



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:38 am GMT

PDB ID : 4IL2
Title : Crystal structure of D-mannonate dehydratase (rspA) from E. coli CFT073 (EFI TARGET EFI-501585)
Authors : Lukk, T.; Wichelecki, D.; Imker, H.J.; Gerlt, J.A.; Nair, S.K.
Deposited on : 2012-12-28
Resolution : 1.95 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

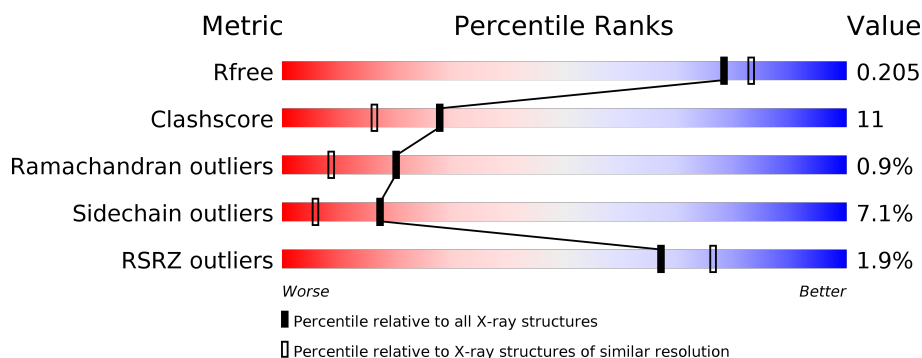
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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	426	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>19%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	426	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>20%</div> <div>5%</div> <div>5%</div> </div> </div>
1	C	426	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>19%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	426	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>20%</div> <div>•</div> <div>11%</div> </div> </div>

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	MG	A	501	-	-	-	X
2	MG	B	501	-	-	-	X
2	MG	C	501	-	-	-	X
2	MG	D	501	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12840 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 Starvation sensing protein rspA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			3031	1942	515	554	20			
1	B	404	Total	C	N	O	S	0	0	0
			3230	2070	547	590	23			
1	C	381	Total	C	N	O	S	0	0	0
			3062	1963	520	558	21			
1	D	380	Total	C	N	O	S	0	0	0
			3041	1947	518	556	20			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP Q8FHC7
A	-9	HIS	-	EXPRESSION TAG	UNP Q8FHC7
A	-8	HIS	-	EXPRESSION TAG	UNP Q8FHC7
A	-7	HIS	-	EXPRESSION TAG	UNP Q8FHC7
A	-6	HIS	-	EXPRESSION TAG	UNP Q8FHC7
A	-5	HIS	-	EXPRESSION TAG	UNP Q8FHC7
A	-4	HIS	-	EXPRESSION TAG	UNP Q8FHC7
A	-3	HIS	-	EXPRESSION TAG	UNP Q8FHC7
A	-2	HIS	-	EXPRESSION TAG	UNP Q8FHC7
A	-1	HIS	-	EXPRESSION TAG	UNP Q8FHC7
A	0	HIS	-	EXPRESSION TAG	UNP Q8FHC7
B	-10	MET	-	EXPRESSION TAG	UNP Q8FHC7
B	-9	HIS	-	EXPRESSION TAG	UNP Q8FHC7
B	-8	HIS	-	EXPRESSION TAG	UNP Q8FHC7
B	-7	HIS	-	EXPRESSION TAG	UNP Q8FHC7
B	-6	HIS	-	EXPRESSION TAG	UNP Q8FHC7
B	-5	HIS	-	EXPRESSION TAG	UNP Q8FHC7
B	-4	HIS	-	EXPRESSION TAG	UNP Q8FHC7
B	-3	HIS	-	EXPRESSION TAG	UNP Q8FHC7
B	-2	HIS	-	EXPRESSION TAG	UNP Q8FHC7
B	-1	HIS	-	EXPRESSION TAG	UNP Q8FHC7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	EXPRESSION TAG	UNP Q8FHC7
C	-10	MET	-	EXPRESSION TAG	UNP Q8FHC7
C	-9	HIS	-	EXPRESSION TAG	UNP Q8FHC7
C	-8	HIS	-	EXPRESSION TAG	UNP Q8FHC7
C	-7	HIS	-	EXPRESSION TAG	UNP Q8FHC7
C	-6	HIS	-	EXPRESSION TAG	UNP Q8FHC7
C	-5	HIS	-	EXPRESSION TAG	UNP Q8FHC7
C	-4	HIS	-	EXPRESSION TAG	UNP Q8FHC7
C	-3	HIS	-	EXPRESSION TAG	UNP Q8FHC7
C	-2	HIS	-	EXPRESSION TAG	UNP Q8FHC7
C	-1	HIS	-	EXPRESSION TAG	UNP Q8FHC7
C	0	HIS	-	EXPRESSION TAG	UNP Q8FHC7
D	-10	MET	-	EXPRESSION TAG	UNP Q8FHC7
D	-9	HIS	-	EXPRESSION TAG	UNP Q8FHC7
D	-8	HIS	-	EXPRESSION TAG	UNP Q8FHC7
D	-7	HIS	-	EXPRESSION TAG	UNP Q8FHC7
D	-6	HIS	-	EXPRESSION TAG	UNP Q8FHC7
D	-5	HIS	-	EXPRESSION TAG	UNP Q8FHC7
D	-4	HIS	-	EXPRESSION TAG	UNP Q8FHC7
D	-3	HIS	-	EXPRESSION TAG	UNP Q8FHC7
D	-2	HIS	-	EXPRESSION TAG	UNP Q8FHC7
D	-1	HIS	-	EXPRESSION TAG	UNP Q8FHC7
D	0	HIS	-	EXPRESSION TAG	UNP Q8FHC7

