Full wwPDB X-ray Structure Validation Report ⓘ

Apr 16, 2025 – 01:16 pm BST

PDB ID	:	9EUX / pdb_00009eux
Title	:	Glycoside hydrolase familiy 191 enzyme from Thermotoga maritima
Authors	:	Roth, C.
Deposited on	:	2024-03-28
Resolution	:	2.40 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:

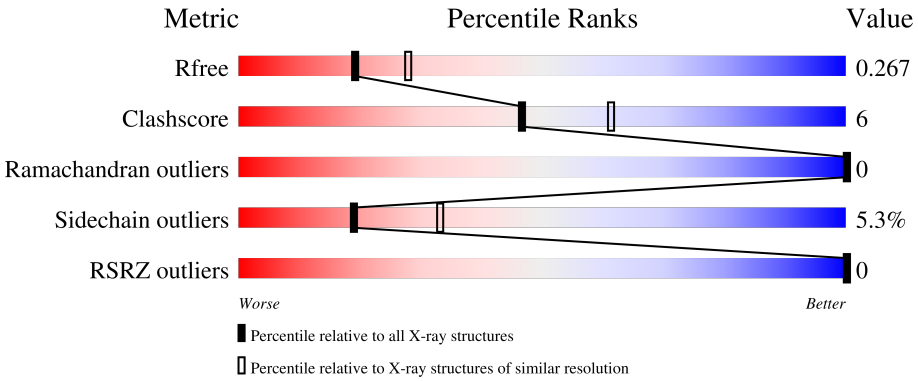
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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 <=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	323	75% 12% • 12%
1	B	323	70% 15% • 12%
1	C	323	69% 15% •• 13%
1	D	323	72% 13% • 13%
1	E	323	76% 9% • 13%

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Mol	Chain	Length	Quality of chain
1	G	323	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 27992 atoms, of which 13354 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 Uncharacterized protein TM_1410.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	G	284	Total	C	H	N	O	S	47	4	0
			4606	1524	2240	376	460	6			
1	E	282	Total	C	H	N	O	S	46	2	0
			4560	1510	2217	372	455	6			
1	C	282	Total	C	H	N	O	S	46	4	0
			4592	1519	2235	376	456	6			
1	D	280	Total	C	H	N	O	S	46	2	0
			4538	1503	2208	370	451	6			
1	B	284	Total	C	H	N	O	S	46	0	0
			4573	1515	2223	373	456	6			
1	A	283	Total	C	H	N	O	S	46	2	0
			4583	1516	2231	376	454	6			

- Molecule 2 is water.

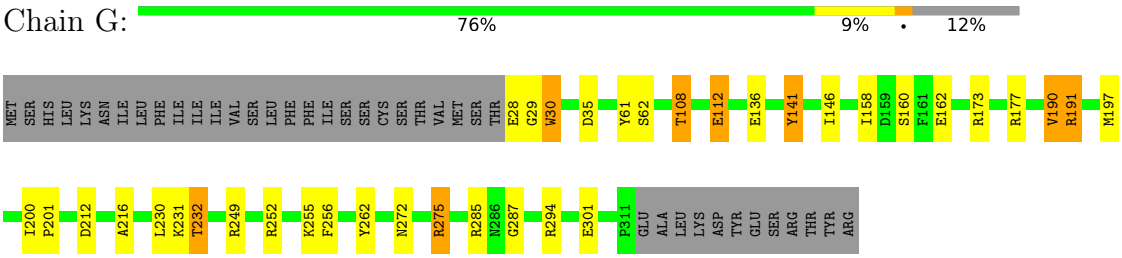
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	83	Total	O	0	0
			83	83		
2	E	92	Total	O	0	0
			92	92		
2	C	75	Total	O	0	0
			75	75		
2	D	93	Total	O	0	0
			93	93		
2	B	94	Total	O	0	0
			94	94		
2	A	103	Total	O	0	0
			103	103		

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.

