Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 10:46 AM EDT

PDB ID	:	5FDF
Title	:	Crystal structure of the monoclinic form of Thermotoga maritima Acetyl Esterase TM0077 (apo structure) at 1.76 Angstrom resolution
Authors	:	Manoj, N.; Singh, M.K.
Deposited on	:	2015-12-16
Resolution	:	1.76 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1
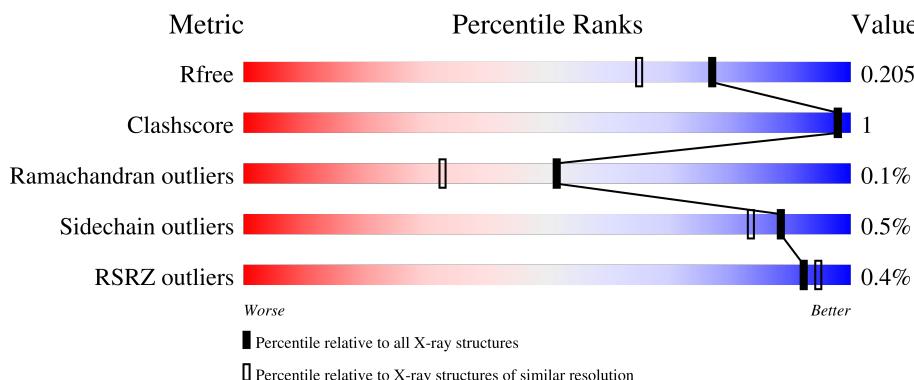
1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.76 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	Percentile Ranks	Value
Rfree		0.205
Clashscore		1
Ramachandran outliers		0.1%
Sidechain outliers		0.5%
RSRZ outliers		0.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▐ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	337	91% · · 5%
1	B	337	90% 5% 5%
1	C	337	90% · · 5%
1	D	337	90% · 5%
1	E	337	91% · 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	337	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	C	401	-	-	X	-

2　Entry composition　ⓘ

There are 4 unique types of molecules in this entry. The entry contains 16780 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 Cephalosporin-C deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2516	1636	410	460	10			
1	B	320	Total	C	N	O	S	0	2	0
			2572	1675	431	456	10			
1	C	320	Total	C	N	O	S	0	2	0
			2541	1654	418	459	10			
1	D	319	Total	C	N	O	S	0	2	0
			2541	1654	422	455	10			
1	E	320	Total	C	N	O	S	0	2	0
			2576	1675	429	462	10			
1	F	320	Total	C	N	O	S	0	2	0
			2542	1653	421	458	10			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q9WXT2
A	-10	GLY	-	expression tag	UNP Q9WXT2
A	-9	SER	-	expression tag	UNP Q9WXT2
A	-8	ASP	-	expression tag	UNP Q9WXT2
A	-7	LYS	-	expression tag	UNP Q9WXT2
A	-6	ILE	-	expression tag	UNP Q9WXT2
A	-5	HIS	-	expression tag	UNP Q9WXT2
A	-4	HIS	-	expression tag	UNP Q9WXT2
A	-3	HIS	-	expression tag	UNP Q9WXT2
A	-2	HIS	-	expression tag	UNP Q9WXT2
A	-1	HIS	-	expression tag	UNP Q9WXT2
A	0	HIS	-	expression tag	UNP Q9WXT2
B	-11	MET	-	initiating methionine	UNP Q9WXT2
B	-10	GLY	-	expression tag	UNP Q9WXT2
B	-9	SER	-	expression tag	UNP Q9WXT2
B	-8	ASP	-	expression tag	UNP Q9WXT2
B	-7	LYS	-	expression tag	UNP Q9WXT2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	ILE	-	expression tag	UNP Q9WXT2
B	-5	HIS	-	expression tag	UNP Q9WXT2
B	-4	HIS	-	expression tag	UNP Q9WXT2
B	-3	HIS	-	expression tag	UNP Q9WXT2
B	-2	HIS	-	expression tag	UNP Q9WXT2
B	-1	HIS	-	expression tag	UNP Q9WXT2
B	0	HIS	-	expression tag	UNP Q9WXT2
C	-11	MET	-	initiating methionine	UNP Q9WXT2
C	-10	GLY	-	expression tag	UNP Q9WXT2
C	-9	SER	-	expression tag	UNP Q9WXT2
C	-8	ASP	-	expression tag	UNP Q9WXT2
C	-7	LYS	-	expression tag	UNP Q9WXT2
C	-6	ILE	-	expression tag	UNP Q9WXT2
C	-5	HIS	-	expression tag	UNP Q9WXT2
C	-4	HIS	-	expression tag	UNP Q9WXT2
C	-3	HIS	-	expression tag	UNP Q9WXT2
C	-2	HIS	-	expression tag	UNP Q9WXT2
C	-1	HIS	-	expression tag	UNP Q9WXT2
C	0	HIS	-	expression tag	UNP Q9WXT2
D	-11	MET	-	initiating methionine	UNP Q9WXT2
D	-10	GLY	-	expression tag	UNP Q9WXT2
D	-9	SER	-	expression tag	UNP Q9WXT2
D	-8	ASP	-	expression tag	UNP Q9WXT2
D	-7	LYS	-	expression tag	UNP Q9WXT2
D	-6	ILE	-	expression tag	UNP Q9WXT2
D	-5	HIS	-	expression tag	UNP Q9WXT2
D	-4	HIS	-	expression tag	UNP Q9WXT2
D	-3	HIS	-	expression tag	UNP Q9WXT2
D	-2	HIS	-	expression tag	UNP Q9WXT2
D	-1	HIS	-	expression tag	UNP Q9WXT2
D	0	HIS	-	expression tag	UNP Q9WXT2
E	-11	MET	-	initiating methionine	UNP Q9WXT2
E	-10	GLY	-	expression tag	UNP Q9WXT2
E	-9	SER	-	expression tag	UNP Q9WXT2
E	-8	ASP	-	expression tag	UNP Q9WXT2
E	-7	LYS	-	expression tag	UNP Q9WXT2
E	-6	ILE	-	expression tag	UNP Q9WXT2
E	-5	HIS	-	expression tag	UNP Q9WXT2
E	-4	HIS	-	expression tag	UNP Q9WXT2
E	-3	HIS	-	expression tag	UNP Q9WXT2
E	-2	HIS	-	expression tag	UNP Q9WXT2
E	-1	HIS	-	expression tag	UNP Q9WXT2

