



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 06:56 AM EDT

PDB ID : 9OTU / pdb_00009otu
Title : Crystal Structure of Salmonella FraB Deglycase, E214A Mutant, Crystal Form 5
Authors : Bell, C.E.; Zakharova, K.
Deposited on : 2025-05-27
Resolution : 1.87 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

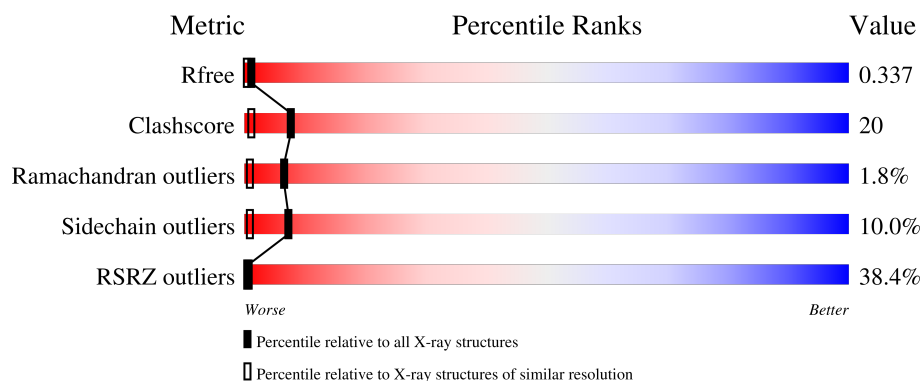
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	
1	B	345	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4709 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	303	Total	C	N	O	S	0	0	0
			2300	1472	379	439	10			
1	B	304	Total	C	N	O	S	0	0	0
			2349	1498	397	443	11			

There are 34 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	214	ALA	GLU	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	GLU	-	expression tag	UNP V7IWJ0
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	214	ALA	GLU	engineered mutation	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	34	Total O 34 34	0	0
2	B	26	Total O 26 26	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.42Å 114.42Å 154.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.09 – 1.87 99.09 – 1.87	Depositor EDS
% Data completeness (in resolution range)	36.7 (99.09-1.87) 36.7 (99.09-1.87)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.268 , 0.333 0.273 , 0.337	Depositor DCC
R_{free} test set	1718 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4709	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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	0.61	0/2355	1.26	13/3204 (0.4%)
1	B	0.59	0/2402	1.23	12/3262 (0.4%)
All	All	0.60	0/4757	1.24	25/6466 (0.4%)

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	1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	PHE	N-CA-CB	-14.87	85.35	110.49
1	B	186	TYR	N-CA-CB	-7.04	99.45	110.44
1	B	211	ILE	CB-CA-C	7.02	117.30	111.05
1	B	210	CYS	CA-C-N	-6.94	115.80	123.16
1	B	210	CYS	C-N-CA	-6.94	115.80	123.16
1	A	233	PHE	CA-CB-CG	6.86	120.66	113.80
1	A	36	PHE	N-CA-CB	-6.17	101.55	110.56
1	A	142	VAL	N-CA-CB	5.83	119.32	110.58
1	A	228	PHE	CA-CB-CG	5.71	119.51	113.80
1	A	286	VAL	CB-CA-C	-5.69	105.07	110.70
1	B	186	TYR	CB-CA-C	5.68	121.07	109.55
1	B	271	VAL	N-CA-CB	5.60	116.63	110.53
1	A	128	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	261	PHE	N-CA-CB	5.54	118.19	109.94
1	A	265	TYR	N-CA-CB	5.54	119.84	110.49
1	A	295	PHE	CB-CA-C	5.53	119.56	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	THR	CA-CB-OG1	-5.48	101.37	109.60
1	B	125	ASP	CB-CA-C	5.40	118.66	109.53
1	A	165	ASN	CA-CB-CG	-5.38	107.22	112.60
1	A	285	THR	CA-CB-OG1	-5.33	101.60	109.60
1	A	26	TYR	CB-CA-C	5.27	118.33	109.48
1	B	5	LYS	CB-CA-C	5.23	119.17	110.90
1	A	134	THR	CA-CB-OG1	-5.12	101.91	109.60
1	B	55	TYR	CB-CA-C	-5.09	99.27	109.35
1	B	243	PHE	CA-CB-CG	5.00	118.81	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	PRO	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	2300	0	2182	96	0
1	B	2349	0	2260	94	0
2	A	34	0	0	0	0
2	B	26	0	0	4	0
All	All	4709	0	4442	183	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 20.

