



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:58 am BST

PDB ID : 5JIB  
Title : Crystal structure of the *Thermotoga maritima* acetyl esterase (TM0077) complex with a substrate analog  
Authors : Manoj, N.  
Deposited on : 2016-04-22  
Resolution : 1.86 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](mailto: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.

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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 : 2.11  
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) : 2.11

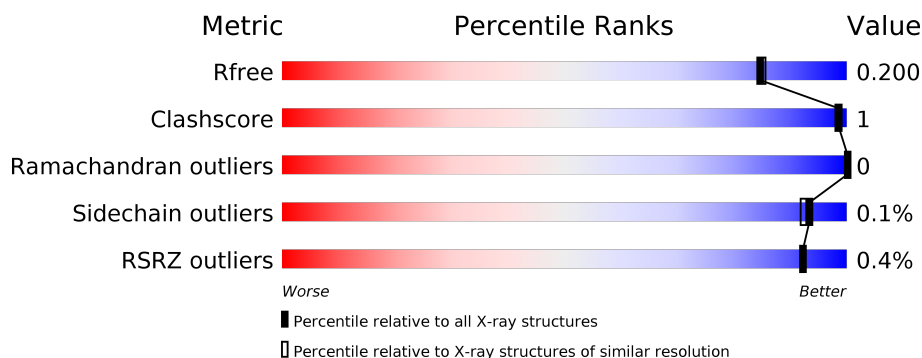
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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))
$R_{free}$	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	337	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>
1	B	337	<div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
1	C	337	<div> <div></div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
1	D	337	<div> <div></div> <div>92%</div> <div>5%</div> </div>
1	E	337	<div> <div></div> <div>91%</div> <div>5%</div> </div>
1	F	337	<div> <div>%</div> <div>91%</div> <div>5%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16248 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
			2497	1626	411	450	10			
1	B	319	Total	C	N	O	S	0	0	0
			2531	1647	425	449	10			
1	C	320	Total	C	N	O	S	0	1	0
			2515	1636	413	456	10			
1	D	319	Total	C	N	O	S	0	0	0
			2515	1637	417	451	10			
1	E	319	Total	C	N	O	S	0	0	0
			2548	1657	426	455	10			
1	F	320	Total	C	N	O	S	0	0	0
			2519	1636	419	454	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

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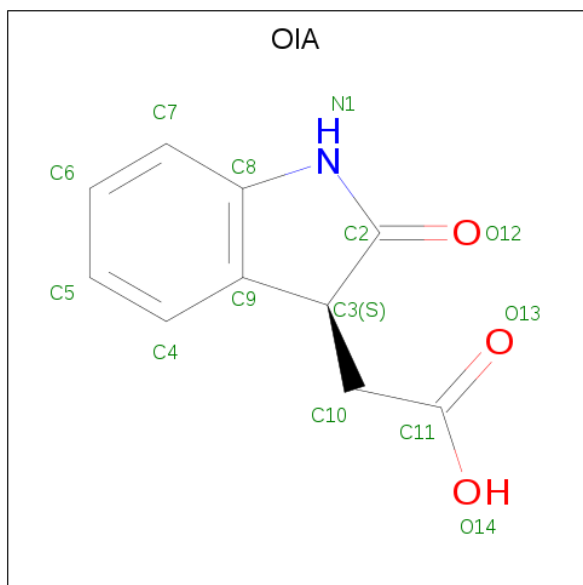
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	ILE	-	expression tag	UNP Q9WXT2
B	-5	HIS	-	expression tag	UNP Q9WXT2
B	-4	HIS	-	expression tag	UNP Q9WXT2
B	-3	HIS	-	expression tag	UNP Q9WXT2
B	-2	HIS	-	expression tag	UNP Q9WXT2
B	-1	HIS	-	expression tag	UNP Q9WXT2
B	0	HIS	-	expression tag	UNP Q9WXT2
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

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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 [(3S)-2-oxo-2,3-dihydro-1H-indol-3-yl]acetic acid (three-letter code: OIA) (formula: C<sub>10</sub>H<sub>9</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	10	1	3		
2	B	1	Total	C	N	O	0	0
			14	10	1	3		
2	C	1	Total	C	N	O	0	0
			14	10	1	3		
2	D	1	Total	C	N	O	0	0
			14	10	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			14	10	1	3		
2	F	1	Total	C	N	O	0	0
			14	10	1	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total	O	0	0
			152	152		
3	B	181	Total	O	0	0
			181	181		
3	C	181	Total	O	0	0
			181	181		
3	D	152	Total	O	0	0
			152	152		
3	E	204	Total	O	0	0
			204	204		
3	F	169	Total	O	0	0
			169	169		

