Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:38 PM GMT

PDB ID	:	4TYP
Title	:	Crystal structure of an adenylate kinase mutant–AKm1
Authors	:	Moon, S.; Bae, E.
Deposited on	:	2014-07-09
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
http://wwpdb.org/validation/2016/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:

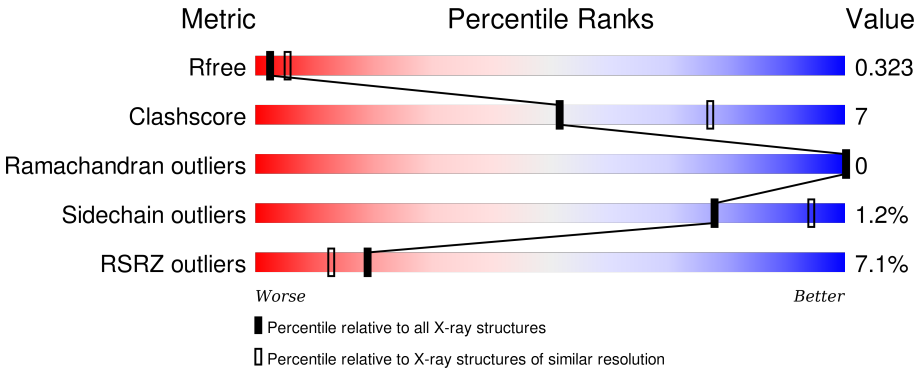
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 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	217	11% 84% 10% • •
1	B	217	3% 87% 7% • 5%
1	C	217	6% 80% 7% 12%
1	D	217	6% 80% 6% 14%

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	ZN	A	301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6504 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 Adenylate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	190	Total	C	N	O	S	0	0	0
			1516	958	263	286	9			
1	B	206	Total	C	N	O	S	0	0	0
			1620	1018	280	310	12			
1	A	208	Total	C	N	O	S	0	0	0
			1640	1029	286	313	12			
1	D	186	Total	C	N	O	S	0	0	0
			1485	938	260	278	9			

There are 164 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	ILE	LEU	engineered mutation	UNP P16304
C	17	ALA	GLY	engineered mutation	UNP P16304
C	19	LYS	ARG	engineered mutation	UNP P16304
C	22	ALA	GLU	engineered mutation	UNP P16304
C	23	LYS	ASP	engineered mutation	UNP P16304
C	69	ARG	LYS	engineered mutation	UNP P16304
C	73	SER	GLY	engineered mutation	UNP P16304
C	75	SER	ASP	engineered mutation	UNP P16304
C	103	MET	TYR	engineered mutation	UNP P16304
C	105	ARG	LYS	engineered mutation	UNP P16304
C	106	LYS	PRO	engineered mutation	UNP P16304
C	107	LEU	ILE	engineered mutation	UNP P16304
C	108	GLU	ASP	engineered mutation	UNP P16304
C	109	HIS	TYR	engineered mutation	UNP P16304
C	112	HIS	ASN	engineered mutation	UNP P16304
C	114	ASP	GLU	engineered mutation	UNP P16304
C	116	ARG	ASP	engineered mutation	UNP P16304
C	117	GLN	LYS	engineered mutation	UNP P16304
C	118	GLU	ASP	engineered mutation	UNP P16304
C	119	GLU	VAL	engineered mutation	UNP P16304
C	169	ALA	SER	engineered mutation	UNP P16304

