Full wwPDB X-ray Structure Validation Report ⓘ

Apr 16, 2025 – 01:14 pm BST

PDB ID	:	9EUZ / pdb_00009euz
Title	:	Glycoside hydrolase family 191 enzyme from Thermotoga maritima
Authors	:	Roth, C.
Deposited on	:	2024-03-28
Resolution	:	2.60 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:

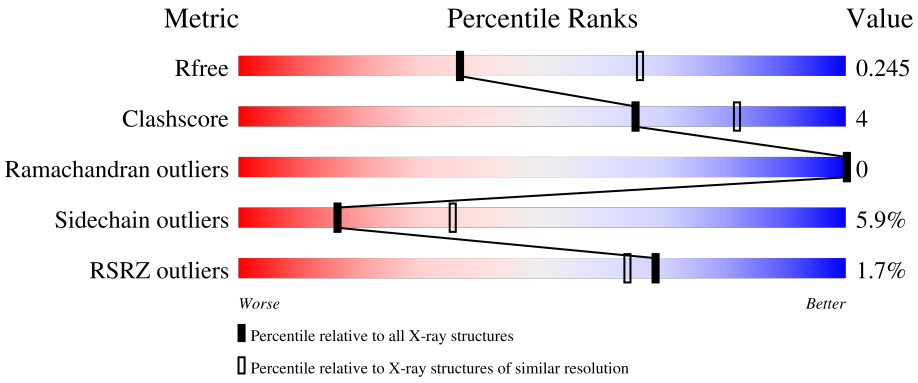
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.60 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	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	297	2% 77% 15%
1	B	297	78% 14% 5%
1	C	297	2% 79% 13% 5%
1	D	297	2% 79% 14% 5%
1	E	297	77% 13% 5%

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Mol	Chain	Length	Quality of chain
1	F	297	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 27953 atoms, of which 13303 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	A	284	Total	C	H	N	O	S	46	2	0
			4586	1519	2228	374	459	6			
1	B	283	Total	C	H	N	O	S	46	0	0
			4558	1510	2217	372	453	6			
1	C	281	Total	C	H	N	O	S	46	0	0
			4530	1500	2203	370	451	6			
1	D	283	Total	C	H	N	O	S	46	0	0
			4558	1510	2217	372	453	6			
1	E	282	Total	C	H	N	O	S	46	0	0
			4551	1508	2214	371	452	6			
1	F	283	Total	C	H	N	O	S	46	2	0
			4574	1515	2224	373	456	6			

- Molecule 2 is water.

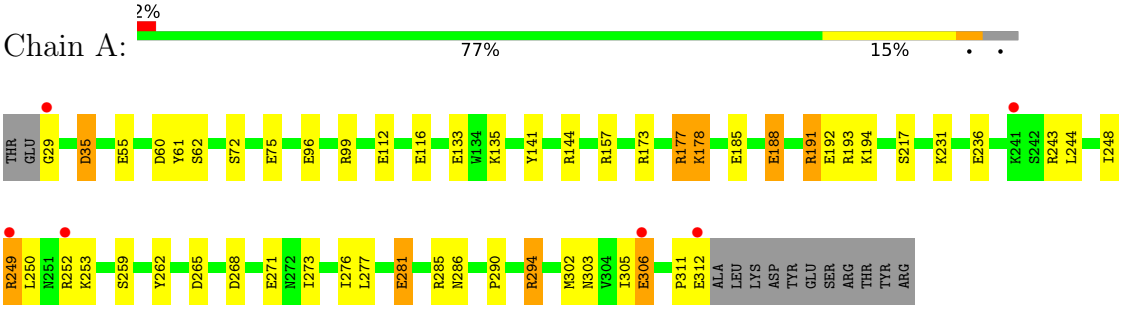
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	110	Total	O	0	0
			110	110		
2	B	107	Total	O	0	0
			107	107		
2	C	94	Total	O	0	0
			94	94		
2	D	106	Total	O	0	0
			106	106		
2	E	88	Total	O	0	0
			88	88		
2	F	91	Total	O	0	0
			91	91		

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.

