



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:49 AM GMT

PDB ID : 3C4W  
Title : Crystal Structure of G protein coupled receptor kinase 1 bound to ATP and magnesium chloride at 2.7Å  
Authors : Singh, P.; Tesmer, J.J.G.  
Deposited on : 2008-01-30  
Resolution : 2.70 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

---

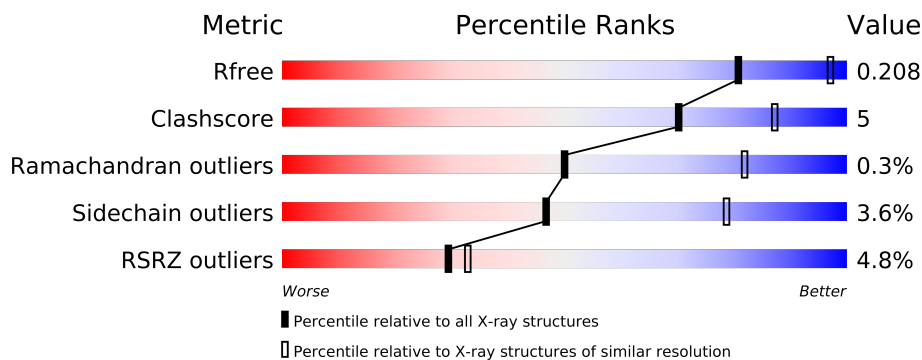
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 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	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. 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	543	
1	B	543	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8390 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 Rhodopsin kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S		0	3	0
			3989	2558	690	722	19				
1	B	519	Total	C	N	O	P	S	0	2	0
			4167	2666	721	760	1	19			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	536	VAL	-	EXPRESSION TAG	UNP P28327
A	537	ASP	-	EXPRESSION TAG	UNP P28327
A	538	HIS	-	EXPRESSION TAG	UNP P28327
A	539	HIS	-	EXPRESSION TAG	UNP P28327
A	540	HIS	-	EXPRESSION TAG	UNP P28327
A	541	HIS	-	EXPRESSION TAG	UNP P28327
A	542	HIS	-	EXPRESSION TAG	UNP P28327
A	543	HIS	-	EXPRESSION TAG	UNP P28327
B	536	VAL	-	EXPRESSION TAG	UNP P28327
B	537	ASP	-	EXPRESSION TAG	UNP P28327
B	538	HIS	-	EXPRESSION TAG	UNP P28327
B	539	HIS	-	EXPRESSION TAG	UNP P28327
B	540	HIS	-	EXPRESSION TAG	UNP P28327
B	541	HIS	-	EXPRESSION TAG	UNP P28327
B	542	HIS	-	EXPRESSION TAG	UNP P28327
B	543	HIS	-	EXPRESSION TAG	UNP P28327

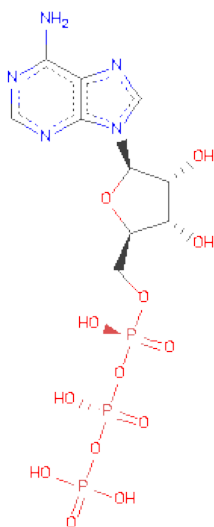
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 31 10 5 13 3	0	0
4	B	1	Total C N O P 31 10 5 13 3	0	0

- Molecule 5 is water.

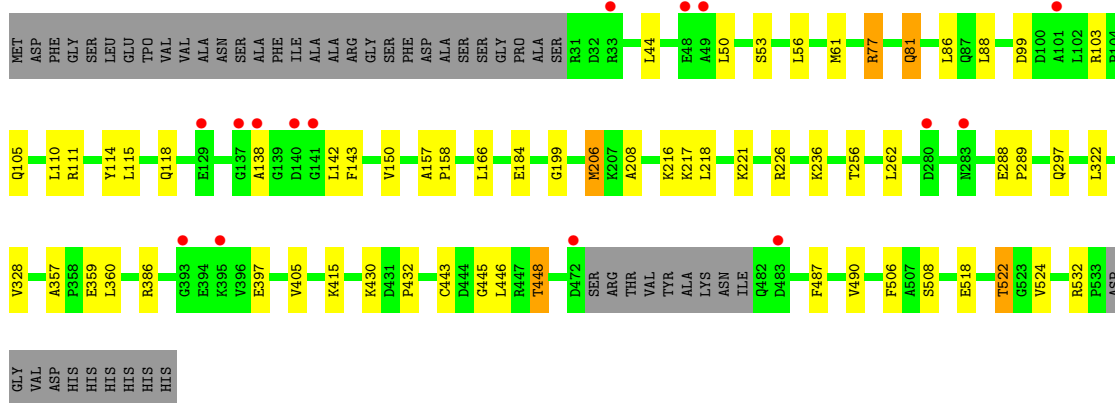
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	109	Total O 109 109	0	0
5	B	57	Total O 57 57	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