Continued on next page...
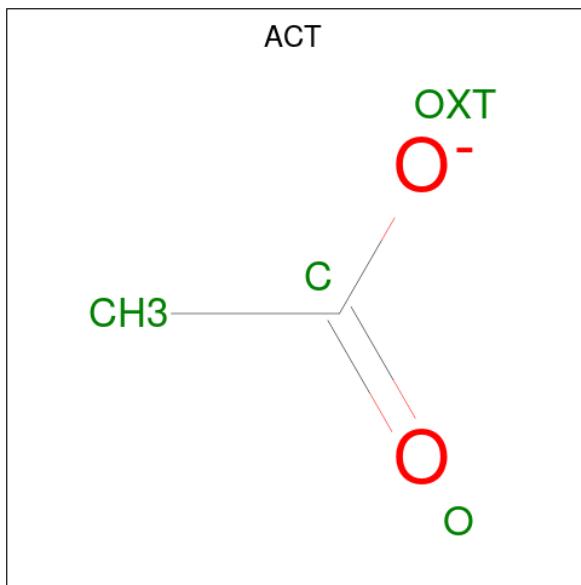
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP Q9WXT2
F	-11	MET	-	initiating methionine	UNP Q9WXT2
F	-10	GLY	-	expression tag	UNP Q9WXT2
F	-9	SER	-	expression tag	UNP Q9WXT2
F	-8	ASP	-	expression tag	UNP Q9WXT2
F	-7	LYS	-	expression tag	UNP Q9WXT2
F	-6	ILE	-	expression tag	UNP Q9WXT2
F	-5	HIS	-	expression tag	UNP Q9WXT2
F	-4	HIS	-	expression tag	UNP Q9WXT2
F	-3	HIS	-	expression tag	UNP Q9WXT2
F	-2	HIS	-	expression tag	UNP Q9WXT2
F	-1	HIS	-	expression tag	UNP Q9WXT2
F	0	HIS	-	expression tag	UNP Q9WXT2

