Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:45 PM GMT

PDB ID	:	4W5J
Title	:	New structural conformations of adenylate kinase from Streptococcus pneumoniae D39 with Ap5A
Authors	:	Thach, T.T.; Lee, S.H.
Deposited on	:	2014-08-18
Resolution	:	1.65 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:

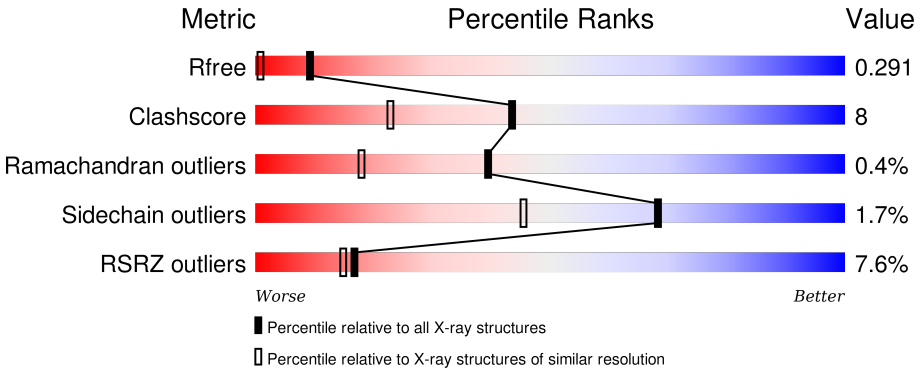
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.65 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	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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	5% 80% 16%
1	B	217	12% 77% 20%
1	C	217	4% 88% 8%
1	D	217	8% 83% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14290 atoms, of which 6608 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	A	211	Total	C	H	N	O	S	0	0	0
			3312	1044	1652	287	324	5			
1	B	211	Total	C	H	N	O	S	0	0	0
			3312	1044	1652	287	324	5			
1	C	211	Total	C	H	N	O	S	0	0	0
			3312	1044	1652	287	324	5			
1	D	211	Total	C	H	N	O	S	0	0	0
			3312	1044	1652	287	324	5			

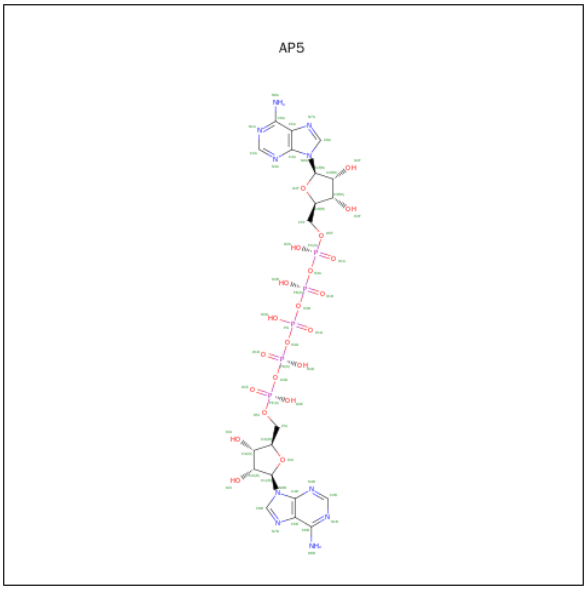
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q04ML5
A	-3	ALA	-	expression tag	UNP Q04ML5
A	-2	MET	-	expression tag	UNP Q04ML5
A	-1	GLY	-	expression tag	UNP Q04ML5
A	0	SER	-	expression tag	UNP Q04ML5
B	-4	GLY	-	expression tag	UNP Q04ML5
B	-3	ALA	-	expression tag	UNP Q04ML5
B	-2	MET	-	expression tag	UNP Q04ML5
B	-1	GLY	-	expression tag	UNP Q04ML5
B	0	SER	-	expression tag	UNP Q04ML5
C	-4	GLY	-	expression tag	UNP Q04ML5
C	-3	ALA	-	expression tag	UNP Q04ML5
C	-2	MET	-	expression tag	UNP Q04ML5
C	-1	GLY	-	expression tag	UNP Q04ML5
C	0	SER	-	expression tag	UNP Q04ML5
D	-4	GLY	-	expression tag	UNP Q04ML5
D	-3	ALA	-	expression tag	UNP Q04ML5
D	-2	MET	-	expression tag	UNP Q04ML5
D	-1	GLY	-	expression tag	UNP Q04ML5
D	0	SER	-	expression tag	UNP Q04ML5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 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
3	A	1	Total C N O P 57 20 10 22 5	0	0
3	B	1	Total C N O P 57 20 10 22 5	0	0
3	C	1	Total C N O P 57 20 10 22 5	0	0
3	D	1	Total C N O P 57 20 10 22 5	0	0