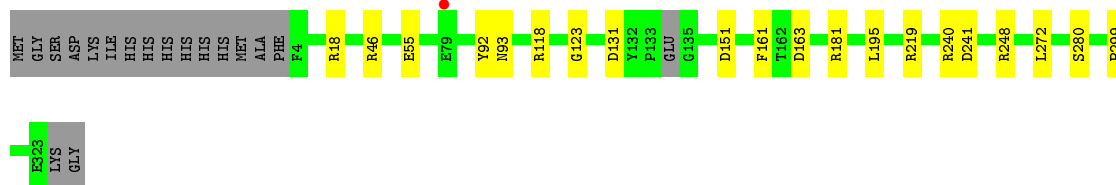
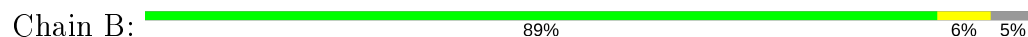
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



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- Molecule 1: Cephalosporin-C deacetylase

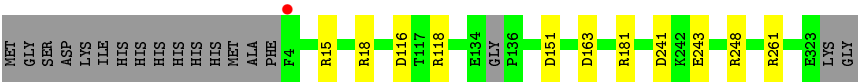


- Molecule 1: Cephalosporin-C deacetylase

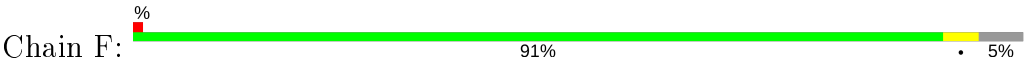


- Molecule 1: Cephalosporin-C deacetylase





● Molecule 1: Cephalosporin-C deacetylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.81Å 115.78Å 103.20Å 90.00° 109.98° 90.00°	Depositor
Resolution (Å)	45.97 – 1.86 39.89 – 1.86	Depositor EDS
% Data completeness (in resolution range)	94.8 (45.97-1.86) 94.8 (39.89-1.86)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.08 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.155 , 0.192 0.167 , 0.200	Depositor DCC
$R_{free}$ test set	7863 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16248	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.93	1/2575 (0.0%)	0.96	8/3507 (0.2%)
1	B	0.98	2/2609 (0.1%)	1.02	14/3545 (0.4%)
1	C	0.95	1/2597 (0.0%)	1.01	15/3539 (0.4%)
1	D	0.96	1/2593 (0.0%)	0.98	8/3528 (0.2%)
1	E	0.98	1/2626 (0.0%)	1.01	13/3565 (0.4%)
1	F	0.94	0/2598	0.96	10/3536 (0.3%)
All	All	0.96	6/15598 (0.0%)	0.99	68/21220 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	243	GLU	CD-OE1	-6.09	1.19	1.25
1	B	280	SER	CB-OG	-5.86	1.34	1.42
1	B	92	TYR	CE1-CZ	5.63	1.45	1.38
1	A	289	TYR	CE1-CZ	5.40	1.45	1.38
1	D	280	SER	CB-OG	-5.18	1.35	1.42
1	C	55	GLU	CD-OE2	-5.07	1.20	1.25

