



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2025 – 10:08 AM JST

PDB ID : 8ZT3
Title : N-acetyltransferase SbzI in the biosynthesis of altemicidin
Authors : Rui, Z.; Mori, T.; Abe, I.
Deposited on : 2024-06-06
Resolution : 2.50 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)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

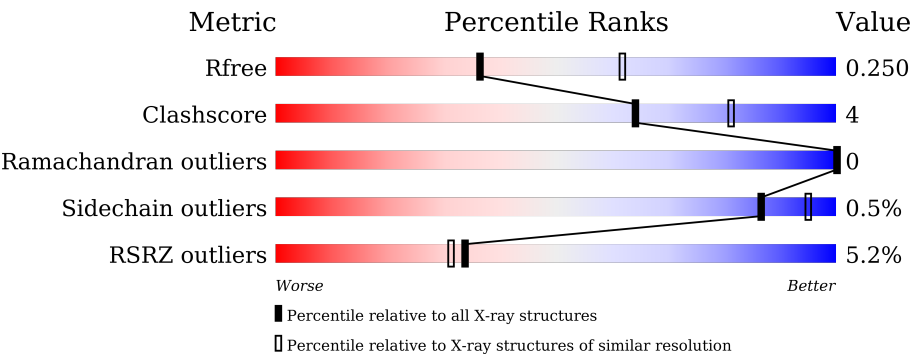
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	208	<div><div>%</div><div><div></div><div>73%</div><div>6%</div><div>21%</div></div></div>
1	B	208	<div><div>3%</div><div><div></div><div>72%</div><div>8%</div><div>21%</div></div></div>
1	C	208	<div><div>5%</div><div><div></div><div>73%</div><div>6%</div><div>21%</div></div></div>
1	D	208	<div><div>%</div><div><div></div><div>80%</div><div>.</div><div>16%</div></div></div>
1	E	208	<div><div>7%</div><div><div></div><div>68%</div><div>11%</div><div>21%</div></div></div>
1	F	208	<div><div>7%</div><div><div></div><div>63%</div><div>12%</div><div>25%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7743 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 GNAT family transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	175	Total	C	N	O	S	0	2	0
			1334	821	258	249	6			
1	A	164	Total	C	N	O	S	0	0	0
			1247	770	242	229	6			
1	B	165	Total	C	N	O	S	0	0	0
			1258	776	246	230	6			
1	C	165	Total	C	N	O	S	0	0	0
			1258	776	246	230	6			
1	E	165	Total	C	N	O	S	0	0	0
			1265	782	246	231	6			
1	F	155	Total	C	N	O	S	0	0	0
			1196	744	232	215	5			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP A0A3T0ZHG5
D	-18	GLY	-	expression tag	UNP A0A3T0ZHG5
D	-17	SER	-	expression tag	UNP A0A3T0ZHG5
D	-16	SER	-	expression tag	UNP A0A3T0ZHG5
D	-15	HIS	-	expression tag	UNP A0A3T0ZHG5
D	-14	HIS	-	expression tag	UNP A0A3T0ZHG5
D	-13	HIS	-	expression tag	UNP A0A3T0ZHG5
D	-12	HIS	-	expression tag	UNP A0A3T0ZHG5
D	-11	HIS	-	expression tag	UNP A0A3T0ZHG5
D	-10	HIS	-	expression tag	UNP A0A3T0ZHG5
D	-9	SER	-	expression tag	UNP A0A3T0ZHG5
D	-8	SER	-	expression tag	UNP A0A3T0ZHG5
D	-7	GLY	-	expression tag	UNP A0A3T0ZHG5
D	-6	LEU	-	expression tag	UNP A0A3T0ZHG5
D	-5	VAL	-	expression tag	UNP A0A3T0ZHG5
D	-4	PRO	-	expression tag	UNP A0A3T0ZHG5
D	-3	ARG	-	expression tag	UNP A0A3T0ZHG5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP A0A3T0ZHG5
D	-1	SER	-	expression tag	UNP A0A3T0ZHG5
D	0	HIS	-	expression tag	UNP A0A3T0ZHG5
D	29	MET	LEU	engineered mutation	UNP A0A3T0ZHG5
D	50	MET	LEU	engineered mutation	UNP A0A3T0ZHG5
