



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:13 pm BST

PDB ID : 2AMX
Title : Crystal structure of Plasmodium Yoelii Adenosine deaminase (PY02076)
Authors : Dong, A.; Vedadi, M.; Wasney, G.; Zhao, Y.; Lew, J.; Alam, Z.; Melone, M.; Koeieradzki, I.; Edwards, A.M.; Arrowsmith, C.H.; Weigelt, J.; Sundstrom, M.; Bochkarev, A.; Hui, R.; Amani, M.; Structural Genomics Consortium (SGC)
Deposited on : 2005-08-10
Resolution : 2.02 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

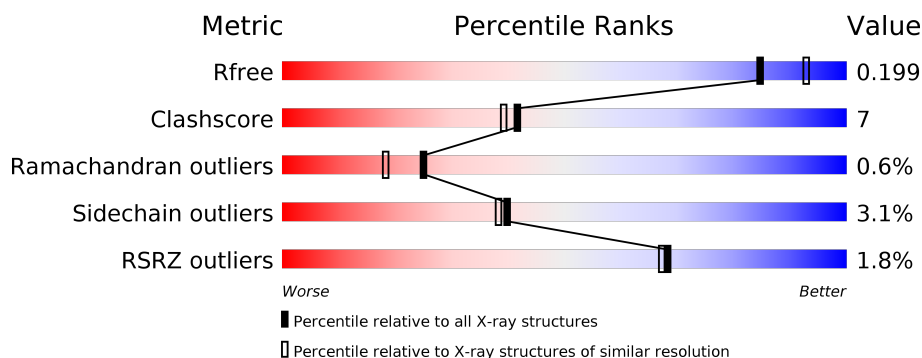
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 on 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	376	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 84%, grey 5%);"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 84%, grey 5%);"></div> </div> <div> 1% 84% 11% • • </div> </div>
1	B	376	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 2%, orange 2%, yellow 13%, green 78%, grey 5%);"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 2%, orange 2%, yellow 13%, green 78%, grey 5%);"></div> </div> <div> 2% 78% 13% • 5% </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UNX	A	2000	-	-	-	X
3	UNX	A	2002	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6372 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 adenosine deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2958	1900	499	549	10			
1	B	356	Total	C	N	O	S	0	0	0
			2908	1870	489	539	10			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP Q7RMV2
A	2	GLY	-	CLONING ARTIFACT	UNP Q7RMV2
A	3	SER	-	CLONING ARTIFACT	UNP Q7RMV2
A	4	SER	-	CLONING ARTIFACT	UNP Q7RMV2
A	5	HIS	-	EXPRESSION TAG	UNP Q7RMV2
A	6	HIS	-	EXPRESSION TAG	UNP Q7RMV2
A	7	HIS	-	EXPRESSION TAG	UNP Q7RMV2
A	8	HIS	-	EXPRESSION TAG	UNP Q7RMV2
A	9	HIS	-	EXPRESSION TAG	UNP Q7RMV2
A	10	HIS	-	EXPRESSION TAG	UNP Q7RMV2
A	11	SER	-	CLONING ARTIFACT	UNP Q7RMV2
A	12	SER	-	CLONING ARTIFACT	UNP Q7RMV2
A	13	GLY	-	CLONING ARTIFACT	UNP Q7RMV2
A	14	LEU	-	CLONING ARTIFACT	UNP Q7RMV2
A	15	VAL	-	CLONING ARTIFACT	UNP Q7RMV2
A	16	PRO	-	CLONING ARTIFACT	UNP Q7RMV2
A	17	ARG	-	CLONING ARTIFACT	UNP Q7RMV2
A	18	GLY	-	CLONING ARTIFACT	UNP Q7RMV2
A	19	SER	-	CLONING ARTIFACT	UNP Q7RMV2
B	1	MET	-	CLONING ARTIFACT	UNP Q7RMV2
B	2	GLY	-	CLONING ARTIFACT	UNP Q7RMV2
B	3	SER	-	CLONING ARTIFACT	UNP Q7RMV2
B	4	SER	-	CLONING ARTIFACT	UNP Q7RMV2
B	5	HIS	-	EXPRESSION TAG	UNP Q7RMV2
B	6	HIS	-	EXPRESSION TAG	UNP Q7RMV2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	EXPRESSION TAG	UNP Q7RMV2
B	8	HIS	-	EXPRESSION TAG	UNP Q7RMV2
B	9	HIS	-	EXPRESSION TAG	UNP Q7RMV2
B	10	HIS	-	EXPRESSION TAG	UNP Q7RMV2
B	11	SER	-	CLONING ARTIFACT	UNP Q7RMV2
B	12	SER	-	CLONING ARTIFACT	UNP Q7RMV2
B	13	GLY	-	CLONING ARTIFACT	UNP Q7RMV2
B	14	LEU	-	CLONING ARTIFACT	UNP Q7RMV2
B	15	VAL	-	CLONING ARTIFACT	UNP Q7RMV2
B	16	PRO	-	CLONING ARTIFACT	UNP Q7RMV2
B	17	ARG	-	CLONING ARTIFACT	UNP Q7RMV2
B	18	GLY	-	CLONING ARTIFACT	UNP Q7RMV2
B	19	SER	-	CLONING ARTIFACT	UNP Q7RMV2

