



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:10 PM GMT

PDB ID : 4BPB  
Title : STRUCTURAL INSIGHTS INTO RNA RECOGNITION BY RIG-I  
Authors : Luo, D.; Pyle, A.M.  
Deposited on : 2013-05-23  
Resolution : 2.58 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

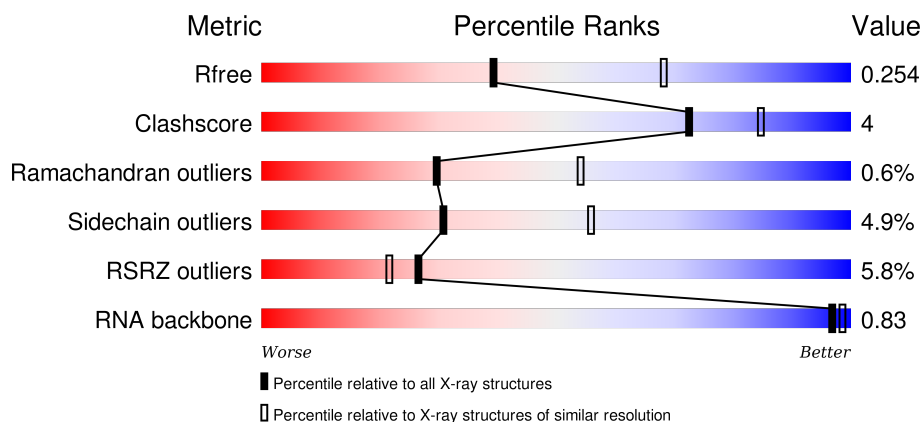
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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))
$R_{free}$	91344	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)
RNA backbone	2183	1042 (3.00-2.16)

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	698	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>• 9%</div> </div> </div>
2	C	10	<div> <div>80%</div> <div>20%</div> </div>
2	D	10	<div> <div>100%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5518 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 PROBABLE ATP-DEPENDENT RNA HELICASE DDX58.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	634	Total	C	N	O	S	3	1	0
			4981	3206	839	906	30			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	ASN	GLN	CONFLICT	UNP O95786
A	419	THR	ASN	CONFLICT	UNP O95786
A	671A	PHE	-	INSERTION	UNP O95786
A	671B	PHE	-	INSERTION	UNP O95786
A	828	ASP	GLU	CONFLICT	UNP O95786

- Molecule 2 is a RNA chain called 5'-R(\*GP\*CP\*GP\*CP\*GP\*CP\*GP\*CP\*GP\*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			212	95	40	68	9			
2	D	10	Total	C	N	O	P	0	0	0
			212	95	40	68	9			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

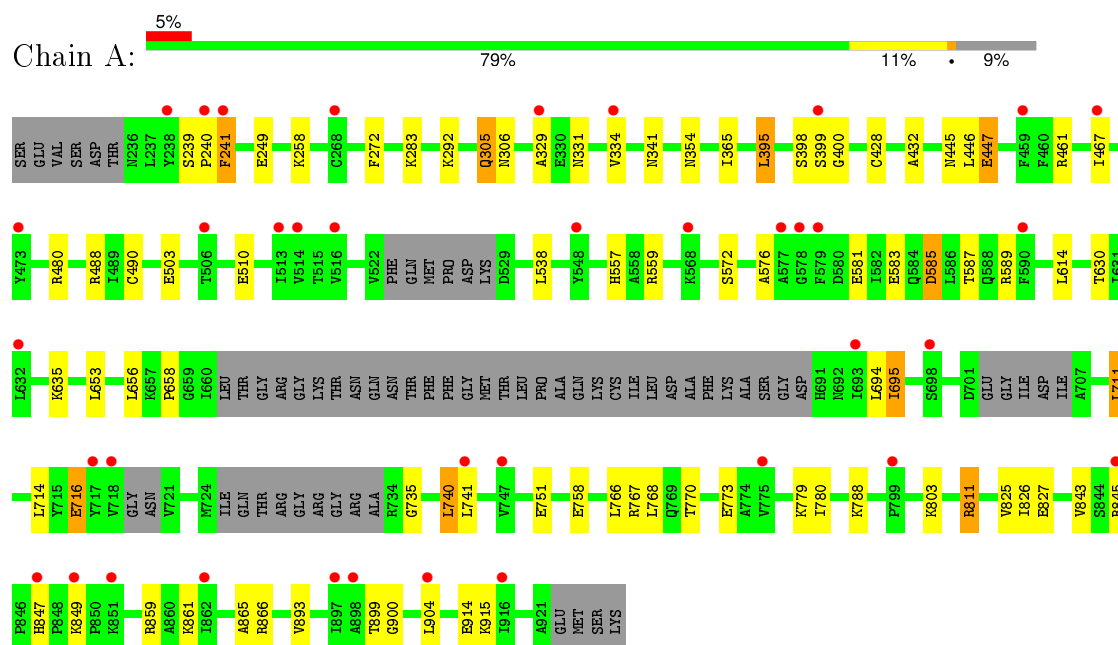
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	95	Total	O	0	0
			95	95		
5	C	6	Total	O	0	0
			6	6		
5	D	6	Total	O	0	0
			6	6		

