



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:23 AM UTC

PDB ID : 1UD9 / pdb_00001ud9
Title : Crystal Structure of Proliferating Cell Nuclear Antigen (PCNA) Homolog From *Sulfolobus tokodaii*
Authors : Tanabe, E.; Yasutake, Y.; Tanaka, Y.; Yao, M.; Tsumoto, K.; Kumagai, I.; Tanaka, I.
Deposited on : 2003-04-28
Resolution : 1.68 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

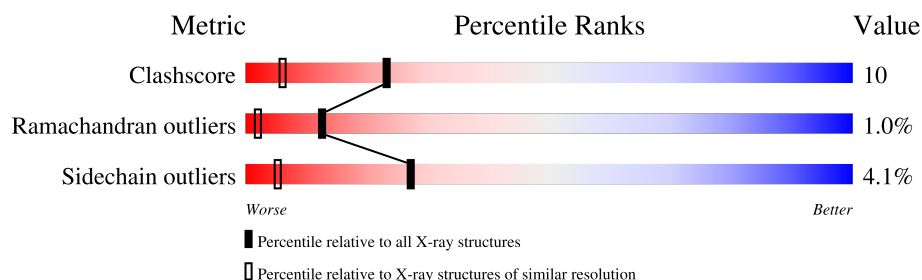
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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))
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	245	
1	B	245	
1	C	245	
1	D	245	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7996 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 DNA polymerase sliding clamp A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1894	1219	297	374	4			
1	B	238	Total	C	N	O	S	0	0	0
			1863	1198	293	368	4			
1	C	239	Total	C	N	O	S	0	0	0
			1871	1204	294	369	4			
1	D	241	Total	C	N	O	S	0	0	0
			1886	1213	297	372	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	SEE REMARK 999	UNP Q975N2
B	1	ALA	-	SEE REMARK 999	UNP Q975N2
C	1	ALA	-	SEE REMARK 999	UNP Q975N2
D	1	ALA	-	SEE REMARK 999	UNP Q975N2

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	Zn	0	0
			8	8		
2	B	4	Total	Zn	0	0
			4	4		
2	C	5	Total	Zn	0	0
			5	5		
2	D	6	Total	Zn	0	0
			6	6		

- Molecule 3 is water.

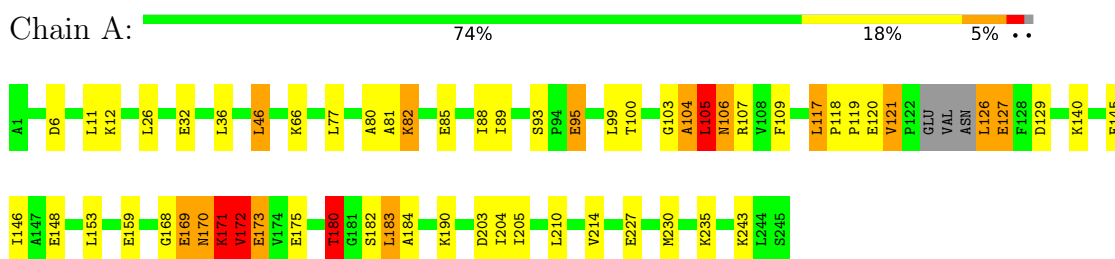
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total 83	O 83	0	0
3	B	120	Total 120	O 120	0	0
3	C	129	Total 129	O 129	0	0
3	D	127	Total 127	O 127	0	0

3 Residue-property plots

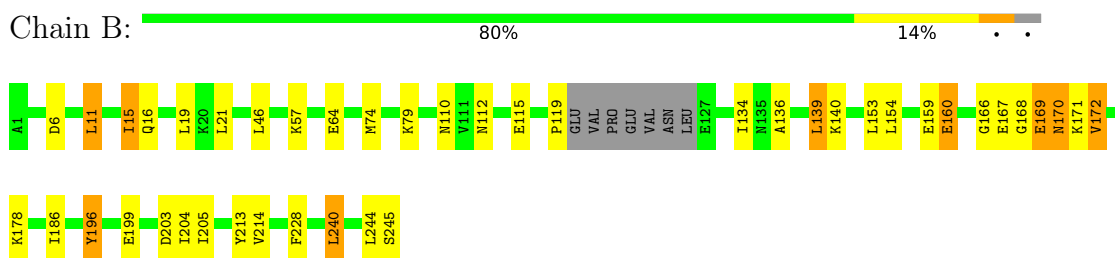
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

