Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:29 AM 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 X-ray Structure 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/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

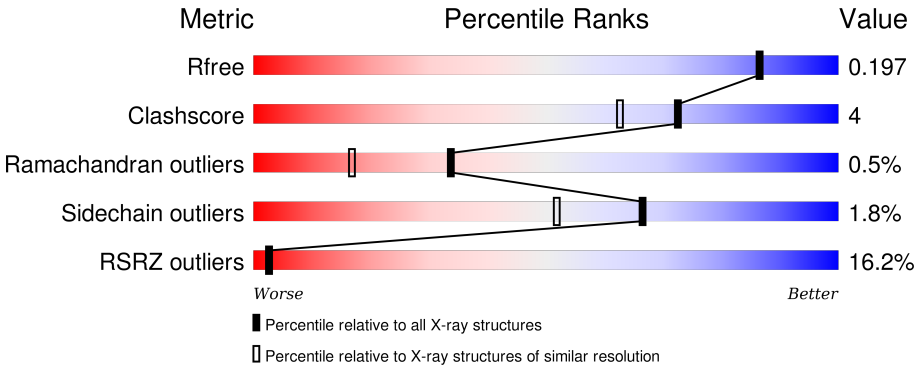
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (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. 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 <=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	9%, 85%, 9%, • 5%
1	B	222	17%, 86%, 7%, • 5%
1	C	222	8%, 83%, 10%, • 5%
1	D	222	28%, 87%, 8%, 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MN	A	301	-	-	-	X
2	MN	B	301	-	-	-	X
2	MN	C	301	-	-	-	X
2	MN	D	301	-	-	-	X

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
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 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 (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.

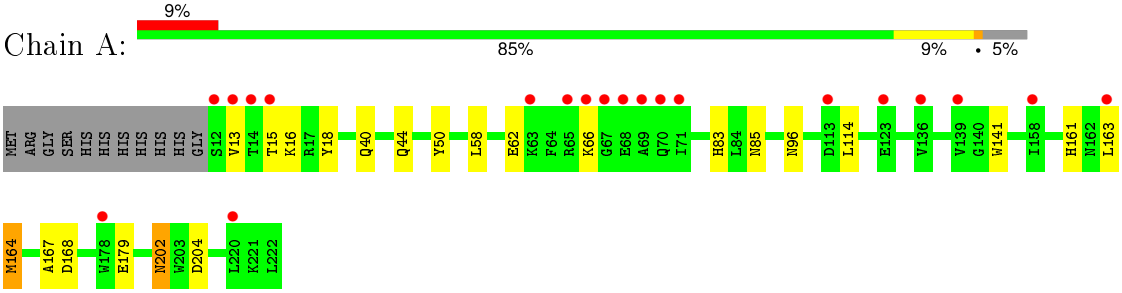
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	60	Total O 60 60	0	0
3	B	38	Total O 38 38	0	0
3	C	60	Total O 60 60	0	0
3	D	19	Total O 19 19	0	0

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.

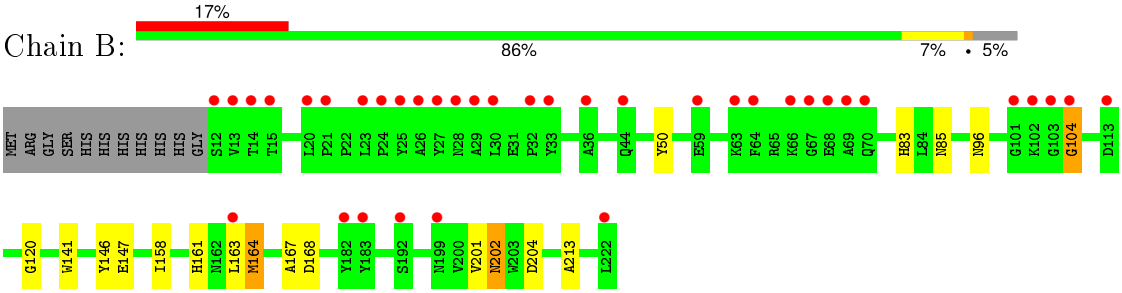
- Molecule 1: Superoxide dismutase [Fe]

Chain A:



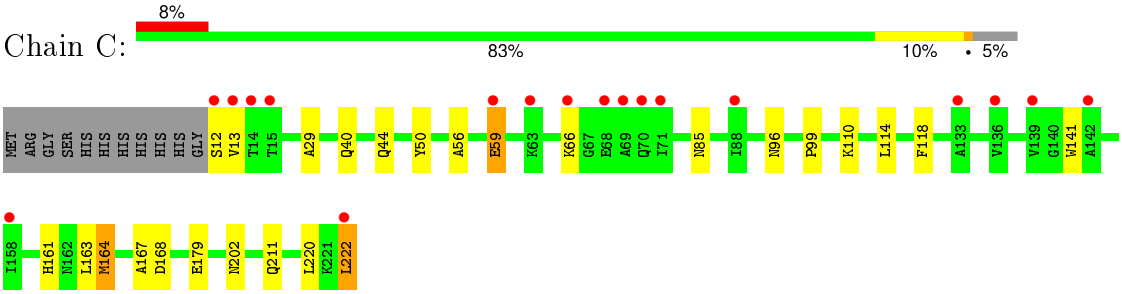
- Molecule 1: Superoxide dismutase [Fe]

