



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:03 AM UTC

PDB ID : 1E9N / pdb_00001e9n
Title : A second divalent metal ion in the active site of a new crystal form of human a purinic/apyrimidinic endonuclease, Ape1, and its implications for the catalytic mechanism
Authors : Beernink, P.T.; Segelke, B.W.; Rupp, B.
Deposited on : 2000-10-24
Resolution : 2.20 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

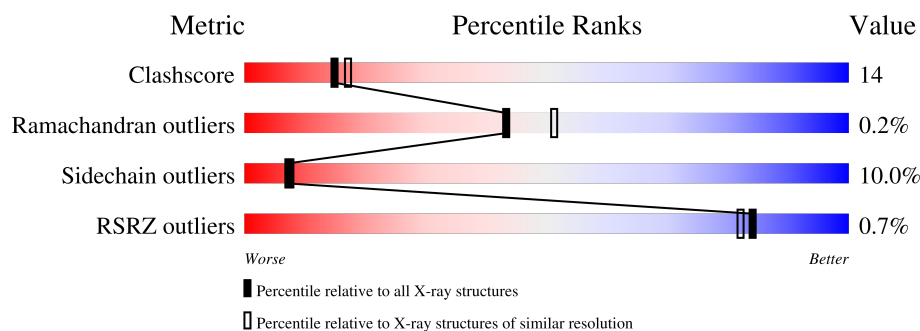
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	318	% 54% 27% 5% 14%
1	B	318	% 56% 24% 5% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4689 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-(APURINIC OR APYRIMIDINIC SITE) LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2166	1385	375	397	9			
1	B	274	Total	C	N	O	S	0	0	0
			2170	1387	375	399	9			

- Molecule 2 is LEAD (II) ION (CCD ID: PB) (formula: Pb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Pb	0	0
			2	2		
2	B	2	Total	Pb	0	0
			2	2		

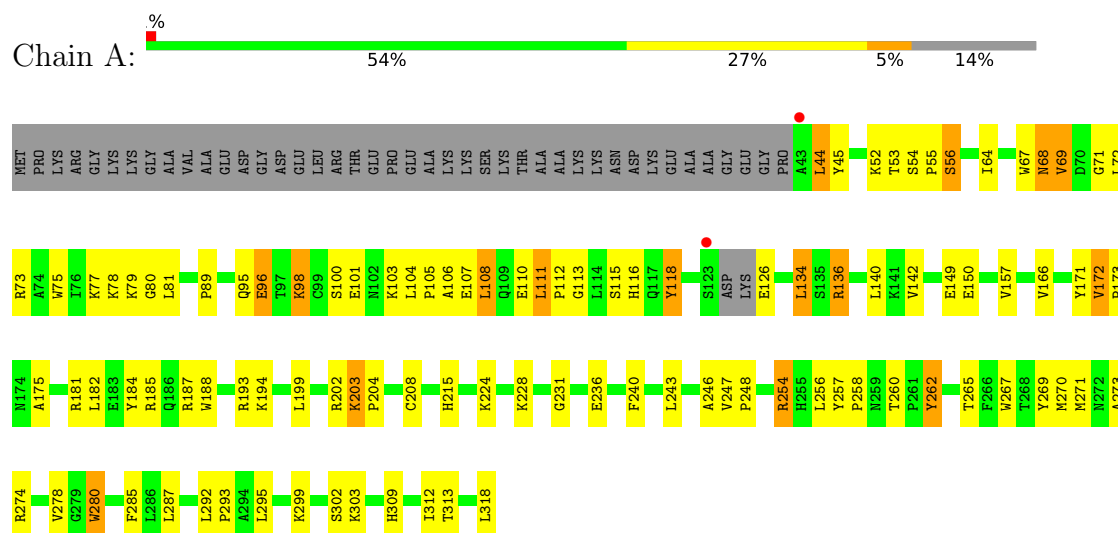
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	168	Total	O	0	0
			168	168		
3	B	181	Total	O	0	0
			181	181		

