



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:16 am GMT

PDB ID : 2A1A  
Title : PKR kinase domain-eIF2alpha Complex  
Authors : Dar, A.C.; Dever, T.E.; Sicheri, F.  
Deposited on : 2005-06-19  
Resolution : 2.80 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

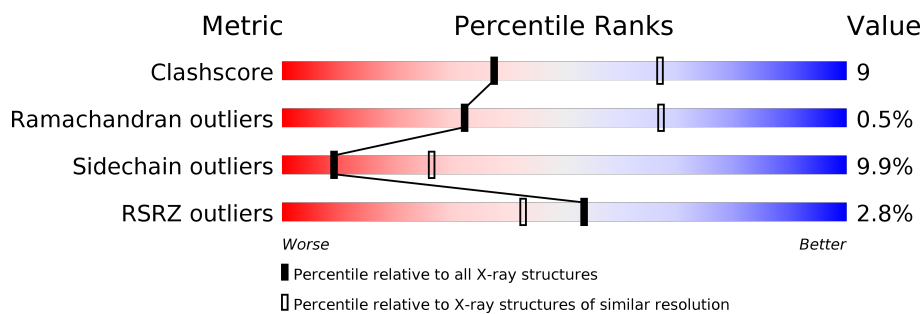
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	 74% 15% • 8%
2	B	284	 4% 68% 22% • 5%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3518 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	161	Total	C	N	O	S	0	0	0
			1314	845	216	248	5			

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	270	Total	C	N	O	P	S	0	0
			2189	1394	377	410	1	7		

There are 19 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
B	?	-	TYR	DELETION	UNP P19525
B	?	-	ASP	DELETION	UNP P19525

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Chain	Residue	Modelled	Actual	Comment	Reference
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

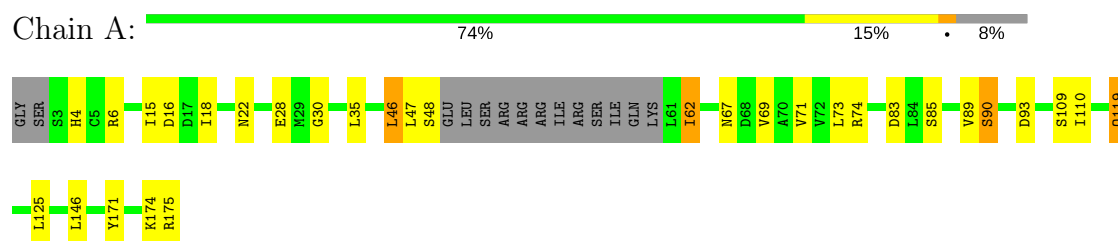
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	7	Total O 7 7	0	0

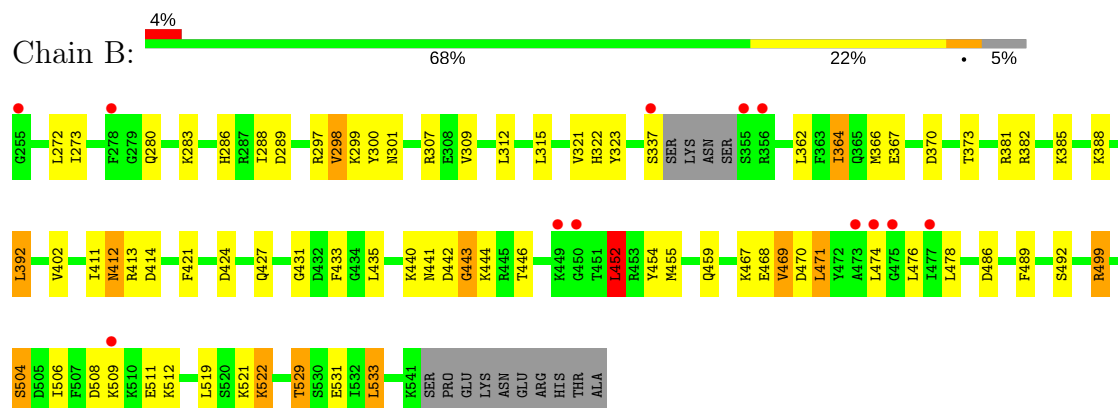
### 3 Residue-property plots [i](#)

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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.30Å 84.30Å 165.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.51 – 2.80 27.59 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.4 (29.51-2.80) 95.9 (27.59-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.207 , 0.268 0.208 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	71.3	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 54.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3518	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO

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	0/1338	0.68	0/1802
2	B	0.58	0/2214	0.73	1/2964 (0.0%)
All	All	0.59	0/3552	0.71	1/4766 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	452	LEU	CA-CB-CG	5.24	127.36	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	1314	0	1320	21	0
2	B	2189	0	2223	42	0
3	A	8	0	0	1	0
3	B	7	0	0	0	0
All	All	3518	0	3543	62	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 9.

