



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:26 PM UTC

PDB ID : 3EVK / pdb\_00003evk  
Title : Crystal structure of the metal-bound superoxide dismutase from *Pyrobaculum aerophilum*  
Authors : Lee, S.  
Deposited on : 2008-10-13  
Resolution : 1.85 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)

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<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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

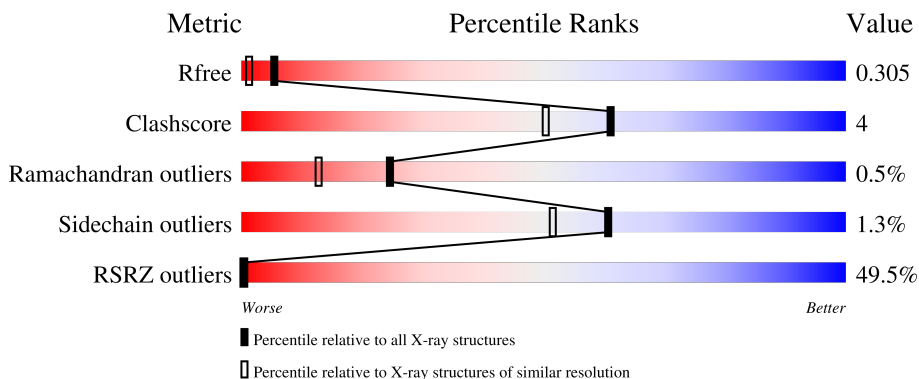
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	222	
1	B	222	
1	C	222	
1	D	222	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7037 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 Superoxide dismutase [Fe].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	211	1714	1109	298	304	3	0	0	0
1	B	211	1714	1109	298	304	3	0	0	0
1	C	211	1714	1109	298	304	3	0	0	0
1	D	211	1714	1109	298	304	3	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O93724
A	2	ARG	-	expression tag	UNP O93724
A	3	GLY	-	expression tag	UNP O93724
A	4	SER	-	expression tag	UNP O93724
A	5	HIS	-	expression tag	UNP O93724
A	6	HIS	-	expression tag	UNP O93724
A	7	HIS	-	expression tag	UNP O93724
A	8	HIS	-	expression tag	UNP O93724
A	9	HIS	-	expression tag	UNP O93724
A	10	HIS	-	expression tag	UNP O93724
A	11	GLY	-	expression tag	UNP O93724
A	12	SER	-	expression tag	UNP O93724
B	1	MET	-	initiating methionine	UNP O93724
B	2	ARG	-	expression tag	UNP O93724
B	3	GLY	-	expression tag	UNP O93724
B	4	SER	-	expression tag	UNP O93724
B	5	HIS	-	expression tag	UNP O93724
B	6	HIS	-	expression tag	UNP O93724
B	7	HIS	-	expression tag	UNP O93724
B	8	HIS	-	expression tag	UNP O93724
B	9	HIS	-	expression tag	UNP O93724

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Chain	Residue	Modelled	Actual	Comment	Reference
B	10	HIS	-	expression tag	UNP O93724
B	11	GLY	-	expression tag	UNP O93724
B	12	SER	-	expression tag	UNP O93724
C	1	MET	-	initiating methionine	UNP O93724
C	2	ARG	-	expression tag	UNP O93724
C	3	GLY	-	expression tag	UNP O93724
C	4	SER	-	expression tag	UNP O93724
C	5	HIS	-	expression tag	UNP O93724
C	6	HIS	-	expression tag	UNP O93724
C	7	HIS	-	expression tag	UNP O93724
C	8	HIS	-	expression tag	UNP O93724
C	9	HIS	-	expression tag	UNP O93724
C	10	HIS	-	expression tag	UNP O93724
C	11	GLY	-	expression tag	UNP O93724
C	12	SER	-	expression tag	UNP O93724
D	1	MET	-	initiating methionine	UNP O93724
D	2	ARG	-	expression tag	UNP O93724
D	3	GLY	-	expression tag	UNP O93724
D	4	SER	-	expression tag	UNP O93724
D	5	HIS	-	expression tag	UNP O93724
D	6	HIS	-	expression tag	UNP O93724
D	7	HIS	-	expression tag	UNP O93724
D	8	HIS	-	expression tag	UNP O93724
D	9	HIS	-	expression tag	UNP O93724
D	10	HIS	-	expression tag	UNP O93724
D	11	GLY	-	expression tag	UNP O93724
D	12	SER	-	expression tag	UNP O93724

