Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:09 PM GMT

PDB ID	:	1E9N
Title	:	A SECOND DIVALENT METAL ION IN THE ACTIVE SITE OF A NEW CRYSTAL FORM OF HUMAN APURINIC/APYRIMIDINIC ENDONUCLEASE, APE1, AND ITS IMPLICATIONS FOR THE CATALYTIC MECHANISM
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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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

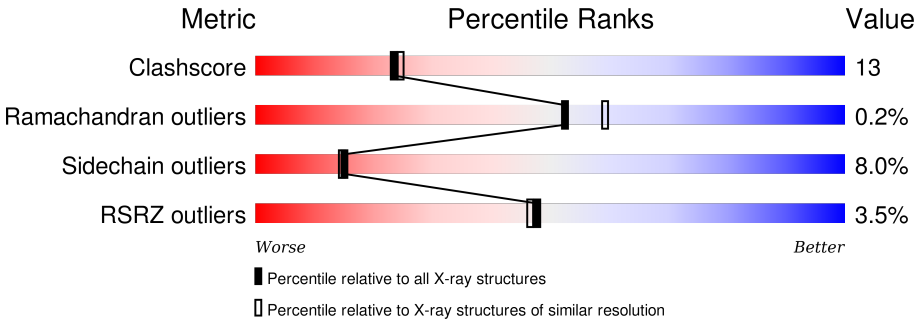
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	4% 55% 26% 14%
1	B	318	2% 56% 26% 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 (three-letter code: PB) (formula: Pb).

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

- Molecule 3 is water.

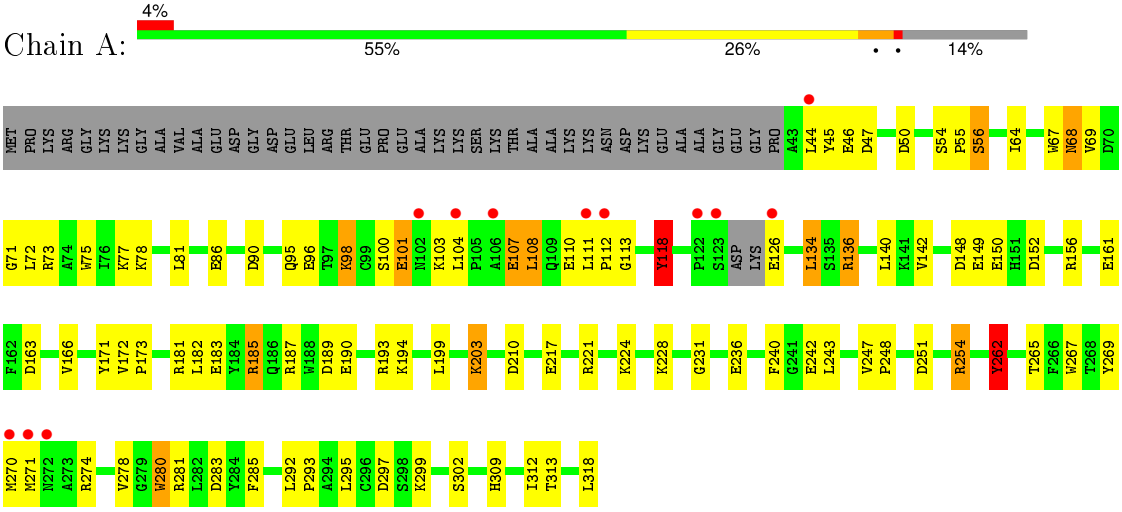
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	168	Total	O	0	0
			168	168		
3	B	181	Total	O	0	0
			181	181		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

