



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:53 am GMT

PDB ID : 4AP0  
Title : The mitotic kinesin Eg5 in complex with Mg-ADP and ispinesib  
Authors : Schuettelkopf, A.W.; Talapatra, S.K.; Kozielski, F.  
Deposited on : 2012-03-30  
Resolution : 2.59 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

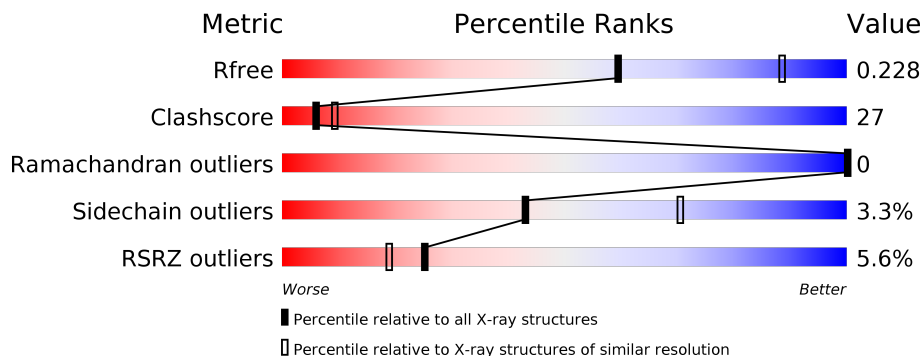
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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  $\geq 3$ , 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	370	<div> <div>5%</div> <div> <div></div> <div>46%</div> <div>41%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	370	<div> <div>7%</div> <div> <div></div> <div>48%</div> <div>34%</div> <div>•</div> <div>16%</div> </div> </div>
1	C	370	<div> <div>5%</div> <div> <div></div> <div>48%</div> <div>34%</div> <div>•</div> <div>16%</div> </div> </div>
1	D	370	<div> <div>2%</div> <div> <div></div> <div>51%</div> <div>31%</div> <div>•</div> <div>16%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9849 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	325	Total	C	N	O	S	0	0	0
			2475	1559	423	484	9			
1	B	312	Total	C	N	O	S	0	0	0
			2374	1492	407	465	10			
1	C	311	Total	C	N	O	S	0	0	0
			2347	1476	405	456	10			
1	D	309	Total	C	N	O	S	0	0	0
			2357	1486	403	459	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P52732
A	0	PRO	-	EXPRESSION TAG	UNP P52732
B	-1	GLY	-	EXPRESSION TAG	UNP P52732
B	0	PRO	-	EXPRESSION TAG	UNP P52732
C	-1	GLY	-	EXPRESSION TAG	UNP P52732
C	0	PRO	-	EXPRESSION TAG	UNP P52732
D	-1	GLY	-	EXPRESSION TAG	UNP P52732
D	0	PRO	-	EXPRESSION TAG	UNP P52732

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

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

- # ADP
- 
- 3D ball-and-stick model of Adenosine Diphosphate (ADP). The molecule consists of an adenine base (blue and purple) attached to a ribose sugar (orange and grey), which is linked via a pyrophosphate group (pink and grey) to another phosphate group. Atoms are labeled with IDs: N16, H17, C6, C5, C4, C3, C2, N11, N13, N14, C11(P), C12(P), C13(P), O4', O5', O2', O3', O1A, O2B, O1B, O3A, PB, PA(5).

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

- Molecule 5 is ISPINESIB MESILATE (three-letter code: G7X) (formula:  $\text{C}_{30}\text{H}_{33}\text{ClN}_4\text{O}_2$ ).