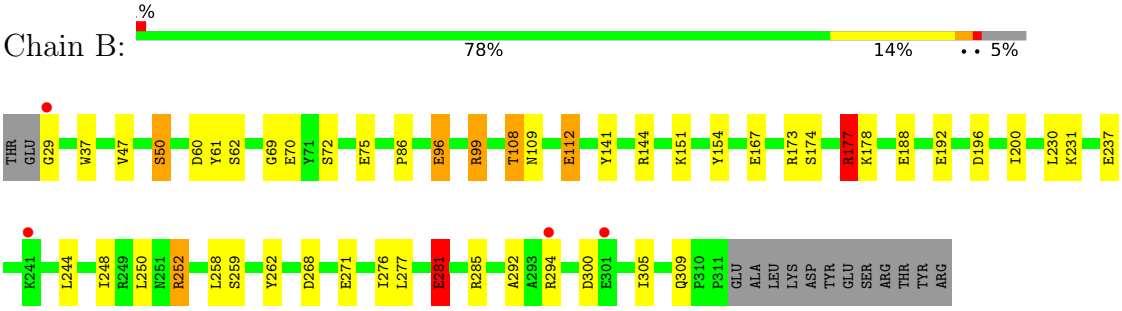
• Molecule 1: Uncharacterized protein TM_1410

Chain A:



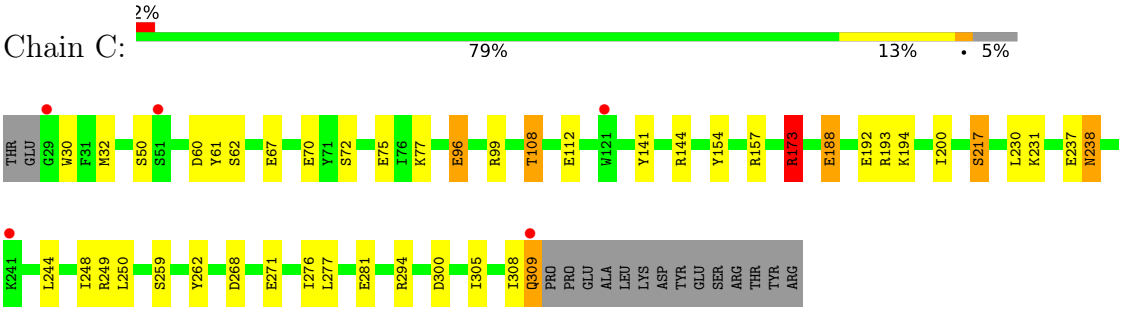
• Molecule 1: Uncharacterized protein TM_1410

Chain B:



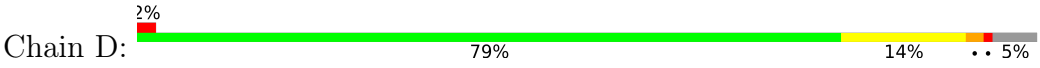
• Molecule 1: Uncharacterized protein TM_1410

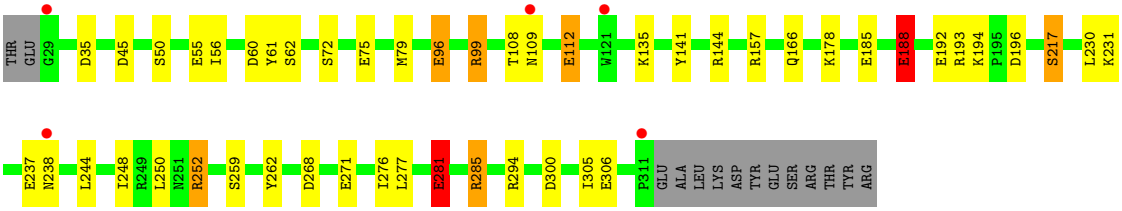
Chain C:



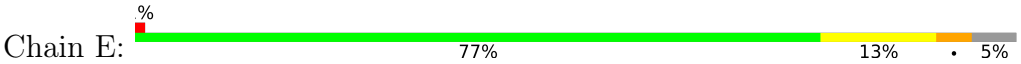
• Molecule 1: Uncharacterized protein TM_1410

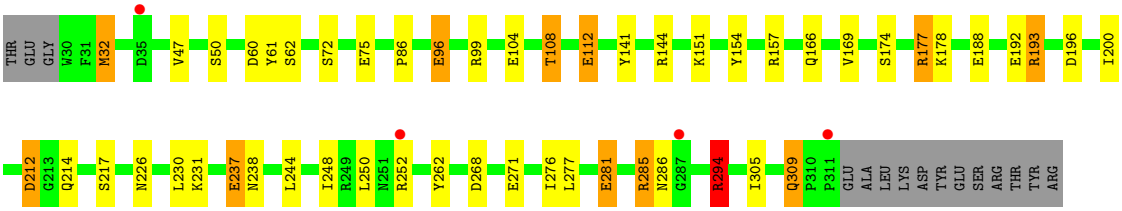
Chain D:



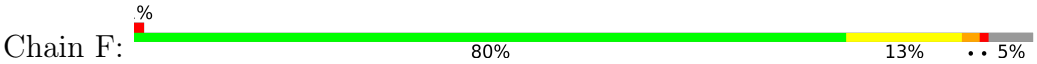


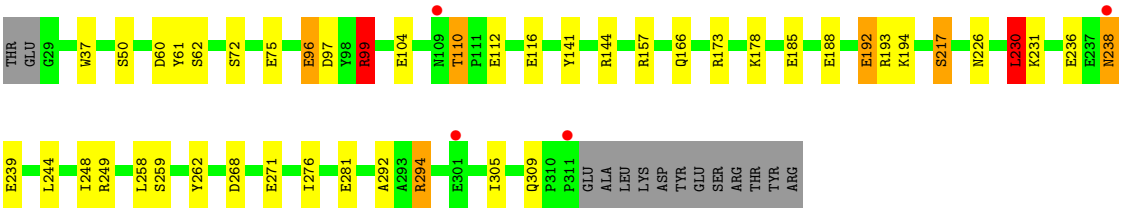
• Molecule 1: Uncharacterized protein TM_1410





• Molecule 1: Uncharacterized protein TM_1410





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	196.06Å 84.50Å 196.63Å 90.00° 119.83° 90.00°	Depositor
Resolution (Å)	49.26 – 2.60 49.26 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.26-2.60) 98.6 (49.26-2.60)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0425, REFMAC 5.8.0425	Depositor
R, R_{free}	0.216 , 0.244 0.218 , 0.245	Depositor DCC
R_{free} test set	8591 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.110 for -h-l,k,h 0.110 for l,k,-h-l 0.055 for h,-k,-h-l 0.054 for -h-l,-k,l 0.055 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	27953	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.87% 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	0.73	1/2431 (0.0%)	1.26	26/3301 (0.8%)
1	B	0.73	1/2406 (0.0%)	1.21	16/3268 (0.5%)
1	C	0.77	2/2390 (0.1%)	1.24	19/3244 (0.6%)
1	D	0.77	4/2406 (0.2%)	1.27	28/3268 (0.9%)
1	E	0.73	2/2402 (0.1%)	1.26	22/3263 (0.7%)
1	F	0.72	2/2431 (0.1%)	1.21	21/3303 (0.6%)
All	All	0.74	12/14466 (0.1%)	1.24	132/19647 (0.7%)

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	5
1	B	0	2
1	C	0	1
1	D	0	2
1	E	0	4
1	F	0	1
All	All	0	15

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	188	GLU	CD-OE2	13.08	1.40	1.25
1	E	192	GLU	CD-OE1	9.69	1.36	1.25
1	F	192	GLU	CD-OE1	8.36	1.34	1.25
1	D	192	GLU	CD-OE1	7.88	1.34	1.25
1	C	192	GLU	CD-OE1	7.79	1.34	1.25
1	B	192	GLU	CD-OE1	7.75	1.34	1.25
1	C	188	GLU	CD-OE2	7.54	1.33	1.25
1	F	185	GLU	CD-OE2	6.01	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	GLU	CD-OE2	5.58	1.31	1.25
1	D	192	GLU	CD-OE2	5.56	1.31	1.25
1	D	185	GLU	CD-OE2	5.06	1.31	1.25
1	E	104	GLU	CD-OE2	5.02	1.31	1.25