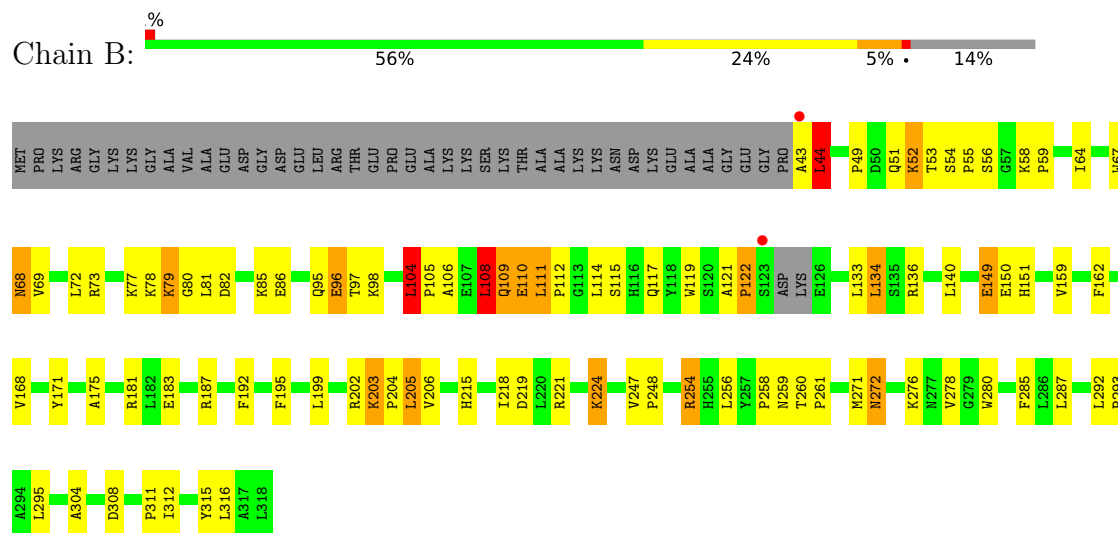
3 Residue-property plots

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: DNA-(APURINIC OR APYRIMIDINIC SITE) LYASE



• Molecule 1: DNA-(APURINIC OR APYRIMIDINIC SITE) LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.52Å 45.02Å 125.70Å 90.00° 108.03° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-2.20) 91.8 (20.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	88.58 (at 2.21Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.186 , 0.252 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 77.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4689	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.64% 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: PB

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	1.42	2/2223 (0.1%)	1.60	29/3013 (1.0%)
1	B	1.42	6/2227 (0.3%)	1.61	30/3018 (1.0%)
All	All	1.42	8/4450 (0.2%)	1.61	59/6031 (1.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	117	GLN	CA-C	-6.97	1.44	1.52
1	B	114	LEU	C-N	-5.53	1.26	1.33
1	B	49	PRO	N-CA	-5.39	1.40	1.47
1	A	184	TYR	CA-C	5.38	1.59	1.52
1	A	53	THR	CA-C	-5.25	1.46	1.52
1	B	218	ILE	C-N	5.17	1.41	1.33
1	B	151	HIS	CA-C	-5.16	1.45	1.52
1	B	64	ILE	CA-CB	-5.10	1.48	1.54