- Molecule 4 is water.

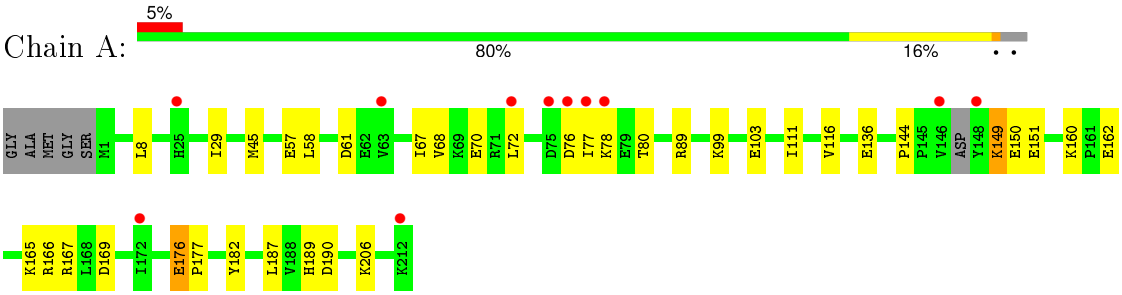
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	218	Total O 218 218	0	0
4	B	191	Total O 191 191	0	0
4	C	209	Total O 209 209	0	0
4	D	192	Total O 192 192	0	0

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 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.

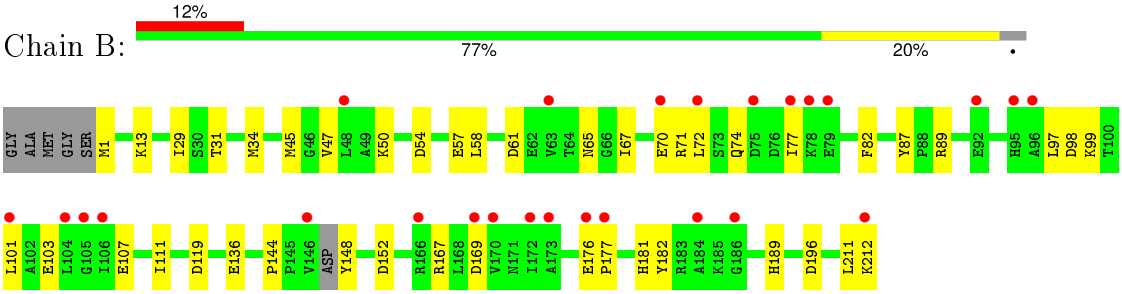
- Molecule 1: Adenylate kinase

Chain A:



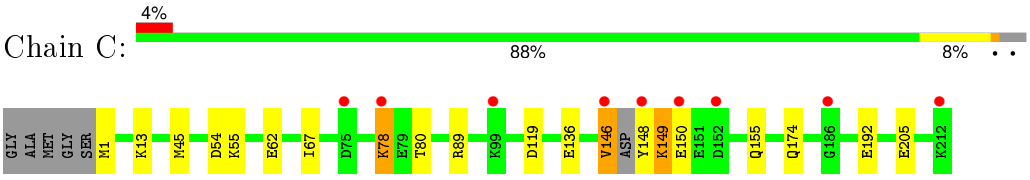
- Molecule 1: Adenylate kinase

Chain B:



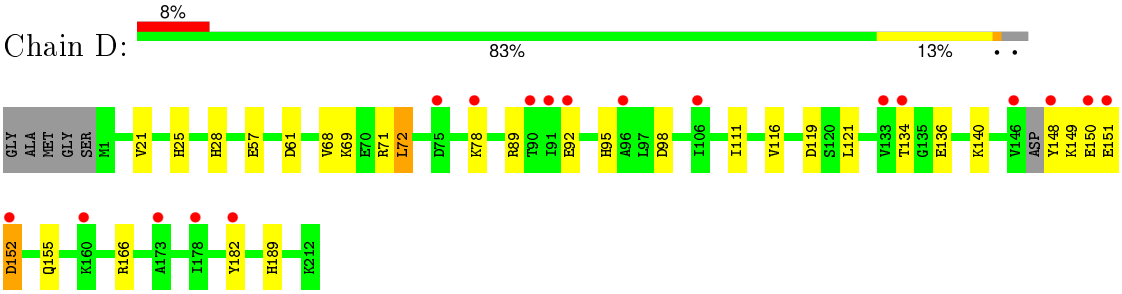
- Molecule 1: Adenylate kinase

Chain C:



- Molecule 1: Adenylate kinase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.91Å 62.30Å 63.02Å 101.89° 112.59° 89.86°	Depositor
Resolution (Å)	46.99 – 1.65 46.99 – 1.65	Depositor EDS
% Data completeness (in resolution range)	95.4 (46.99-1.65) 83.5 (46.99-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.66 (at 1.65Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, R_{free}	0.257 , 0.286 0.264 , 0.291	Depositor DCC
R_{free} test set	4279 reflections (5.67%)	DCC
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.52 , 63.2	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 85172 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14290	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 80.49 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.4202e-07.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: MG, 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	0.31	0/1685	0.48	0/2274
1	B	0.31	0/1685	0.48	0/2274
1	C	0.31	0/1685	0.48	0/2274
1	D	0.31	0/1685	0.50	0/2274
All	All	0.31	0/6740	0.48	0/9096

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	211	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1660	1652	1660	30	1
1	B	1660	1652	1660	32	0
1	C	1660	1652	1660	18	1
1	D	1660	1652	1660	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	57	0	23	2	0
3	B	57	0	22	2	0
3	C	57	0	22	2	0
3	D	57	0	23	3	0
4	A	218	0	0	19	4
4	B	191	0	0	15	4
4	C	209	0	0	12	4
4	D	192	0	0	20	2
All	All	7682	6608	6730	110	8

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 8.

