



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:10 PM UTC

PDB ID : 2IZO / pdb_00002izo
Title : Structure of an Archaeal PCNA1-PCNA2-FEN1 Complex
Authors : Dore, A.S.; Kilkenny, M.L.; Roe, S.M.; Pearl, L.H.
Deposited on : 2006-07-25
Resolution : 2.90 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

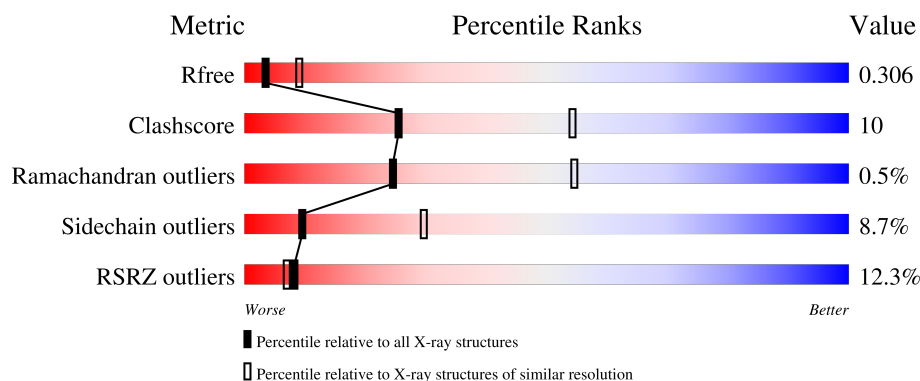
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	346	18% 63% 13% • 23%
2	B	246	10% 71% 25% • •
3	C	249	2% 74% 21% • •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5811 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 FLAP STRUCTURE-SPECIFIC ENDONUCLEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2043	1308	350	381	4			

- Molecule 2 is a protein called DNA POLYMERASE SLIDING CLAMP C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	245	Total	C	N	O	S	0	0	1
			1866	1201	294	366	5			

- Molecule 3 is a protein called DNA POLYMERASE SLIDING CLAMP B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	244	Total	C	N	O	S	0	0	0
			1816	1158	288	361	9			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	C	2	Total	Zn	0	0
			2	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total 1	Mg 1	0	0

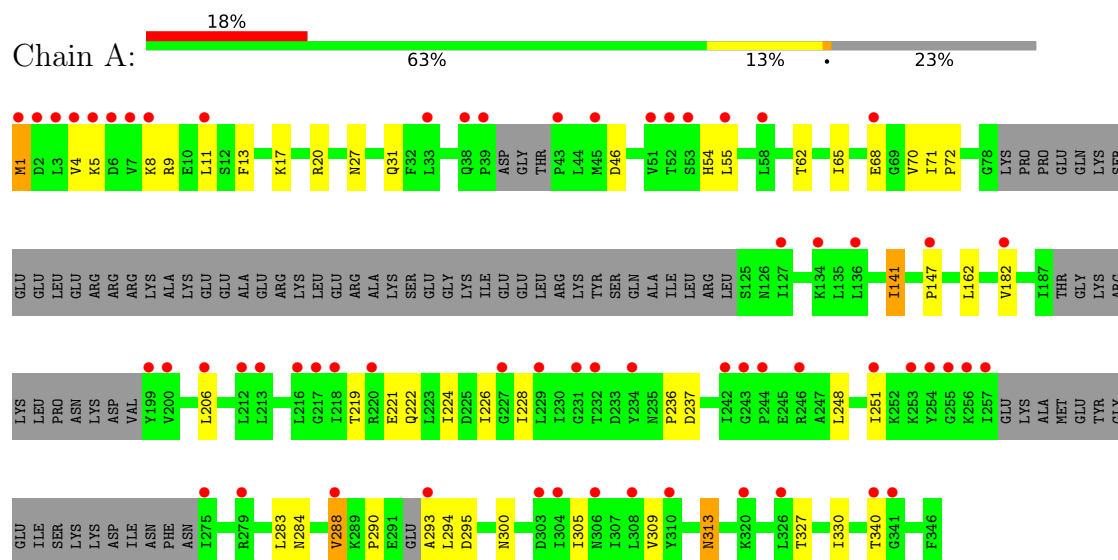
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	26	Total 26	O 26	0	0
6	B	23	Total 23	O 23	0	0
6	C	29	Total 29	O 29	0	0