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Chain	Residue	Modelled	Actual	Comment	Reference
C	179	MET	THR	engineered mutation	UNP P16304
C	180	LYS	GLN	engineered mutation	UNP P16304
C	184	ALA	ASP	engineered mutation	UNP P16304
C	187	ASP	SER	engineered mutation	UNP P16304
C	188	SER	GLU	engineered mutation	UNP P16304
C	190	GLU	GLY	engineered mutation	UNP P16304
C	191	VAL	TYR	engineered mutation	UNP P16304
C	193	ARG	ALA	engineered mutation	UNP P16304
C	198	GLU	GLN	engineered mutation	UNP P16304
C	201	MET	ILE	engineered mutation	UNP P16304
C	202	GLU	GLN	engineered mutation	UNP P16304
C	203	LYS	ASP	engineered mutation	UNP P16304
C	205	PHE	TYR	engineered mutation	UNP P16304
C	206	LYS	ALA	engineered mutation	UNP P16304
C	208	LEU	VAL	engineered mutation	UNP P16304
C	209	ARG	LYS	engineered mutation	UNP P16304
C	210	GLU	ASP	engineered mutation	UNP P16304
C	213	GLN	GLY	engineered mutation	UNP P16304
C	216	ALA	LYS	engineered mutation	UNP P16304
C	217	ARG	LYS	engineered mutation	UNP P16304
B	3	ILE	LEU	engineered mutation	UNP P16304
B	17	ALA	GLY	engineered mutation	UNP P16304
B	19	LYS	ARG	engineered mutation	UNP P16304
B	22	ALA	GLU	engineered mutation	UNP P16304
B	23	LYS	ASP	engineered mutation	UNP P16304
B	69	ARG	LYS	engineered mutation	UNP P16304
B	73	SER	GLY	engineered mutation	UNP P16304
B	75	SER	ASP	engineered mutation	UNP P16304
B	103	MET	TYR	engineered mutation	UNP P16304
B	105	ARG	LYS	engineered mutation	UNP P16304
B	106	LYS	PRO	engineered mutation	UNP P16304
B	107	LEU	ILE	engineered mutation	UNP P16304
B	108	GLU	ASP	engineered mutation	UNP P16304
B	109	HIS	TYR	engineered mutation	UNP P16304
B	112	HIS	ASN	engineered mutation	UNP P16304
B	114	ASP	GLU	engineered mutation	UNP P16304
B	116	ARG	ASP	engineered mutation	UNP P16304
B	117	GLN	LYS	engineered mutation	UNP P16304
B	118	GLU	ASP	engineered mutation	UNP P16304
B	119	GLU	VAL	engineered mutation	UNP P16304
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Chain	Residue	Modelled	Actual	Comment	Reference
B	180	LYS	GLN	engineered mutation	UNP P16304
B	184	ALA	ASP	engineered mutation	UNP P16304
B	187	ASP	SER	engineered mutation	UNP P16304
B	188	SER	GLU	engineered mutation	UNP P16304
B	190	GLU	GLY	engineered mutation	UNP P16304
B	191	VAL	TYR	engineered mutation	UNP P16304
B	193	ARG	ALA	engineered mutation	UNP P16304
B	198	GLU	GLN	engineered mutation	UNP P16304
B	201	MET	ILE	engineered mutation	UNP P16304
B	202	GLU	GLN	engineered mutation	UNP P16304
B	203	LYS	ASP	engineered mutation	UNP P16304
B	205	PHE	TYR	engineered mutation	UNP P16304
B	206	LYS	ALA	engineered mutation	UNP P16304
B	208	LEU	VAL	engineered mutation	UNP P16304
B	209	ARG	LYS	engineered mutation	UNP P16304
B	210	GLU	ASP	engineered mutation	UNP P16304
B	213	GLN	GLY	engineered mutation	UNP P16304
B	216	ALA	LYS	engineered mutation	UNP P16304
B	217	ARG	LYS	engineered mutation	UNP P16304
A	3	ILE	LEU	engineered mutation	UNP P16304
A	17	ALA	GLY	engineered mutation	UNP P16304
A	19	LYS	ARG	engineered mutation	UNP P16304
A	22	ALA	GLU	engineered mutation	UNP P16304
A	23	LYS	ASP	engineered mutation	UNP P16304
A	69	ARG	LYS	engineered mutation	UNP P16304