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	LEU	CA-C-N	9.12	131.24	119.84
1	B	111	LEU	C-N-CA	9.12	131.24	119.84
1	B	108	LEU	N-CA-C	8.85	123.38	112.23
1	A	111	LEU	CA-C-N	8.32	130.24	119.84
1	A	111	LEU	C-N-CA	8.32	130.24	119.84
1	A	172	VAL	N-CA-C	8.17	116.62	109.02
1	B	260	THR	CA-C-N	7.73	129.20	120.85
1	B	260	THR	C-N-CA	7.73	129.20	120.85
1	B	79	LYS	N-CA-C	7.48	121.83	111.74
1	B	271	MET	N-CA-C	7.17	121.42	112.24
1	A	115	SER	CA-C-N	-7.02	112.10	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	SER	C-N-CA	-7.02	112.10	122.41
1	B	111	LEU	O-C-N	6.89	127.40	121.20
1	B	67	TRP	N-CA-C	6.64	119.21	108.32
1	A	69	VAL	N-CA-C	6.59	122.10	113.07
1	A	257	TYR	CA-C-N	6.39	126.61	119.32
1	A	257	TYR	C-N-CA	6.39	126.61	119.32
1	B	80	GLY	CA-C-N	6.34	130.84	120.63
1	B	80	GLY	C-N-CA	6.34	130.84	120.63
1	A	273	ALA	N-CA-C	6.20	118.59	111.02
1	A	106	ALA	N-CA-C	6.14	117.98	111.28
1	B	44	LEU	N-CA-C	6.03	119.91	110.32
1	A	52	LYS	N-CA-C	6.00	119.91	112.59
1	A	80	GLY	CA-C-O	5.99	126.89	120.30
1	A	157	VAL	N-CA-C	5.99	116.92	108.17
1	B	175	ALA	CA-C-N	5.97	129.25	121.85
1	B	175	ALA	C-N-CA	5.97	129.25	121.85
1	A	116	HIS	CA-CB-CG	-5.94	107.86	113.80
1	A	204	PRO	N-CA-CB	5.92	108.57	103.31
1	B	204	PRO	N-CA-CB	5.87	108.53	103.31
1	B	78	LYS	CA-C-N	5.80	130.37	122.19
1	B	78	LYS	C-N-CA	5.80	130.37	122.19
1	A	44	LEU	N-CA-C	5.67	118.87	110.48
1	A	175	ALA	CA-C-N	5.54	128.72	121.85
1	A	175	ALA	C-N-CA	5.54	128.72	121.85
1	B	72	LEU	N-CA-C	5.47	116.94	110.97
1	B	82	ASP	CA-C-O	5.46	126.31	120.24
1	A	215	HIS	N-CA-C	5.45	116.91	110.97
1	B	68	ASN	CA-C-N	5.45	129.58	120.64
1	B	68	ASN	C-N-CA	5.45	129.58	120.64
1	B	104	LEU	N-CA-C	5.42	116.48	109.65
1	B	117	GLN	N-CA-C	5.39	117.68	108.90
1	A	111	LEU	O-C-N	5.36	127.48	121.32
1	A	246	ALA	N-CA-C	5.32	118.24	111.69
1	A	260	THR	CA-C-N	5.31	126.48	119.84
1	A	260	THR	C-N-CA	5.31	126.48	119.84
1	A	79	LYS	N-CA-C	5.31	122.11	110.80
1	A	208	CYS	CA-C-N	-5.24	115.02	121.83
1	A	208	CYS	C-N-CA	-5.24	115.02	121.83
1	A	105	PRO	N-CA-CB	5.18	108.16	103.34
1	B	122	PRO	O-C-N	5.17	128.88	123.03
1	B	67	TRP	CA-C-N	5.14	129.25	122.42
1	B	67	TRP	C-N-CA	5.14	129.25	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	TRP	N-CA-C	5.12	117.51	108.75
1	A	89	PRO	CB-CA-C	-5.09	103.21	110.75
1	B	52	LYS	N-CA-C	5.08	118.79	112.59
1	B	115	SER	N-CA-C	5.08	118.74	112.54
1	B	205	LEU	N-CA-C	5.04	117.61	109.40
1	B	110	GLU	CB-CA-C	5.01	119.28	110.37

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	2166	0	2130	62	0
1	B	2170	0	2134	57	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	168	0	0	11	0
3	B	181	0	0	10	0
All	All	4689	0	4264	119	0

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 14.

