



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 04:36 AM GMT

PDB ID : 3K5E
Title : The structure of human kinesin-like motor protein Kif11/KSP/Eg5 in complex with ADP and enastrol.
Authors : Crawley, L.; Cheng, R.K.Y.; Wood, M.; Barker, J.; Felicetti, B.; Whittaker, M.
Deposited on : 2009-10-07
Resolution : 1.97 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

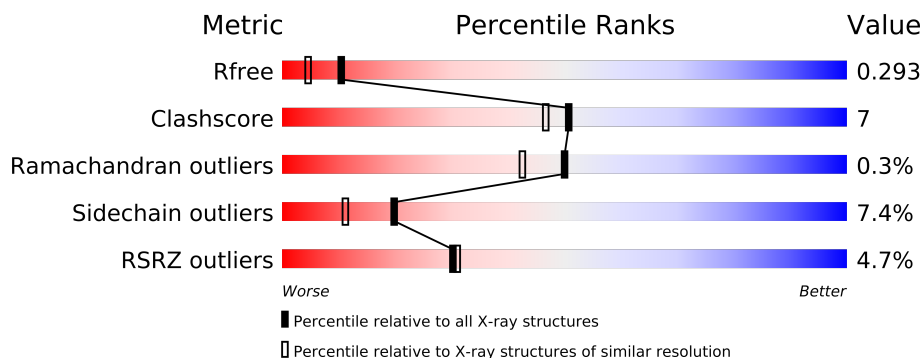
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.97 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}	66092	6577 (2.00-1.96)
Clashscore	79885	8091 (2.00-1.96)
Ramachandran outliers	78287	7989 (2.00-1.96)
Sidechain outliers	78261	7987 (2.00-1.96)
RSRZ outliers	66119	6578 (2.00-1.96)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	368	
1	B	368	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MG	A	604	-	X

2 Entry composition i

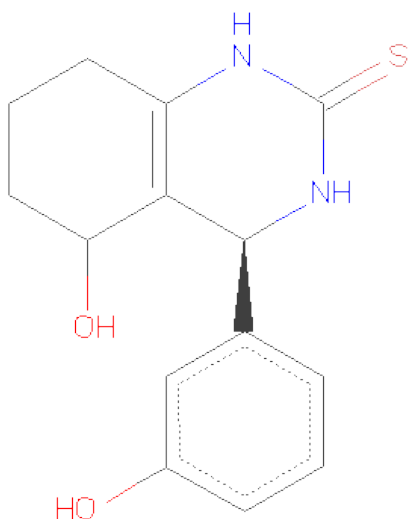
There are 5 unique types of molecules in this entry. The entry contains 5701 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Kinesin-like protein KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2588	1620	451	507	10			
1	B	324	Total	C	N	O	S	0	2	0
			2565	1607	447	501	10			

- Molecule 2 is (4S,5R)-5-HYDROXY-4-(3-HYDROXYPHENYL)-3,4,5,6,7,8-HEXAHYDRO QUINAZOLINE-2(1H)-THIONE (three-letter code: K5E) (formula: C₁₄H₁₆N₂O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			19	14	2	2	1		
2	B	1	Total	C	N	O	S	0	0
			19	14	2	2	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	230	Total	O	0	0
			230	230		
5	B	224	Total	O	0	0
			224	224		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.58Å 79.80Å 69.19Å 90.00° 96.93° 90.00°	Depositor
Resolution (Å)	39.90 – 1.97 39.90 – 1.97	Depositor EDS
% Data completeness (in resolution range)	96.7 (39.90-1.97) 96.6 (39.90-1.97)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.81 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.241 , 0.295 0.241 , 0.293	Depositor DCC
R_{free} test set	3024 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 59446 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5701	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K5E, MG, ADP

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	0.50	0/2626	0.63	0/3550
1	B	0.49	0/2605	0.63	0/3514
All	All	0.49	0/5231	0.63	0/7064