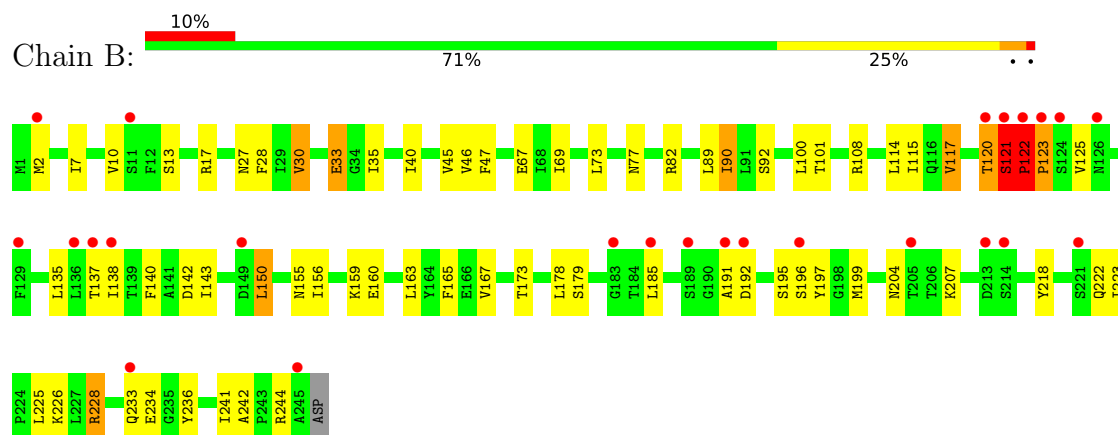
3 Residue-property plots [i](#)

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.

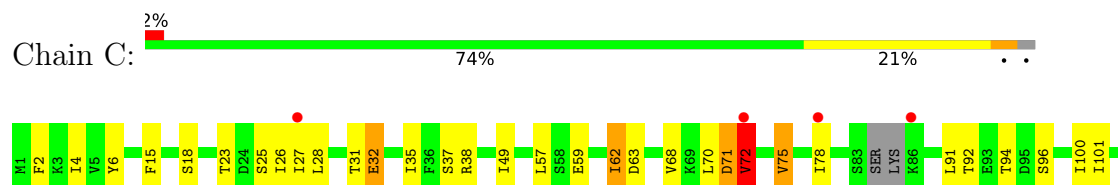
• Molecule 1: FLAP STRUCTURE-SPECIFIC ENDONUCLEASE

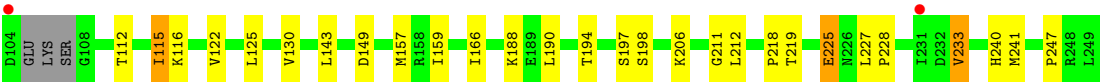


• Molecule 2: DNA POLYMERASE SLIDING CLAMP C



• Molecule 3: DNA POLYMERASE SLIDING CLAMP B





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.99Å 99.77Å 99.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.00-2.90) 98.8 (30.00-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.250 , 0.312 0.246 , 0.306	Depositor DCC
R_{free} test set	1088 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 87.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for -h,l,k	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5811	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.45	0/2070	0.82	3/2795 (0.1%)
2	B	0.48	1/1901 (0.1%)	0.86	6/2583 (0.2%)
3	C	0.46	0/1842	0.77	0/2498
All	All	0.46	1/5813 (0.0%)	0.82	9/7876 (0.1%)

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
2	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	244	ARG	C-N	-6.87	1.23	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	122	PRO	N-CA-C	10.89	140.41	112.10
2	B	125	VAL	N-CA-C	6.88	118.20	108.36
2	B	121	SER	N-CA-CB	-6.11	99.49	110.37
1	A	141	ILE	CA-C-N	5.77	125.79	119.90
1	A	141	ILE	C-N-CA	5.77	125.79	119.90
2	B	223	ILE	CA-C-N	5.77	127.05	119.84
2	B	223	ILE	C-N-CA	5.77	127.05	119.84
2	B	122	PRO	CB-CA-C	-5.15	99.13	112.00
1	A	313	ASN	N-CA-C	5.04	117.32	111.02