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	60	Total O 60 60	0	0
3	B	38	Total O 38 38	0	0
3	C	60	Total O 60 60	0	0
3	D	19	Total O 19 19	0	0





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.91Å 94.91Å 171.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.54 – 1.85 41.54 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.6 (41.54-1.85) 96.6 (41.54-1.85)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.30 (at 1.86Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.202 , 0.230 (Not available) , 0.305	Depositor DCC
$R_{free}$ test set	7528 reflections (9.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7037	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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 39.19 % 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 3.2955e-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: MN

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	0.55	0/1762	0.75	0/2387
1	B	0.54	0/1762	0.79	0/2387
1	C	0.58	0/1762	0.77	0/2387
1	D	0.57	2/1762 (0.1%)	0.78	0/2387
All	All	0.56	2/7048 (0.0%)	0.78	0/9548

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	37	GLU	CD-OE2	7.74	1.40	1.25
1	D	103	GLY	C-O	5.41	1.30	1.23

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	1714	0	1688	18	0
1	B	1714	0	1688	15	0
1	C	1714	0	1688	21	0
1	D	1714	0	1688	14	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	60	0	0	0	0
3	B	38	0	0	0	0
3	C	60	0	0	1	0
3	D	19	0	0	1	0
All	All	7037	0	6752	57	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 (57) 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:C:141:TRP:HE1	1:C:161:HIS:HD2	1.22	0.86
1:D:146:TYR:OH	3:D:310:HOH:O	1.96	0.84
1:A:167:ALA:H	1:D:85:ASN:HD21	1.26	0.83
1:D:141:TRP:HE1	1:D:161:HIS:HD2	1.27	0.81
1:A:85:ASN:HD21	1:D:167:ALA:H	1.28	0.81
1:A:141:TRP:HE1	1:A:161:HIS:HD2	1.25	0.81
1:B:141:TRP:HE1	1:B:161:HIS:HD2	1.28	0.78
1:B:167:ALA:H	1:C:85:ASN:HD21	1.28	0.78
1:B:85:ASN:HD21	1:C:167:ALA:H	1.33	0.75
1:C:56:ALA:O	1:C:59:GLU:HG3	1.85	0.74
1:C:110:LYS:HG3	1:C:211:GLN:NE2	2.07	0.69
1:C:110:LYS:HG3	1:C:211:GLN:HE22	1.57	0.69
1:D:212:LYS:HD2	1:D:222:LEU:HB3	1.75	0.68
1:A:141:TRP:HE1	1:A:161:HIS:CD2	2.15	0.61
1:B:167:ALA:H	1:C:85:ASN:ND2	1.99	0.60
1:A:85:ASN:ND2	1:D:167:ALA:H	1.99	0.60
1:C:13:VAL:HB	1:C:66:LYS:HE3	1.83	0.59
1:A:167:ALA:H	1:D:85:ASN:ND2	1.97	0.59