All (119) 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:71:GLY:HA2	1:A:98:LYS:HG3	1.50	0.92
1:A:78:LYS:CE	3:A:2026:HOH:O	2.34	0.75
1:B:54:SER:HB2	1:B:55:PRO:HD2	1.67	0.75
1:B:104:LEU:HD21	1:B:119:TRP:CE2	2.25	0.72
1:B:134:LEU:HD12	1:B:134:LEU:N	2.05	0.72
1:A:269:TYR:CB	1:A:270:MET:HE2	2.20	0.72
1:A:134:LEU:N	1:A:134:LEU:HD12	2.06	0.71
1:B:315:TYR:O	1:B:316:LEU:HD23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:HB3	3:A:2153:HOH:O	1.92	0.68
1:A:269:TYR:HB2	1:A:270:MET:HE2	1.76	0.68
1:B:44:LEU:HD12	3:B:2002:HOH:O	1.94	0.68
1:B:96:GLU:HG3	1:B:171:TYR:CZ	2.29	0.67
1:A:68:ASN:HD22	1:A:68:ASN:C	2.03	0.66
1:A:71:GLY:HA2	1:A:98:LYS:CG	2.24	0.66
1:A:54:SER:HB2	1:A:55:PRO:HD2	1.78	0.66
1:A:78:LYS:HE3	3:A:2026:HOH:O	1.92	0.66
1:B:108:LEU:HD12	1:B:119:TRP:CZ2	2.32	0.65
1:B:56:SER:HB3	3:B:2013:HOH:O	1.97	0.65
1:A:81:LEU:HD11	1:A:108:LEU:CD1	2.29	0.63
1:A:45:TYR:HB2	1:A:262:TYR:O	2.00	0.61
1:A:81:LEU:HD11	1:A:108:LEU:HD12	1.82	0.61
1:A:166:VAL:HG23	1:A:203:LYS:HG2	1.83	0.60
1:A:78:LYS:HG3	3:A:2026:HOH:O	2.03	0.59
1:B:121:ALA:HB1	1:B:122:PRO:HD2	1.86	0.57
1:A:118:TYR:N	1:A:118:TYR:CD1	2.72	0.57
1:A:318:LEU:HB2	3:A:2020:HOH:O	2.04	0.57
1:B:149:GLU:HG2	3:B:2069:HOH:O	2.04	0.57
1:A:95:GLN:HB3	1:A:171:TYR:HB2	1.87	0.57
1:B:162:PHE:O	1:B:203:LYS:HE3	2.05	0.57
1:A:113:GLY:O	1:A:136:ARG:HG3	2.04	0.57
1:B:81:LEU:O	1:B:85:LYS:CG	2.53	0.56
1:A:110:GLU:O	1:A:111:LEU:C	2.49	0.55
1:A:81:LEU:HB2	3:A:2029:HOH:O	2.08	0.54
1:A:172:VAL:HG13	1:A:173:PRO:HD2	1.88	0.54
1:A:96:GLU:OE2	3:A:2039:HOH:O	2.19	0.54
1:A:72:LEU:HD22	1:A:108:LEU:HD21	1.90	0.53
1:B:150:GLU:OE2	1:B:187:ARG:NH1	2.38	0.52
1:B:259:ASN:O	1:B:261:PRO:HD3	2.10	0.51
1:A:110:GLU:O	1:A:112:PRO:N	2.43	0.51
1:B:105:PRO:O	1:B:108:LEU:HB2	2.10	0.51
1:A:78:LYS:HE2	3:A:2026:HOH:O	2.03	0.51
1:A:107:GLU:H	1:A:107:GLU:CD	2.17	0.51
1:A:107:GLU:OE1	1:A:107:GLU:N	2.29	0.51
1:B:44:LEU:HD13	1:B:44:LEU:N	2.25	0.51
1:B:81:LEU:O	1:B:85:LYS:HG3	2.11	0.50
1:B:183:GLU:HB2	3:B:2087:HOH:O	2.11	0.50
1:B:308:ASP:OD1	3:B:2178:HOH:O	2.20	0.50
1:B:108:LEU:HD12	1:B:119:TRP:HZ2	1.75	0.49
1:A:68:ASN:C	1:A:68:ASN:ND2	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ALA:HB3	1:B:311:PRO:HD2	1.93	0.49
1:B:109:GLN:HG2	1:B:110:GLU:OE2	2.12	0.49
1:A:285:PHE:CD2	1:A:312:ILE:HD12	2.48	0.49
1:A:240:PHE:O	1:A:243:LEU:HB3	2.13	0.49
1:A:113:GLY:O	1:A:136:ARG:HA	2.13	0.49
1:A:292:LEU:N	1:A:293:PRO:HD2	2.28	0.49
1:B:81:LEU:O	1:B:85:LYS:HG2	2.12	0.49
1:A:101:GLU:HA	1:A:104:LEU:HG	1.95	0.48
1:A:269:TYR:HB2	1:A:270:MET:CE	2.40	0.48
1:B:136:ARG:NH2	3:B:2047:HOH:O	2.43	0.48