All (62) 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:71:VAL:HG22	1:A:89:VAL:HG23	1.52	0.89
2:B:424:ASP:HB3	2:B:427:GLN:HB2	1.61	0.82
1:A:71:VAL:CG2	1:A:89:VAL:HG23	2.14	0.75
1:A:119:GLN:HA	1:A:119:GLN:HE21	1.52	0.74
1:A:174:LYS:HG3	1:A:175:ARG:H	1.51	0.74
2:B:412:ASN:O	2:B:470:ASP:OD2	2.08	0.72
2:B:286:HIS:CD2	2:B:288:ILE:H	2.08	0.71
1:A:73:LEU:HD11	1:A:85:SER:HB2	1.77	0.67
2:B:322:HIS:HB2	2:B:367:GLU:HB2	1.78	0.64
2:B:454:TYR:HA	2:B:476:LEU:CD1	2.28	0.64
2:B:455:MET:O	2:B:499:ARG:NH2	2.30	0.63
2:B:299:LYS:HE3	2:B:301:ASN:HB3	1.83	0.60
2:B:286:HIS:HD2	2:B:289:ASP:H	1.48	0.60
2:B:321:VAL:HG22	2:B:431:GLY:HA2	1.83	0.60
2:B:286:HIS:HD2	2:B:288:ILE:H	1.47	0.60
1:A:30:GLY:HA2	1:A:47:LEU:HG	1.83	0.59
2:B:286:HIS:CD2	2:B:289:ASP:H	2.20	0.58
1:A:22:ASN:HD22	1:A:67:ASN:HD22	1.52	0.57
2:B:454:TYR:HA	2:B:476:LEU:HD13	1.88	0.56
2:B:442:ASP:O	2:B:444:LYS:N	2.39	0.56
2:B:273:ILE:HD13	2:B:283:LYS:HB2	1.91	0.53
2:B:321:VAL:CG2	2:B:431:GLY:HA2	2.39	0.53
2:B:468:GLU:H	2:B:468:GLU:CD	2.13	0.53
2:B:312:LEU:HB3	2:B:323:TYR:HB2	1.90	0.52
1:A:119:GLN:CA	1:A:119:GLN:HE21	2.22	0.52
1:A:28:GLU:OE1	2:B:452:LEU:HD22	2.11	0.51
1:A:74:ARG:HB2	1:A:83:ASP:HB2	1.92	0.50
2:B:412:ASN:C	2:B:412:ASN:HD22	2.15	0.50
2:B:454:TYR:HA	2:B:476:LEU:HD12	1.94	0.48
1:A:90:SER:HB3	1:A:93:ASP:OD1	2.13	0.48
2:B:298:VAL:HG12	2:B:362:LEU:HB3	1.97	0.46
2:B:508:ASP:O	2:B:512:LYS:HB2	2.16	0.46
2:B:309:VAL:HG12	2:B:364:ILE:HD12	1.98	0.45
1:A:62:ILE:N	1:A:62:ILE:HD13	2.31	0.45
2:B:402:VAL:HG21	2:B:474:LEU:HD21	1.98	0.45
1:A:15:ILE:O	1:A:16:ASP:HB2	2.16	0.45
2:B:280:GLN:OE1	2:B:297:ARG:NH1	2.44	0.45
1:A:174:LYS:O	1:A:175:ARG:CB	2.64	0.45
2:B:468:GLU:HA	2:B:471:LEU:HD22	1.98	0.45
2:B:504:SER:HB3	2:B:506:ILE:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ILE:HG12	1:A:171:TYR:CE1	2.52	0.44
2:B:373:THR:HG22	2:B:421:PHE:CD2	2.53	0.44
1:A:46:LEU:N	1:A:46:LEU:HD23	2.33	0.43
2:B:459:GLN:HB2	2:B:469:VAL:CG2	2.49	0.43
1:A:22:ASN:HD22	1:A:67:ASN:ND2	2.15	0.43
2:B:414:ASP:HB2	2:B:435:LEU:HD12	2.01	0.42
2:B:508:ASP:HB2	2:B:511:GLU:CG	2.49	0.42
1:A:174:LYS:CG	1:A:175:ARG:H	2.26	0.42
2:B:382:ARG:O	2:B:486:ASP:OD2	2.36	0.42
2:B:307:ARG:HH22	2:B:446:TPO:P	2.43	0.42
2:B:412:ASN:C	2:B:412:ASN:ND2	2.73	0.42
2:B:411:ILE:HG21	2:B:467:LYS:HA	2.02	0.41
1:A:18:ILE:HG22	1:A:69:VAL:CG1	2.51	0.41
2:B:421:PHE:CE1	2:B:431:GLY:HA3	2.55	0.41
2:B:312:LEU:HD21	2:B:433:PHE:CD1	2.56	0.41
2:B:442:ASP:O	2:B:443:GLY:C	2.59	0.41
1:A:47:LEU:O	1:A:48:SER:HB2	2.21	0.41
2:B:412:ASN:HD22	2:B:414:ASP:H	1.69	0.41
2:B:529:THR:O	2:B:533:LEU:HB2	2.21	0.41
2:B:392:LEU:HD12	2:B:392:LEU:HA	1.94	0.41
1:A:6:ARG:HD3	3:A:177:HOH:O	2.20	0.41
2:B:521:LYS:HG3	2:B:522:LYS:HE2	2.04	0.40

