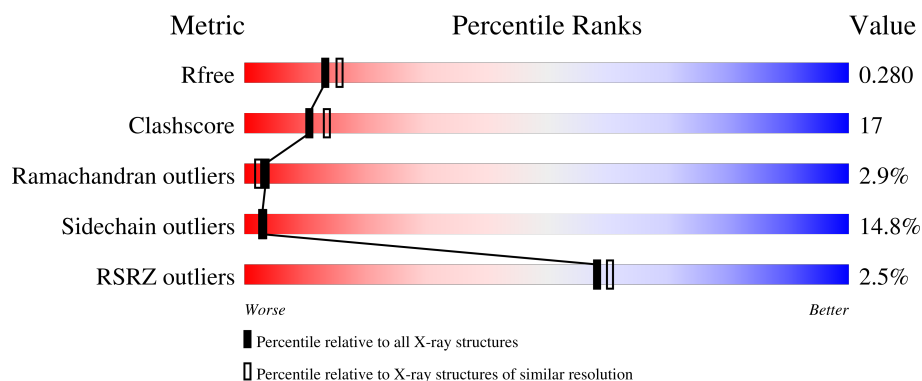
1 Overall quality at a glance

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	3% 68% 23% 5% ..
1	B	261	3% 62% 26% 8% ..
1	C	261	% 69% 22% 6% ..

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			

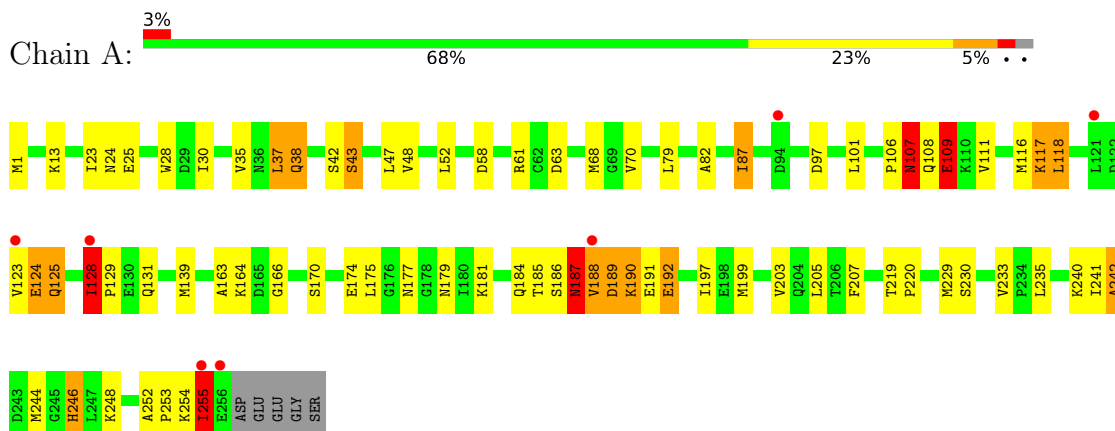
- Molecule 2 is water.

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		

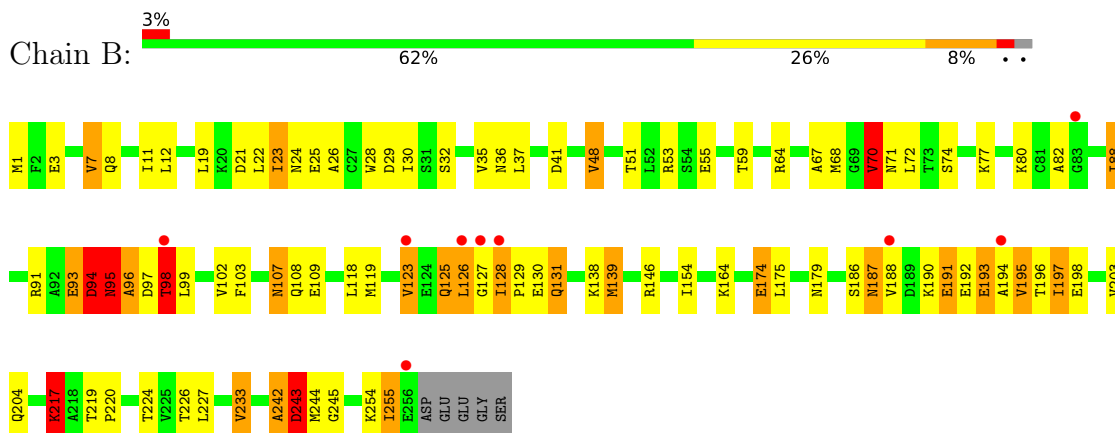
3 Residue-property plots [i](#)

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.