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	188	GLU	CG-CD-OE1	-11.41	95.47	118.30
1	E	309	GLN	N-CA-CB	11.34	131.01	110.60
1	D	188	GLU	CG-CD-OE2	9.98	138.26	118.30
1	E	157	ARG	NE-CZ-NH2	-9.89	115.36	120.30
1	C	108	THR	CA-CB-OG1	-9.06	89.97	109.00
1	A	188	GLU	OE1-CD-OE2	8.26	133.21	123.30
1	E	309	GLN	CB-CA-C	-8.12	94.15	110.40
1	F	144	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	F	110	THR	CA-CB-OG1	-7.89	92.43	109.00
1	A	144	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	C	188	GLU	CG-CD-OE1	-7.73	102.84	118.30
1	F	249	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	E	108	THR	CA-CB-OG1	-7.46	93.33	109.00
1	A	188	GLU	CG-CD-OE2	-7.43	103.44	118.30
1	F	178	LYS	CD-CE-NZ	-7.30	94.91	111.70
1	E	294	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	F	96	GLU	CG-CD-OE2	-7.07	104.16	118.30
1	D	79	MET	CG-SD-CE	-7.00	88.99	100.20
1	E	144	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	A	217	SER	N-CA-CB	6.89	120.83	110.50
1	F	238	ASN	CB-CA-C	-6.84	96.72	110.40
1	F	268	ASP	CB-CA-C	6.83	124.07	110.40
1	D	217	SER	N-CA-CB	6.79	120.69	110.50
1	E	192	GLU	CG-CD-OE2	-6.67	104.95	118.30
1	E	144	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	D	285	ARG	NE-CZ-NH2	6.55	123.58	120.30
1	C	294	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	281	GLU	CG-CD-OE1	6.53	131.36	118.30
1	F	99	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	A	303	ASN	N-CA-CB	6.48	122.26	110.60
1	D	112	GLU	OE1-CD-OE2	-6.47	115.53	123.30
1	C	144	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	E	238	ASN	CB-CA-C	-6.40	97.61	110.40
1	B	281	GLU	CB-CA-C	6.38	123.17	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	281	GLU	CB-CA-C	6.38	123.16	110.40
1	F	281	GLU	CB-CA-C	6.38	123.16	110.40
1	D	112	GLU	CG-CD-OE1	6.37	131.04	118.30
1	A	252	ARG	NE-CZ-NH2	6.33	123.47	120.30
1	A	177	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	F	104	GLU	CG-CD-OE2	-6.28	105.73	118.30
1	A	281	GLU	CB-CA-C	6.26	122.92	110.40
1	D	185	GLU	OE1-CD-OE2	6.26	130.81	123.30
1	D	268	ASP	CB-CA-C	6.25	122.90	110.40
1	B	250	LEU	N-CA-CB	-6.22	97.96	110.40
1	A	193	ARG	CD-NE-CZ	-6.21	114.91	123.60
1	E	281	GLU	CB-CA-C	6.21	122.81	110.40
1	C	268	ASP	CB-CA-C	6.19	122.78	110.40
1	C	249	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	185	GLU	OE1-CD-OE2	6.16	130.69	123.30
1	B	173	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	D	250	LEU	N-CA-CB	-6.12	98.16	110.40
1	C	108	THR	N-CA-CB	-6.08	98.74	110.30
1	D	238	ASN	CB-CA-C	-6.07	98.25	110.40
1	E	193	ARG	CD-NE-CZ	-6.06	115.12	123.60
1	D	157	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	191	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	C	238	ASN	CB-CA-C	-5.96	98.48	110.40
1	B	96	GLU	CG-CD-OE1	5.95	130.21	118.30
1	D	96	GLU	CG-CD-OE2	-5.93	106.45	118.30
1	A	116	GLU	CG-CD-OE2	5.85	130.00	118.30
1	E	32	MET	CG-SD-CE	5.85	109.56	100.20
1	F	96	GLU	CG-CD-OE1	5.85	129.99	118.30
1	A	250	LEU	N-CA-CB	-5.84	98.72	110.40
1	D	178	LYS	CD-CE-NZ	-5.84	98.27	111.70
1	B	96	GLU	CG-CD-OE2	-5.83	106.64	118.30
1	D	193	ARG	CA-CB-CG	-5.80	100.63	113.40
1	E	277	LEU	CB-CG-CD2	5.77	120.81	111.00
1	D	108	THR	N-CA-CB	-5.76	99.36	110.30
1	D	277	LEU	CB-CG-CD2	5.75	120.78	111.00
1	D	99	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	D	45	ASP	CB-CG-OD2	-5.72	113.16	118.30
1	D	135	LYS	CD-CE-NZ	-5.71	98.56	111.70
1	D	259	SER	N-CA-CB	5.71	119.07	110.50
1	B	109	ASN	CB-CA-C	5.71	121.81	110.40
