



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:19 am GMT

PDB ID : 2A19  
Title : PKR kinase domain- eIF2alpha- AMP-PNP complex.  
Authors : Dar, A.C.; Dever, T.E.; Sicheri, F.  
Deposited on : 2005-06-19  
Resolution : 2.50 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](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

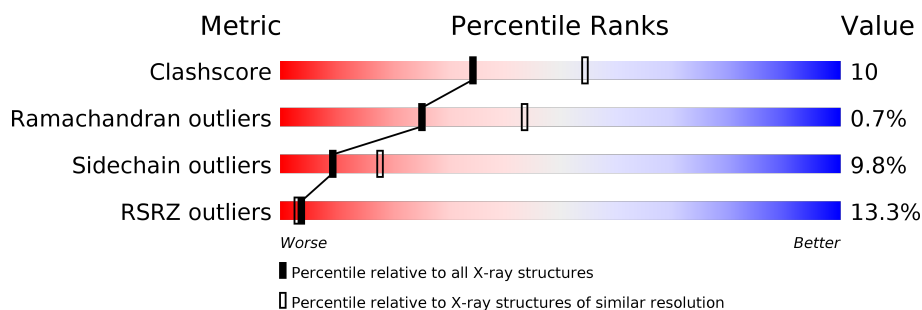
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	175	<div> <div>5%</div> <div>74%</div> <div>18%</div> <div>• 6%</div> </div>
2	B	284	<div> <div>12%</div> <div>71%</div> <div>18%</div> <div>• 7%</div> </div>
2	C	284	<div> <div>14%</div> <div>49%</div> <div>19%</div> <div>• 29%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5216 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 Eukaryotic translation initiation factor 2 alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1342	862	220	254	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP P20459
A	2	SER	-	CLONING ARTIFACT	UNP P20459

- Molecule 2 is a protein called Interferon-induced, double-stranded RNA-activated protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	264	Total	C	N	O	P S	0	0	0
			2137	1363	366	400	1 7			
2	C	203	Total	C	N	O	S	0	0	0
			1594	1027	265	297	5			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	255	GLY	-	CLONING ARTIFACT	UNP P19525
B	256	ALA	-	CLONING ARTIFACT	UNP P19525
B	257	HIS	-	CLONING ARTIFACT	UNP P19525
B	?	-	ASP	DELETION	UNP P19525
B	?	-	ASP	DELETION	UNP P19525
B	?	-	SER	DELETION	UNP P19525
B	?	-	LEU	DELETION	UNP P19525
B	?	-	GLU	DELETION	UNP P19525
B	?	-	SER	DELETION	UNP P19525
B	?	-	SER	DELETION	UNP P19525
B	?	-	ASP	DELETION	UNP P19525

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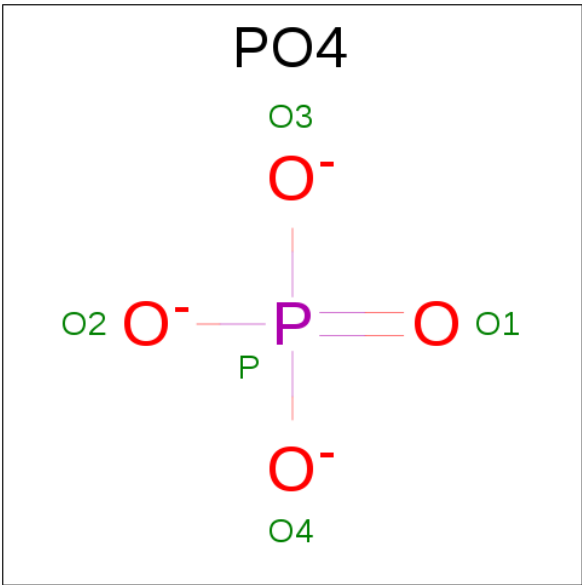
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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	TYR	DELETION	UNP P19525
B	?	-	ASP	DELETION	UNP P19525
B	?	-	PRO	DELETION	UNP P19525
B	?	-	GLU	DELETION	UNP P19525
B	?	-	ASN	DELETION	UNP P19525
B	412	ASN	HIS	ENGINEERED	UNP P19525
B	446	TPO	THR	MODIFIED RESIDUE	UNP P19525
B	551	ALA	CYS	ENGINEERED	UNP P19525
C	255	GLY	-	CLONING ARTIFACT	UNP P19525
C	256	ALA	-	CLONING ARTIFACT	UNP P19525
C	257	HIS	-	CLONING ARTIFACT	UNP P19525
C	?	-	ASP	DELETION	UNP P19525
C	?	-	ASP	DELETION	UNP P19525
C	?	-	SER	DELETION	UNP P19525
C	?	-	LEU	DELETION	UNP P19525
C	?	-	GLU	DELETION	UNP P19525
C	?	-	SER	DELETION	UNP P19525
C	?	-	SER	DELETION	UNP P19525
C	?	-	ASP	DELETION	UNP P19525
C	?	-	TYR	DELETION	UNP P19525
C	?	-	ASP	DELETION	UNP P19525
C	?	-	PRO	DELETION	UNP P19525
C	?	-	GLU	DELETION	UNP P19525
C	?	-	ASN	DELETION	UNP P19525
C	412	ASN	HIS	ENGINEERED	UNP P19525
C	446	TPO	THR	MODIFIED RESIDUE	UNP P19525
C	551	ALA	CYS	ENGINEERED	UNP P19525