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2588	0	2607	45	0
1	B	2565	0	2593	34	0
2	A	19	0	16	0	0
2	B	19	0	16	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	230	0	0	6	0
5	B	224	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5701	0	5256	78	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (78) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:326:GLY:O	1:A:361:ASN:HB2	1.69	0.93
1:B:326:GLY:O	1:B:361:ASN:HB2	1.68	0.92
1:A:89:ILE:HD11	1:A:99:CYS:HB3	1.63	0.79
1:B:323:SER:O	1:B:330:THR:HG21	1.82	0.78
1:A:287:ASN:ND2	5:A:516:HOH:O	2.18	0.74
1:A:48:LYS:HD2	1:A:69:ASP:O	1.93	0.69
1:A:89:ILE:CD1	1:A:99:CYS:HB3	2.25	0.67
1:B:173:ASN:C	1:B:173:ASN:HD22	1.98	0.66
1:A:362:LYS:HE3	1:A:363:PRO:HD2	1.77	0.65
1:A:45:PRO:HA	1:A:71:VAL:HG23	1.79	0.65
1:A:81:VAL:O	1:A:85:VAL:HG22	1.97	0.65
1:B:170:ASP:HB2	1:B:182:LEU:HD11	1.79	0.63
1:A:85:VAL:O	1:A:89:ILE:HG22	2.02	0.60
1:B:173:ASN:ND2	1:B:175:SER:H	2.00	0.59
1:A:161:LEU:HD21	1:A:168:LEU:HG	1.83	0.59
1:A:299:ILE:HG23	1:A:359:ILE:HD11	1.84	0.58
1:A:53:ARG:HD3	1:A:56:GLY:HA2	1.84	0.58
1:B:339:ALA:HB1	1:B:341:LEU:HD13	1.86	0.57
1:B:92:GLU:HA	1:B:95:MET:HE3	1.87	0.55
1:B:299:ILE:HG23	1:B:359:ILE:HD11	1.87	0.55
1:A:170:ASP:HB2	1:A:182:LEU:HD11	1.89	0.55
1:A:116:GLU:OE2	1:A:221:ARG:NH1	2.36	0.54
1:A:99:CYS:O	1:A:261:LEU:HA	2.09	0.53
1:B:341:LEU:H	1:B:341:LEU:HD12	1.71	0.53
1:B:167:GLU:HG2	1:B:181:ARG:HH21	1.73	0.53
1:B:234:ARG:NH1	5:B:585:HOH:O	2.33	0.52
1:A:28:PHE:HB3	1:A:32:GLU:HG3	1.90	0.52
1:A:260:LYS:HE2	1:A:262:ASN:HD21	1.75	0.52
1:A:327:ARG:HB3	1:A:363:PRO:HD3	1.91	0.52
1:A:175:SER:HB3	1:B:34:LYS:HD3	1.92	0.51
1:B:341:LEU:H	1:B:341:LEU:CD1	2.24	0.51
1:A:315:LYS:NZ	5:A:506:HOH:O	2.43	0.51
1:B:18:ASN:HB3	1:B:360:LEU:HA	1.93	0.51
1:A:54:THR:HG21	1:A:64:LYS:HD3	1.92	0.51
1:B:173:ASN:HD22	1:B:174:PRO:N	2.09	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:173:ASN:HB2	1:B:200:GLU:HG3	1.93	0.50
1:B:154:PHE:HA	1:B:244:HIS:O	2.11	0.50
1:B:40:ILE:HG21	1:B:340:SER:HB3	1.94	0.50
1:A:222:THR:O	1:A:226:THR:HG23	2.12	0.49
1:A:323:SER:O	1:A:330:THR:HG21	2.12	0.49
5:A:395:HOH:O	1:B:208:ASP:HB3	2.12	0.49
1:A:247:GLU:HB3	1:A:255:LEU:HD23	1.94	0.48
1:A:86:VAL:HG21	1:A:135:ILE:HG12	1.94	0.48
1:A:362:LYS:CE	1:A:363:PRO:HD2	2.43	0.48
1:B:90:LEU:HD13	1:B:139:THR:HG23	1.94	0.48
1:A:289:ASN:HD22	1:A:292:LEU:H	1.61	0.47
1:B:173:ASN:C	1:B:173:ASN:ND2	2.65	0.47
1:A:289:ASN:ND2	1:A:292:LEU:H	2.12	0.47
1:B:190:ASN:ND2	1:B:190:ASN:O	2.48	0.47
1:B:289:ASN:HD22	1:B:292:LEU:H	1.61	0.47
1:A:173:ASN:CG	1:A:200:GLU:HG3	2.36	0.46
1:A:89:ILE:HD12	5:A:560:HOH:O	2.16	0.46
1:A:327:ARG:HA	1:A:362:LYS:HA	1.97	0.46
1:B:162:GLU:HG3	1:B:171:LEU:HD23	1.97	0.46
1:A:18:ASN:N	5:A:595:HOH:O	2.48	0.46
1:A:128:GLU:HB2	1:A:141:HIS:CD2	2.51	0.45
1:A:327:ARG:CB	1:A:363:PRO:HD3	2.46	0.45
1:A:241:VAL:CG1	1:A:261:LEU:HB3	2.47	0.45
1:A:163:ILE:HG12	1:A:168:LEU:HD12	2.00	0.44
1:B:54:THR:HG22	1:B:343:LEU:HD11	1.98	0.44
1:B:325:GLY:HA2	1:B:361:ASN:HB3	2.00	0.43
1:A:18:ASN:HB3	1:A:360:LEU:HA	2.00	0.43
1:B:287:ASN:HB3	1:B:288:ILE:H	1.46	0.43
1:A:82:TYR:OH	1:A:142:GLN:HG3	2.19	0.43
1:B:222:THR:O	1:B:226:THR:HG23	2.19	0.42
1:A:191:LYS:O	1:A:192:ARG:HG2	2.19	0.42
1:A:93:VAL:HG21	1:A:261:LEU:HB2	2.01	0.42
1:A:86:VAL:O	1:A:89:ILE:HG23	2.20	0.41
1:A:187:ASP:OD2	1:A:189:ARG:NH1	2.50	0.41
1:B:142:GLN:HG2	5:B:455:HOH:O	2.20	0.41
1:A:48:LYS:HA	1:A:71:VAL:HG22	2.03	0.41
1:B:90:LEU:O	1:B:94:ILE:HD13	2.20	0.41
1:A:31:ALA:HB2	5:B:559:HOH:O	2.21	0.41
1:B:83:ARG:NH2	5:B:589:HOH:O	2.42	0.41
1:A:287:ASN:ND2	5:A:546:HOH:O	2.51	0.40
1:B:289:ASN:ND2	1:B:292:LEU:H	2.19	0.40
1:B:77:LYS:HG3	5:B:501:HOH:O	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:111:LYS:HB2	1:B:111:LYS:HE2	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	323/368 (88%)	309 (96%)	13 (4%)	1 (0%)	50	42
1	B	315/368 (86%)	311 (99%)	3 (1%)	1 (0%)	50	42
All	All	638/736 (87%)	620 (97%)	16 (2%)	2 (0%)	50	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	189	ARG
1	A	362	LYS