A	73	SER	GLY	engineered mutation	UNP P16304
A	75	SER	ASP	engineered mutation	UNP P16304
A	103	MET	TYR	engineered mutation	UNP P16304
A	105	ARG	LYS	engineered mutation	UNP P16304
A	106	LYS	PRO	engineered mutation	UNP P16304
A	107	LEU	ILE	engineered mutation	UNP P16304
A	108	GLU	ASP	engineered mutation	UNP P16304
A	109	HIS	TYR	engineered mutation	UNP P16304
A	112	HIS	ASN	engineered mutation	UNP P16304
A	114	ASP	GLU	engineered mutation	UNP P16304
A	116	ARG	ASP	engineered mutation	UNP P16304
A	117	GLN	LYS	engineered mutation	UNP P16304
A	118	GLU	ASP	engineered mutation	UNP P16304
A	119	GLU	VAL	engineered mutation	UNP P16304
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A	187	ASP	SER	engineered mutation	UNP P16304
A	188	SER	GLU	engineered mutation	UNP P16304
A	190	GLU	GLY	engineered mutation	UNP P16304
A	191	VAL	TYR	engineered mutation	UNP P16304
A	193	ARG	ALA	engineered mutation	UNP P16304
A	198	GLU	GLN	engineered mutation	UNP P16304
A	201	MET	ILE	engineered mutation	UNP P16304
A	202	GLU	GLN	engineered mutation	UNP P16304
A	203	LYS	ASP	engineered mutation	UNP P16304
A	205	PHE	TYR	engineered mutation	UNP P16304
A	206	LYS	ALA	engineered mutation	UNP P16304
A	208	LEU	VAL	engineered mutation	UNP P16304
A	209	ARG	LYS	engineered mutation	UNP P16304
A	210	GLU	ASP	engineered mutation	UNP P16304
A	213	GLN	GLY	engineered mutation	UNP P16304
A	216	ALA	LYS	engineered mutation	UNP P16304
A	217	ARG	LYS	engineered mutation	UNP P16304
D	3	ILE	LEU	engineered mutation	UNP P16304
D	17	ALA	GLY	engineered mutation	UNP P16304
D	19	LYS	ARG	engineered mutation	UNP P16304
D	22	ALA	GLU	engineered mutation	UNP P16304
D	23	LYS	ASP	engineered mutation	UNP P16304
D	69	ARG	LYS	engineered mutation	UNP P16304
D	73	SER	GLY	engineered mutation	UNP P16304
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D	105	ARG	LYS	engineered mutation	UNP P16304
D	106	LYS	PRO	engineered mutation	UNP P16304
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D	109	HIS	TYR	engineered mutation	UNP P16304
D	112	HIS	ASN	engineered mutation	UNP P16304
D	114	ASP	GLU	engineered mutation	UNP P16304
D	116	ARG	ASP	engineered mutation	UNP P16304
D	117	GLN	LYS	engineered mutation	UNP P16304
D	118	GLU	ASP	engineered mutation	UNP P16304
D	119	GLU	VAL	engineered mutation	UNP P16304
D	169	ALA	SER	engineered mutation	UNP P16304
D	179	MET	THR	engineered mutation	UNP P16304
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Chain	Residue	Modelled	Actual	Comment	Reference
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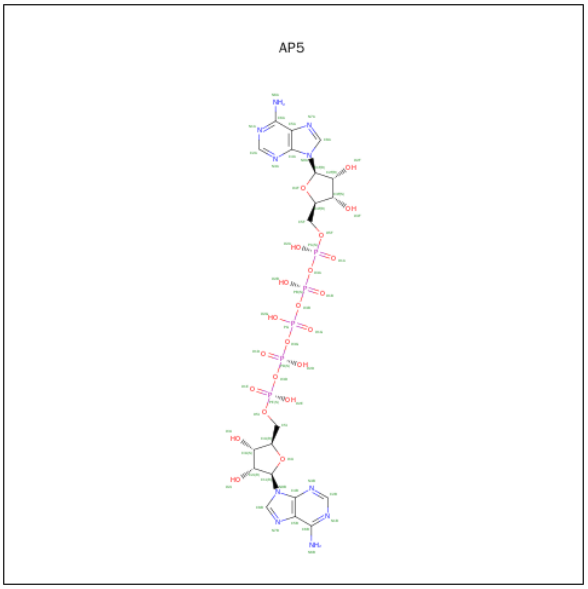
D	193	ARG	ALA	engineered mutation	UNP P16304
D	198	GLU	GLN	engineered mutation	UNP P16304
D	201	MET	ILE	engineered mutation	UNP P16304
D	202	GLU	GLN	engineered mutation	UNP P16304
D	203	LYS	ASP	engineered mutation	UNP P16304
D	205	PHE	TYR	engineered mutation	UNP P16304
D	206	LYS	ALA	engineered mutation	UNP P16304
D	208	LEU	VAL	engineered mutation	UNP P16304
D	209	ARG	LYS	engineered mutation	UNP P16304
D	210	GLU	ASP	engineered mutation	UNP P16304
D	213	GLN	GLY	engineered mutation	UNP P16304
D	216	ALA	LYS	engineered mutation	UNP P16304
D	217	ARG	LYS	engineered mutation	UNP P16304