1	B	281	GLU	CG-CD-OE2	-5.69	106.92	118.30
1	C	217	SER	N-CA-CB	5.67	119.01	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	188	GLU	CG-CD-OE2	-5.67	106.97	118.30
1	A	157	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	E	268	ASP	CB-CA-C	5.63	121.65	110.40
1	E	250	LEU	N-CA-CB	-5.62	99.16	110.40
1	A	249	ARG	CD-NE-CZ	5.60	131.44	123.60
1	C	250	LEU	N-CA-CB	-5.59	99.22	110.40
1	A	135	LYS	CD-CE-NZ	-5.58	98.86	111.70
1	A	277	LEU	CB-CG-CD2	5.54	120.42	111.00
1	B	144	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	96	GLU	CG-CD-OE2	-5.53	107.24	118.30
1	B	294	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	C	193	ARG	CA-CB-CG	-5.50	101.31	113.40
1	A	178	LYS	CG-CD-CE	-5.48	95.47	111.90
1	C	32	MET	CG-SD-CE	5.47	108.95	100.20
1	D	252	ARG	CG-CD-NE	-5.45	100.36	111.80
1	F	104	GLU	CG-CD-OE1	5.42	129.14	118.30
1	F	217	SER	CB-CA-C	-5.41	99.82	110.10
1	B	177	ARG	CD-NE-CZ	5.39	131.15	123.60
1	A	243	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	A	306	GLU	CG-CD-OE1	5.39	129.07	118.30
1	C	157	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	268	ASP	CB-CA-C	5.34	121.08	110.40
1	E	96	GLU	CG-CD-OE2	-5.33	107.64	118.30
1	F	178	LYS	CG-CD-CE	-5.33	95.92	111.90
1	B	268	ASP	CB-CA-C	5.32	121.05	110.40
1	F	217	SER	N-CA-CB	5.32	118.48	110.50
1	E	285	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	F	259	SER	N-CA-CB	5.30	118.45	110.50
1	D	109	ASN	CB-CA-C	5.28	120.96	110.40
1	C	259	SER	N-CA-CB	5.27	118.41	110.50
1	E	193	ARG	CA-CB-CG	-5.27	101.80	113.40
1	D	144	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	F	230	LEU	CB-CG-CD2	5.26	119.94	111.00
1	C	277	LEU	CB-CG-CD2	5.25	119.92	111.00
1	E	96	GLU	CG-CD-OE1	5.21	128.73	118.30
1	A	277	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	A	193	ARG	CA-CB-CG	-5.20	101.95	113.40
1	C	188	GLU	CG-CD-OE2	5.20	128.69	118.30
1	E	237	GLU	CG-CD-OE2	-5.19	107.92	118.30
1	C	96	GLU	CG-CD-OE1	5.18	128.66	118.30
1	F	110	THR	CA-CB-CG2	5.18	119.65	112.40
1	B	108	THR	CA-CB-OG1	-5.18	98.13	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	192	GLU	CG-CD-OE2	-5.17	107.96	118.30
1	D	99	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	F	193	ARG	CA-CB-CG	-5.15	102.06	113.40
1	D	178	LYS	CG-CD-CE	-5.15	96.45	111.90
1	A	116	GLU	CG-CD-OE1	-5.15	108.00	118.30
1	E	108	THR	N-CA-CB	-5.15	100.52	110.30
1	D	96	GLU	CG-CD-OE1	5.14	128.59	118.30
1	B	277	LEU	CB-CG-CD2	5.13	119.72	111.00
1	C	281	GLU	CB-CA-C	5.13	120.66	110.40
1	A	259	SER	N-CA-CB	5.11	118.17	110.50
1	F	173	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	259	SER	N-CA-CB	5.07	118.10	110.50
1	E	177	ARG	N-CA-CB	5.07	119.72	110.60
1	A	306	GLU	CG-CD-OE2	-5.04	108.22	118.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	ARG	Sidechain
1	A	191	ARG	Sidechain
1	A	249	ARG	Sidechain
1	A	294	ARG	Sidechain
1	A	302	MET	Mainchain
1	B	252	ARG	Sidechain
1	B	29	GLY	Peptide
1	C	173	ARG	Sidechain
1	D	252	ARG	Sidechain
1	D	294	ARG	Sidechain
1	E	177	ARG	Sidechain
1	E	193	ARG	Sidechain
1	E	212	ASP	Mainchain
1	E	294	ARG	Sidechain
1	F	294	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	2358	2228	2217	15	0
1	B	2341	2217	2216	28	0
1	C	2327	2203	2202	12	0
1	D	2341	2217	2216	13	0
1	E	2337	2214	2213	17	0
1	F	2350	2224	2212	17	0
2	A	110	0	0	5	0
2	B	107	0	0	8	0
2	C	94	0	0	2	0
2	D	106	0	0	4	0
2	E	88	0	0	4	0
2	F	91	0	0	5	0
All	All	14650	13303	13276	101	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 4.