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	157/175 (90%)	151 (96%)	6 (4%)	0	100	100
2	B	265/284 (93%)	246 (93%)	17 (6%)	2 (1%)	22	55
All	All	422/459 (92%)	397 (94%)	23 (6%)	2 (0%)	32	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	443	GLY
2	B	441	ASN

### 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	145/161 (90%)	136 (94%)	9 (6%)	21	52
2	B	239/254 (94%)	210 (88%)	29 (12%)	6	17
All	All	384/415 (92%)	346 (90%)	38 (10%)	9	26

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	35	LEU
1	A	46	LEU
1	A	62	ILE
1	A	90	SER
1	A	109	SER
1	A	119	GLN
1	A	125	LEU
1	A	146	LEU
2	B	272	LEU
2	B	298	VAL
2	B	300	TYR
2	B	315	LEU
2	B	337	SER
2	B	364	ILE
2	B	366	MET
2	B	370	ASP
2	B	381	ARG
2	B	385	LYS
2	B	388	LYS
2	B	392	LEU

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Mol	Chain	Res	Type
2	B	412	ASN
2	B	413	ARG
2	B	440	LYS
2	B	452	LEU
2	B	469	VAL
2	B	471	LEU
2	B	478	LEU
2	B	489	PHE
2	B	492	SER
2	B	499	ARG
2	B	504	SER
2	B	509	LYS
2	B	519	LEU
2	B	522	LYS
2	B	529	THR
2	B	531	GLU
2	B	533	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) 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	319	ASN
2	B	324	ASN
2	B	412	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	0.82	0	10,14,16	1.06	1 (10%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	446	TPO	O3P-P-O2P	2.10	116.08	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	446	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	161/175 (92%)	-0.25	0 100 100	46, 62, 73, 82	0
2	B	269/284 (94%)	0.03	12 (4%) 34 24	46, 61, 74, 83	0
All	All	430/459 (93%)	-0.08	12 (2%) 53 43	46, 61, 74, 83	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	356	ARG	3.2
2	B	474	LEU	2.7
2	B	473	ALA	2.6
2	B	355	SER	2.5
2	B	255	GLY	2.5
2	B	450	GLY	2.4
2	B	509	LYS	2.3
2	B	475	GLY	2.2
2	B	449	LYS	2.2
2	B	337	SER	2.2
2	B	278	PHE	2.1
2	B	477	ILE	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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	TPO	B	446	11/12	0.96	0.10	-	57,60,64,64	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.