1:C:141:TRP:HE1	1:C:161:HIS:CD2	2.13	0.56
1:B:85:ASN:ND2	1:C:167:ALA:H	2.02	0.56
1:C:222:LEU:HA	3:C:347:HOH:O	2.06	0.56
1:C:40:GLN:HE21	1:C:44:GLN:HE22	1.53	0.55
1:A:40:GLN:HE21	1:A:44:GLN:HE22	1.55	0.55
1:C:50:TYR:CZ	1:C:161:HIS:HE1	2.27	0.53
1:D:50:TYR:CZ	1:D:161:HIS:HE1	2.26	0.53
1:C:29:ALA:HB1	1:C:99:PRO:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:GLU:HG2	1:D:66:LYS:HE3	1.91	0.52
1:D:38:ILE:O	1:D:42:HIS:HB2	2.10	0.51
1:A:50:TYR:CZ	1:A:161:HIS:HE1	2.28	0.51
1:B:50:TYR:CZ	1:B:161:HIS:HE1	2.28	0.51
1:C:50:TYR:CZ	1:C:161:HIS:CE1	3.02	0.48
1:A:163:LEU:O	1:A:164:MET:HB2	2.13	0.48
1:A:16:LYS:H	1:D:152:GLN:NE2	2.12	0.47
1:A:202:ASN:HD21	1:A:204:ASP:HB2	1.79	0.47
1:A:13:VAL:HB	1:A:66:LYS:HE3	1.97	0.47
1:B:104:GLY:HA2	1:B:201:VAL:O	2.15	0.47
1:C:114:LEU:HD12	1:C:118:PHE:HE2	1.79	0.47
1:D:50:TYR:CZ	1:D:161:HIS:CE1	3.04	0.46
1:B:163:LEU:O	1:B:164:MET:HB2	2.16	0.45
1:A:50:TYR:HA	1:A:83:HIS:HD2	1.81	0.45
1:A:167:ALA:O	1:A:168:ASP:HB2	2.15	0.45
1:B:202:ASN:HD21	1:B:204:ASP:HB2	1.81	0.45
1:B:141:TRP:HB2	1:B:158:ILE:HB	1.98	0.45
1:B:146:TYR:CD2	1:B:213:ALA:HB1	2.52	0.44
1:A:18:TYR:HE2	1:A:58:LEU:HD11	1.82	0.43
1:C:167:ALA:O	1:C:168:ASP:HB2	2.18	0.43
1:B:120:GLY:HA2	1:C:12:SER:O	2.19	0.43
1:B:50:TYR:CZ	1:B:161:HIS:CE1	3.07	0.43
1:D:212:LYS:HA	1:D:217:GLN:HE21	1.83	0.43
1:A:15:THR:OG1	1:A:62:GLU:OE2	2.35	0.42
1:C:141:TRP:NE1	1:C:161:HIS:HD2	2.04	0.42
1:B:167:ALA:O	1:B:168:ASP:HB2	2.19	0.42
1:A:50:TYR:CZ	1:A:161:HIS:CE1	3.08	0.41
1:C:163:LEU:O	1:C:164:MET:HB2	2.20	0.41
1:D:141:TRP:HE1	1:D:161:HIS:CD2	2.19	0.41
1:B:50:TYR:HA	1:B:83:HIS:HD2	1.86	0.40
1:A:179:GLU:HB2	1:C:179:GLU:HB2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	209/222 (94%)	202 (97%)	6 (3%)	1 (0%)	24	13
1	B	209/222 (94%)	200 (96%)	7 (3%)	2 (1%)	12	4
1	C	209/222 (94%)	199 (95%)	9 (4%)	1 (0%)	24	13
1	D	209/222 (94%)	200 (96%)	9 (4%)	0	100	100
All	All	836/888 (94%)	801 (96%)	31 (4%)	4 (0%)	24	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	MET
1	B	164	MET
1	B	104	GLY
1	C	164	MET

### 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	176/185 (95%)	174 (99%)	2 (1%)	65	57
1	B	176/185 (95%)	175 (99%)	1 (1%)	78	73
1	C	176/185 (95%)	172 (98%)	4 (2%)	44	30
1	D	176/185 (95%)	174 (99%)	2 (1%)	65	57
All	All	704/740 (95%)	695 (99%)	9 (1%)	61	51

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	114	LEU
1	B	96	ASN
1	C	59	GLU