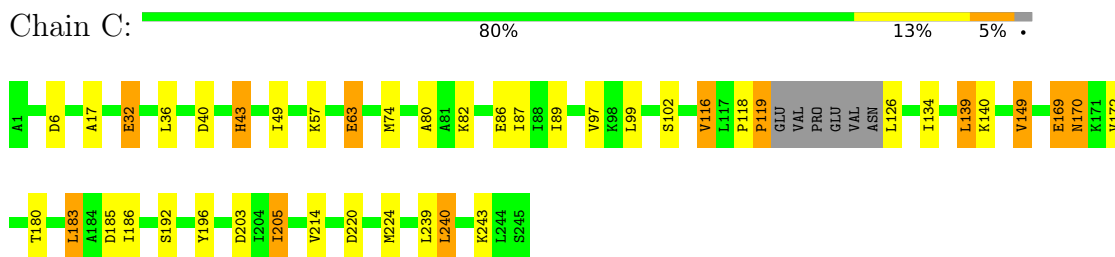
• Molecule 1: DNA polymerase sliding clamp A



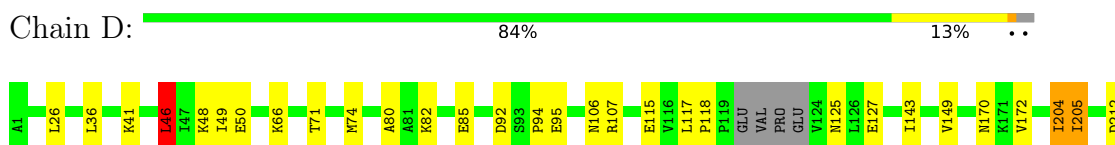
• Molecule 1: DNA polymerase sliding clamp A



• Molecule 1: DNA polymerase sliding clamp A



• Molecule 1: DNA polymerase sliding clamp A



E231	L239	P242	K243	L244	S245
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.40Å 75.44Å 88.14Å 90.00° 98.83° 90.00°	Depositor
Resolution (Å)	10.00 – 1.68	Depositor
% Data completeness (in resolution range)	97.8 (10.00-1.68)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.202 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7996	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	1.05	1/1921 (0.1%)	1.28	16/2591 (0.6%)
1	B	1.23	2/1889 (0.1%)	1.27	6/2546 (0.2%)
1	C	1.34	7/1897 (0.4%)	1.27	6/2557 (0.2%)
1	D	1.17	1/1912 (0.1%)	1.21	6/2578 (0.2%)
All	All	1.20	11/7619 (0.1%)	1.26	34/10272 (0.3%)

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	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	43	HIS	CA-CB	17.55	1.79	1.53
1	C	43	HIS	CA-C	10.77	1.66	1.53
1	C	43	HIS	CB-CG	8.59	1.62	1.50
1	C	43	HIS	ND1-CE1	6.79	1.39	1.32
1	C	17	ALA	CA-CB	6.75	1.64	1.53
1	B	74	MET	SD-CE	6.34	1.95	1.79
1	D	204	ILE	CA-CB	6.10	1.62	1.54
1	B	15	ILE	CA-CB	6.06	1.62	1.54
1	C	87	ILE	C-O	5.41	1.29	1.24
1	C	224	MET	SD-CE	-5.19	1.66	1.79
1	A	184	ALA	CA-CB	-5.06	1.45	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	HIS	CB-CA-C	9.99	125.91	111.73
1	A	121	VAL	N-CA-C	9.00	117.77	108.95
1	A	95	GLU	N-CA-C	8.73	122.92	111.75
1	A	82	LYS	N-CA-C	7.69	119.67	111.28
1	C	149	VAL	N-CA-C	7.02	119.91	113.10
1	A	180	THR	N-CA-C	-7.01	103.05	112.94
1	A	106	ASN	N-CA-C	6.89	125.47	110.80
1	A	117	LEU	CA-C-N	6.46	127.03	120.38
1	A	117	LEU	C-N-CA	6.46	127.03	120.38
1	C	43	HIS	N-CA-C	-6.44	103.04	111.74
1	A	105	LEU	N-CA-C	6.34	124.31	110.80
1	D	71	THR	N-CA-C	6.10	117.93	111.28
1	A	6	ASP	N-CA-C	5.95	120.15	113.01
1	A	129	ASP	N-CA-C	-5.93	105.13	112.90
1	C	149	VAL	CB-CA-C	-5.76	104.59	110.93
1	B	6	ASP	N-CA-C	5.67	120.04	113.18
1	A	171	LYS	N-CA-C	5.66	118.33	108.76
1	D	95	GLU	N-CA-C	5.66	118.22	111.71
1	A	173	GLU	N-CA-C	5.55	122.62	110.80
1	D	94	PRO	N-CA-C	5.48	121.04	113.65
1	A	93	SER	CA-C-N	5.45	124.90	119.24
1	A	93	SER	C-N-CA	5.45	124.90	119.24
1	B	112	ASN	CB-CA-C	5.43	118.70	109.84
1	D	46	LEU	CA-CB-CG	5.34	134.98	116.30
1	B	166	GLY	N-CA-C	-5.28	103.35	111.64
1	B	110	ASN	CA-C-N	-5.28	116.08	123.10
1	B	110	ASN	C-N-CA	-5.28	116.08	123.10
1	A	127	GLU	N-CA-C	-5.23	102.74	110.48
1	A	243	LYS	N-CA-C	-5.18	103.08	110.59
1	C	6	ASP	N-CA-C	5.11	119.36	113.18
1	D	149	VAL	N-CA-C	5.09	117.79	112.90
1	C	43	HIS	ND1-CE1-NE2	-5.04	103.36	108.40
1	B	199	GLU	CB-CA-C	-5.04	102.43	110.79
1	D	243	LYS	N-CA-C	-5.02	103.32	110.59