All (101) 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:D:188:GLU:HG2	2:D:479:HOH:O	1.61	0.97
1:B:177:ARG:HH11	1:B:177:ARG:HG3	1.38	0.88
1:F:116:GLU:HB3	2:F:459:HOH:O	1.74	0.85
1:C:300:ASP:OD1	2:C:401:HOH:O	1.91	0.85
1:B:300:ASP:OD1	2:B:401:HOH:O	1.95	0.85
1:D:188:GLU:CG	2:D:479:HOH:O	2.23	0.81
1:D:281:GLU:OE2	1:D:285:ARG:NH1	2.14	0.80
1:B:281:GLU:OE2	1:B:285:ARG:NH1	2.14	0.80
1:C:308:ILE:O	1:C:309:GLN:NE2	2.16	0.78
1:B:292:ALA:H	1:B:309:GLN:HE22	1.36	0.69
1:E:169:VAL:HG13	2:E:428:HOH:O	1.93	0.68
1:F:292:ALA:H	1:F:309:GLN:HE22	1.44	0.63
1:B:177:ARG:HG2	2:B:426:HOH:O	1.97	0.63
1:A:281:GLU:OE2	1:A:285:ARG:NH1	2.30	0.63
1:A:35:ASP:HB2	1:A:55:GLU:OE2	2.00	0.62
1:B:177:ARG:CG	2:B:426:HOH:O	2.47	0.62
1:F:236:GLU:OE1	1:F:239:GLU:OE1	2.18	0.62
1:B:177:ARG:HG3	1:B:177:ARG:NH1	2.11	0.61
1:D:35:ASP:HB2	1:D:55:GLU:OE2	2.00	0.61
1:E:174:SER:OG	1:E:178:LYS:HE2	2.01	0.61
1:B:96:GLU:HB2	1:B:99:ARG:HG3	1.83	0.61
1:E:281:GLU:OE2	1:E:285:ARG:NH1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLU:HB2	1:A:99:ARG:HG3	1.84	0.59
1:E:96:GLU:HB2	1:E:99:ARG:HG3	1.85	0.59
1:C:96:GLU:HB2	1:C:99:ARG:HG3	1.85	0.58
1:F:96:GLU:HB2	1:F:99:ARG:HG3	1.85	0.58
1:A:192:GLU:OE2	2:A:401:HOH:O	2.17	0.57
1:A:29:GLY:N	2:A:407:HOH:O	2.37	0.57
1:D:96:GLU:HB2	1:D:99:ARG:HG3	1.87	0.57
1:E:212:ASP:OD1	1:E:214:GLN:HG3	2.05	0.56
1:B:252:ARG:HD2	2:B:402:HOH:O	2.05	0.56
1:B:112:GLU:HG2	2:B:479:HOH:O	2.05	0.55
1:F:292:ALA:H	1:F:309:GLN:NE2	2.04	0.55
1:B:167:GLU:O	2:B:403:HOH:O	2.18	0.55
1:F:226:ASN:ND2	2:F:405:HOH:O	2.35	0.55
1:B:86:PRO:HD2	1:B:151:LYS:HG3	1.88	0.54
1:B:292:ALA:H	1:B:309:GLN:NE2	2.03	0.54
1:D:306:GLU:HB2	2:D:434:HOH:O	2.08	0.53
1:F:236:GLU:H	1:F:236:GLU:CD	2.12	0.53
1:A:244:LEU:O	1:A:248:ILE:HG12	2.09	0.53
1:E:75:GLU:OE1	2:E:401:HOH:O	2.19	0.53
1:F:157:ARG:NH1	2:F:403:HOH:O	2.23	0.53
1:A:311:PRO:O	1:A:312:GLU:C	2.49	0.51
1:F:244:LEU:O	1:F:248:ILE:HG12	2.12	0.50
1:C:276:ILE:HD13	1:C:305:ILE:HD13	1.94	0.50
1:C:244:LEU:O	1:C:248:ILE:HG12	2.11	0.50
1:B:177:ARG:HH11	1:B:177:ARG:CG	2.16	0.49
1:A:265:ASP:OD2	2:A:402:HOH:O	2.19	0.49
1:F:60:ASP:CG	1:F:99:ARG:HH22	2.15	0.49
1:B:244:LEU:O	1:B:248:ILE:HG12	2.12	0.49
1:F:97:ASP:OD1	2:F:401:HOH:O	2.19	0.49
1:E:244:LEU:O	1:E:248:ILE:HG12	2.13	0.48
1:B:231:LYS:HA	1:B:262:TYR:O	2.14	0.48
1:D:244:LEU:O	1:D:248:ILE:HG12	2.14	0.47
1:F:72:SER:OG	1:F:75:GLU:HG3	2.15	0.47
1:B:177:ARG:HG3	2:B:426:HOH:O	2.13	0.47
1:F:230:LEU:O	1:F:231:LYS:HB2	2.14	0.47
1:F:231:LYS:HA	1:F:262:TYR:O	2.15	0.47
1:A:276:ILE:HD13	1:A:305:ILE:HD13	1.97	0.46
1:D:231:LYS:HA	1:D:262:TYR:O	2.15	0.46
1:A:194:LYS:NZ	2:A:410:HOH:O	2.48	0.46
1:B:60:ASP:CG	1:B:99:ARG:HH22	2.18	0.46
1:E:226:ASN:ND2	2:E:405:HOH:O	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASP:CG	1:A:99:ARG:HH22	2.19	0.46
1:B:174:SER:OG	1:B:178:LYS:CE	2.64	0.46
1:D:72:SER:OG	1:D:75:GLU:HG3	2.16	0.46
1:D:276:ILE:HD13	1:D:305:ILE:HD13	1.98	0.46
1:C:60:ASP:CG	1:C:99:ARG:HH22	2.19	0.46
1:C:72:SER:OG	1:C:75:GLU:HG3	2.16	0.46
1:E:72:SER:OG	1:E:75:GLU:HG3	2.16	0.46
1:D:60:ASP:CG	1:D:99:ARG:HH22	2.19	0.45
1:A:72:SER:OG	1:A:75:GLU:HG3	2.16	0.45
1:D:300:ASP:OD1	2:D:401:HOH:O	2.21	0.45
1:A:231:LYS:HA	1:A:262:TYR:O	2.16	0.45
1:B:72:SER:OG	1:B:75:GLU:HG3	2.17	0.45
1:E:60:ASP:CG	1:E:99:ARG:HH22	2.20	0.45
1:B:154:TYR:HA	1:B:200:ILE:O	2.18	0.44
1:E:154:TYR:HA	1:E:200:ILE:O	2.19	0.43
1:E:276:ILE:HD13	1:E:305:ILE:HD13	2.00	0.42
1:C:30:TRP:CH2	1:C:248:ILE:HD12	2.54	0.42
1:E:231:LYS:HA	1:E:262:TYR:O	2.18	0.42
1:E:86:PRO:HD2	1:E:151:LYS:HG3	2.01	0.42
1:B:69:GLY:O	1:B:70:GLU:C	2.58	0.42
1:C:231:LYS:HA	1:C:262:TYR:O	2.19	0.42
1:A:178:LYS:O	2:A:403:HOH:O	2.21	0.42
1:F:192:GLU:HG3	2:F:488:HOH:O	2.20	0.42
1:B:174:SER:OG	1:B:178:LYS:HE3	2.19	0.41
1:B:196:ASP:OD1	1:B:196:ASP:N	2.53	0.41
1:C:173:ARG:NE	2:C:407:HOH:O	2.48	0.41
1:F:276:ILE:HD13	1:F:305:ILE:HD13	2.02	0.41
1:B:252:ARG:NH1	2:B:402:HOH:O	2.04	0.41
1:A:133:GLU:CG	1:E:112:GLU:HG3	2.50	0.41
1:B:276:ILE:HD13	1:B:305:ILE:HD13	2.03	0.41
1:E:47:VAL:O	1:E:50:SER:HB2	2.21	0.40
1:E:169:VAL:HA	2:E:428:HOH:O	2.20	0.40
1:B:37:TRP:CE2	1:B:258:LEU:HB3	2.57	0.40
1:B:47:VAL:O	1:B:50:SER:HB2	2.22	0.40
1:C:67:GLU:O	1:C:70:GLU:HG3	2.21	0.40
1:C:154:TYR:HA	1:C:200:ILE:O	2.20	0.40
1:D:56:ILE:HG21	1:D:56:ILE:HD13	1.76	0.40
1:F:37:TRP:CE2	1:F:258:LEU:HB3	2.56	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	284/297 (96%)	274 (96%)	10 (4%)	0	100	100
1	B	281/297 (95%)	271 (96%)	10 (4%)	0	100	100
1	C	279/297 (94%)	270 (97%)	9 (3%)	0	100	100
1	D	281/297 (95%)	272 (97%)	9 (3%)	0	100	100
1	E	280/297 (94%)	270 (96%)	10 (4%)	0	100	100
1	F	283/297 (95%)	275 (97%)	8 (3%)	0	100	100
All	All	1688/1782 (95%)	1632 (97%)	56 (3%)	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	253/263 (96%)	238 (94%)	15 (6%)	16	35
1	B	250/263 (95%)	237 (95%)	13 (5%)	19	41
1	C	248/263 (94%)	232 (94%)	16 (6%)	14	31
1	D	250/263 (95%)	236 (94%)	14 (6%)	17	38
1	E	250/263 (95%)	233 (93%)	17 (7%)	13	28
1	F	252/263 (96%)	238 (94%)	14 (6%)	17	38
All	All	1503/1578 (95%)	1414 (94%)	89 (6%)	16	35

