



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 5, 2023 – 02:19 PM EST

PDB ID : 8EHV  
Title : Kelch domain of human KEAP1 bound to Nrf2 cyclic peptide, c[DhA-GDPET(bAla)E]  
Authors : Muellers, S.N.; Allen, K.N.  
Deposited on : 2022-09-14  
Resolution : 2.29 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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 : 2.36  
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) : 2.36

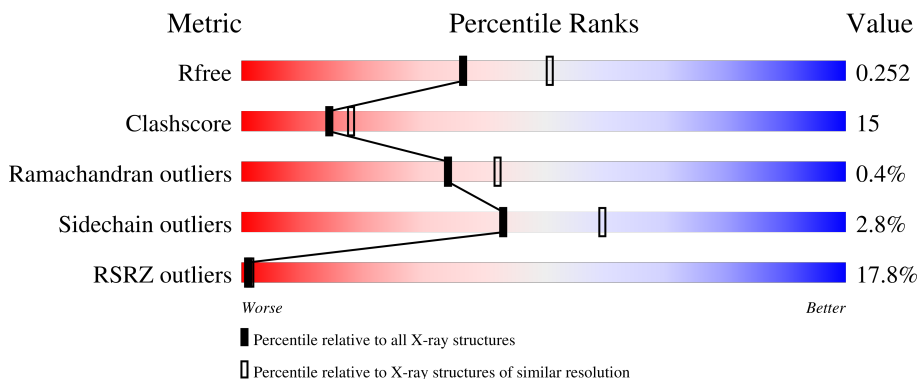
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	336	
1	B	336	
2	P	7	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	B3A	P	76	X	X	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4608 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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	289	2222	1381	404	421	16	0	0	0
1	B	279	2145	1337	388	405	15	0	0	0

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	MET	-	expression tag	UNP Q14145
A	290	GLY	-	expression tag	UNP Q14145
A	291	SER	-	expression tag	UNP Q14145
A	292	SER	-	expression tag	UNP Q14145
A	293	HIS	-	expression tag	UNP Q14145
A	294	HIS	-	expression tag	UNP Q14145
A	295	HIS	-	expression tag	UNP Q14145
A	296	HIS	-	expression tag	UNP Q14145
A	297	HIS	-	expression tag	UNP Q14145
A	298	HIS	-	expression tag	UNP Q14145
A	299	SER	-	expression tag	UNP Q14145
A	300	SER	-	expression tag	UNP Q14145
A	301	GLY	-	expression tag	UNP Q14145
A	302	GLY	-	expression tag	UNP Q14145
A	303	GLU	-	expression tag	UNP Q14145
A	304	ASN	-	expression tag	UNP Q14145
A	305	LEU	-	expression tag	UNP Q14145
A	306	TYR	-	expression tag	UNP Q14145
A	307	PHE	-	expression tag	UNP Q14145
A	308	GLN	-	expression tag	UNP Q14145
A	309	GLY	-	expression tag	UNP Q14145
A	310	HIS	-	expression tag	UNP Q14145
A	311	MET	-	expression tag	UNP Q14145
A	319	SER	CYS	conflict	UNP Q14145
A	540	ALA	GLU	engineered mutation	UNP Q14145

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	ALA	GLU	engineered mutation	UNP Q14145
A	613	SER	CYS	engineered mutation	UNP Q14145
A	622	SER	CYS	conflict	UNP Q14145
A	624	SER	CYS	conflict	UNP Q14145
B	289	MET	-	expression tag	UNP Q14145
B	290	GLY	-	expression tag	UNP Q14145
B	291	SER	-	expression tag	UNP Q14145
B	292	SER	-	expression tag	UNP Q14145
B	293	HIS	-	expression tag	UNP Q14145
B	294	HIS	-	expression tag	UNP Q14145
B	295	HIS	-	expression tag	UNP Q14145
B	296	HIS	-	expression tag	UNP Q14145
B	297	HIS	-	expression tag	UNP Q14145
B	298	HIS	-	expression tag	UNP Q14145
B	299	SER	-	expression tag	UNP Q14145
B	300	SER	-	expression tag	UNP Q14145
B	301	GLY	-	expression tag	UNP Q14145
B	302	GLY	-	expression tag	UNP Q14145
B	303	GLU	-	expression tag	UNP Q14145
B	304	ASN	-	expression tag	UNP Q14145
B	305	LEU	-	expression tag	UNP Q14145
B	306	TYR	-	expression tag	UNP Q14145
B	307	PHE	-	expression tag	UNP Q14145
B	308	GLN	-	expression tag	UNP Q14145
B	309	GLY	-	expression tag	UNP Q14145
B	310	HIS	-	expression tag	UNP Q14145
B	311	MET	-	expression tag	UNP Q14145
B	319	SER	CYS	conflict	UNP Q14145
B	540	ALA	GLU	engineered mutation	UNP Q14145
B	542	ALA	GLU	engineered mutation	UNP Q14145
B	613	SER	CYS	engineered mutation	UNP Q14145
B	622	SER	CYS	conflict	UNP Q14145
B	624	SER	CYS	conflict	UNP Q14145

- Molecule 2 is a protein called cyclic peptide c[DhA-GDPET(bAla)E].