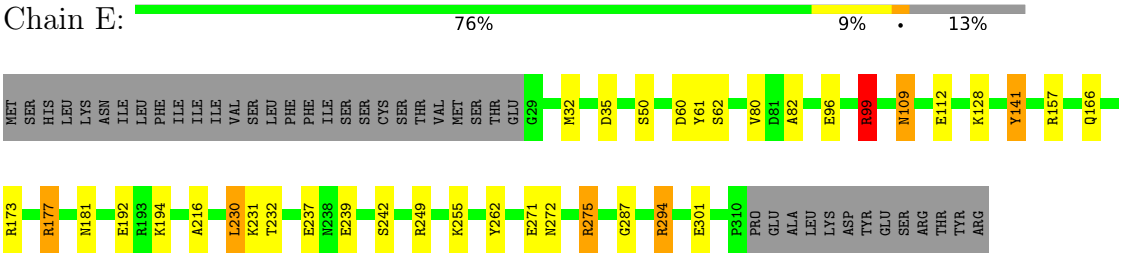
• Molecule 1: Uncharacterized protein TM_1410

Chain G:



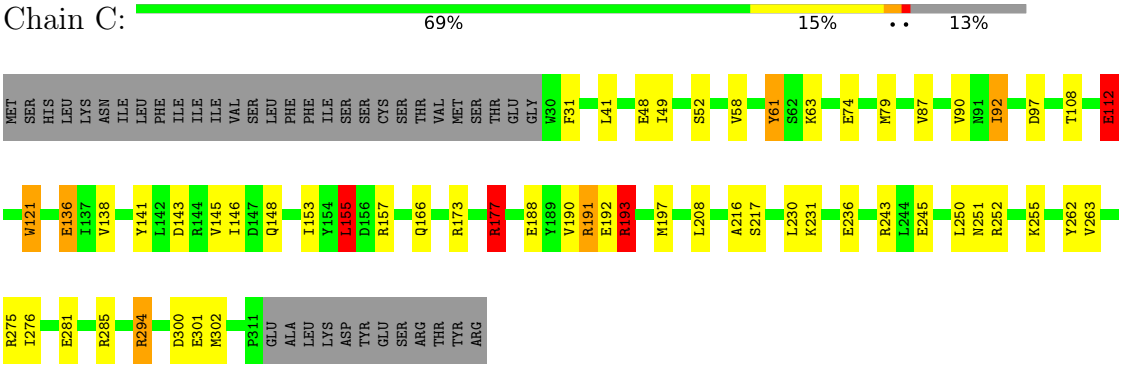
• Molecule 1: Uncharacterized protein TM_1410

Chain E:



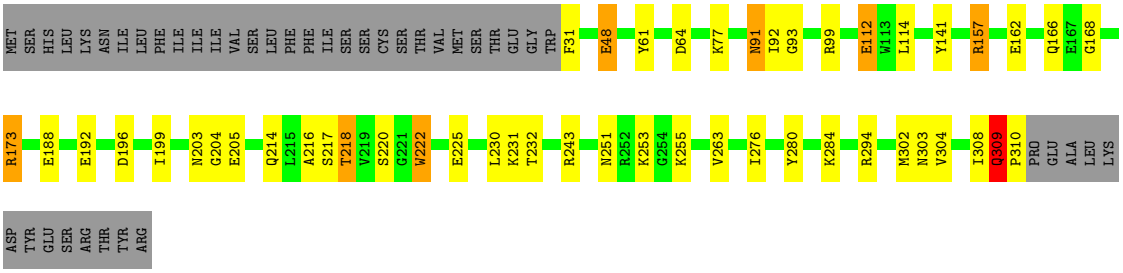
• Molecule 1: Uncharacterized protein TM_1410

Chain C:



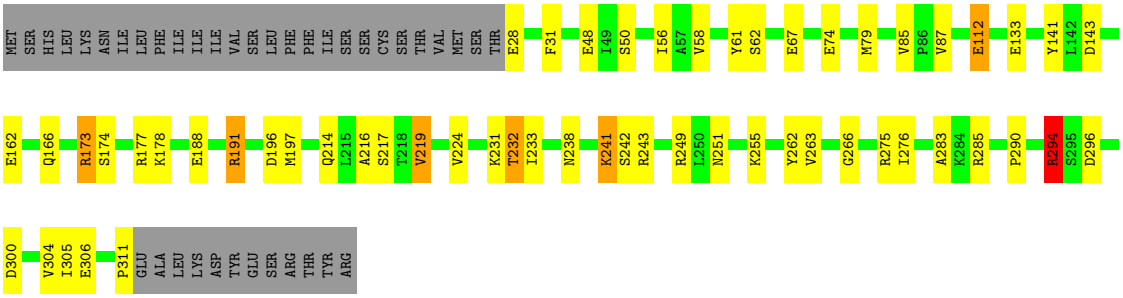
• Molecule 1: Uncharacterized protein TM_1410

Chain D:



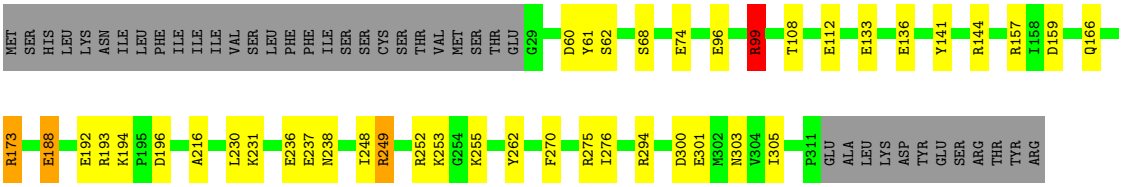
• Molecule 1: Uncharacterized protein TM_1410

Chain B:



• Molecule 1: Uncharacterized protein TM_1410

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	195.19Å 84.50Å 195.48Å 90.00° 119.91° 90.00°	Depositor
Resolution (Å)	48.95 – 2.40 48.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.95-2.40) 99.4 (48.95-2.40)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0425, REFMAC 5.8.0425	Depositor
R, R_{free}	0.236 , 0.264 0.237 , 0.267	Depositor DCC
R_{free} test set	11154 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 22.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.207 for -h-l,k,h 0.207 for l,k,-h-l 0.098 for h,-k,-h-l 0.096 for -h-l,-k,l 0.098 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	27992	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 7.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.68	2/2423 (0.1%)	1.19	11/3290 (0.3%)
1	B	0.68	1/2415 (0.0%)	1.16	16/3280 (0.5%)
1	C	0.70	3/2444 (0.1%)	1.18	24/3319 (0.7%)
1	D	0.70	3/2399 (0.1%)	1.15	9/3258 (0.3%)
1	E	0.64	3/2423 (0.1%)	1.13	10/3291 (0.3%)
1	G	0.68	3/2448 (0.1%)	1.12	13/3326 (0.4%)
All	All	0.68	15/14552 (0.1%)	1.15	83/19764 (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	3
1	B	0	3
1	C	0	3
1	D	0	4
1	E	0	1
1	G	0	1
All	All	0	15

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	192	GLU	CD-OE2	10.04	1.36	1.25
1	D	192	GLU	CD-OE1	7.15	1.33	1.25
1	E	192	GLU	CD-OE1	7.03	1.33	1.25
1	G	136	GLU	CD-OE2	6.97	1.33	1.25
1	C	136	GLU	CD-OE2	6.87	1.33	1.25
1	C	136	GLU	CD-OE1	6.19	1.32	1.25
1	E	192	GLU	CD-OE2	5.97	1.32	1.25
1	B	28	GLU	CD-OE1	5.91	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	192	GLU	CG-CD	5.73	1.60	1.51
1	G	162	GLU	CD-OE2	5.73	1.31	1.25
1	G	136	GLU	CD-OE1	5.61	1.31	1.25
1	A	136	GLU	CD-OE1	5.60	1.31	1.25
1	D	112	GLU	CD-OE1	5.37	1.31	1.25
1	A	136	GLU	CD-OE2	5.36	1.31	1.25
1	C	192	GLU	CD-OE2	5.13	1.31	1.25