- Molecule 2 is BIS(ADENOSINE)-5'-PENTAPHOSPHATE (three-letter code: AP5) (formula: $C_{20}H_{29}N_{10}O_{22}P_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			57	20	10	22	5		
2	B	1	Total	C	N	O	P	0	0
			57	20	10	22	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			57	20	10	22	5		
2	D	1	Total	C	N	O	P	0	0
			57	20	10	22	5		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

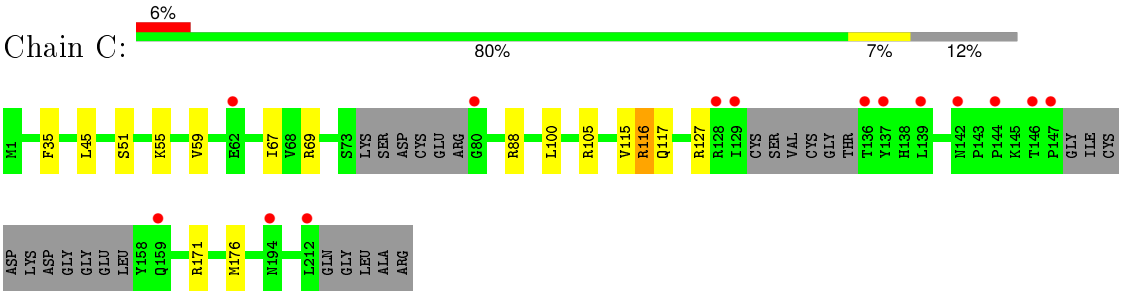
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	7	Total	O	0	0
			7	7		
4	B	4	Total	O	0	0
			4	4		
4	A	2	Total	O	0	0
			2	2		

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.

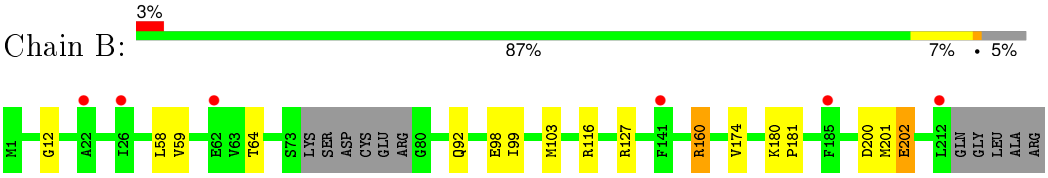
- Molecule 1: Adenylate kinase

Chain C:



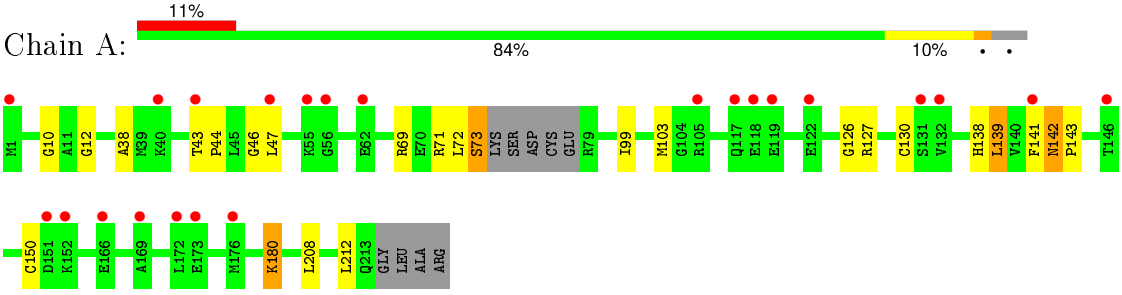
- Molecule 1: Adenylate kinase

Chain B:



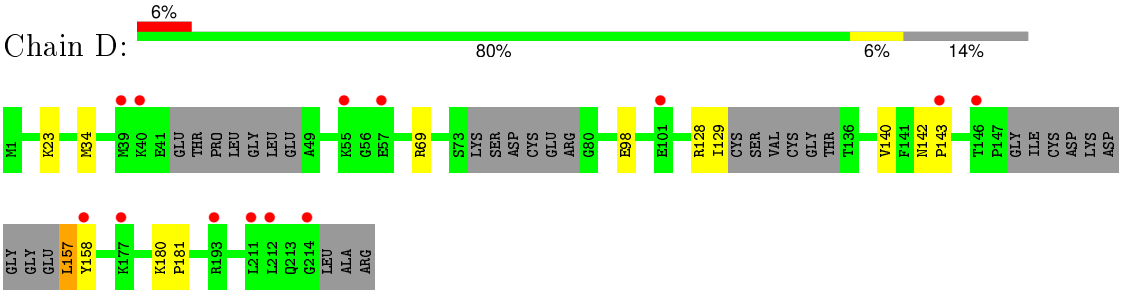
- Molecule 1: Adenylate kinase

Chain A:



- Molecule 1: Adenylate kinase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.64Å 123.34Å 86.69Å 90.00° 98.28° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 35.21 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.7 (50.00-2.90) 93.8 (35.21-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.288 , 0.329 0.287 , 0.323	Depositor DCC
R_{free} test set	969 reflections (5.40%)	DCC
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 32.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 18918 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	6504	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: ZN, AP5

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	0.53	0/1662	0.66	1/2231 (0.0%)
1	B	0.45	0/1642	0.58	0/2205
1	C	0.44	0/1536	0.57	0/2060
1	D	0.47	0/1503	0.60	0/2012
All	All	0.48	0/6343	0.61	1/8508 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	142	ASN	C-N-CD	5.57	140.09	128.40

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	1640	0	1666	47	1
1	B	1620	0	1642	20	0
1	C	1516	0	1546	16	1
1	D	1485	0	1516	9	0
2	A	57	0	24	3	0
2	B	57	0	24	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	57	0	24	6	0
2	D	57	0	24	0	0
3	A	1	0	0	2	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	4	0	0	0	0
4	C	7	0	0	0	0
All	All	6504	0	6466	88	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 7.