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	196	TYR	Sidechain
1	B	213	TYR	Sidechain

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	1894	0	1937	53	0
1	B	1863	0	1904	33	0
1	C	1871	0	1915	48	0
1	D	1886	0	1930	23	0
2	A	8	0	0	0	0
2	B	4	0	0	0	0
2	C	5	0	0	0	0
2	D	6	0	0	0	0
3	A	83	0	0	3	1
3	B	120	0	0	5	0
3	C	129	0	0	4	0
3	D	127	0	0	4	1
All	All	7996	0	7686	156	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 10.

All (156) 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:43:HIS:CA	1:C:43:HIS:CB	1.79	1.59
1:A:171:LYS:HD3	1:A:171:LYS:H	1.17	1.07
1:C:170:ASN:HD22	1:C:172:VAL:HG23	1.22	1.01
1:B:140:LYS:HA	1:B:205:ILE:HD11	1.47	0.95
1:A:227:GLU:HG3	1:A:235:LYS:HE3	1.52	0.91
1:A:171:LYS:HD3	1:A:171:LYS:N	1.82	0.91
1:A:26:LEU:HD11	1:A:66:LYS:HB3	1.58	0.86
1:C:118:PRO:HB2	1:C:119:PRO:HD2	1.55	0.86
1:B:136:ALA:HB2	1:B:214:VAL:HG23	1.59	0.84
1:C:140:LYS:HG3	1:C:205:ILE:CD1	2.08	0.84
1:A:85:GLU:OE2	1:A:103:GLY:HA3	1.78	0.83
1:A:26:LEU:CD2	1:A:118:PRO:HG3	2.12	0.78
1:A:175:GLU:O	1:A:180:THR:HG21	1.84	0.77
1:B:171:LYS:O	1:B:172:VAL:HG12	1.84	0.77
1:A:227:GLU:CG	1:A:235:LYS:HE3	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:HIS:CB	1:C:43:HIS:HA	2.11	0.75
1:C:170:ASN:HD22	1:C:172:VAL:CG2	1.97	0.75
1:A:103:GLY:O	1:A:105:LEU:N	2.20	0.74
1:C:203:ASP:OD1	3:C:1040:HOH:O	2.06	0.74
1:B:140:LYS:CA	1:B:205:ILE:HD11	2.17	0.72
1:B:140:LYS:HG3	1:B:205:ILE:CD1	2.21	0.70
1:C:169:GLU:OE1	1:C:169:GLU:N	2.24	0.70
1:A:103:GLY:O	1:A:104:ALA:C	2.36	0.69
1:C:169:GLU:O	1:C:170:ASN:HB3	1.91	0.67
1:B:203:ASP:OD2	3:B:1051:HOH:O	2.11	0.67
1:C:149:VAL:HG21	1:C:172:VAL:HG21	1.77	0.67
1:C:118:PRO:HB2	1:C:119:PRO:CD	2.25	0.66
1:C:170:ASN:ND2	1:C:172:VAL:HG23	2.03	0.66
1:B:79:LYS:HD2	3:B:1448:HOH:O	1.96	0.65
1:C:118:PRO:CB	1:C:119:PRO:CD	2.75	0.65
1:A:227:GLU:CD	1:A:235:LYS:HE3	2.22	0.64
1:A:26:LEU:HD23	1:A:118:PRO:HG3	1.79	0.64
1:C:118:PRO:CB	1:C:119:PRO:HD2	2.30	0.61
1:A:77:LEU:HD22	1:A:109:PHE:CD2	2.35	0.61
1:A:12:LYS:NZ	1:A:81:ALA:O	2.30	0.60
1:B:46:LEU:C	1:B:46:LEU:HD23	2.26	0.60
1:C:36:LEU:HD22	1:C:49:ILE:HD12	1.82	0.60
1:A:171:LYS:C	1:A:173:GLU:H	2.09	0.59
1:C:180:THR:HG21	3:C:1358:HOH:O	2.02	0.59
1:A:12:LYS:HZ1	1:A:81:ALA:C	2.11	0.59
1:A:103:GLY:C	1:A:105:LEU:N	2.56	0.59
1:B:119:PRO:HG3	3:B:1050:HOH:O	2.02	0.59
1:C:32:GLU:H	1:C:32:GLU:CD	2.11	0.59
1:A:80:ALA:O	1:A:107:ARG:NH1	2.32	0.59
1:D:117:LEU:HD23	1:D:118:PRO:CD	2.32	0.59