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	99	ARG	NE-CZ-NH1	15.12	127.86	120.30
1	C	300	ASP	CB-CA-C	-13.09	84.22	110.40
1	D	309	GLN	N-CA-CB	12.43	132.98	110.60
1	A	300	ASP	CB-CA-C	-12.12	86.17	110.40
1	A	99	ARG	NE-CZ-NH2	-12.10	114.25	120.30
1	E	99	ARG	NE-CZ-NH1	11.99	126.30	120.30
1	B	300	ASP	CB-CA-C	-11.98	86.44	110.40
1	D	99	ARG	NE-CZ-NH1	-11.63	114.49	120.30
1	E	99	ARG	NE-CZ-NH2	-11.62	114.49	120.30
1	A	99	ARG	CD-NE-CZ	11.31	139.43	123.60
1	B	191	ARG	NE-CZ-NH2	10.86	125.73	120.30
1	C	191	ARG	NE-CZ-NH2	10.23	125.41	120.30
1	D	157	ARG	NE-CZ-NH1	-10.15	115.23	120.30
1	E	99	ARG	CD-NE-CZ	9.69	137.17	123.60
1	D	64	ASP	CB-CA-C	-9.59	91.22	110.40
1	E	275	ARG	NE-CZ-NH2	-9.49	115.56	120.30
1	G	191	ARG	CG-CD-NE	9.39	131.52	111.80
1	E	157	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	B	191	ARG	CG-CD-NE	9.01	130.72	111.80
1	C	191	ARG	CG-CD-NE	8.35	129.34	111.80
1	C	155	LEU	CB-CG-CD1	7.72	124.12	111.00
1	A	275	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	B	214	GLN	N-CA-CB	7.66	124.39	110.60
1	C	173	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	B	191	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	D	243	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	B	173	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	G	177	ARG	NE-CZ-NH2	6.99	123.80	120.30
1	G	177	ARG	NE-CZ-NH1	-6.83	116.88	120.30
1	C	193[A]	ARG	CD-NE-CZ	6.82	133.15	123.60
1	C	193[B]	ARG	CD-NE-CZ	6.82	133.15	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	136	GLU	OE1-CD-OE2	6.82	131.48	123.30
1	E	109	ASN	CB-CA-C	6.72	123.85	110.40
1	G	108	THR	CA-CB-OG1	6.70	123.08	109.00
1	C	275	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	C	79	MET	CG-SD-CE	-6.64	89.57	100.20
1	C	108	THR	CA-CB-OG1	6.55	122.76	109.00
1	A	136	GLU	OE1-CD-OE2	6.55	131.16	123.30
1	A	157	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	G	173	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	G	275	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	D	157	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	A	144	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	C	121	TRP	CA-CB-CG	6.10	125.29	113.70
1	C	285	ARG	CA-CB-CG	6.10	126.82	113.40
1	C	74	GLU	CG-CD-OE1	6.06	130.41	118.30
1	A	99	ARG	CG-CD-NE	5.94	124.27	111.80
1	G	173	ARG	CD-NE-CZ	5.89	131.84	123.60
1	E	173	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	219	VAL	N-CA-CB	-5.82	98.71	111.50
1	E	173	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	D	48	GLU	OE1-CD-OE2	-5.73	116.42	123.30
1	C	275	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	D	218	THR	CA-CB-OG1	-5.70	97.04	109.00
1	B	173	ARG	CD-NE-CZ	5.64	131.49	123.60
1	C	188	GLU	CG-CD-OE2	-5.62	107.07	118.30
1	B	275	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	155	LEU	CB-CG-CD2	-5.57	101.53	111.00
1	B	294	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	D	173	ARG	CB-CG-CD	5.56	126.05	111.60
1	B	173	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	B	143	ASP	CB-CG-OD2	-5.42	113.43	118.30
1	G	136	GLU	OE1-CD-OE2	5.32	129.68	123.30
1	C	157	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	112	GLU	CG-CD-OE1	5.27	128.85	118.30
1	G	232[A]	THR	CA-CB-OG1	-5.23	98.01	109.00
1	G	232[B]	THR	CA-CB-OG1	-5.23	98.01	109.00
1	B	306	GLU	CB-CA-C	5.23	120.85	110.40
1	B	296	ASP	N-CA-CB	-5.21	101.22	110.60
1	C	112	GLU	CG-CD-OE1	5.21	128.72	118.30
1	B	67	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	G	177	ARG	CD-NE-CZ	5.17	130.84	123.60
1	A	74	GLU	CG-CD-OE1	5.16	128.62	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	121	TRP	CB-CG-CD1	5.16	133.71	127.00
1	G	191	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	G	141	TYR	N-CA-CB	-5.14	101.35	110.60
1	C	177	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	E	141	TYR	N-CA-CB	-5.10	101.42	110.60
1	A	159	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	C	193[A]	ARG	CA-CB-CG	5.07	124.55	113.40
1	C	193[B]	ARG	CA-CB-CG	5.07	124.55	113.40
1	C	177	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	E	239	GLU	OE1-CD-OE2	5.04	129.35	123.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173[A]	ARG	Sidechain
1	A	193	ARG	Sidechain
1	A	99	ARG	Sidechain
1	B	177	ARG	Sidechain
1	B	285	ARG	Sidechain
1	B	294	ARG	Sidechain
1	C	193[A]	ARG	Sidechain
1	C	243	ARG	Sidechain
1	C	294	ARG	Sidechain
1	D	157	ARG	Sidechain
1	D	173	ARG	Sidechain
1	D	309	GLN	Peptide,Sidechain
1	E	177	ARG	Sidechain
1	G	249	ARG	Sidechain