All (183) 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	1.34	1.04
1:A:228:PHE:O	1:A:233:PHE:HB2	1.58	1.02
1:A:28:ALA:HB1	1:A:32:SER:HB3	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:THR:O	1:A:85:GLU:N	2.03	0.90
1:B:134:THR:HG21	1:B:292:HIS:CD2	2.11	0.85
1:B:21:VAL:HG12	1:B:50:LEU:HD11	1.60	0.83
1:A:7:THR:O	1:A:11:ILE:HG13	1.77	0.83
1:B:183:ALA:HB1	1:B:305:ALA:O	1.80	0.82
1:B:4:MET:O	1:B:8:VAL:HG23	1.80	0.82
1:A:3:GLY:O	1:A:7:THR:OG1	2.00	0.79
1:B:8:VAL:HG13	1:B:144:LEU:HD23	1.70	0.74
1:B:24:VAL:O	1:B:52:VAL:HA	1.89	0.72
1:A:221:ALA:HB2	1:B:221:ALA:HB2	1.72	0.71
1:A:62:ASN:HB3	1:B:250:ASN:O	1.92	0.70
1:A:61:ILE:HG21	1:A:88:LYS:HB2	1.73	0.69
1:A:178:ARG:HH11	1:A:181:ALA:HB3	1.57	0.68
1:A:264:LYS:O	1:A:265:TYR:CD2	2.47	0.68
1:A:128:ASP:HA	1:A:165:ASN:HD21	1.60	0.66
1:B:183:ALA:CB	1:B:305:ALA:O	2.42	0.66
1:A:30:GLY:HA2	1:B:227:GLU:OE2	1.96	0.66
1:A:112:VAL:HG13	1:A:118:VAL:HG21	1.79	0.65
1:B:14:SER:OG	1:B:15:GLN:HG2	1.96	0.65
1:B:42:PHE:O	1:B:46:GLU:HG2	1.98	0.64
1:A:211:ILE:HG21	1:A:303:ASN:OD1	1.97	0.64
1:B:224:HIS:O	1:B:225:SER:C	2.42	0.63
1:B:245:GLN:HG3	1:B:295:PHE:CE1	2.34	0.63
1:A:211:ILE:HG21	1:A:303:ASN:CG	2.24	0.63
1:B:6:GLU:OE1	1:B:10:ASN:OD1	2.17	0.62
1:A:175:VAL:CG1	1:A:175:VAL:O	2.47	0.62
1:B:300:PRO:CB	1:B:304:ARG:HH12	2.13	0.62
1:B:36:PHE:CZ	1:B:77:ALA:HB2	2.35	0.62
1:A:33:TYR:C	1:A:33:TYR:CD1	2.77	0.61
1:A:178:ARG:NH2	1:A:270:GLU:OE2	2.32	0.61
1:B:169:TRP:CE3	1:B:169:TRP:HA	2.35	0.60
1:B:300:PRO:HB3	1:B:304:ARG:HH12	1.66	0.60
1:A:51:THR:HG22	1:B:51:THR:CG2	2.21	0.60
1:A:218:ILE:CG2	1:A:219:HIS:N	2.65	0.60
1:B:136:LYS:HD2	1:B:136:LYS:N	2.16	0.60
1:A:178:ARG:HH11	1:A:181:ALA:CB	2.14	0.60
1:A:159:ASP:O	1:A:160:GLY:C	2.45	0.60
1:A:117:TYR:O	1:A:118:VAL:HG23	2.02	0.59
1:A:192:ILE:O	1:A:220:SER:HA	2.03	0.59
1:A:104:THR:HB	1:A:111:LEU:HD23	1.85	0.58
1:B:249:GLY:HA3	1:B:288:ASP:OD1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:THR:CG2	1:B:121:TYR:H	2.16	0.58
1:A:145:LEU:HD23	1:A:151:TYR:HB2	1.86	0.58
1:B:23:HIS:HA	1:B:51:THR:OG1	2.02	0.58
1:A:28:ALA:HB1	1:A:32:SER:CB	2.26	0.58
1:A:232:PRO:HA	1:B:213:MET:HE2	1.85	0.57
1:A:61:ILE:HD13	1:A:85:GLU:HA	1.86	0.56
1:A:232:PRO:O	1:A:235:ILE:HD12	2.04	0.56
1:B:23:HIS:O	1:B:72:ALA:HA	2.05	0.56
1:B:169:TRP:HA	1:B:169:TRP:HE3	1.69	0.56
1:A:206:LEU:HD23	1:A:210:CYS:HB2	1.88	0.56
1:A:237:ASP:HB2	1:A:240:THR:OG1	2.05	0.56
1:B:113:ALA:O	1:B:114:HIS:CG	2.58	0.56
1:A:107:MET:HA	1:A:112:VAL:HG21	1.89	0.55
1:A:138:LEU:O	1:A:142:VAL:HG13	2.06	0.55
1:A:213:MET:O	1:A:214:ALA:HB2	2.07	0.55
1:B:245:GLN:HG3	1:B:295:PHE:CZ	2.42	0.55
1:B:241:PRO:HA	1:B:268:ARG:O	2.07	0.54
1:B:120:THR:CG2	1:B:121:TYR:N	2.71	0.53
