



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2025 – 02:39 PM EDT

PDB ID : 9OTR / pdb_00009otr
Title : Crystal Structure of Salmonella FraB Deglycase, Crystal Form 4 with deletion of C-terminal residues 313-325.
Authors : Bell, C.E.; Zakharova, K.
Deposited on : 2025-05-27
Resolution : 1.84 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	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

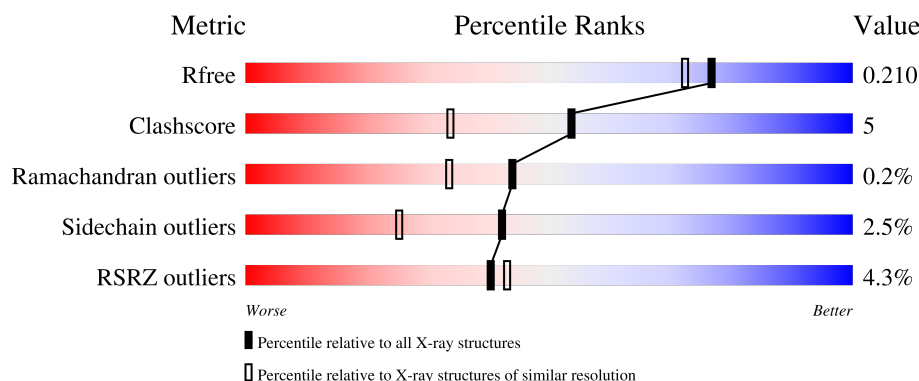
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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}	164625	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

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	332	
1	B	332	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5007 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 SIS domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2386	1525	400	451	10			
1	B	299	Total	C	N	O	S	0	0	0
			2311	1479	385	437	10			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP V7IWJ0
A	-18	ASP	-	expression tag	UNP V7IWJ0
A	-17	HIS	-	expression tag	UNP V7IWJ0
A	-16	HIS	-	expression tag	UNP V7IWJ0
A	-15	HIS	-	expression tag	UNP V7IWJ0
A	-14	HIS	-	expression tag	UNP V7IWJ0
A	-13	HIS	-	expression tag	UNP V7IWJ0
A	-12	HIS	-	expression tag	UNP V7IWJ0
A	-11	GLU	-	expression tag	UNP V7IWJ0
A	-10	ASN	-	expression tag	UNP V7IWJ0
A	-9	LEU	-	expression tag	UNP V7IWJ0
A	-8	TYR	-	expression tag	UNP V7IWJ0
A	-7	PHE	-	expression tag	UNP V7IWJ0
A	-6	GLN	-	expression tag	UNP V7IWJ0
A	275	ALA	LYS	engineered mutation	UNP V7IWJ0
A	276	ALA	GLU	engineered mutation	UNP V7IWJ0
B	-19	MET	-	expression tag	UNP V7IWJ0
B	-18	ASP	-	expression tag	UNP V7IWJ0
B	-17	HIS	-	expression tag	UNP V7IWJ0
B	-16	HIS	-	expression tag	UNP V7IWJ0
B	-15	HIS	-	expression tag	UNP V7IWJ0
B	-14	HIS	-	expression tag	UNP V7IWJ0
B	-13	HIS	-	expression tag	UNP V7IWJ0
B	-12	HIS	-	expression tag	UNP V7IWJ0
B	-11	GLU	-	expression tag	UNP V7IWJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	ASN	-	expression tag	UNP V7IWJ0
B	-9	LEU	-	expression tag	UNP V7IWJ0
B	-8	TYR	-	expression tag	UNP V7IWJ0
B	-7	PHE	-	expression tag	UNP V7IWJ0
B	-6	GLN	-	expression tag	UNP V7IWJ0
B	275	ALA	LYS	engineered mutation	UNP V7IWJ0
B	276	ALA	GLU	engineered mutation	UNP V7IWJ0

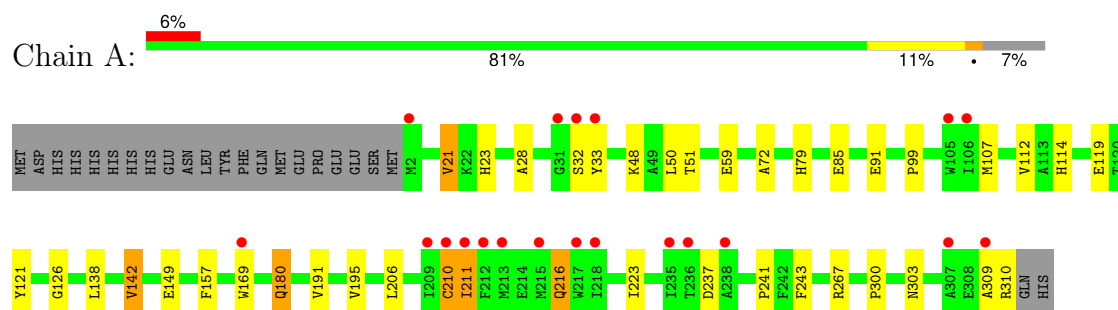
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	150	Total	O	0	0
			150	150		
2	B	160	Total	O	0	0
			160	160		