A	-19	MET	-	initiating methionine	UNP A0A3T0ZHG5
A	-18	GLY	-	expression tag	UNP A0A3T0ZHG5
A	-17	SER	-	expression tag	UNP A0A3T0ZHG5
A	-16	SER	-	expression tag	UNP A0A3T0ZHG5
A	-15	HIS	-	expression tag	UNP A0A3T0ZHG5
A	-14	HIS	-	expression tag	UNP A0A3T0ZHG5
A	-13	HIS	-	expression tag	UNP A0A3T0ZHG5
A	-12	HIS	-	expression tag	UNP A0A3T0ZHG5
A	-11	HIS	-	expression tag	UNP A0A3T0ZHG5
A	-10	HIS	-	expression tag	UNP A0A3T0ZHG5
A	-9	SER	-	expression tag	UNP A0A3T0ZHG5
A	-8	SER	-	expression tag	UNP A0A3T0ZHG5
A	-7	GLY	-	expression tag	UNP A0A3T0ZHG5
A	-6	LEU	-	expression tag	UNP A0A3T0ZHG5
A	-5	VAL	-	expression tag	UNP A0A3T0ZHG5
A	-4	PRO	-	expression tag	UNP A0A3T0ZHG5
A	-3	ARG	-	expression tag	UNP A0A3T0ZHG5
A	-2	GLY	-	expression tag	UNP A0A3T0ZHG5
A	-1	SER	-	expression tag	UNP A0A3T0ZHG5
A	0	HIS	-	expression tag	UNP A0A3T0ZHG5
A	29	MET	LEU	engineered mutation	UNP A0A3T0ZHG5
A	50	MET	LEU	engineered mutation	UNP A0A3T0ZHG5
B	-19	MET	-	initiating methionine	UNP A0A3T0ZHG5
B	-18	GLY	-	expression tag	UNP A0A3T0ZHG5
B	-17	SER	-	expression tag	UNP A0A3T0ZHG5
B	-16	SER	-	expression tag	UNP A0A3T0ZHG5
B	-15	HIS	-	expression tag	UNP A0A3T0ZHG5
B	-14	HIS	-	expression tag	UNP A0A3T0ZHG5
B	-13	HIS	-	expression tag	UNP A0A3T0ZHG5
B	-12	HIS	-	expression tag	UNP A0A3T0ZHG5
B	-11	HIS	-	expression tag	UNP A0A3T0ZHG5
B	-10	HIS	-	expression tag	UNP A0A3T0ZHG5
B	-9	SER	-	expression tag	UNP A0A3T0ZHG5
B	-8	SER	-	expression tag	UNP A0A3T0ZHG5
B	-7	GLY	-	expression tag	UNP A0A3T0ZHG5
B	-6	LEU	-	expression tag	UNP A0A3T0ZHG5
B	-5	VAL	-	expression tag	UNP A0A3T0ZHG5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	PRO	-	expression tag	UNP A0A3T0ZHG5
B	-3	ARG	-	expression tag	UNP A0A3T0ZHG5
B	-2	GLY	-	expression tag	UNP A0A3T0ZHG5
B	-1	SER	-	expression tag	UNP A0A3T0ZHG5
B	0	HIS	-	expression tag	UNP A0A3T0ZHG5
B	29	MET	LEU	engineered mutation	UNP A0A3T0ZHG5
B	50	MET	LEU	engineered mutation	UNP A0A3T0ZHG5
C	-19	MET	-	initiating methionine	UNP A0A3T0ZHG5
C	-18	GLY	-	expression tag	UNP A0A3T0ZHG5
C	-17	SER	-	expression tag	UNP A0A3T0ZHG5
C	-16	SER	-	expression tag	UNP A0A3T0ZHG5
C	-15	HIS	-	expression tag	UNP A0A3T0ZHG5
C	-14	HIS	-	expression tag	UNP A0A3T0ZHG5
C	-13	HIS	-	expression tag	UNP A0A3T0ZHG5
C	-12	HIS	-	expression tag	UNP A0A3T0ZHG5
C	-11	HIS	-	expression tag	UNP A0A3T0ZHG5
C	-10	HIS	-	expression tag	UNP A0A3T0ZHG5
C	-9	SER	-	expression tag	UNP A0A3T0ZHG5
C	-8	SER	-	expression tag	UNP A0A3T0ZHG5
C	-7	GLY	-	expression tag	UNP A0A3T0ZHG5
C	-6	LEU	-	expression tag	UNP A0A3T0ZHG5