1:A:83:THR:O	1:A:84:PRO:C	2.51	0.53
1:B:120:THR:HG22	1:B:121:TYR:N	2.24	0.53
1:A:128:ASP:HA	1:A:165:ASN:ND2	2.24	0.53
1:B:13:THR:O	1:B:14:SER:C	2.52	0.53
1:B:306:LEU:HD22	1:B:310:ARG:HD2	1.91	0.53
1:B:175:VAL:HG23	1:B:301:VAL:HG11	1.90	0.53
1:A:37:TYR:N	1:A:38:PRO:CD	2.72	0.52
1:A:249:GLY:HA3	1:A:288:ASP:OD1	2.09	0.52
1:B:135:MET:SD	1:B:161:VAL:HG22	2.49	0.52
1:A:105:TRP:CE3	1:A:106:ILE:HD11	2.46	0.51
1:B:43:LEU:O	1:B:44:GLU:C	2.52	0.51
1:B:8:VAL:HG13	1:B:144:LEU:CD2	2.40	0.51
1:B:192:ILE:O	1:B:220:SER:HB2	2.10	0.51
1:B:35:ALA:O	1:B:134:THR:HG23	2.11	0.51
1:B:91:GLU:HG2	1:B:114:HIS:CE1	2.46	0.51
1:B:313:PRO:C	1:B:315:THR:N	2.67	0.51
1:B:279:LEU:HD22	1:B:282:ILE:HD12	1.93	0.50
1:A:30:GLY:O	1:A:34:ALA:N	2.44	0.50
1:A:175:VAL:O	1:A:175:VAL:HG13	2.10	0.50
1:A:108:ASP:OD1	1:A:108:ASP:N	2.37	0.50
1:A:7:THR:HG22	1:A:117:TYR:CD2	2.47	0.50
1:B:239:ASN:O	1:B:268:ARG:HD3	2.12	0.49
1:B:18:LYS:HG2	1:B:70:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ILE:HG22	1:A:219:HIS:N	2.27	0.49
1:B:44:GLU:OE1	2:B:401:HOH:O	2.20	0.49
1:A:78:SER:HB2	1:A:86:THR:HG21	1.94	0.49
1:B:95:GLN:C	1:B:96:HIS:HD1	2.20	0.49
1:B:192:ILE:O	1:B:220:SER:CB	2.61	0.49
1:A:51:THR:CG2	1:B:51:THR:HG22	2.24	0.49
1:A:82:ASN:OD1	1:A:82:ASN:N	2.46	0.49
1:B:4:MET:O	1:B:8:VAL:CG2	2.58	0.49
1:A:4:MET:O	1:A:8:VAL:HG23	2.12	0.48
1:A:115:CYS:HB3	1:A:117:TYR:O	2.13	0.48
1:A:42:PHE:HA	1:A:289:TYR:CE1	2.48	0.48
1:A:69:GLY:O	1:A:98:ALA:HB2	2.13	0.48
1:A:143:GLU:OE2	1:A:154:TYR:OH	2.22	0.48
1:B:21:VAL:HG22	2:B:419:HOH:O	2.14	0.48
1:A:83:THR:HB	1:A:86:THR:HB	1.95	0.48
1:A:197:SER:HB3	1:A:225:SER:OG	2.14	0.47
1:B:215:MET:HG2	1:B:317:ARG:HH12	1.79	0.47
1:A:112:VAL:HG12	1:A:112:VAL:O	2.14	0.47
1:B:129:ILE:HB	1:B:165:ASN:HA	1.96	0.47
1:A:192:ILE:O	1:A:220:SER:OG	2.32	0.47
1:B:105:TRP:CZ3	1:B:123:PHE:HB3	2.49	0.47
1:A:299:TYR:N	1:A:300:PRO:CD	2.77	0.47
1:B:245:GLN:HG3	1:B:295:PHE:CD1	2.49	0.47
1:A:25:TYR:HB2	1:A:74:VAL:HG22	1.96	0.47
1:A:74:VAL:HG12	1:A:100:VAL:HG22	1.96	0.47
1:B:216:GLN:OE1	1:B:310:ARG:HD3	2.15	0.47
1:A:195:VAL:HG22	1:A:223:ILE:HB	1.97	0.47
1:A:224:HIS:HB3	1:A:227:GLU:HB2	1.96	0.47
1:B:268:ARG:C	1:B:269:ILE:HG13	2.39	0.47
1:B:42:PHE:CZ	1:B:142:VAL:HG22	2.50	0.47
1:B:207:GLN:NE2	1:B:211:ILE:HD11	2.30	0.47
1:B:94:ARG:HD3	1:B:116:ASP:OD1	2.15	0.47
1:B:182:PHE:CD1	1:B:186:TYR:CD2	3.03	0.47
1:A:252:ARG:NH2	1:A:273:ASP:OD2	2.43	0.46
1:B:73:VAL:HG22	1:B:99:PRO:HG2	1.98	0.46
1:A:103:LEU:HD21	1:A:136:LYS:CB	2.45	0.46
1:A:127:LYS:HE3	1:A:129:ILE:HD13	1.98	0.46
1:B:273:ASP:HB3	1:B:276:ALA:HB3	1.98	0.46
1:A:206:LEU:O	1:A:210:CYS:HB2	2.16	0.45
1:A:258:ALA:O	1:A:262:LEU:HD12	2.17	0.45