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

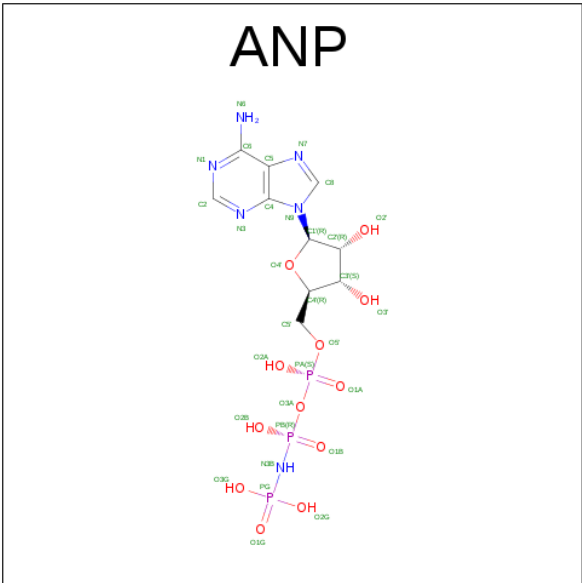
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

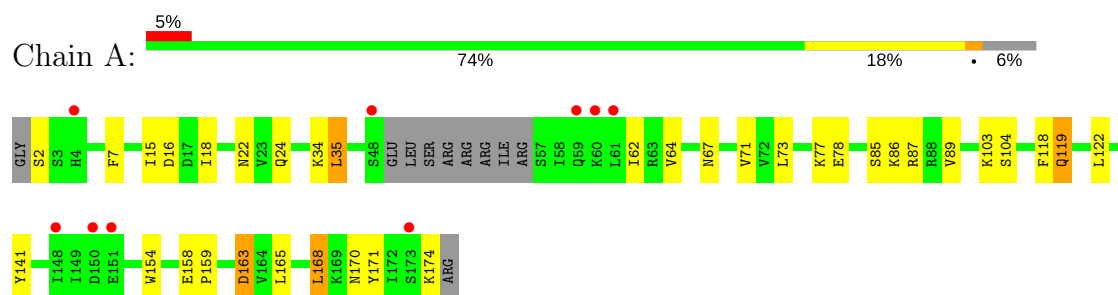
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total 32	O 32	0	0
6	B	33	Total 33	O 33	0	0
6	C	7	Total 7	O 7	0	0