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total X 1 1	0	0
3	A	5	Total X 5 5	0	0

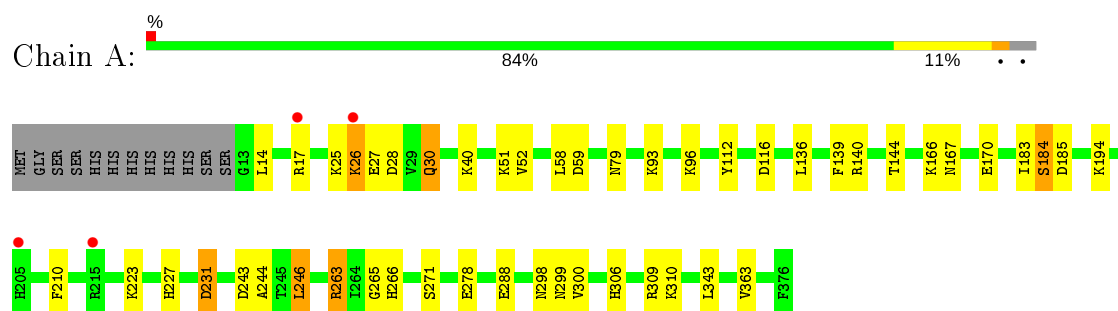
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	233	Total O 233 233	0	0
4	B	262	Total O 262 262	0	0

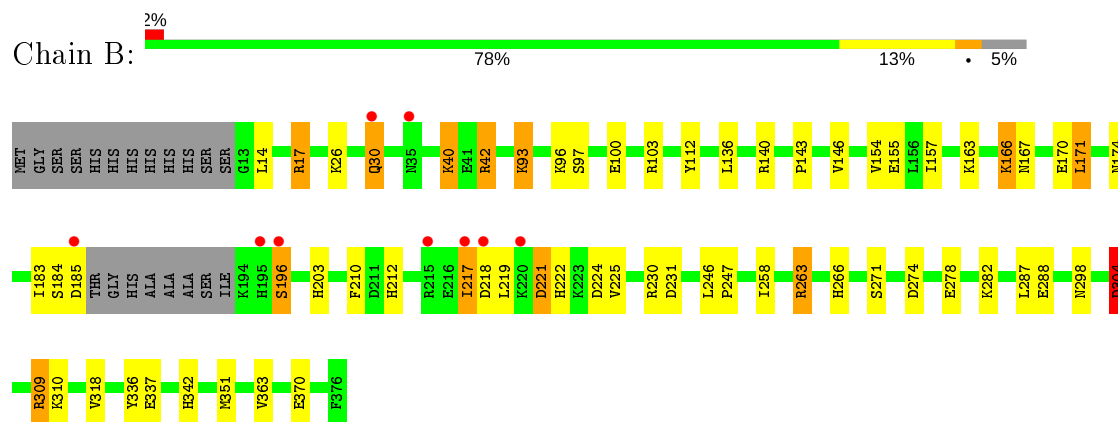
3 Residue-property plots [i](#)