All (88) 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:126:GLY:O	1:A:139:LEU:CD2	1.72	1.35
1:A:138:HIS:N	1:A:142:ASN:O	1.68	1.26
1:A:138:HIS:O	1:A:143:PRO:HA	1.13	1.23
1:A:138:HIS:O	1:A:143:PRO:CA	1.87	1.22
1:C:117:GLN:NE2	1:C:176:MET:SD	2.12	1.22
1:A:138:HIS:CD2	1:A:141:PHE:HD2	1.58	1.20
1:A:126:GLY:O	1:A:139:LEU:HD21	1.29	1.19
1:A:72:LEU:O	1:A:103:MET:HE1	1.49	1.12
1:A:138:HIS:NE2	1:A:141:PHE:HD2	1.48	1.12
1:A:138:HIS:NE2	1:A:141:PHE:CD2	2.24	1.04
1:A:138:HIS:HB3	1:A:142:ASN:H	1.19	1.02
1:A:138:HIS:CA	1:A:142:ASN:O	2.10	0.99
1:A:138:HIS:CD2	1:A:141:PHE:CD2	2.50	0.98
1:B:202:GLU:N	1:B:202:GLU:OE1	1.97	0.96
1:A:126:GLY:O	1:A:139:LEU:HD23	1.69	0.93
1:A:72:LEU:O	1:A:103:MET:CE	2.19	0.91
1:D:140:VAL:O	1:D:143:PRO:HD3	1.70	0.91
1:A:150:CYS:SG	3:A:301:ZN:ZN	1.67	0.82
1:A:138:HIS:O	1:A:142:ASN:O	1.99	0.81
1:C:116:ARG:HH12	1:B:116:ARG:HA	1.46	0.79
1:D:142:ASN:OD1	1:D:142:ASN:O	2.03	0.77
1:A:138:HIS:HB3	1:A:142:ASN:N	1.98	0.76
1:A:43:THR:OG1	1:A:44:PRO:HD2	1.88	0.74
1:A:138:HIS:C	1:A:142:ASN:O	2.28	0.72
1:D:128:ARG:HB3	1:D:157:LEU:HD13	1.74	0.70
1:B:201:MET:HB2	1:B:202:GLU:OE1	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:CYS:HG	3:A:301:ZN:ZN	1.05	0.69
1:A:126:GLY:C	1:A:139:LEU:HD21	2.13	0.69
1:A:69:ARG:O	1:A:73:SER:OG	2.11	0.68
1:A:138:HIS:CB	1:A:142:ASN:H	2.04	0.67
1:A:180:LYS:HD3	1:A:180:LYS:O	1.95	0.65
1:D:128:ARG:HB3	1:D:157:LEU:CD1	2.28	0.64
1:A:43:THR:OG1	1:A:44:PRO:CD	2.45	0.63
1:A:208:LEU:O	1:A:212:LEU:HD12	2.02	0.60
1:C:45:LEU:HD21	1:C:67:ILE:HD12	1.84	0.59
1:C:127:ARG:NH2	2:C:301:AP5:O2A	2.34	0.59
1:A:138:HIS:NE2	1:A:141:PHE:CE2	2.69	0.59
1:B:99:ILE:O	1:B:103:MET:HG3	2.03	0.58
1:A:127:ARG:NH1	2:A:302:AP5:O1G	2.36	0.57
1:C:115:VAL:HG12	1:C:116:ARG:H	1.68	0.57
1:A:138:HIS:O	1:A:142:ASN:C	2.42	0.57
1:C:51:SER:O	1:C:55:LYS:HG3	2.04	0.57
1:A:138:HIS:CE1	1:A:141:PHE:CD2	2.92	0.56
1:A:130:CYS:HG	1:A:150:CYS:HG	1.53	0.56
1:A:138:HIS:CB	1:A:142:ASN:O	2.54	0.55
1:A:43:THR:O	1:A:47:LEU:HD23	2.06	0.55
1:A:138:HIS:O	1:A:143:PRO:N	2.39	0.55
1:B:127:ARG:HD3	2:B:302:AP5:H52A	1.89	0.53
1:A:139:LEU:CD2	1:A:139:LEU:N	2.72	0.52
1:C:116:ARG:NH1	1:B:116:ARG:HG2	2.25	0.52
1:C:116:ARG:HH12	1:B:116:ARG:CA	2.19	0.52
1:D:180:LYS:HB2	1:D:181:PRO:HD3	1.93	0.51
1:B:180:LYS:HB2	1:B:181:PRO:HD3	1.92	0.50
1:A:99:ILE:O	1:A:103:MET:HG3	2.11	0.50
1:C:88:ARG:CD	2:C:301:AP5:C6B	2.90	0.50
1:C:88:ARG:HD3	2:C:301:AP5:C6B	2.42	0.49
1:B:127:ARG:HD3	2:B:302:AP5:C5F	2.42	0.49
1:D:129:ILE:O	1:D:158:TYR:CD1	2.65	0.49
1:D:128:ARG:CB	1:D:157:LEU:CD1	2.91	0.48
1:C:100:LEU:HB3	1:C:105:ARG:O	2.13	0.48
1:B:12:GLY:HA2	2:B:302:AP5:O1A	2.14	0.48
1:B:160:ARG:NH1	2:B:302:AP5:O1E	2.48	0.47
1:D:69:ARG:NH1	1:D:98:GLU:OE1	2.48	0.47
1:B:202:GLU:CD	1:B:202:GLU:H	2.13	0.46
1:C:88:ARG:HD3	2:C:301:AP5:C5B	2.46	0.46
1:C:35:PHE:CZ	1:C:59:VAL:HG21	2.51	0.45
1:A:130:CYS:SG	1:A:150:CYS:HB2	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ARG:CZ	1:B:116:ARG:HG2	2.48	0.44
1:A:43:THR:HG23	1:A:46:GLY:H	1.82	0.44
1:B:92:GLN:NE2	2:B:302:AP5:H62B	2.16	0.44
1:A:126:GLY:C	1:A:139:LEU:CD2	2.72	0.43
1:A:10:GLY:HA2	2:A:302:AP5:H51A	2.01	0.43
1:B:58:LEU:HG	1:B:174:VAL:CG1	2.49	0.43
1:A:139:LEU:H	1:A:139:LEU:HD23	1.83	0.42
1:A:130:CYS:SG	1:A:150:CYS:SG	3.15	0.42
1:B:98:GLU:OE2	1:D:34:MET:HA	2.20	0.42
1:A:139:LEU:CD2	1:A:139:LEU:H	2.32	0.42
1:A:180:LYS:HD3	1:A:180:LYS:C	2.34	0.42
1:B:200:ASP:O	1:B:201:MET:C	2.57	0.42
1:A:12:GLY:HA2	2:A:302:AP5:O1A	2.19	0.42
1:A:138:HIS:CD2	1:A:141:PHE:HB2	2.55	0.41
1:A:38:ALA:HB1	1:A:43:THR:CG2	2.50	0.41
2:C:301:AP5:H2F	2:C:301:AP5:H8A	1.91	0.41
1:B:64:THR:HG21	2:B:302:AP5:N6B	2.36	0.41
1:C:115:VAL:HG12	1:C:116:ARG:N	2.33	0.40
1:B:59:VAL:N	2:B:302:AP5:H2B	2.35	0.40
1:B:59:VAL:O	2:B:302:AP5:H2B	2.21	0.40
1:C:171:ARG:NH1	2:C:301:AP5:O1G	2.54	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)
1:C:69:ARG:CD	1:A:71:ARG:NH2[2_557]	2.13	0.07