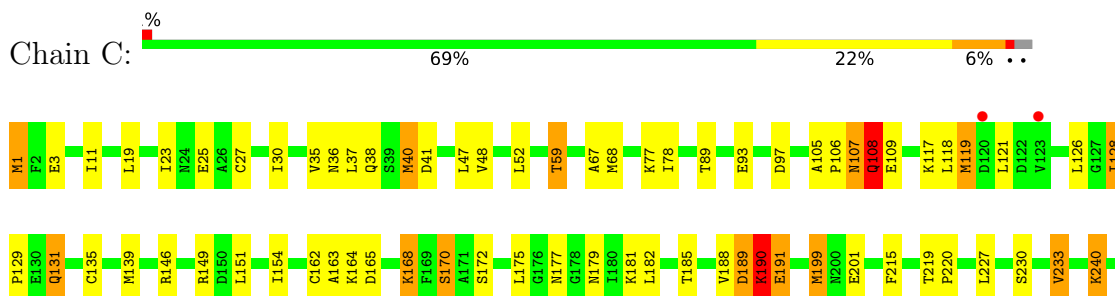
• Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN

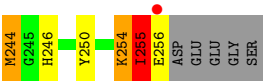


• Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN



• Molecule 1: PROLIFERATING CELL NUCLEAR ANTIGEN





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.65Å 83.27Å 71.63Å 90.00° 117.49° 90.00°	Depositor
Resolution (Å)	14.00 – 2.30 14.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (14.00-2.30) 98.9 (14.00-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.06%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6033	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	0.76	2/1990 (0.1%)	1.08	3/2689 (0.1%)
1	B	0.82	2/1990 (0.1%)	1.18	10/2689 (0.4%)
1	C	0.89	3/1990 (0.2%)	1.17	2/2689 (0.1%)
All	All	0.83	7/5970 (0.1%)	1.14	15/8067 (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	A	0	3
1	B	0	2
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	139	MET	SD-CE	-7.84	1.59	1.79
1	B	139	MET	SD-CE	-7.80	1.60	1.79
1	A	139	MET	SD-CE	-7.68	1.60	1.79
1	C	255	ILE	C-N	-7.54	1.22	1.33
1	A	255	ILE	C-N	-7.52	1.22	1.33
1	B	255	ILE	C-N	-7.52	1.22	1.33
1	C	68	MET	SD-CE	-5.38	1.66	1.79

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	LYS	CG-CD-CE	7.29	128.07	111.30
1	A	166	GLY	N-CA-C	6.67	118.89	110.96
1	B	94	ASP	CA-CB-CG	6.49	119.09	112.60
1	C	108	GLN	N-CA-C	6.18	120.61	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	ILE	CB-CA-C	-5.77	104.92	111.55
1	C	89	THR	N-CA-C	5.62	117.90	108.73
1	B	243	ASP	N-CA-C	5.56	122.64	110.80
1	B	70	VAL	CB-CA-C	-5.55	101.80	110.69
1	B	32	SER	N-CA-C	-5.48	106.44	113.23
1	B	48	VAL	CB-CA-C	-5.45	102.42	110.82
1	B	7	VAL	CB-CA-C	-5.37	105.17	111.94
1	A	38	GLN	N-CA-C	5.30	116.84	107.61
1	B	242	ALA	N-CA-C	5.23	117.56	111.02
1	B	233	VAL	N-CA-C	5.16	113.56	107.84
1	A	177	ASN	N-CA-C	5.09	117.15	109.41

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	62	0
1	B	1964	0	1973	75	1
1	C	1964	0	1973	65	1
2	A	39	0	0	4	0
2	B	44	0	0	12	0
2	C	58	0	0	6	0
All	All	6033	0	5919	196	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 17.