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



- Molecule 1: adenosine deaminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.72Å 90.33Å 137.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.90 – 2.02 42.90 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.90-2.02) 99.7 (42.90-2.02)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.196 , 0.246 0.196 , 0.199	Depositor DCC
R_{free} test set	803 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6372	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 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: UNX, CO

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	0.87	0/3024	0.83	7/4080 (0.2%)
1	B	0.98	5/2972 (0.2%)	1.16	10/4007 (0.2%)
All	All	0.92	5/5996 (0.1%)	1.01	17/8087 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	ASP	CB-CG	10.06	1.72	1.51
1	B	304	ASP	CG-OD1	8.67	1.45	1.25
1	B	166	LYS	CE-NZ	6.51	1.65	1.49
1	B	166	LYS	CD-CE	5.52	1.65	1.51
1	B	336	TYR	CE1-CZ	5.16	1.45	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	ASP	CB-CG-OD1	31.60	146.74	118.30
1	B	304	ASP	CB-CG-OD2	-26.41	94.53	118.30
1	B	263	ARG	NE-CZ-NH2	-18.32	111.14	120.30
1	B	263	ARG	NE-CZ-NH1	15.36	127.98	120.30
1	A	263	ARG	NE-CZ-NH2	-13.68	113.46	120.30
1	A	263	ARG	NE-CZ-NH1	10.15	125.37	120.30
1	A	263	ARG	CB-CG-CD	-6.56	94.54	111.60
1	A	309	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	263	ARG	CB-CG-CD	-6.18	95.52	111.60
1	B	42	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	309	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	304	ASP	CB-CA-C	5.87	122.13	110.40
1	B	224	ASP	CB-CG-OD1	5.63	123.36	118.30
1	B	171	LEU	CA-CB-CG	5.31	127.51	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	A	116	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	231	ASP	CB-CG-OD1	5.11	122.90	118.30

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	2958	0	2939	31	2
1	B	2908	0	2891	49	3
2	A	2	0	0	0	0
2	B	3	0	0	0	0
3	A	5	0	0	1	0
3	B	1	0	0	1	0
4	A	233	0	0	6	0
4	B	262	0	0	11	0
All	All	6372	0	5830	82	3

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 7.