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	241	ASP	CB-CG-OD1	9.66	127.00	118.30
1	D	248	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	E	118	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	C	241	ASP	CB-CG-OD1	8.22	125.70	118.30
1	B	241	ASP	CB-CG-OD1	8.16	125.65	118.30
1	C	18	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	E	118	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	C	151	ASP	CB-CG-OD1	7.72	125.25	118.30
1	C	18	ARG	NE-CZ-NH2	-7.53	116.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	261	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	D	241	ASP	CB-CG-OD1	7.25	124.82	118.30
1	F	151	ASP	CB-CG-OD1	7.21	124.79	118.30
1	D	261	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	B	240	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	F	241	ASP	CB-CG-OD1	7.06	124.65	118.30
1	C	68	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	C	219	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	F	46	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	E	248	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	219	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	F	248	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	240	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	151	ASP	CB-CG-OD1	6.53	124.17	118.30
1	B	151	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	C	163	ASP	CB-CG-OD1	6.41	124.07	118.30
1	B	18	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	E	15	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	B	161	PHE	CB-CG-CD1	6.34	125.24	120.80
1	C	118	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	219	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	D	25	ASP	CB-CG-OD1	6.17	123.86	118.30
1	C	240	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	D	163	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	241	ASP	CB-CG-OD1	6.14	123.83	118.30
1	E	163	ASP	CB-CG-OD1	6.12	123.81	118.30
1	F	65	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	E	151	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	163	ASP	CB-CG-OD1	6.04	123.74	118.30
1	C	261	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	B	181	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	248	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	248	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	195	LEU	CA-CB-CG	5.66	128.33	115.30
1	E	18	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	E	163	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	B	118	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	18	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	219	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	D	248	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	D	58	ASP	CB-CG-OD1	5.54	123.29	118.30
1	C	58	ASP	CB-CG-OD1	5.47	123.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	248	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	163	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	F	46	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	E	181	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	151	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	65	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	E	116	ASP	CB-CG-OD2	-5.21	113.62	118.30
1	C	151	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	F	101	ASP	CB-CG-OD2	5.16	122.94	118.30
1	F	296	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	118	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	F	195	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	A	163	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	E	241	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	B	131	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	C	240	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	F	138	ASP	CB-CG-OD1	5.02	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	2497	0	2346	4	0
1	B	2531	0	2424	4	0
1	C	2515	0	2362	3	0
1	D	2515	0	2384	1	0
1	E	2548	0	2447	0	0
1	F	2519	0	2377	3	0
2	A	14	0	0	0	0
2	B	14	0	0	0	0
2	C	14	0	0	0	0
2	D	14	0	0	0	0
2	E	14	0	0	0	0
2	F	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	152	0	0	1	0
3	B	181	0	0	1	0
3	C	181	0	0	0	0
3	D	152	0	0	1	0
3	E	204	0	0	0	0
3	F	169	0	0	0	0
All	All	16248	0	14340	15	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 (15) 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:B:55:GLU:OE1	3:B:501:HOH:O	2.12	0.68
1:F:93:ASN:HB3	1:F:123:GLY:HA3	1.88	0.55
1:B:46:ARG:NH2	1:B:55:GLU:HG2	2.23	0.53
1:C:93:ASN:HB3	1:C:123:GLY:HA3	1.96	0.48
3:A:568:HOH:O	1:C:237:LYS:HD3	2.15	0.46
1:A:93:ASN:HB3	1:A:123:GLY:HA3	1.97	0.45
1:B:93:ASN:HB3	1:B:123:GLY:HA3	2.00	0.44
1:F:106:PRO:HA	1:F:110:TYR:O	2.18	0.44
1:F:272:LEU:HB2	1:F:299:PRO:HA	1.99	0.43
1:A:259:ALA:HB1	1:A:289:TYR:HA	2.02	0.42
1:C:146:THR:HG21	1:C:235:PHE:HB2	2.01	0.42
1:D:176:GLN:HG3	3:D:627:HOH:O	2.19	0.42
1:A:106:PRO:HA	1:A:110:TYR:O	2.19	0.42
1:B:272:LEU:HB2	1:B:299:PRO:HA	2.02	0.41
1:A:130:PRO:HG2	1:A:132:TYR:CZ	2.56	0.41