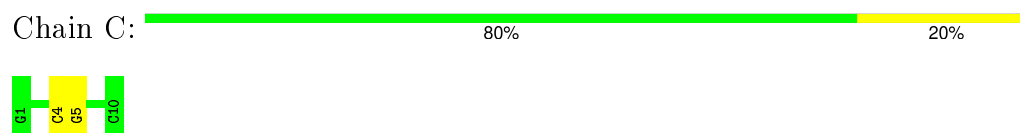
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: PROBABLE ATP-DEPENDENT RNA HELICASE DDX58



- Molecule 2: 5'-R(\*GP\*CP\*GP\*CP\*GP\*CP\*GP\*CP\*GP\*CP)-3'



- Molecule 2: 5'-R(\*GP\*CP\*GP\*CP\*GP\*CP\*GP\*CP\*GP\*CP)-3'



There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.62Å 76.21Å 219.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.93 – 2.58 43.69 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.93-2.58) 99.0 (43.69-2.58)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.58Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.195 , 0.255 0.192 , 0.254	Depositor DCC
$R_{free}$ test set	1310 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.9	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 25750 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5518	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, SO4

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	0.25	0/5087	0.43	0/6877
2	C	0.23	0/236	0.68	0/367
2	D	0.21	0/236	0.71	0/367
All	All	0.25	0/5559	0.46	0/7611

There are no bond length outliers.

There are no bond angle outliers.

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	4981	0	4910	42	0
2	C	212	0	112	2	0
2	D	212	0	112	0	0
3	A	1	0	0	0	0
4	A	5	0	0	0	0
5	A	95	0	0	4	0
5	C	6	0	0	0	0
5	D	6	0	0	0	0
All	All	5518	0	5134	44	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 4.

All (44) 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:480:ARG:NH2	5:A:2048:HOH:O	2.25	0.70
1:A:398:SER:O	1:A:400:GLY:N	2.30	0.65
1:A:803:LYS:HG2	1:A:914:GLU:HB2	1.82	0.61
1:A:656:LEU:HB3	1:A:695:ILE:HD11	1.81	0.61
1:A:714:LEU:HB2	1:A:740:LEU:HD23	1.83	0.61
1:A:826:ILE:HG22	1:A:827:GLU:HG2	1.84	0.59
1:A:557:HIS:CE1	1:A:716:GLU:HG2	2.38	0.58
1:A:767:ARG:O	1:A:770:THR:OG1	2.20	0.58
1:A:292:LYS:NZ	1:A:341:ASN:O	2.37	0.57
1:A:899:THR:OG1	1:A:900:GLY:N	2.34	0.57
1:A:461:ARG:HB2	1:A:741:LEU:HD23	1.86	0.57
1:A:653:LEU:HG	1:A:656:LEU:HD12	1.87	0.55
1:A:258:LYS:NZ	1:A:773:GLU:OE1	2.36	0.54
1:A:490:CYS:SG	5:A:2052:HOH:O	2.59	0.53
1:A:861:LYS:NZ	5:A:2089:HOH:O	2.37	0.50
1:A:241:PHE:HB3	1:A:272:PHE:CE1	2.46	0.50
1:A:767:ARG:NH1	5:A:2070:HOH:O	2.34	0.48
1:A:893:VAL:HG22	1:A:904:LEU:HD21	1.94	0.48
1:A:843:VAL:HG13	1:A:865:ALA:HA	1.96	0.47
1:A:583:GLU:O	1:A:587:THR:HG23	2.15	0.47
1:A:825:VAL:HG21	1:A:915:LYS:HB3	1.97	0.47
1:A:334:VAL:HG11	1:A:354:ASN:OD1	2.15	0.46
1:A:447:GLU:H	1:A:447:GLU:CD	2.17	0.46
1:A:239:SER:O	1:A:241:PHE:N	2.49	0.45
1:A:585:ASP:O	1:A:589:ARG:HG3	2.16	0.45
1:A:557:HIS:CD2	1:A:635:LYS:HE2	2.51	0.45
1:A:658:PRO:HB3	1:A:695:ILE:HD12	1.99	0.45
1:A:249:GLU:OE1	1:A:445:ASN:ND2	2.46	0.44
1:A:305:GLN:HG3	1:A:306:ASN:N	2.31	0.44
1:A:845:ARG:HA	1:A:845:ARG:HD2	1.91	0.44
1:A:630:THR:HB	1:A:695:ILE:HG23	1.99	0.44
1:A:656:LEU:HA	1:A:694:LEU:HD12	2.00	0.43
1:A:656:LEU:HD22	1:A:695:ILE:HG12	2.00	0.43
1:A:329:ALA:HA	1:A:331:ASN:H	1.84	0.43
1:A:467:ILE:HD13	1:A:467:ILE:HA	1.92	0.43
1:A:811:ARG:HA	1:A:893:VAL:HG23	2.01	0.43
2:C:4:C:H2'	2:C:5:G:C8	2.54	0.42
1:A:847:HIS:CE1	1:A:849:LYS:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:ARG:HH11	1:A:866:ARG:HA	1.85	0.42
1:A:428:CYS:SG	1:A:779:LYS:NZ	2.68	0.41
1:A:630:THR:HG23	1:A:711:LEU:HB3	2.02	0.41
1:A:432:ALA:HA	1:A:780:ILE:HG23	2.02	0.41
2:C:4:C:H2'	2:C:5:G:H8	1.87	0.40
1:A:395:LEU:HD23	1:A:788:LYS:HD2	2.03	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	623/698 (89%)	585 (94%)	34 (6%)	4 (1%)	30 54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	399	SER
1	A	240	PRO
1	A	735	GLY
1	A	576	ALA