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	2352	2231	2224	22	0
1	B	2350	2223	2222	34	0
1	C	2357	2235	2210	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2330	2208	2201	27	0
1	E	2343	2217	2205	18	0
1	G	2366	2240	2220	15	0
2	A	103	0	0	8	0
2	B	94	0	0	4	0
2	C	75	0	0	8	0
2	D	93	0	0	3	0
2	E	92	0	0	4	0
2	G	83	0	0	0	0
All	All	14638	13354	13282	154	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 (154) 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:G:191:ARG:NH1	1:G:197:MET:O	1.91	1.04
1:C:191:ARG:NH1	1:C:197:MET:O	1.90	1.02
1:B:191:ARG:NH1	1:B:197:MET:O	1.92	1.02
1:B:58:VAL:HG22	1:B:87:VAL:CG2	2.04	0.87
1:B:56:ILE:HG13	1:B:85:VAL:HG23	1.56	0.85
1:C:31:PHE:H	1:C:251:ASN:HD21	1.25	0.83
1:C:146:ILE:HG21	1:C:193[A]:ARG:HD3	1.58	0.83
1:C:58:VAL:HG22	1:C:87:VAL:CG2	2.08	0.82
1:B:58:VAL:HG22	1:B:87:VAL:HG21	1.63	0.80
1:E:32:MET:HE2	1:E:287:GLY:HA2	1.62	0.80
1:D:205:GLU:HA	1:D:222[A]:TRP:CH2	2.16	0.80
1:B:31:PHE:H	1:B:251:ASN:HD21	1.29	0.79
1:D:203:ASN:HD21	1:D:225:GLU:H	1.31	0.79
1:D:203:ASN:O	1:D:222[A]:TRP:CZ3	2.38	0.76
1:C:63:LYS:NZ	2:C:402:HOH:O	2.18	0.75
1:A:68:SER:OG	2:A:401:HOH:O	2.03	0.74
1:B:224:VAL:HG23	1:B:243:ARG:NH2	2.04	0.73
1:C:58:VAL:HG22	1:C:87:VAL:HG21	1.71	0.71
1:C:90:VAL:HG12	1:C:92:ILE:CD1	2.20	0.71
1:E:32:MET:CE	1:E:287:GLY:HA2	2.19	0.71
1:C:190:VAL:HG11	1:C:197:MET:HG2	1.74	0.68
1:B:58:VAL:HA	1:B:87:VAL:HG22	1.76	0.68
1:A:270:PHE:HE2	2:A:485:HOH:O	1.76	0.67
1:C:294:ARG:HG3	1:C:294:ARG:HH11	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ILE:HD13	1:A:305:ILE:HD13	1.76	0.66
1:E:194:LYS:CE	2:E:482:HOH:O	2.44	0.66
1:B:58:VAL:HG22	1:B:87:VAL:HG22	1.80	0.63
1:C:58:VAL:HA	1:C:87:VAL:HG22	1.79	0.63
1:C:58:VAL:HG22	1:C:87:VAL:HG22	1.81	0.61
1:G:28:GLU:N	1:G:285:ARG:O	2.33	0.61
1:D:162:GLU:O	1:D:166:GLN:HG2	2.01	0.61
1:G:112:GLU:HG2	1:A:133:GLU:CD	2.21	0.60
1:D:214:GLN:O	1:D:218:THR:HG23	2.00	0.60
1:C:31:PHE:N	1:C:251:ASN:HD21	1.97	0.60
1:B:162:GLU:O	1:B:166:GLN:HG2	2.01	0.60
1:C:31:PHE:H	1:C:251:ASN:ND2	1.98	0.59
1:B:56:ILE:CG1	1:B:85:VAL:HG23	2.29	0.59
1:D:168:GLY:HA2	2:D:426:HOH:O	2.02	0.59
1:B:174:SER:O	1:B:178:LYS:HG3	2.02	0.59
1:C:208:LEU:CD1	1:C:250:LEU:HD21	2.33	0.58
1:C:90:VAL:HG12	1:C:92:ILE:HD13	1.86	0.57
1:C:145:VAL:HA	1:C:148:GLN:HE21	1.69	0.57
1:B:31:PHE:N	1:B:251:ASN:HD21	2.00	0.57
1:G:200:ILE:HD11	1:G:256:PHE:CZ	2.41	0.56
1:C:121:TRP:CG	2:C:448:HOH:O	2.58	0.56
1:B:133:GLU:HB2	2:B:475:HOH:O	2.06	0.56
1:E:216:ALA:O	1:E:255:LYS:HE3	2.05	0.55
1:D:199:ILE:H	1:D:220:SER:HB3	1.71	0.55
1:C:121:TRP:CD2	2:C:448:HOH:O	2.53	0.55
1:E:194:LYS:HE3	2:E:482:HOH:O	2.05	0.55
1:C:216:ALA:O	1:C:255:LYS:HE3	2.06	0.55
1:D:205:GLU:CA	1:D:222[A]:TRP:CH2	2.89	0.55
1:E:50:SER:OG	1:E:82:ALA:HB2	2.05	0.55
1:C:190:VAL:CG1	1:C:197:MET:HG2	2.37	0.54
1:C:97:ASP:OD2	2:C:401:HOH:O	2.17	0.54
1:B:216:ALA:O	1:B:255:LYS:HE3	2.07	0.54
1:C:252:ARG:NH1	2:C:404:HOH:O	2.35	0.53
1:A:252:ARG:HG2	1:A:252:ARG:O	2.09	0.53
1:D:304:VAL:HG23	1:D:310:PRO:O	2.08	0.53
1:B:56:ILE:HB	1:B:85:VAL:CG2	2.38	0.53
1:A:216:ALA:O	1:A:255:LYS:HE3	2.10	0.52
1:D:203:ASN:O	1:D:222[A]:TRP:CH2	2.63	0.52
1:D:216:ALA:O	1:D:255:LYS:HE3	2.10	0.52
1:C:49:ILE:HA	1:C:302:MET:HE2	1.92	0.52
1:C:236:GLU:HG2	2:C:446:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:VAL:HG23	1:B:85:VAL:O	2.09	0.52
1:A:60:ASP:CG	1:A:99:ARG:HH22	2.12	0.51
1:B:56:ILE:CG1	1:B:85:VAL:CG2	2.88	0.51
1:E:128:LYS:NZ	1:C:136:GLU:OE1	2.42	0.51
1:G:216:ALA:O	1:G:255:LYS:HE3	2.11	0.50
1:D:48:GLU:HG2	1:D:302:MET:CE	2.42	0.50
1:B:56:ILE:CB	1:B:85:VAL:CG2	2.89	0.50
1:E:60:ASP:CG	1:E:99:ARG:HH22	2.15	0.50
1:B:263:VAL:HG23	1:B:276:ILE:HD13	1.93	0.50
1:D:294:ARG:NE	1:D:303:ASN:OD1	2.40	0.50
1:B:56:ILE:HA	1:B:85:VAL:HG22	1.93	0.49
1:D:203:ASN:O	1:D:222[A]:TRP:HZ3	1.93	0.49
1:B:238:ASN:O	1:B:241:LYS:HG2	2.12	0.49
1:A:236:GLU:H	1:A:236:GLU:CD	2.16	0.49
