



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:53 AM UTC

PDB ID : 3IFV / pdb_00003ifv
Title : Crystal structure of the Haloferax volcanii proliferating cell nuclear antigen
Authors : Winter, J.A.; Christofi, P.; Morroll, S.; Bunting, K.A.
Deposited on : 2009-07-26
Resolution : 2.00 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

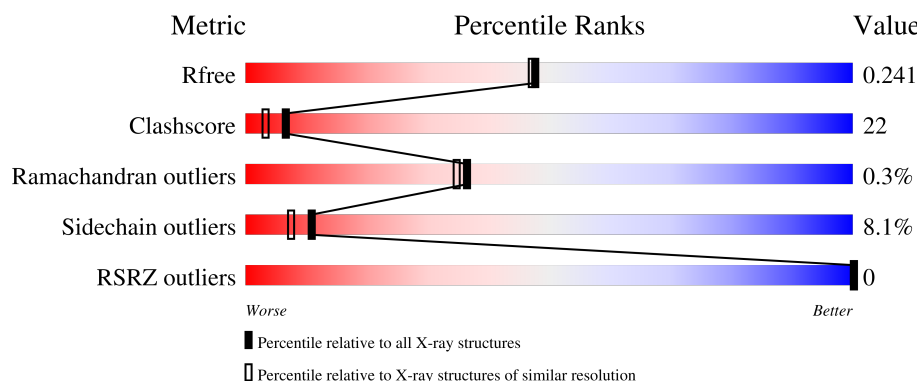
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	247	
1	B	247	
1	C	247	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5498 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 PCNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1633	1027	265	334	7			
1	B	234	Total	C	N	O	S	0	0	0
			1762	1106	291	358	7			
1	C	240	Total	C	N	O	S	0	0	0
			1821	1139	300	375	7			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Na	0	0
			3	3		
2	B	3	Total	Na	0	0
			3	3		
2	C	3	Total	Na	0	0
			3	3		

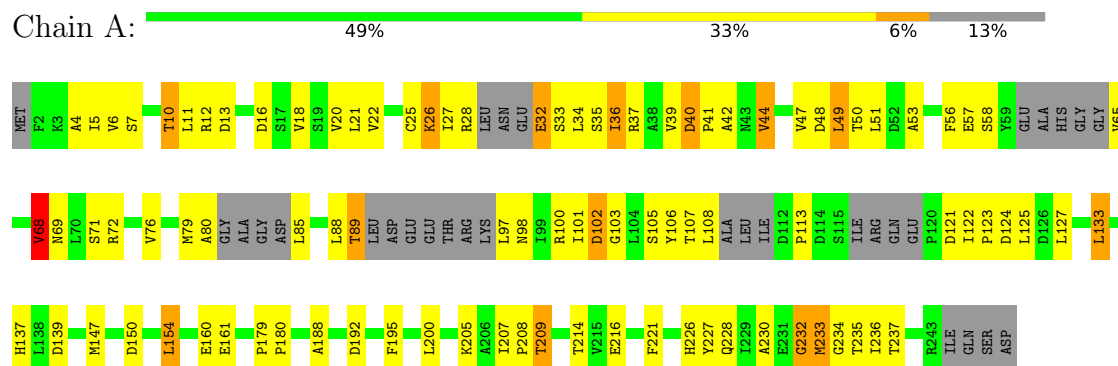
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	79	Total	O	0	0
			79	79		
3	B	73	Total	O	0	0
			73	73		
3	C	121	Total	O	0	0
			121	121		