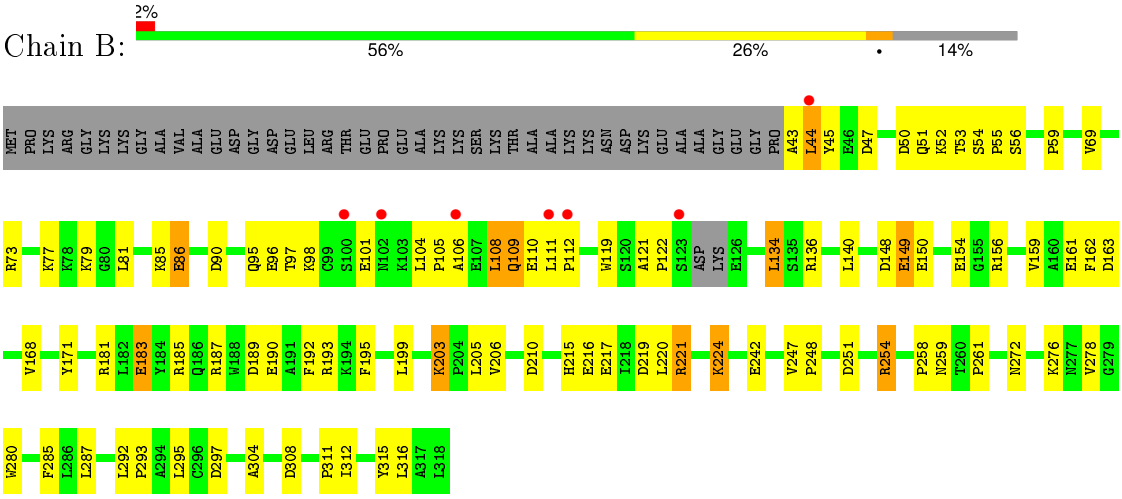
- Molecule 1: DNA-(APURINIC OR APYRIMIDINIC SITE) LYASE

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

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 12.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-2.20) 92.5 (12.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	88.58 (at 2.21Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.186 , 0.252 0.191 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 64.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 34641 reflections	Xtriage
F_o,F_c correlation	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.10	9/2223 (0.4%)	1.36	26/3013 (0.9%)
1	B	1.11	9/2227 (0.4%)	1.35	21/3018 (0.7%)
All	All	1.11	18/4450 (0.4%)	1.36	47/6031 (0.8%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	183	GLU	CD-OE2	7.60	1.34	1.25
1	A	183	GLU	CD-OE2	7.49	1.33	1.25
1	A	107	GLU	CD-OE2	7.28	1.33	1.25
1	B	101	GLU	CD-OE2	7.11	1.33	1.25
1	B	86	GLU	CD-OE2	7.07	1.33	1.25
1	A	101	GLU	CD-OE2	6.81	1.33	1.25
1	B	217	GLU	CD-OE2	6.42	1.32	1.25
1	B	154	GLU	CD-OE2	6.26	1.32	1.25
1	B	242	GLU	CD-OE2	6.03	1.32	1.25
1	A	161	GLU	CD-OE2	5.58	1.31	1.25
1	A	46	GLU	CD-OE2	5.46	1.31	1.25
1	B	161	GLU	CD-OE2	5.42	1.31	1.25
1	B	190	GLU	CD-OE2	5.41	1.31	1.25
1	A	242	GLU	CD-OE2	5.29	1.31	1.25
1	A	217	GLU	CD-OE2	5.28	1.31	1.25
1	B	216	GLU	CD-OE2	5.18	1.31	1.25
1	A	86	GLU	CD-OE2	5.12	1.31	1.25
1	A	190	GLU	CD-OE2	5.09	1.31	1.25

