



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:08 PM UTC

PDB ID : 9OTJ / pdb_00009otj
Title : Crystal Structure of Salmonella FraB Deglycase, Crystal Form 1
Authors : Bell, C.E.; Zakharova, K.
Deposited on : 2025-05-27
Resolution : 1.85 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 Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

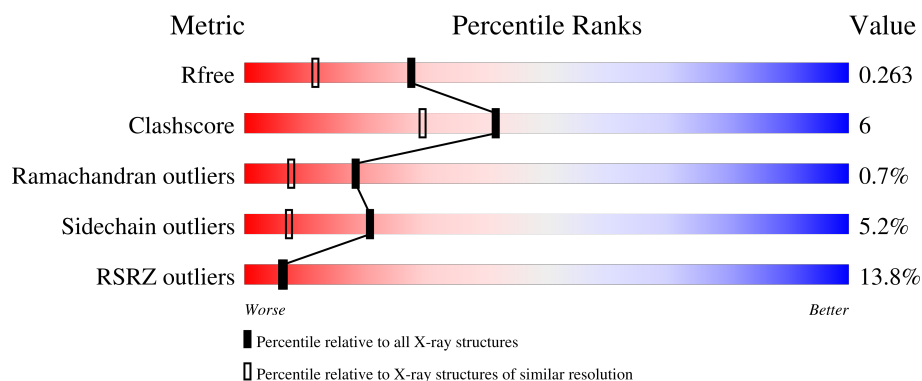
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	345	10% 77% 11% • 9%
1	B	345	15% 69% 16% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5074 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	313	Total	C	N	O	S	0	0	0
			2420	1553	402	453	12			
1	B	308	Total	C	N	O	S	0	0	0
			2381	1522	399	450	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	137	Total	O	0	0
			137	137		
2	B	136	Total	O	0	0
			136	136		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.29Å 108.52Å 120.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.74 – 1.85 80.74 – 1.85	Depositor EDS
% Data completeness (in resolution range)	85.7 (80.74-1.85) 85.7 (80.74-1.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.196 , 0.254 0.205 , 0.263	Depositor DCC
R_{free} test set	2620 reflections (4.17%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5074	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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	0.69	0/2479	1.20	7/3363 (0.2%)
1	B	0.71	0/2438	1.30	16/3310 (0.5%)
All	All	0.70	0/4917	1.25	23/6673 (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	4
All	All	0	6

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	MET	CG-SD-CE	-9.82	79.30	100.90
1	B	21	VAL	N-CA-CB	7.70	119.11	110.72
1	B	248	GLU	N-CA-CB	-7.55	98.54	110.69
1	B	149	GLU	CB-CA-C	-7.15	97.06	109.07
1	A	142	VAL	N-CA-CB	6.80	120.78	110.58
1	B	248	GLU	CB-CA-C	6.64	121.33	109.38
1	B	288	ASP	CA-CB-CG	6.33	118.93	112.60
1	B	142	VAL	N-CA-CB	5.92	119.45	110.58
1	A	267	ARG	CG-CD-NE	5.88	124.93	112.00
1	A	80	LYS	CB-CA-C	5.76	120.79	109.72
1	B	18	LYS	CB-CA-C	5.70	120.19	110.56
1	B	138	LEU	N-CA-CB	-5.64	101.81	110.16
1	B	188	ASP	CA-CB-CG	5.63	118.23	112.60
1	B	134	THR	CA-CB-OG1	-5.56	101.25	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	THR	CA-CB-OG1	-5.53	101.30	109.60
1	A	288	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	284	THR	CA-CB-OG1	-5.46	101.41	109.60
1	B	246	PHE	CA-CB-CG	5.25	119.05	113.80
1	A	138	LEU	N-CA-CB	-5.13	102.56	110.16
1	B	7	THR	CA-CB-OG1	-5.10	101.94	109.60
1	A	62	ASN	CA-CB-CG	-5.09	107.51	112.60
1	B	245	GLN	N-CA-CB	-5.07	102.80	110.35
1	B	173	GLU	N-CA-C	-5.03	105.51	111.69

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267	ARG	Sidechain
1	A	94	ARG	Sidechain
1	B	170	ARG	Sidechain
1	B	257	ARG	Sidechain
1	B	304	ARG	Sidechain
1	B	94	ARG	Sidechain

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	2420	0	2310	25	0
1	B	2381	0	2290	41	0
2	A	137	0	0	1	0
2	B	136	0	0	4	0
All	All	5074	0	4600	60	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 6.

