



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2021 – 07:34 PM EDT

PDB ID : 5RP1  
Title : PanDDA analysis group deposition – Proteinase K crystal structure Apo36  
Authors : Lima, G.M.A.; Talibov, V.; Benz, L.S.; Jagudin, E.; Mueller, U.  
Deposited on : 2020-09-23  
Resolution : 1.11 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

<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 : 2.20  
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) : 2.20

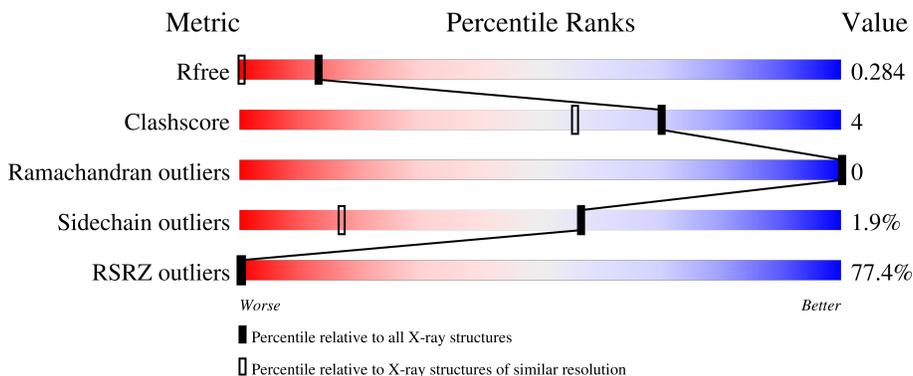
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.11 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	1168 (1.14-1.10)
Clashscore	141614	1205 (1.14-1.10)
Ramachandran outliers	138981	1168 (1.14-1.10)
Sidechain outliers	138945	1165 (1.14-1.10)
RSRZ outliers	127900	1146 (1.14-1.10)

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	279	<p>77% 92% 8%</p>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2213 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.

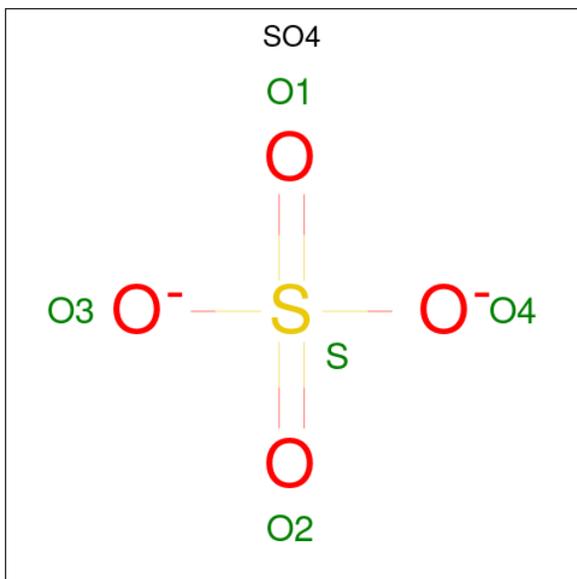
- Molecule 1 is a protein called Proteinase K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	279	2023	1244	355	414	10	0	17	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	ASP	SER	conflict	UNP P06873