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%)	306 (97%)	9 (3%)	0	100	100
1	B	315/337 (94%)	307 (98%)	8 (2%)	0	100	100
1	C	319/337 (95%)	310 (97%)	9 (3%)	0	100	100
1	D	315/337 (94%)	306 (97%)	9 (3%)	0	100	100
1	E	315/337 (94%)	307 (98%)	8 (2%)	0	100	100
1	F	318/337 (94%)	312 (98%)	6 (2%)	0	100	100
All	All	1897/2022 (94%)	1848 (97%)	49 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	250/285 (88%)	250 (100%)	0	100	100
1	B	257/285 (90%)	257 (100%)	0	100	100
1	C	253/285 (89%)	252 (100%)	1 (0%)	91	89
1	D	254/285 (89%)	254 (100%)	0	100	100
1	E	261/285 (92%)	261 (100%)	0	100	100
1	F	254/285 (89%)	254 (100%)	0	100	100
All	All	1529/1710 (89%)	1528 (100%)	1 (0%)	93	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	46	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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
2	OIA	D	400	-	11,15,15	1.46	2 (18%)	14,21,21	1.87	5 (35%)
2	OIA	F	400	-	11,15,15	1.45	2 (18%)	14,21,21	2.32	3 (21%)
2	OIA	B	400	-	11,15,15	1.32	0	14,21,21	2.01	3 (21%)
2	OIA	E	400	-	11,15,15	1.56	2 (18%)	14,21,21	2.01	3 (21%)
2	OIA	A	400	-	11,15,15	1.95	5 (45%)	14,21,21	2.41	6 (42%)
2	OIA	C	400	-	11,15,15	1.64	3 (27%)	14,21,21	1.65	3 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OIA	D	400	-	-	0/2/16/16	0/2/2/2
2	OIA	F	400	-	-	0/2/16/16	0/2/2/2
2	OIA	B	400	-	-	0/2/16/16	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OIA	E	400	-	-	0/2/16/16	0/2/2/2
2	OIA	A	400	-	-	0/2/16/16	0/2/2/2
2	OIA	C	400	-	-	0/2/16/16	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	OIA	C9-C3	-3.43	1.45	1.51
2	C	400	OIA	C2-N1	3.25	1.38	1.35
2	E	400	OIA	C5-C4	3.00	1.45	1.38
2	D	400	OIA	C4-C9	-2.72	1.36	1.39
2	F	400	OIA	C4-C9	-2.60	1.36	1.39
2	A	400	OIA	C4-C9	-2.59	1.36	1.39
2	A	400	OIA	C8-C9	-2.49	1.37	1.39
2	F	400	OIA	C10-C3	2.20	1.62	1.54
2	E	400	OIA	C10-C3	2.19	1.62	1.54
2	A	400	OIA	C6-C7	2.16	1.43	1.38
2	A	400	OIA	C5-C4	2.12	1.43	1.38
2	C	400	OIA	C4-C9	-2.11	1.37	1.39
2	C	400	OIA	C9-C3	-2.06	1.48	1.51
2	D	400	OIA	C9-C3	-2.05	1.48	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	400	OIA	C10-C3-C9	6.08	129.59	115.01
2	E	400	OIA	C8-N1-C2	-4.89	109.18	111.85
2	A	400	OIA	C9-C3-C2	4.88	104.03	102.40
2	B	400	OIA	C9-C3-C2	4.57	103.93	102.40
2	A	400	OIA	C8-N1-C2	-4.14	109.59	111.85
2	F	400	OIA	C4-C9-C8	-3.67	117.67	119.95
2	B	400	OIA	C4-C9-C8	-3.61	117.70	119.95
2	A	400	OIA	C4-C9-C8	-3.31	117.89	119.95
2	F	400	OIA	C8-N1-C2	-3.28	110.06	111.85
2	C	400	OIA	C9-C3-C2	3.27	103.49	102.40
2	D	400	OIA	C4-C9-C8	-3.24	117.93	119.95
2	D	400	OIA	C9-C8-N1	-3.23	107.81	109.31
2	E	400	OIA	C4-C9-C8	-3.14	117.99	119.95
2	D	400	OIA	C8-N1-C2	-3.14	110.14	111.85
2	C	400	OIA	C4-C9-C8	-3.00	118.08	119.95
2	A	400	OIA	O12-C2-N1	-2.79	123.61	125.95
2	B	400	OIA	O12-C2-N1	-2.74	123.65	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	OIA	C8-N1-C2	-2.69	110.38	111.85
2	A	400	OIA	C11-C10-C3	2.49	119.53	113.94
2	D	400	OIA	C5-C6-C7	-2.31	116.67	120.19
2	E	400	OIA	C5-C6-C7	-2.24	116.78	120.19
2	A	400	OIA	C5-C4-C9	2.07	123.63	121.01
2	D	400	OIA	C9-C3-C2	2.00	103.07	102.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	319/337 (94%)	-0.54	2 (0%) 89 89	12, 19, 33, 53	0
1	B	319/337 (94%)	-0.41	1 (0%) 94 93	11, 16, 31, 51	0
1	C	320/337 (94%)	-0.55	0 100 100	10, 17, 32, 48	0
1	D	319/337 (94%)	-0.50	1 (0%) 94 93	12, 18, 33, 52	0
1	E	319/337 (94%)	-0.57	1 (0%) 94 93	10, 15, 29, 48	0
1	F	320/337 (94%)	-0.53	2 (0%) 89 89	11, 17, 33, 55	0
All	All	1916/2022 (94%)	-0.52	7 (0%) 92 92	10, 17, 32, 55	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	GLU	3.6
1	D	4	PHE	3.0
1	B	79	GLU	2.8
1	E	4	PHE	2.7
1	A	4	PHE	2.3
1	F	4	PHE	2.2
1	F	79	GLU	2.1

### 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 carbohydrates 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	OIA	A	400	14/14	0.83	0.15	20,32,38,41	0
2	OIA	B	400	14/14	0.85	0.15	15,32,38,38	0
2	OIA	E	400	14/14	0.86	0.17	15,34,36,37	0
2	OIA	F	400	14/14	0.86	0.15	18,36,40,41	0
2	OIA	C	400	14/14	0.87	0.15	17,30,33,33	0
2	OIA	D	400	14/14	0.88	0.14	17,33,39,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.