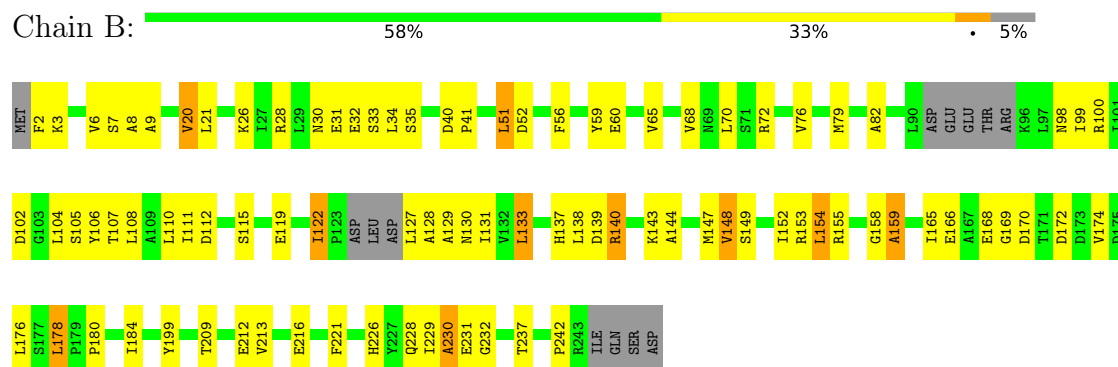
3 Residue-property plots

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 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.

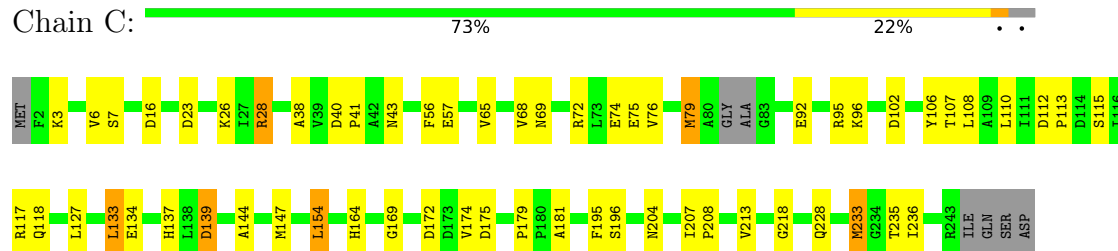
• Molecule 1: PCNA



• Molecule 1: PCNA



• Molecule 1: PCNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.36Å 143.76Å 78.03Å 90.00° 121.56° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 25.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.1 (25.00-2.00) 91.8 (25.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.214 , 0.259 (Not available) , 0.241	Depositor DCC
R_{free} test set	2580 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 23.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.901 for H, K, L 0.099 for -H, -K, H+L	Depositor
Outliers	0 of 50128 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5498	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.06% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.26	4/1650 (0.2%)	1.38	15/2236 (0.7%)
1	B	1.28	2/1784 (0.1%)	1.36	11/2422 (0.5%)
1	C	1.38	5/1844 (0.3%)	1.35	7/2505 (0.3%)
All	All	1.31	11/5278 (0.2%)	1.37	33/7163 (0.5%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	38	ALA	CA-CB	7.47	1.67	1.53
1	A	209	THR	CA-C	6.38	1.61	1.52
1	C	181	ALA	CA-CB	6.08	1.64	1.53
1	B	129	ALA	CA-CB	5.74	1.62	1.53
1	C	218	GLY	N-CA	5.73	1.49	1.44
1	C	213	VAL	C-O	5.71	1.30	1.24
1	A	47	VAL	N-CA	5.41	1.52	1.46
1	A	18	VAL	CA-CB	5.32	1.61	1.54
1	C	28	ARG	CA-C	-5.28	1.46	1.52
1	B	178	LEU	N-CA	-5.15	1.41	1.46
1	A	200	LEU	N-CA	5.07	1.52	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	CYS	N-CA-C	9.50	122.58	108.14
1	B	159	ALA	N-CA-C	-8.76	100.60	111.11
1	B	170	ASP	N-CA-C	-8.67	101.15	112.68
1	B	99	ILE	CB-CA-C	-7.97	100.63	110.99
1	A	33	SER	N-CA-C	7.51	119.98	108.42
1	A	39	VAL	N-CA-C	-7.27	97.03	108.81
1	B	122	ILE	N-CA-C	-7.17	101.92	108.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	GLU	N-CA-C	-7.09	103.29	112.23
1	A	68	VAL	N-CA-C	6.74	118.75	108.71
1	C	102	ASP	CB-CA-C	-6.60	108.97	116.63
1	A	44	VAL	CB-CA-C	6.43	117.21	110.91
1	C	169	GLY	N-CA-C	-6.18	105.37	112.79
1	A	139	ASP	CB-CA-C	-6.09	101.23	110.92
1	C	74	GLU	N-CA-C	5.93	117.42	111.07
1	C	139	ASP	CB-CA-C	-5.72	101.66	110.81
1	A	26	LYS	N-CA-C	5.67	117.97	108.73
1	A	188	ALA	N-CA-C	5.60	118.46	110.68
1	A	13	ASP	N-CA-C	-5.56	105.30	111.36
1	A	192	ASP	N-CA-C	-5.55	98.97	110.80
1	B	230	ALA	N-CA-C	-5.50	103.70	111.56
1	A	205	LYS	CB-CA-C	-5.40	101.49	110.68
1	B	159	ALA	O-C-N	5.38	127.69	122.09
1	B	102	ASP	CB-CA-C	-5.38	110.39	116.63
1	A	50	THR	N-CA-C	5.34	117.53	108.02
1	A	232	GLY	N-CA-C	-5.27	108.00	115.43
1	B	139	ASP	CB-CA-C	-5.26	102.55	110.92
1	B	139	ASP	N-CA-CB	5.25	117.80	109.82
1	C	233	MET	CA-CB-CG	-5.20	103.70	114.10
1	B	105	SER	N-CA-C	5.14	117.28	108.90
1	B	128	ALA	N-CA-C	5.07	116.89	111.36
1	A	98	ASN	N-CA-C	5.06	116.77	108.52
1	A	150	ASP	N-CA-C	-5.05	106.36	112.88
1	C	179	PRO	CB-CA-C	5.05	117.08	110.92