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Mol	Chain	Res	Type
1	C	96	ASN
1	C	220	LEU
1	C	222	LEU
1	D	96	ASN
1	D	127	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	83	HIS
1	A	85	ASN
1	A	131	GLN
1	A	161	HIS
1	A	185	GLN
1	A	199	ASN
1	A	202	ASN
1	B	48	GLN
1	B	83	HIS
1	B	85	ASN
1	B	131	GLN
1	B	161	HIS
1	B	196	ASN
1	B	199	ASN
1	B	202	ASN
1	C	40	GLN
1	C	83	HIS
1	C	85	ASN
1	C	161	HIS
1	C	199	ASN
1	C	202	ASN
1	C	211	GLN
1	D	40	GLN
1	D	83	HIS
1	D	85	ASN
1	D	152	GLN
1	D	161	HIS
1	D	199	ASN
1	D	202	ASN
1	D	211	GLN
1	D	217	GLN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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	211/222 (95%)	1.10	28 (13%) <b>7</b> <b>6</b>	26, 29, 41, 44	0
1	B	211/222 (95%)	2.94	172 (81%) <b>0</b> <b>0</b>	24, 30, 39, 44	0
1	C	211/222 (95%)	1.09	26 (12%) <b>8</b> <b>8</b>	25, 29, 40, 45	0
1	D	211/222 (95%)	3.61	192 (90%) <b>0</b> <b>0</b>	25, 30, 38, 45	0
All	All	844/888 (95%)	2.18	418 (49%) <b>0</b> <b>0</b>	24, 30, 39, 45	0