1:D:263:VAL:HG23	1:D:276:ILE:HD13	1.94	0.49
1:A:96:GLU:OE1	1:A:99:ARG:NH1	2.42	0.49
1:E:294:ARG:HG2	1:E:294:ARG:HH11	1.77	0.49
1:C:49:ILE:HG12	1:C:302:MET:HE2	1.95	0.48
1:E:50:SER:OG	1:E:82:ALA:CB	2.61	0.48
1:D:77:LYS:NZ	2:D:405:HOH:O	2.46	0.48
1:D:284:LYS:HD3	2:D:485:HOH:O	2.13	0.47
1:E:272:ASN:OD1	1:E:275:ARG:NH1	2.48	0.47
1:G:158:ILE:HD11	1:G:201:PRO:HB3	1.97	0.47
1:B:266:GLY:HA2	1:B:294:ARG:CZ	2.45	0.47
1:A:249:ARG:HB2	1:A:249:ARG:HH11	1.79	0.47
1:D:31:PHE:N	1:D:251:ASN:HD21	2.13	0.46
1:C:145:VAL:HA	1:C:148:GLN:NE2	2.30	0.46
1:C:263:VAL:HG23	1:C:276:ILE:HD13	1.97	0.46
1:B:31:PHE:H	1:B:251:ASN:ND2	2.04	0.46
1:A:294:ARG:HE	1:A:303:ASN:ND2	2.13	0.46
1:C:153:ILE:HD12	1:C:155:LEU:HD11	1.98	0.46
1:E:96:GLU:OE1	1:E:99:ARG:NH1	2.46	0.46
1:G:30:TRP:HA	1:G:30:TRP:CE3	2.51	0.46
1:D:308:ILE:O	1:D:310:PRO:HD2	2.16	0.46
1:A:249:ARG:NH1	2:A:419:HOH:O	2.49	0.46
1:A:173[A]:ARG:NH2	2:A:418:HOH:O	2.48	0.45
1:D:205:GLU:CA	1:D:222[A]:TRP:CZ3	3.00	0.45
1:C:112:GLU:HG2	1:B:133:GLU:CD	2.36	0.45
1:B:48:GLU:OE1	2:B:402:HOH:O	2.21	0.45
1:G:272:ASN:OD1	1:G:275:ARG:NH1	2.48	0.45
1:C:121:TRP:HZ3	2:C:441:HOH:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ARG:CG	2:C:460:HOH:O	2.63	0.45
1:D:91:ASN:HD22	1:D:92:ILE:N	2.14	0.45
1:G:29:GLY:HA2	1:G:287:GLY:CA	2.47	0.45
1:A:237:GLU:H	1:A:237:GLU:CD	2.20	0.45
1:B:56:ILE:HB	1:B:85:VAL:HG22	1.98	0.44
1:A:252:ARG:HD2	2:A:411:HOH:O	2.16	0.44
1:C:230:LEU:O	1:C:231:LYS:HB2	2.16	0.44
1:B:249:ARG:NH2	2:B:405:HOH:O	2.27	0.44
1:D:91:ASN:HD22	1:D:91:ASN:C	2.21	0.44
1:A:253:LYS:HA	2:A:451:HOH:O	2.18	0.44
1:E:112[A]:GLU:O	1:E:112[A]:GLU:HG3	2.14	0.44
1:A:238:ASN:ND2	2:A:413:HOH:O	2.50	0.44
1:D:280:TYR:OH	1:D:309:GLN:HB3	2.18	0.43
1:G:112:GLU:HG2	1:A:133:GLU:CG	2.49	0.43
1:C:48:GLU:HG2	1:C:302:MET:HE1	1.99	0.43
1:E:230:LEU:O	1:E:231:LYS:HB2	2.18	0.43
1:A:303:ASN:HD22	1:A:303:ASN:HA	1.63	0.43
1:G:230:LEU:O	1:G:231:LYS:HB2	2.19	0.43
1:E:194:LYS:HE2	2:E:482:HOH:O	2.15	0.43
1:D:205:GLU:HB3	1:D:222[A]:TRP:CZ3	2.54	0.43
1:G:158:ILE:CD1	1:G:201:PRO:HB3	2.49	0.43
1:B:304:VAL:O	1:B:305:ILE:HD13	2.19	0.42
1:C:92:ILE:HD11	1:C:138:VAL:HG13	2.00	0.42
1:B:231:LYS:HA	1:B:262:TYR:O	2.20	0.42
1:B:173:ARG:NE	2:B:408:HOH:O	2.38	0.42
1:A:231:LYS:HA	1:A:262:TYR:O	2.20	0.42
1:G:231:LYS:HA	1:G:262:TYR:O	2.19	0.42
1:C:48:GLU:O	1:C:52:SER:OG	2.38	0.41
1:C:231:LYS:HA	1:C:262:TYR:O	2.19	0.41
1:G:146:ILE:HD11	1:G:190:VAL:HG23	2.02	0.41
1:C:92:ILE:HD11	1:C:138:VAL:CG1	2.50	0.41
1:D:91:ASN:HD22	1:D:93:GLY:H	1.68	0.41
1:C:49:ILE:HA	1:C:302:MET:CE	2.50	0.41
1:D:204:GLY:C	1:D:222[A]:TRP:HH2	2.24	0.41
1:B:50:SER:OG	1:B:79:MET:HA	2.19	0.41
1:D:230:LEU:O	1:D:231:LYS:HB2	2.21	0.41
1:A:188:GLU:CD	2:A:436:HOH:O	2.59	0.41
1:G:212:ASP:OD1	1:G:212:ASP:C	2.60	0.41
1:A:230:LEU:O	1:A:231:LYS:HB2	2.20	0.41
1:E:249:ARG:HD2	2:E:485:HOH:O	2.21	0.41
1:C:61:TYR:HB2	1:C:148:GLN:HE22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ASP:OD1	1:C:193[B]:ARG:NH2	2.55	0.40
1:B:56:ILE:HA	1:B:85:VAL:CG2	2.51	0.40
1:B:232:THR:HG22	1:B:233:ILE:HG13	2.03	0.40
1:E:177:ARG:HH21	1:E:181:ASN:HD21	1.69	0.40
1:E:231:LYS:HA	1:E:262:TYR:O	2.21	0.40
1:B:283:ALA:CB	1:B:290:PRO:HB3	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	283/323 (88%)	273 (96%)	10 (4%)	0	100	100
1	B	282/323 (87%)	271 (96%)	11 (4%)	0	100	100
1	C	284/323 (88%)	275 (97%)	9 (3%)	0	100	100
1	D	280/323 (87%)	269 (96%)	11 (4%)	0	100	100
1	E	282/323 (87%)	273 (97%)	9 (3%)	0	100	100
1	G	286/323 (88%)	273 (96%)	13 (4%)	0	100	100
All	All	1697/1938 (88%)	1634 (96%)	63 (4%)	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	252/289 (87%)	238 (94%)	14 (6%)	17	30
1	B	251/289 (87%)	237 (94%)	14 (6%)	17	30
1	C	254/289 (88%)	239 (94%)	15 (6%)	16	28
1	D	249/289 (86%)	237 (95%)	12 (5%)	21	37
1	E	251/289 (87%)	236 (94%)	15 (6%)	16	27
1	G	255/289 (88%)	241 (94%)	14 (6%)	18	31
All	All	1512/1734 (87%)	1428 (94%)	84 (6%)	19	30