There are no chirality outliers.

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	1633	0	1615	96	0
1	B	1762	0	1750	85	0
1	C	1821	0	1798	59	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
3	A	79	0	0	2	1
3	B	73	0	0	3	1
3	C	121	0	0	9	0
All	All	5498	0	5163	224	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 22.

All (224) 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:28:ARG:NH1	1:C:65:VAL:HG21	1.54	1.21
1:B:140:ARG:HG3	1:B:140:ARG:HH11	1.05	1.18
1:C:133:LEU:HD12	1:C:134:GLU:O	1.39	1.17
1:A:28:ARG:HG2	1:A:65:VAL:HG23	1.22	1.12
1:A:65:VAL:HG13	1:A:65:VAL:O	1.50	1.10
1:A:233:MET:HE3	1:A:233:MET:HA	1.27	1.10
1:C:133:LEU:CD1	1:C:134:GLU:O	2.05	1.03
1:A:121:ASP:O	1:A:123:PRO:HD3	1.61	1.01
1:A:65:VAL:O	1:A:65:VAL:CG1	2.10	1.00
1:B:140:ARG:HH11	1:B:140:ARG:CG	1.75	1.00
1:C:28:ARG:HH11	1:C:65:VAL:CG2	1.75	0.98
1:C:28:ARG:HH11	1:C:65:VAL:HG21	1.21	0.96
1:B:40:ASP:OD2	1:B:199:TYR:OH	1.83	0.95
1:B:28:ARG:NH1	1:B:65:VAL:HG11	1.83	0.93
1:A:28:ARG:CG	1:A:65:VAL:HG23	2.00	0.90
1:A:147:MET:HE3	1:C:75:GLU:HB3	1.51	0.90
1:A:233:MET:HA	1:A:233:MET:CE	2.00	0.90
1:A:89:THR:HG22	1:A:89:THR:O	1.70	0.89
1:B:140:ARG:HG3	1:B:140:ARG:NH1	1.88	0.89
1:B:28:ARG:HD3	1:B:65:VAL:HG12	1.55	0.88
1:B:76:VAL:HG22	1:C:147:MET:HE1	1.56	0.87
1:A:27:ILE:HG12	1:A:36:ILE:HD11	1.55	0.87
1:A:32:GLU:OE2	1:A:32:GLU:HA	1.73	0.86
1:C:118:GLN:HB2	3:C:291:HOH:O	1.75	0.86
1:B:176:LEU:CD1	1:B:178:LEU:HG	2.08	0.83
1:B:153:ARG:C	1:B:154:LEU:HD12	2.03	0.83
1:B:169:GLY:N	1:B:172:ASP:O	2.12	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:LEU:HD11	1:B:178:LEU:HD21	1.61	0.82
1:C:72:ARG:O	1:C:76:VAL:HG23	1.80	0.81
1:C:133:LEU:CD1	1:C:137:HIS:HB2	2.11	0.81
1:C:72:ARG:HD2	1:C:106:TYR:OH	1.81	0.81
1:A:97:LEU:N	1:A:108:LEU:O	2.15	0.79
1:B:28:ARG:HH11	1:B:65:VAL:HG11	1.47	0.78
1:B:176:LEU:HD11	1:B:178:LEU:CD2	2.14	0.77
1:C:28:ARG:NH1	1:C:65:VAL:CG2	2.37	0.77
1:B:28:ARG:HD3	1:B:65:VAL:CG1	2.14	0.77
1:A:147:MET:HE1	1:C:76:VAL:HG22	1.67	0.76
