



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 01:39 PM BST

PDB ID : 3MXB  
Title : Molecular basis of engineered meganuclease targeting of the endogenous human RAG1 locus  
Authors : Munoz, I.G.; Prieto, J.; Subramanian, S.; Coloma, J.; Montoya, G.  
Deposited on : 2010-05-07  
Resolution : 2.30 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	:	2.13.1
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)	:	2.13.1

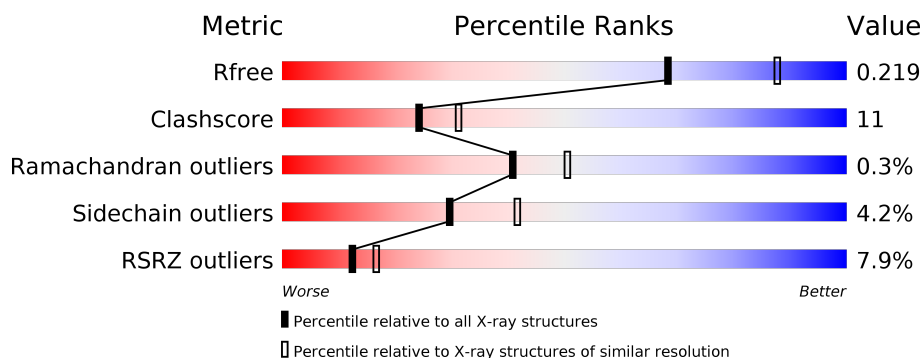
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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 on 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	175	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>14%</div> <div>•</div> <div>13%</div> </div> </div>
1	R	175	<div> <div>7%</div> <div> <div></div> <div>64%</div> <div>21%</div> <div>•</div> <div>12%</div> </div> </div>
2	B	173	<div> <div>9%</div> <div> <div></div> <div>68%</div> <div>21%</div> <div></div> <div>12%</div> </div> </div>
2	S	173	<div> <div>8%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>12%</div> </div> </div>
3	C	24	<div> <div></div> <div> <div></div> <div>71%</div> <div>25%</div> <div>•</div> </div> </div>
3	T	24	<div> <div></div> <div> <div></div> <div>50%</div> <div>42%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	E	24	 42% 54% .
4	V	24	 4% 33% 50% 17%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7005 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 V3(E8K).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1199	772	207	219	1			
1	R	154	Total	C	N	O	S	0	0	0
			1221	786	211	223	1			

- Molecule 2 is a protein called V2(K7E-G19S).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1214	780	205	228	1			
2	S	152	Total	C	N	O	S	0	0	0
			1212	780	205	226	1			

- Molecule 3 is a DNA chain called DNA (5'-D(\*TP\*TP\*GP\*TP\*TP\*CP\*TP\*CP\*AP\*GP\*GP\*TP\*AP\*CP\*CP\*TP\*CP\*AP\*GP\*CP\*CP\*AP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	24	Total	C	N	O	P	0	0	0
			485	233	85	144	23			
3	T	24	Total	C	N	O	P	0	0	0
			485	233	85	144	23			

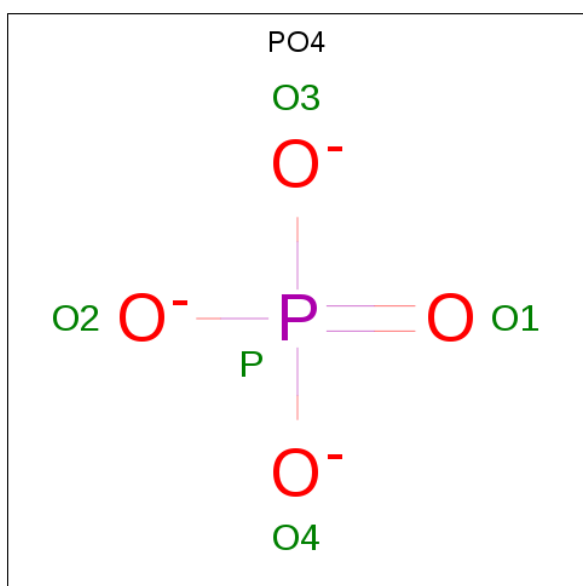
- Molecule 4 is a DNA chain called DNA (5'-D(\*TP\*CP\*TP\*GP\*GP\*CP\*TP\*GP\*AP\*GP\*GP\*TP\*AP\*CP\*CP\*TP\*GP\*AP\*GP\*AP\*AP\*CP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	24	Total	C	N	O	P	0	0	0
			493	235	95	140	23			
4	V	24	Total	C	N	O	P	2	0	0
			493	235	95	140	23			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Ca 1 1	0	0
5	A	1	Total Ca 1 1	0	0
5	R	1	Total Ca 1 1	0	0
5	S	1	Total Ca 1 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	32	Total O 32 32	0	0
7	B	27	Total O 27 27	0	0

