



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 12:54 am GMT

PDB ID : 2X7C
Title : Crystal structure of human kinesin Eg5 in complex with (S)-enastron
Authors : Kaan, H.Y.K.; Ulaganathan, V.; Rath, O.; Laggner, C.; Prokopcova, H.;
Dallinger, D.; Kappe, C.O.; Kozielski, F.
Deposited on : 2010-02-26
Resolution : 1.90 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

<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
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

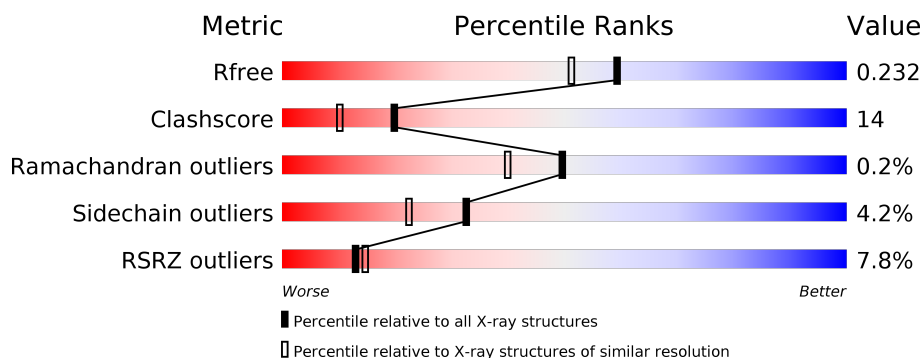
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	111664	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (1.90-1.90)

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 $\leq 5\%$. 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	368	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	368	<div> <div>8%</div> <div> <div></div> <div>73%</div> <div>15%</div> <div>•</div> <div>9%</div> </div> </div>

2 Entry composition [i](#)

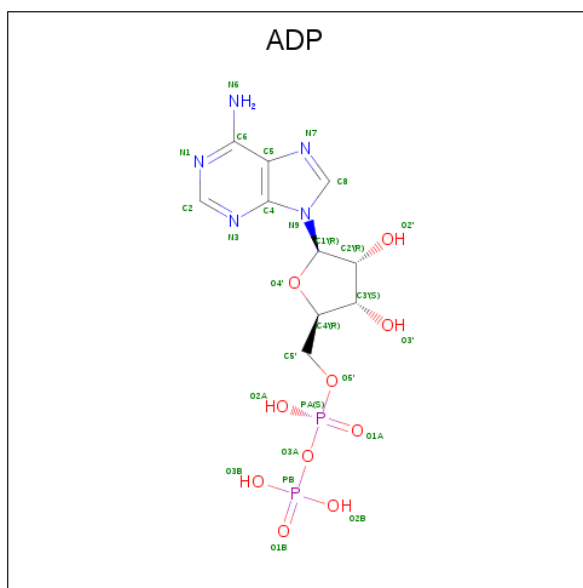
There are 5 unique types of molecules in this entry. The entry contains 6228 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 KINESIN-LIKE PROTEIN KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	19	0
			2705	1707	461	526	11			
1	B	334	Total	C	N	O	S	0	22	0
			2745	1733	473	527	12			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

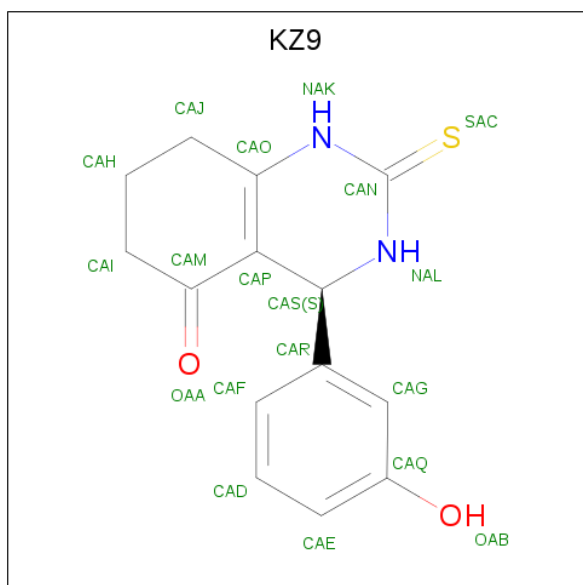


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is (S)-4-(3-HYDROXYPHENYL)-2-THIOXO-1,2,3,4,7,8-HEXAHYDROQUINA ZOLIN-5(6H)-ONE (three-letter code: KZ9) (formula: C₁₄H₁₄N₂O₂S).