1:B:292:LEU:N	1:B:293:PRO:HD2	2.28	0.48
1:A:182:LEU:O	1:A:185:ARG:HB3	2.14	0.48
1:B:106:ALA:C	1:B:108:LEU:N	2.70	0.48
1:B:55:PRO:HD3	1:B:295:LEU:O	2.12	0.48
1:B:43:ALA:C	1:B:44:LEU:HD13	2.38	0.48
1:A:247:VAL:N	1:A:248:PRO:HA	2.27	0.47
1:B:272:ASN:O	1:B:276:LYS:HG3	2.15	0.47
1:B:215:HIS:HB3	1:B:219:ASP:OD2	2.14	0.47
1:B:292:LEU:N	1:B:293:PRO:CD	2.77	0.47
1:A:193:ARG:HD3	3:A:2124:HOH:O	2.13	0.47
1:B:81:LEU:HB2	3:B:2020:HOH:O	2.15	0.47
1:B:258:PRO:HD2	3:B:2141:HOH:O	2.14	0.47
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.66	0.46
1:A:111:LEU:HA	1:A:112:PRO:HD3	1.51	0.46
1:A:194:LYS:HD3	3:A:2098:HOH:O	2.15	0.46
1:B:221:ARG:HG2	1:B:278:VAL:HA	1.97	0.46
1:B:304:ALA:HB3	1:B:311:PRO:CD	2.44	0.46
1:B:254:ARG:HD3	1:B:254:ARG:HA	1.61	0.46
1:A:292:LEU:N	1:A:293:PRO:CD	2.78	0.46
1:A:270:MET:HE2	1:A:270:MET:N	2.31	0.46
1:B:192:PHE:O	1:B:195:PHE:HB3	2.16	0.46
1:B:224:LYS:HG2	3:B:2118:HOH:O	2.15	0.46
1:B:247:VAL:N	1:B:248:PRO:HA	2.29	0.46
1:A:267:TRP:CD1	1:A:274:ARG:HA	2.50	0.46
1:A:231:GLY:H	1:A:236:GLU:CD	2.24	0.46
1:A:150:GLU:OE2	1:A:187:ARG:NH1	2.48	0.45
1:B:150:GLU:OE1	1:B:187:ARG:NH1	2.49	0.45
1:A:134:LEU:N	1:A:134:LEU:CD1	2.79	0.44
1:A:278:VAL:O	1:A:278:VAL:HG12	2.17	0.44
1:B:54:SER:HB2	1:B:55:PRO:CD	2.43	0.44
1:B:59:PRO:HD2	3:B:2014:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:THR:O	1:A:309:HIS:HA	2.18	0.44
1:A:64:ILE:O	1:A:313:THR:HA	2.18	0.44
1:B:111:LEU:HA	1:B:112:PRO:HD3	1.49	0.44
1:A:280:TRP:CD1	1:A:280:TRP:N	2.85	0.44
1:B:133:LEU:C	1:B:133:LEU:HD23	2.43	0.44
1:B:68:ASN:OD1	1:B:68:ASN:C	2.61	0.44
1:B:159:VAL:HG22	1:B:168:VAL:HG22	1.99	0.43
1:A:73:ARG:NH1	1:A:103:LYS:O	2.42	0.43
1:A:55:PRO:HD3	1:A:295:LEU:O	2.18	0.43
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.64	0.42
1:B:256:LEU:C	1:B:258:PRO:HD3	2.44	0.42
1:B:285:PHE:CD2	1:B:312:ILE:HD12	2.54	0.42
1:A:188:TRP:CD1	1:A:188:TRP:C	2.97	0.42
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.60	0.42
1:A:254:ARG:HD3	1:A:254:ARG:HA	1.58	0.42
1:A:69:VAL:HB	1:A:75:TRP:CG	2.54	0.42
1:B:81:LEU:HA	1:B:81:LEU:HD23	1.58	0.42
1:B:104:LEU:HD21	1:B:119:TRP:CD2	2.54	0.42
1:B:205:LEU:HD12	1:B:206:VAL:N	2.35	0.42
1:B:73:ARG:HG2	1:B:105:PRO:HG3	2.02	0.41
1:B:51:GLN:HE21	1:B:53:THR:H	1.68	0.41
1:A:299:LYS:HE3	1:A:299:LYS:HB3	1.75	0.41
1:A:73:ARG:HG3	3:A:2041:HOH:O	2.21	0.41
1:B:97:THR:O	1:B:98:LYS:HB2	2.21	0.41
1:B:121:ALA:HB1	1:B:122:PRO:CD	2.51	0.41
1:A:118:TYR:CE2	1:A:142:VAL:HG21	2.56	0.41
1:A:256:LEU:C	1:A:258:PRO:HD3	2.46	0.41
1:B:69:VAL:HG22	1:B:95:GLN:O	2.20	0.41
1:A:54:SER:HB2	1:A:55:PRO:CD	2.49	0.40

