WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 02:39 am BST

PDB ID : 2RAD

Title : Crystal structure of the succinoglycan biosynthesis protein. Northeast structural Genomics Consortium target BcR135

Authors : Kuzin, A.P.; Abashidze, M.; Seetharaman, J.; Wang, H.; Mao, L.; Cunningham, K.; Xiao, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)

Deposited on : 2007-09-14

Resolution : 2.75 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
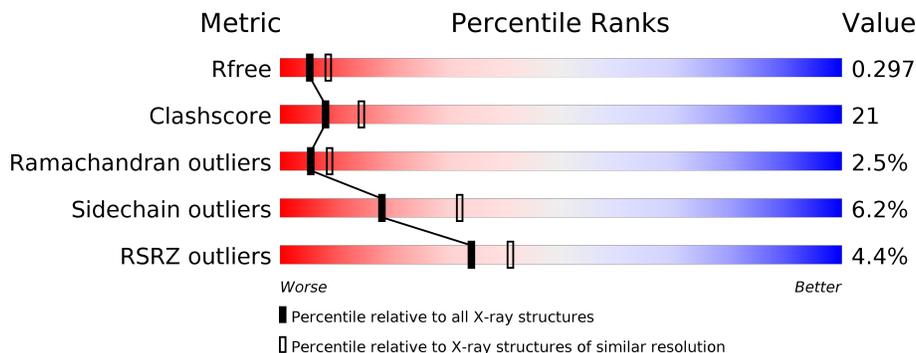with specific help available everywhere you see the ⓘ symbol.