All (418) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	222	LEU	7.9
1	D	32	PRO	7.5
1	B	192	SER	7.0
1	D	103	GLY	7.0
1	D	77	LEU	6.8
1	D	12	SER	6.8
1	D	26	ALA	6.6
1	C	222	LEU	6.6
1	B	222	LEU	6.5
1	D	23	LEU	6.3
1	D	14	THR	6.3
1	D	204	ASP	6.1
1	D	167	ALA	6.1
1	B	44	GLN	6.1
1	B	103	GLY	6.0
1	D	98	ALA	6.0
1	D	73	ILE	6.0
1	D	108	GLY	5.9
1	D	168	ASP	5.9
1	D	104	GLY	5.8
1	B	167	ALA	5.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	56	ALA	5.8
1	D	31	GLU	5.7
1	D	75	ALA	5.7
1	B	32	PRO	5.7
1	D	203	TRP	5.5
1	D	58	LEU	5.5
1	D	149	LEU	5.4
1	B	28	ASN	5.4
1	B	183	TYR	5.4
1	D	163	LEU	5.4
1	D	24	PRO	5.4
1	D	15	THR	5.4
1	C	13	VAL	5.3
1	D	33	TYR	5.3
1	D	166	ALA	5.3
1	B	149	LEU	5.3
1	D	54	ALA	5.3
1	B	102	LYS	5.2
1	D	123	GLU	5.2
1	D	13	VAL	5.2
1	B	13	VAL	5.2
1	D	218	ILE	5.1
1	D	192	SER	5.1
1	D	100	PRO	5.1
1	D	219	ALA	5.0
1	B	36	ALA	5.0
1	D	82	PHE	5.0
1	D	105	GLY	5.0
1	D	216	GLY	4.9
1	B	73	ILE	4.9
1	B	12	SER	4.9
1	D	25	TYR	4.9
1	D	220	LEU	4.8
1	B	104	GLY	4.8
1	D	51	VAL	4.7
1	D	118	PHE	4.7
1	B	27	TYR	4.7
1	B	139	VAL	4.7
1	B	184	LEU	4.7
1	D	154	LEU	4.6
1	D	67	GLY	4.6
1	D	34	ILE	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	163	LEU	4.6
1	B	166	ALA	4.6
1	D	107	PRO	4.6
1	D	162	ASN	4.5
1	B	191	GLY	4.4
1	D	146	TYR	4.4
1	B	71	ILE	4.4
1	D	119	PHE	4.4
1	B	154	LEU	4.4
1	D	164	MET	4.4
1	D	201	VAL	4.4
1	D	20	LEU	4.3
1	D	196	ASN	4.3
1	D	40	GLN	4.3
1	B	41	LEU	4.3
1	D	41	LEU	4.3
1	B	158	ILE	4.3
1	B	20	LEU	4.3
1	D	88	ILE	4.3
1	D	60	LYS	4.2
1	B	169	ALA	4.2
1	B	216	GLY	4.2
1	B	15	THR	4.2
1	D	145	VAL	4.2
1	D	111	ILE	4.2
1	B	178	TRP	4.2
1	D	115	ILE	4.2
1	D	169	ALA	4.1
1	B	74	ARG	4.1
1	D	80	LEU	4.1
1	D	101	GLY	4.1
1	D	221	LYS	4.1
1	B	181	ALA	4.1
1	D	57	ALA	4.1
1	B	33	TYR	4.1
1	D	95	PRO	4.1
1	D	214	LEU	4.1
1	D	71	ILE	4.0
1	B	182	TYR	4.0
1	D	191	GLY	4.0
1	B	141	TRP	4.0
1	D	213	ALA	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	18	TYR	4.0
1	D	61	LEU	4.0
1	B	29	ALA	4.0
1	D	28	ASN	4.0
1	D	126	LYS	3.9
1	B	14	THR	3.9
1	D	49	GLY	3.9
1	D	27	TYR	3.9
1	A	220	LEU	3.9
1	D	35	SER	3.9
1	D	112	ALA	3.9
1	B	25	TYR	3.8
1	B	186	TYR	3.8
1	B	198	TRP	3.8
1	D	198	TRP	3.8
1	D	63	LYS	3.8
1	B	23	LEU	3.8
1	B	69	ALA	3.8
1	B	145	VAL	3.8
1	B	150	GLU	3.8
1	D	64	PHE	3.8
1	D	189	ASP	3.8
1	D	44	GLN	3.8
1	D	188	ASN	3.8
1	A	13	VAL	3.8
1	D	148	PRO	3.7
1	D	171	VAL	3.7
1	D	86	GLY	3.7
1	B	153	LEU	3.7
1	D	17	ARG	3.7
1	B	115	ILE	3.7
1	B	24	PRO	3.7
1	B	179	GLU	3.7
1	D	109	GLY	3.7
1	D	21	PRO	3.7
1	C	12	SER	3.6
1	B	146	TYR	3.6
1	D	66	LYS	3.6
1	D	110	LYS	3.6
1	B	119	PHE	3.6