1:B:140:LYS:HG3	1:B:205:ILE:HD13	1.85	0.58
1:B:154:LEU:HD11	1:B:167:GLU:HG3	1.84	0.58
1:B:136:ALA:CB	1:B:214:VAL:HG23	2.30	0.58
1:C:40:ASP:O	1:C:43:HIS:HD2	1.87	0.58
1:C:63:GLU:O	1:C:63:GLU:HG2	2.02	0.57
1:A:12:LYS:NZ	1:A:81:ALA:C	2.63	0.57
1:A:180:THR:HG22	1:A:182:SER:OG	2.05	0.57
1:B:178:LYS:NZ	1:B:186:ILE:HG22	2.19	0.57
1:D:92:ASP:OD2	3:D:1045:HOH:O	2.17	0.57
1:B:244:LEU:O	1:B:245:SER:HB3	2.05	0.57
1:A:169:GLU:CG	1:A:170:ASN:H	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ILE:HD11	1:C:139:LEU:HG	1.87	0.56
1:D:36:LEU:HD22	1:D:49:ILE:HD12	1.85	0.56
1:B:172:VAL:O	1:B:172:VAL:HG13	2.04	0.56
1:C:140:LYS:HG3	1:C:205:ILE:CG1	2.37	0.55
1:C:140:LYS:HG3	1:C:205:ILE:HD13	1.86	0.55
1:A:140:LYS:HG2	1:A:205:ILE:HG12	1.87	0.55
1:A:180:THR:CG2	1:A:182:SER:OG	2.54	0.55
1:C:32:GLU:CD	1:C:32:GLU:N	2.65	0.54
1:D:172:VAL:O	1:D:172:VAL:HG23	2.07	0.54
1:D:85:GLU:OE1	1:D:85:GLU:HA	2.07	0.54
1:B:57:LYS:HD2	3:B:1325:HOH:O	2.07	0.54
1:B:214:VAL:HG22	1:B:228:PHE:CE2	2.42	0.53
1:D:74:MET:HA	1:D:74:MET:HE2	1.89	0.53
1:D:117:LEU:HD23	1:D:118:PRO:HD3	1.90	0.53
1:D:143:ILE:HD12	1:D:205:ILE:HD11	1.91	0.53
1:C:140:LYS:HG3	1:C:205:ILE:HG12	1.90	0.53
1:B:196:TYR:HB3	1:B:240:LEU:HD13	1.90	0.53
1:C:116:VAL:O	1:C:116:VAL:CG2	2.57	0.52
1:C:57:LYS:NZ	1:C:86:GLU:OE2	2.32	0.52
1:D:107:ARG:NH2	3:D:1235:HOH:O	2.42	0.52
1:D:26:LEU:HD11	1:D:66:LYS:HB3	1.91	0.52
1:C:86:GLU:HB2	1:C:102:SER:HB3	1.92	0.52
1:A:126:LEU:HD12	1:A:127:GLU:HG3	1.92	0.51
1:A:26:LEU:HD22	1:A:118:PRO:HG3	1.92	0.51
1:C:63:GLU:O	1:C:63:GLU:CG	2.58	0.51
1:C:220:ASP:OD2	3:C:1077:HOH:O	2.19	0.51
1:A:227:GLU:OE1	1:A:235:LYS:NZ	2.38	0.51
1:C:43:HIS:CB	1:C:43:HIS:N	2.67	0.51
1:A:169:GLU:HG3	1:A:170:ASN:N	2.27	0.50
1:D:46:LEU:HD13	1:D:239:LEU:HD12	1.94	0.50
1:D:212:ASP:OD2	3:D:1145:HOH:O	2.19	0.50
1:A:159:GLU:HG2	3:A:1416:HOH:O	2.12	0.49
1:B:169:GLU:O	1:B:170:ASN:C	2.54	0.49
1:A:183:LEU:C	1:A:183:LEU:HD13	2.37	0.49
1:A:140:LYS:HG2	1:A:205:ILE:CG1	2.43	0.48
1:B:214:VAL:HG22	1:B:228:PHE:CD2	2.47	0.48
1:C:63:GLU:H	1:C:63:GLU:CD	2.22	0.48
1:B:159:GLU:O	1:B:178:LYS:HE2	2.14	0.48
1:B:153:LEU:C	1:B:153:LEU:HD23	2.39	0.47
1:A:89:ILE:HG12	1:A:99:LEU:CD2	2.45	0.47
1:D:41:LYS:HG3	3:D:1168:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:CG	1:A:170:ASN:N	2.77	0.47
1:C:140:LYS:HG3	1:C:205:ILE:HD11	1.95	0.47
1:A:119:PRO:HG3	3:A:1029:HOH:O	2.14	0.47
1:B:171:LYS:O	1:B:172:VAL:CG1	2.60	0.47