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

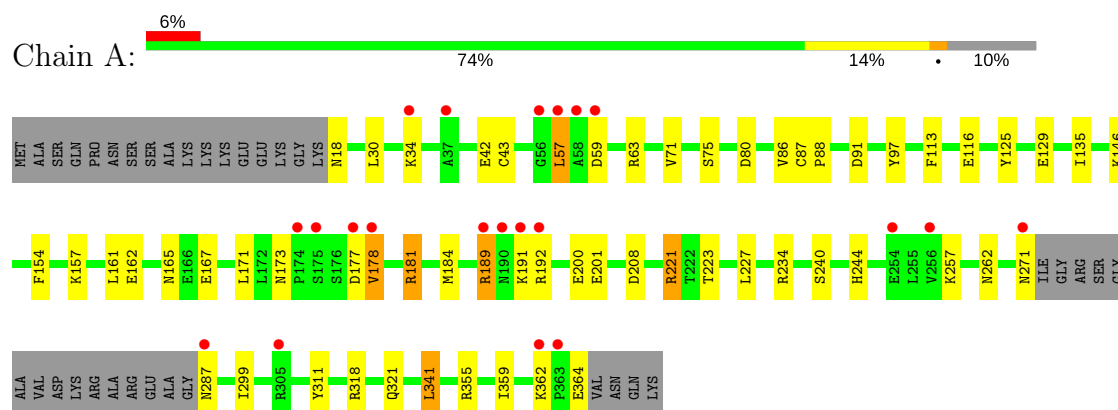
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	342	Total O 342 342	0	0
5	B	341	Total O 341 341	0	0

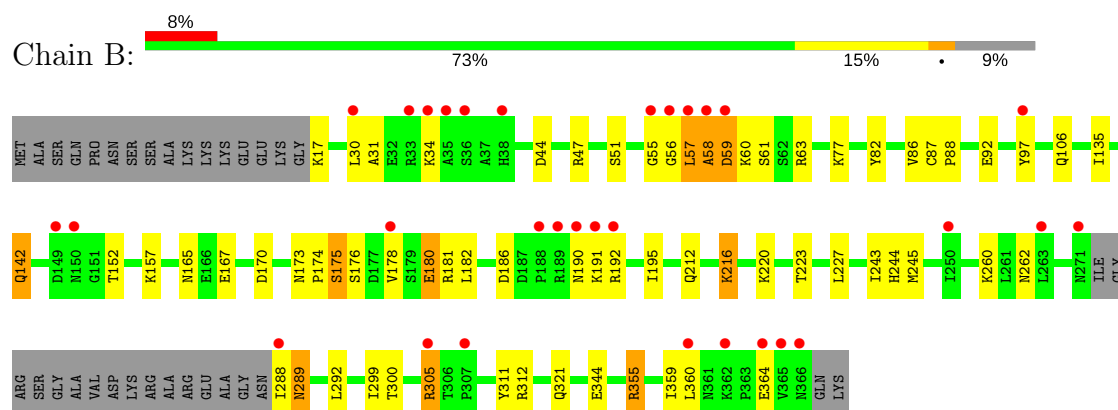
3 Residue-property plots [i](#)

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: KINESIN-LIKE PROTEIN KIF11