### 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	533/626 (85%)	507 (95%)	26 (5%)	31 56

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	PHE
1	A	283	LYS
1	A	305	GLN
1	A	365	ILE
1	A	395	LEU
1	A	446	LEU
1	A	447	GLU
1	A	488	ARG
1	A	503	GLU
1	A	510	GLU
1	A	538	LEU
1	A	559	ARG
1	A	572	SER
1	A	581	GLU
1	A	585	ASP
1	A	614	LEU
1	A	695	ILE
1	A	711	LEU
1	A	716	GLU
1	A	740	LEU
1	A	751	GLU
1	A	758	GLU
1	A	766	LEU
1	A	768	LEU
1	A	811	ARG
1	A	859	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	9/10 (90%)	0	0
2	D	9/10 (90%)	0	0
All	All	18/20 (90%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	SO4	A	1923	-	4,4,4	0.31	0	6,6,6	0.10	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
4	SO4	A	1923	-	-	0/0/0/0	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.

## 5.7 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	634/698 (90%)	0.45	38 (5%) 25 20	14, 49, 92, 134	1 (0%)
2	C	10/10 (100%)	-0.31	0 100 100	31, 35, 84, 99	0
2	D	10/10 (100%)	-0.20	0 100 100	41, 54, 70, 80	0
All	All	654/718 (91%)	0.43	38 (5%) 26 22	14, 49, 92, 134	1 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	PHE	7.7
1	A	399	SER	6.1
1	A	579	PHE	5.5
1	A	240	PRO	5.3
1	A	851	LYS	5.2
1	A	577	ALA	5.1
1	A	578	GLY	4.1
1	A	898	ALA	3.7
1	A	513	ILE	3.6
1	A	718	VAL	3.5
1	A	904	LEU	3.5
1	A	268[A]	CYS	3.3
1	A	467	ILE	3.1
1	A	799	PRO	3.0
1	A	329	ALA	2.9
1	A	632	LEU	2.8
1	A	238	TYR	2.8
1	A	916	ILE	2.7
1	A	849	LYS	2.7
1	A	847	HIS	2.6
1	A	862	ILE	2.5
1	A	717	TYR	2.4
1	A	845	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	741	LEU	2.3
1	A	516	VAL	2.3
1	A	775	VAL	2.3
1	A	897	ILE	2.3
1	A	568	LYS	2.3
1	A	548	TYR	2.2
1	A	459	PHE	2.2
1	A	747	VAL	2.2
1	A	473	TYR	2.1
1	A	698	SER	2.1
1	A	590	PHE	2.1
1	A	334	VAL	2.1
1	A	506	THR	2.1
1	A	514	VAL	2.0
1	A	693	ILE	2.0

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

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

## 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
4	SO4	A	1923	5/5	0.99	0.12	-0.85	52,55,59,61	0
3	ZN	A	927	1/1	0.99	0.10	-1.39	66,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.