All (196) 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:37:LEU:HD23	1:A:37:LEU:C	1.95	0.92
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: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:C:117:LYS:HA	2:C:2030:HOH:O	1.86	0.74
1:B:125:GLN:O	1:B:126:LEU:HB2	1.86	0.74
1:A:187:ASN:HB3	1:A:190:LYS:HZ2	1.53	0.73
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:B:174:GLU:H	1:B:174:GLU:CD	1.99	0.70
1:C:106:PRO:HD2	2:C:2024:HOH:O	1.92	0.69
1:B:97:ASP:OD2	1:B:98:THR:HG23	1.93	0.69
1:C:126:LEU:HG	1:C:128:ILE:H	1.57	0.69
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:C:107:ASN:C	1:C:107:ASN:HD22	2.04	0.66
1:A:246:HIS:CE1	1:A:248:LYS:HE3	2.30	0.66
1:C:11:ILE:HG21	1:C:244:MET:HE2	1.77	0.66
1:C:190:LYS:O	1:C:191:GLU:HB3	1.96	0.65
1:B:107:ASN:C	1:B:108:GLN:HG2	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ALA:HB1	1:B:123:VAL:HG23	1.79	0.63
1:C:189:ASP:O	1:C:189:ASP:CG	2.42	0.63
1:A:187:ASN:CB	1:A:190:LYS:HZ2	2.13	0.62
1:A:187:ASN:HB3	1:A:190:LYS:HZ1	1.62	0.62
1:B:93:GLU:O	1:B:94:ASP:CB	2.47	0.62
1:C:59:THR:CG2	2:C:2001:HOH:O	2.46	0.62
1:C:154:ILE:HD13	1:C:175:LEU:HD11	1.82	0.62
1:B:59:THR:HG22	2:B:2001:HOH:O	1.99	0.61
1:A:1:MET:SD	1:A:61:ARG:NH1	2.73	0.61
1:B:23:ILE:HD11	1:B:26:ALA:HB2	1.82	0.61
1:A:117:LYS:O	1:A:118:LEU:CB	2.49	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:O	1:B:191:GLU:HG2	2.03	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:A:187:ASN:CG	1:A:190:LYS:HZ2	2.12	0.56
1:B:93:GLU:O	1:B:94:ASP:HB2	2.06	0.56
1:A:13:LYS:NZ	1:A:82:ALA:O	2.38	0.56
1:A:123:VAL:HG22	1:A:124:GLU:H	1.71	0.56
1:B:77:LYS:O	1:B:80:LYS:HB2	2.06	0.55
1:C:190:LYS:O	1:C:191:GLU:CB	2.54	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:A:37:LEU:C	1:A:37:LEU:CD2	2.68	0.54
1:A:163:ALA:HA	1:A:199:MET:HE2	1.90	0.54
1:B:41:ASP:OD1	1:B:41:ASP:C	2.49	0.53
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:B:226:THR:C	2:B:2039:HOH:O	2.51	0.53
1:A:23:ILE:HD11	1:A:48:VAL:CG2	2.38	0.53
1:B:174:GLU:CD	1:B:174:GLU:N	2.65	0.53
1:C:189:ASP:O	1:C:190:LYS:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:52:LEU:HD22	1:C:244:MET:HE3	1.92	0.52
1:A:254:LYS:O	1:A:255:ILE:C	2.53	0.52
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:A:175:LEU:C	1:A:175:LEU:HD12	2.35	0.51
1:C:154:ILE:HG21	1:C:177:ASN:HA	1.92	0.51
1:C:185:THR:HB	1:C:188:VAL:CG2	2.38	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: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:246:HIS:C	1:A:246:HIS:CD2	2.90	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:C:37:LEU:C	1:C:37:LEU:HD23	2.38	0.49
1:A:185:THR:HG21	1:C:109:GLU:HG2	1.93	0.49
1:A:241:ILE:O	1:A:242:ALA:C	2.55	0.49
1:C:219:THR:N	1:C:220:PRO:CD	2.74	0.49
1:A:30:ILE:CG1	1:A:68:MET:HE2	2.43	0.48
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:30:ILE:HG13	1:A:68:MET:HE2	1.95	0.47