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	61	TYR
1	A	62	SER
1	A	112	GLU
1	A	141	TYR
1	A	177	ARG
1	A	188	GLU
1	A	236	GLU
1	A	253	LYS
1	A	271	GLU
1	A	273	ILE
1	A	286	ASN
1	A	290	PRO
1	A	294	ARG
1	A	306	GLU
1	B	50	SER
1	B	61	TYR
1	B	62	SER
1	B	99	ARG
1	B	108	THR
1	B	112	GLU
1	B	141	TYR
1	B	177	ARG
1	B	188	GLU
1	B	230	LEU
1	B	237	GLU
1	B	271	GLU
1	B	281	GLU
1	C	50	SER
1	C	61	TYR
1	C	62	SER
1	C	77	LYS
1	C	108	THR
1	C	112	GLU
1	C	141	TYR
1	C	173	ARG
1	C	188	GLU
1	C	194	LYS
1	C	217	SER
1	C	230	LEU
1	C	237	GLU
1	C	238	ASN

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Mol	Chain	Res	Type
1	C	271	GLU
1	C	309	GLN
1	D	50	SER
1	D	61	TYR
1	D	62	SER
1	D	112	GLU
1	D	141	TYR
1	D	166	GLN
1	D	188	GLU
1	D	194	LYS
1	D	196	ASP
1	D	217	SER
1	D	230	LEU
1	D	237	GLU
1	D	271	GLU
1	D	281	GLU
1	E	32	MET
1	E	61	TYR
1	E	62	SER
1	E	108	THR
1	E	112	GLU
1	E	141	TYR
1	E	166	GLN
1	E	188	GLU
1	E	196	ASP
1	E	217	SER
1	E	230	LEU
1	E	237	GLU
1	E	252	ARG
1	E	271	GLU
1	E	286	ASN
1	E	294	ARG
1	E	309	GLN
1	F	50	SER
1	F	61	TYR
1	F	62	SER
1	F	99	ARG
1	F	110	THR
1	F	112	GLU
1	F	141	TYR
1	F	166	GLN
1	F	194	LYS