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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 2.75 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	Percentile Ranks	Value
Rfree		0.297
Clashscore		21
Ramachandran outliers		2.5%
Sidechain outliers		6.2%
RSRZ outliers		4.4%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 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 <=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	451	5% 52% 33% • 11%
1	B	451	2% 46% 41% • 10%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 6506 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 Succinoglycan biosynthesis protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total 3230	C 2071	N 547	O 604	Se 8	0	0	0
1	B	405	Total 3245	C 2079	N 550	O 608	Se 8	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	THR	GLN	CONFLICT	UNP Q81BN2
A	444	LEU	-	EXPRESSION TAG	UNP Q81BN2
A	445	GLU	-	EXPRESSION TAG	UNP Q81BN2
A	446	HIS	-	EXPRESSION TAG	UNP Q81BN2
A	447	HIS	-	EXPRESSION TAG	UNP Q81BN2
A	448	HIS	-	EXPRESSION TAG	UNP Q81BN2
A	449	HIS	-	EXPRESSION TAG	UNP Q81BN2
A	450	HIS	-	EXPRESSION TAG	UNP Q81BN2
A	451	HIS	-	EXPRESSION TAG	UNP Q81BN2
B	233	THR	GLN	CONFLICT	UNP Q81BN2
B	444	LEU	-	EXPRESSION TAG	UNP Q81BN2
B	445	GLU	-	EXPRESSION TAG	UNP Q81BN2
B	446	HIS	-	EXPRESSION TAG	UNP Q81BN2
B	447	HIS	-	EXPRESSION TAG	UNP Q81BN2
B	448	HIS	-	EXPRESSION TAG	UNP Q81BN2
B	449	HIS	-	EXPRESSION TAG	UNP Q81BN2
B	450	HIS	-	EXPRESSION TAG	UNP Q81BN2
B	451	HIS	-	EXPRESSION TAG	UNP Q81BN2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total 21	O 21	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	10	Total O 10 10		0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Succinoglycan biosynthesis protein
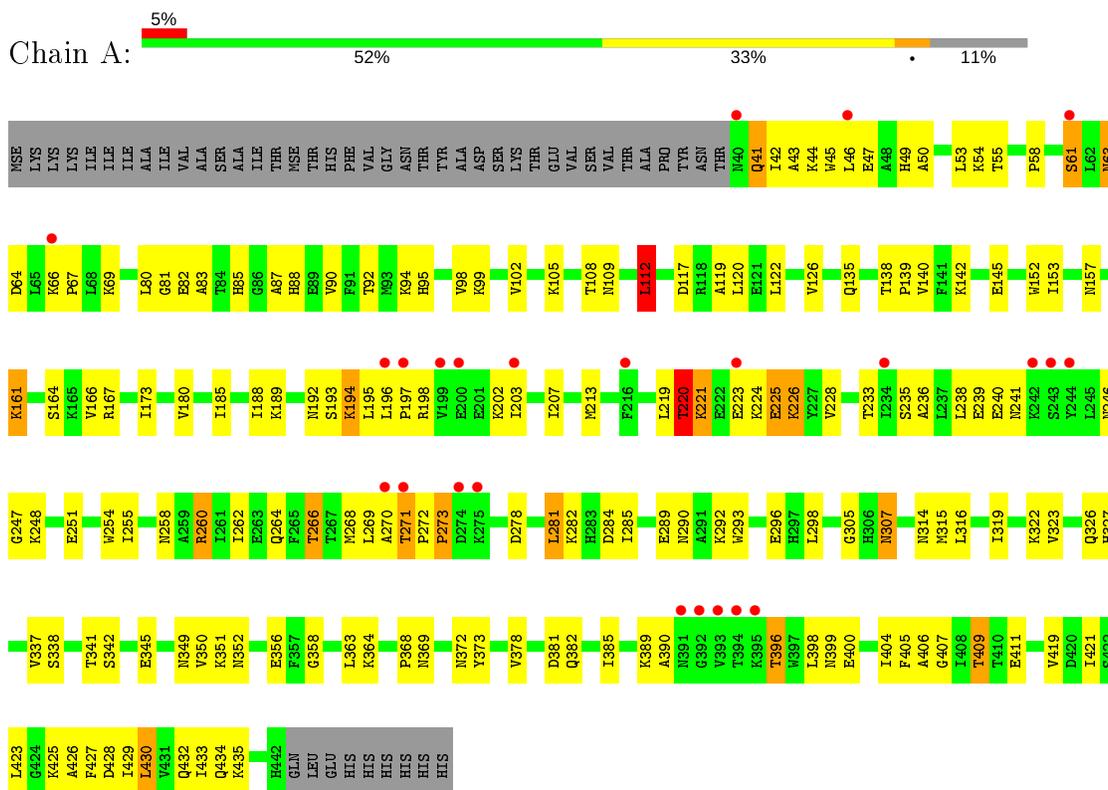
• Molecule 1: Succinoglycan biosynthesis protein
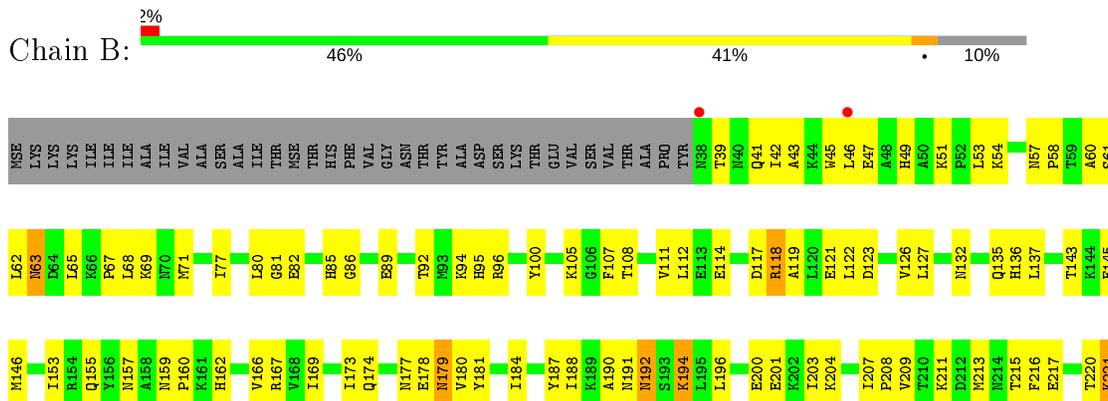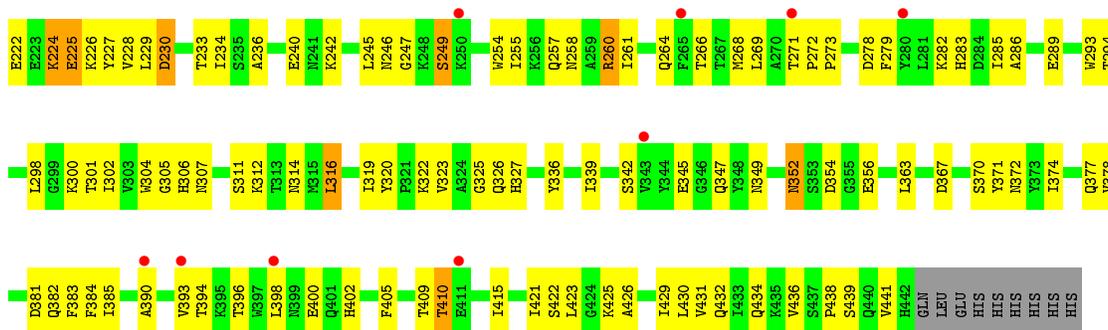
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	87.79Å 54.19Å 98.91Å	Depositor
a, b, c, α, β, γ	90.00° 97.20° 90.00°	
Resolution (Å)	19.93 – 2.75	Depositor
	46.01 – 2.75	EDS
% Data completeness	82.1 (19.93-2.75)	Depositor
(in resolution range)	94.9 (46.01-2.75)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.35 (at 2.77Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.209 , 0.281	Depositor
	0.225 , 0.297	DCC
R_{free} test set	4462 reflections (9.76%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.726	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.5	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6506	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.44	0/3298	0.67	1/4450 (0.0%)
1	B	0.40	0/3313	0.63	1/4471 (0.0%)
All	All	0.42	0/6611	0.65	2/8921 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	112	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	43	ALA	N-CA-C	-5.02	97.44	111.00