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	251	ASP	CB-CG-OD2	-10.20	109.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	251	ASP	CB-CG-OD1	8.75	126.18	118.30
1	B	210	ASP	CB-CG-OD2	-8.62	110.54	118.30
1	A	210	ASP	CB-CG-OD2	-8.61	110.55	118.30
1	B	156	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	A	47	ASP	CB-CG-OD1	8.02	125.52	118.30
1	B	193	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	47	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	A	156	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	156	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	B	185	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	118	TYR	CB-CG-CD2	-7.21	116.67	121.00
1	B	193	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	B	210	ASP	CB-CG-OD1	7.03	124.63	118.30
1	A	251	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	A	90	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	A	148	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	A	67	TRP	CD1-CG-CD2	-6.90	100.78	106.30
1	A	251	ASP	CB-CG-OD1	6.75	124.37	118.30
1	A	221	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	B	50	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	A	163	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	A	185	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	B	297	ASP	CB-CG-OD1	6.38	124.04	118.30
1	B	47	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	B	90	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	A	281	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	283	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	A	90	ASP	CB-CG-OD1	5.84	123.56	118.30
1	B	148	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	210	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	262	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	A	189	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	152	ASP	CB-CG-OD2	-5.50	113.36	118.30
1	A	281	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	297	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	50	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	297	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	A	50	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	287	LEU	CB-CA-C	-5.27	100.18	110.20
1	B	163	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	221	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	47	ASP	CB-CG-OD1	5.15	122.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	189	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	A	148	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	50	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	B	45	TYR	CB-CG-CD1	-5.04	117.97	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	60	0
1	B	2170	0	2134	54	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	114	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 13.

All (114) 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:N	1:B:134:LEU:HD12	2.05	0.72
1:A:134:LEU:HD12	1:A:134:LEU:N	2.06	0.71
1:B:315:TYR:O	1:B:316:LEU:HD23	1.92	0.69
1:A:56:SER:HB3	3:A:2153:HOH:O	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:68:ASN:HD22	1:A:68:ASN:C	2.03	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:CD1	1:A:118:TYR:N	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: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:269:TYR:HB2	1:A:270:MET:HE2	1.89	0.53
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:N	1:A:107:GLU:OE1	2.29	0.51
1:B:44:LEU:HD13	1:B:44:LEU:N	2.25	0.51
1:A:269:TYR:HB3	1:A:270:MET:HE1	1.93	0.51
1:B:81:LEU:O	1:B:85:LYS:HG3	2.11	0.50
1:A:269:TYR:HB2	1:A:270:MET:CE	2.40	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:A:110:GLU:O	1:A:111:LEU:C	2.49	0.50
1:B:108:LEU:HD12	1:B:119:TRP:HZ2	1.75	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:81:LEU:O	1:B:85:LYS:HG2	2.12	0.49
1:A:292:LEU:N	1:A:293:PRO:HD2	2.28	0.49
1:A:101:GLU:HA	1:A:104:LEU:HG	1.95	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:55:PRO:HD3	1:B:295:LEU:O	2.12	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:292:LEU:N	1:B:293:PRO:CD	2.77	0.47
1:B:215:HIS:HB3	1:B:219:ASP:OD2	2.14	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:B:304:ALA:HB3	1:B:311:PRO:CD	2.44	0.46
1:B:221:ARG:HG2	1:B:278:VAL:HA	1.97	0.46
1:A:194:LYS:HD3	3:A:2098:HOH:O	2.15	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:B:224:LYS:HG2	3:B:2118:HOH:O	2.15	0.46
1:B:192:PHE:O	1:B:195:PHE:HB3	2.16	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:150:GLU:OE2	1:A:187:ARG:NH1	2.48	0.45
1:A:68:ASN:ND2	1:A:68:ASN:C	2.70	0.45
1:B:150:GLU:OE1	1:B:187:ARG:NH1	2.49	0.45
1:B:54:SER:HB2	1:B:55:PRO:CD	2.43	0.44
1:A:134:LEU:CD1	1:A:134:LEU:N	2.79	0.44
1:B:59:PRO:HD2	3:B:2014:HOH:O	2.18	0.44
1:A:278:VAL:O	1:A:278:VAL:HG12	2.17	0.44
1:A:265:THR:O	1:A:309:HIS:HA	2.18	0.44
1:A:269:TYR:CB	1:A:270:MET:HE1	2.48	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:106:ALA:C	1:B:108:LEU:N	2.70	0.43
1:B:159:VAL:HG22	1:B:168:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ARG:NH1	1:A:103:LYS:O	2.42	0.43
1:B:43:ALA:C	1:B:44:LEU:HD13	2.38	0.43
1:A:55:PRO:HD3	1:A:295:LEU:O	2.18	0.43
1:A:269:TYR:CB	1:A:270:MET:CE	2.97	0.43
1:B:285:PHE:CD2	1:B:312:ILE:HD12	2.54	0.42
1:B:199:LEU:HA	1:B:199:LEU:HD23	1.64	0.42
1:A:254:ARG:HA	1:A:254:ARG:HD3	1.58	0.42
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.60	0.42
1:B:104:LEU:HD21	1:B:119:TRP:CD2	2.54	0.42
1:B:81:LEU:HA	1:B:81:LEU:HD23	1.58	0.42
1:A:69:VAL:HB	1:A:75:TRP:CG	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:HB3	1:A:299:LYS:HE3	1.75	0.41
1:B:121:ALA:HB1	1:B:122:PRO:CD	2.51	0.41
1:A:73:ARG:HG3	3:A:2041:HOH:O	2.21	0.41
1:A:231:GLY:H	1:A:236:GLU:CD	2.24	0.41
1:B:97:THR:O	1:B:98:LYS:HB2	2.21	0.41
1:A:118:TYR:CE2	1:A:142:VAL:HG21	2.56	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 (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	270/318 (85%)	256 (95%)	13 (5%)	1 (0%)	39 42
1	B	270/318 (85%)	261 (97%)	9 (3%)	0	100 100
All	All	540/636 (85%)	517 (96%)	22 (4%)	1 (0%)	52 59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	TYR