All (110) 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:C:55:LYS:NZ	4:C:402:HOH:O	1.90	1.04
1:A:76:ASP:OD2	4:A:592:HOH:O	1.83	0.95
1:C:89:ARG:NH2	3:C:302:AP5:O1B	2.00	0.94
1:D:119:ASP:OD2	4:D:401:HOH:O	1.88	0.91
1:C:119:ASP:OD2	4:C:401:HOH:O	1.88	0.91
1:B:107:GLU:OE2	4:B:401:HOH:O	1.91	0.89
1:B:176:GLU:OE2	4:B:561:HOH:O	1.92	0.86
1:C:174:GLN:NE2	4:C:404:HOH:O	2.10	0.85
1:A:165:LYS:NZ	4:A:403:HOH:O	2.08	0.84
1:D:21:VAL:O	4:D:554:HOH:O	1.96	0.84
1:D:25:HIS:N	4:D:554:HOH:O	2.12	0.83
1:A:187:LEU:O	4:A:401:HOH:O	1.97	0.82
1:A:70:GLU:OE1	4:A:402:HOH:O	1.98	0.80
1:A:61:ASP:OD2	4:A:567:HOH:O	1.98	0.79
1:D:69:LYS:NZ	4:D:542:HOH:O	2.16	0.79
1:A:189:HIS:ND1	4:A:401:HOH:O	2.19	0.76
1:D:57:GLU:OE2	4:D:567:HOH:O	2.03	0.75
1:D:166:ARG:NH1	4:D:404:HOH:O	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LYS:NZ	1:B:54:ASP:OD2	2.20	0.73
1:B:196:ASP:OD2	4:B:534:HOH:O	2.07	0.72
1:B:119:ASP:OD2	4:B:570:HOH:O	2.08	0.72
1:D:95:HIS:ND1	4:D:485:HOH:O	2.23	0.71
1:C:192:GLU:OE2	4:C:403:HOH:O	2.09	0.70
1:D:155:GLN:OE1	4:D:402:HOH:O	2.09	0.70
1:A:116:VAL:O	4:A:580:HOH:O	2.10	0.69
1:B:152:ASP:OD2	4:B:537:HOH:O	2.08	0.69
1:A:57:GLU:OE2	4:A:573:HOH:O	2.11	0.69
1:A:99:LYS:NZ	1:A:103:GLU:OE2	2.25	0.68
1:D:98:ASP:OD1	4:D:533:HOH:O	2.10	0.68
1:B:13:LYS:NZ	4:B:555:HOH:O	2.26	0.68
1:B:148:TYR:N	4:B:544:HOH:O	2.26	0.67
1:A:169:ASP:OD1	4:A:404:HOH:O	2.13	0.66
1:B:196:ASP:OD1	4:B:402:HOH:O	2.13	0.66
1:C:89:ARG:NH1	3:C:302:AP5:N7A	2.43	0.65
1:D:148:TYR:HA	4:D:580:HOH:O	1.96	0.65
1:C:155:GLN:OE1	4:C:405:HOH:O	2.15	0.65
1:B:169:ASP:OD1	4:B:576:HOH:O	2.14	0.64
1:B:29:ILE:HG23	1:B:34:MET:HE1	1.81	0.63
1:A:189:HIS:CE1	4:A:401:HOH:O	2.51	0.63
1:A:190:ASP:OD2	4:A:406:HOH:O	2.16	0.61
1:B:144:PRO:O	4:B:539:HOH:O	2.16	0.61
1:D:89:ARG:NH2	3:D:302:AP5:O1B	2.35	0.59
1:C:54:ASP:OD2	4:C:406:HOH:O	2.17	0.58
1:D:155:GLN:OE1	4:D:403:HOH:O	2.18	0.57
1:D:189:HIS:HE1	4:D:421:HOH:O	1.89	0.56
1:C:148:TYR:OH	1:C:150:GLU:OE1	2.16	0.56
1:A:136:GLU:OE1	4:A:540:HOH:O	2.17	0.55
1:C:136:GLU:OE1	4:C:407:HOH:O	2.18	0.55
1:A:166:ARG:NH1	4:A:408:HOH:O	2.26	0.54
1:B:97:LEU:CD1	1:B:101:LEU:HD21	2.38	0.53
1:D:89:ARG:NH2	3:D:302:AP5:O2A	2.43	0.52
1:D:111:ILE:HD12	1:D:182:TYR:HB3	1.91	0.52
1:A:111:ILE:HD12	1:A:182:TYR:CB	2.40	0.51
1:C:148:TYR:CD2	1:C:149:LYS:N	2.78	0.51
1:B:29:ILE:HG23	1:B:34:MET:CE	2.40	0.51
