



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 11, 2021 – 04:05 pm BST

PDB ID : 6YZH  
Title : Crystal structure of P8C9 bound to CK2alpha  
Authors : Atkinson, E.; Iegre, J.; Brear, P.; Baker, D.; Sore, H.; Hyvonen, M.; Spring, D.  
Deposited on : 2020-05-07  
Resolution : 1.19 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.18

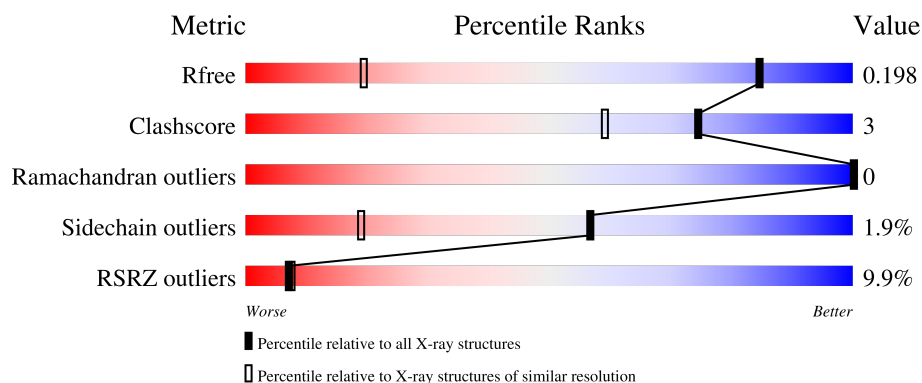
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.19 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))
$R_{free}$	130704	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	398	<div> <div>9%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div>
2	D	10	<div> <div>80%</div> <div>20%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3481 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 Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	344	3011	1920	535	544	12	0	16	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-46	MET	-	initiating methionine	UNP P68400
A	-45	ASN	-	expression tag	UNP P68400
A	-44	THR	-	expression tag	UNP P68400
A	-43	ILE	-	expression tag	UNP P68400
A	-42	HIS	-	expression tag	UNP P68400
A	-41	HIS	-	expression tag	UNP P68400
A	-40	HIS	-	expression tag	UNP P68400
A	-39	HIS	-	expression tag	UNP P68400
A	-38	HIS	-	expression tag	UNP P68400
A	-37	HIS	-	expression tag	UNP P68400
A	-36	ASN	-	expression tag	UNP P68400
A	-35	THR	-	expression tag	UNP P68400
A	-34	SER	-	expression tag	UNP P68400
A	-33	GLY	-	expression tag	UNP P68400
A	-32	SER	-	expression tag	UNP P68400
A	-31	GLY	-	expression tag	UNP P68400
A	-30	GLY	-	expression tag	UNP P68400
A	-29	GLY	-	expression tag	UNP P68400
A	-28	GLY	-	expression tag	UNP P68400
A	-27	GLY	-	expression tag	UNP P68400
A	-26	ARG	-	expression tag	UNP P68400
A	-25	LEU	-	expression tag	UNP P68400
A	-24	VAL	-	expression tag	UNP P68400
A	-23	PRO	-	expression tag	UNP P68400
A	-22	ARG	-	expression tag	UNP P68400
A	-21	GLY	-	expression tag	UNP P68400
A	-20	SER	-	expression tag	UNP P68400

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P68400
A	-18	SER	-	expression tag	UNP P68400
A	-17	GLU	-	expression tag	UNP P68400
A	-16	ASN	-	expression tag	UNP P68400
A	-15	LEU	-	expression tag	UNP P68400
A	-14	TYR	-	expression tag	UNP P68400
A	-13	PHE	-	expression tag	UNP P68400
A	-12	GLN	-	expression tag	UNP P68400
A	-11	GLY	-	expression tag	UNP P68400
A	-10	SER	-	expression tag	UNP P68400
A	-9	MET	-	expression tag	UNP P68400
A	-8	ASP	-	expression tag	UNP P68400
A	-7	ILE	-	expression tag	UNP P68400
A	-6	GLU	-	expression tag	UNP P68400
A	-5	PHE	-	expression tag	UNP P68400
A	-4	GLY	-	expression tag	UNP P68400
A	-3	GLU	-	expression tag	UNP P68400
A	-2	GLY	-	expression tag	UNP P68400
A	-1	GLU	-	expression tag	UNP P68400
A	0	GLY	-	expression tag	UNP P68400
A	1	SER	-	expression tag	UNP P68400
A	2	GLU	-	expression tag	UNP P68400
A	21	SER	ARG	conflict	UNP P68400
A	330	GLU	-	expression tag	UNP P68400
A	331	ASN	-	expression tag	UNP P68400
A	332	LEU	-	expression tag	UNP P68400
A	333	TYR	-	expression tag	UNP P68400
A	334	PHE	-	expression tag	UNP P68400
A	335	GLN	-	expression tag	UNP P68400
A	336	GLY	-	expression tag	UNP P68400
A	337	SER	-	expression tag	UNP P68400
A	338	SER	-	expression tag	UNP P68400
A	339	GLY	-	expression tag	UNP P68400
A	340	SER	-	expression tag	UNP P68400
A	341	GLY	-	expression tag	UNP P68400
A	342	SER	-	expression tag	UNP P68400
A	343	GLY	-	expression tag	UNP P68400
A	344	SER	-	expression tag	UNP P68400
A	345	SER	-	expression tag	UNP P68400
A	346	HIS	-	expression tag	UNP P68400
A	347	HIS	-	expression tag	UNP P68400
A	348	HIS	-	expression tag	UNP P68400