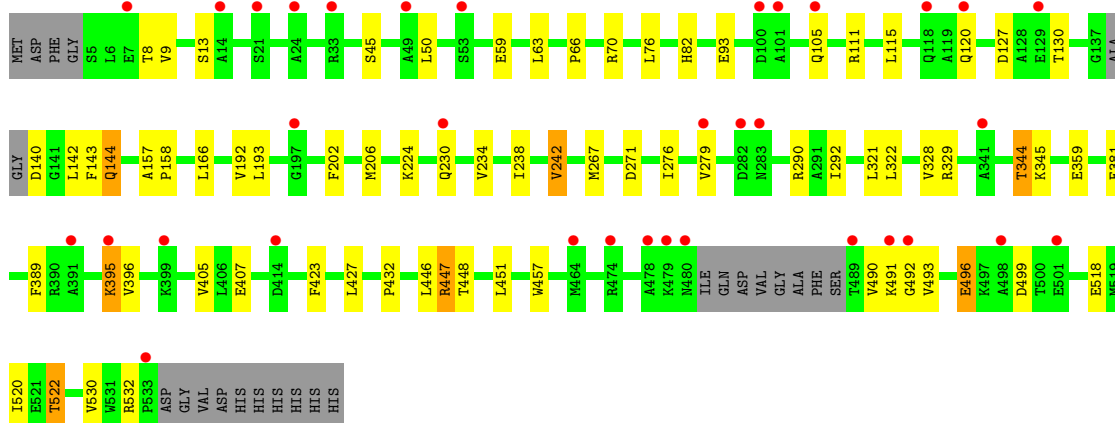
- Molecule 1: Rhodopsin kinase

Chain A: 



- Molecule 1: Rhodopsin kinase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	202.89Å 55.05Å 122.70Å 90.00° 100.82° 90.00°	Depositor
Resolution (Å)	19.98 – 2.70 19.97 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.98-2.70) 99.8 (19.97-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.20 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.192 , (Not available) 0.194 , 0.208	Depositor DCC
$R_{free}$ test set	1859 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.1	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 25.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 36930 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8390	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: TPO, MG, ATP, 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	0.60	1/4084 (0.0%)	0.68	0/5509
1	B	0.53	0/4253	0.65	1/5736 (0.0%)
All	All	0.57	1/8337 (0.0%)	0.66	1/11245 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	CYS	CB-SG	-6.04	1.72	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	447	ARG	NE-CZ-NH2	-6.57	117.01	120.30

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	3989	0	3948	40	0
1	B	4167	0	4116	37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	3	0	0	0	0
4	A	31	0	12	0	0
4	B	31	0	12	1	0
5	A	109	0	0	0	0
5	B	57	0	0	0	0
All	All	8390	0	8088	75	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 5.