There are no symmetry-related clashes.

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	270/318 (85%)	256 (95%)	13 (5%)	1 (0%)	30	34
1	B	270/318 (85%)	261 (97%)	9 (3%)	0	100	100
All	All	540/636 (85%)	517 (96%)	22 (4%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	TYR

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	230/266 (86%)	205 (89%)	25 (11%)	6	6
1	B	231/266 (87%)	210 (91%)	21 (9%)	9	9
All	All	461/532 (87%)	415 (90%)	46 (10%)	7	7

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

Mol	Chain	Res	Type
1	A	44	LEU
1	A	56	SER
1	A	68	ASN
1	A	77	LYS
1	A	96	GLU
1	A	98	LYS
1	A	100	SER
1	A	108	LEU
1	A	118	TYR
1	A	126	GLU
1	A	134	LEU
1	A	136	ARG
1	A	140	LEU
1	A	149	GLU
1	A	181	ARG

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Mol	Chain	Res	Type
1	A	202	ARG
1	A	203	LYS
1	A	224	LYS
1	A	228	LYS
1	A	254	ARG
1	A	271	MET
1	A	280	TRP
1	A	287	LEU
1	A	302	SER
1	A	303	LYS
1	B	44	LEU
1	B	52	LYS
1	B	58	LYS
1	B	77	LYS
1	B	79	LYS
1	B	86	GLU
1	B	96	GLU
1	B	104	LEU
1	B	108	LEU
1	B	109	GLN
1	B	134	LEU
1	B	140	LEU
1	B	149	GLU
1	B	181	ARG
1	B	202	ARG
1	B	203	LYS
1	B	224	LYS
1	B	254	ARG
1	B	272	ASN
1	B	280	TRP
1	B	287	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	68	ASN
1	A	153	GLN
1	A	229	ASN
1	A	255	HIS
1	B	51	GLN
1	B	109	GLN

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Mol	Chain	Res	Type
1	B	116	HIS
1	B	153	GLN
1	B	186	GLN
1	B	229	ASN
1	B	272	ASN
1	B	277	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 4 ligands modelled in this entry, 4 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 [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	274/318 (86%)	-0.37	2 (0%) 84 82	19, 32, 65, 80	0
1	B	274/318 (86%)	-0.45	2 (0%) 84 82	19, 31, 61, 78	0
All	All	548/636 (86%)	-0.41	4 (0%) 84 82	19, 32, 64, 80	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	SER	4.0
1	B	123	SER	2.9
1	A	43	ALA	2.5
1	B	43	ALA	2.4

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	PB	A	1319	1/1	0.96	0.05	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PB	B	1320	1/1	0.98	0.04	58,58,58,58	0
2	PB	A	1320	1/1	0.99	0.02	56,56,56,56	0
2	PB	B	1319	1/1	1.00	0.02	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.