1:C:126:LEU:C	1:C:126:LEU:HD13	2.39	0.47
1:C:196:TYR:HB3	1:C:240:LEU:HD13	1.97	0.47
1:D:48:LYS:HE2	1:D:50:GLU:OE2	2.15	0.47
1:C:186:ILE:O	1:C:186:ILE:HG23	2.15	0.46
1:A:145:GLU:HA	1:A:148:GLU:HG2	1.96	0.46
1:B:134:ILE:HD11	1:B:139:LEU:HG	1.97	0.46
1:B:204:ILE:C	1:B:204:ILE:HD12	2.41	0.46
1:C:116:VAL:O	1:C:116:VAL:HG22	2.14	0.46
1:A:105:LEU:H	1:A:105:LEU:CD2	2.27	0.46
1:A:210:LEU:HD22	1:A:230:MET:HE3	1.98	0.46
1:C:170:ASN:ND2	1:C:172:VAL:CG2	2.70	0.46
1:A:171:LYS:HG2	1:A:173:GLU:HB2	1.98	0.45
1:A:227:GLU:CD	1:A:235:LYS:CE	2.89	0.45
1:A:153:LEU:C	1:A:153:LEU:HD23	2.42	0.45
1:B:19:LEU:C	1:B:19:LEU:HD12	2.42	0.45
1:A:171:LYS:N	1:A:171:LYS:CD	2.66	0.45
1:A:146:ILE:HA	1:A:172:VAL:HG21	1.99	0.45
1:B:214:VAL:CG2	1:B:228:PHE:CE2	3.00	0.44
1:B:178:LYS:HZ1	1:B:186:ILE:HG22	1.80	0.44
1:D:80:ALA:O	1:D:82:LYS:HG3	2.18	0.44
1:C:89:ILE:HG12	1:C:99:LEU:CD2	2.48	0.44
1:A:190:LYS:HE2	1:D:106:ASN:OD1	2.18	0.44
1:C:80:ALA:O	1:C:82:LYS:HG3	2.18	0.43
1:C:89:ILE:HG23	1:C:97:VAL:HG13	1.99	0.43
1:D:125:ASN:OD1	1:D:127:GLU:HB3	2.18	0.43
1:B:11:LEU:O	1:B:15:ILE:HG12	2.17	0.43
1:C:169:GLU:O	1:C:170:ASN:CB	2.63	0.43
1:D:170:ASN:OD1	1:D:172:VAL:HG22	2.18	0.43
1:A:214:VAL:HG13	1:A:214:VAL:O	2.18	0.43
1:C:63:GLU:CD	1:C:63:GLU:N	2.77	0.43
1:D:117:LEU:HD23	1:D:117:LEU:HA	1.79	0.43
1:A:88:ILE:HB	1:A:100:THR:HB	2.01	0.42
1:C:89:ILE:HG12	1:C:99:LEU:HD22	2.00	0.42
1:A:168:GLY:O	1:A:169:GLU:O	2.37	0.42
1:D:117:LEU:CD2	1:D:118:PRO:HD2	2.50	0.42
1:A:140:LYS:HG2	1:A:205:ILE:CD1	2.50	0.42
1:A:203:ASP:OD1	3:A:1443:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:LEU:HD23	1:D:118:PRO:HD2	2.01	0.41
1:A:140:LYS:HG2	1:A:205:ILE:HD11	2.01	0.41
1:C:139:LEU:HD12	1:C:214:VAL:HG11	2.01	0.41
1:C:185:ASP:OD1	1:C:186:ILE:N	2.53	0.41
1:D:204:ILE:C	1:D:204:ILE:HD12	2.45	0.41
1:A:36:LEU:C	1:A:36:LEU:HD23	2.46	0.41
1:A:82:LYS:O	1:A:82:LYS:HD2	2.21	0.41
1:A:117:LEU:HA	1:A:118:PRO:HD3	1.76	0.41
1:B:21:LEU:HD12	1:B:21:LEU:N	2.36	0.41
1:D:117:LEU:HA	1:D:118:PRO:HD3	1.92	0.41
1:A:46:LEU:C	1:A:46:LEU:HD23	2.45	0.41
1:A:204:ILE:C	1:A:204:ILE:HD12	2.46	0.41
1:B:160:GLU:HA	1:B:178:LYS:HE2	2.03	0.40
1:C:183:LEU:C	1:C:183:LEU:HD13	2.46	0.40
1:C:74:MET:HE3	1:C:74:MET:HB3	1.90	0.40
1:C:243:LYS:HD3	3:C:1422:HOH:O	2.20	0.40
1:B:16:GLN:OE1	3:B:1450:HOH:O	2.22	0.40
1:B:168:GLY:O	1:B:170:ASN:N	2.55	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)
3:A:1250:HOH:O	3:D:1214:HOH:O[1_554]	2.08	0.12