1:A:76:ASP:N	1:A:76:ASP:OD1	2.44	0.50
1:D:61:ASP:OD1	4:D:507:HOH:O	2.20	0.50
1:A:206:LYS:NZ	4:A:405:HOH:O	2.15	0.49
1:A:29:ILE:HD11	1:A:77:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:LEU:HD22	1:B:89:ARG:HD2	1.95	0.49
1:B:57:GLU:O	3:B:302:AP5:O2J	2.30	0.49
1:C:1:MET:N	4:C:590:HOH:O	2.27	0.48
1:B:98:ASP:OD2	1:B:181:HIS:NE2	2.44	0.48
1:D:166:ARG:CZ	4:D:404:HOH:O	2.59	0.48
1:D:71:ARG:NH1	4:D:519:HOH:O	2.46	0.48
1:B:136:GLU:OE1	4:B:404:HOH:O	2.20	0.47
1:D:151:GLU:OE1	4:D:541:HOH:O	2.20	0.47
1:D:166:ARG:NH2	4:D:404:HOH:O	2.48	0.47
1:D:140:LYS:NZ	4:D:412:HOH:O	2.46	0.47
1:B:34:MET:HE2	1:B:71:ARG:NH1	2.30	0.46
1:D:150:GLU:C	1:D:152:ASP:H	2.17	0.46
1:B:111:ILE:HD12	1:B:182:TYR:CB	2.46	0.46
1:A:149:LYS:HD3	1:A:151:GLU:OE2	2.16	0.46
1:B:70:GLU:O	1:B:74:GLN:HG2	2.16	0.46
1:B:47:VAL:O	4:B:405:HOH:O	2.21	0.46
1:B:176:GLU:HB3	1:B:177:PRO:CD	2.46	0.45
1:D:116:VAL:HG21	1:D:121:LEU:HD21	1.98	0.45
1:D:134:THR:HG23	1:D:136:GLU:H	1.81	0.45
1:A:45:MET:SD	1:A:67:ILE:HG21	2.56	0.45
1:A:8:LEU:HD12	4:A:580:HOH:O	2.16	0.44
1:C:13:LYS:HE2	4:C:589:HOH:O	2.18	0.44
1:B:61:ASP:CA	4:B:541:HOH:O	2.64	0.44
1:C:150:GLU:HB3	4:C:438:HOH:O	2.17	0.43
1:C:146:VAL:HA	4:C:415:HOH:O	2.17	0.43
1:A:176:GLU:HB3	1:A:177:PRO:CD	2.49	0.43
1:C:78:LYS:HD2	1:C:78:LYS:H	1.84	0.43
1:B:87:TYR:HE2	1:B:97:LEU:HD13	1.84	0.43
1:A:144:PRO:O	4:A:536:HOH:O	2.22	0.42
1:A:58:LEU:HD22	1:A:89:ARG:HD2	2.01	0.42
1:B:189:HIS:HE1	4:B:435:HOH:O	2.02	0.42
1:D:21:VAL:HG21	1:D:28:HIS:HB2	2.01	0.42
1:B:45:MET:SD	1:B:67:ILE:HG21	2.60	0.42
1:B:77:ILE:HG23	1:B:82:PHE:HD2	1.84	0.42
1:A:160:LYS:HD3	1:A:162:GLU:OE2	2.20	0.42
1:D:89:ARG:HH22	3:D:302:AP5:PA	2.43	0.41
1:A:150:GLU:O	4:A:407:HOH:O	2.22	0.41
1:B:65:ASN:ND2	4:B:541:HOH:O	2.54	0.41
1:A:89:ARG:NH1	4:A:549:HOH:O	2.53	0.41
1:C:45:MET:SD	1:C:67:ILE:HG21	2.59	0.41
1:C:62:GLU:CD	4:C:417:HOH:O	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:VAL:HG12	1:D:72:LEU:CD2	2.50	0.41
1:A:206:LYS:NZ	4:A:416:HOH:O	2.49	0.41
1:B:167:ARG:NH2	3:B:302:AP5:O1G	2.54	0.41
1:A:68:VAL:O	1:A:72:LEU:HD23	2.20	0.41
1:B:72:LEU:HA	1:B:77:ILE:HG13	2.03	0.41
1:A:167:ARG:NH2	3:A:302:AP5:O2G	2.54	0.41
1:B:99:LYS:O	1:B:103:GLU:HG3	2.21	0.40
3:A:302:AP5:O5F	3:A:302:AP5:H8A	2.21	0.40
1:D:78:LYS:HE3	4:D:460:HOH:O	2.21	0.40
1:D:155:GLN:NE2	4:D:497:HOH:O	2.55	0.40