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	30	TRP
1	G	35	ASP
1	G	61	TYR
1	G	62	SER
1	G	108	THR
1	G	112	GLU
1	G	141	TYR
1	G	160	SER
1	G	190	VAL
1	G	232[A]	THR
1	G	232[B]	THR
1	G	252	ARG
1	G	294	ARG
1	G	301	GLU
1	E	35	ASP
1	E	61	TYR
1	E	62	SER
1	E	80	VAL
1	E	99	ARG
1	E	109	ASN
1	E	141	TYR
1	E	166	GLN
1	E	230	LEU
1	E	232	THR
1	E	237	GLU
1	E	242	SER
1	E	271	GLU
1	E	294	ARG
1	E	301	GLU
1	C	41	LEU

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Mol	Chain	Res	Type
1	C	61	TYR
1	C	92	ILE
1	C	112	GLU
1	C	141	TYR
1	C	155	LEU
1	C	166	GLN
1	C	177	ARG
1	C	193[A]	ARG
1	C	193[B]	ARG
1	C	217	SER
1	C	245[A]	GLU
1	C	245[B]	GLU
1	C	281	GLU
1	C	301	GLU
1	D	61	TYR
1	D	91	ASN
1	D	112	GLU
1	D	114	LEU
1	D	141	TYR
1	D	188	GLU
1	D	196	ASP
1	D	217	SER
1	D	222[A]	TRP
1	D	222[B]	TRP
1	D	232	THR
1	D	253	LYS
1	B	61	TYR
1	B	62	SER
1	B	74	GLU
1	B	112	GLU
1	B	141	TYR
1	B	188	GLU
1	B	196	ASP
1	B	217	SER
1	B	219	VAL
1	B	232	THR
1	B	241	LYS
1	B	242	SER
1	B	294	ARG
1	B	311	PRO
1	A	61	TYR
1	A	62	SER