All (60) 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	1.29	1.07
1:B:191:VAL:HG23	1:B:240:THR:HG23	1.59	0.84
1:A:91:GLU:OE1	1:A:114:HIS:ND1	2.10	0.83
1:B:270:GLU:HA	1:B:270:GLU:OE1	1.82	0.80
1:A:239:ASN:HA	1:A:267:ARG:HH22	1.55	0.72
1:B:119:GLU:OE1	2:B:401:HOH:O	2.11	0.68
1:A:95:GLN:NE2	2:A:402:HOH:O	2.28	0.65
1:A:133:LYS:NZ	1:A:325:TYR:O	2.32	0.62
1:A:233:PHE:CZ	1:A:267:ARG:HD2	2.38	0.58
1:A:181:ALA:O	1:A:182:PHE:C	2.46	0.58
1:B:222:CYS:SG	2:B:482:HOH:O	2.57	0.58
1:A:189:ASP:CG	1:A:268:ARG:HH22	2.12	0.58
1:A:309:ALA:O	1:A:310:ARG:CB	2.51	0.57
1:B:82:ASN:OD1	1:B:82:ASN:N	2.39	0.56
1:B:94:ARG:HG2	2:B:443:HOH:O	2.05	0.55
1:B:248:GLU:HG2	1:B:287:ILE:HD11	1.88	0.55
1:A:4:MET:HE2	1:A:119:GLU:HG3	1.88	0.55
1:B:91:GLU:OE1	1:B:114:HIS:ND1	2.31	0.55
1:A:243:PHE:HE2	1:A:299:TYR:CE1	2.26	0.53
1:A:29:CYS:SG	1:A:57:SER:HB2	2.50	0.52
1:B:108:ASP:O	1:B:109:SER:O	2.27	0.52
1:B:178:ARG:NH1	1:B:270:GLU:OE2	2.43	0.51
1:B:248:GLU:HG2	1:B:287:ILE:CD1	2.41	0.51
1:B:241:PRO:HG3	1:B:268:ARG:HH12	1.76	0.50
1:B:185:GLU:OE1	1:B:185:GLU:N	2.44	0.50
1:A:63:ASN:OD1	1:B:45:LYS:HE3	2.12	0.50
1:B:299:TYR:HB2	1:B:300:PRO:HD3	1.93	0.49
1:B:107:MET:SD	1:B:120:THR:HB	2.52	0.49
1:B:181:ALA:O	1:B:182:PHE:C	2.56	0.48
1:B:184:GLN:HE21	1:B:184:GLN:HA	1.78	0.48
1:A:230:HIS:HE1	1:B:85:GLU:OE1	1.97	0.47
1:B:108:ASP:O	1:B:109:SER:C	2.57	0.47
1:B:120:THR:O	1:B:136:LYS:NZ	2.48	0.47
1:A:185:GLU:N	1:A:185:GLU:OE1	2.48	0.47
1:B:112:VAL:HG13	1:B:118:VAL:HG21	1.96	0.47
1:A:214:GLU:HG2	1:A:306:LEU:HD12	1.97	0.47
1:B:245:GLN:HG3	1:B:295:PHE:CG	2.50	0.47
1:B:31:GLY:HA2	1:B:206:LEU:HD21	1.97	0.46
1:B:268:ARG:HB2	1:B:268:ARG:HH11	1.80	0.46
1:A:321:TRP:HB3	1:B:232:PRO:HA	1.96	0.46
1:B:185:GLU:HB2	1:B:186:TYR:CD1	2.51	0.45
1:B:193:TYR:CE2	1:B:234:GLU:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:O	1:A:180:GLN:HB2	2.17	0.44
1:B:185:GLU:CB	1:B:186:TYR:CD1	3.01	0.43
1:A:191:VAL:HG23	1:A:240:THR:HB	1.99	0.43
1:A:169:TRP:HA	1:A:169:TRP:CE3	2.53	0.43
1:B:56:ASN:HD22	1:B:59:GLU:H	1.65	0.43
1:B:182:PHE:CD1	1:B:270:GLU:HG2	2.54	0.43
1:A:178:ARG:HH21	1:A:181:ALA:CB	2.31	0.43
1:B:44:GLU:CD	2:B:449:HOH:O	2.62	0.43
1:B:183:ALA:HB1	1:B:305:ALA:O	2.18	0.43
1:B:309:ALA:O	1:B:310:ARG:HG3	2.19	0.42
1:A:51:THR:HG22	1:B:51:THR:CG2	2.22	0.42
1:A:63:ASN:OD1	1:B:45:LYS:CE	2.67	0.42
1:A:239:ASN:OD1	1:A:267:ARG:NH2	2.53	0.41
1:B:184:GLN:HB2	1:B:185:GLU:OE1	2.20	0.41
1:A:204:ALA:HB2	1:A:245:GLN:NE2	2.36	0.41
1:B:105:TRP:CE3	1:B:106:ILE:HD11	2.56	0.41
1:B:31:GLY:HA2	1:B:206:LEU:CD2	2.50	0.40
1:B:181:ALA:O	1:B:184:GLN:N	2.54	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	307/345 (89%)	295 (96%)	12 (4%)	0	100	100
1	B	306/345 (89%)	290 (95%)	12 (4%)	4 (1%)	9	2
All	All	613/690 (89%)	585 (95%)	24 (4%)	4 (1%)	18	8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	231	GLY
1	B	181	ALA
1	B	109	SER
1	B	266	GLY