All (8) 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)
4:A:403:HOH:O	4:B:413:HOH:O[1_656]	1.95	0.25
4:A:486:HOH:O	4:B:465:HOH:O[1_656]	2.02	0.18
4:A:474:HOH:O	4:C:471:HOH:O[1_546]	2.03	0.17
4:A:473:HOH:O	4:D:471:HOH:O[1_656]	2.05	0.15
4:C:466:HOH:O	4:D:425:HOH:O[1_655]	2.15	0.05
4:B:431:HOH:O	4:C:469:HOH:O[1_556]	2.16	0.04
4:B:466:HOH:O	4:C:463:HOH:O[1_556]	2.17	0.03
1:A:150:GLU:OE2	1:C:205:GLU:OE2[1_546]	2.19	0.01

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	207/217 (95%)	204 (99%)	2 (1%)	1 (0%)	34 12
1	B	207/217 (95%)	206 (100%)	1 (0%)	0	100 100
1	C	207/217 (95%)	206 (100%)	0	1 (0%)	34 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	207/217 (95%)	203 (98%)	3 (1%)	1 (0%)	34 12
All	All	828/868 (95%)	819 (99%)	6 (1%)	3 (0%)	39 18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	149	LYS
1	A	149	LYS
1	D	149	LYS

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	180/183 (98%)	177 (98%)	3 (2%)	68 45
1	B	180/183 (98%)	177 (98%)	3 (2%)	68 45
1	C	180/183 (98%)	177 (98%)	3 (2%)	68 45
1	D	180/183 (98%)	177 (98%)	3 (2%)	68 45
All	All	720/732 (98%)	708 (98%)	12 (2%)	68 45

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LYS
1	A	80	THR
1	A	176	GLU
1	B	1	MET
1	B	31	THR
1	B	212	LYS
1	C	78	LYS
1	C	80	THR
1	C	146	VAL
1	D	72	LEU
1	D	92	GLU

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Mol	Chain	Res	Type
1	D	152	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	189	HIS
1	B	189	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 8 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
3	AP5	A	302	2	44,62,62	3.78	13 (29%)	55,98,98	2.75	7 (12%)
3	AP5	B	302	2	44,62,62	3.78	15 (34%)	55,98,98	2.67	11 (20%)
3	AP5	C	302	2	44,62,62	3.71	13 (29%)	55,98,98	2.74	7 (12%)
3	AP5	D	302	2	44,62,62	3.86	13 (29%)	55,98,98	2.73	8 (14%)

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
3	AP5	A	302	2	-	0/36/76/76	0/6/6/6
3	AP5	B	302	2	-	0/36/76/76	0/6/6/6
3	AP5	C	302	2	-	0/36/76/76	0/6/6/6
3	AP5	D	302	2	-	0/36/76/76	0/6/6/6

