



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 07:12 AM EDT

PDB ID : 4GXA
Title : Crystal structure of Sulfate free form of CYSB, a member of LysR family from Salmonella typhimurium LT2
Authors : Mittal, M.; Singh, A.K.; Kumaran, S.
Deposited on : 2012-09-04
Resolution : 2.81 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

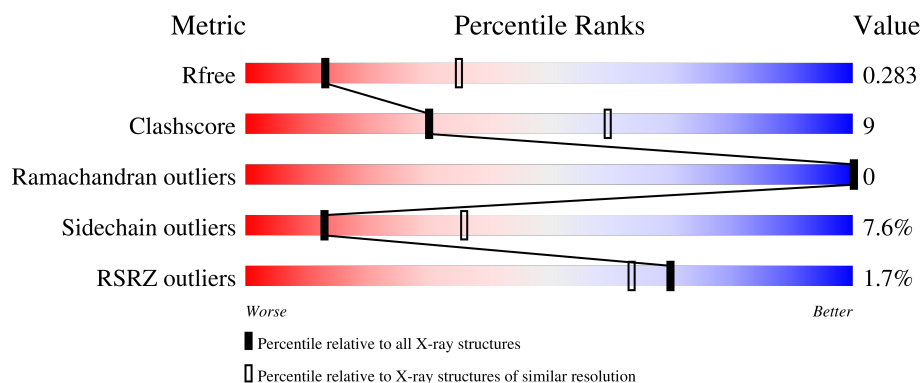
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 of 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 $\leq 5\%$. 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	239	
1	B	239	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3635 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 HTH-type transcriptional regulator CysB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1792	1148	308	331	5			
1	B	239	Total	C	N	O	S	0	0	0
			1833	1172	318	337	6			

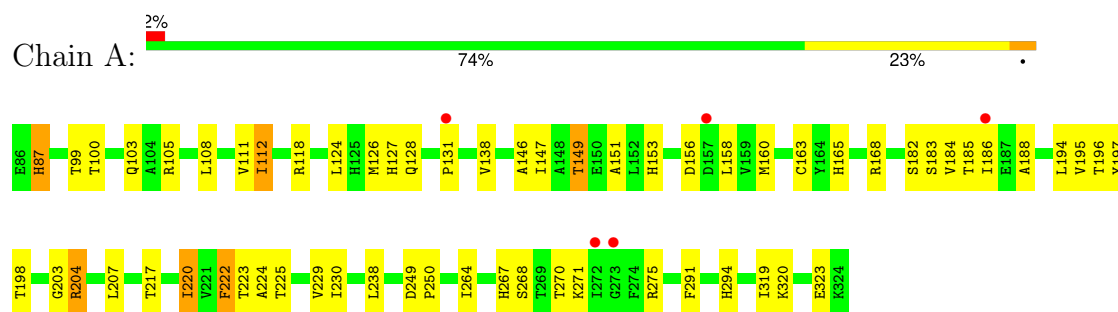
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	O	0	0
			7	7		
2	B	3	Total	O	0	0
			3	3		

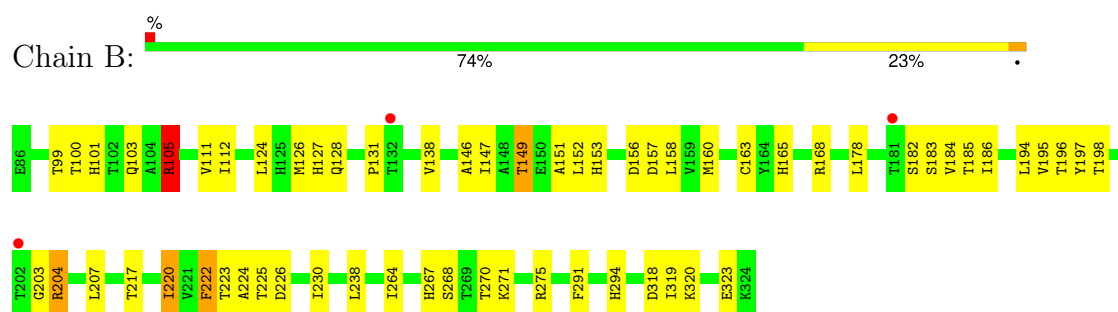
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: HTH-type transcriptional regulator CysB



- Molecule 1: HTH-type transcriptional regulator CysB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.48Å 104.83Å 46.51Å 90.00° 102.67° 90.00°	Depositor
Resolution (Å)	45.37 – 2.81 45.37 – 2.81	Depositor EDS
% Data completeness (in resolution range)	90.3 (45.37-2.81) 90.4 (45.37-2.81)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.94 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.194 , 0.257 0.238 , 0.283	Depositor DCC
R_{free} test set	459 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	57.7	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.478 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3635	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.49% 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