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

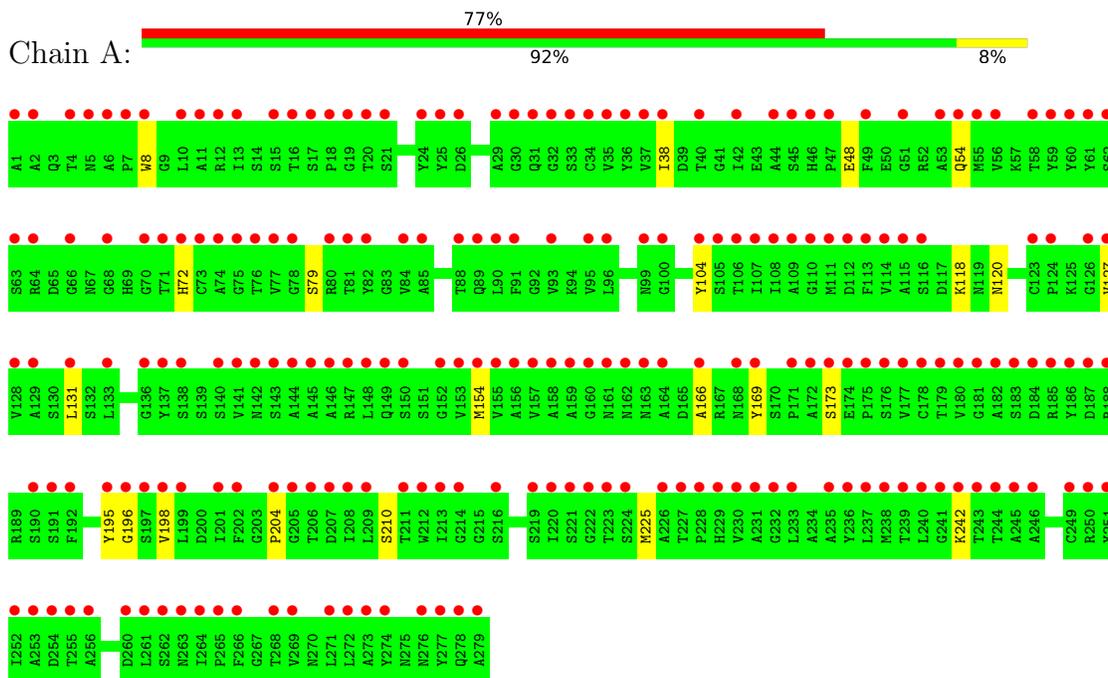
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	185	Total 185	O 185	0	0

### 3 Residue-property plots

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: Proteinase K



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.08Å 68.08Å 102.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 1.11 48.14 – 1.11	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.14-1.11) 97.3 (48.14-1.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.96 (at 1.11Å)	Xtrriage
Refinement program	PHENIX 1.19.1	Depositor
R, $R_{free}$	0.285 , 0.287 0.281 , 0.284	Depositor DCC
$R_{free}$ test set	4417 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.4	Xtrriage
Anisotropy	0.124	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	2213	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% 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: 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	0.31	0/2062	0.61	0/2804

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 [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	2023	0	1900	14	0
2	A	5	0	0	0	0
3	A	185	0	0	9	2
All	All	2213	0	1900	14	2

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 (14) 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:166:ALA:O	3:A:1101:HOH:O	1.86	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:TYR:HB2	3:A:1101:HOH:O	1.70	0.89
1:A:195:TYR:O	3:A:1102:HOH:O	1.98	0.82
1:A:127:VAL:HG21	3:A:1249:HOH:O	1.88	0.74
1:A:120:ASN:ND2	3:A:1104:HOH:O	2.28	0.66
1:A:118:LYS:HB2	3:A:1249:HOH:O	1.97	0.64
1:A:196:GLY:HA3	3:A:1102:HOH:O	2.06	0.56
1:A:242[A]:LYS:NZ	3:A:1105:HOH:O	2.34	0.50
1:A:173:SER:HA	1:A:198:VAL:HG21	1.96	0.47
1:A:38:ILE:HD12	1:A:131[A]:LEU:HD11	1.98	0.45
1:A:127:VAL:CG2	3:A:1249:HOH:O	2.55	0.42
1:A:48:GLU:HB3	1:A:79:SER:HB2	2.01	0.42
1:A:8:TRP:CH2	1:A:204:PRO:HB3	2.56	0.41
1:A:72:HIS:CD2	1:A:210:SER:HB3	2.55	0.41

All (2) 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)
3:A:1105:HOH:O	3:A:1226:HOH:O[3_644]	1.85	0.35
3:A:1118:HOH:O	3:A:1196:HOH:O[5_655]	2.13	0.07

## 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	277/279 (99%)	269 (97%)	8 (3%)	0	<a href="#">100</a> <a href="#">100</a>

There are no Ramachandran outliers to report.

