



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:28 PM GMT

PDB ID : 3EVK
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

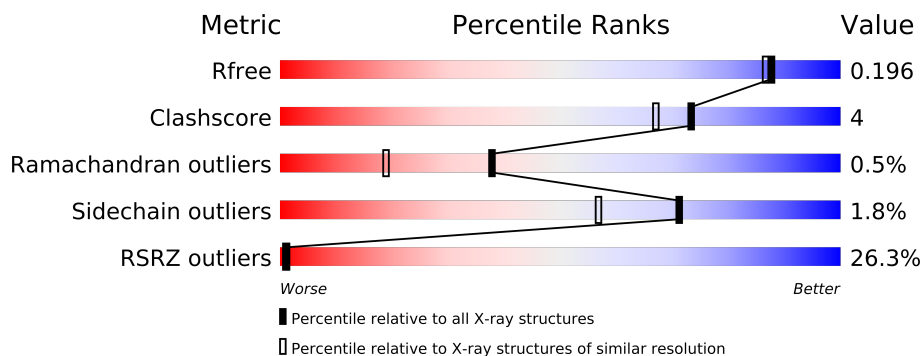
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	222	
1	B	222	
1	C	222	
1	D	222	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7037 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	211	Total	C	N	O	S	0	0	0
			1714	1109	298	304	3			
1	B	211	Total	C	N	O	S	0	0	0
			1714	1109	298	304	3			
1	C	211	Total	C	N	O	S	0	0	0
			1714	1109	298	304	3			
1	D	211	Total	C	N	O	S	0	0	0
			1714	1109	298	304	3			

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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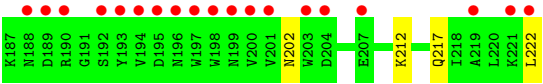
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	HIS	-	EXPRESSION TAG	UNP 093724
B	11	GLY	-	EXPRESSION TAG	UNP 093724
B	12	SER	-	EXPRESSION TAG	UNP 093724
C	1	MET	-	INITIATING METHIONINE	UNP 093724
C	2	ARG	-	EXPRESSION TAG	UNP 093724
C	3	GLY	-	EXPRESSION TAG	UNP 093724
C	4	SER	-	EXPRESSION TAG	UNP 093724
C	5	HIS	-	EXPRESSION TAG	UNP 093724
C	6	HIS	-	EXPRESSION TAG	UNP 093724
C	7	HIS	-	EXPRESSION TAG	UNP 093724
C	8	HIS	-	EXPRESSION TAG	UNP 093724
C	9	HIS	-	EXPRESSION TAG	UNP 093724
C	10	HIS	-	EXPRESSION TAG	UNP 093724
C	11	GLY	-	EXPRESSION TAG	UNP 093724
C	12	SER	-	EXPRESSION TAG	UNP 093724
D	1	MET	-	INITIATING METHIONINE	UNP 093724
D	2	ARG	-	EXPRESSION TAG	UNP 093724
D	3	GLY	-	EXPRESSION TAG	UNP 093724
D	4	SER	-	EXPRESSION TAG	UNP 093724
D	5	HIS	-	EXPRESSION TAG	UNP 093724
D	6	HIS	-	EXPRESSION TAG	UNP 093724
D	7	HIS	-	EXPRESSION TAG	UNP 093724
D	8	HIS	-	EXPRESSION TAG	UNP 093724
D	9	HIS	-	EXPRESSION TAG	UNP 093724
D	10	HIS	-	EXPRESSION TAG	UNP 093724
D	11	GLY	-	EXPRESSION TAG	UNP 093724
D	12	SER	-	EXPRESSION TAG	UNP 093724

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is water.

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.230 0.202 , 0.196	Depositor DCC
R_{free} test set	7524 reflections (10.10%)	DCC
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 32.3	EDS
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 74509 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7037	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.47	0/1762	0.53	0/2387
1	B	0.44	0/1762	0.52	0/2387
1	C	0.48	0/1762	0.54	0/2387
1	D	0.53	1/1762 (0.1%)	0.53	0/2387
All	All	0.48	1/7048 (0.0%)	0.53	0/9548

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	37	GLU	CD-OE2	13.09	1.40	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (57) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:D:62:GLU:HG2	1:D:66:LYS:HE3	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:A:13:VAL:HB	1:A:66:LYS:HE3	1.97	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:C:167:ALA:O	1:C:168:ASP:HB2	2.18	0.43
1:A:18:TYR:HE2	1:A:58:LEU:HD11	1.82	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%)	38	19
1	B	209/222 (94%)	200 (96%)	7 (3%)	2 (1%)	22	7
1	C	209/222 (94%)	199 (95%)	9 (4%)	1 (0%)	38	19
1	D	209/222 (94%)	200 (96%)	9 (4%)	0	100	100
All	All	836/888 (94%)	801 (96%)	31 (4%)	4 (0%)	38	19