1:A:241:ILE:O	1:A:241:ILE:HG22	2.14	0.47
1:B:95:ASN:O	1:B:96:ALA:C	2.57	0.47
1:C:19:LEU:HD21	1:C:48:VAL:HG11	1.96	0.47
1:C:52:LEU:HD22	1:C:244:MET:CE	2.45	0.47
1:C:107:ASN:O	1:C:108:GLN:HG2	2.14	0.47
1:B:127:GLY:O	1:B:128:ILE:C	2.58	0.47
1:B:11:ILE:HD13	1:B:244:MET:HE1	1.97	0.46
1:B:130:GLU:C	1:B:131:GLN:HG2	2.41	0.46
1:A:37:LEU:HD23	1:A:38:GLN:CA	2.45	0.46
1:C:185:THR:CB	1:C:188:VAL:CG2	2.94	0.46
1:A:52:LEU:HD22	1:A:244:MET:HE3	1.97	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:A:255:ILE:O	1:A:255:ILE:HG22	2.16	0.46
1:B:139:MET:HE3	1:B:227:LEU:HD11	1.97	0.46
1:B:11:ILE:HD13	1:B:244:MET:CE	2.46	0.45
1:B:226:THR:HG23	2:B:2038:HOH:O	2.17	0.45
1:A:229:MET:HG3	1:A:235:LEU:HD13	1.98	0.45
1:B:125:GLN:O	1:B:126:LEU:CB	2.58	0.45
1:B:53:ARG:NH1	1:B:243:ASP:O	2.49	0.45
1:B:93:GLU:O	1:B:94:ASP:CG	2.59	0.45
1:C:37:LEU:HD23	1:C:38:GLN:N	2.32	0.45
1:A:70:VAL:HG13	1:A:116:MET:CE	2.47	0.45
1:B:19:LEU:CD2	1:B:48:VAL:HG11	2.46	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:203:VAL:HG12	1:A:205:LEU:HG	1.98	0.45
1:A:246:HIS:HD2	1:A:246:HIS:O	1.98	0.45
1:B:244:MET:HE2	2:B:2013:HOH:O	2.16	0.45
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:128:ILE:HG13	1:A:129:PRO:HD2	1.99	0.44
1:A:174:GLU:O	1:C:117:LYS:HD2	2.17	0.44
1:C:131:GLN:HE22	1:C:233:VAL:HG21	1.83	0.44
1:A:111:VAL:HG22	2:A:2018:HOH:O	2.16	0.44
1:B:68:MET:HE1	1:B:99:LEU:HD13	1.99	0.44
1:C:47:LEU:HB3	1:C:250:TYR:HB2	2.00	0.44
1:A:203:VAL:CG1	1:A:205:LEU:HD11	2.46	0.44
1:C:107:ASN:ND2	1:C:109:GLU:H	2.15	0.44
1:C:164:LYS:HG2	1:C:199:MET:HE2	1.98	0.44
1:A:61:ARG:NH2	1:A:63:ASP:OD2	2.51	0.43
1:A:123:VAL:HG13	1:A:124:GLU:H	1.79	0.43
1:B:3:GLU:OE2	1:B:91:ARG:NH1	2.51	0.43
1:B:219:THR:HB	1:B:220:PRO:HD3	2.01	0.43
1:C:105:ALA:HB1	1:C:106:PRO:HD2	2.01	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:C:25:GLU:CG	1:C:119:MET:SD	3.04	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:O	1:A:255:ILE:CG2	2.65	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:C:41:ASP:OD1	1:C:41:ASP:C	2.61	0.42
1:C:25:GLU:CD	1:C:119:MET:SD	3.02	0.42
1:B:128:ILE:HA	1:B:129:PRO:HD3	1.80	0.42
1:A:28:TRP:CZ3	1:A:35:VAL:HG11	2.55	0.42
1:B:12:LEU:HD12	1:B:12:LEU:HA	1.84	0.42
1:B:23:ILE:HG13	1:B:24:ASN:N	2.35	0.42
1:A:70:VAL:HG13	1:A:116:MET:HE2	2.01	0.42
1:B:242:ALA:C	1:B:244:MET:H	2.25	0.42
1:C:30:ILE:HD13	1:C:35:VAL:HG13	2.02	0.42
1:C:126:LEU:HG	1:C:128:ILE:N	2.30	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:97:ASP:O	1:B:98:THR:C	2.61	0.41
1:B:11:ILE:CD1	1:B:244:MET:HE1	2.50	0.41
1:C:40:MET:HE3	1:C:47:LEU:HD13	2.02	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:B:194:ALA:O	1:B:195:VAL:C	2.64	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:B:194:ALA:O	1:B:196:THR:CG2	2.68	0.41
1:C:151:LEU:HD23	1:C:151:LEU:HA	1.93	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