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	204/217 (94%)	196 (96%)	8 (4%)	0	100	100
1	B	202/217 (93%)	196 (97%)	6 (3%)	0	100	100
1	C	182/217 (84%)	177 (97%)	5 (3%)	0	100	100
1	D	176/217 (81%)	171 (97%)	5 (3%)	0	100	100
All	All	764/868 (88%)	740 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	178/185 (96%)	175 (98%)	3 (2%)	68	91
1	B	176/185 (95%)	174 (99%)	2 (1%)	80	95
1	C	164/185 (89%)	163 (99%)	1 (1%)	90	97
1	D	160/185 (86%)	158 (99%)	2 (1%)	76	94
All	All	678/740 (92%)	670 (99%)	8 (1%)	78	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	116	ARG
1	B	160	ARG
1	B	202	GLU
1	A	73	SER
1	A	139	LEU
1	A	180	LYS
1	D	23	LYS
1	D	157	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AP5	A	302	-	44,62,62	1.11	4 (9%)	55,98,98	2.22	13 (23%)
2	AP5	B	302	-	44,62,62	1.30	4 (9%)	55,98,98	2.49	17 (30%)
2	AP5	C	301	-	44,62,62	1.18	3 (6%)	55,98,98	2.08	11 (20%)
2	AP5	D	301	-	44,62,62	0.95	2 (4%)	55,98,98	2.19	13 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AP5	A	302	-	-	0/36/76/76	0/6/6/6
2	AP5	B	302	-	-	0/36/76/76	0/6/6/6
2	AP5	C	301	-	-	0/36/76/76	0/6/6/6
2	AP5	D	301	-	-	0/36/76/76	0/6/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	AP5	C4B-N3B	-2.76	1.31	1.35
2	C	301	AP5	C5B-N7B	-2.67	1.30	1.39
2	B	302	AP5	C2J-C3J	-2.33	1.47	1.53
2	A	302	AP5	C5B-N7B	-2.32	1.31	1.39
2	A	302	AP5	C4A-N3A	-2.22	1.32	1.35
2	B	302	AP5	C5A-N7A	-2.15	1.32	1.39
2	A	302	AP5	C5A-N7A	-2.03	1.32	1.39
2	A	302	AP5	C5A-C4A	2.17	1.45	1.40
2	C	301	AP5	C5A-C4A	2.31	1.45	1.40
2	B	302	AP5	C5B-C4B	2.55	1.46	1.40
2	B	302	AP5	C5A-C4A	2.78	1.46	1.40
2	D	301	AP5	C5A-C4A	2.81	1.46	1.40
2	D	301	AP5	C5B-C4B	2.90	1.47	1.40