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

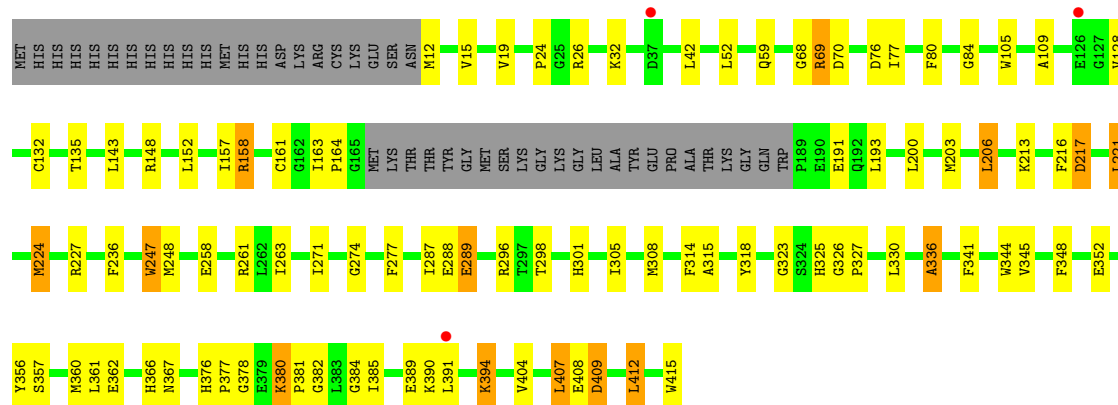
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	100	Total O 100 100	0	0

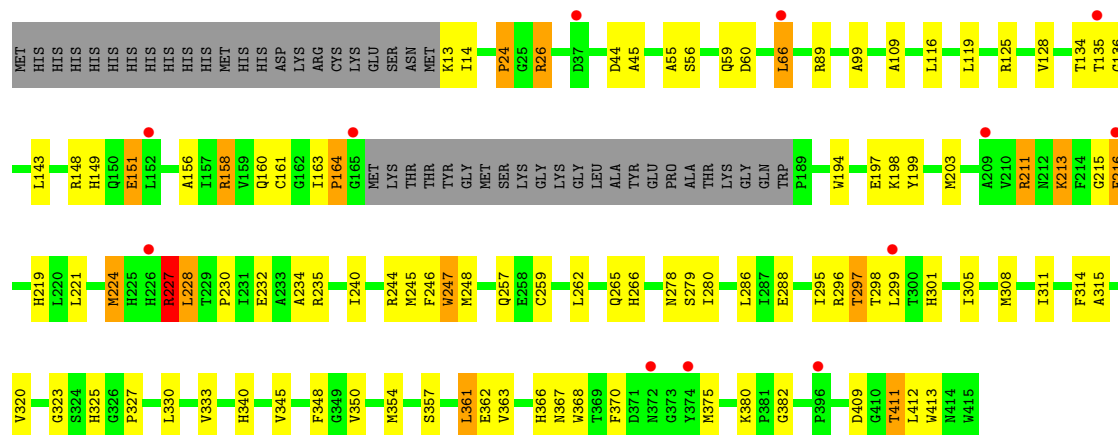
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	152	Total 152	O 152	0	0
3	C	142	Total 142	O 142	0	0
3	D	78	Total 78	O 78	0	0