1:B:294:LEU:O	1:B:295:PHE:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:GLY:HA3	1:B:71:ASN:HD21	1.81	0.45
1:A:292:HIS:C	1:A:292:HIS:CD2	2.94	0.45
1:B:135:MET:O	1:B:139:LEU:HG	2.17	0.45
1:B:154:TYR:C	1:B:154:TYR:CD1	2.94	0.45
1:A:28:ALA:HB3	1:A:32:SER:C	2.42	0.45
1:B:76:VAL:HG11	1:B:90:ALA:HB2	1.98	0.45
1:A:4:MET:HA	1:A:7:THR:OG1	2.17	0.44
1:B:216:GLN:CB	1:B:218:ILE:HD12	2.48	0.44
1:A:79:HIS:HA	1:A:121:TYR:OH	2.17	0.44
1:B:159:ASP:O	1:B:162:SER:OG	2.30	0.44
1:A:104:THR:HG21	1:A:112:VAL:CG2	2.47	0.44
1:A:237:ASP:HB3	1:A:239:ASN:H	1.83	0.44
1:B:122:THR:HB	1:B:127:LYS:HB2	2.00	0.44
1:B:279:LEU:O	1:B:281:THR:N	2.50	0.44
1:A:186:TYR:CE1	1:A:241:PRO:HB3	2.52	0.43
1:B:171:ALA:O	1:B:175:VAL:HG22	2.19	0.43
1:B:47:ALA:HB2	1:B:145:LEU:HD13	2.01	0.43
1:A:176:ALA:C	1:A:178:ARG:N	2.75	0.43
1:A:61:ILE:CG2	1:A:88:LYS:HB2	2.47	0.43
1:A:170:ARG:HG3	1:A:170:ARG:HH11	1.82	0.43
1:B:181:ALA:O	1:B:182:PHE:C	2.60	0.43
1:B:200:GLY:C	2:B:402:HOH:O	2.60	0.43
1:B:30:GLY:O	1:B:33:TYR:HB3	2.19	0.42
1:A:129:ILE:C	1:A:131:GLY:N	2.76	0.42
1:B:191:VAL:O	1:B:241:PRO:HG2	2.18	0.42
1:A:186:TYR:O	1:A:187:LYS:C	2.61	0.42
1:A:211:ILE:HG22	1:A:212:PHE:N	2.33	0.42
1:B:82:ASN:HB3	1:B:110:PRO:HD2	2.00	0.42
1:B:224:HIS:O	1:B:225:SER:O	2.37	0.42
1:B:313:PRO:C	1:B:315:THR:H	2.27	0.42
1:A:231:GLY:N	1:A:232:PRO:CD	2.83	0.41
1:A:7:THR:HG22	1:A:117:TYR:CG	2.54	0.41
1:B:8:VAL:HA	1:B:11:ILE:HD12	2.02	0.41
1:B:49:ALA:HB3	1:B:149:GLU:OE1	2.20	0.41
1:A:78:SER:OG	1:A:79:HIS:N	2.53	0.41
1:A:38:PRO:HB2	1:A:138:LEU:HD13	2.01	0.41
1:A:107:MET:O	1:A:112:VAL:HB	2.21	0.41
1:A:175:VAL:HG12	1:A:301:VAL:HG11	2.03	0.41
1:A:60:PHE:CE1	1:A:65:PRO:CD	3.04	0.41
1:A:177:GLU:C	1:A:178:ARG:HG2	2.46	0.41
1:B:102:GLY:CA	1:B:115:CYS:SG	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ILE:HB	1:A:165:ASN:OD1	2.21	0.41
1:A:135:MET:HE3	1:A:135:MET:HA	2.03	0.41
1:A:164:ILE:HD12	1:A:164:ILE:HA	1.94	0.41
1:B:300:PRO:HB2	1:B:304:ARG:HH12	1.85	0.41
1:B:300:PRO:HB3	1:B:304:ARG:NH1	2.34	0.40
1:A:207:GLN:HE22	1:A:211:ILE:HG21	1.85	0.40
1:B:10:ASN:HB3	1:B:117:TYR:OH	2.21	0.40
1:B:164:ILE:O	1:B:165:ASN:C	2.62	0.40
1:B:195:VAL:O	1:B:245:GLN:HB3	2.21	0.40
1:A:176:ALA:C	1:A:178:ARG:H	2.28	0.40
1:B:94:ARG:HA	2:B:408:HOH:O	2.20	0.40
1:A:93:ALA:HB3	1:A:100:VAL:HG21	2.04	0.40
1:B:94:ARG:NH2	1:B:114:HIS:HA	2.36	0.40
1:B:104:THR:O	1:B:120:THR:OG1	2.19	0.40
1:B:274:ALA:HB2	1:B:295:PHE:CE2	2.57	0.40
1:A:61:ILE:CD1	1:A:85:GLU:HA	2.52	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	301/345 (87%)	257 (85%)	38 (13%)	6 (2%)	6	0
1	B	298/345 (86%)	264 (89%)	29 (10%)	5 (2%)	7	1
All	All	599/690 (87%)	521 (87%)	67 (11%)	11 (2%)	6	1