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	AP5	N3A-C2A-N1A	-8.32	122.52	128.89
2	D	301	AP5	N3B-C2B-N1B	-8.17	122.64	128.89
2	C	301	AP5	N3B-C2B-N1B	-7.65	123.04	128.89
2	A	302	AP5	N3B-C2B-N1B	-7.47	123.18	128.89
2	B	302	AP5	N3B-C2B-N1B	-6.81	123.68	128.89
2	A	302	AP5	N3A-C2A-N1A	-6.19	124.16	128.89
2	C	301	AP5	N3A-C2A-N1A	-5.91	124.37	128.89
2	B	302	AP5	N3A-C2A-N1A	-5.70	124.53	128.89
2	A	302	AP5	PB-O3A-PA	-5.68	116.79	132.73
2	B	302	AP5	PD-O3G-PG	-5.44	117.45	132.73
2	B	302	AP5	PG-O3B-PB	-5.14	118.30	132.73
2	B	302	AP5	PB-O3A-PA	-5.12	118.35	132.73
2	B	302	AP5	C4F-O4F-C1F	-4.86	104.38	109.72
2	A	302	AP5	PG-O3B-PB	-4.78	119.31	132.73
2	B	302	AP5	C4B-C5B-N7B	-4.29	105.53	109.48
2	A	302	AP5	C2F-C1F-N9A	-4.23	107.83	114.29
2	C	301	AP5	PG-O3B-PB	-4.15	121.07	132.73
2	B	302	AP5	O2J-C2J-C3J	-4.12	98.42	111.83
2	D	301	AP5	C2J-C1J-N9B	-4.04	108.12	114.29
2	C	301	AP5	PD-O3G-PG	-3.89	121.79	132.73
2	C	301	AP5	PE-O3D-PD	-3.80	122.05	132.73
2	B	302	AP5	C2J-C1J-N9B	-3.77	108.53	114.29
2	B	302	AP5	O3J-C3J-C2J	-3.73	99.68	111.83
2	C	301	AP5	C4A-C5A-N7A	-3.65	106.12	109.48
2	A	302	AP5	PE-O3D-PD	-3.60	122.61	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	AP5	PB-O3A-PA	-3.55	122.77	132.73
2	D	301	AP5	PG-O3B-PB	-3.54	122.79	132.73
2	A	302	AP5	C2J-C1J-N9B	-3.44	109.04	114.29
2	A	302	AP5	C4B-C5B-N7B	-2.97	106.75	109.48
2	A	302	AP5	C4A-C5A-N7A	-2.96	106.75	109.48
2	D	301	AP5	PD-O3G-PG	-2.92	124.52	132.73
2	D	301	AP5	C1F-N9A-C4A	-2.91	122.55	126.94
2	D	301	AP5	C4B-C5B-N7B	-2.78	106.92	109.48
2	D	301	AP5	PE-O3D-PD	-2.69	125.18	132.73
2	A	302	AP5	O2J-C2J-C3J	-2.64	103.25	111.83
2	D	301	AP5	C4A-C5A-N7A	-2.61	107.08	109.48
2	C	301	AP5	O2J-C2J-C3J	-2.60	103.37	111.83
2	C	301	AP5	C2F-C1F-N9A	-2.47	110.51	114.29
2	B	302	AP5	C4A-C5A-N7A	-2.45	107.22	109.48
2	A	302	AP5	O2F-C2F-C3F	-2.42	103.94	111.83
2	C	301	AP5	O5F-PA-O1A	-2.26	100.85	109.62
2	D	301	AP5	C1J-N9B-C4B	-2.19	123.63	126.94
2	B	302	AP5	O5J-PE-O1E	-2.16	101.24	109.62
2	A	302	AP5	O3F-C3F-C2F	-2.12	104.94	111.83
2	D	301	AP5	PB-O3A-PA	-2.02	127.06	132.73
2	D	301	AP5	C2B-N1B-C6B	2.14	122.59	118.77
2	D	301	AP5	C2A-N1A-C6A	2.29	122.86	118.77
2	B	302	AP5	C2B-N1B-C6B	2.42	123.09	118.77
2	A	302	AP5	O2G-PG-O3G	2.43	116.13	105.09
2	B	302	AP5	O3A-PA-O5F	2.47	109.48	102.94
2	C	301	AP5	C4F-O4F-C1F	2.60	112.58	109.72
2	B	302	AP5	O2E-PE-O3D	2.75	117.56	105.09
2	B	302	AP5	C1F-N9A-C4A	2.92	131.35	126.94
2	B	302	AP5	O4F-C1F-N9A	3.71	115.86	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	AP5	3	0
2	B	302	AP5	8	0
2	C	301	AP5	6	0