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	P	7	51	30	7	14	0	0	0

- Molecule 3 is water.

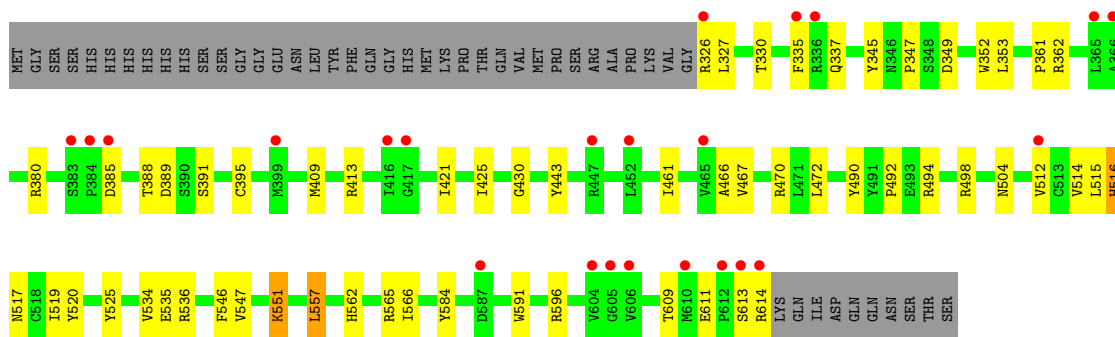
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	137	Total 137	O 137	0	0
3	B	53	Total 53	O 53	0	0

### 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.

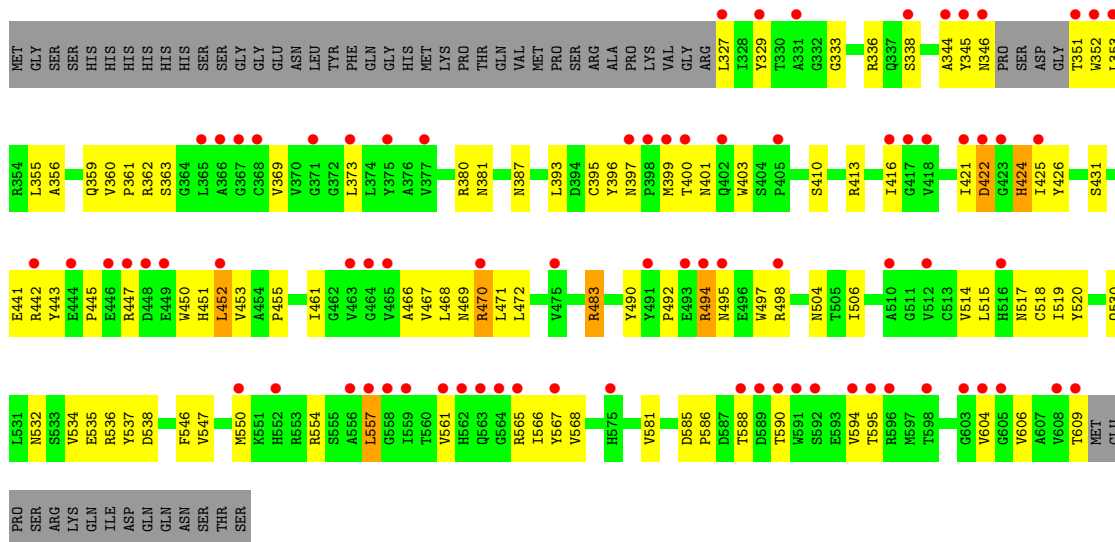
- Molecule 1: Kelch-like ECH-associated protein 1

Chain A: 



- Molecule 1: Kelch-like ECH-associated protein 1

Chain B: 



- Molecule 2: cyclic peptide c[DhA-GDPET(bAla)E

Chain P: 

A76  
D77  
P78  
E79  
T80  
BAL81  
E82



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.35Å 68.85Å 77.22Å 90.00° 117.63° 90.00°	Depositor
Resolution (Å)	29.58 – 2.29 29.59 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.58-2.29) 99.3 (29.59-2.29)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.203 , 0.253 0.203 , 0.252	Depositor DCC
$R_{free}$ test set	1996 reflections (5.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtrriage
Anisotropy	0.565	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.012 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4608	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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: B3A, BAL