• Molecule 1: KINESIN-LIKE PROTEIN KIF11



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.62Å 79.76Å 159.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 29.62 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (30.00-1.90) 97.9 (29.62-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.84 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.163 , 0.232 0.164 , 0.232	Depositor DCC
R_{free} test set	3498 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6228	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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 46.49 % 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 1.1360e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, KZ9, 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	0.59	0/2803	0.73	2/3791 (0.1%)
1	B	0.60	0/2850	0.74	0/3848
All	All	0.60	0/5653	0.73	2/7639 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	161	LEU	CB-CG-CD2	-5.34	101.92	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2705	0	2777	58	0
1	B	2745	0	2844	92	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	19	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	19	0	13	0	0
5	A	342	0	0	25	0
5	B	341	0	0	30	0
All	All	6228	0	5672	152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (152) 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:B:212[B]:GLN:HE22	1:B:216[B]:LYS:CD	1.17	1.55
1:B:212[B]:GLN:NE2	1:B:216[B]:LYS:HD2	1.03	1.35
1:B:82[B]:TYR:OH	1:B:142[B]:GLN:HG3	1.22	1.33
1:B:61:SER:OG	1:B:63[A]:ARG:NH1	1.64	1.31
1:B:212[B]:GLN:NE2	1:B:216[B]:LYS:CD	1.82	1.24
1:B:157:LYS:HE2	5:B:2154:HOH:O	1.40	1.15
1:A:113:PHE:HB2	5:A:2338:HOH:O	1.49	1.08
1:A:364:GLU:HA	5:A:2331:HOH:O	1.54	1.07
1:B:58:ALA:O	1:B:59:ASP:HB2	1.56	1.04
1:A:57:LEU:H	1:A:57:LEU:HD23	1.19	1.03
1:B:212[B]:GLN:HE21	1:B:216[B]:LYS:HD2	1.23	1.02
1:A:287:ASN:HB3	5:A:2265:HOH:O	1.59	1.01
1:B:56:GLY:HA3	1:B:61:SER:HA	1.41	1.00
1:B:31:ALA:O	1:B:34[B]:LYS:HD3	1.65	0.97
1:B:61:SER:HG	1:B:63[A]:ARG:HH12	1.07	0.94
1:B:82[B]:TYR:OH	1:B:142[B]:GLN:CG	2.15	0.93
1:A:91:ASP:OD1	1:A:146:LYS:HE2	1.70	0.92
1:B:17:LYS:N	5:B:2001:HOH:O	2.04	0.91
1:A:18:ASN:N	5:A:2001:HOH:O	2.04	0.90
1:A:287:ASN:HA	5:A:2263:HOH:O	1.71	0.90
1:A:184:MET:HE3	1:A:318:ARG:CZ	2.02	0.89
1:B:212[B]:GLN:HE22	1:B:216[B]:LYS:CE	1.86	0.89
1:A:116:GLU:OE2	1:A:221:ARG:NH2	2.05	0.88
1:B:82[B]:TYR:HH	1:B:142[B]:GLN:HG3	1.37	0.86
1:B:55:GLY:HA2	5:B:2038:HOH:O	1.75	0.85
1:B:58:ALA:O	1:B:59:ASP:CB	2.25	0.84
1:B:305:ARG:HG3	1:B:305:ARG:HH11	1.45	0.82
1:B:212[B]:GLN:NE2	1:B:216[B]:LYS:HD3	1.96	0.80
1:B:305:ARG:CG	1:B:305:ARG:HH11	1.94	0.80