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	B	1	1	1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	C	1	4	2	2	0	0
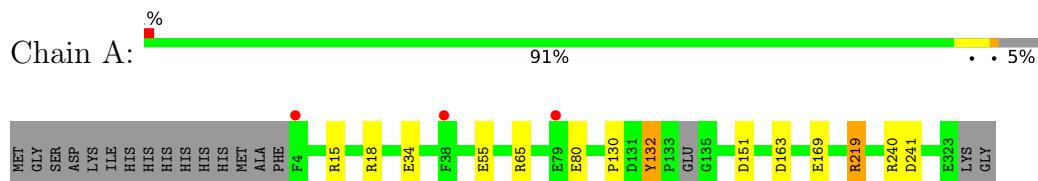
- Molecule 4 is water.

| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	213	Total 213 O 213	0	0
4	B	253	Total 253 O 253	0	0
4	C	255	Total 255 O 255	0	0
4	D	230	Total 230 O 230	0	0
4	E	282	Total 282 O 282	0	0
4	F	254	Total 254 O 254	0	0
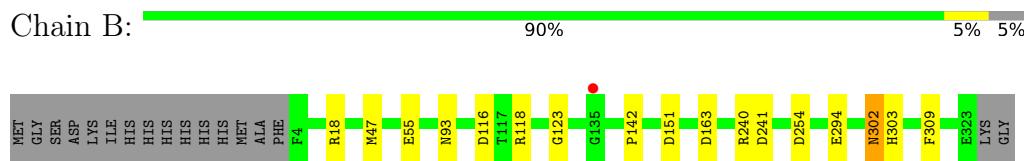
3 Residue-property plots ⓘ

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.
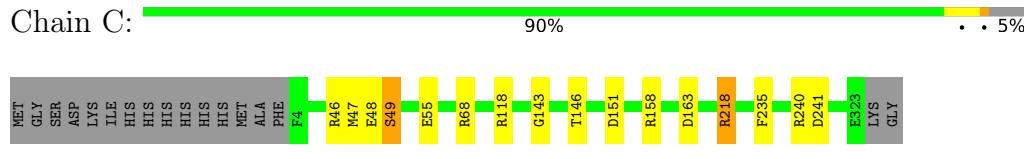
- Molecule 1: Cephalosporin-C deacetylase
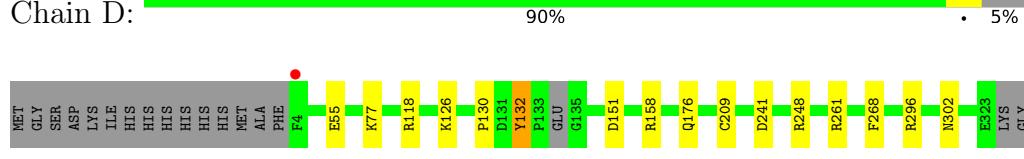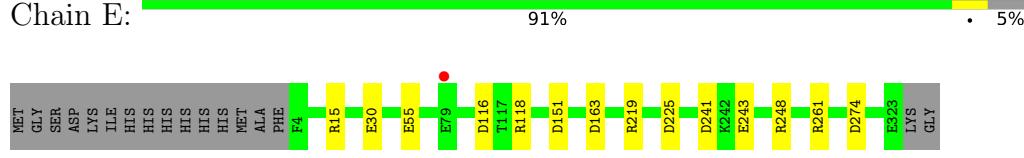
Chain A:

- Molecule 1: Cephalosporin-C deacetylase

Chain B:

- Molecule 1: Cephalosporin-C deacetylase

Chain C:

- Molecule 1: Cephalosporin-C deacetylase

Chain D:
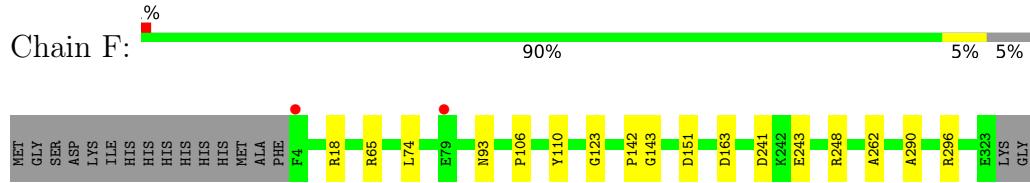
- Molecule 1: Cephalosporin-C deacetylase

Chain E:

- Molecule 1: Cephalosporin-C deacetylase

Chain F:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.76Å 116.20Å 103.29Å 90.00° 109.97° 90.00°	Depositor
Resolution (Å)	39.96 – 1.76 37.95 – 1.76	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.96-1.76) 98.8 (37.95-1.76)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.160 , 0.195 0.173 , 0.205	Depositor DCC
R_{free} test set	9696 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.5	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16780	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, CL