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%)	2	1
1	B	254/261 (97%)	229 (90%)	17 (7%)	8 (3%)	3	2
1	C	254/261 (97%)	238 (94%)	13 (5%)	3 (1%)	10	12
All	All	762/783 (97%)	690 (91%)	50 (7%)	22 (3%)	3	2

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%)	193 (86%)	30 (14%)	4	4
1	B	223/228 (98%)	187 (84%)	36 (16%)	2	2
1	C	223/228 (98%)	190 (85%)	33 (15%)	3	3
All	All	669/684 (98%)	570 (85%)	99 (15%)	3	3

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	25	GLU
1	A	37	LEU
1	A	42	SER
1	A	43	SER
1	A	47	LEU
1	A	58	ASP
1	A	79	LEU
1	A	87	ILE
1	A	107	ASN
1	A	109	GLU
1	A	124	GLU
1	A	125	GLN
1	A	128	ILE
1	A	131	GLN
1	A	164	LYS
1	A	170	SER
1	A	179	ASN
1	A	181	LYS
1	A	184	GLN
1	A	187	ASN
1	A	190	LYS
1	A	191	GLU
1	A	192	GLU
1	A	197	ILE
1	A	230	SER

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Mol	Chain	Res	Type
1	A	233	VAL
1	A	240	LYS
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	25	GLU
1	B	55	GLU
1	B	64	ARG
1	B	70	VAL
1	B	88	ILE
1	B	93	GLU
1	B	107	ASN
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	217	LYS
1	B	224	THR
1	B	233	VAL
1	B	254	LYS
1	B	255	ILE
1	C	1	MET
1	C	23	ILE

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Mol	Chain	Res	Type
1	C	36	ASN
1	C	40	MET
1	C	59	THR
1	C	77	LYS
1	C	97	ASP
1	C	107	ASN
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	227	LEU
1	C	230	SER
1	C	233	VAL
1	C	240	LYS
1	C	244	MET
1	C	254	LYS
1	C	255	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	204	GLN
1	A	246	HIS
1	B	84	ASN
1	B	108	GLN
1	B	125	GLN
1	B	177	ASN

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Mol	Chain	Res	Type
1	B	187	ASN
1	C	36	ASN
1	C	49	GLN
1	C	65	ASN
1	C	84	ASN
1	C	107	ASN
1	C	108	GLN
1	C	131	GLN
1	C	177	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 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	256/261 (98%)	-0.12	7 (2%) 56 58	20, 46, 110, 134	0
1	B	256/261 (98%)	-0.10	9 (3%) 47 49	20, 44, 114, 137	0
1	C	256/261 (98%)	-0.22	3 (1%) 76 77	20, 40, 93, 120	0
All	All	768/783 (98%)	-0.15	19 (2%) 58 60	20, 44, 108, 137	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	ILE	6.0
1	B	256	GLU	5.9
1	A	256	GLU	4.7
1	C	256	GLU	4.4
1	B	123	VAL	4.1
1	A	121	LEU	2.9
1	C	123	VAL	2.7
1	A	128	ILE	2.6
1	B	127	GLY	2.5
1	A	188	VAL	2.3
1	B	126	LEU	2.3
1	B	98	THR	2.3
1	B	194	ALA	2.2
1	B	188	VAL	2.2
1	B	128	ILE	2.1
1	A	94	ASP	2.1
1	B	83	GLY	2.1
1	C	120	ASP	2.1
1	A	123	VAL	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 oligosaccharides 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.