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	120	THR	Peptide
2	B	122	PRO	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	2043	0	2051	34	0
2	B	1866	0	1805	43	0
3	C	1816	0	1778	34	1
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	26	0	0	0	0
6	B	23	0	0	1	0
6	C	29	0	0	1	1
All	All	5811	0	5634	109	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 (109) 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:A:1:MET:CE	1:A:4:VAL:HG21	1.61	1.28
2:B:122:PRO:HB2	2:B:123:PRO:CA	1.69	1.23
1:A:1:MET:HE3	1:A:4:VAL:CG2	1.73	1.17
2:B:122:PRO:CB	2:B:123:PRO:HA	1.78	1.14
2:B:40:ILE:CD1	2:B:123:PRO:HD2	1.84	1.06
3:C:225:GLU:OE1	6:C:2025:HOH:O	1.82	0.97
2:B:40:ILE:HD11	2:B:123:PRO:HD2	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:PRO:HB2	2:B:123:PRO:HA	0.92	0.91
2:B:233:GLN:OE1	6:B:2022:HOH:O	1.89	0.90
1:A:5:LYS:HZ1	1:A:226:ILE:HG21	1.42	0.83
2:B:40:ILE:HD11	2:B:123:PRO:CD	2.11	0.81
2:B:17:ARG:HA	2:B:77:ASN:HD21	1.48	0.79
2:B:120:THR:HA	2:B:121:SER:O	1.83	0.77
1:A:5:LYS:NZ	1:A:226:ILE:HG21	2.01	0.76
2:B:17:ARG:HA	2:B:77:ASN:ND2	2.02	0.73
1:A:13:PHE:CG	1:A:68:GLU:HG2	2.26	0.70
2:B:135:LEU:HD11	2:B:140:PHE:HB2	1.75	0.69
1:A:293:ALA:HB1	1:A:294:LEU:HD23	1.75	0.68
1:A:1:MET:HE3	1:A:4:VAL:HG21	0.77	0.68
2:B:178:LEU:HB3	2:B:185:LEU:HD13	1.78	0.66
1:A:46:ASP:HB2	1:A:313:ASN:HB3	1.78	0.66
2:B:90:ILE:HG23	2:B:101:THR:HB	1.77	0.66
1:A:20:ARG:NH1	1:A:294:LEU:O	2.26	0.65
3:C:219:THR:HG23	3:C:233:VAL:HG12	1.80	0.64
3:C:32:GLU:H	3:C:32:GLU:CD	2.04	0.63
1:A:54:HIS:CD2	1:A:55:LEU:HG	2.32	0.63
2:B:40:ILE:CD1	2:B:123:PRO:CD	2.68	0.62
3:C:18:SER:HB3	3:C:241:MET:HE3	1.82	0.62
3:C:70:LEU:O	3:C:72:VAL:N	2.34	0.61
2:B:218:TYR:HB2	2:B:226:LYS:HB3	1.85	0.58
1:A:54:HIS:HD2	1:A:55:LEU:H	1.50	0.58
3:C:15:PHE:HD2	3:C:241:MET:HE2	1.69	0.57
3:C:2:PHE:HB3	3:C:62:ILE:HG23	1.87	0.56
1:A:162:LEU:HD13	1:A:290:PRO:HG3	1.87	0.55
2:B:156:ILE:HG22	2:B:165:PHE:HA	1.87	0.55
2:B:120:THR:HG23	2:B:120:THR:O	2.07	0.54
3:C:166:ILE:CD1	3:C:190:LEU:HD11	2.37	0.54
1:A:65:ILE:HG23	1:A:70:VAL:HB	1.90	0.54
2:B:30:VAL:HG13	2:B:67:GLU:HB3	1.90	0.54
3:C:31:THR:HG22	3:C:122:VAL:HG21	1.90	0.54
1:A:219:THR:H	1:A:222:GLN:HE21	1.57	0.53
1:A:1:MET:CE	1:A:4:VAL:CG2	2.55	0.53
1:A:54:HIS:HD2	1:A:55:LEU:N	2.06	0.53
2:B:28:PHE:HB2	2:B:69:ILE:HB	1.91	0.53
1:A:13:PHE:CD1	1:A:68:GLU:HG2	2.44	0.53
2:B:40:ILE:HD12	2:B:123:PRO:HD2	1.82	0.52
3:C:6:TYR:HD1	3:C:57:LEU:HD23	1.74	0.52
3:C:26:ILE:HD11	3:C:70:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HD22	1:A:206:LEU:HB2	1.92	0.52
1:A:5:LYS:HE3	1:A:248:LEU:HB2	1.92	0.51