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Mol	Chain	Res	Type
1	F	217	SER
1	F	230	LEU
1	F	238	ASN
1	F	271	GLU
1	F	294	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	309	GLN
1	C	238	ASN
1	E	181	ASN
1	E	226	ASN
1	F	309	GLN

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, 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	284/297 (95%)	-0.70	6 (2%)	63	58	15, 34, 64, 108	1 (0%)
1	B	283/297 (95%)	-0.60	4 (1%)	73	68	18, 36, 66, 96	0
1	C	281/297 (94%)	-0.46	5 (1%)	67	62	16, 38, 69, 96	0
1	D	283/297 (95%)	-0.41	5 (1%)	67	62	20, 40, 68, 93	0
1	E	282/297 (94%)	-0.50	4 (1%)	73	68	19, 39, 69, 94	0
1	F	283/297 (95%)	-0.50	4 (1%)	73	68	12, 40, 68, 96	1 (0%)
All	All	1696/1782 (95%)	-0.53	28 (1%)	69	64	12, 38, 69, 108	2 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	29	GLY	7.1
1	A	312	GLU	5.6
1	B	29	GLY	5.3
1	C	29	GLY	5.0
1	F	311	PRO	4.2
1	A	29	GLY	4.1
1	E	311	PRO	4.0
1	D	109	ASN	3.3
1	F	301	GLU	3.1
1	C	51	SER	2.9
1	E	35	ASP	2.9
1	C	241	LYS	2.8
1	B	301	GLU	2.7
1	F	109	ASN	2.6
1	D	311	PRO	2.6
1	A	252	ARG	2.6
1	A	306	GLU	2.5
1	D	238	ASN	2.3
1	B	294	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	238	ASN	2.2
1	C	309	GLN	2.2
1	C	121	TRP	2.2
1	E	252	ARG	2.2
1	B	241	LYS	2.1
1	A	249	ARG	2.1
1	A	241	LYS	2.0
1	E	287	GLY	2.0
1	D	121	TRP	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 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.