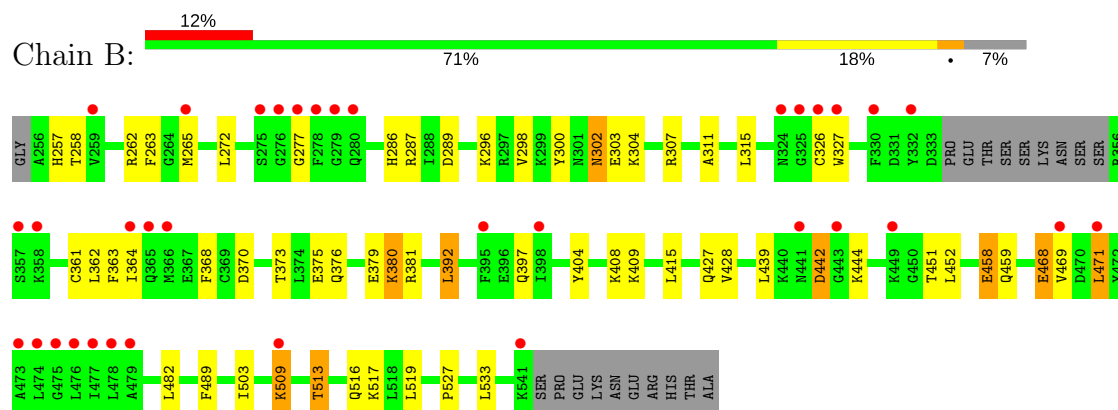
### 3 Residue-property plots

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

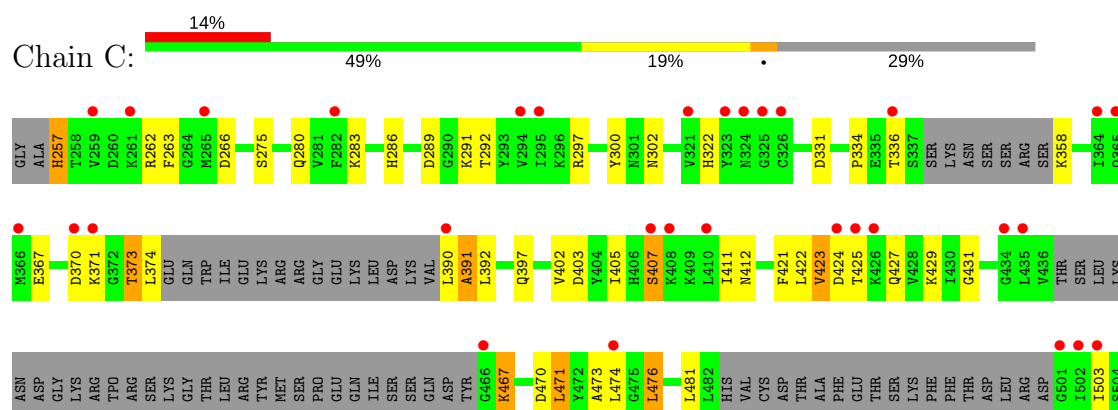
- Molecule 1: Eukaryotic translation initiation factor 2 alpha subunit

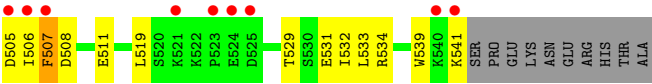


- Molecule 2: Interferon-induced, double-stranded RNA-activated protein kinase



- Molecule 2: Interferon-induced, double-stranded RNA-activated protein kinase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.66Å 48.75Å 133.43Å 90.00° 98.44° 90.00°	Depositor
Resolution (Å)	27.33 – 2.50 27.33 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.9 (27.33-2.50) 94.7 (27.33-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.228 , 0.286 0.233 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	56.8	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5216	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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: TPO, PO4, ANP, MG

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	0/1366	0.68	2/1839 (0.1%)
2	B	0.52	0/2161	0.64	0/2895
2	C	0.46	0/1618	0.59	0/2174
All	All	0.53	0/5145	0.64	2/6908 (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	35	LEU	CA-CB-CG	7.49	132.52	115.30
1	A	168	LEU	CA-CB-CG	5.65	128.29	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	1342	0	1350	23	0
2	B	2137	0	2160	33	0
2	C	1594	0	1588	37	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	31	0	13	6	0
5	C	31	0	13	0	0
6	A	32	0	0	0	0
6	B	33	0	0	1	0
6	C	7	0	0	0	0
All	All	5216	0	5124	98	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 10.