All (75) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:81:GLN:HE21	1:A:81:GLN:H	1.14	0.93
1:B:423:PHE:CE2	1:B:427:LEU:HD11	2.27	0.68
1:A:88:LEU:HD12	1:A:110:LEU:HD11	1.78	0.64
1:A:157:ALA:HB3	1:A:158:PRO:HD3	1.79	0.64
1:A:297:GLN:OE1	1:A:328:VAL:HG22	1.98	0.62
1:B:344:THR:HG23	1:B:345:LYS:HG3	1.81	0.62
1:A:110:LEU:HD12	1:A:114:TYR:CE1	2.35	0.62
1:A:88:LEU:HD23	1:A:150:VAL:CG2	2.30	0.60
1:A:522:THR:HG23	1:A:524:VAL:HG23	1.83	0.60
1:A:138:ALA:HA	1:A:142:LEU:HD22	1.85	0.59
1:B:193:LEU:HD13	4:B:562:ATP:C2	2.39	0.58
1:A:405:VAL:O	1:A:430:LYS:HE3	2.04	0.57
1:A:56:LEU:HA	1:A:61:MET:HE2	1.87	0.56
1:A:166:LEU:HD22	1:B:166:LEU:HD22	1.86	0.56
1:B:446:LEU:HD23	1:B:446:LEU:C	2.26	0.56
1:A:142:LEU:HD12	1:A:142:LEU:O	2.06	0.56
1:A:81:GLN:NE2	1:A:81:GLN:H	1.96	0.56
1:B:279:VAL:HG21	1:B:290:ARG:HH12	1.71	0.55
1:A:359:GLU:HG2	1:A:432:PRO:HG3	1.88	0.55
1:B:111:ARG:HG2	1:B:115:LEU:HD12	1.89	0.54
1:B:447:ARG:HG2	1:B:457:TRP:CZ2	2.43	0.53
1:A:88:LEU:HD23	1:A:150:VAL:HG21	1.90	0.53
1:B:157:ALA:HB3	1:B:158:PRO:HD3	1.92	0.52
1:B:142:LEU:HD23	1:B:143:PHE:CE1	2.45	0.51
1:A:360:LEU:HD23	1:A:360:LEU:C	2.30	0.51
1:B:292:ILE:HD13	1:B:451:LEU:O	2.11	0.50
1:B:59:GLU:HG3	1:B:63:LEU:HD12	1.94	0.50
1:A:288:GLU:HB3	1:A:289:PRO:HD3	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:322:LEU:HG	1:B:328:VAL:HG12	1.93	0.49
1:A:110:LEU:HD12	1:A:114:TYR:HE1	1.73	0.49
1:A:262:LEU:HD21	1:A:506:PHE:CZ	2.47	0.49
1:B:395:LYS:HE2	1:B:395:LYS:HA	1.94	0.49
1:B:142:LEU:HD23	1:B:143:PHE:CZ	2.48	0.48
1:B:396:VAL:O	1:B:396:VAL:HG13	2.13	0.48
1:B:447:ARG:HG2	1:B:457:TRP:CH2	2.49	0.48
1:A:445:GLY:O	1:A:448:THR:HB	2.13	0.48
1:B:238:ILE:O	1:B:242:VAL:HG13	2.14	0.48
1:B:491:LYS:O	1:B:493:VAL:HG23	2.14	0.48
1:A:221:LYS:HB3	1:A:490:VAL:CG2	2.44	0.47
1:A:99:ASP:O	1:A:103:ARG:HG3	2.16	0.46
1:A:77[B]:ARG:HG3	1:A:86:LEU:HD21	1.98	0.46
1:B:8:TPO:O2P	1:B:93:GLU:OE1	2.34	0.45
1:A:111:ARG:HG2	1:A:115:LEU:HD12	1.97	0.45
1:B:518:GLU:O	1:B:522:THR:HB	2.16	0.45
1:B:66:PRO:O	1:B:70:ARG:HB2	2.16	0.45
1:A:322:LEU:HD12	1:A:328:VAL:HG12	1.98	0.45
1:A:110:LEU:HD23	1:A:143:PHE:CZ	2.52	0.45
1:A:532:ARG:HH21	1:B:530:VAL:HG12	1.82	0.45
1:A:522:THR:CG2	1:A:524:VAL:HG23	2.45	0.45
1:B:447:ARG:HD3	1:B:457:TRP:CE3	2.52	0.44
1:B:76:LEU:HD22	1:B:82:HIS:HB3	1.98	0.44
1:B:271:ASP:HB3	1:B:321:LEU:HD23	2.00	0.43
1:B:230:GLN:O	1:B:234:VAL:HG23	2.18	0.43
1:B:276:ILE:HD13	1:B:381:GLU:HG2	1.99	0.43
1:B:127:ASP:HB2	1:B:130:THR:H	1.84	0.43
1:A:446:LEU:HD23	1:A:446:LEU:C	2.39	0.43
1:A:216:LYS:HE2	1:A:218:LEU:HD21	2.00	0.43
1:A:405:VAL:O	1:A:430:LYS:CE	2.66	0.43
1:A:206:MET:SD	1:A:208:ALA:HB3	2.59	0.43
1:B:192:VAL:HG22	1:B:202:PHE:CE2	2.54	0.42
1:B:144:GLN:N	1:B:144:GLN:HE21	2.18	0.42
1:B:144:GLN:NE2	1:B:144:GLN:CA	2.83	0.42
1:A:518:GLU:O	1:A:522:THR:HB	2.19	0.42
1:A:110:LEU:HD23	1:A:143:PHE:CE2	2.55	0.41
1:B:267:MET:HE2	1:B:329:ARG:HB2	2.01	0.41
1:A:199:GLY:HA2	1:A:487:PHE:CE1	2.55	0.41
1:A:77[B]:ARG:HG3	1:A:86:LEU:CD2	2.50	0.41
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.90	0.41
1:A:357:ALA:HB1	1:A:359:GLU:OE2	2.21	0.41
1:A:236:LYS:NZ	1:A:508:SER:OG	2.51	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:184:GLU:HB2	1:A:256:THR:HG22	2.03	0.41
1:B:9:VAL:O	1:B:520:ILE:HG21	2.21	0.41
1:B:389:PHE:CD1	1:B:405:VAL:HG22	2.56	0.40
1:B:224:LYS:NZ	1:B:499:ASP:OD2	2.47	0.40
1:B:359:GLU:HG2	1:B:432:PRO:HG3	2.03	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	493/543 (91%)	473 (96%)	20 (4%)	0	100	100
1	B	514/543 (95%)	494 (96%)	17 (3%)	3 (1%)	33	66
All	All	1007/1086 (93%)	967 (96%)	37 (4%)	3 (0%)	50	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	496	GLU
1	B	490	VAL
1	B	492	GLY