1:A:37:ARG:CD	1:A:48:ASP:OD2	2.33	0.76
1:A:76:VAL:HG22	1:B:147:MET:HE1	1.68	0.76
1:B:108:LEU:HD12	1:C:172:ASP:OD2	1.85	0.76
1:A:76:VAL:CG2	1:B:147:MET:HE1	2.15	0.75
1:A:49:LEU:HA	1:A:236:ILE:HD13	1.67	0.74
1:C:133:LEU:HD13	1:C:137:HIS:HB2	1.68	0.74
1:A:37:ARG:HD2	1:A:48:ASP:OD2	1.88	0.74
1:A:57:GLU:HG3	1:A:85:LEU:HD22	1.67	0.74
1:B:154:LEU:HD12	1:B:154:LEU:N	2.02	0.73
1:B:184:ILE:HD11	1:B:212:GLU:HG2	1.70	0.73
1:A:27:ILE:HG12	1:A:36:ILE:CD1	2.19	0.72
1:B:133:LEU:HD23	1:B:137:HIS:HB2	1.72	0.72
1:B:154:LEU:N	1:B:154:LEU:CD1	2.53	0.70
1:A:7:SER:HB3	1:A:10:THR:HB	1.73	0.70
1:B:140:ARG:CG	1:B:140:ARG:NH1	2.41	0.70
1:A:36:ILE:HG13	1:A:49:LEU:HD23	1.73	0.70
1:C:164:HIS:HD2	1:C:175:ASP:OD1	1.75	0.70
1:B:40:ASP:HB2	1:B:41:PRO:HD2	1.74	0.69
1:A:89:THR:O	1:A:89:THR:CG2	2.41	0.68
1:A:106:TYR:HE2	1:A:108:LEU:HB2	1.56	0.68
1:B:169:GLY:HA3	1:B:172:ASP:O	1.94	0.68
1:A:230:ALA:O	1:A:233:MET:CG	2.43	0.66
1:B:169:GLY:CA	1:B:172:ASP:O	2.43	0.66
1:B:56:PHE:HB2	1:B:59:TYR:HB2	1.78	0.66
1:B:176:LEU:HD13	1:B:176:LEU:C	2.20	0.66
1:B:2:PHE:C	1:B:3:LYS:HG3	2.18	0.66
1:A:21:LEU:O	1:A:22:VAL:HG13	1.95	0.66
1:A:230:ALA:O	1:A:233:MET:HG2	1.96	0.66
1:C:16:ASP:OD2	3:C:358:HOH:O	2.13	0.65
1:C:133:LEU:HD12	1:C:134:GLU:C	2.19	0.65
1:A:107:THR:O	1:B:172:ASP:HB3	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LEU:CD2	1:B:137:HIS:HB2	2.26	0.65
1:B:158:GLY:O	1:B:159:ALA:C	2.40	0.64
1:A:27:ILE:HA	1:A:36:ILE:HD13	1.80	0.64
1:C:68:VAL:HG12	1:C:69:ASN:C	2.23	0.64
1:B:176:LEU:CD1	1:B:178:LEU:CG	2.76	0.64
1:C:118:GLN:CB	3:C:291:HOH:O	2.41	0.64
1:A:100:ARG:HG2	1:A:100:ARG:HH11	1.62	0.63
1:C:23:ASP:OD1	3:C:317:HOH:O	2.15	0.63
1:C:92:GLU:O	1:C:95:ARG:CZ	2.47	0.63
1:A:26:LYS:HE3	1:A:113:PRO:O	1.98	0.63
1:A:147:MET:HE3	1:C:75:GLU:CB	2.27	0.63
1:C:133:LEU:HD11	1:C:137:HIS:HB2	1.80	0.63
1:A:49:LEU:HD13	1:A:236:ILE:HD11	1.81	0.63
1:C:68:VAL:HG12	1:C:69:ASN:N	2.14	0.63
1:A:147:MET:HE1	1:C:76:VAL:CG2	2.30	0.62
1:A:57:GLU:HG3	1:A:85:LEU:CD2	2.29	0.62