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	208/217 (95%)	0.60	23 (11%) 7 4	36, 65, 99, 115	0
1	B	206/217 (94%)	0.33	6 (2%) 55 49	33, 57, 82, 94	0
1	C	190/217 (87%)	0.43	14 (7%) 17 11	39, 56, 82, 107	0
1	D	186/217 (85%)	0.52	13 (6%) 19 13	41, 62, 87, 103	0
All	All	790/868 (91%)	0.47	56 (7%) 19 13	33, 60, 89, 115	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	139	LEU	4.5
1	A	118	GLU	4.4
1	C	129	ILE	4.3
1	A	55	LYS	4.2
1	A	122	GLU	4.1
1	D	40	LYS	4.1
1	A	166	GLU	4.0
1	A	146	THR	3.8
1	A	172	LEU	3.7
1	A	173	GLU	3.7
1	C	159	GLN	3.6
1	A	151	ASP	3.6
1	A	117	GLN	3.4
1	C	212	LEU	3.3
1	B	212	LEU	3.1
1	C	142	ASN	3.1
1	A	119	GLU	3.0
1	D	158	TYR	3.0
1	A	176	MET	2.9
1	D	211	LEU	2.9
1	A	56	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	55	LYS	2.9
1	C	136	THR	2.9
1	D	146	THR	2.9
1	C	147	PRO	2.8
1	C	144	PRO	2.8
1	B	141	PHE	2.8
1	B	26	ILE	2.7
1	D	143	PRO	2.7
1	A	131	SER	2.6
1	A	47	LEU	2.6
1	B	22	ALA	2.6
1	A	141	PHE	2.5
1	D	212	LEU	2.5
1	D	57	GLU	2.5
1	B	62	GLU	2.4
1	A	132	VAL	2.4
1	C	146	THR	2.4
1	C	80	GLY	2.4
1	C	137	TYR	2.4
1	A	169	ALA	2.4
1	A	62	GLU	2.3
1	D	214	GLY	2.3
1	A	43	THR	2.3
1	C	62	GLU	2.3
1	D	39	MET	2.2
1	A	152	LYS	2.2
1	D	101	GLU	2.2
1	A	105	ARG	2.2
1	A	1	MET	2.2
1	D	177	LYS	2.2
1	C	194	ASN	2.2
1	D	193	ARG	2.1
1	C	128	ARG	2.0
1	A	40	LYS	2.0
1	B	185	PHE	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 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	AP5	B	302	57/57	0.94	0.24	0.74	70,80,103,108	0
2	AP5	A	302	57/57	0.91	0.27	0.50	73,83,100,102	0
3	ZN	B	301	1/1	0.95	0.16	0.15	112,112,112,112	0
2	AP5	D	301	57/57	0.93	0.24	0.09	76,94,119,121	0
2	AP5	C	301	57/57	0.94	0.22	0.01	65,79,90,90	0
3	ZN	A	301	1/1	0.94	0.07	-1.49	139,139,139,139	0

6.5 Other polymers (i)

There are no such residues in this entry.