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	AP5	O4J-C4J	-6.44	1.30	1.45
3	D	302	AP5	O4F-C4F	-6.17	1.30	1.45
3	A	302	AP5	O4F-C4F	-6.01	1.31	1.45
3	C	302	AP5	O4F-C4F	-5.97	1.31	1.45
3	D	302	AP5	O4J-C4J	-5.71	1.31	1.45
3	C	302	AP5	O4J-C4J	-5.68	1.31	1.45
3	B	302	AP5	O4F-C4F	-5.47	1.32	1.45
3	A	302	AP5	O4J-C4J	-5.41	1.32	1.45
3	D	302	AP5	O3F-C3F	-3.51	1.34	1.43
3	A	302	AP5	O3F-C3F	-3.50	1.34	1.43
3	C	302	AP5	O3F-C3F	-3.31	1.35	1.43
3	B	302	AP5	O3F-C3F	-3.06	1.35	1.43
3	D	302	AP5	C5A-C4A	-2.93	1.33	1.40
3	B	302	AP5	O3J-C3J	-2.87	1.36	1.43
3	C	302	AP5	O3J-C3J	-2.74	1.36	1.43
3	C	302	AP5	C5A-C4A	-2.64	1.34	1.40
3	D	302	AP5	C5B-C4B	-2.55	1.34	1.40
3	A	302	AP5	C5B-C4B	-2.51	1.34	1.40
3	A	302	AP5	C5A-C4A	-2.49	1.34	1.40
3	B	302	AP5	C5A-C4A	-2.48	1.34	1.40
3	B	302	AP5	C5B-C4B	-2.46	1.35	1.40
3	C	302	AP5	C5B-C4B	-2.32	1.35	1.40
3	D	302	AP5	O3J-C3J	-2.27	1.37	1.43
3	B	302	AP5	O2F-C2F	2.02	1.47	1.43
3	B	302	AP5	C2A-N3A	2.13	1.36	1.32
3	B	302	AP5	C2B-N1B	2.14	1.38	1.33
3	D	302	AP5	C2A-N3A	2.22	1.36	1.32
3	C	302	AP5	O2J-C2J	2.28	1.48	1.43
3	A	302	AP5	O2F-C2F	2.31	1.48	1.43
3	B	302	AP5	O2J-C2J	2.44	1.48	1.43
3	A	302	AP5	C2A-N3A	2.45	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	AP5	O2J-C2J	2.55	1.49	1.43
3	C	302	AP5	C2A-N3A	2.55	1.36	1.32
3	A	302	AP5	O2J-C2J	2.55	1.49	1.43
3	C	302	AP5	C6A-N6A	2.59	1.42	1.34
3	D	302	AP5	C6A-N6A	2.61	1.43	1.34
3	B	302	AP5	C6A-N6A	2.73	1.43	1.34
3	A	302	AP5	C6A-N6A	2.74	1.43	1.34
3	A	302	AP5	C6B-N6B	3.68	1.46	1.34
3	B	302	AP5	C2B-N3B	3.73	1.38	1.32
3	D	302	AP5	C6B-N6B	3.78	1.46	1.34
3	C	302	AP5	C6B-N6B	3.92	1.47	1.34
3	D	302	AP5	C2B-N3B	3.94	1.39	1.32
3	A	302	AP5	C2B-N3B	4.00	1.39	1.32
3	C	302	AP5	C2B-N3B	4.03	1.39	1.32
3	B	302	AP5	C6B-N6B	4.12	1.47	1.34
3	C	302	AP5	O4J-C1J	13.72	1.58	1.41
3	D	302	AP5	O4J-C1J	14.54	1.59	1.41
3	A	302	AP5	O4J-C1J	14.73	1.59	1.41
3	B	302	AP5	O4F-C1F	14.90	1.60	1.41
3	B	302	AP5	O4J-C1J	15.14	1.60	1.41
3	A	302	AP5	O4F-C1F	15.47	1.60	1.41
3	C	302	AP5	O4F-C1F	15.59	1.60	1.41
3	D	302	AP5	O4F-C1F	16.27	1.61	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	302	AP5	N3B-C2B-N1B	-12.73	119.14	128.89
3	A	302	AP5	N3B-C2B-N1B	-12.21	119.55	128.89
3	D	302	AP5	N3B-C2B-N1B	-12.04	119.68	128.89
3	A	302	AP5	N3A-C2A-N1A	-11.73	119.92	128.89
3	B	302	AP5	N3A-C2A-N1A	-11.56	120.04	128.89
3	B	302	AP5	N3B-C2B-N1B	-11.21	120.31	128.89
3	C	302	AP5	N3A-C2A-N1A	-11.13	120.37	128.89
3	D	302	AP5	N3A-C2A-N1A	-11.10	120.39	128.89
3	B	302	AP5	N6B-C6B-N1B	-6.89	104.41	119.20
3	D	302	AP5	N6B-C6B-N1B	-6.65	104.92	119.20
3	A	302	AP5	N6B-C6B-N1B	-6.44	105.39	119.20
3	C	302	AP5	N6B-C6B-N1B	-6.28	105.72	119.20
3	D	302	AP5	C1J-N9B-C4B	-4.52	120.12	126.94
3	C	302	AP5	C1J-N9B-C4B	-3.93	121.01	126.94
3	B	302	AP5	C1J-N9B-C4B	-3.92	121.02	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	AP5	C1J-N9B-C4B	-3.86	121.12	126.94
3	C	302	AP5	PG-O3B-PB	-3.31	123.42	132.73
3	C	302	AP5	N6A-C6A-N1A	-3.21	112.32	119.20
3	D	302	AP5	N6A-C6A-N1A	-3.20	112.34	119.20
3	A	302	AP5	N6A-C6A-N1A	-3.09	112.56	119.20
3	A	302	AP5	C4F-O4F-C1F	-3.02	106.40	109.72
3	B	302	AP5	N6A-C6A-N1A	-2.97	112.82	119.20
3	B	302	AP5	C2J-C1J-N9B	-2.85	109.93	114.29
3	D	302	AP5	PG-O3B-PB	-2.82	124.81	132.73
3	D	302	AP5	PB-O3A-PA	-2.16	126.66	132.73
3	B	302	AP5	PD-O3G-PG	-2.08	126.89	132.73
3	B	302	AP5	O3J-C3J-C2J	-2.04	105.19	111.83
3	B	302	AP5	C2J-C3J-C4J	2.12	106.97	102.61
3	C	302	AP5	O2D-PD-O3G	2.27	115.41	105.09
3	B	302	AP5	O2B-PB-O3B	2.30	115.52	105.09
3	B	302	AP5	O2E-PE-O3D	2.30	115.53	105.09
3	D	302	AP5	O2D-PD-O3G	2.54	116.62	105.09
3	A	302	AP5	O2D-PD-O3G	2.66	117.14	105.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	AP5	2	0
3	B	302	AP5	2	0
3	C	302	AP5	2	0
3	D	302	AP5	3	0