3:C:228:PRO:HA	3:C:247:PRO:HD3	1.91	0.51
3:C:227:LEU:HB3	3:C:228:PRO:HD2	1.91	0.51
3:C:94:THR:HG22	3:C:96:SER:H	1.76	0.51
2:B:228:ARG:O	2:B:228:ARG:HG3	2.10	0.50
3:C:197:SER:H	3:C:225:GLU:HG2	1.77	0.50
1:A:5:LYS:HZ1	1:A:226:ILE:HD13	1.77	0.50
1:A:27:ASN:O	1:A:31:GLN:HG2	2.10	0.50
2:B:82:ARG:HD3	3:C:149:ASP:OD2	2.12	0.50
2:B:47:PHE:CD2	2:B:122:PRO:O	2.65	0.50
1:A:224:ILE:O	1:A:228:ILE:HG12	2.12	0.50
3:C:166:ILE:HD13	3:C:190:LEU:HD11	1.94	0.49
2:B:228:ARG:HD3	2:B:236:TYR:HB2	1.93	0.49
3:C:4:ILE:HG21	3:C:35:ILE:HD11	1.94	0.49
1:A:236:PRO:O	1:A:237:ASP:HB2	2.13	0.49
3:C:38:ARG:HG3	3:C:49:ILE:HG12	1.94	0.49
2:B:155:ASN:HA	2:B:196:SER:HA	1.95	0.48
3:C:157:MET:HE3	3:C:159:ILE:HB	1.96	0.48
1:A:54:HIS:CD2	1:A:55:LEU:N	2.82	0.48
2:B:2:MET:HG3	2:B:30:VAL:HG21	1.95	0.47
1:A:62:THR:HG21	1:A:141:ILE:HD13	1.97	0.47
2:B:135:LEU:CD1	2:B:140:PHE:HB2	2.43	0.47
2:B:197:TYR:CZ	2:B:225:LEU:HB2	2.50	0.47
2:B:33:GLU:H	2:B:33:GLU:HG2	1.51	0.47
3:C:101:ILE:HG12	3:C:112:THR:HG22	1.97	0.47
2:B:46:VAL:HG22	2:B:241:ILE:HG12	1.96	0.47
2:B:122:PRO:CB	2:B:123:PRO:CA	2.51	0.47
1:A:327:THR:HA	1:A:330:ILE:HD12	1.97	0.46
3:C:2:PHE:HB3	3:C:62:ILE:CG2	2.45	0.46
1:A:305:ILE:HG23	1:A:309:VAL:HB	1.97	0.46
2:B:2:MET:O	2:B:92:SER:HA	2.16	0.45
3:C:100:ILE:O	3:C:112:THR:HA	2.16	0.45
3:C:91:LEU:HD23	3:C:100:ILE:HG12	1.98	0.45
1:A:13:PHE:HB3	1:A:68:GLU:HG2	1.99	0.44
3:C:71:ASP:HB2	3:C:116:LYS:O	2.18	0.44
2:B:150:LEU:O	2:B:167:VAL:HG11	2.18	0.44
3:C:130:VAL:HG21	3:C:227:LEU:HD22	1.99	0.44
2:B:27:ASN:ND2	2:B:117:VAL:HG13	2.33	0.44
2:B:30:VAL:HB	2:B:35:ILE:HG12	2.00	0.44
2:B:179:SER:HA	2:B:185:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ALA:HA	1:A:294:LEU:HA	1.70	0.43
1:A:13:PHE:CB	1:A:68:GLU:HG2	2.48	0.42
3:C:70:LEU:HD22	3:C:115:ILE:HG21	2.00	0.42
2:B:45:VAL:HG13	2:B:242:ALA:HB3	2.00	0.42
1:A:221:GLU:HG2	1:A:283:LEU:HD21	2.01	0.42
2:B:204:ASN:HD22	2:B:204:ASN:HA	1.65	0.42
2:B:89:LEU:HD11	2:B:100:LEU:HB3	2.02	0.41
3:C:212:LEU:HD22	3:C:233:VAL:HG13	2.02	0.41
3:C:28:LEU:HB2	3:C:68:VAL:HG13	2.02	0.41
3:C:75:VAL:HA	3:C:78:ILE:HD12	2.02	0.41
2:B:120:THR:CA	2:B:121:SER:O	2.63	0.41
3:C:23:THR:C	3:C:25:SER:H	2.28	0.41
3:C:188:LYS:NZ	3:C:218:PRO:HB3	2.35	0.41
3:C:18:SER:OG	3:C:211:GLY:O	2.34	0.41
1:A:71:ILE:HA	1:A:72:PRO:HD3	1.91	0.41
2:B:121:SER:HA	2:B:122:PRO:HA	1.52	0.41
2:B:138:ILE:H	2:B:138:ILE:HG13	1.74	0.41
1:A:147:PRO:HD3	1:A:288:VAL:HG22	2.04	0.40
1:A:340:THR:HG22	3:C:247:PRO:O	2.20	0.40
2:B:191:ALA:HA	2:B:192:ASP:HA	1.92	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:C:59:GLU:OE1	6:C:2025:HOH:O[2_454]	1.99	0.21