All (98) 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)
2:C:507:PHE:HD1	2:C:507:PHE:H	1.04	1.01
5:B:1640:ANP:H5'2	5:B:1640:ANP:HNB1	1.33	0.93
2:B:373:THR:H	2:B:376:GLN:HE21	1.22	0.85
5:B:1640:ANP:HNB1	5:B:1640:ANP:C5'	1.90	0.83
5:B:1640:ANP:H5'2	5:B:1640:ANP:N3B	1.92	0.83
1:A:119:GLN:HA	1:A:119:GLN:HE21	1.44	0.81
5:B:1640:ANP:O5'	5:B:1640:ANP:H8	1.86	0.75
2:B:286:HIS:HD2	2:B:289:ASP:H	1.36	0.71
2:B:397:GLN:HE22	2:B:427:GLN:HA	1.56	0.71
1:A:15:ILE:O	1:A:16:ASP:HB2	1.96	0.65
2:C:507:PHE:N	2:C:507:PHE:CD1	2.55	0.64
2:C:507:PHE:HD1	2:C:507:PHE:N	1.85	0.64
2:C:322:HIS:HB3	2:C:367:GLU:HB3	1.80	0.63
2:B:300:TYR:HB2	2:B:362:LEU:HB2	1.79	0.62
2:B:381:ARG:HB3	6:B:59:HOH:O	1.99	0.61
2:B:503:ILE:HG13	2:B:516:GLN:HG2	1.83	0.61
2:C:424:ASP:OD1	2:C:425:THR:N	2.35	0.59
2:C:529:THR:HA	2:C:532:ILE:HD12	1.83	0.59
1:A:2:SER:N	1:A:122:LEU:H	2.01	0.59
2:B:509:LYS:O	2:B:513:THR:HG23	2.03	0.58
2:B:442:ASP:HB3	2:B:444:LYS:H	1.68	0.58
2:C:507:PHE:HB2	2:C:511:GLU:OE2	2.04	0.58
2:C:331:ASP:O	2:C:358:LYS:HA	2.03	0.57
2:B:262:ARG:HG2	2:B:327:TRP:CD1	2.40	0.56
2:C:390:LEU:HG	2:C:391:ALA:H	1.69	0.56
1:A:119:GLN:CA	1:A:119:GLN:HE21	2.17	0.56
2:C:397:GLN:HE22	2:C:427:GLN:HA	1.70	0.56
2:C:280:GLN:HE21	2:C:297:ARG:HH11	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:286:HIS:CD2	2:C:289:ASP:H	2.24	0.55
5:B:1640:ANP:N3B	5:B:1640:ANP:C5'	2.60	0.54
2:B:368:PHE:CE2	2:B:370:ASP:HB3	2.42	0.54
2:C:286:HIS:HD2	2:C:289:ASP:H	1.55	0.54
2:C:423:VAL:HG23	2:C:427:GLN:HB3	1.89	0.53
2:C:473:ALA:O	2:C:476:LEU:HB2	2.10	0.51
1:A:171:TYR:O	1:A:174:LYS:HG2	2.09	0.51
2:B:326:CYS:HA	2:B:363:PHE:O	2.10	0.51
1:A:154:TRP:HH2	1:A:168:LEU:HD11	1.75	0.51
2:B:517:LYS:HB3	2:B:527:PRO:HD3	1.93	0.51
1:A:22:ASN:HD22	1:A:67:ASN:ND2	2.09	0.50
2:B:409:LYS:HD2	2:B:439:LEU:HD23	1.93	0.50
2:B:392:LEU:HD13	2:B:482:LEU:HD21	1.93	0.50
2:B:397:GLN:NE2	2:B:428:VAL:H	2.10	0.49
2:B:404:TYR:O	2:B:408:LYS:HG2	2.12	0.49
1:A:18:ILE:HD13	1:A:71:VAL:HG22	1.94	0.49
2:C:402:VAL:HA	2:C:405:ILE:HD12	1.94	0.49
2:C:471:LEU:HA	2:C:474:LEU:HD12	1.95	0.49
2:C:291:LYS:HG2	2:C:292:THR:N	2.28	0.48
2:C:390:LEU:C	2:C:392:LEU:H	2.15	0.48
2:C:423:VAL:HG11	2:C:429:LYS:HD2	1.95	0.48
2:B:265:MET:O	2:B:287:ARG:HD2	2.13	0.48
2:B:257:HIS:CE1	2:B:272:LEU:HD22	2.48	0.48
1:A:119:GLN:HA	1:A:119:GLN:NE2	2.22	0.48
2:C:291:LYS:HG2	2:C:292:THR:H	1.78	0.48
1:A:22:ASN:HD22	1:A:67:ASN:HD22	1.60	0.47