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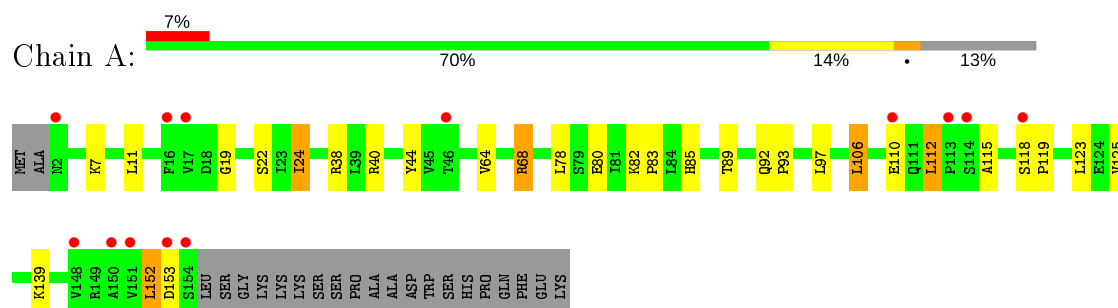
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	12	Total 12	O 12	0	0
7	E	9	Total 9	O 9	0	0
7	R	21	Total 21	O 21	0	0
7	S	37	Total 37	O 37	0	0
7	T	21	Total 21	O 21	0	0
7	V	20	Total 20	O 20	0	0

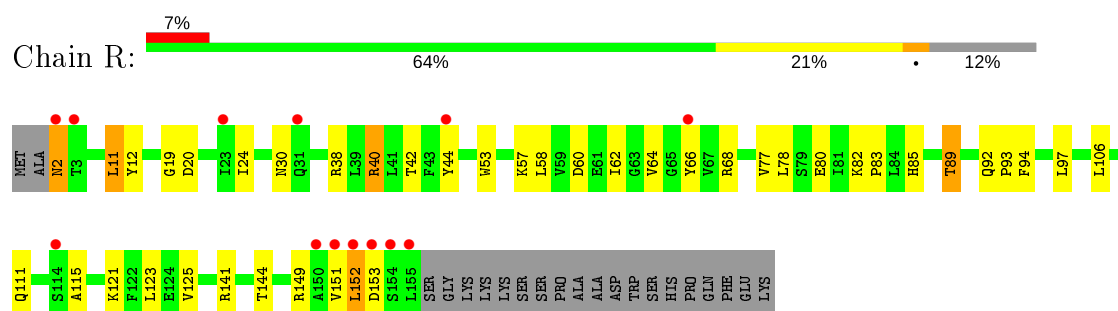
### 3 Residue-property plots [i](#)

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.

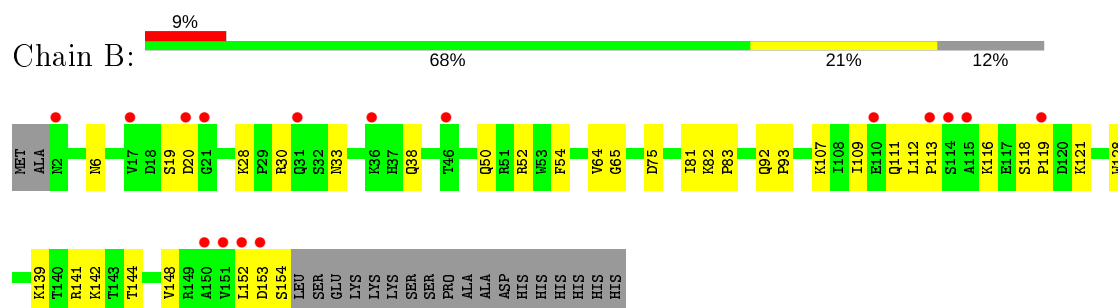
- Molecule 1: V3(E8K)



