



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:20 AM GMT

PDB ID : 3E82
Title : Crystal structure of a putative oxidoreductase from *Klebsiella pneumoniae*
Authors : Eswaramoorthy, S.; Mohammad, M.B.; Thomas, C.A.; Brown, A.C.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-08-19
Resolution : 2.04 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

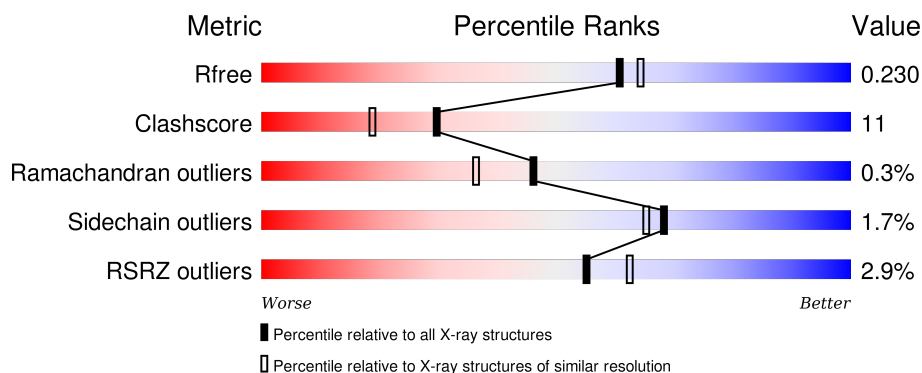
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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 $\leq 5\%$. 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	364	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>6%</div> </div> </div>
1	B	364	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>5%</div> </div> </div>
1	D	364	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div></div> </div> </div>
1	E	364	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>5%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11358 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 Putative oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	Se	0	0	0
			2645	1669	475	495	1	5			
1	B	347	Total	C	N	O	S	Se	0	0	0
			2675	1686	481	502	1	5			
1	D	350	Total	C	N	O	S	Se	0	0	0
			2712	1710	492	504	1	5			
1	E	344	Total	C	N	O	S	Se	0	0	0
			2638	1664	472	496	1	5			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MSE	-	expression tag	UNP A6T882
A	10	SER	-	expression tag	UNP A6T882
A	11	LEU	-	expression tag	UNP A6T882
A	365	GLU	-	expression tag	UNP A6T882
A	366	GLY	-	expression tag	UNP A6T882
A	367	HIS	-	expression tag	UNP A6T882
A	368	HIS	-	expression tag	UNP A6T882
A	369	HIS	-	expression tag	UNP A6T882
A	370	HIS	-	expression tag	UNP A6T882
A	371	HIS	-	expression tag	UNP A6T882
A	372	HIS	-	expression tag	UNP A6T882
B	9	MSE	-	expression tag	UNP A6T882
B	10	SER	-	expression tag	UNP A6T882
B	11	LEU	-	expression tag	UNP A6T882
B	365	GLU	-	expression tag	UNP A6T882
B	366	GLY	-	expression tag	UNP A6T882
B	367	HIS	-	expression tag	UNP A6T882
B	368	HIS	-	expression tag	UNP A6T882
B	369	HIS	-	expression tag	UNP A6T882
B	370	HIS	-	expression tag	UNP A6T882
B	371	HIS	-	expression tag	UNP A6T882

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Chain	Residue	Modelled	Actual	Comment	Reference
B	372	HIS	-	expression tag	UNP A6T882
D	9	MSE	-	expression tag	UNP A6T882
D	10	SER	-	expression tag	UNP A6T882
D	11	LEU	-	expression tag	UNP A6T882
D	365	GLU	-	expression tag	UNP A6T882
D	366	GLY	-	expression tag	UNP A6T882
D	367	HIS	-	expression tag	UNP A6T882
D	368	HIS	-	expression tag	UNP A6T882
D	369	HIS	-	expression tag	UNP A6T882
D	370	HIS	-	expression tag	UNP A6T882
D	371	HIS	-	expression tag	UNP A6T882
D	372	HIS	-	expression tag	UNP A6T882
E	9	MSE	-	expression tag	UNP A6T882
E	10	SER	-	expression tag	UNP A6T882
E	11	LEU	-	expression tag	UNP A6T882
E	365	GLU	-	expression tag	UNP A6T882
E	366	GLY	-	expression tag	UNP A6T882
E	367	HIS	-	expression tag	UNP A6T882
E	368	HIS	-	expression tag	UNP A6T882
E	369	HIS	-	expression tag	UNP A6T882
E	370	HIS	-	expression tag	UNP A6T882
E	371	HIS	-	expression tag	UNP A6T882
E	372	HIS	-	expression tag	UNP A6T882