1:A:24:GLN:NE2	1:A:34:LYS:HD3	2.29	0.47
2:C:280:GLN:NE2	2:C:297:ARG:HH11	2.12	0.47
1:A:159:PRO:HG3	1:A:165:LEU:HB2	1.95	0.47
2:B:380:LYS:HE3	2:B:380:LYS:HA	1.97	0.47
2:C:411:ILE:HG13	2:C:411:ILE:O	2.15	0.47
1:A:154:TRP:CH2	1:A:168:LEU:CD1	2.97	0.47
2:C:297:ARG:HD3	2:C:334:PRO:HG3	1.97	0.47
1:A:154:TRP:CH2	1:A:168:LEU:HD11	2.50	0.46
2:B:458:GLU:CD	2:B:458:GLU:H	2.19	0.46
2:B:311:ALA:O	2:B:315:LEU:HG	2.16	0.46
2:B:302:ASN:O	2:B:304:LYS:N	2.49	0.46
2:B:302:ASN:N	2:B:302:ASN:HD22	2.14	0.46
2:C:286:HIS:HD2	2:C:289:ASP:N	2.13	0.45
1:A:103:LYS:HG2	1:A:141:TYR:CG	2.51	0.45
2:C:531:GLU:HA	2:C:534:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LYS:HG2	1:A:141:TYR:CD2	2.51	0.45
2:B:459:GLN:HB2	2:B:469:VAL:HG22	1.99	0.45
2:C:421:PHE:CE1	2:C:431:GLY:HA3	2.52	0.44
2:B:262:ARG:NH2	2:C:266:ASP:OD1	2.48	0.44
1:A:71:VAL:HG23	1:A:89:VAL:HG22	1.99	0.44
2:B:373:THR:H	2:B:376:GLN:NE2	2.02	0.44
5:B:1640:ANP:H5'1	5:B:1640:ANP:HNB1	1.79	0.43
2:C:257:HIS:O	2:C:297:ARG:NH2	2.35	0.43
1:A:15:ILE:O	1:A:16:ASP:CB	2.65	0.43
2:C:421:PHE:HE1	2:C:431:GLY:HA3	1.82	0.43
1:A:118:PHE:CE2	1:A:163:ASP:HB3	2.54	0.43
2:B:468:GLU:HA	2:B:471:LEU:HD22	2.01	0.43
1:A:86:LYS:O	1:A:87:ARG:C	2.55	0.43
2:B:262:ARG:HG2	2:B:327:TRP:NE1	2.33	0.43
2:B:468:GLU:CD	2:B:468:GLU:H	2.22	0.42
2:C:539:TRP:CD1	2:C:539:TRP:N	2.87	0.42
2:B:375:GLU:O	2:B:379:GLU:HG3	2.19	0.42
2:B:370:ASP:N	2:B:370:ASP:OD1	2.50	0.42
1:A:7:PHE:CD2	1:A:104:SER:HB3	2.55	0.42
1:A:73:LEU:HD11	1:A:85:SER:HB2	2.01	0.42
2:C:411:ILE:CG2	2:C:467:LYS:HB3	2.50	0.41
2:C:403:ASP:O	2:C:407:SER:HB2	2.20	0.41
2:C:467:LYS:H	2:C:467:LYS:HD3	1.85	0.41
2:B:302:ASN:H	2:B:302:ASN:HD22	1.68	0.41
2:C:373:THR:HG23	2:C:374:LEU:N	2.35	0.41
2:B:296:LYS:HB3	2:B:364:ILE:HB	2.02	0.41
2:C:412:ASN:O	2:C:470:ASP:OD1	2.39	0.41
2:C:373:THR:CG2	2:C:374:LEU:N	2.84	0.40
1:A:24:GLN:CD	1:A:34:LYS:HD3	2.42	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	161/175 (92%)	151 (94%)	10 (6%)	0	100	100
2	B	259/284 (91%)	250 (96%)	7 (3%)	2 (1%)	22	39
2	C	193/284 (68%)	177 (92%)	14 (7%)	2 (1%)	18	32
All	All	613/743 (82%)	578 (94%)	31 (5%)	4 (1%)	25	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	303	GLU
2	B	277	GLY
2	C	371	LYS
2	C	391	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	149/161 (92%)	140 (94%)	9 (6%)	22	41
2	B	232/254 (91%)	212 (91%)	20 (9%)	12	23
2	C	170/254 (67%)	145 (85%)	25 (15%)	3	6
All	All	551/669 (82%)	497 (90%)	54 (10%)	9	18