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	293/322 (91%)	274 (94%)	19 (6%)	24	15
1	B	292/322 (91%)	268 (92%)	24 (8%)	17	9
All	All	585/644 (91%)	542 (93%)	43 (7%)	20	11

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	64	LYS
1	A	65	THR
1	A	89	ILE
1	A	161	LEU
1	A	168	LEU
1	A	173	ASN
1	A	179	SER
1	A	189	ARG
1	A	190	ASN
1	A	192	ARG
1	A	207	LYS
1	A	216	LYS
1	A	254	GLU
1	A	255	LEU
1	A	289	ASN
1	A	330	THR
1	A	337	SER
1	A	361	ASN
1	B	34	LYS
1	B	46	VAL
1	B	49	GLU
1	B	61	SER
1	B	65	THR
1	B	85	VAL
1	B	87	CYS
1	B	128	GLU
1	B	148	THR
1	B	161	LEU
1	B	168	LEU
1	B	173	ASN
1	B	179	SER
1	B	190	ASN
1	B	192	ARG
1	B	216	LYS
1	B	226	THR
1	B	241	VAL
1	B	287	ASN
1	B	289	ASN
1	B	330	THR
1	B	337	SER
1	B	341	LEU
1	B	361	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	142	GLN
1	A	173	ASN
1	A	205	HIS
1	A	212	GLN
1	A	229	ASN
1	A	262	ASN
1	A	287	ASN
1	A	289	ASN
1	A	361	ASN
1	B	18	ASN
1	B	173	ASN
1	B	190	ASN
1	B	229	ASN
1	B	262	ASN
1	B	289	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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	K5E	A	369	-	21,21,21	5.76	4 (19%)	30,30,30	2.18	7 (23%)
3	ADP	A	603	4	29,29,29	1.10	2 (6%)	45,45,45	2.01	8 (17%)
2	K5E	B	369	-	21,21,21	5.76	4 (19%)	30,30,30	1.86	4 (13%)
3	ADP	B	605	4	29,29,29	1.09	3 (10%)	45,45,45	1.98	9 (20%)