Chain B:



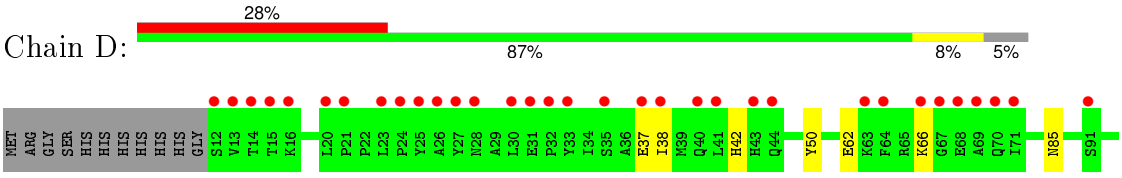
- Molecule 1: Superoxide dismutase [Fe]

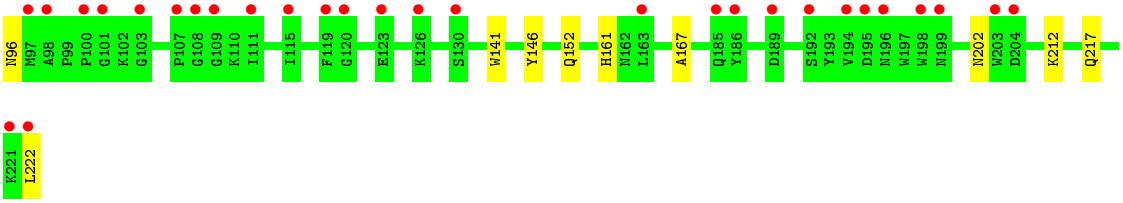
Chain C:



- Molecule 1: Superoxide dismutase [Fe]

Chain D:




N96
N97
A98
P99
P100
G101
K102
G103
P107
G108
G109
K110
I111
I115
F119
G120
E123
K126
S130
W141
Y146
Q152
H161
N162
L163
A167
Q185
Y186
D189
S192
Y193
V194
D195
N196
W197
W198
N199
N202
W203
D204
K212
Q217
K221
L222

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.30 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.230 0.205 , 0.197	Depositor DCC
R_{free} test set	7528 reflections (11.24%)	DCC
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.1	EDS
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 74509 reflections	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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 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	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
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
1:D:62:GLU:HG2	1:D:66:LYS:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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 (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	209/222 (94%)	202 (97%)	6 (3%)	1 (0%)	34 17
1	B	209/222 (94%)	200 (96%)	7 (3%)	2 (1%)	19 6
1	C	209/222 (94%)	199 (95%)	9 (4%)	1 (0%)	34 17
1	D	209/222 (94%)	200 (96%)	9 (4%)	0	100 100
All	All	836/888 (94%)	801 (96%)	31 (4%)	4 (0%)	34 17

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%)	173 (98%)	3 (2%)	68 54
1	B	176/185 (95%)	173 (98%)	3 (2%)	68 54
1	C	176/185 (95%)	171 (97%)	5 (3%)	51 33
1	D	176/185 (95%)	174 (99%)	2 (1%)	80 72
All	All	704/740 (95%)	691 (98%)	13 (2%)	66 52

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

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Mol	Chain	Res	Type
1	B	147	GLU
1	B	202	ASN
1	C	59	GLU
1	C	96	ASN
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 molecules 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.