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	62	ILE
1	A	64	VAL
1	A	77	LYS
1	A	78	GLU
1	A	119	GLN
1	A	158	GLU
1	A	163	ASP
1	A	170	ASN

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Mol	Chain	Res	Type
2	B	258	THR
2	B	263	PHE
2	B	298	VAL
2	B	302	ASN
2	B	307	ARG
2	B	361	CYS
2	B	380	LYS
2	B	392	LEU
2	B	415	LEU
2	B	442	ASP
2	B	451	THR
2	B	452	LEU
2	B	458	GLU
2	B	468	GLU
2	B	471	LEU
2	B	489	PHE
2	B	509	LYS
2	B	513	THR
2	B	519	LEU
2	B	533	LEU
2	C	257	HIS
2	C	262	ARG
2	C	263	PHE
2	C	275	SER
2	C	283	LYS
2	C	300	TYR
2	C	302	ASN
2	C	336	THR
2	C	370	ASP
2	C	373	THR
2	C	407	SER
2	C	422	LEU
2	C	423	VAL
2	C	467	LYS
2	C	471	LEU
2	C	476	LEU
2	C	481	LEU
2	C	503	ILE
2	C	505	ASP
2	C	506	ILE
2	C	507	PHE
2	C	508	ASP

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Mol	Chain	Res	Type
2	C	519	LEU
2	C	533	LEU
2	C	541	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	67	ASN
1	A	119	GLN
2	B	286	HIS
2	B	302	ASN
2	B	319	ASN
2	B	322	HIS
2	B	376	GLN
2	B	397	GLN
2	B	463	GLN
2	C	280	GLN
2	C	286	HIS
2	C	301	ASN
2	C	302	ASN
2	C	319	ASN
2	C	397	GLN
2	C	528	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	TPO	B	446	2	9,10,11	0.77	0	10,14,16	1.26	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
2	TPO	B	446	2	-	0/8/11/13	0/0/0/0

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.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\# Z  > 2$
5	ANP	B	1640	3	29,33,33	2.10	7 (24%)	28,52,52	2.04	6 (21%)
5	ANP	C	2640	3	29,33,33	2.11	5 (17%)	28,52,52	2.04	6 (21%)
4	PO4	C	901	-	4,4,4	0.71	0	6,6,6	0.50	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
5	ANP	B	1640	3	-	0/13/38/38	0/3/3/3
5	ANP	C	2640	3	-	1/13/38/38	0/3/3/3
4	PO4	C	901	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1640	ANP	O4'-C1'	2.11	1.44	1.41
5	B	1640	ANP	C2-N3	2.29	1.36	1.32
5	B	1640	ANP	C5-C4	2.88	1.47	1.40
5	C	2640	ANP	C5-C4	3.09	1.47	1.40
5	B	1640	ANP	PB-N3B	4.13	1.74	1.63
5	B	1640	ANP	PG-N3B	4.22	1.74	1.63
5	C	2640	ANP	PG-O1G	4.72	1.51	1.46
5	B	1640	ANP	PB-O1B	4.73	1.51	1.46
5	C	2640	ANP	PB-N3B	4.90	1.76	1.63
5	C	2640	ANP	PG-N3B	4.98	1.76	1.63
5	C	2640	ANP	PB-O1B	5.14	1.51	1.46
5	B	1640	ANP	PG-O1G	5.62	1.52	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2640	ANP	N3-C2-N1	-6.70	123.02	128.86
5	B	1640	ANP	N3-C2-N1	-6.55	123.15	128.86
5	C	2640	ANP	O1G-PG-N3B	-3.69	106.27	111.79
5	C	2640	ANP	PA-O3A-PB	-3.24	120.94	132.38
5	B	1640	ANP	O1G-PG-N3B	-3.22	106.97	111.79
5	C	2640	ANP	C4-C5-N7	-2.50	107.00	109.41
5	B	1640	ANP	PA-O3A-PB	-2.28	124.34	132.38
5	B	1640	ANP	C4-C5-N7	-2.05	107.43	109.41
5	C	2640	ANP	C2-N1-C6	2.07	122.40	118.77
5	B	1640	ANP	O3G-PG-O2G	2.83	115.61	107.69
5	C	2640	ANP	O2B-PB-O1B	4.01	118.20	109.87
5	B	1640	ANP	O2B-PB-O1B	5.19	120.65	109.87