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	K5E	A	369	-	-	0/4/30/30	0/1/3/3
3	ADP	A	603	4	-	0/16/32/32	0/1/3/3
2	K5E	B	369	-	-	0/4/30/30	0/1/3/3
3	ADP	B	605	4	-	0/16/32/32	0/1/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	369	K5E	C10-C9	25.64	1.49	1.33
2	B	369	K5E	C10-C9	25.60	1.49	1.33
2	A	369	K5E	C8-S	-3.79	1.58	1.68
2	B	369	K5E	C8-S	-3.06	1.60	1.68
3	B	605	ADP	C5-C4	2.88	1.47	1.40
2	B	369	K5E	C11-C10	-2.84	1.49	1.52
3	A	603	ADP	C5-C4	2.83	1.46	1.40
3	A	603	ADP	C4-N9	-2.69	1.33	1.37
3	B	605	ADP	C4-N9	-2.63	1.33	1.37
2	B	369	K5E	C14-C9	2.31	1.52	1.49
2	A	369	K5E	C14-C9	2.25	1.52	1.49
2	A	369	K5E	C11-C10	-2.15	1.50	1.52
3	B	605	ADP	O4'-C1'	2.13	1.44	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	369	K5E	N2-C8-N1	9.51	122.64	116.27
3	A	603	ADP	N3-C2-N1	-7.96	122.05	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	369	K5E	N2-C8-N1	7.66	121.40	116.27
3	B	605	ADP	N3-C2-N1	-7.24	122.66	128.71
3	A	603	ADP	N3-C4-N9	5.51	135.38	125.43
3	B	605	ADP	N3-C4-N9	5.30	135.01	125.43
3	B	605	ADP	O4'-C1'-N9	4.31	112.45	108.44
3	A	603	ADP	C8-N9-C4	4.08	110.02	106.90
2	A	369	K5E	S-C8-N1	-3.09	118.92	122.76
2	B	369	K5E	S-C8-N1	-3.06	118.95	122.76
3	B	605	ADP	C5-C4-N3	-3.01	119.15	125.70
3	B	605	ADP	C4-C5-N7	-2.86	107.07	109.52
3	A	603	ADP	C5-C4-N3	-2.78	119.64	125.70
2	B	369	K5E	C5-C7-N1	-2.66	108.14	110.83
3	B	605	ADP	C8-N9-C4	2.66	108.93	106.90
2	A	369	K5E	S-C8-N2	-2.65	118.44	121.99
3	B	605	ADP	C3'-C2'-C1'	2.63	105.03	100.91
3	A	603	ADP	C4-C5-N7	-2.59	107.31	109.52
2	A	369	K5E	C10-C7-N1	2.52	111.78	109.39
3	B	605	ADP	C2-N3-C4	2.52	121.18	114.01
3	A	603	ADP	C2-N3-C4	2.49	121.11	114.01
3	A	603	ADP	O4'-C1'-N9	2.41	110.68	108.44
2	B	369	K5E	C14-C9-N2	2.39	119.05	115.27
2	A	369	K5E	C14-C9-N2	2.35	118.97	115.27
3	A	603	ADP	PA-O3A-PB	-2.23	125.14	131.68
2	A	369	K5E	C8-N2-C9	-2.21	121.98	123.61
2	A	369	K5E	O2-C11-C10	2.08	112.34	109.12
3	B	605	ADP	O3A-PA-O5'	-2.06	94.19	103.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	329/368 (89%)	0.50	20 (6%) 21 21	10, 24, 46, 51	0
1	B	324/368 (88%)	0.37	11 (3%) 43 44	11, 25, 44, 53	0
All	All	653/736 (88%)	0.44	31 (4%) 30 31	10, 25, 45, 53	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	ILE	5.7
1	A	36	SER	4.8
1	B	37	ALA	4.6
1	A	34	LYS	4.5
1	A	38	HIS	4.2
1	A	249	THR	3.8
1	A	363	PRO	3.8
1	B	38	HIS	3.7
1	A	31	ALA	3.5
1	A	178	VAL	3.3
1	A	149	ASP	3.2
1	A	190	ASN	3.2
1	B	34	LYS	3.1
1	A	341	LEU	3.0
1	A	192	ARG	3.0
1	A	151	GLY	3.0
1	B	33	ARG	2.8
1	B	175	SER	2.8
1	A	188	PRO	2.7
1	A	360	LEU	2.7
1	A	150	ASN	2.6
1	A	55	GLY	2.4
1	A	191	LYS	2.4
1	B	31	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	192	ARG	2.3
1	A	30	LEU	2.3
1	B	360	LEU	2.3
1	A	152	THR	2.2
1	B	181	ARG	2.1
1	B	190	ASN	2.1
1	B	191	LYS	2.1

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	A	604	1/1	0.19	2.92	26,26,26,26	0
2	K5E	B	369	19/19	0.12	0.80	19,23,27,29	0
3	ADP	B	605	27/27	0.12	0.03	14,31,35,36	0
3	ADP	A	603	27/27	0.11	-0.03	16,26,29,31	0
2	K5E	A	369	19/19	0.10	-0.10	16,20,27,27	0
4	MG	B	606	1/1	0.07	-1.44	17,17,17,17	0

6.5 Other polymers ⓘ

There are no such residues in this entry.