• Molecule 1: Starvation sensing protein *rspA*



4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	123.78Å 123.78Å 112.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 1.95 29.83 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.83-1.95) 100.0 (29.83-1.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.178 , 0.209 0.173 , 0.205	Depositor DCC
R_{free} test set	6075 reflections (4.94%)	DCC
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12840	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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, 0.333 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: MG

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	0.46	0/3118	0.68	0/4232
1	B	0.53	1/3324 (0.0%)	0.76	5/4510 (0.1%)
1	C	0.49	1/3150 (0.0%)	0.74	2/4272 (0.0%)
1	D	0.44	0/3128	0.71	2/4244 (0.0%)
All	All	0.49	2/12720 (0.0%)	0.72	9/17258 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	GLU	CD-OE1	-5.51	1.19	1.25
1	C	336	ALA	CA-CB	-5.34	1.41	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	224	MET	CG-SD-CE	-6.51	89.79	100.20
1	B	158	ARG	CG-CD-NE	6.43	125.30	111.80
1	B	261	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	224	MET	CG-SD-CE	-5.97	90.64	100.20
1	D	224	MET	CG-SD-CE	-5.63	91.20	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	68	GLY	Peptide
1	D	247	TRP	Peptide

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	3031	0	2898	65	0
1	B	3230	0	3103	83	0
1	C	3062	0	2947	68	0
1	D	3041	0	2913	62	0
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	100	0	0	3	0
3	B	152	0	0	8	0
3	C	142	0	0	1	0
3	D	78	0	0	3	0
All	All	12840	0	11861	272	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 272 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:B:224:MET:HE3	1:B:248:MET:HB2	1.34	1.08
1:C:224:MET:HE3	1:C:248:MET:HB2	1.36	1.03
1:A:22:THR:HG21	1:A:392:ALA:HB1	1.55	0.87
1:D:14:ILE:HD13	1:D:66:LEU:HD11	1.56	0.87
1:B:380:LYS:HG2	1:B:384:GLY:HA2	1.58	0.85

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	376/426 (88%)	355 (94%)	20 (5%)	1 (0%)	44	33
1	B	402/426 (94%)	383 (95%)	13 (3%)	6 (2%)	12	3
1	C	377/426 (88%)	358 (95%)	17 (4%)	2 (0%)	32	19
1	D	376/426 (88%)	349 (93%)	22 (6%)	5 (1%)	14	4
All	All	1531/1704 (90%)	1445 (94%)	72 (5%)	14 (1%)	20	9

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	PRO
1	B	24	PRO
1	B	215	GLY
1	C	24	PRO
1	D	24	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	315/360 (88%)	292 (93%)	23 (7%)	16	5
1	B	336/360 (93%)	310 (92%)	26 (8%)	15	4
1	C	321/360 (89%)	301 (94%)	20 (6%)	21	8
1	D	317/360 (88%)	294 (93%)	23 (7%)	16	5
All	All	1289/1440 (90%)	1197 (93%)	92 (7%)	17	6

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	244	ARG
1	C	52	LEU
1	D	361	LEU
1	B	247	TRP
1	B	380	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	150	GLN
1	D	285	GLN
1	C	325	HIS
1	B	187	GLN
1	C	226	HIS

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 [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	380/426 (89%)	0.26	11 (2%) 52 62	8, 18, 34, 52	0
1	B	404/426 (94%)	0.09	3 (0%) 87 92	5, 14, 27, 44	0
1	C	381/426 (89%)	0.04	3 (0%) 86 91	6, 13, 25, 47	0
1	D	380/426 (89%)	0.33	12 (3%) 48 59	9, 19, 36, 47	0
All	All	1545/1704 (90%)	0.18	29 (1%) 67 76	5, 16, 33, 52	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	126	GLU	5.2
1	D	152	LEU	4.5
1	A	125	ARG	4.4
1	A	126	GLU	4.0
1	D	135	THR	4.0

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 [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	MG	D	501	1/1	0.49	0.29	19.46	35,35,35,35	0
2	MG	C	501	1/1	0.88	0.20	5.58	11,11,11,11	0
2	MG	A	501	1/1	0.91	0.20	4.26	19,19,19,19	0
2	MG	B	501	1/1	0.95	0.18	2.74	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.