1:C:92:GLU:O	1:C:95:ARG:NE	2.32	0.62
1:B:31:GLU:OE1	1:B:32:GLU:HG2	2.00	0.61
1:A:108:LEU:C	1:B:172:ASP:OD1	2.44	0.60
1:A:147:MET:CE	1:C:75:GLU:HB3	2.26	0.60
1:B:221:PHE:C	1:B:242:PRO:HG3	2.25	0.60
1:A:108:LEU:HA	1:B:172:ASP:OD1	2.02	0.60
1:C:139:ASP:OD1	1:C:204:ASN:ND2	2.23	0.60
1:A:49:LEU:HA	1:A:236:ILE:CD1	2.32	0.60
1:A:37:ARG:HG2	1:A:48:ASP:OD2	2.01	0.59
1:A:228:GLN:HG2	1:A:235:THR:HG22	1.84	0.59
1:A:40:ASP:O	1:A:41:PRO:C	2.44	0.58
1:C:28:ARG:HD3	1:C:65:VAL:HG22	1.85	0.58
1:A:27:ILE:HG23	1:A:34:LEU:HD21	1.84	0.58
1:A:106:TYR:CE2	1:A:108:LEU:HB2	2.36	0.58
1:B:230:ALA:O	1:B:232:GLY:N	2.37	0.58
1:B:72:ARG:HD2	1:B:106:TYR:OH	2.04	0.58
1:B:106:TYR:HE2	1:B:108:LEU:HD13	1.68	0.58
1:A:28:ARG:NH1	1:A:65:VAL:HG21	2.19	0.58
1:C:118:GLN:CG	3:C:291:HOH:O	2.52	0.58
1:A:100:ARG:HG2	1:A:100:ARG:NH1	2.19	0.57
1:B:226:HIS:HD2	1:B:237:THR:OG1	1.87	0.57
1:C:68:VAL:CG1	1:C:69:ASN:N	2.67	0.57
1:B:184:ILE:CD1	1:B:212:GLU:HG2	2.33	0.57
1:B:138:LEU:HD11	1:B:213:VAL:HG11	1.87	0.57
1:B:176:LEU:HD11	1:B:178:LEU:CG	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ARG:CD	1:C:65:VAL:HG22	2.34	0.56
1:A:65:VAL:HG13	1:A:113:PRO:HG3	1.86	0.56
1:C:118:GLN:CD	3:C:291:HOH:O	2.48	0.56
1:A:37:ARG:CG	1:A:48:ASP:OD2	2.53	0.56
1:B:106:TYR:CE2	1:B:108:LEU:HD13	2.40	0.56
1:B:106:TYR:HE2	1:B:108:LEU:CD1	2.18	0.55
1:A:125:LEU:HD12	1:A:127:LEU:HD11	1.88	0.55
1:B:34:LEU:HB3	1:B:51:LEU:HB3	1.88	0.55
1:C:117:ARG:NH1	3:C:303:HOH:O	2.37	0.55
1:A:125:LEU:HD13	1:A:127:LEU:HD21	1.88	0.55
1:A:36:ILE:CG1	1:A:49:LEU:HD23	2.35	0.55
1:A:76:VAL:HG23	1:B:147:MET:HE1	1.89	0.55
1:A:27:ILE:CG1	1:A:36:ILE:CD1	2.84	0.55
1:A:40:ASP:O	1:A:42:ALA:N	2.40	0.55
1:A:4:ALA:N	1:A:88:LEU:O	2.31	0.53
1:B:155:ARG:NE	1:B:166:GLU:OE2	2.36	0.53
1:B:176:LEU:HD11	1:B:178:LEU:HG	1.91	0.53
1:C:204:ASN:HA	1:C:207:ILE:HD12	1.89	0.53
1:B:216:GLU:OE2	1:B:226:HIS:HE1	1.92	0.53
1:B:144:ALA:HB1	1:B:174:VAL:HG21	1.91	0.52
1:B:2:PHE:C	1:B:3:LYS:CG	2.82	0.52
1:C:133:LEU:HD13	1:C:137:HIS:CD2	2.45	0.52