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

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	211/217 (97%)	0.42	11 (5%) 31 28	13, 26, 53, 69	0
1	B	211/217 (97%)	0.74	26 (12%) 5 4	12, 28, 55, 81	0
1	C	211/217 (97%)	0.43	9 (4%) 39 38	13, 28, 54, 90	0
1	D	211/217 (97%)	0.65	18 (8%) 13 12	14, 30, 61, 85	0
All	All	844/868 (97%)	0.56	64 (7%) 17 15	12, 28, 57, 90	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	148	TYR	8.1
1	D	146	VAL	7.2
1	D	148	TYR	6.7
1	A	146	VAL	5.8
1	D	152	ASP	4.6
1	B	78	LYS	4.1
1	D	151	GLU	4.0
1	B	146	VAL	3.8
1	C	146	VAL	3.6
1	B	75	ASP	3.6
1	B	173	ALA	3.6
1	B	212	LYS	3.6
1	D	173	ALA	3.5
1	B	172	ILE	3.5
1	C	152	ASP	3.4
1	B	106	ILE	3.4
1	A	78	LYS	3.3
1	B	92	GLU	3.3
1	B	176	GLU	3.3
1	B	105	GLY	3.3
1	B	79	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	148	TYR	3.1
1	A	25	HIS	3.0
1	C	150	GLU	3.0
1	B	184	ALA	3.0
1	B	170	VAL	3.0
1	D	150	GLU	2.9
1	A	72	LEU	2.9
1	C	212	LYS	2.9
1	A	77	ILE	2.9
1	A	212	LYS	2.8
1	B	177	PRO	2.8
1	D	91	ILE	2.6
1	B	104	LEU	2.6
1	B	169	ASP	2.6
1	B	186	GLY	2.6
1	D	75	ASP	2.6
1	A	172	ILE	2.5
1	D	90	THR	2.5
1	B	48	LEU	2.5
1	D	134	THR	2.5
1	B	101	LEU	2.5
1	A	76	ASP	2.4
1	D	160	LYS	2.4
1	B	77	ILE	2.3
1	B	70	GLU	2.3
1	D	178	ILE	2.3
1	A	75	ASP	2.3
1	C	75	ASP	2.3
1	B	63	VAL	2.3
1	B	95	HIS	2.2
1	B	166	ARG	2.2
1	D	92	GLU	2.2
1	D	96	ALA	2.2
1	D	133	VAL	2.2
1	B	72	LEU	2.1
1	B	96	ALA	2.1
1	C	99	LYS	2.1
1	C	186	GLY	2.1
1	D	182	TYR	2.1
1	A	63	VAL	2.0
1	D	78	LYS	2.0
1	D	106	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	78	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no 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	MG	D	301	1/1	0.93	0.11	1.23	25,25,25,25	0
3	AP5	B	302	57/57	0.96	0.11	0.12	10,16,33,49	0
3	AP5	D	302	57/57	0.95	0.10	0.11	13,19,29,35	0
3	AP5	C	302	57/57	0.96	0.10	0.09	12,17,29,32	0
3	AP5	A	302	57/57	0.97	0.09	-0.22	11,16,26,26	0
2	MG	C	301	1/1	0.97	0.09	-0.33	24,24,24,24	0
2	MG	B	301	1/1	0.99	0.06	-1.61	20,20,20,20	0
2	MG	A	301	1/1	0.98	0.05	-2.94	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.