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	0.98	2/2594 (0.1%)	0.97	12/3532 (0.3%)
1	B	0.98	4/2655 (0.2%)	1.02	13/3604 (0.4%)
1	C	0.98	0/2627	1.05	13/3576 (0.4%)
1	D	0.95	0/2623	0.95	10/3567 (0.3%)
1	E	0.99	1/2659 (0.0%)	1.00	14/3611 (0.4%)
1	F	0.99	1/2625 (0.0%)	0.98	8/3574 (0.2%)
All	All	0.98	8/15783 (0.1%)	1.00	70/21464 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	GLU	CD-OE1	7.33	1.33	1.25
1	A	169	GLU	CG-CD	6.63	1.61	1.51
1	A	55	GLU	CD-OE2	5.77	1.31	1.25
1	B	302[A]	ASN	CB-CG	5.67	1.64	1.51
1	B	302[B]	ASN	CB-CG	5.67	1.64	1.51
1	B	294	GLU	CD-OE2	-5.64	1.19	1.25
1	F	243	GLU	CD-OE2	-5.54	1.19	1.25
1	E	243	GLU	CD-OE1	-5.14	1.20	1.25

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	ASP	CB-CG-OD1	12.96	129.97	118.30
1	D	241	ASP	CB-CG-OD1	12.02	129.12	118.30
1	E	241	ASP	CB-CG-OD1	10.87	128.09	118.30
1	C	151	ASP	CB-CG-OD1	9.45	126.80	118.30
1	F	241	ASP	CB-CG-OD1	9.37	126.73	118.30
1	B	118	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	D	248	ARG	NE-CZ-NH1	8.80	124.70	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	B	118	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	C	163	ASP	CB-CG-OD1	7.99	125.49	118.30
1	E	261	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	B	241	ASP	CB-CG-OD1	7.40	124.96	118.30
1	C	151	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	A	18	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	241	ASP	CB-CG-OD1	7.23	124.81	118.30
1	C	241	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	B	47	MET	CG-SD-CE	-7.21	88.67	100.20
1	C	47	MET	CB-CG-SD	-7.15	90.96	112.40
1	A	240	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	F	18	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	D	241	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	C	68	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	E	163	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	15	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	C	118	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	E	116	ASP	CB-CG-OD2	-6.38	112.55	118.30
1	A	15	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	E	241	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	E	248	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	D	296	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	E	116	ASP	CB-CG-OD1	6.01	123.71	118.30
1	E	118	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	163	ASP	CB-CG-OD1	5.92	123.63	118.30
1	E	118	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	E	219	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	F	151	ASP	CB-CG-OD1	5.84	123.56	118.30
1	D	151	ASP	CB-CG-OD1	5.83	123.55	118.30
1	D	261	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	241	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	A	240	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	F	241	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	F	296	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	219	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	240	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	296	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	18	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	219	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	169	GLU	OE1-CD-OE2	-5.48	116.72	123.30
1	B	241	ASP	CB-CG-OD2	-5.48	113.37	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	219	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	F	248	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	C	49	SER	CB-CA-C	5.38	120.33	110.10
1	F	163	ASP	CB-CG-OD1	5.38	123.14	118.30
1	D	248	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	151	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	163	ASP	CB-CG-OD1	5.33	123.10	118.30
1	B	151	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	151	ASP	CB-CG-OD1	5.33	123.09	118.30
1	E	151	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	240	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	18	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	F	65	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	118	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	E	225	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	48	GLU	N-CA-C	-5.07	97.31	111.00
1	B	254	ASP	CB-CG-OD1	5.06	122.85	118.30
1	D	158	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	C	158	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	116	ASP	CB-CG-OD1	5.02	122.82	118.30
1	E	274	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2516	0	2360	3	0
1	B	2572	0	2482	5	0
1	C	2541	0	2403	4	0
1	D	2541	0	2413	5	0
1	E	2576	0	2472	1	0
1	F	2542	0	2398	5	0
2	B	1	0	0	0	0
3	C	4	0	3	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	213	0	0	1	0
4	B	253	0	0	1	0
4	C	255	0	0	1	0
4	D	230	0	0	1	0
4	E	282	0	0	1	0
4	F	254	0	0	0	0
All	All	16780	0	14531	22	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 1.