### 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	414/448 (92%)	399 (96%)	15 (4%)	47	79
1	B	432/448 (96%)	416 (96%)	16 (4%)	45	78

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	846/896 (94%)	815 (96%)	31 (4%)	47 78

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

Mol	Chain	Res	Type
1	A	50	LEU
1	A	53	SER
1	A	77[A]	ARG
1	A	77[B]	ARG
1	A	81	GLN
1	A	105	GLN
1	A	118	GLN
1	A	206	MET
1	A	217	LYS
1	A	226	ARG
1	A	386	ARG
1	A	397	GLU
1	A	415	LYS
1	A	448	THR
1	A	522	THR
1	B	13	SER
1	B	45	SER
1	B	50	LEU
1	B	105	GLN
1	B	120	GLN
1	B	140	ASP
1	B	144	GLN
1	B	206	MET
1	B	242	VAL
1	B	344	THR
1	B	395	LYS
1	B	407	GLU
1	B	448	THR
1	B	496	GLU
1	B	522	THR
1	B	532	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	87	GLN
1	A	105	GLN
1	A	118	GLN
1	A	309	ASN
1	A	429	GLN
1	B	73	GLN
1	B	87	GLN
1	B	108	GLN
1	B	120	GLN
1	B	144	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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$
1	TPO	B	8	1	10,10,11	5.46	1 (10%)	12,14,16	1.60	2 (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
1	TPO	B	8	1	-	0/9/11/13	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	8	TPO	O-C	17.08	1.23	1.11

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	TPO	C-CA-N	-3.70	105.92	111.94
1	B	8	TPO	O2P-P-OG1	-2.85	98.89	107.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 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	ATP	A	562	2	33,33,33	1.10	2 (6%)	52,52,52	1.88	9 (17%)
4	ATP	B	562	2	33,33,33	0.99	2 (6%)	52,52,52	2.01	12 (23%)