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0

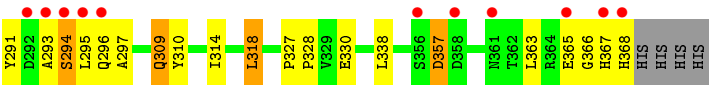
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	210	Total O 210 210	0	0

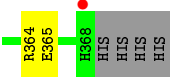
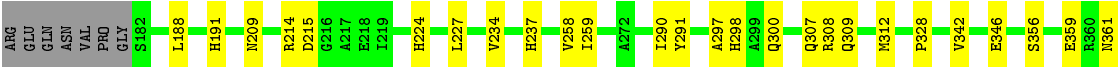
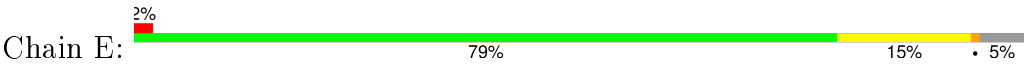
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	181	Total 181	O 181	0	0
3	D	118	Total 118	O 118	0	0
3	E	175	Total 175	O 175	0	0



● Molecule 1: Putative oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.91Å 79.75Å 209.14Å 90.00° 94.00° 90.00°	Depositor
Resolution (Å)	35.87 – 2.04 35.87 – 2.04	Depositor EDS
% Data completeness (in resolution range)	94.0 (35.87-2.04) 93.8 (35.87-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.03Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.232 0.207 , 0.230	Depositor DCC
R_{free} test set	4166 reflections (4.01%)	DCC
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 109352 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11358	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
CL

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	0.33	0/2696	0.61	0/3660
1	B	0.34	0/2726	0.62	0/3701
1	D	0.33	0/2765	0.61	0/3752
1	E	0.33	0/2689	0.62	1/3653 (0.0%)
All	All	0.33	0/10876	0.61	1/14766 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	15	THR	N-CA-C	-5.72	95.55	111.00

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	2645	0	2618	68	0
1	B	2675	0	2646	57	0
1	D	2712	0	2685	72	0
1	E	2638	0	2595	60	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	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	210	0	0	2	0
3	B	181	0	0	3	0
3	D	118	0	0	4	0
3	E	175	0	0	3	0
All	All	11358	0	10544	237	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 11.

The worst 5 of 237 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:E:361:ASN:HD22	1:E:364:ARG:HH12	1.08	0.98
1:A:101:HIS:HD2	1:A:128:LEU:H	1.12	0.97
1:A:224:HIS:CE1	1:B:224:HIS:HE1	1.82	0.96
1:A:224:HIS:HE1	1:B:224:HIS:CE1	1.84	0.96
1:D:224:HIS:HE1	1:E:224:HIS:HE1	0.98	0.95

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	339/364 (93%)	331 (98%)	7 (2%)	1 (0%)	46	36
1	B	343/364 (94%)	334 (97%)	9 (3%)	0	100	100
1	D	346/364 (95%)	328 (95%)	16 (5%)	2 (1%)	30	18
1	E	340/364 (93%)	329 (97%)	10 (3%)	1 (0%)	46	36
All	All	1368/1456 (94%)	1322 (97%)	42 (3%)	4 (0%)	46	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	294	SER
1	E	14	ASN
1	A	367	HIS
1	D	74	PRO

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	280/294 (95%)	277 (99%)	3 (1%)	80	79
1	B	284/294 (97%)	280 (99%)	4 (1%)	74	72
1	D	286/294 (97%)	278 (97%)	8 (3%)	51	44
1	E	278/294 (95%)	274 (99%)	4 (1%)	74	72
All	All	1128/1176 (96%)	1109 (98%)	19 (2%)	68	65

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	113	GLN
1	D	153	LEU
1	E	13	ASN
1	D	60	ASP
1	E	105	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	300	GLN
1	D	150	GLN
1	E	298	HIS
1	B	309	GLN
1	D	97	ASN

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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	338/364 (92%)	-0.18	6 (1%) 71 76	14, 24, 39, 50	0
1	B	342/364 (93%)	-0.21	8 (2%) 64 70	14, 24, 40, 57	0
1	D	345/364 (94%)	0.22	18 (5%) 31 36	16, 33, 49, 59	0
1	E	339/364 (93%)	-0.06	8 (2%) 62 68	15, 27, 41, 52	0
All	All	1364/1456 (93%)	-0.06	40 (2%) 55 62	14, 27, 46, 59	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	368	HIS	4.4
1	D	60	ASP	4.2
1	B	368	HIS	4.1
1	D	368	HIS	4.1
1	E	13	ASN	4.1

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, 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CL	E	4	1/1	0.97	0.12	-0.72	36,36,36,36	0
2	CL	B	2	1/1	0.99	0.10	-1.93	29,29,29,29	0
2	CL	A	1	1/1	0.99	0.10	-2.48	24,24,24,24	0
2	CL	D	3	1/1	0.97	0.09	-3.13	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.