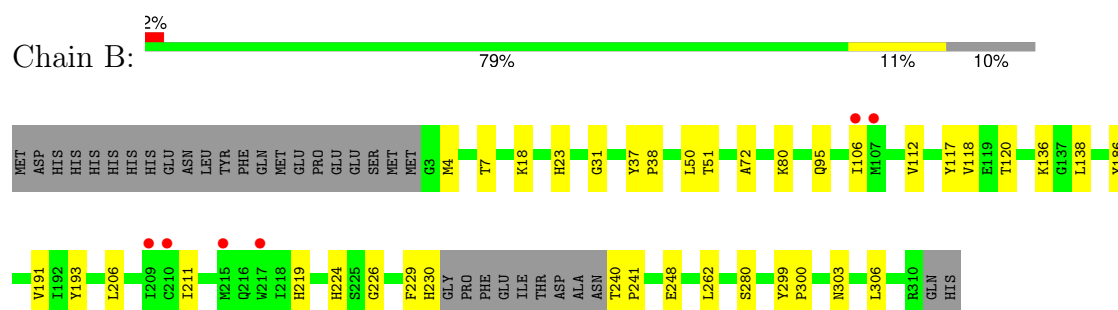
3 Residue-property plots [i](#)

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: SIS domain protein



• Molecule 1: SIS domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.48Å 108.36Å 119.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 1.84 49.43 – 1.84	Depositor EDS
% Data completeness (in resolution range)	71.2 (49.43-1.84) 71.3 (49.43-1.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.172 , 0.204 0.182 , 0.210	Depositor DCC
R_{free} test set	2238 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5007	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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](#)

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	0.60	0/2443	1.10	7/3317 (0.2%)
1	B	0.62	0/2364	1.07	3/3206 (0.1%)
All	All	0.61	0/4807	1.09	10/6523 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	GLU	CB-CA-C	-7.55	96.86	109.55
1	B	4	MET	CG-SD-CE	-7.35	84.73	100.90
1	A	142	VAL	N-CA-CB	7.26	121.47	110.58
1	B	50	LEU	N-CA-CB	-7.21	98.66	109.69
1	A	157	PHE	CA-CB-CG	-6.06	107.74	113.80
1	A	85	GLU	N-CA-CB	5.96	118.88	110.12
1	A	243	PHE	CB-CA-C	5.93	120.28	110.78
1	A	21	VAL	N-CA-CB	5.83	117.08	110.72
1	B	120	THR	CA-CB-OG1	-5.75	100.98	109.60
1	A	85	GLU	CB-CA-C	-5.23	102.11	110.79

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	2386	0	2292	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2311	0	2230	21	0
2	A	150	0	0	4	0
2	B	160	0	0	2	0
All	All	5007	0	4522	44	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 5.