1:A:57:LEU:H	1:A:57:LEU:CD2	1.93	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97[B]:TYR:CD1	1:A:364:GLU:HB2	2.19	0.76
1:A:191:LYS:O	1:A:192:ARG:HG2	1.87	0.74
1:B:305:ARG:HG3	1:B:305:ARG:NH1	2.02	0.74
1:B:55:GLY:O	1:B:61:SER:HB2	1.89	0.73
1:A:184:MET:HE3	1:A:318:ARG:NH1	2.04	0.72
1:B:44:ASP:OD2	1:B:47[B]:ARG:HD2	1.89	0.72
1:B:51:SER:C	1:B:63[B]:ARG:NH1	2.43	0.72
1:B:60:LYS:O	1:B:61:SER:HB3	1.90	0.72
1:B:223[B]:THR:HG21	5:B:2215:HOH:O	1.88	0.71
1:B:63[B]:ARG:NH2	5:B:2054:HOH:O	2.22	0.70
1:B:142[A]:GLN:HE21	1:B:142[A]:GLN:HA	1.57	0.70
1:B:288:ILE:N	5:B:2269:HOH:O	2.24	0.69
1:A:192:ARG:HG3	5:A:2181:HOH:O	1.94	0.67
1:A:287:ASN:CA	5:A:2263:HOH:O	2.36	0.67
1:B:57:LEU:O	1:B:58:ALA:CB	2.42	0.67
1:B:288:ILE:N	5:B:2268:HOH:O	2.26	0.66
1:B:175[B]:SER:OG	5:B:2166:HOH:O	1.97	0.66
1:B:195:ILE:HD13	5:B:2177:HOH:O	1.97	0.64
1:B:244:HIS:HD2	5:B:2237:HOH:O	1.82	0.63
1:A:184:MET:CE	1:A:318:ARG:NH1	2.62	0.63
1:A:97[B]:TYR:HD1	1:A:364:GLU:HB2	1.61	0.63
1:A:162:GLU:HG3	1:A:171:LEU:HD23	1.81	0.62
1:B:56:GLY:O	1:B:60:LYS:O	2.17	0.62
1:B:195:ILE:CD1	5:B:2177:HOH:O	2.48	0.61
1:B:152:THR:N	5:B:2145:HOH:O	2.33	0.61
1:B:220:LYS:O	1:B:223[B]:THR:CG2	2.49	0.60
1:B:31:ALA:O	1:B:34[B]:LYS:CD	2.45	0.60
1:B:51:SER:C	1:B:63[B]:ARG:HH12	2.05	0.60
1:B:167:GLU:OE1	1:B:181:ARG:CZ	2.51	0.59
1:B:165:ASN:HB2	5:B:2157:HOH:O	2.02	0.59
1:A:341:LEU:HD22	5:A:2303:HOH:O	2.03	0.59
1:B:82[A]:TYR:CE2	1:B:86:VAL:HG11	2.36	0.59
1:B:165:ASN:CB	5:B:2157:HOH:O	2.51	0.58
1:A:192:ARG:CD	5:A:2292:HOH:O	2.51	0.58
1:B:170:ASP:HB2	1:B:182:LEU:HD11	1.85	0.58
1:B:57:LEU:O	1:B:58:ALA:HB2	2.04	0.58
1:B:31:ALA:HA	1:B:34[B]:LYS:HD2	1.84	0.57
1:B:82[B]:TYR:CZ	1:B:142[B]:GLN:HG3	2.33	0.57
1:B:220:LYS:O	1:B:223[B]:THR:HG23	2.06	0.56
1:A:184:MET:HE3	1:A:318:ARG:NE	2.21	0.55
1:B:186:ASP:OD2	1:B:312:ARG:NH2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:PRO:HB3	1:B:216[B]:LYS:HE3	1.88	0.55
1:B:87[B]:CYS:HB3	1:B:88:PRO:HD3	1.88	0.55
1:A:157:LYS:HE2	5:A:2160:HOH:O	2.06	0.55
1:B:57:LEU:HG	5:B:2038:HOH:O	2.06	0.55
1:A:244[B]:HIS:HE1	5:A:2240:HOH:O	1.90	0.54
1:B:51:SER:OG	1:B:63[B]:ARG:HD3	2.08	0.54
1:B:321:GLN:NE2	5:B:2292:HOH:O	2.38	0.53
1:A:42:GLU:CD	1:A:63:ARG:HH12	2.11	0.53
1:B:142[B]:GLN:HG2	5:B:2137:HOH:O	2.08	0.53
1:A:157:LYS:HE3	5:A:2066:HOH:O	2.08	0.53
1:A:208:ASP:HB3	5:A:2199:HOH:O	2.08	0.53
1:B:106:GLN:CG	5:B:2091:HOH:O	2.57	0.52
1:B:243:ILE:HG22	1:B:245:MET:HG3	1.92	0.51
1:B:51:SER:O	1:B:63[B]:ARG:NH1	2.36	0.50
1:B:157:LYS:CE	5:B:2154:HOH:O	2.22	0.50
1:A:43:CYS:HB3	1:A:71[A]:VAL:HG12	1.94	0.50
1:A:240:SER:OG	1:A:262:ASN:ND2	2.45	0.49
1:A:57:LEU:HD12	1:A:59:ASP:OD2	2.13	0.49
1:B:176:SER:OG	1:B:180[B]:GLU:OE1	2.25	0.49