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	243/282 (86%)	232 (96%)	11 (4%)	24	10
1	B	242/282 (86%)	228 (94%)	14 (6%)	18	6
All	All	485/564 (86%)	460 (95%)	25 (5%)	21	7

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	138	LEU
1	A	142	VAL
1	A	166	ARG
1	A	178	ARG
1	A	185	GLU
1	A	208	SER
1	A	220	SER
1	A	240	THR
1	A	306	LEU
1	A	320	MET
1	B	21	VAL
1	B	40	LYS
1	B	45	LYS
1	B	50	LEU
1	B	138	LEU
1	B	142	VAL
1	B	184	GLN
1	B	185	GLU
1	B	239	ASN

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Mol	Chain	Res	Type
1	B	240	THR
1	B	264	LYS
1	B	268	ARG
1	B	270	GLU
1	B	306	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	15	GLN
1	A	95	GLN
1	A	153	HIS
1	A	230	HIS
1	B	10	ASN
1	B	15	GLN
1	B	23	HIS
1	B	56	ASN
1	B	95	GLN
1	B	153	HIS
1	B	184	GLN
1	B	224	HIS
1	B	292	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	313/345 (90%)	0.73	35 (11%) 10 9	30, 46, 93, 123	0
1	B	308/345 (89%)	0.90	51 (16%) 4 4	30, 47, 99, 137	0
All	All	621/690 (90%)	0.81	86 (13%) 6 6	30, 47, 97, 137	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	203	ALA	5.4
1	A	218	ILE	5.2
1	A	217	TRP	4.8
1	B	192	ILE	4.7
1	A	323	VAL	4.7
1	A	191	VAL	4.7
1	B	191	VAL	4.6
1	A	220	SER	4.6
1	B	186	TYR	4.4
1	B	212	PHE	4.3
1	A	221	ALA	4.3
1	A	321	TRP	4.3
1	B	241	PRO	4.2
1	A	1	MET	4.1
1	B	211	ILE	4.0
1	A	325	TYR	4.0
1	B	309	ALA	3.9
1	B	213	MET	3.9
1	A	319	TYR	3.8
1	B	229	PHE	3.8
1	B	205	TYR	3.7
1	B	204	ALA	3.7
1	B	233	PHE	3.7
1	B	225	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	201	TYR	3.6
1	A	2	MET	3.6
1	B	106	ILE	3.6
1	B	235	ILE	3.5
1	B	243	PHE	3.4
1	B	223	ILE	3.4
1	B	306	LEU	3.4
1	A	233	PHE	3.4
1	B	221	ALA	3.2
1	B	240	THR	3.2
1	A	234	GLU	3.2
1	B	202	GLY	3.2
1	B	299	TYR	3.2
1	B	3	GLY	3.2
1	A	182	PHE	3.2
1	A	322	LYS	3.1
1	B	206	LEU	3.1
1	B	183	ALA	3.1
1	B	209	ILE	3.0
1	B	193	TYR	3.0
1	B	182	PHE	3.0
1	A	219	HIS	3.0
1	B	198	GLY	3.0
1	B	217	TRP	3.0
1	B	231	GLY	3.0
1	B	232	PRO	3.0
1	B	228	PHE	3.0
1	B	181	ALA	2.9
1	B	226	GLY	2.9
1	B	219	HIS	2.9
1	B	222	CYS	2.9
1	A	239	ASN	2.8
1	A	169	TRP	2.8
1	B	218	ILE	2.8
1	A	306	LEU	2.8
1	B	194	THR	2.8
1	A	105	TRP	2.8
1	B	197	SER	2.7
1	A	229	PHE	2.7
1	B	230	HIS	2.7
1	A	212	PHE	2.6
1	B	215	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	199	ALA	2.6
1	A	184	GLN	2.6
1	A	213	MET	2.5
1	B	195	VAL	2.5
1	B	224	HIS	2.5
1	B	242	PHE	2.5
1	A	230	HIS	2.3
1	A	240	THR	2.3
1	A	320	MET	2.3
1	A	215	MET	2.2
1	A	194	THR	2.2
1	A	106	ILE	2.2
1	A	228	PHE	2.2
1	A	190	LYS	2.2
1	B	178	ARG	2.1
1	B	187	LYS	2.1
1	B	268	ARG	2.1
1	A	222	CYS	2.0
1	A	209	ILE	2.0
1	A	186	TYR	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.