1	D	153	LEU	3.6
1	B	168	ASP	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	177	VAL	3.6
1	D	122	PHE	3.6
1	D	69	ALA	3.6
1	B	58	LEU	3.6
1	D	197	TRP	3.5
1	D	165	HIS	3.5
1	A	12	SER	3.5
1	B	34	ILE	3.5
1	D	158	ILE	3.5
1	D	76	VAL	3.5
1	D	215	ASN	3.5
1	B	77	LEU	3.5
1	B	124	LYS	3.5
1	D	55	ASN	3.5
1	D	207	GLU	3.5
1	B	64	PHE	3.5
1	B	75	ALA	3.5
1	B	213	ALA	3.5
1	D	84	LEU	3.5
1	D	172	LEU	3.5
1	D	182	TYR	3.5
1	B	40	GLN	3.5
1	B	136	VAL	3.5
1	B	30	LEU	3.5
1	B	66	LYS	3.5
1	D	185	GLN	3.4
1	B	164	MET	3.4
1	D	94	TRP	3.4
1	D	136	VAL	3.4
1	D	200	VAL	3.4
1	D	206	VAL	3.4
1	B	140	GLY	3.4
1	D	79	ASP	3.4
1	D	195	ASP	3.4
1	D	29	ALA	3.4
1	C	71	ILE	3.4
1	B	57	ALA	3.4
1	B	112	ALA	3.4
1	D	65	ARG	3.4
1	D	50	TYR	3.3
1	D	199	ASN	3.3
1	D	74	ARG	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	39	MET	3.3
1	B	42	HIS	3.3
1	C	70	GLN	3.3
1	B	101	GLY	3.3
1	D	59	GLU	3.3
1	D	70	GLN	3.3
1	A	14	THR	3.3
1	C	15	THR	3.3
1	D	19	THR	3.3
1	B	118	PHE	3.3
1	A	120	GLY	3.3
1	B	162	ASN	3.3
1	D	217	GLN	3.2
1	D	194	VAL	3.2
1	B	61	LEU	3.2
1	B	214	LEU	3.2
1	D	125	PHE	3.2
1	D	22	PRO	3.2
1	B	187	LYS	3.2
1	D	140	GLY	3.2
1	D	157	GLN	3.2
1	D	78	ARG	3.2
1	A	71	ILE	3.1
1	B	143	ILE	3.1
1	B	35	SER	3.1
1	D	89	LEU	3.1
1	D	114	LEU	3.1
1	D	210	LEU	3.1
1	B	137	GLU	3.1
1	B	135	ASN	3.1
1	D	52	ASN	3.1
1	A	75	ALA	3.1
1	D	36	ALA	3.1
1	B	218	ILE	3.1
1	D	143	ILE	3.1
1	D	155	ILE	3.1
1	D	186	TYR	3.1
1	B	156	LEU	3.1
1	C	69	ALA	3.1
1	D	99	PRO	3.1
1	B	111	ILE	3.1
1	D	156	LEU	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	193	TYR	3.1
1	B	67	GLY	3.1
1	B	157	GLN	3.0
1	B	78	ARG	3.0
1	B	165	HIS	3.0
1	D	72	ASP	3.0
1	D	43	HIS	3.0
1	B	45	LYS	3.0
1	C	221	LYS	3.0
1	D	92	ILE	3.0
1	D	127	GLU	3.0
1	D	184	LEU	3.0
1	D	113	ASP	3.0
1	B	199	ASN	3.0
1	D	147	GLU	3.0
1	B	38	ILE	3.0
1	D	81	SER	2.9
1	D	102	LYS	2.9
1	D	142	ALA	2.9
1	B	155	ILE	2.9
1	D	30	LEU	2.9
1	B	190	ARG	2.9
1	B	125	PHE	2.9
1	A	69	ALA	2.9
1	D	16	LYS	2.9
1	D	121	SER	2.9
1	D	93	PHE	2.9
1	B	26	ALA	2.9
1	D	45	LYS	2.9
1	B	72	ASP	2.9
1	B	159	GLU	2.9
1	B	210	LEU	2.9
1	B	138	GLY	2.9
1	B	215	ASN	2.8
1	B	114	LEU	2.8
1	C	114	LEU	2.8
1	D	53	GLY	2.8
1	D	106	LYS	2.8
1	B	197	TRP	2.8
1	C	67	GLY	2.8
1	D	117	LYS	2.8
1	D	120	GLY	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	123	GLU	2.8
1	B	80	LEU	2.8
1	B	99	PRO	2.8
1	D	97	MET	2.8
1	B	188	ASN	2.7
1	B	59	GLU	2.7
1	B	144	LEU	2.7
1	D	173	LEU	2.7
1	B	113	ASP	2.7
1	B	70	GLN	2.7
1	D	96	ASN	2.7
1	D	202	ASN	2.7
1	B	82	PHE	2.7
1	D	91	SER	2.7
1	D	116	ASN	2.7
1	B	63	LYS	2.7
1	D	187	LYS	2.7