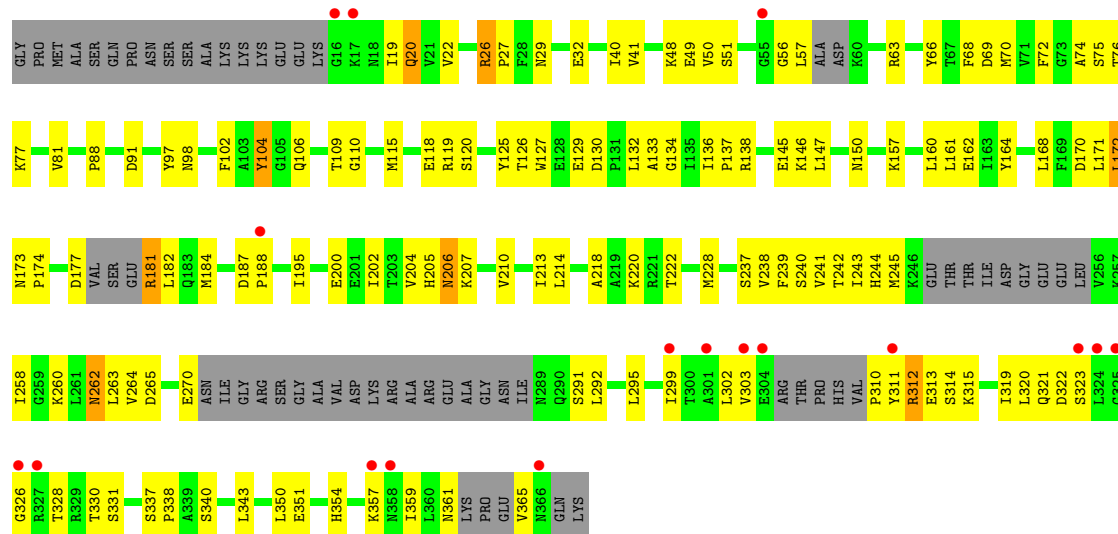
- Molecule 6 is water.