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	0.94	5/2276 (0.2%)	0.89	1/3099 (0.0%)
1	B	0.74	0/2196	0.87	4/2990 (0.1%)
2	P	1.52	0/39	1.18	0/51
All	All	0.86	5/4511 (0.1%)	0.88	5/6140 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	P	1	1
All	All	1	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	391	SER	CB-OG	7.13	1.51	1.42
1	A	535	GLU	CG-CD	6.05	1.61	1.51
1	A	395	CYS	CB-SG	-5.97	1.72	1.81
1	A	349	ASP	CB-CG	-5.61	1.40	1.51
1	A	525	TYR	CD2-CE2	5.21	1.47	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	ARG	NE-CZ-NH1	-7.36	116.62	120.30
1	B	538	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	422	ASP	CB-CG-OD1	5.98	123.68	118.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	483	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	B	494	ARG	NE-CZ-NH1	-5.03	117.78	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	P	76	B3A	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	609	THR	Mainchain
2	P	80	THR	Peptide

## 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	2222	0	2119	41	3
1	B	2145	0	2046	90	3
2	P	51	0	33	3	0
3	A	137	0	0	4	0
3	B	53	0	0	8	0
All	All	4608	0	4198	133	3

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 15.

The worst 5 of 133 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:B:393:LEU:HD12	1:B:450:TRP:HZ2	1.09	1.14
1:B:441:GLU:HB3	1:B:452:LEU:HD23	1.39	1.03
1:B:393:LEU:HD12	1:B:450:TRP:CZ2	1.94	1.03
1:B:346:ASN:HD22	1:B:351:THR:HG22	1.26	1.00
1:B:441:GLU:HB3	1:B:452:LEU:CD2	1.92	1.00

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:ASN:OD1	1:B:470:ARG:NH1[2_555]	0.37	1.83
1:A:517:ASN:CG	1:B:470:ARG:NH1[2_555]	1.54	0.66
1:A:517:ASN:OD1	1:B:470:ARG:CZ[2_555]	1.55	0.65

### 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	287/336 (85%)	274 (96%)	12 (4%)	1 (0%)	41	50
1	B	275/336 (82%)	263 (96%)	11 (4%)	1 (0%)	34	42
2	P	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
All	All	566/679 (83%)	540 (95%)	24 (4%)	2 (0%)	34	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	516	HIS
1	B	453	VAL

#### 5.3.2 Protein sidechains [i](#)

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	234/275 (85%)	228 (97%)	6 (3%)	46	63

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	225/275 (82%)	218 (97%)	7 (3%)	40	55
2	P	5/5 (100%)	5 (100%)	0	100	100
All	All	464/555 (84%)	451 (97%)	13 (3%)	43	60

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	424	HIS
1	B	447	ARG
1	B	557	LEU
1	B	470	ARG
1	B	494	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	346	ASN
1	B	387	ASN
1	B	401	ASN
1	B	517	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues are 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	B3A	P	76	2	5,5,6	9.75	4 (80%)	5,5,7	7.78	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BAL	P	81	2	4,4,5	1.98	1 (25%)	3,3,5	14.05	1 (33%)

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	B3A	P	76	2	1/1/1/2	0/3/3/4	-
2	BAL	P	81	2	-	0/1/2/3	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	76	B3A	CB-CA	-20.98	1.25	1.53
2	P	76	B3A	CA-N	-5.02	1.35	1.49
2	P	81	BAL	CB-CA	-3.58	1.35	1.51
2	P	76	B3A	O-C	2.41	1.33	1.19
2	P	76	B3A	CB-C	-2.14	1.44	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	81	BAL	CB-CA-C	24.32	147.54	111.42
2	P	76	B3A	CA-CB-C	16.83	146.96	113.37
2	P	76	B3A	CB-CA-N	-3.09	102.28	110.72
2	P	76	B3A	CG-CA-N	2.00	117.39	108.81

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	P	76	B3A	CA

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	81:BAL	C	82:GLU	N	1.16

## 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	289/336 (86%)	0.35	23 (7%) 12 16	22, 34, 56, 79	0
1	B	279/336 (83%)	1.30	78 (27%) 0 0	28, 63, 108, 132	0
2	P	5/7 (71%)	0.90	1 (20%) 1 1	55, 56, 68, 79	0
All	All	573/679 (84%)	0.82	102 (17%) 1 1	22, 43, 102, 132	0

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	351	THR	6.3
1	A	613	SER	6.1
1	B	567	TYR	5.6
1	A	614	ARG	5.5
1	B	399	MET	5.3

### 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	B3A	P	76	6/7	0.71	0.50	76,77,80,83	0
2	BAL	P	81	5/6	0.85	0.18	68,68,75,75	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.