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^{th} 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%)	0.78	20 (9%) 10 10	26, 29, 41, 44	0
1	B	211/222 (95%)	1.13	37 (17%) 2 2	24, 30, 39, 44	0
1	C	211/222 (95%)	0.81	18 (8%) 13 13	25, 29, 40, 45	0
1	D	211/222 (95%)	1.66	62 (29%) 1 0	25, 30, 38, 45	0
All	All	844/888 (95%)	1.10	137 (16%) 3 3	24, 30, 39, 45	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	108	GLY	8.8
1	C	12	SER	8.3
1	D	32	PRO	7.4
1	D	14	THR	7.3
1	D	12	SER	7.1
1	C	222	LEU	7.0
1	C	13	VAL	6.8
1	D	119	PHE	6.8
1	B	13	VAL	6.5
1	D	222	LEU	6.5
1	C	70	GLN	6.5
1	A	12	SER	6.4
1	D	26	ALA	6.4
1	A	13	VAL	5.9
1	D	70	GLN	5.9
1	D	31	GLU	5.7
1	A	69	ALA	5.6
1	D	13	VAL	5.6
1	B	12	SER	5.5
1	D	25	TYR	5.4
1	B	102	LYS	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	14	THR	5.0
1	B	222	LEU	5.0
1	D	98	ALA	5.0
1	D	123	GLU	5.0
1	B	32	PRO	4.9
1	D	196	ASN	4.6
1	B	69	ALA	4.6
1	D	67	GLY	4.6
1	D	101	GLY	4.6
1	D	28	ASN	4.5
1	C	69	ALA	4.5
1	B	28	ASN	4.5
1	A	65	ARG	4.5
1	D	24	PRO	4.5
1	B	23	LEU	4.5
1	D	69	ALA	4.5
1	B	67	GLY	4.4
1	B	20	LEU	4.4
1	A	70	GLN	4.3
1	A	67	GLY	4.2
1	B	70	GLN	4.1
1	C	14	THR	4.1
1	C	68	GLU	4.1
1	C	66	LYS	4.1
1	D	23	LEU	4.1
1	D	15	THR	4.0
1	A	66	LYS	4.0
1	C	63	LYS	4.0
1	B	63	LYS	3.7
1	A	68	GLU	3.7
1	B	68	GLU	3.7
1	B	15	THR	3.7
1	D	27	TYR	3.6
1	D	204	ASP	3.6
1	B	103	GLY	3.5
1	D	198	TRP	3.5
1	B	25	TYR	3.5
1	B	27	TYR	3.5
1	D	115	ILE	3.5
1	D	103	GLY	3.4
1	A	63	LYS	3.3
1	D	41	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	139	VAL	3.3
1	D	35	SER	3.2
1	D	68	GLU	3.2
1	D	189	ASP	3.1
1	C	71	ILE	3.1
1	D	63	LYS	3.1
1	B	192	SER	3.1
1	B	24	PRO	3.1
1	D	126	LYS	3.0
1	B	66	LYS	3.0
1	C	59	GLU	3.0
1	B	29	ALA	3.0
1	A	14	THR	2.9
1	D	66	LYS	2.9
1	D	221	LYS	2.9
1	D	120	GLY	2.9
1	C	158	ILE	2.9
1	B	44	GLN	2.9
1	D	33	TYR	2.9
1	D	43	HIS	2.9
1	D	40	GLN	2.8
1	D	185	GLN	2.8
1	B	101	GLY	2.7
1	A	71	ILE	2.7
1	A	15	THR	2.7
1	B	21	PRO	2.7
1	D	100	PRO	2.7
1	A	220	LEU	2.7
1	D	21	PRO	2.7
1	D	64	PHE	2.7
1	A	123	GLU	2.6
1	B	64	PHE	2.6
1	B	30	LEU	2.6
1	D	20	LEU	2.6
1	B	26	ALA	2.6
1	A	158	ILE	2.6
1	D	203	TRP	2.6
1	D	163	LEU	2.6
1	D	111	ILE	2.5
1	C	15	THR	2.5
1	D	37	GLU	2.5
1	D	16	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	130	SER	2.4
1	C	142	ALA	2.4
1	D	199	ASN	2.4
1	D	194	VAL	2.4
1	D	195	ASP	2.4
1	B	33	TYR	2.4
1	B	183	TYR	2.4
1	B	59	GLU	2.4
1	A	178	TRP	2.3
1	D	44	GLN	2.3
1	D	91	SER	2.3
1	C	136	VAL	2.3
1	D	107	PRO	2.3
1	B	163	LEU	2.3
1	D	109	GLY	2.3
1	C	133	ALA	2.3
1	C	139	VAL	2.2
1	D	30	LEU	2.2
1	B	104	GLY	2.2
1	D	186	TYR	2.2
1	B	199	ASN	2.2
1	C	88	ILE	2.2
1	D	38	ILE	2.2
1	A	163	LEU	2.2
1	D	192	SER	2.2
1	D	71	ILE	2.1
1	A	113	ASP	2.1
1	A	136	VAL	2.1
1	D	97	MET	2.1
1	B	113	ASP	2.1
1	B	36	ALA	2.0
1	B	182	TYR	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

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^{th} 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(Å^2)	Q<0.9
2	MN	B	301	1/1	0.95	0.33	9.30	48,48,48,48	0
2	MN	C	301	1/1	0.98	0.29	8.03	35,35,35,35	0
2	MN	D	301	1/1	0.98	0.31	6.27	47,47,47,47	0
2	MN	A	301	1/1	0.98	0.26	5.85	33,33,33,33	0

6.5 Other polymers

There are no such residues in this entry.