1	D	47	HIS	2.7
1	B	81	SER	2.7
1	B	76	VAL	2.7
1	B	86	GLY	2.6
1	B	122	PHE	2.6
1	D	129	PHE	2.6
1	D	130	SER	2.6
1	B	105	GLY	2.6
1	B	17	ARG	2.6
1	B	142	ALA	2.6
1	B	21	PRO	2.6
1	D	161	HIS	2.6
1	D	208	ARG	2.6
1	C	120	GLY	2.6
1	C	14	THR	2.6
1	D	42	HIS	2.6
1	C	220	LEU	2.6
1	B	31	GLU	2.6
1	D	212	LYS	2.6
1	B	51	VAL	2.6
1	B	18	TYR	2.5
1	B	50	TYR	2.5
1	B	107	PRO	2.5
1	B	152	GLN	2.5
1	B	193	TYR	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	108	GLY	2.5
1	B	130	SER	2.5
1	D	150	GLU	2.5
1	D	176	ASP	2.5
1	A	222	LEU	2.5
1	D	83	HIS	2.5
1	B	68	GLU	2.5
1	B	39	MET	2.5
1	D	178	TRP	2.5
1	B	133	ALA	2.5
1	A	139	VAL	2.5
1	D	177	VAL	2.5
1	D	183	TYR	2.4
1	B	93	PHE	2.4
1	B	129	PHE	2.4
1	B	180	HIS	2.4
1	D	46	HIS	2.4
1	D	38	ILE	2.4
1	A	66	LYS	2.4
1	B	171	VAL	2.4
1	B	47	HIS	2.4
1	B	176	ASP	2.4
1	C	219	ALA	2.4
1	D	209	ARG	2.4
1	B	46	HIS	2.4
1	B	49	GLY	2.4
1	B	90	HIS	2.4
1	A	221	LYS	2.4
1	B	204	ASP	2.4
1	A	76	VAL	2.4
1	B	203	TRP	2.4
1	A	113	ASP	2.3
1	B	48	GLN	2.3
1	B	116	ASN	2.3
1	B	100	PRO	2.3
1	A	110	LYS	2.3
1	C	66	LYS	2.3
1	D	138	GLY	2.3
1	B	194	VAL	2.3
1	C	139	VAL	2.3
1	D	37	GLU	2.3
1	D	68	GLU	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	220	LEU	2.3
1	D	141	TRP	2.3
1	B	52	ASN	2.3
1	A	27	TYR	2.3
1	B	120	GLY	2.3
1	B	147	GLU	2.3
1	C	102	LYS	2.3
1	A	92	ILE	2.2
1	D	85	ASN	2.2
1	B	60	LYS	2.2
1	B	208	ARG	2.2
1	B	84	LEU	2.2
1	B	170	GLN	2.2
1	B	217	GLN	2.2
1	B	98	ALA	2.2
1	D	90	HIS	2.2
1	D	139	VAL	2.2
1	D	151	GLU	2.2
1	B	131	GLN	2.2
1	D	211	GLN	2.2
1	B	79	ASP	2.2
1	B	148	PRO	2.2
1	B	56	ALA	2.2
1	C	29	ALA	2.2
1	C	33	TYR	2.2
1	B	55	ASN	2.2
1	B	126	LYS	2.2
1	B	200	VAL	2.2
1	A	102	LYS	2.2
1	B	189	ASP	2.1
1	C	204	ASP	2.1
1	A	208	ARG	2.1
1	B	16	LYS	2.1
1	C	127	GLU	2.1
1	B	54	ALA	2.1
1	B	85	ASN	2.1
1	A	73	ILE	2.1
1	A	182	TYR	2.1
1	C	27	TYR	2.1
1	B	94	TRP	2.1
1	B	201	VAL	2.1
1	B	221	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	135	ASN	2.1
1	C	57	ALA	2.1
1	D	152	GLN	2.1
1	C	118	PHE	2.1
1	B	195	ASP	2.1
1	A	109	GLY	2.1
1	B	43	HIS	2.1
1	B	83	HIS	2.1
1	D	180	HIS	2.1
1	C	100	PRO	2.1
1	D	48	GLN	2.1
1	B	132	ALA	2.1
1	A	204	ASP	2.1
1	A	64	PHE	2.0
1	A	103	GLY	2.0
1	A	108	GLY	2.0
1	A	57	ALA	2.0
1	B	65	ARG	2.0
1	C	56	ALA	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 oligosaccharides 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
2	MN	D	301	1/1	0.91	0.29	47,47,47,47	0
2	MN	B	301	1/1	0.92	0.33	48,48,48,48	0
2	MN	C	301	1/1	0.96	0.34	35,35,35,35	0
2	MN	A	301	1/1	0.99	0.31	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.