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 ⓘ

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%)	173 (98%)	3 (2%)	73	59
1	B	176/185 (95%)	173 (98%)	3 (2%)	73	59
1	C	176/185 (95%)	171 (97%)	5 (3%)	56	37
1	D	176/185 (95%)	174 (99%)	2 (1%)	84	77
All	All	704/740 (95%)	691 (98%)	13 (2%)	71	57

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	114	LEU
1	A	202	ASN
1	B	96	ASN
1	B	147	GLU
1	B	202	ASN
1	C	59	GLU
1	C	96	ASN

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Mol	Chain	Res	Type
1	C	202	ASN
1	C	220	LEU
1	C	222	LEU
1	D	96	ASN
1	D	202	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	83	HIS
1	A	85	ASN
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	161	HIS
1	B	202	ASN
1	B	211	GLN
1	C	44	GLN
1	C	83	HIS
1	C	85	ASN
1	C	161	HIS
1	C	202	ASN
1	C	211	GLN
1	C	215	ASN
1	D	40	GLN
1	D	83	HIS
1	D	85	ASN
1	D	152	GLN
1	D	161	HIS
1	D	202	ASN
1	D	211	GLN
1	D	217	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

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, 95th 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 ²)	Q<0.9
1	A	211/222 (95%)	1.17	41 (19%) 2 1	26, 29, 41, 44	0
1	B	211/222 (95%)	1.43	48 (22%) 1 1	24, 30, 39, 44	0
1	C	211/222 (95%)	1.19	43 (20%) 1 1	25, 29, 40, 45	0
1	D	211/222 (95%)	2.09	91 (43%) 1 1	25, 30, 38, 45	0
All	All	844/888 (95%)	1.47	223 (26%) 1 1	24, 30, 39, 45	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	32	PRO	9.7
1	A	13	VAL	8.2
1	D	222	LEU	8.2
1	D	14	THR	7.0
1	D	26	ALA	6.2
1	C	222	LEU	6.1
1	D	108	GLY	6.1
1	B	13	VAL	5.9
1	D	31	GLU	5.7
1	D	119	PHE	5.7
1	D	123	GLU	5.7
1	B	102	LYS	5.6
1	B	12	SER	5.6
1	D	12	SER	5.4
1	B	69	ALA	5.4
1	C	13	VAL	5.3
1	D	24	PRO	5.3
1	D	101	GLY	5.3
1	A	12	SER	5.3
1	B	14	THR	5.3
1	D	33	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	12	SER	5.2
1	D	25	TYR	5.2
1	D	13	VAL	5.0
1	C	70	GLN	5.0
1	D	27	TYR	5.0
1	D	28	ASN	4.9
1	B	23	LEU	4.9
1	D	198	TRP	4.8
1	B	28	ASN	4.8
1	B	222	LEU	4.7
1	B	24	PRO	4.6
1	A	71	ILE	4.6
1	B	44	GLN	4.6
1	D	34	ILE	4.5
1	D	30	LEU	4.5
1	A	67	GLY	4.5
1	C	139	VAL	4.4
1	B	25	TYR	4.4
1	A	69	ALA	4.4
1	D	70	GLN	4.2
1	D	107	PRO	4.2
1	B	183	TYR	4.2
1	B	32	PRO	4.2
1	C	68	GLU	4.2
1	D	203	TRP	4.1
1	D	100	PRO	4.1
1	A	158	ILE	4.1
1	A	178	TRP	4.1
1	A	139	VAL	4.1
1	D	102	LYS	4.0
1	D	67	GLY	4.0
1	D	23	LEU	4.0
1	B	70	GLN	4.0
1	D	43	HIS	3.9
1	B	192	SER	3.9
1	D	189	ASP	3.9
1	D	196	ASN	3.9
1	B	27	TYR	3.9
1	D	41	LEU	3.9
1	B	68	GLU	3.9
1	D	204	ASP	3.9
1	C	178	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	140	GLY	3.8
1	D	201	VAL	3.8
1	D	15	THR	3.8
1	B	66	LYS	3.8
1	C	158	ILE	3.7
1	D	192	SER	3.7
1	D	98	ALA	3.7
1	D	104	GLY	3.7
1	D	40	GLN	3.6
1	C	140	GLY	3.6
1	A	68	GLU	3.6
1	D	37	GLU	3.6
1	C	141	TRP	3.6
1	D	109	GLY	3.6
1	C	142	ALA	3.6
1	D	106	LYS	3.6
1	A	141	TRP	3.5