- Molecule 1: V3(E8K)

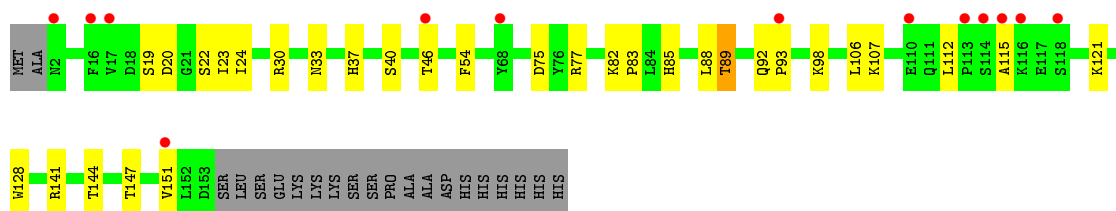


- Molecule 2: V2(K7E-G19S)



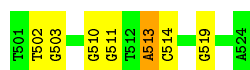
- Molecule 2: V2(K7E-G19S)





- Molecule 3: DNA (5'-D(\*TP\*TP\*GP\*TP\*TP\*CP\*TP\*CP\*AP\*GP\*GP\*TP\*AP\*CP\*CP\*TP\*CP\*AP\*GP\*CP\*CP\*AP\*GP\*A)-3')

Chain C: 71% 25% .



- Molecule 3: DNA (5'-D(\*TP\*TP\*GP\*TP\*TP\*CP\*TP\*CP\*AP\*GP\*GP\*TP\*AP\*CP\*CP\*TP\*CP\*AP\*GP\*CP\*CP\*AP\*GP\*A)-3')

Chain T: 50% 42% 8% .



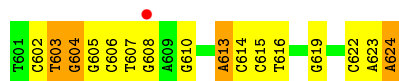
- Molecule 4: DNA (5'-D(\*TP\*CP\*TP\*GP\*GP\*CP\*TP\*GP\*AP\*GP\*GP\*TP\*AP\*CP\*CP\*TP\*GP\*AP\*GP\*AP\*AP\*CP\*AP\*A)-3')

Chain E: 42% 54% .



- Molecule 4: DNA (5'-D(\*TP\*CP\*TP\*GP\*GP\*CP\*TP\*GP\*AP\*GP\*GP\*TP\*AP\*CP\*CP\*TP\*GP\*AP\*GP\*AP\*AP\*CP\*AP\*A)-3')

Chain V: 4% 33% 50% 17% .





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.05Å 89.36Å 86.34Å 90.00° 99.51° 90.00°	Depositor
Resolution (Å)	35.84 – 2.30 37.36 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (35.84-2.30) 97.8 (37.36-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.180 , 0.231 0.169 , 0.219	Depositor DCC
$R_{free}$ test set	2300 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtrriage
Anisotropy	0.112	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 63.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7005	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9354e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: CA, PO4

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	0.35	0/1222	0.50	0/1660
1	R	0.37	0/1244	0.52	0/1685
2	B	0.38	0/1237	0.49	0/1677
2	S	0.41	0/1235	0.54	0/1673
3	C	0.75	0/542	1.41	4/834 (0.5%)
3	T	0.80	0/542	1.54	8/834 (1.0%)
4	E	0.73	0/554	1.36	4/854 (0.5%)
4	V	0.86	0/554	1.52	9/854 (1.1%)
All	All	0.54	0/7130	0.94	25/10071 (0.2%)

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	613	DA	O4'-C1'-N9	-9.54	101.32	108.00
3	C	513	DA	O4'-C1'-N9	-8.77	101.86	108.00
3	T	513	DA	O4'-C1'-N9	-7.93	102.45	108.00
4	E	613	DA	O4'-C1'-N9	-7.89	102.47	108.00
3	C	510	DG	O4'-C1'-N9	-7.60	102.68	108.00

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	1199	0	1191	25	0
1	R	1221	0	1233	42	0
2	B	1214	0	1213	33	0
2	S	1212	0	1219	24	0
3	C	485	0	273	3	0
3	T	485	0	273	8	0
4	E	493	0	271	12	0
4	V	493	0	271	17	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	R	1	0	0	0	0
5	S	1	0	0	0	0
6	B	10	0	0	0	0
6	C	5	0	0	0	0
6	S	5	0	0	1	0
7	A	32	0	0	2	0
7	B	27	0	0	1	0
7	C	12	0	0	0	0
7	E	9	0	0	0	0
7	R	21	0	0	2	0
7	S	37	0	0	2	0
7	T	21	0	0	0	0
7	V	20	0	0	2	0
All	All	7005	0	5944	140	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 11.