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	238/245 (97%)	228 (96%)	5 (2%)	5 (2%)	5	0
1	B	234/245 (96%)	226 (97%)	5 (2%)	3 (1%)	9	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	235/245 (96%)	227 (97%)	7 (3%)	1 (0%)	30	13
1	D	237/245 (97%)	235 (99%)	2 (1%)	0	100	100
All	All	944/980 (96%)	916 (97%)	19 (2%)	9 (1%)	12	2

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ALA
1	A	105	LEU
1	A	106	ASN
1	A	169	GLU
1	B	170	ASN
1	B	169	GLU
1	C	170	ASN
1	B	172	VAL
1	A	172	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/213 (99%)	198 (94%)	12 (6%)	18	2
1	B	206/213 (97%)	200 (97%)	6 (3%)	37	11
1	C	207/213 (97%)	196 (95%)	11 (5%)	20	2
1	D	209/213 (98%)	204 (98%)	5 (2%)	43	17
All	All	832/852 (98%)	798 (96%)	34 (4%)	27	5

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

Mol	Chain	Res	Type
1	A	11	LEU
1	A	32	GLU
1	A	46	LEU

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Mol	Chain	Res	Type
1	A	95	GLU
1	A	120	GLU
1	A	121	VAL
1	A	126	LEU
1	A	170	ASN
1	A	171	LYS
1	A	172	VAL
1	A	180	THR
1	A	183	LEU
1	B	11	LEU
1	B	64	GLU
1	B	115	GLU
1	B	139	LEU
1	B	160	GLU
1	B	240	LEU
1	C	32	GLU
1	C	63	GLU
1	C	116	VAL
1	C	119	PRO
1	C	139	LEU
1	C	169	GLU
1	C	183	LEU
1	C	192	SER
1	C	205	ILE
1	C	239	LEU
1	C	240	LEU
1	D	46	LEU
1	D	115	GLU
1	D	205	ILE
1	D	231	GLU
1	D	242	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	110	ASN
1	A	170	ASN
1	B	16	GLN
1	B	202	ASN
1	C	43	HIS
1	C	112	ASN

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Mol	Chain	Res	Type
1	C	170	ASN
1	C	202	ASN
1	D	110	ASN
1	D	202	ASN
1	D	225	GLN

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](#)

Of 23 ligands modelled in this entry, 23 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.