All (44) 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:51:THR:HG22	1:B:51:THR:HG22	1.33	1.03
1:A:211:ILE:HG21	1:A:303:ASN:CG	2.06	0.80
1:B:248:GLU:OE1	1:B:280:SER:HB3	1.85	0.76
1:A:211:ILE:HG21	1:A:303:ASN:ND2	2.05	0.71
1:B:229:PHE:O	1:B:230:HIS:CB	2.41	0.69
1:A:23:HIS:HE1	2:A:535:HOH:O	1.75	0.69
1:A:59:GLU:OE1	1:B:224:HIS:HE1	1.77	0.66
2:A:537:HOH:O	1:B:23:HIS:HE1	1.80	0.64
1:A:237:ASP:O	1:A:267:ARG:NH2	2.35	0.59
1:A:59:GLU:OE1	1:B:224:HIS:CE1	2.57	0.58
1:A:309:ALA:O	1:A:310:ARG:HG3	2.04	0.57
1:A:119:GLU:OE2	2:A:401:HOH:O	2.17	0.57
1:B:112:VAL:HG13	1:B:118:VAL:HG21	1.89	0.55
1:B:224:HIS:CD2	1:B:226:GLY:H	2.26	0.53
1:A:79:HIS:HA	1:A:121:TYR:OH	2.09	0.53
1:A:206:LEU:O	1:A:210:CYS:HB2	2.09	0.52
1:A:91:GLU:OE1	1:A:114:HIS:ND1	2.26	0.52
1:A:72:ALA:O	1:A:99:PRO:HD2	2.12	0.49
1:A:180:GLN:HE21	1:A:180:GLN:HA	1.79	0.48
1:B:80:LYS:HA	1:B:106:ILE:HD12	1.96	0.47
1:A:48:LYS:NZ	2:A:405:HOH:O	2.48	0.46
1:B:211:ILE:HG21	1:B:303:ASN:ND2	2.32	0.45
1:B:23:HIS:O	1:B:72:ALA:HA	2.17	0.45
1:B:193:TYR:CE2	1:B:240:THR:HG21	2.52	0.44
1:A:28:ALA:HB1	1:A:32:SER:HB2	2.00	0.44
1:B:95:GLN:NE2	2:B:405:HOH:O	2.48	0.44
1:B:31:GLY:HA2	1:B:206:LEU:HD21	2.00	0.44
1:B:23:HIS:HD2	1:B:51:THR:OG1	2.01	0.43
1:B:37:TYR:HB3	1:B:38:PRO:HD3	2.00	0.43
1:A:195:VAL:HA	1:A:223:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LYS:HE2	2:B:467:HOH:O	2.18	0.42
1:A:23:HIS:HD2	1:A:51:THR:OG1	2.01	0.42
1:B:191:VAL:HG22	1:B:219:HIS:HB2	2.01	0.42
1:A:126:GLY:HA2	1:A:169:TRP:CZ2	2.55	0.42
1:A:210:CYS:O	1:A:211:ILE:C	2.62	0.42
1:B:299:TYR:N	1:B:300:PRO:CD	2.83	0.42
1:A:216:GLN:HB3	1:A:310:ARG:HH12	1.84	0.41
1:A:107:MET:O	1:A:112:VAL:HG21	2.20	0.41
1:A:191:VAL:O	1:A:241:PRO:HD2	2.20	0.41
1:A:33:TYR:CD1	1:A:33:TYR:C	2.99	0.41
1:B:7:THR:HG23	1:B:117:TYR:CG	2.55	0.41
1:A:309:ALA:O	1:A:310:ARG:CG	2.69	0.41
1:B:186:TYR:HE1	1:B:241:PRO:CB	2.34	0.41
1:A:216:GLN:HB3	1:A:310:ARG:NH1	2.36	0.41

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	307/332 (92%)	295 (96%)	11 (4%)	1 (0%)	37	25
1	B	295/332 (89%)	292 (99%)	3 (1%)	0	100	100
All	All	602/664 (91%)	587 (98%)	14 (2%)	1 (0%)	44	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	CYS

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	242/269 (90%)	234 (97%)	8 (3%)	33	16
1	B	235/269 (87%)	231 (98%)	4 (2%)	56	41
All	All	477/538 (89%)	465 (98%)	12 (2%)	42	25

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	50	LEU
1	A	138	LEU
1	A	142	VAL
1	A	180	GLN
1	A	211	ILE
1	A	216	GLN
1	A	300	PRO
1	B	18	LYS
1	B	138	LEU
1	B	262	LEU
1	B	306	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	15	GLN
1	A	23	HIS
1	A	95	GLN
1	A	153	HIS
1	A	180	GLN
1	A	184	GLN
1	A	219	HIS
1	A	297	ASN
1	B	10	ASN

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Mol	Chain	Res	Type
1	B	15	GLN
1	B	23	HIS
1	B	95	GLN
1	B	114	HIS
1	B	153	HIS
1	B	207	GLN
1	B	224	HIS
1	B	245	GLN
1	B	303	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 oligosaccharides 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

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, 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	309/332 (93%)	0.30	20 (6%) 26 28	22, 35, 69, 115	0
1	B	299/332 (90%)	0.08	6 (2%) 64 71	20, 33, 57, 78	0
All	All	608/664 (91%)	0.19	26 (4%) 40 43	20, 34, 63, 115	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	TRP	6.4
1	B	209	ILE	5.4
1	A	209	ILE	5.2
1	A	235	ILE	4.5
1	B	215	MET	4.3
1	A	2	MET	4.0
1	A	218	ILE	3.7
1	A	210	CYS	3.6
1	A	212	PHE	3.3
1	A	105	TRP	3.3
1	A	215	MET	3.2
1	A	106	ILE	3.1
1	B	217	TRP	3.1
1	A	211	ILE	3.0
1	A	32	SER	3.0
1	A	169	TRP	2.9
1	A	236	THR	2.7
1	A	213	MET	2.7
1	B	107	MET	2.7
1	B	106	ILE	2.6
1	A	31	GLY	2.6
1	A	309	ALA	2.5
1	A	33	TYR	2.3
1	A	238	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	307	ALA	2.1
1	B	210	CYS	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 oligosaccharides 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.