### 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	210/213 (99%)	206 (98%)	4 (2%)	57 17

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54[A]	GLN
1	A	104	TYR
1	A	154[A]	MET
1	A	225	MET

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

### 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](#)

1 ligand 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	SO4	A	1001	-	4,4,4	0.19	0	6,6,6	0.22	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 [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	279/279 (100%)	2.87	216 (77%) <b>0</b> <b>0</b>	7, 9, 13, 20	11 (3%)

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	TRP	6.1
1	A	35	VAL	6.1
1	A	128	VAL	5.8
1	A	37	VAL	5.7
1	A	239	THR	5.6
1	A	144	ALA	5.5
1	A	11	ALA	5.5
1	A	279	ALA	5.5
1	A	109	ALA	5.3
1	A	233	LEU	5.2
1	A	220	ILE	5.1
1	A	77	VAL	5.1
1	A	114	VAL	5.0
1	A	164	ALA	4.9
1	A	202	PHE	4.9
1	A	2	ALA	4.8
1	A	73	CYS	4.8
1	A	195	TYR	4.8
1	A	228	PRO	4.6
1	A	261	LEU	4.5
1	A	105	SER	4.5
1	A	157	VAL	4.5
1	A	231	ALA	4.5
1	A	237	LEU	4.4
1	A	131[A]	LEU	4.4
1	A	38	ILE	4.4
1	A	222	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	93	VAL	4.3
1	A	269	VAL	4.3
1	A	249	CYS	4.3
1	A	90	LEU	4.3
1	A	141	VAL	4.3
1	A	18	PRO	4.3
1	A	162	ASN	4.3
1	A	196	GLY	4.2
1	A	56	VAL	4.2
1	A	137	TYR	4.2
1	A	70	GLY	4.2
1	A	198	VAL	4.2
1	A	201	ILE	4.2
1	A	155	VAL	4.1
1	A	8	TRP	4.1
1	A	54[A]	GLN	4.1
1	A	127	VAL	4.0
1	A	230	VAL	4.0
1	A	113	PHE	4.0
1	A	266	PHE	4.0
1	A	16	THR	4.0
1	A	107	ILE	4.0
1	A	59	TYR	4.0
1	A	277	TYR	4.0
1	A	148	LEU	4.0
1	A	235	ALA	4.0
1	A	274	TYR	3.9
1	A	240	LEU	3.9
1	A	232	GLY	3.9
1	A	10	LEU	3.9
1	A	104	TYR	3.9
1	A	182	ALA	3.9
1	A	245	ALA	3.8
1	A	13[A]	ILE	3.8
1	A	256	ALA	3.8
1	A	49	PHE	3.8
1	A	160	GLY	3.8
1	A	108	ILE	3.8
1	A	213	ILE	3.8
1	A	74	ALA	3.8
1	A	197	SER	3.7
1	A	123	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	21	SER	3.7
1	A	236	TYR	3.7
1	A	227	THR	3.7
1	A	244	THR	3.7
1	A	96	LEU	3.7
1	A	76	THR	3.6
1	A	126	GLY	3.6
1	A	175	PRO	3.6
1	A	64	ARG	3.6
1	A	192	PHE	3.6
1	A	211	THR	3.6
1	A	251	TYR	3.6
1	A	204	PRO	3.6
1	A	110	GLY	3.6
1	A	24	TYR	3.6
1	A	36	TYR	3.6
1	A	95	VAL	3.6
1	A	106	THR	3.5
1	A	246	ALA	3.5
1	A	199	LEU	3.5
1	A	25	TYR	3.5
1	A	216[A]	SER	3.4
1	A	82	TYR	3.4
1	A	252	ILE	3.4
1	A	58	THR	3.4
1	A	84	VAL	3.4