1	C	136	VAL	3.5
1	B	67	GLY	3.5
1	D	182	TYR	3.5
1	D	120	GLY	3.4
1	B	26	ALA	3.4
1	D	126	LYS	3.4
1	C	71	ILE	3.4
1	C	66	LYS	3.4
1	D	113	ASP	3.4
1	C	163	LEU	3.4
1	A	177	VAL	3.3
1	A	65	ARG	3.3
1	D	221	LYS	3.3
1	D	44	GLN	3.3
1	A	70	GLN	3.3
1	D	183	TYR	3.3
1	B	103	GLY	3.3
1	A	182	TYR	3.2
1	B	15	THR	3.2
1	D	185	GLN	3.2
1	C	177	VAL	3.2
1	B	29	ALA	3.2
1	A	136	VAL	3.1
1	A	14	THR	3.1
1	D	68	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	63	LYS	3.1
1	B	198	TRP	3.1
1	B	30	LEU	3.1
1	C	175	LEU	3.1
1	D	35	SER	3.1
1	D	186	TYR	3.1
1	A	66	LYS	3.1
1	C	14	THR	3.1
1	D	194	VAL	3.0
1	D	103	GLY	3.0
1	D	36	ALA	3.0
1	C	15	THR	3.0
1	A	163	LEU	3.0
1	B	59	GLU	3.0
1	D	200	VAL	2.9
1	D	163	LEU	2.9
1	D	188	ASN	2.9
1	D	195	ASP	2.9
1	C	88	ILE	2.9
1	D	193	TYR	2.9
1	D	29	ALA	2.9
1	C	182	TYR	2.9
1	D	97	MET	2.9
1	C	133	ALA	2.8
1	C	82	PHE	2.8
1	B	20	LEU	2.8
1	D	199	ASN	2.8
1	A	175	LEU	2.8
1	B	163	LEU	2.8
1	C	69	ALA	2.8
1	C	120	GLY	2.8
1	B	33	TYR	2.7
1	B	71	ILE	2.7
1	D	66	LYS	2.7
1	D	130	SER	2.7
1	D	94	TRP	2.6
1	D	121	SER	2.6
1	B	158	ILE	2.6
1	A	89	LEU	2.6
1	B	41	LEU	2.6
1	A	138	GLY	2.6
1	D	111	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	183	TYR	2.6
1	D	16	LYS	2.6
1	B	64	PHE	2.5
1	A	88	ILE	2.5
1	D	158	ILE	2.5
1	D	69	ALA	2.5
1	C	160	LYS	2.5
1	D	71	ILE	2.5
1	A	181	ALA	2.5
1	C	167	ALA	2.5
1	D	127	GLU	2.5
1	A	93	PHE	2.4
1	A	142	ALA	2.4
1	B	39	MET	2.4
1	D	184	LEU	2.4
1	D	207	GLU	2.4
1	C	85	ASN	2.3
1	C	81	SER	2.3
1	D	38	ILE	2.3
1	A	220	LEU	2.3
1	B	98	ALA	2.3
1	D	99	PRO	2.3
1	C	63	LYS	2.3
1	D	178	TRP	2.3
1	A	92	ILE	2.3
1	D	63	LYS	2.3
1	D	190	ARG	2.3
1	C	93	PHE	2.3
1	B	36	ALA	2.3
1	D	197	TRP	2.3
1	A	63	LYS	2.3
1	C	161	HIS	2.3
1	D	122	PHE	2.2
1	D	136	VAL	2.2
1	B	100	PRO	2.2
1	A	132	ALA	2.2
1	C	181	ALA	2.2
1	A	161	HIS	2.2
1	C	138	GLY	2.2
1	A	64	PHE	2.2
1	A	133	ALA	2.2
1	C	174	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	64	PHE	2.2
1	D	118	PHE	2.2
1	B	31	GLU	2.2
1	B	65	ARG	2.2
1	B	21	PRO	2.2
1	D	219	ALA	2.2
1	D	52	ASN	2.2
1	D	20	LEU	2.2
1	A	143	ILE	2.1
1	A	180	HIS	2.1
1	A	183	TYR	2.1
1	A	82	PHE	2.1
1	A	123	GLU	2.1
1	B	123	GLU	2.1
1	C	156	LEU	2.1
1	B	166	ALA	2.1
1	D	115	ILE	2.1
1	C	171	VAL	2.1
1	A	16	LYS	2.1
1	B	105	GLY	2.1
1	C	50	TYR	2.1
1	C	89	LEU	2.1
1	B	164	MET	2.1
1	B	167	ALA	2.1
1	D	105	GLY	2.1
1	C	193	TYR	2.1
1	D	134	LYS	2.0
1	B	104	GLY	2.0
1	A	186	TYR	2.0
1	D	22	PRO	2.0
1	C	92	ILE	2.0
1	C	84	LEU	2.0
1	A	15	THR	2.0
1	B	40	GLN	2.0

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 carbohydrates in this entry.

6.4 Ligands

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MN	B	301	1/1	0.18	0.17	48,48,48,48	0
2	MN	D	301	1/1	0.18	0.04	47,47,47,47	0
2	MN	C	301	1/1	0.16	-1.72	35,35,35,35	0
2	MN	A	301	1/1	0.14	-2.90	33,33,33,33	0

6.5 Other polymers

There are no such residues in this entry.