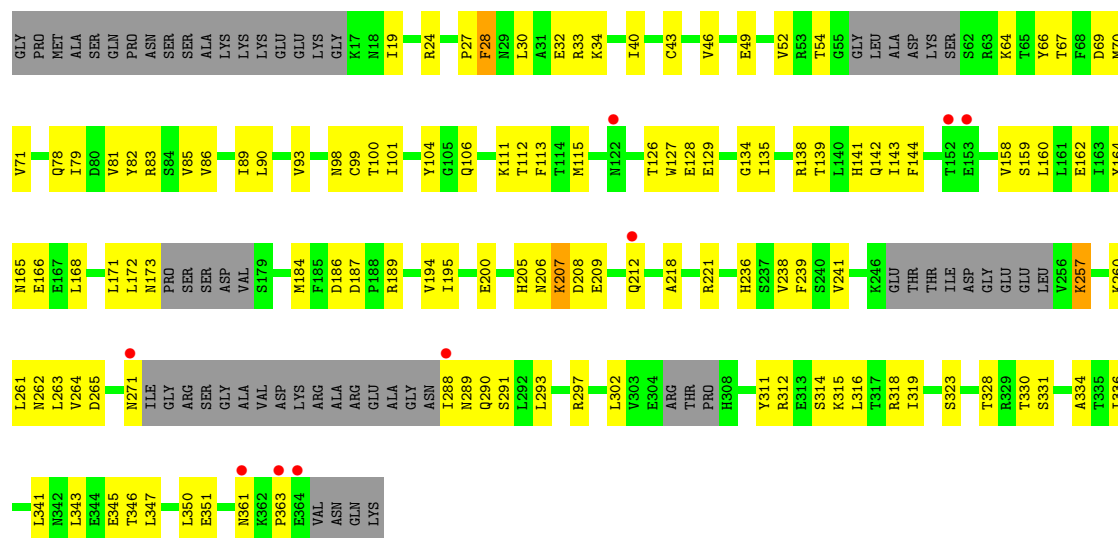




• Molecule 1: KINESIN-LIKE PROTEIN KIF11



• Molecule 1: KINESIN-LIKE PROTEIN KIF11



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.72Å 112.61Å 106.91Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	29.86 – 2.59 29.86 – 2.59	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.86-2.59) 95.7 (29.86-2.59)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.203 , 0.253 0.186 , 0.228	Depositor DCC
$R_{free}$ test set	2297 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.3	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 18.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.019 for -h,-l,-k 0.012 for -h,l,k 0.430 for h,-k,-l	Xtriage
Reported twinning fraction	0.452 for H,-K,-L	Depositor
Outliers	1 of 45505 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9849	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	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 32.28 % 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 9.6433e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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, G7X, 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	0.46	0/2512	0.69	0/3410
1	B	0.45	0/2406	0.69	0/3259
1	C	0.48	0/2377	0.73	0/3217
1	D	0.49	0/2389	0.73	1/3237 (0.0%)
All	All	0.47	0/9684	0.71	1/13123 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	341	LEU	CA-CB-CG	5.58	128.13	115.30

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	2475	0	2424	153	0
1	B	2374	0	2333	127	0
1	C	2347	0	2297	126	0
1	D	2357	0	2312	109	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
3	C	27	0	12	2	0
3	D	27	0	12	2	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
4	D	1	0	0	0	0
5	A	34	0	25	6	0
5	B	37	0	33	13	0
5	C	37	0	33	12	0
5	D	37	0	33	11	0
6	A	9	0	0	0	0
6	B	6	0	0	0	0
6	C	10	0	0	0	0
6	D	8	0	0	0	0
All	All	9849	0	9538	532	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 27.

The worst 5 of 532 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:312:ARG:HG2	1:C:312:ARG:HH11	1.19	1.05
1:B:148:THR:HA	1:B:152:THR:HG22	1.43	1.00
1:C:50:VAL:HG12	1:C:66:TYR:HB2	1.43	0.99
1:A:143:ILE:HD13	1:A:243:ILE:HD11	1.45	0.98
1:A:86:VAL:HG21	1:A:135:ILE:HG12	1.45	0.98

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	317/370 (86%)	309 (98%)	8 (2%)	0	100	100
1	B	302/370 (82%)	295 (98%)	7 (2%)	0	100	100
1	C	297/370 (80%)	294 (99%)	3 (1%)	0	100	100
1	D	297/370 (80%)	287 (97%)	10 (3%)	0	100	100
All	All	1213/1480 (82%)	1185 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	268/323 (83%)	263 (98%)	5 (2%)	62	84
1	B	257/323 (80%)	241 (94%)	16 (6%)	21	42
1	C	252/323 (78%)	243 (96%)	9 (4%)	40	68
1	D	255/323 (79%)	251 (98%)	4 (2%)	68	87
All	All	1032/1292 (80%)	998 (97%)	34 (3%)	43	70

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	182	LEU
1	B	241	VAL
1	D	207	LYS
1	B	234	ARG
1	B	24	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	262	ASN
1	B	321	GLN
1	C	354	HIS
1	B	229	ASN
1	B	236	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 18 ligands modelled in this entry, 10 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
3	ADP	A	1003	2	25,29,29	1.15	2 (8%)	24,45,45	1.78	2 (8%)
5	G7X	A	2001	-	35,37,40	1.24	3 (8%)	44,53,56	1.30	3 (6%)
3	ADP	B	1003	2	25,29,29	1.01	1 (4%)	24,45,45	1.74	3 (12%)
5	G7X	B	2001	-	38,40,40	1.07	3 (7%)	45,56,56	1.49	3 (6%)
3	ADP	C	1003	2	25,29,29	1.10	2 (8%)	24,45,45	2.03	4 (16%)
5	G7X	C	2001	-	38,40,40	0.99	2 (5%)	45,56,56	1.60	9 (20%)
3	ADP	D	1003	2	25,29,29	1.15	3 (12%)	24,45,45	1.57	2 (8%)
5	G7X	D	2001	-	38,40,40	1.00	0	45,56,56	1.49	5 (11%)