1:A:18:ASN:CA	5:A:2001:HOH:O	2.56	0.49
1:A:244[B]:HIS:CE1	5:A:2240:HOH:O	2.65	0.49
1:B:300:THR:OG1	1:B:355:ARG:NH2	2.44	0.49
1:B:61:SER:OG	1:B:63[A]:ARG:CZ	2.50	0.49
1:B:220:LYS:O	1:B:223[B]:THR:HG22	2.13	0.49
1:A:91:ASP:OD1	1:A:146:LYS:CE	2.53	0.48
1:B:311:TYR:CD1	1:B:321:GLN:HG3	2.49	0.47
1:B:57:LEU:CG	5:B:2038:HOH:O	2.61	0.47
1:B:299:ILE:HG23	1:B:359:ILE:HD11	1.97	0.47
1:B:92:GLU:HG3	1:B:97:TYR:CD2	2.50	0.47
1:A:192:ARG:HD3	5:A:2292:HOH:O	2.14	0.46
1:A:234:ARG:NH1	5:A:2233:HOH:O	2.41	0.46
1:A:271:ASN:HA	5:A:2261:HOH:O	2.16	0.46
1:A:57:LEU:CD1	1:A:59:ASP:OD2	2.63	0.46
1:B:289:ASN:HD22	1:B:292:LEU:H	1.63	0.45
1:B:82[A]:TYR:CE2	1:B:86:VAL:CG1	3.00	0.45
1:B:289:ASN:ND2	1:B:292:LEU:H	2.15	0.45
1:A:167[A]:GLU:OE1	1:A:181:ARG:NE	2.50	0.45
1:A:178:VAL:HG21	1:A:223:THR:HB	1.98	0.45
1:A:201:GLU:OE2	5:A:2187:HOH:O	2.21	0.45
1:B:174:PRO:HB3	1:B:216[C]:LYS:HD3	1.99	0.45
1:B:260:LYS:HE2	1:B:262:ASN:HD21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ILE:HG23	1:A:359:ILE:HD11	2.00	0.44
1:B:106:GLN:HG3	5:B:2091:HOH:O	2.16	0.44
1:A:173:ASN:HA	1:A:200:GLU:HG3	1.99	0.44
1:A:87[A]:CYS:HB2	1:A:88:PRO:HD3	1.99	0.44
1:A:287:ASN:N	5:A:2263:HOH:O	2.49	0.43
1:B:344:GLU:HG2	5:B:2309:HOH:O	2.18	0.43
1:A:189:ARG:HD2	5:A:2178:HOH:O	2.18	0.43
1:B:57:LEU:HD11	5:B:2038:HOH:O	2.19	0.43
1:B:56:GLY:HA3	1:B:61:SER:CA	2.29	0.43
1:A:125:TYR:HD2	1:A:129:GLU:HG3	1.84	0.42
1:A:97[B]:TYR:CE1	1:A:364:GLU:OE1	2.72	0.42
1:B:61:SER:HG	1:B:63[A]:ARG:NH1	1.84	0.42
1:B:87[A]:CYS:HB2	1:B:88:PRO:HD3	2.00	0.42
1:B:190:ASN:HB3	5:B:2179:HOH:O	2.19	0.42
1:A:257:LYS:HB2	1:A:257:LYS:HE3	1.85	0.42
1:B:77:LYS:NZ	5:B:2063:HOH:O	2.34	0.42
1:A:43:CYS:HB3	1:A:71[A]:VAL:CG1	2.49	0.42
1:B:244:HIS:HE1	5:B:2239:HOH:O	2.02	0.42
1:B:56:GLY:CA	1:B:61:SER:HA	2.29	0.42
1:B:173:ASN:HA	1:B:174:PRO:HD3	1.82	0.42
1:A:86:VAL:HG21	1:A:135:ILE:HG12	2.02	0.41
1:A:75:SER:HA	5:A:2056:HOH:O	2.20	0.41
1:A:311:TYR:CD1	1:A:321:GLN:HG3	2.56	0.41
1:A:42:GLU:OE1	1:A:63:ARG:NH1	2.42	0.41
1:B:142[B]:GLN:NE2	5:B:2140:HOH:O	2.49	0.41
1:B:173:ASN:C	1:B:173:ASN:OD1	2.59	0.41
1:B:17:LYS:CA	5:B:2001:HOH:O	2.61	0.41
1:A:97[B]:TYR:CE1	1:A:364:GLU:HB2	2.55	0.41
1:A:80:ASP:OD2	5:A:2062:HOH:O	2.22	0.41
1:A:362:LYS:HB3	1:A:362:LYS:NZ	2.36	0.40
1:A:355:ARG:HG3	5:A:2317:HOH:O	2.21	0.40
1:B:86:VAL:HG21	1:B:135:ILE:HG12	2.04	0.40
1:A:189:ARG:NH1	5:A:2178:HOH:O	2.32	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	347/368 (94%)	339 (98%)	8 (2%)	0	100	100
1	B	351/368 (95%)	345 (98%)	5 (1%)	1 (0%)	43	33
All	All	698/736 (95%)	684 (98%)	13 (2%)	1 (0%)	49	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	58	ALA