All (82) 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)
3:B:2005:UNX:UNK	4:B:2019:HOH:O	1.44	0.96
1:A:271:SER:O	1:A:310:LYS:HE2	1.67	0.94
1:B:26:LYS:HA	1:B:351:MET:CE	2.00	0.92
1:A:30:GLN:H	1:A:30:GLN:CD	1.76	0.89
1:B:219:LEU:HD22	1:B:222:HIS:HD2	1.40	0.86
3:A:2004:UNX:UNK	4:A:2047:HOH:O	1.56	0.85
1:B:26:LYS:HA	1:B:351:MET:HE2	1.59	0.82
1:B:219:LEU:HD22	1:B:222:HIS:CD2	2.18	0.78
1:B:17:ARG:HH11	1:B:17:ARG:CG	1.96	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ARG:NH1	1:B:17:ARG:HG3	2.01	0.74
1:B:263:ARG:HD2	1:B:288:GLU:OE2	1.87	0.73
1:B:17:ARG:HH11	1:B:17:ARG:HG3	1.53	0.73
1:B:26:LYS:HA	1:B:351:MET:HE3	1.72	0.71
1:B:96:LYS:O	1:B:298:ASN:ND2	2.23	0.71
1:A:27:GLU:O	1:A:30:GLN:NE2	2.24	0.69
1:B:184:SER:HB3	1:B:210:PHE:CZ	2.28	0.69
1:B:155:GLU:OE2	1:B:203:HIS:HE1	1.78	0.66
1:B:136:LEU:HD11	1:B:363:VAL:HG11	1.77	0.65
1:A:30:GLN:HG3	4:A:2195:HOH:O	1.96	0.65
1:A:30:GLN:CD	1:A:30:GLN:N	2.47	0.65
1:B:274:ASP:O	1:B:278:GLU:HG2	1.97	0.65
1:A:144:THR:HG21	1:A:185:ASP:HB3	1.78	0.64
1:B:304:ASP:OD1	1:B:342:HIS:ND1	2.18	0.64
1:A:166:LYS:HE2	1:A:167:ASN:ND2	2.12	0.64
1:B:100:GLU:CD	1:B:103:ARG:HE	2.01	0.64
1:B:40:LYS:HE3	4:B:2223:HOH:O	1.97	0.64
1:B:185:ASP:HB2	1:B:196:SER:HB2	1.79	0.63
1:A:96:LYS:O	1:A:298:ASN:ND2	2.28	0.62
1:B:42:ARG:HD2	1:B:337:GLU:OE1	2.00	0.61
1:B:203:HIS:HD2	4:B:2074:HOH:O	1.85	0.59
1:B:17:ARG:NH1	1:B:17:ARG:CG	2.59	0.59
1:B:271:SER:HB2	1:B:310:LYS:HD3	1.84	0.58
1:B:185:ASP:H	1:B:196:SER:HB2	1.68	0.57
1:A:79:ASN:ND2	4:A:2144:HOH:O	2.35	0.57
1:A:263:ARG:HD2	1:A:288:GLU:OE2	2.06	0.55
1:B:304:ASP:HB2	4:B:2036:HOH:O	2.04	0.55
1:B:309:ARG:HD3	4:B:2102:HOH:O	2.07	0.55
1:A:27:GLU:C	1:A:30:GLN:HE22	2.10	0.55
1:B:230:ARG:NH1	1:B:231:ASP:OD1	2.39	0.55
1:A:194:LYS:HE3	4:A:2233:HOH:O	2.07	0.54
1:A:52:VAL:HG22	1:A:136:LEU:HB3	1.89	0.54
1:B:221:ASP:N	1:B:221:ASP:OD1	2.29	0.53
1:A:25:LYS:HG3	1:A:28:ASP:OD2	2.09	0.53
1:A:136:LEU:HD11	1:A:363:VAL:HG11	1.91	0.52
1:A:184:SER:HB2	1:A:210:PHE:CZ	2.44	0.52
1:B:174:ASN:ND2	1:B:370:GLU:OE2	2.38	0.52
1:B:93:LYS:HD2	1:B:93:LYS:N	2.27	0.50
1:B:258:ILE:O	4:B:2253:HOH:O	2.19	0.50
1:B:26:LYS:HD2	4:B:2155:HOH:O	2.12	0.49
1:A:244:ALA:H	1:A:299:ASN:ND2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LYS:HA	1:B:166:LYS:HE2	1.94	0.49
1:B:30:GLN:HB2	4:B:2070:HOH:O	2.13	0.49
1:A:26:LYS:HG3	4:A:2226:HOH:O	2.11	0.49
1:A:265:GLY:HA2	1:A:288:GLU:HB2	1.94	0.49
1:B:212:HIS:CE1	1:B:219:LEU:HD21	2.48	0.48
1:A:243:ASP:HB3	1:A:246:LEU:HD22	1.95	0.48
1:A:306:HIS:HB3	1:A:343:LEU:HD11	1.95	0.47
1:B:184:SER:HA	1:B:196:SER:HB3	1.96	0.47
1:A:140:ARG:HG3	1:A:183:ILE:HD11	1.98	0.46
1:A:30:GLN:CG	4:A:2195:HOH:O	2.61	0.46
1:B:154:VAL:HA	1:B:157:ILE:HD12	1.98	0.46
1:B:155:GLU:OE2	1:B:203:HIS:CE1	2.65	0.45
1:A:166:LYS:O	1:A:170:GLU:HG3	2.16	0.45
1:B:166:LYS:O	1:B:170:GLU:HG3	2.17	0.45
1:B:140:ARG:HG3	1:B:183:ILE:HD11	2.00	0.44
1:B:225:VAL:HG12	4:B:2232:HOH:O	2.18	0.43
1:A:223:LYS:HB3	1:A:223:LYS:HE3	1.77	0.42
1:B:246:LEU:HA	1:B:247:PRO:HD3	1.76	0.42
1:A:51:LYS:HE2	1:A:51:LYS:HB2	1.87	0.42
1:B:166:LYS:HE2	1:B:166:LYS:HB3	1.90	0.42
1:B:143:PRO:HD2	4:B:2117:HOH:O	2.19	0.41
1:A:244:ALA:H	1:A:299:ASN:HD22	1.69	0.41
1:A:58:LEU:HB2	1:A:139:PHE:HB3	2.01	0.41
1:B:112:TYR:CD1	1:B:146:VAL:HG13	2.55	0.41
1:A:59:ASP:O	1:A:112:TYR:OH	2.32	0.41
1:B:287:LEU:HB2	1:B:318:VAL:HG12	2.03	0.40
1:B:42:ARG:NH1	1:B:337:GLU:OE2	2.54	0.40
1:A:300:VAL:HG11	1:A:306:HIS:CD2	2.56	0.40
1:B:103:ARG:HD2	4:B:2244:HOH:O	2.20	0.40
1:B:185:ASP:H	1:B:196:SER:CB	2.33	0.40
1:A:271:SER:O	1:A:310:LYS:CE	2.53	0.40
1:B:167:ASN:HD22	1:B:167:ASN:HA	1.67	0.40