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Chain	Residue	Modelled	Actual	Comment	Reference
A	349	HIS	-	expression tag	UNP P68400
A	350	HIS	-	expression tag	UNP P68400
A	351	HIS	-	expression tag	UNP P68400

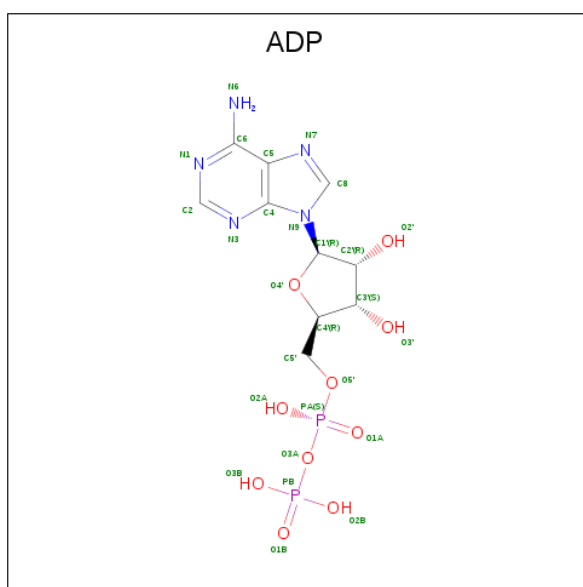
- Molecule 2 is a protein called P8C9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	10	Total	C	N	O	S	0	0	1
			80	55	14	10	1			

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

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

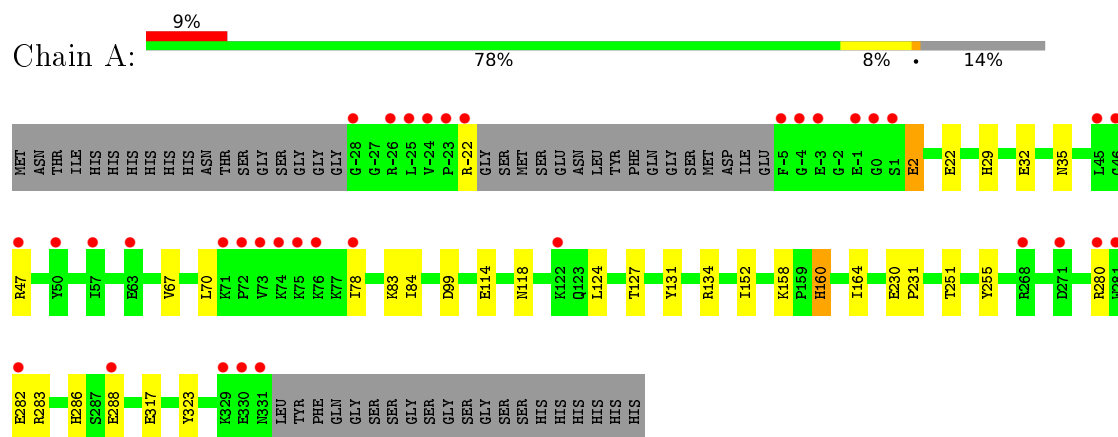
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	348	Total	O	0	0
			348	348		
7	D	6	Total	O	0	0
			6	6		