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	314/322 (98%)	302 (96%)	12 (4%)	36	26
1	B	319/322 (99%)	300 (94%)	19 (6%)	21	11
All	All	633/644 (98%)	602 (95%)	31 (5%)	32	17

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30[A]	LEU
1	A	30[B]	LEU
1	A	34	LYS
1	A	57	LEU
1	A	165	ASN

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Mol	Chain	Res	Type
1	A	177	ASP
1	A	178	VAL
1	A	181	ARG
1	A	189	ARG
1	A	227[A]	LEU
1	A	227[B]	LEU
1	A	341	LEU
1	B	30	LEU
1	B	57	LEU
1	B	59	ASP
1	B	142[A]	GLN
1	B	142[B]	GLN
1	B	175[A]	SER
1	B	175[B]	SER
1	B	178	VAL
1	B	180[A]	GLU
1	B	180[B]	GLU
1	B	191	LYS
1	B	192	ARG
1	B	216[B]	LYS
1	B	216[C]	LYS
1	B	289	ASN
1	B	305	ARG
1	B	355	ARG
1	B	360	LEU
1	B	364	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	ASN
1	A	287	ASN
1	B	165	ASN
1	B	244	HIS
1	B	262	ASN
1	B	289	ASN
1	B	290	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 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$
4	KZ9	A	1365	-	21,21,21	2.20	6 (28%)	29,30,30	2.30	10 (34%)
2	ADP	A	601	3	25,29,29	0.99	2 (8%)	25,45,45	1.79	3 (12%)
4	KZ9	B	1367	-	21,21,21	2.32	6 (28%)	29,30,30	2.40	11 (37%)
2	ADP	B	602	3	25,29,29	1.10	2 (8%)	25,45,45	1.88	4 (16%)

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
4	KZ9	A	1365	-	-	0/4/30/30	0/3/3/3
2	ADP	A	601	3	-	0/12/32/32	0/3/3/3
4	KZ9	B	1367	-	-	0/4/30/30	0/3/3/3
2	ADP	B	602	3	-	0/12/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1365	KZ9	CAM-CAP	-3.03	1.40	1.45
4	B	1367	KZ9	CAM-CAP	-2.77	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	ADP	C2-N3	2.02	1.35	1.32
2	A	601	ADP	O4'-C1'	2.08	1.44	1.41
4	B	1367	KZ9	CAN-NAK	2.14	1.38	1.36
4	B	1367	KZ9	CAJ-CAO	2.28	1.53	1.49
4	B	1367	KZ9	CAI-CAM	2.46	1.54	1.50
4	A	1365	KZ9	CAJ-CAO	2.48	1.54	1.49
2	A	601	ADP	C5-C4	2.50	1.46	1.40
4	A	1365	KZ9	CAI-CAM	2.56	1.54	1.50
4	A	1365	KZ9	CAN-NAK	2.64	1.39	1.36
2	B	602	ADP	C5-C4	2.87	1.47	1.40
4	A	1365	KZ9	CAS-CAP	3.05	1.54	1.51
4	B	1367	KZ9	CAS-CAP	4.76	1.56	1.51
4	A	1365	KZ9	CAN-NAL	6.45	1.39	1.33
4	B	1367	KZ9	CAN-NAL	7.11	1.40	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ADP	N3-C2-N1	-7.04	122.84	128.86
2	B	602	ADP	N3-C2-N1	-6.84	123.01	128.86
4	B	1367	KZ9	CAR-CAS-NAL	-5.28	104.95	110.81
4	A	1365	KZ9	SAC-CAN-NAK	-4.03	116.94	122.06
4	B	1367	KZ9	CAM-CAP-CAO	-3.42	116.26	119.50
4	B	1367	KZ9	OAA-CAM-CAP	-3.11	118.17	121.28
4	A	1365	KZ9	CAR-CAS-NAL	-3.10	107.37	110.81
4	A	1365	KZ9	OAA-CAM-CAP	-3.05	118.24	121.28
4	B	1367	KZ9	CAN-NAK-CAO	-2.93	122.08	123.84
2	A	601	ADP	O3'-C3'-C4'	-2.66	103.36	111.06
4	B	1367	KZ9	OAA-CAM-CAI	-2.52	116.62	120.86
4	A	1365	KZ9	CAS-NAL-CAN	-2.47	121.55	125.23
2	B	602	ADP	O3'-C3'-C4'	-2.43	104.03	111.06
4	B	1367	KZ9	SAC-CAN-NAK	-2.38	119.03	122.06
4	B	1367	KZ9	CAR-CAS-CAP	-2.16	110.05	112.87
4	A	1365	KZ9	CAR-CAS-CAP	-2.07	110.17	112.87
4	A	1365	KZ9	OAA-CAM-CAI	-2.05	117.42	120.86
2	A	601	ADP	C4-C5-N7	-2.03	107.44	109.41
4	A	1365	KZ9	CAH-CAI-CAM	-2.01	110.02	113.55
2	B	602	ADP	N6-C6-N1	2.10	122.94	118.57
2	B	602	ADP	C2-N1-C6	2.66	123.27	118.75
4	B	1367	KZ9	CAS-CAP-CAM	3.01	121.89	117.61
4	B	1367	KZ9	CAP-CAS-NAL	3.33	111.80	109.11
4	A	1365	KZ9	CAI-CAM-CAP	3.87	123.78	117.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1367	KZ9	CAI-CAM-CAP	4.78	125.14	117.99
4	A	1365	KZ9	CAP-CAS-NAL	5.51	113.55	109.11
4	A	1365	KZ9	NAK-CAN-NAL	5.71	120.35	116.20
4	B	1367	KZ9	NAK-CAN-NAL	5.72	120.35	116.20

