



wwPDB X-ray Structure Validation Summary Report

Feb 1, 2016 – 02:40 PM GMT

PDB ID : 4A5Y
Title : Intermediate state of human kinesin Eg5 in complex with Ispinesib
Authors : Kaan, H.Y.K.; Kozielski, F.
Deposited on : 2011-10-29
Resolution : 2.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

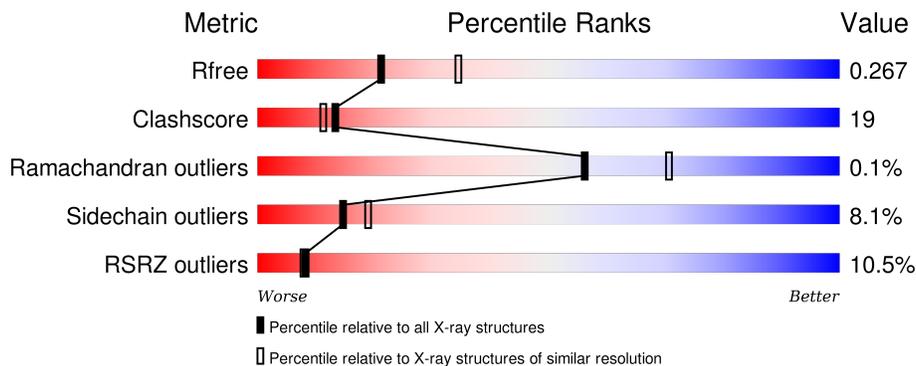
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	
1	B	368	
1	C	368	

2 Entry composition [i](#)

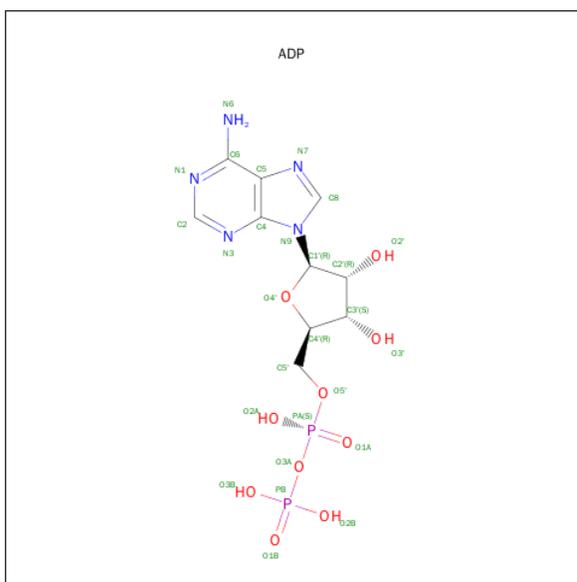
There are 7 unique types of molecules in this entry. The entry contains 8127 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	334	Total	C	N	O	S	0	4	0
			2598	1631	448	509	10			
1	B	302	Total	C	N	O	S	0	0	0
			2364	1489	404	461	10			
1	C	339	Total	C	N	O	S	0	1	0
			2618	1643	458	507	10			

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

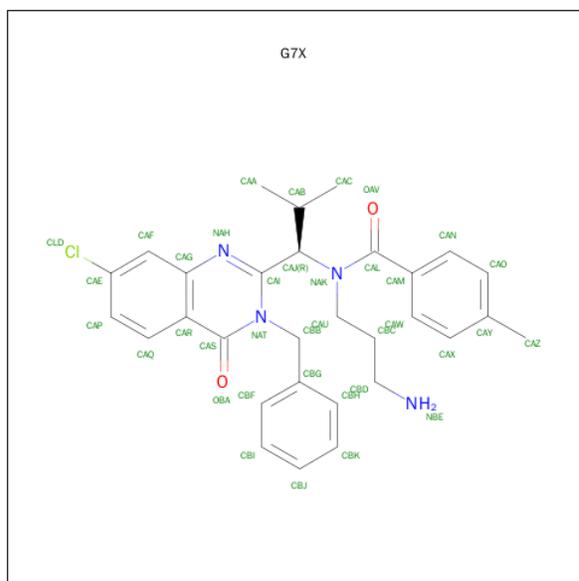


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0

- Molecule 4 is ISPINESIB MESILATE (three-letter code: G7X) (formula: C₃₀H₃₃ClN₄O₂).