1:B:32:GLU:O	1:B:52:ASP:OD1	2.28	0.52
1:B:176:LEU:HD13	1:B:178:LEU:HG	1.90	0.52
1:A:228:GLN:HA	1:A:234:GLY:O	2.09	0.52
1:B:72:ARG:O	1:B:76:VAL:HG23	2.10	0.52
1:C:228:GLN:HG2	1:C:235:THR:HG22	1.92	0.52
1:B:6:VAL:HG22	1:B:7:SER:N	2.25	0.52
1:A:21:LEU:O	1:A:22:VAL:CG1	2.59	0.51
1:A:216:GLU:OE1	1:A:226:HIS:HE1	1.93	0.51
1:C:112:ASP:O	1:C:115:SER:HB3	2.10	0.51
1:A:34:LEU:HD23	1:A:35:SER:N	2.26	0.51
3:A:275:HOH:O	1:C:96:LYS:HD3	2.10	0.51
1:B:230:ALA:C	1:B:232:GLY:H	2.18	0.51
1:A:69:ASN:OD1	1:A:69:ASN:C	2.54	0.51
1:C:117:ARG:NH1	3:C:249:HOH:O	2.44	0.50
1:A:27:ILE:HD11	1:A:68:VAL:HB	1.94	0.50
1:A:27:ILE:CD1	1:A:68:VAL:HB	2.41	0.49
1:A:106:TYR:C	1:A:106:TYR:CD2	2.90	0.49
1:A:79:MET:SD	1:B:143:LYS:HD3	2.53	0.49
1:A:5:ILE:HG22	1:A:57:GLU:HB2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:VAL:HG22	1:A:7:SER:O	2.13	0.49
1:B:76:VAL:CG2	1:C:147:MET:HE1	2.34	0.49
1:B:130:ASN:C	1:B:131:ILE:HG13	2.38	0.49
1:B:30:ASN:HB2	1:B:33:SER:O	2.13	0.49
1:B:34:LEU:N	1:B:51:LEU:O	2.40	0.48
1:C:144:ALA:HB1	1:C:174:VAL:HG21	1.95	0.48
1:A:28:ARG:HH11	1:A:65:VAL:HG21	1.79	0.47
1:A:72:ARG:HG2	1:A:108:LEU:HD13	1.96	0.47
1:A:207:ILE:HG12	1:A:227:TYR:CE2	2.50	0.47
1:B:229:ILE:O	1:B:230:ALA:HB3	2.14	0.47
1:A:226:HIS:HD2	1:A:237:THR:OG1	1.96	0.47
1:A:179:PRO:HB2	1:A:180:PRO:CD	2.46	0.47
1:B:152:ILE:HD11	1:B:165:ILE:CG2	2.45	0.46
1:A:26:LYS:HB2	3:A:303:HOH:O	2.15	0.46
1:B:20:VAL:HG12	1:B:21:LEU:HG	1.97	0.46
1:C:79:MET:HE3	1:C:79:MET:HB3	1.79	0.46
1:A:230:ALA:O	1:A:233:MET:CB	2.64	0.46
1:C:133:LEU:HD12	1:C:133:LEU:C	2.41	0.46
1:A:230:ALA:O	1:A:233:MET:HB2	2.16	0.46
1:B:72:ARG:HG2	1:B:72:ARG:HH11	1.81	0.46
1:A:80:ALA:HB2	1:A:101:ILE:HD13	1.98	0.45
1:A:108:LEU:CA	1:B:172:ASP:OD1	2.65	0.45
1:A:11:LEU:O	1:A:11:LEU:HG	2.15	0.45
1:B:140:ARG:CD	3:B:258:HOH:O	2.64	0.45
1:A:37:ARG:HG2	1:A:48:ASP:CG	2.41	0.45
1:A:233:MET:HE3	1:A:233:MET:CA	2.19	0.45
1:A:102:ASP:HB3	1:A:103:GLY:H	1.50	0.45
1:C:26:LYS:HE2	1:C:113:PRO:O	2.17	0.45
1:A:21:LEU:C	1:A:22:VAL:HG13	2.42	0.45