1	A	133	LEU	3.4
1	A	71	THR	3.3
1	A	99	ASN	3.3
1	A	145	ALA	3.3
1	A	271	LEU	3.3
1	A	150	SER	3.3
1	A	163	ASN	3.2
1	A	272	LEU	3.2
1	A	75	GLY	3.2
1	A	186	TYR	3.1
1	A	243	THR	3.1
1	A	169	TYR	3.1
1	A	26	ASP	3.1
1	A	88	THR	3.0
1	A	278	GLN	3.0
1	A	112	ASP	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	159	ALA	2.9
1	A	42	ILE	2.9
1	A	153	VAL	2.9
1	A	209	LEU	2.9
1	A	143[A]	SER	2.9
1	A	224	SER	2.9
1	A	31[A]	GLN	2.9
1	A	34[A]	CYS	2.9
1	A	208	ILE	2.9
1	A	91[A]	PHE	2.9
1	A	176	SER	2.8
1	A	89	GLN	2.8
1	A	260	ASP	2.8
1	A	221	SER	2.8
1	A	19	GLY	2.8
1	A	172	ALA	2.8
1	A	205	GLY	2.8
1	A	179	THR	2.7
1	A	124	PRO	2.7
1	A	78	GLY	2.7
1	A	219[A]	SER	2.7
1	A	115	ALA	2.7
1	A	226	ALA	2.7
1	A	40	THR	2.7
1	A	1	ALA	2.7
1	A	273	ALA	2.7
1	A	4	THR	2.6
1	A	223	THR	2.6
1	A	147	ARG	2.6
1	A	149	GLN	2.6
1	A	142	ASN	2.5
1	A	60	TYR	2.5
1	A	206	THR	2.5
1	A	214	GLY	2.5
1	A	154[A]	MET	2.5
1	A	156	ALA	2.5
1	A	250[A]	ARG	2.5
1	A	61	TYR	2.5
1	A	100	GLY	2.5
1	A	136	GLY	2.5
1	A	263	ASN	2.5
1	A	33	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	184	ASP	2.5
1	A	20	THR	2.5
1	A	68	GLY	2.5
1	A	242[A]	LYS	2.5
1	A	187	ASP	2.5
1	A	111	MET	2.4
1	A	238[A]	MET	2.4
1	A	47	PRO	2.4
1	A	255	THR	2.4
1	A	30	GLY	2.4
1	A	32	GLY	2.4
1	A	45	SER	2.4
1	A	140[A]	SER	2.4
1	A	178	CYS	2.4
1	A	81	THR	2.4
1	A	276	ASN	2.4
1	A	264	ILE	2.4
1	A	181	GLY	2.4
1	A	6	ALA	2.3
1	A	183	SER	2.3
1	A	152	GLY	2.3
1	A	207	ASP	2.3
1	A	44	ALA	2.3
1	A	138	SER	2.3
1	A	268	THR	2.3
1	A	254	ASP	2.3
1	A	129	ALA	2.2
1	A	161[A]	ASN	2.2
1	A	191	SER	2.2
1	A	72	HIS	2.2
1	A	158	ALA	2.2
1	A	265	PRO	2.2
1	A	66	GLY	2.2
1	A	185	ARG	2.2
1	A	17	SER	2.2
1	A	85	ALA	2.2
1	A	46	HIS	2.1
1	A	29	ALA	2.1
1	A	174	GLU	2.1
1	A	188	ARG	2.1
1	A	5	ASN	2.1
1	A	177	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	62	SER	2.1
1	A	51	GLY	2.1
1	A	7	PRO	2.1
1	A	229	HIS	2.1
1	A	12	ARG	2.1
1	A	80	ARG	2.1
1	A	53	ALA	2.1
1	A	253	ALA	2.1
1	A	116	SER	2.1
1	A	173	SER	2.1
1	A	262	SER	2.1
1	A	171	PRO	2.1
1	A	190	SER	2.0
1	A	146	ALA	2.0
1	A	15	SER	2.0
1	A	63	SER	2.0
1	A	168	ASN	2.0
1	A	55	MET	2.0
1	A	241	GLY	2.0
1	A	166	ALA	2.0
1	A	180	VAL	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 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	1001	5/5	0.92	0.16	10,11,13,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.