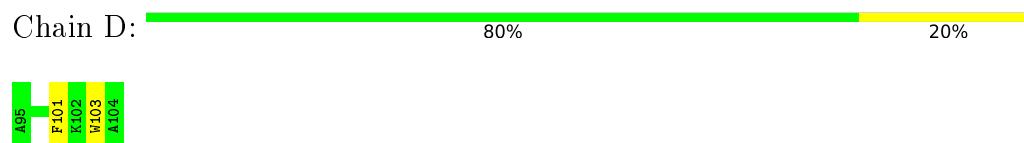
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Casein kinase II subunit alpha



- Molecule 2: P8C9



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.37Å 65.02Å 59.20Å 90.00° 111.20° 90.00°	Depositor
Resolution (Å)	55.19 – 1.19 55.19 – 1.19	Depositor EDS
% Data completeness (in resolution range)	91.7 (55.19-1.19) 91.7 (55.19-1.19)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 1.19Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.172 , 0.190 0.182 , 0.198	Depositor DCC
$R_{free}$ test set	5925 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.2	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3481	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: GOL, MG, NA, ADP, Q2E

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	0.78	3/3086 (0.1%)	0.91	2/4167 (0.0%)
2	D	0.66	0/64	0.88	0/83
All	All	0.78	3/3150 (0.1%)	0.91	2/4250 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	GLU	CD-OE1	6.07	1.32	1.25
1	A	114	GLU	CD-OE2	-5.25	1.19	1.25
1	A	317	GLU	CD-OE2	5.05	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	131	TYR	CB-CG-CD2	5.06	124.04	121.00

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	3011	0	2951	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	80	0	63	1	0
3	A	2	0	0	0	0
4	A	27	0	12	0	0
5	A	6	0	8	0	0
6	A	1	0	0	0	0
7	A	348	0	0	5	0
7	D	6	0	0	0	0
All	All	3481	0	3034	20	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 3.

The worst 5 of 20 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:A:2:GLU:HG2	7:A:594:HOH:O	1.83	0.77
1:A:118:ASN:HD22	1:A:164:ILE:H	1.35	0.72
1:A:124:LEU:O	1:A:127[B]:THR:HG22	1.98	0.63
1:A:127[B]:THR:HG21	7:A:720:HOH:O	2.01	0.60
1:A:29:HIS:HE1	7:A:793:HOH:O	1.82	0.60

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	356/398 (89%)	347 (98%)	9 (2%)	0	100	100
2	D	6/10 (60%)	6 (100%)	0	0	100	100
All	All	362/408 (89%)	353 (98%)	9 (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	328/357 (92%)	321 (98%)	7 (2%)	53	15
2	D	5/5 (100%)	5 (100%)	0	100	100
All	All	333/362 (92%)	326 (98%)	7 (2%)	57	15

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	160	HIS
1	A	283[B]	ARG
1	A	283[A]	ARG
1	A	35	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	A	262	ASN
1	A	286	HIS
1	A	270	ASN
1	A	118	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	Q2E	D	103	2	13,17,17	1.18	1 (7%)	12,23,23	0.91	1 (8%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Q2E	D	103	2	-	2/3/8/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	103	Q2E	CB-C8	-2.77	1.48	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	103	Q2E	C-S-C1	2.21	104.02	101.72

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	103	Q2E	N1-CA-CB-C8
2	D	103	Q2E	C9-CA-CB-C8

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	ADP	A	403	3	24,29,29	0.75	0	29,45,45	0.79	0
5	GOL	A	404	-	5,5,5	0.07	0	5,5,5	0.65	0

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	ADP	A	403	3	-	0/12/32/32	0/3/3/3
5	GOL	A	404	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

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, 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	344/398 (86%)	0.76	35 (10%) 6 7	9, 18, 43, 77	0
2	D	9/10 (90%)	0.50	0 100 100	16, 22, 29, 29	0
All	All	353/408 (86%)	0.75	35 (9%) 7 7	9, 18, 43, 77	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-5	PHE	23.4
1	A	-4	GLY	7.4
1	A	47	ARG	7.2
1	A	73	VAL	6.2
1	A	-22	ARG	5.8

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	Q2E	D	103	16/16	0.93	0.09	20,21,26,29	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	A	404	6/6	0.94	0.10	16,20,20,21	0
6	NA	A	405	1/1	0.96	0.45	33,33,33,33	0
3	MG	A	402	1/1	0.99	0.05	13,13,13,13	0
4	ADP	A	403	27/27	0.99	0.06	10,12,14,16	0
3	MG	A	401	1/1	1.00	0.07	10,10,10,10	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.