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	256/346 (74%)	233 (91%)	23 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	243/246 (99%)	224 (92%)	17 (7%)	2 (1%)	16	44
3	C	238/249 (96%)	226 (95%)	10 (4%)	2 (1%)	16	44
All	All	737/841 (88%)	683 (93%)	50 (7%)	4 (0%)	24	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	123	PRO
3	C	71	ASP
3	C	72	VAL
2	B	122	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/297 (70%)	199 (95%)	10 (5%)	23	55
2	B	202/220 (92%)	176 (87%)	26 (13%)	4	13
3	C	196/220 (89%)	179 (91%)	17 (9%)	9	30
All	All	607/737 (82%)	554 (91%)	53 (9%)	9	30

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	LYS
1	A	9	ARG
1	A	17	LYS
1	A	182	VAL
1	A	251	ILE
1	A	284	ASN
1	A	288	VAL
1	A	295	ASP
1	A	300	ASN

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Mol	Chain	Res	Type
2	B	7	ILE
2	B	10	VAL
2	B	13	SER
2	B	30	VAL
2	B	33	GLU
2	B	73	LEU
2	B	90	ILE
2	B	108	ARG
2	B	114	LEU
2	B	115	ILE
2	B	117	VAL
2	B	121	SER
2	B	137	THR
2	B	142	ASP
2	B	143	ILE
2	B	150	LEU
2	B	159	LYS
2	B	160	GLU
2	B	163	LEU
2	B	173	THR
2	B	195	SER
2	B	199	MET
2	B	207	LYS
2	B	222	GLN
2	B	228	ARG
2	B	234	GLU
3	C	27	ILE
3	C	32	GLU
3	C	37	SER
3	C	62	ILE
3	C	63	ASP
3	C	72	VAL
3	C	75	VAL
3	C	92	THR
3	C	115	ILE
3	C	125	LEU
3	C	143	LEU
3	C	194	THR
3	C	198	SER
3	C	206	LYS
3	C	225	GLU
3	C	233	VAL

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Mol	Chain	Res	Type
3	C	240	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	54	HIS
1	A	222	GLN
1	A	284	ASN
1	A	312	HIS
2	B	27	ASN
2	B	77	ASN
2	B	204	ASN
2	B	233	GLN
3	C	8	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](#)

Of 8 ligands modelled in this entry, 8 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