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	PRO
1	A	177	GLU

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Mol	Chain	Res	Type
1	A	214	ALA
1	A	233	PHE
1	A	265	TYR
1	B	114	HIS
1	A	85	GLU
1	B	115	CYS
1	B	314	LEU
1	B	280	SER
1	B	263	LYS

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	231/281 (82%)	207 (90%)	24 (10%)	7	1
1	B	239/281 (85%)	216 (90%)	23 (10%)	8	1
All	All	470/562 (84%)	423 (90%)	47 (10%)	7	1

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	14	SER
1	A	17	GLU
1	A	21	VAL
1	A	57	SER
1	A	74	VAL
1	A	86	THR
1	A	103	LEU
1	A	108	ASP
1	A	120	THR
1	A	122	THR
1	A	134	THR
1	A	142	VAL
1	A	164	ILE

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Mol	Chain	Res	Type
1	A	172	CYS
1	A	175	VAL
1	A	178	ARG
1	A	211	ILE
1	A	225	SER
1	A	235	ILE
1	A	248	GLU
1	A	280	SER
1	A	281	THR
1	A	283	LYS
1	B	7	THR
1	B	17	GLU
1	B	82	ASN
1	B	117	TYR
1	B	120	THR
1	B	122	THR
1	B	155	ASP
1	B	159	ASP
1	B	168	VAL
1	B	169	TRP
1	B	187	LYS
1	B	189	ASP
1	B	208	SER
1	B	211	ILE
1	B	243	PHE
1	B	248	GLU
1	B	262	LEU
1	B	271	VAL
1	B	279	LEU
1	B	293	SER
1	B	298	VAL
1	B	306	LEU
1	B	315	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	56	ASN
1	A	71	ASN
1	A	146	GLN
1	A	174	GLN