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Mol	Chain	Res	Type
1	A	99	ARG
1	A	108	THR
1	A	112	GLU
1	A	141	TYR
1	A	166	GLN
1	A	188	GLU
1	A	192	GLU
1	A	194	LYS
1	A	196	ASP
1	A	248	ILE
1	A	249	ARG
1	A	301	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	132	ASN
1	E	181	ASN
1	E	214	GLN
1	C	42	GLN
1	C	148	GLN
1	C	251	ASN
1	D	91	ASN
1	D	94	GLN
1	D	203	ASN
1	B	251	ASN
1	B	303	ASN
1	A	303	ASN

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	283/323 (87%)	-1.48	0	100	100	20, 47, 76, 100	1 (0%)
1	B	284/323 (87%)	-1.46	0	100	100	28, 47, 75, 100	0
1	C	282/323 (87%)	-1.36	0	100	100	23, 53, 81, 105	2 (0%)
1	D	280/323 (86%)	-1.38	0	100	100	26, 53, 86, 109	1 (0%)
1	E	282/323 (87%)	-1.39	0	100	100	23, 53, 86, 101	1 (0%)
1	G	284/323 (87%)	-1.37	0	100	100	25, 52, 83, 138	2 (0%)
All	All	1695/1938 (87%)	-1.41	0	100	100	20, 51, 82, 138	7 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.