1:B:9:ALA:HB2	1:B:82:ALA:HB1	1.98	0.45
1:A:154:LEU:HD22	1:A:195:PHE:CE1	2.51	0.45
1:A:179:PRO:HB2	1:A:180:PRO:HD2	1.98	0.45
1:A:160:GLU:O	1:A:161:GLU:C	2.59	0.45
1:C:68:VAL:HG12	1:C:69:ASN:O	2.16	0.45
1:A:49:LEU:HB2	1:A:236:ILE:CD1	2.47	0.44
1:A:97:LEU:O	1:A:108:LEU:N	2.35	0.44
1:A:51:LEU:HD23	1:A:51:LEU:HA	1.87	0.44
1:B:115:SER:O	1:B:115:SER:OG	2.27	0.44
1:B:56:PHE:CB	1:B:59:TYR:HB2	2.45	0.44
1:C:133:LEU:HD13	1:C:137:HIS:CB	2.45	0.44
1:C:43:ASN:OD1	1:C:117:ARG:NH2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ARG:O	1:A:16:ASP:HB2	2.18	0.43
1:B:98:ASN:ND2	3:B:319:HOH:O	2.44	0.43
1:C:204:ASN:HA	1:C:207:ILE:CD1	2.47	0.43
1:B:230:ALA:C	1:B:232:GLY:N	2.74	0.43
1:A:27:ILE:CG2	1:A:34:LEU:HD21	2.48	0.43
1:A:214:THR:HB	1:A:226:HIS:HB2	2.00	0.43
1:B:6:VAL:CG2	1:B:7:SER:N	2.82	0.43
1:C:28:ARG:HH11	1:C:65:VAL:HG22	1.77	0.43
1:C:154:LEU:HD22	1:C:195:PHE:CE1	2.54	0.43
1:A:228:GLN:HB3	1:A:232:GLY:HA2	2.01	0.42
1:B:100:ARG:HA	1:B:104:LEU:O	2.20	0.42
1:C:110:LEU:HA	1:C:110:LEU:HD23	1.61	0.42
1:B:112:ASP:O	1:B:115:SER:HB3	2.20	0.42
1:C:6:VAL:HB	1:C:56:PHE:CD1	2.55	0.42
1:B:70:LEU:HD12	1:B:70:LEU:HA	1.88	0.41
1:C:40:ASP:HB2	1:C:41:PRO:HD2	2.02	0.41
1:A:26:LYS:CE	1:A:113:PRO:O	2.66	0.41
1:A:28:ARG:HG2	1:A:65:VAL:CG2	2.16	0.41
1:C:96:LYS:HD2	1:C:107:THR:CG2	2.51	0.41
1:C:208:PRO:HG2	3:C:296:HOH:O	2.20	0.41
1:B:148:VAL:O	1:B:149:SER:HB2	2.21	0.41
1:B:176:LEU:CD1	1:B:176:LEU:C	2.91	0.41
1:C:113:PRO:C	1:C:115:SER:H	2.28	0.41
1:A:53:ALA:O	1:A:56:PHE:HB2	2.21	0.41
1:A:233:MET:CE	1:A:233:MET:CA	2.75	0.41
1:B:40:ASP:CB	1:B:41:PRO:HD2	2.48	0.41
1:C:133:LEU:HD12	1:C:134:GLU:N	2.36	0.41
1:B:26:LYS:HD2	1:B:119:GLU:HG3	2.03	0.41
1:A:133:LEU:HD22	1:A:137:HIS:HB2	2.03	0.40
1:B:79:MET:HE3	1:B:79:MET:HB3	1.88	0.40
1:B:111:ILE:HG22	1:B:112:ASP:N	2.36	0.40
1:B:8:ALA:HB3	1:B:82:ALA:HA	2.04	0.40
1:B:228:GLN:N	3:B:304:HOH:O	2.45	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:319:HOH:O	3:B:320:HOH:O[2_656]	1.97	0.23