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Mol	Chain	Res	Type
1	A	216	GLN
1	A	297	ASN
1	B	23	HIS
1	B	62	ASN
1	B	71	ASN
1	B	82	ASN
1	B	95	GLN
1	B	219	HIS
1	B	224	HIS
1	B	239	ASN
1	B	292	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 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	303/345 (87%)	1.63	99 (32%) 1 1	14, 37, 70, 93	0
1	B	304/345 (88%)	1.96	134 (44%) 0 0	20, 45, 64, 79	0
All	All	607/690 (87%)	1.80	233 (38%) 1 0	14, 42, 68, 93	0

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	LEU	7.9
1	B	105	TRP	7.1
1	A	115	CYS	6.6
1	A	126	GLY	6.3
1	B	169	TRP	6.2
1	A	110	PRO	6.0
1	B	106	ILE	6.0
1	A	105	TRP	5.7
1	B	262	LEU	5.6
1	A	69	GLY	5.6
1	B	171	ALA	5.5
1	A	60	PHE	5.4
1	B	103	LEU	5.0
1	A	180	GLN	5.0
1	B	271	VAL	5.0
1	A	82	ASN	5.0
1	B	251	THR	4.9
1	A	96	HIS	4.9
1	A	106	ILE	4.9
1	A	114	HIS	4.7
1	A	176	ALA	4.6
1	B	170	ARG	4.6
1	A	118	VAL	4.6
1	A	181	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	123	PHE	4.6
1	B	265	TYR	4.5
1	B	244	PHE	4.5
1	A	113	ALA	4.5
1	B	112	VAL	4.4
1	B	111	LEU	4.4
1	A	61	ILE	4.4
1	A	209	ILE	4.4
1	B	264	LYS	4.4
1	B	294	LEU	4.4
1	B	320	MET	4.4
1	A	84	PRO	4.4
1	A	124	GLY	4.3
1	A	120	THR	4.2
1	A	168	VAL	4.2
1	A	92	ILE	4.2
1	A	103	LEU	4.1
1	A	112	VAL	4.1
1	B	100	VAL	4.1
1	B	295	PHE	4.1
1	A	68	LEU	4.1
1	B	261	PHE	4.0
1	B	272	VAL	4.0
1	A	217	TRP	4.0
1	B	246	PHE	4.0
1	B	177	GLU	4.0
1	A	93	ALA	4.0
1	A	78	SER	3.9
1	B	281	THR	3.9
1	B	157	PHE	3.9
1	A	86	THR	3.9
1	B	102	GLY	3.9
1	A	88	LYS	3.9
1	A	218	ILE	3.9
1	A	90	ALA	3.8
1	A	183	ALA	3.8
1	B	113	ALA	3.8
1	B	118	VAL	3.8
1	A	279	LEU	3.8
1	A	214	ALA	3.8
1	B	287	ILE	3.8
1	B	301	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	117	TYR	3.7
1	A	305	ALA	3.7
1	A	87	ILE	3.7
1	B	168	VAL	3.7
1	B	145	LEU	3.7
1	A	94	ARG	3.7
1	A	116	ASP	3.6
1	A	167	ILE	3.6
1	B	90	ALA	3.6
1	B	172	CYS	3.6
1	A	91	GLU	3.6
1	A	107	MET	3.6
1	B	276	ALA	3.5
1	A	29	CYS	3.5
1	B	180	GLN	3.5
1	B	269	ILE	3.5
1	B	196	ALA	3.5
1	B	139	LEU	3.4
1	B	4	MET	3.4
1	B	247	SER	3.3
1	B	284	THR	3.3
1	B	73	VAL	3.3
1	B	107	MET	3.3
1	A	123	PHE	3.3
1	A	187	LYS	3.3
1	A	125	ASP	3.3
1	A	304	ARG	3.3
1	A	184	GLN	3.2
1	A	122	THR	3.2
1	B	259	LEU	3.2
1	B	182	PHE	3.2
1	B	173	GLU	3.2
1	B	239	ASN	3.2
1	B	94	ARG	3.2
1	B	223	ILE	3.2
1	B	305	ALA	3.2
1	B	144	LEU	3.2