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	0.26	0/1837	0.69	6/2515 (0.2%)
1	B	0.27	0/1879	0.72	7/2567 (0.3%)
All	All	0.27	0/3716	0.70	13/5082 (0.3%)

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	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ARG	NE-CZ-NH2	-12.58	114.01	120.30
1	B	105	ARG	NE-CZ-NH1	-12.44	114.08	120.30
1	A	204	ARG	NE-CZ-NH2	-12.18	114.21	120.30
1	B	204	ARG	NE-CZ-NH1	-12.07	114.27	120.30
1	B	105	ARG	NE-CZ-NH2	11.97	126.29	120.30
1	A	204	ARG	NE-CZ-NH1	11.97	126.28	120.30
1	A	105	ARG	NE-CZ-NH1	11.71	126.16	120.30
1	B	204	ARG	NE-CZ-NH2	11.59	126.09	120.30
1	B	105	ARG	CD-NE-CZ	6.23	132.33	123.60
1	A	105	ARG	CD-NE-CZ	6.10	132.14	123.60
1	A	204	ARG	CD-NE-CZ	6.02	132.03	123.60
1	B	204	ARG	CD-NE-CZ	5.92	131.89	123.60
1	B	207	LEU	CA-CB-CG	5.41	127.74	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	HIS	Peptide
1	A	184	VAL	Peptide
1	B	153	HIS	Peptide
1	B	184	VAL	Peptide

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	1792	0	1712	35	0
1	B	1833	0	1788	34	0
2	A	7	0	0	1	0
2	B	3	0	0	0	0
All	All	3635	0	3500	66	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 9.