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	202/247 (82%)	189 (94%)	13 (6%)	0	100	100
1	B	228/247 (92%)	216 (95%)	10 (4%)	2 (1%)	14	9
1	C	236/247 (96%)	231 (98%)	5 (2%)	0	100	100
All	All	666/741 (90%)	636 (96%)	28 (4%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	110	LEU
1	B	231	GLU

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	179/203 (88%)	158 (88%)	21 (12%)	5	3
1	B	190/203 (94%)	175 (92%)	15 (8%)	11	8
1	C	198/203 (98%)	188 (95%)	10 (5%)	21	19
All	All	567/609 (93%)	521 (92%)	46 (8%)	11	7

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	20	VAL
1	A	32	GLU
1	A	36	ILE
1	A	40	ASP
1	A	44	VAL
1	A	49	LEU
1	A	58	SER
1	A	68	VAL
1	A	71	SER
1	A	89	THR
1	A	102	ASP
1	A	105	SER
1	A	122	ILE
1	A	124	ASP
1	A	133	LEU
1	A	154	LEU
1	A	208	PRO
1	A	209	THR
1	A	221	PHE
1	A	233	MET
1	B	20	VAL
1	B	35	SER
1	B	51	LEU
1	B	60	GLU
1	B	68	VAL
1	B	107	THR
1	B	122	ILE
1	B	127	LEU
1	B	133	LEU
1	B	140	ARG
1	B	148	VAL
1	B	154	LEU
1	B	168	GLU
1	B	180	PRO
1	B	209	THR
1	C	3	LYS
1	C	7	SER
1	C	79	MET
1	C	108	LEU
1	C	127	LEU
1	C	133	LEU
1	C	154	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	196	SER
1	C	233	MET
1	C	236	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	226	HIS
1	B	30	ASN
1	B	226	HIS
1	C	30	ASN
1	C	87	HIS
1	C	164	HIS

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 9 ligands modelled in this entry, 9 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	216/247 (87%)	-0.76	0 100 100	13, 27, 45, 50	0
1	B	234/247 (94%)	-0.75	0 100 100	18, 28, 41, 49	0
1	C	240/247 (97%)	-1.09	0 100 100	11, 20, 33, 41	0
All	All	690/741 (93%)	-0.87	0 100 100	11, 24, 41, 50	0

There are no RSRZ outliers to report.

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NA	A	401	1/1	0.99	0.04	13,13,13,13	0
2	NA	A	403	1/1	0.99	0.02	27,27,27,27	0
2	NA	B	405	1/1	0.99	0.02	28,28,28,28	0
2	NA	B	406	1/1	0.99	0.04	24,24,24,24	0
2	NA	C	408	1/1	0.99	0.02	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	C	409	1/1	0.99	0.03	22,22,22,22	0
2	NA	C	407	1/1	1.00	0.01	14,14,14,14	0
2	NA	A	402	1/1	1.00	0.03	22,22,22,22	0
2	NA	B	404	1/1	1.00	0.06	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.