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	230/266 (86%)	209 (91%)	21 (9%)	12 11
1	B	231/266 (87%)	215 (93%)	16 (7%)	19 20
All	All	461/532 (87%)	424 (92%)	37 (8%)	15 15

All (37) 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	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
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	302	SER
1	B	44	LEU

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Mol	Chain	Res	Type
1	B	52	LYS
1	B	77	LYS
1	B	79	LYS
1	B	86	GLU
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	203	LYS
1	B	220	LEU
1	B	224	LYS
1	B	254	ARG
1	B	280	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	68	ASN
1	A	153	GLN
1	A	212	ASN
1	A	229	ASN
1	A	255	HIS
1	B	51	GLN
1	B	109	GLN
1	B	116	HIS
1	B	153	GLN
1	B	212	ASN
1	B	229	ASN
1	B	272	ASN
1	B	277	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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, 95^{th} 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%)	-0.10	12 (4%) 38 37	19, 32, 65, 80	0
1	B	274/318 (86%)	-0.19	7 (2%) 59 58	19, 31, 61, 78	0
All	All	548/636 (86%)	-0.15	19 (3%) 48 46	19, 32, 64, 80	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	MET	4.9
1	A	270	MET	4.7
1	B	44	LEU	3.9
1	B	123	SER	3.3
1	A	44	LEU	3.1
1	A	112	PRO	3.0
1	B	106	ALA	2.9
1	B	102	ASN	2.7
1	B	100	SER	2.6
1	A	102	ASN	2.5
1	A	106	ALA	2.4
1	A	123	SER	2.3
1	B	112	PRO	2.3
1	A	272	ASN	2.3
1	A	126	GLU	2.2
1	A	104	LEU	2.2
1	A	111	LEU	2.2
1	A	122	PRO	2.0
1	B	111	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	PB	A	1320	1/1	1.00	0.05	-2.92	56,56,56,56	0
2	PB	B	1319	1/1	1.00	0.03	-3.84	53,53,53,53	0
2	PB	B	1320	1/1	0.99	0.03	-	58,58,58,58	0
2	PB	A	1319	1/1	0.98	0.05	-	63,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.