All (3) 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)
1:A:227:HIS:NE2	1:B:304:ASP:OD1[4_555]	1.82	0.38
1:B:17:ARG:NH2	1:B:282:LYS:O[4_445]	1.91	0.29
1:A:231:ASP:OD1	1:B:304:ASP:OD1[4_555]	2.01	0.19

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	362/376 (96%)	352 (97%)	8 (2%)	2 (1%)	25	18
1	B	352/376 (94%)	343 (97%)	7 (2%)	2 (1%)	25	18
All	All	714/752 (95%)	695 (97%)	15 (2%)	4 (1%)	25	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	266	HIS
1	B	217	ILE
1	B	266	HIS

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	327/338 (97%)	319 (98%)	8 (2%)	49	49
1	B	323/338 (96%)	311 (96%)	12 (4%)	34	31
All	All	650/676 (96%)	630 (97%)	20 (3%)	40	38

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	17	ARG

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Mol	Chain	Res	Type
1	A	30	GLN
1	A	40	LYS
1	A	93	LYS
1	A	184	SER
1	A	246	LEU
1	A	278	GLU
1	B	14	LEU
1	B	17	ARG
1	B	30	GLN
1	B	40	LYS
1	B	93	LYS
1	B	97	SER
1	B	171	LEU
1	B	196	SER
1	B	217	ILE
1	B	218	ASP
1	B	221	ASP
1	B	304	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	167	ASN
1	A	222	HIS
1	A	260	ASN
1	A	299	ASN
1	B	75	ASN
1	B	167	ASN
1	B	203	HIS

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 11 ligands modelled in this entry, 6 are unknown and 5 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	364/376 (96%)	-0.10	4 (1%) 80 80	15, 25, 42, 56	0
1	B	356/376 (94%)	-0.01	9 (2%) 57 57	13, 23, 43, 53	0
All	All	720/752 (95%)	-0.06	13 (1%) 68 67	13, 24, 43, 56	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	HIS	4.0
1	B	35	ASN	3.6
1	B	185	ASP	3.5
1	A	215	ARG	3.4
1	B	218	ASP	3.3
1	B	217	ILE	3.2
1	B	196	SER	3.0
1	B	215	ARG	2.9
1	B	30	GLN	2.8
1	A	17	ARG	2.6
1	A	26	LYS	2.5
1	A	205	HIS	2.3
1	B	220	LYS	2.2

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 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. 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(\AA^2)	Q<0.9
3	UNX	A	2003	1/1	-0.02	0.36	500,500,500,500	0
3	UNX	A	2002	1/1	0.44	0.54	500,500,500,500	0
3	UNX	A	2000	1/1	0.46	3.44	493,493,493,493	0
3	UNX	A	2001	1/1	0.88	0.32	500,500,500,500	0
2	CO	A	1002	1/1	0.93	0.24	84,84,84,84	0
2	CO	B	1002	1/1	0.96	0.08	68,68,68,68	0
3	UNX	A	2004	1/1	0.97	1.05	500,500,500,500	0
2	CO	B	1001	1/1	0.97	0.07	44,44,44,44	0
3	UNX	B	2005	1/1	0.99	1.06	500,500,500,500	0
2	CO	A	1000	1/1	0.99	0.08	24,24,24,24	0
2	CO	B	1000	1/1	0.99	0.08	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.