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	268/346 (77%)	1.35	62 (23%) 2 2	30, 50, 54, 56	2 (0%)
2	B	245/246 (99%)	0.79	25 (10%) 12 10	45, 50, 54, 59	0
3	C	244/249 (97%)	0.43	6 (2%) 58 48	44, 50, 54, 56	0
All	All	757/841 (90%)	0.87	93 (12%) 8 7	30, 50, 54, 59	2 (0%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	TYR	7.6
1	A	1	MET	6.0
1	A	246	ARG	5.6
1	A	257	ILE	5.6
2	B	123	PRO	5.0
2	B	122	PRO	4.9
1	A	7	VAL	4.8
1	A	51	VAL	4.5
1	A	320	LYS	4.0
1	A	255	GLY	3.9
1	A	304	ILE	3.7
2	B	121	SER	3.6
2	B	191	ALA	3.5
1	A	6	ASP	3.5
2	B	192	ASP	3.5
1	A	229	LEU	3.3
1	A	136	LEU	3.2
1	A	45	MET	3.2
1	A	147	PRO	3.2
1	A	39	PRO	3.2
1	A	58	LEU	3.1
1	A	253	LYS	3.1
1	A	3	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	256	LYS	3.1
2	B	196	SER	3.0
1	A	43	PRO	3.0
1	A	275	ILE	3.0
2	B	2	MET	3.0
1	A	251	ILE	2.9
1	A	341	GLY	2.8
2	B	149	ASP	2.8
2	B	138	ILE	2.7
1	A	244	PRO	2.7
1	A	308	LEU	2.7
1	A	232	THR	2.7
3	C	104	ASP	2.7
1	A	340	THR	2.6
1	A	4	VAL	2.6
1	A	212	LEU	2.6
1	A	38	GLN	2.6
1	A	5	LYS	2.6
2	B	183	GLY	2.6
1	A	200	VAL	2.5
1	A	218	ILE	2.5
1	A	303	ASP	2.5
1	A	11	LEU	2.5
2	B	213	ASP	2.5
1	A	326	LEU	2.5
2	B	124	SER	2.5
1	A	293	ALA	2.5
1	A	220	ARG	2.4
1	A	52	THR	2.4
3	C	231	ILE	2.4
2	B	245	ALA	2.4
1	A	2	ASP	2.3
2	B	189	SER	2.3
2	B	221	SER	2.3
1	A	243	GLY	2.3
1	A	216	LEU	2.3
1	A	234	TYR	2.3
1	A	213	LEU	2.3
2	B	120	THR	2.3
1	A	33	LEU	2.3
1	A	134	LYS	2.3
1	A	127	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	53	SER	2.2
3	C	78	ILE	2.2
1	A	217	GLY	2.2
1	A	68	GLU	2.2
2	B	136	LEU	2.2
2	B	185	LEU	2.2
3	C	27	ILE	2.2
1	A	306	ASN	2.2
1	A	231	GLY	2.2
1	A	55	LEU	2.1
1	A	242	ILE	2.1
2	B	233	GLN	2.1
2	B	126	ASN	2.1
1	A	288	VAL	2.1
1	A	206	LEU	2.1
2	B	214	SER	2.1
1	A	227	GLY	2.1
1	A	199	TYR	2.1
2	B	11	SER	2.1
2	B	137	THR	2.1
3	C	72	VAL	2.0
1	A	279	ARG	2.0
2	B	129	PHE	2.0
2	B	205	THR	2.0
1	A	310	TYR	2.0
3	C	86	LYS	2.0
1	A	182	VAL	2.0
1	A	8	LYS	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 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($\text{\AA}^2$)	Q<0.9
4	ZN	B	1246	1/1	0.87	0.07	87,87,87,87	0
5	MG	A	1349	1/1	0.90	0.14	50,50,50,50	0
5	MG	A	1348	1/1	0.93	0.05	20,20,20,20	0
4	ZN	A	1347	1/1	0.94	0.07	83,83,83,83	0
4	ZN	C	1252	1/1	0.94	0.10	75,75,75,75	0
5	MG	B	1247	1/1	0.94	0.05	39,39,39,39	0
5	MG	C	1250	1/1	0.94	0.09	42,42,42,42	0
4	ZN	C	1251	1/1	0.96	0.07	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.