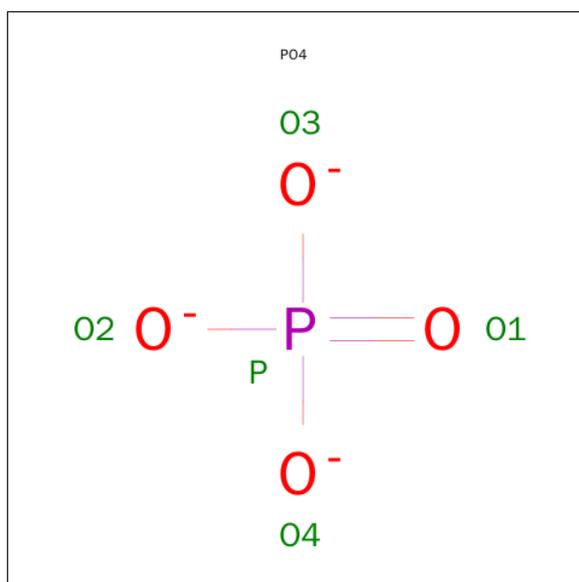


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Cl N O 37 30 1 4 2	0	0
4	B	1	Total C Cl N O 37 30 1 4 2	0	0
4	C	1	Total C Cl N O 37 30 1 4 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Mg 1 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0

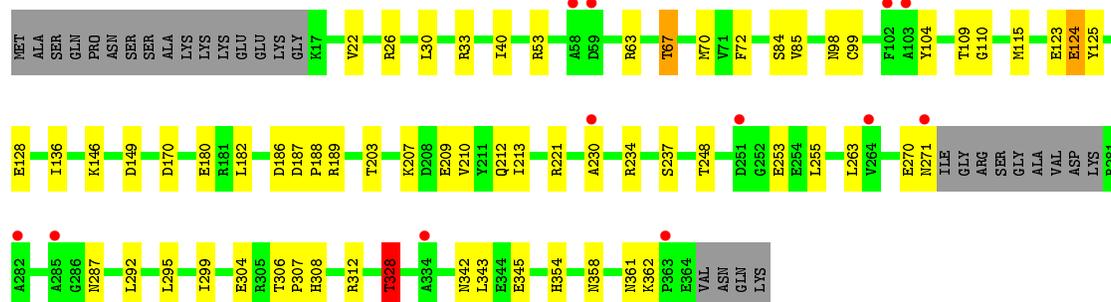
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	93	Total O 93 93	0	0
7	B	81	Total O 81 81	0	0
7	C	168	Total O 168 168	0	0

ASN
GLN
LYS

• Molecule 1: KINESIN-LIKE PROTEIN KIF11

Chain C:  3% 74% 17% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.63Å 91.93Å 163.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 2.45 29.60 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.60-2.45) 99.6 (29.60-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 2.45Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.201 , 0.268 0.201 , 0.267	Depositor DCC
R_{free} test set	2429 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	45.3	Xtrriage
Anisotropy	0.112	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.6	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Outliers	0 of 48117 reflections	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8127	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.27 % 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 2.7156e-03. 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, 0.375 respectively for untwinned datasets, and 0.333, 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: G7X, MG, PO4, ADP, CL

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	0.67	0/2648	0.81	0/3586
1	B	0.58	0/2399	0.71	1/3245 (0.0%)
1	C	0.78	0/2661	0.81	2/3603 (0.1%)
All	All	0.68	0/7708	0.78	3/10434 (0.0%)

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	A	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	328	THR	CB-CA-C	-5.59	96.50	111.60
1	C	110	GLY	N-CA-C	5.50	126.84	113.10
1	B	326	GLY	N-CA-C	-5.03	100.52	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	PRO	Peptide
1	A	122	ASN	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	2598	0	2588	102	0
1	B	2364	0	2363	125	0
1	C	2618	0	2612	59	0
2	A	27	0	12	2	0
2	B	27	0	12	2	0
2	C	27	0	12	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	37	0	33	2	0
4	B	37	0	33	8	0
4	C	37	0	33	3	0
5	C	1	0	0	0	0
6	C	10	0	0	0	0
7	A	93	0	0	5	0
7	B	81	0	0	9	0
7	C	168	0	0	8	0
All	All	8127	0	7698	291	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 19.

The worst 5 of 291 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:244:HIS:HD2	1:B:258:ILE:HG12	1.21	1.04
1:B:153:GLU:HG3	1:B:246:LYS:HB3	1.39	1.01
1:A:227:LEU:HG	1:A:228:MET:HG3	1.48	0.96
1:A:344:GLU:H	1:A:344:GLU:CD	1.68	0.93
1:B:304:GLU:HG3	1:B:306:THR:HG23	1.48	0.92

There are no symmetry-related clashes.