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	2640	ANP	O1B-PB-N3B-PG

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1640	ANP	6	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

### 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	165/175 (94%)	0.14	9 (5%) 26 27	43, 51, 65, 71	0
2	B	263/284 (92%)	0.52	35 (13%) 4 3	45, 57, 77, 86	0
2	C	203/284 (71%)	0.98	40 (19%) 1 1	52, 67, 79, 82	0
All	All	631/743 (84%)	0.57	84 (13%) 4 3	43, 59, 77, 86	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	278	PHE	8.8
2	C	523	PRO	7.7
2	C	502	ILE	7.5
2	C	506	ILE	7.0
2	C	425	THR	6.2
2	B	279	GLY	5.7
2	C	466	GLY	5.5
2	B	332	TYR	5.0
2	B	277	GLY	4.2
2	B	473	ALA	4.0
1	A	59	GLN	3.7
2	C	265	MET	3.7
2	C	261	LYS	3.6
2	B	325	GLY	3.6
2	B	326	CYS	3.6
2	C	541	LYS	3.6
2	C	521	LYS	3.6
2	C	325	GLY	3.6
2	C	505	ASP	3.5
2	B	365	GLN	3.5
2	C	295	ILE	3.5
2	C	503	ILE	3.5
2	C	540	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	477	ILE	3.3
2	B	330	PHE	3.3
2	C	507	PHE	3.2
1	A	61	LEU	3.2
2	C	501	GLY	3.1
2	B	449	LYS	3.0
2	B	474	LEU	3.0
2	C	321	VAL	3.0
1	A	60	LYS	2.9
2	C	407	SER	2.9
2	B	259	VAL	2.9
2	C	294	VAL	2.8
2	B	509	LYS	2.8
2	B	475	GLY	2.8
2	B	476	LEU	2.7
2	B	441	ASN	2.7
2	B	276	GLY	2.7
2	C	434	GLY	2.7
1	A	173	SER	2.7
2	C	435	LEU	2.6
2	C	366	MET	2.6
2	C	426	LYS	2.6
2	C	365	GLN	2.6
2	B	357	SER	2.6
2	C	524	GLU	2.5
2	B	275	SER	2.5
2	B	280	GLN	2.5
2	C	336	THR	2.5
1	A	150	ASP	2.4
2	B	327	TRP	2.4
1	A	48	SER	2.4
1	A	151	GLU	2.4
2	B	478	LEU	2.4
2	C	525	ASP	2.3
2	B	364	ILE	2.3
2	C	259	VAL	2.3
2	B	443	GLY	2.3
2	B	265	MET	2.3
2	B	395	PHE	2.3
2	B	541	LYS	2.3
2	C	364	ILE	2.3
2	B	471	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	370	ASP	2.2
1	A	4	HIS	2.2
2	B	366	MET	2.2
2	C	410	LEU	2.2
2	B	398	ILE	2.2
2	C	408	LYS	2.2
2	B	324	ASN	2.2
2	C	324	ASN	2.1
2	B	358	LYS	2.1
2	B	469	VAL	2.1
2	C	323	TYR	2.1
2	C	424	ASP	2.1
2	B	479	ALA	2.1
2	C	371	LYS	2.1
1	A	148	ILE	2.0
2	C	282	PHE	2.0
2	C	390	LEU	2.0
2	C	474	LEU	2.0
2	C	326	CYS	2.0

## 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. 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(Å <sup>2</sup> )	Q<0.9
2	TPO	B	446	11/12	0.96	0.11	-	51,54,57,57	0

## 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	ANP	C	2640	31/31	0.80	0.19	-0.26	75,77,79,80	12
5	ANP	B	1640	31/31	0.89	0.16	-0.66	70,76,90,91	0
3	MG	C	2641	1/1	0.96	0.06	-	75,75,75,75	0
3	MG	B	1642	1/1	0.90	0.14	-	44,44,44,44	0
4	PO4	C	901	5/5	0.89	0.15	-	108,108,108,108	0
3	MG	B	1641	1/1	0.93	0.18	-	63,63,63,63	0
3	MG	C	2642	1/1	0.87	0.09	-	79,79,79,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.