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	3230	0	3239	131	0
1	B	3245	0	3252	145	0
2	A	21	0	0	1	0
2	B	10	0	0	0	0
All	All	6506	0	6491	276	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 21.

The worst 5 of 276 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:A:323:VAL:H	1:A:326:GLN:HE21	1.14	0.95
1:B:67:PRO:HG2	1:B:384:PHE:HZ	1.31	0.94
1:B:372:ASN:HD21	1:B:405:PHE:H	1.00	0.92
1:A:372:ASN:HD21	1:A:405:PHE:H	1.19	0.91
1:B:268:MSE:HE3	1:B:269:LEU:HG	1.56	0.88

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	401/451 (89%)	350 (87%)	39 (10%)	12 (3%)	4	6
1	B	403/451 (89%)	355 (88%)	40 (10%)	8 (2%)	7	13
All	All	804/902 (89%)	705 (88%)	79 (10%)	20 (2%)	5	9

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	THR
1	A	273	PRO
1	B	220	THR
1	B	249	SER
1	B	273	PRO

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	354/386 (92%)	330 (93%)	24 (7%)	16	28
1	B	356/386 (92%)	336 (94%)	20 (6%)	21	36
All	All	710/772 (92%)	666 (94%)	44 (6%)	18	32

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	363	LEU
1	B	53	LEU
1	B	409	THR
1	A	369	ASN
1	A	409	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	399	ASN
1	B	136	HIS
1	B	349	ASN
1	A	432	GLN
1	B	155	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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(Å²)	Q<0.9
1	A	395/451 (87%)	0.27	24 (6%)	21	26	33, 56, 90, 103	0
1	B	397/451 (88%)	0.18	11 (2%)	53	62	33, 64, 91, 104	0
All	All	792/902 (87%)	0.22	35 (4%)	34	41	33, 61, 91, 104	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	391	ASN	4.9
1	A	199	VAL	4.3
1	A	244	TYR	4.0
1	A	392	GLY	4.0
1	A	275	LYS	3.7

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.