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	332/368 (90%)	319 (96%)	12 (4%)	1 (0%)	46	57
1	B	292/368 (79%)	280 (96%)	12 (4%)	0	100	100
1	C	336/368 (91%)	332 (99%)	4 (1%)	0	100	100
All	All	960/1104 (87%)	931 (97%)	28 (3%)	1 (0%)	56	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU

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	287/322 (89%)	264 (92%)	23 (8%)	15	19
1	B	266/322 (83%)	236 (89%)	30 (11%)	7	7
1	C	287/322 (89%)	272 (95%)	15 (5%)	29	40
All	All	840/966 (87%)	772 (92%)	68 (8%)	15	19

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	111	LYS
1	B	212	GLN

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Mol	Chain	Res	Type
1	C	212	GLN
1	B	119	ARG
1	B	183	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	98	ASN
1	B	262	ASN
1	B	106	GLN
1	A	142	GLN
1	B	244	HIS

5.3.3 RNA [i](#)

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 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	G7X	A	1365	-	39,40,40	1.03	4 (10%)	41,56,56	1.37	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	A	601	-	22,29,29	1.14	3 (13%)	27,45,45	2.32	5 (18%)
4	G7X	B	1363	-	39,40,40	1.22	4 (10%)	41,56,56	1.02	2 (4%)
2	ADP	B	601	-	22,29,29	1.04	1 (4%)	27,45,45	1.99	7 (25%)
6	PO4	C	1366	-	4,4,4	0.27	0	6,6,6	0.32	0
6	PO4	C	1367	-	4,4,4	0.36	0	6,6,6	0.28	0
4	G7X	C	1369	-	39,40,40	1.28	4 (10%)	41,56,56	1.16	4 (9%)
2	ADP	C	601	5	22,29,29	0.96	1 (4%)	27,45,45	1.90	7 (25%)

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	G7X	A	1365	-	-	0/24/28/28	0/4/4/4
2	ADP	A	601	-	-	0/12/32/32	0/3/3/3
4	G7X	B	1363	-	-	0/24/28/28	0/4/4/4
2	ADP	B	601	-	-	0/12/32/32	0/3/3/3
6	PO4	C	1366	-	-	0/0/0/0	0/0/0/0
6	PO4	C	1367	-	-	0/0/0/0	0/0/0/0
4	G7X	C	1369	-	-	0/24/28/28	0/4/4/4
2	ADP	C	601	5	-	0/12/32/32	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1365	G7X	CAF-CAG	-2.31	1.38	1.41
4	A	1365	G7X	CAS-CAR	-2.09	1.37	1.41
4	B	1363	G7X	CAI-NAT	2.10	1.41	1.36
4	A	1365	G7X	CAS-NAT	2.12	1.41	1.38
4	A	1365	G7X	CAM-CAL	2.20	1.53	1.50

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ADP	N3-C2-N1	-7.38	123.24	128.89
2	B	601	ADP	N3-C2-N1	-7.32	123.29	128.89
2	C	601	ADP	N3-C2-N1	-6.44	123.97	128.89
2	A	601	ADP	PA-O3A-PB	-4.40	117.92	132.67
2	A	601	ADP	C2'-C1'-N9	-4.38	107.60	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1365	G7X	2	0
2	A	601	ADP	2	0
4	B	1363	G7X	8	0
2	B	601	ADP	2	0
4	C	1369	G7X	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 [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	334/368 (90%)	0.42	39 (11%) 6 6	26, 49, 91, 110	0
1	B	302/368 (82%)	0.67	51 (16%) 2 2	37, 62, 98, 118	0
1	C	339/368 (92%)	-0.01	12 (3%) 48 51	18, 37, 65, 99	0
All	All	975/1104 (88%)	0.35	102 (10%) 8 8	18, 49, 91, 118	0

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	ALA	9.3
1	B	46	VAL	7.9
1	B	343	LEU	6.8
1	A	360	LEU	6.4
1	A	285	ALA	6.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	G7X	A	1365	37/37	0.93	0.15	0.07	30,38,47,51	0
4	G7X	B	1363	37/37	0.95	0.13	-0.50	36,45,53,56	0
4	G7X	C	1369	37/37	0.97	0.11	-0.69	22,27,37,39	0
3	CL	C	1368	1/1	0.99	0.12	-0.86	38,38,38,38	0
6	PO4	C	1366	5/5	0.95	0.11	-0.88	53,54,57,60	0
2	ADP	B	601	27/27	0.92	0.11	-1.02	69,76,84,88	0
2	ADP	C	601	27/27	0.97	0.13	-1.22	26,36,45,48	0
2	ADP	A	601	27/27	0.94	0.12	-1.54	42,52,61,62	0
3	CL	A	1364	1/1	0.94	0.11	-	74,74,74,74	0
6	PO4	C	1367	5/5	0.95	0.12	-	63,71,86,86	0
5	MG	C	1365	1/1	0.91	0.13	-	48,48,48,48	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.