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 [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 [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	332/368 (90%)	0.23	21 (6%)	20 23	4, 17, 41, 56	0
1	B	334/368 (90%)	0.30	31 (9%)	8 10	5, 16, 39, 59	0
All	All	666/736 (90%)	0.27	52 (7%)	13 15	4, 16, 41, 59	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	ALA	11.8
1	A	57	LEU	10.1
1	A	178	VAL	7.4
1	B	57	LEU	6.7
1	B	191	LYS	5.9
1	B	149	ASP	5.9
1	B	56	GLY	5.7
1	A	192	ARG	4.9
1	B	192	ARG	4.5
1	A	271	ASN	4.5
1	B	190	ASN	4.3
1	A	58	ALA	4.3
1	A	287	ASN	4.1
1	B	365	VAL	4.1
1	A	56	GLY	3.9
1	A	191	LYS	3.9
1	B	178	VAL	3.8
1	B	366	ASN	3.6
1	A	190	ASN	3.1
1	B	271[A]	ASN	3.0
1	A	256	VAL	3.0
1	A	175	SER	3.0
1	B	250	ILE	2.9
1	A	177	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	150	ASN	2.9
1	A	362	LYS	2.8
1	B	305	ARG	2.8
1	B	188	PRO	2.8
1	A	34	LYS	2.7
1	B	59	ASP	2.6
1	B	34[A]	LYS	2.6
1	A	254	GLU	2.5
1	A	189	ARG	2.5
1	B	30	LEU	2.4
1	A	305	ARG	2.4
1	B	36	SER	2.3
1	B	38	HIS	2.3
1	B	189	ARG	2.3
1	B	55	GLY	2.3
1	B	33[A]	ARG	2.3
1	A	37	ALA	2.2
1	B	97	TYR	2.2
1	B	35	ALA	2.2
1	B	288	ILE	2.2
1	A	363	PRO	2.2
1	B	362	LYS	2.2
1	B	360	LEU	2.1
1	B	263	LEU	2.1
1	B	307	PRO	2.1
1	B	364	GLU	2.1
1	A	59	ASP	2.0
1	A	174	PRO	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. 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
4	KZ9	A	1365	19/19	0.98	0.10	7,11,19,23	0
4	KZ9	B	1367	19/19	0.98	0.10	4,9,14,17	0
2	ADP	B	602	27/27	0.99	0.07	4,11,16,21	0
2	ADP	A	601	27/27	0.99	0.08	4,13,20,20	0
3	MG	B	702	1/1	0.99	0.10	7,7,7,7	0
3	MG	A	701	1/1	1.00	0.12	7,7,7,7	0
3	MG	B	703	1/1	1.00	0.10	7,7,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.