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	ADP	A	1003	2	-	0/12/32/32	0/3/3/3
5	G7X	A	2001	-	-	0/20/24/28	0/4/4/4
3	ADP	B	1003	2	-	0/12/32/32	0/3/3/3
5	G7X	B	2001	-	-	0/24/28/28	0/4/4/4
3	ADP	C	1003	2	-	0/12/32/32	0/3/3/3
5	G7X	C	2001	-	-	0/24/28/28	0/4/4/4
3	ADP	D	1003	2	-	0/12/32/32	0/3/3/3
5	G7X	D	2001	-	-	0/24/28/28	0/4/4/4

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1003	ADP	C2-N3	2.05	1.35	1.32
5	C	2001	G7X	CAI-CAJ	2.12	1.53	1.50
5	B	2001	G7X	CAI-NAT	2.19	1.41	1.36
3	C	1003	ADP	PB-O3A	2.19	1.63	1.60
5	A	2001	G7X	CAM-CAL	2.57	1.54	1.50

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	ADP	N3-C2-N1	-6.29	123.38	128.86
3	B	1003	ADP	N3-C2-N1	-6.10	123.54	128.86
5	C	2001	G7X	CAR-CAG-NAH	-5.84	120.34	123.67
5	D	2001	G7X	CAR-CAG-NAH	-5.83	120.34	123.67
3	D	1003	ADP	N3-C2-N1	-5.73	123.87	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2001	G7X	6	0
3	B	1003	ADP	1	0
5	B	2001	G7X	13	0
3	C	1003	ADP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2001	G7X	12	0
3	D	1003	ADP	2	0
5	D	2001	G7X	11	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	325/370 (87%)	0.30	17 (5%) 28 21	22, 56, 102, 129	0
1	B	312/370 (84%)	0.45	27 (8%) 11 7	28, 58, 105, 137	0
1	C	311/370 (84%)	0.36	17 (5%) 26 19	23, 51, 102, 153	0
1	D	309/370 (83%)	0.19	9 (2%) 52 45	21, 50, 89, 112	0
All	All	1257/1480 (84%)	0.32	70 (5%) 25 19	21, 54, 101, 153	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	325	GLY	8.6
1	A	363	PRO	8.3
1	C	301	ALA	8.1
1	B	178	VAL	7.3
1	B	57	LEU	7.1

### 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	G7X	C	2001	37/37	0.92	0.19	1.33	18,39,56,58	0
4	CL	A	1368	1/1	0.89	0.16	0.46	65,65,65,65	0
5	G7X	B	2001	37/37	0.90	0.19	0.26	26,46,64,69	0
5	G7X	A	2001	34/37	0.93	0.18	0.25	12,42,74,80	0
3	ADP	D	1003	27/27	0.95	0.16	0.10	15,31,45,55	0
5	G7X	D	2001	37/37	0.89	0.17	0.03	25,43,61,69	0
3	ADP	C	1003	27/27	0.96	0.16	0.02	15,30,47,50	0
3	ADP	A	1003	27/27	0.97	0.15	0.01	15,33,42,45	0
4	CL	D	1365	1/1	0.87	0.16	-0.19	51,51,51,51	0
4	CL	B	1362	1/1	0.86	0.14	-0.69	53,53,53,53	0
3	ADP	B	1003	27/27	0.95	0.15	-0.76	18,36,45,54	0
4	CL	B	1360	1/1	0.92	0.12	-2.00	59,59,59,59	0
4	CL	A	1367	1/1	0.97	0.08	-4.87	38,38,38,38	0
2	MG	B	1001	1/1	0.70	0.17	-	35,35,35,35	0
2	MG	D	1001	1/1	0.69	0.24	-	50,50,50,50	0
2	MG	A	1001	1/1	0.88	0.13	-	30,30,30,30	0
4	CL	B	1361	1/1	0.83	0.12	-	60,60,60,60	0
2	MG	C	1001	1/1	0.90	0.18	-	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.