The worst 5 of 140 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:S:22:SER:OG	2:S:24:ILE:HD11	1.76	0.85
1:R:38:ARG:NH2	4:V:604:DG:C8	2.45	0.84
2:S:92:GLN:HG3	2:S:93:PRO:HD3	1.61	0.83
2:B:30:ARG:HD3	2:B:33:ASN:ND2	1.94	0.82
7:R:182:HOH:O	4:V:603:DT:H71	1.86	0.74

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	151/175 (86%)	142 (94%)	8 (5%)	1 (1%)	22	26
1	R	152/175 (87%)	143 (94%)	9 (6%)	0	100	100
2	B	151/173 (87%)	142 (94%)	8 (5%)	1 (1%)	22	26
2	S	150/173 (87%)	145 (97%)	5 (3%)	0	100	100
All	All	604/696 (87%)	572 (95%)	30 (5%)	2 (0%)	41	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	LEU
2	B	153	ASP

### 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	128/158 (81%)	123 (96%)	5 (4%)	32	46
1	R	133/158 (84%)	124 (93%)	9 (7%)	16	21
2	B	133/157 (85%)	129 (97%)	4 (3%)	41	57
2	S	133/157 (85%)	129 (97%)	4 (3%)	41	57
All	All	527/630 (84%)	505 (96%)	22 (4%)	30	42

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	2	ASN
1	R	58	LEU
2	S	89	THR
1	R	11	LEU
1	R	40	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	111	GLN
2	S	92	GLN
1	R	111	GLN
2	B	92	GLN
1	R	103	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z  > 2$
6	PO4	C	3	-	4,4,4	0.87	0	6,6,6	0.48	0
6	PO4	B	175	-	4,4,4	0.88	0	6,6,6	0.60	0
6	PO4	B	174	-	4,4,4	0.90	0	6,6,6	0.43	0
6	PO4	S	174	-	4,4,4	0.92	0	6,6,6	0.27	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	S	174	PO4	1	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	153/175 (87%)	0.72	13 (8%) 10 14	19, 44, 76, 95	0
1	R	154/175 (88%)	0.80	13 (8%) 11 15	20, 45, 76, 95	0
2	B	153/173 (88%)	0.72	16 (10%) 6 8	19, 39, 63, 91	0
2	S	152/173 (87%)	0.61	13 (8%) 10 14	18, 36, 63, 81	0
3	C	24/24 (100%)	0.18	0 100 100	26, 45, 88, 93	0
3	T	24/24 (100%)	0.25	0 100 100	26, 46, 88, 94	0
4	E	24/24 (100%)	0.39	0 100 100	23, 53, 80, 82	0
4	V	24/24 (100%)	0.40	1 (4%) 36 43	22, 51, 67, 78	1 (4%)
All	All	708/792 (89%)	0.66	56 (7%) 12 17	18, 41, 74, 95	1 (0%)

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	153	ASP	8.4
1	A	154	SER	4.6
2	B	113	PRO	4.4
1	A	151	VAL	4.2
1	R	2	ASN	4.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

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
6	PO4	C	3	5/5	0.62	0.32	130,134,135,135	0
6	PO4	B	174	5/5	0.81	0.32	94,100,104,109	0
6	PO4	S	174	5/5	0.89	0.32	81,91,93,97	0
6	PO4	B	175	5/5	0.90	0.27	73,89,90,90	0
5	CA	B	173	1/1	0.99	0.24	23,23,23,23	0
5	CA	A	175	1/1	0.99	0.19	19,19,19,19	0
5	CA	R	175	1/1	0.99	0.21	20,20,20,20	0
5	CA	S	173	1/1	0.99	0.17	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.