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	ATP	A	562	2	-	0/22/38/38	0/1/3/3
4	ATP	B	562	2	-	0/22/38/38	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	562	ATP	C4-N9	-3.27	1.33	1.37
4	B	562	ATP	C4-N9	-2.88	1.33	1.37
4	A	562	ATP	C5-C4	2.77	1.46	1.40
4	B	562	ATP	C5-C4	2.29	1.45	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	562	ATP	N3-C2-N1	-7.69	122.28	128.71
4	B	562	ATP	N3-C2-N1	-7.49	122.44	128.71
4	B	562	ATP	O4'-C1'-N9	5.17	113.25	108.44
4	B	562	ATP	N3-C4-N9	4.87	134.22	125.43
4	A	562	ATP	O4'-C1'-N9	-4.60	104.16	108.44
4	A	562	ATP	N3-C4-N9	4.53	133.62	125.43
4	B	562	ATP	C8-N9-C4	3.22	109.35	106.90
4	B	562	ATP	PB-O3B-PG	-3.19	122.32	131.68
4	B	562	ATP	C1'-N9-C4	-2.95	121.53	126.64
4	A	562	ATP	C1'-N9-C4	-2.92	121.59	126.64
4	B	562	ATP	C5-C4-N3	-2.78	119.65	125.70
4	A	562	ATP	C5-C4-N3	-2.66	119.91	125.70
4	B	562	ATP	C4-C5-N7	-2.61	107.29	109.52
4	A	562	ATP	C2-N3-C4	2.51	121.15	114.01
4	A	562	ATP	C8-N9-C4	2.46	108.78	106.90
4	B	562	ATP	C2-N3-C4	2.44	120.97	114.01
4	B	562	ATP	PA-O3A-PB	-2.41	124.60	131.68
4	B	562	ATP	C2'-C1'-N9	-2.37	107.17	113.27
4	B	562	ATP	O2B-PB-O1B	2.36	125.38	112.21
4	A	562	ATP	C4-C5-N7	-2.29	107.56	109.52
4	A	562	ATP	O3G-PG-O1G	2.07	117.21	110.44

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, 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	494/543 (90%)	0.04	15 (3%)	48 54	11, 24, 49, 68	0
1	B	519/543 (95%)	0.20	34 (6%)	18 20	11, 24, 49, 60	0
All	All	1013/1086 (93%)	0.13	49 (4%)	29 33	11, 24, 49, 68	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	474	ARG	5.6
1	A	140	ASP	5.0
1	B	279	VAL	4.7
1	A	395	LYS	4.3
1	B	341	ALA	4.1
1	B	33	ARG	4.1
1	B	478	ALA	4.0
1	B	479	LYS	3.9
1	B	21	SER	3.9
1	B	395	LYS	3.8
1	B	491	LYS	3.5
1	A	33	ARG	3.5
1	B	282	ASP	3.3
1	B	414	ASP	3.3
1	B	498	ALA	3.2
1	B	24	ALA	3.0
1	B	120	GLN	2.9
1	A	393	GLY	2.8
1	A	101	ALA	2.8
1	B	480	ASN	2.8
1	A	138	ALA	2.8
1	B	129	GLU	2.7
1	A	483	ASP	2.7
1	B	501	GLU	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	141	GLY	2.7
1	B	533	PRO	2.6
1	A	137	GLY	2.6
1	B	197	GLY	2.6
1	A	48	GLU	2.5
1	A	472	ASP	2.4
1	B	399	LYS	2.4
1	B	489	THR	2.4
1	B	492	GLY	2.4
1	B	49	ALA	2.4
1	B	7	GLU	2.4
1	A	49	ALA	2.3
1	B	464	MET	2.3
1	B	391	ALA	2.3
1	B	100	ASP	2.3
1	B	283	ASN	2.3
1	B	230	GLN	2.2
1	A	280	ASP	2.2
1	B	105	GLN	2.2
1	A	129	GLU	2.2
1	A	283	ASN	2.1
1	B	101	ALA	2.1
1	B	53	SER	2.1
1	B	118	GLN	2.1
1	B	14	ALA	2.1

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPO	B	8	11/12	0.13	-0.90	22,31,38,40	0

## 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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CL	A	566	1/1	0.22	0.46	23,23,23,23	0
2	MG	B	563	1/1	0.14	-0.16	49,49,49,49	0
4	ATP	A	562	31/31	0.14	-0.25	6,16,19,20	0
2	MG	B	564	1/1	0.10	-0.69	24,24,24,24	0
3	CL	A	567	1/1	0.13	-0.76	16,16,16,16	0
4	ATP	B	562	31/31	0.10	-0.93	6,17,23,25	0
2	MG	A	564	1/1	0.07	-2.33	18,18,18,18	0
3	CL	A	565	1/1	0.12	-3.56	21,21,21,21	0

## 6.5 Other polymers

There are no such residues in this entry.