All (22) 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:E:55:GLU:OE1	4:E:401:HOH:O	2.13	0.65
1:B:302[A]:ASN:CG	1:B:303:HIS:N	2.50	0.64
1:D:176:GLN:HG3	4:D:489:HOH:O	2.04	0.57
1:A:34:GLU:OE2	1:A:65:ARG:NH1	2.42	0.52
1:C:49:SER:HB2	4:C:505:HOH:O	2.10	0.52
1:F:262:ALA:O	1:F:290:ALA:HB3	2.13	0.49
3:C:401:ACT:H1	1:F:142:PRO:HA	1.95	0.49
1:B:93:ASN:HB3	1:B:123:GLY:HA3	1.95	0.49
1:F:93:ASN:HB3	1:F:123:GLY:HA3	1.97	0.46
1:A:80:GLU:O	4:A:401:HOH:O	2.20	0.46
1:B:309[A]:PHE:CZ	1:D:126:LYS:HD3	2.50	0.46
3:C:401:ACT:H1	1:F:143:GLY:H	1.82	0.43
1:D:55:GLU:HG3	1:D:77:LYS:HE3	2.01	0.42
1:D:130:PRO:HG2	1:D:132:TYR:CZ	2.55	0.42
1:C:143:GLY:H	3:C:401:ACT:H1	1.85	0.42
1:A:130:PRO:HG2	1:A:132:TYR:CZ	2.54	0.41
1:B:309[B]:PHE:HE1	4:B:686:HOH:O	2.03	0.41
1:D:209:CYS:O	1:D:268:PHE:HA	2.21	0.41
1:F:106:PRO:HA	1:F:110:TYR:O	2.20	0.41
1:C:46:ARG:NE	1:C:55:GLU:OE2	2.37	0.40
1:C:146:THR:HG21	1:C:235:PHE:HB2	2.03	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	315/337 (94%)	308 (98%)	7 (2%)	0	100	100
1	B	320/337 (95%)	310 (97%)	10 (3%)	0	100	100
1	C	320/337 (95%)	308 (96%)	12 (4%)	0	100	100
1	D	317/337 (94%)	308 (97%)	7 (2%)	2 (1%)	25	10
1	E	320/337 (95%)	311 (97%)	9 (3%)	0	100	100
1	F	320/337 (95%)	307 (96%)	13 (4%)	0	100	100
All	All	1912/2022 (95%)	1852 (97%)	58 (3%)	2 (0%)	51	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	302[A]	ASN
1	D	302[B]	ASN

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	254/285 (89%)	252 (99%)	2 (1%)	81	72
1	B	264/285 (93%)	263 (100%)	1 (0%)	91	87
1	C	258/285 (90%)	257 (100%)	1 (0%)	91	87
1	D	258/285 (90%)	257 (100%)	1 (0%)	91	87
1	E	265/285 (93%)	263 (99%)	2 (1%)	81	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	257/285 (90%)	256 (100%)	1 (0%)	91	87
All	All	1556/1710 (91%)	1548 (100%)	8 (0%)	88	83

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	TYR
1	A	219	ARG
1	B	142	PRO
1	C	218	ARG
1	D	132	TYR
1	E	15	ARG
1	E	30	GLU
1	F	74	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	222	GLN
1	C	179	GLN
1	E	222	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	ACT	C	401	-	3,3,3	1.18	0	3,3,3	1.28	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	ACT	3	0

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, 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(Å²)	Q<0.9
1	A	319/337 (94%)	-0.36	3 (0%)	84	89	14, 21, 34, 47	0
1	B	320/337 (94%)	-0.37	1 (0%)	94	95	13, 19, 33, 56	0
1	C	320/337 (94%)	-0.35	0	100	100	13, 20, 36, 57	0
1	D	319/337 (94%)	-0.36	1 (0%)	94	95	14, 20, 35, 48	0
1	E	320/337 (94%)	-0.46	1 (0%)	94	95	12, 17, 31, 47	0
1	F	320/337 (94%)	-0.48	2 (0%)	89	92	14, 19, 33, 52	0
All	All	1918/2022 (94%)	-0.40	8 (0%)	92	94	12, 19, 34, 57	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	PHE	3.2
1	A	79	GLU	2.9
1	F	4	PHE	2.5
1	A	38	PHE	2.5
1	B	135	GLY	2.5
1	A	4	PHE	2.1
1	F	79	GLU	2.1
1	E	79	GLU	2.1

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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACT	C	401	4/4	0.87	0.14	26,29,40,40	0
2	CL	B	401	1/1	0.98	0.03	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.