All (66) 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:149:THR:HG23	2:A:403:HOH:O	1.92	0.68
1:A:112:ILE:HG23	1:A:124:LEU:HD21	1.79	0.65
1:B:101:HIS:CD2	1:B:226:ASP:HB2	2.32	0.65
1:B:168:ARG:NH2	1:B:203:GLY:O	2.31	0.63
1:A:168:ARG:NH2	1:A:203:GLY:O	2.31	0.63
1:B:168:ARG:NH2	1:B:268:SER:OG	2.32	0.63
1:A:138:VAL:HG21	1:A:146:ALA:HB2	1.81	0.62
1:A:168:ARG:NH2	1:A:268:SER:OG	2.32	0.62
1:B:138:VAL:HG21	1:B:146:ALA:HB2	1.81	0.61
1:A:112:ILE:CG2	1:A:124:LEU:HD21	2.33	0.58
1:B:112:ILE:HD12	1:B:124:LEU:HD21	1.86	0.57
1:A:196:THR:OG1	1:A:197:TYR:N	2.37	0.57
1:B:195:VAL:HG13	1:B:222:PHE:HB3	1.87	0.56
1:A:195:VAL:HG13	1:A:222:PHE:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:HIS:CD2	1:B:226:ASP:CB	2.91	0.54
1:B:149:THR:HA	1:B:270:THR:HA	1.90	0.54
1:B:196:THR:OG1	1:B:197:TYR:N	2.37	0.54
1:A:149:THR:HA	1:A:270:THR:HA	1.89	0.53
1:B:157:ASP:O	1:B:158:LEU:HD12	2.07	0.53
1:B:149:THR:O	1:B:149:THR:OG1	2.27	0.53
1:A:225:THR:N	1:B:128:GLN:OE1	2.38	0.52
1:A:149:THR:O	1:A:149:THR:OG1	2.27	0.52
1:B:220:ILE:H	1:B:220:ILE:HD13	1.75	0.52
1:A:126:MET:O	1:A:127:HIS:ND1	2.44	0.51
1:B:126:MET:O	1:B:127:HIS:ND1	2.44	0.51
1:A:220:ILE:H	1:A:220:ILE:HD13	1.76	0.50
1:B:195:VAL:HG12	1:B:230:ILE:HG23	1.94	0.50
1:A:195:VAL:HG12	1:A:230:ILE:HG23	1.94	0.48
1:A:182:SER:HA	1:A:183:SER:HA	1.61	0.48
1:A:160:MET:HB3	1:A:271:LYS:HE2	1.94	0.48
1:B:156:ASP:HA	1:B:157:ASP:C	2.34	0.48
1:A:185:THR:OG1	1:A:186:ILE:N	2.46	0.48
1:B:160:MET:HB3	1:B:271:LYS:HE2	1.95	0.48
1:B:99:THR:OG1	1:B:100:THR:N	2.46	0.48
1:B:182:SER:HA	1:B:183:SER:HA	1.59	0.47
1:A:165:HIS:HB2	1:A:323:GLU:HG2	1.97	0.47
1:B:165:HIS:HB2	1:B:323:GLU:HG2	1.97	0.47
1:B:198:THR:N	1:B:224:ALA:O	2.47	0.46
1:A:99:THR:OG1	1:A:100:THR:N	2.46	0.46
1:A:198:THR:N	1:A:224:ALA:O	2.47	0.46
1:A:112:ILE:CG2	1:A:124:LEU:CD2	2.93	0.46
1:B:185:THR:OG1	1:B:186:ILE:N	2.49	0.46
1:B:103:GLN:HG2	1:B:147:ILE:HG22	1.97	0.45
1:B:111:VAL:HG21	1:B:291:PHE:HD1	1.81	0.45
1:A:103:GLN:HG2	1:A:147:ILE:HG22	1.97	0.45
1:A:111:VAL:HG21	1:A:291:PHE:HD1	1.81	0.45
1:A:128:GLN:OE1	1:B:225:THR:N	2.37	0.45
1:A:131:PRO:HB3	1:A:151:ALA:HB1	1.98	0.45
1:B:163:CYS:O	1:B:294:HIS:HE1	2.01	0.44
1:B:131:PRO:HB3	1:B:151:ALA:HB1	1.98	0.44
1:A:186:ILE:HB	1:A:264:ILE:HG23	1.99	0.44
1:A:163:CYS:O	1:A:294:HIS:HE1	2.01	0.44
1:A:229:VAL:HG12	1:B:105:ARG:HB2	2.00	0.43
1:B:186:ILE:HB	1:B:264:ILE:HG23	2.00	0.43
1:B:198:THR:HA	1:B:223:THR:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:THR:HA	1:A:223:THR:HB	2.01	0.42
1:B:156:ASP:HA	1:B:158:LEU:N	2.34	0.42
1:A:220:ILE:HG12	1:A:220:ILE:O	2.20	0.42
1:B:220:ILE:O	1:B:220:ILE:HG12	2.20	0.42
1:B:101:HIS:NE2	1:B:226:ASP:HB2	2.35	0.41
1:A:185:THR:HG23	1:A:188:ALA:H	1.86	0.41
1:A:156:ASP:C	1:A:158:LEU:H	2.25	0.41
1:B:178:LEU:HD23	1:B:178:LEU:HA	1.92	0.41
1:A:108:LEU:O	1:A:112:ILE:HG12	2.21	0.40
1:A:87:HIS:O	1:A:118:ARG:HG3	2.22	0.40
1:A:249:ASP:HA	1:A:250:PRO:HD3	1.93	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	237/239 (99%)	225 (95%)	12 (5%)	0	100	100
1	B	237/239 (99%)	224 (94%)	13 (6%)	0	100	100
All	All	474/478 (99%)	449 (95%)	25 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	179/202 (89%)	165 (92%)	14 (8%)	12	35
1	B	190/202 (94%)	176 (93%)	14 (7%)	13	37
All	All	369/404 (91%)	341 (92%)	28 (8%)	13	36

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	112	ILE
1	A	149	THR
1	A	194	LEU
1	A	204	ARG
1	A	207	LEU
1	A	217	THR
1	A	220	ILE
1	A	222	PHE
1	A	238	LEU
1	A	267	HIS
1	A	275	ARG
1	A	319	ILE
1	A	320	LYS
1	B	105	ARG
1	B	149	THR
1	B	152	LEU
1	B	194	LEU
1	B	204	ARG
1	B	217	THR
1	B	220	ILE
1	B	222	PHE
1	B	238	LEU
1	B	267	HIS
1	B	275	ARG
1	B	318	ASP
1	B	319	ILE
1	B	320	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	101	HIS

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 monosaccharides 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(Å ²)	Q<0.9
1	A	239/239 (100%)	0.10	5 (2%) 63 54	66, 85, 110, 125	0
1	B	239/239 (100%)	0.14	3 (1%) 77 72	67, 85, 112, 127	0
All	All	478/478 (100%)	0.12	8 (1%) 70 63	66, 85, 112, 127	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	132	THR	3.2
1	B	181	THR	2.7
1	A	273	GLY	2.7
1	B	202	THR	2.7
1	A	131	PRO	2.6
1	A	272	ILE	2.4
1	A	186	ILE	2.3
1	A	157	ASP	2.2

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 monosaccharides 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.