1	B	242	PHE	3.2
1	B	184	GLN	3.2
1	A	102	GLY	3.1
1	A	277	LEU	3.1
1	B	8	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	282	ILE	3.1
1	A	127	LYS	3.1
1	B	99	PRO	3.1
1	A	301	VAL	3.1
1	B	142	VAL	3.1
1	B	110	PRO	3.0
1	B	286	VAL	3.0
1	B	148	THR	3.0
1	A	95	GLN	3.0
1	A	66	VAL	3.0
1	A	298	VAL	3.0
1	A	109	SER	3.0
1	A	17	GLU	3.0
1	B	6	GLU	3.0
1	B	76	VAL	2.9
1	B	186	TYR	2.9
1	B	124	GLY	2.9
1	B	249	GLY	2.9
1	A	215	MET	2.9
1	A	177	GLU	2.9
1	B	98	ALA	2.9
1	B	304	ARG	2.9
1	A	213	MET	2.9
1	A	3	GLY	2.9
1	B	254	VAL	2.8
1	A	243	PHE	2.8
1	A	32	SER	2.8
1	A	164	ILE	2.8
1	B	101	ILE	2.8
1	B	167	ILE	2.8
1	B	289	TYR	2.8
1	B	183	ALA	2.8
1	B	298	VAL	2.8
1	A	274	ALA	2.8
1	B	257	ARG	2.8
1	B	161	VAL	2.8
1	A	178	ARG	2.7
1	A	179	ALA	2.7
1	B	268	ARG	2.7
1	A	79	HIS	2.7
1	B	79	HIS	2.7
1	B	291	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	128	ASP	2.7
1	B	134	THR	2.7
1	B	9	SER	2.7
1	A	104	THR	2.7
1	B	20	GLY	2.6
1	A	169	TRP	2.6
1	A	85	GLU	2.6
1	B	138	LEU	2.6
1	B	314	LEU	2.6
1	A	175	VAL	2.6
1	B	166	ARG	2.6
1	B	116	ASP	2.6
1	B	179	ALA	2.6
1	A	271	VAL	2.6
1	A	275	ALA	2.6
1	B	16	ALA	2.6
1	B	121	TYR	2.5
1	B	243	PHE	2.5
1	B	185	GLU	2.5
1	B	277	LEU	2.5
1	A	81	GLY	2.5
1	B	274	ALA	2.5
1	B	309	ALA	2.5
1	B	155	ASP	2.5
1	B	126	GLY	2.5
1	B	200	GLY	2.5
1	A	265	TYR	2.5
1	B	212	PHE	2.5
1	A	269	ILE	2.5
1	A	70	GLU	2.5
1	B	260	ASN	2.4
1	B	306	LEU	2.4
1	A	238	ALA	2.4
1	B	120	THR	2.4
1	A	71	ASN	2.4
1	B	240	THR	2.4
1	B	18	LYS	2.4
1	B	154	TYR	2.4
1	A	233	PHE	2.4
1	A	166	ARG	2.4
1	B	156	ASP	2.3
1	B	49	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	253	ALA	2.3
1	B	10	ASN	2.3
1	B	97	GLY	2.3
1	B	175	VAL	2.3
1	A	89	ALA	2.3
1	B	226	GLY	2.3
1	A	294	LEU	2.3
1	A	121	TYR	2.3
1	A	278	GLY	2.3
1	A	77	ALA	2.2
1	A	212	PHE	2.2
1	B	275	ALA	2.2
1	B	87	ILE	2.2
1	B	164	ILE	2.2
1	A	18	LYS	2.2
1	A	100	VAL	2.2
1	B	125	ASP	2.2
1	B	197	SER	2.2
1	B	135	MET	2.2
1	B	195	VAL	2.2
1	B	302	TYR	2.1
1	A	101	ILE	2.1
1	B	129	ILE	2.1
1	B	147	GLN	2.1
1	B	19	GLY	2.1
1	B	300	PRO	2.1
1	B	258	ALA	2.1
1	B	95	GLN	2.1
1	B	81	GLY	2.1
1	B	163	LYS	2.1
1	B	78	SER	2.1
1	A	83	THR	2.1
1	B	46	GLU	2.1
1	A	28	ALA	2.1
1	B	130	ALA	2.1
1	A	211	ILE	2.0
1	A	280	SER	2.0
1	B	136	LYS	2.0
1	B	74	VAL	2.0
1	B	279	LEU	2.0
1	B	151	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.