C	-5	VAL	-	expression tag	UNP A0A3T0ZHG5
C	-4	PRO	-	expression tag	UNP A0A3T0ZHG5
C	-3	ARG	-	expression tag	UNP A0A3T0ZHG5
C	-2	GLY	-	expression tag	UNP A0A3T0ZHG5
C	-1	SER	-	expression tag	UNP A0A3T0ZHG5
C	0	HIS	-	expression tag	UNP A0A3T0ZHG5
C	29	MET	LEU	engineered mutation	UNP A0A3T0ZHG5
C	50	MET	LEU	engineered mutation	UNP A0A3T0ZHG5
E	-19	MET	-	initiating methionine	UNP A0A3T0ZHG5
E	-18	GLY	-	expression tag	UNP A0A3T0ZHG5
E	-17	SER	-	expression tag	UNP A0A3T0ZHG5
E	-16	SER	-	expression tag	UNP A0A3T0ZHG5
E	-15	HIS	-	expression tag	UNP A0A3T0ZHG5
E	-14	HIS	-	expression tag	UNP A0A3T0ZHG5
E	-13	HIS	-	expression tag	UNP A0A3T0ZHG5
E	-12	HIS	-	expression tag	UNP A0A3T0ZHG5
E	-11	HIS	-	expression tag	UNP A0A3T0ZHG5
E	-10	HIS	-	expression tag	UNP A0A3T0ZHG5
E	-9	SER	-	expression tag	UNP A0A3T0ZHG5
E	-8	SER	-	expression tag	UNP A0A3T0ZHG5
E	-7	GLY	-	expression tag	UNP A0A3T0ZHG5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	LEU	-	expression tag	UNP A0A3T0ZHG5
E	-5	VAL	-	expression tag	UNP A0A3T0ZHG5
E	-4	PRO	-	expression tag	UNP A0A3T0ZHG5
E	-3	ARG	-	expression tag	UNP A0A3T0ZHG5
E	-2	GLY	-	expression tag	UNP A0A3T0ZHG5
E	-1	SER	-	expression tag	UNP A0A3T0ZHG5
E	0	HIS	-	expression tag	UNP A0A3T0ZHG5
E	29	MET	LEU	engineered mutation	UNP A0A3T0ZHG5
E	50	MET	LEU	engineered mutation	UNP A0A3T0ZHG5
F	-19	MET	-	initiating methionine	UNP A0A3T0ZHG5
F	-18	GLY	-	expression tag	UNP A0A3T0ZHG5
F	-17	SER	-	expression tag	UNP A0A3T0ZHG5
F	-16	SER	-	expression tag	UNP A0A3T0ZHG5
F	-15	HIS	-	expression tag	UNP A0A3T0ZHG5
F	-14	HIS	-	expression tag	UNP A0A3T0ZHG5
F	-13	HIS	-	expression tag	UNP A0A3T0ZHG5
F	-12	HIS	-	expression tag	UNP A0A3T0ZHG5
F	-11	HIS	-	expression tag	UNP A0A3T0ZHG5
F	-10	HIS	-	expression tag	UNP A0A3T0ZHG5
F	-9	SER	-	expression tag	UNP A0A3T0ZHG5
F	-8	SER	-	expression tag	UNP A0A3T0ZHG5
F	-7	GLY	-	expression tag	UNP A0A3T0ZHG5
F	-6	LEU	-	expression tag	UNP A0A3T0ZHG5
F	-5	VAL	-	expression tag	UNP A0A3T0ZHG5
F	-4	PRO	-	expression tag	UNP A0A3T0ZHG5
F	-3	ARG	-	expression tag	UNP A0A3T0ZHG5
F	-2	GLY	-	expression tag	UNP A0A3T0ZHG5
F	-1	SER	-	expression tag	UNP A0A3T0ZHG5
F	0	HIS	-	expression tag	UNP A0A3T0ZHG5
F	29	MET	LEU	engineered mutation	UNP A0A3T0ZHG5
F	50	MET	LEU	engineered mutation	UNP A0A3T0ZHG5

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	46	Total 46	O 46	0	0
3	A	52	Total 52	O 52	0	0
3	B	34	Total 34	O 34	0	0
3	C	23	Total 23	O 23	0	0
3	E	21	Total 21	O 21	0	0
3	F	8	Total 8	O 8	0	0

- Molecule 1: GNAT family transferase

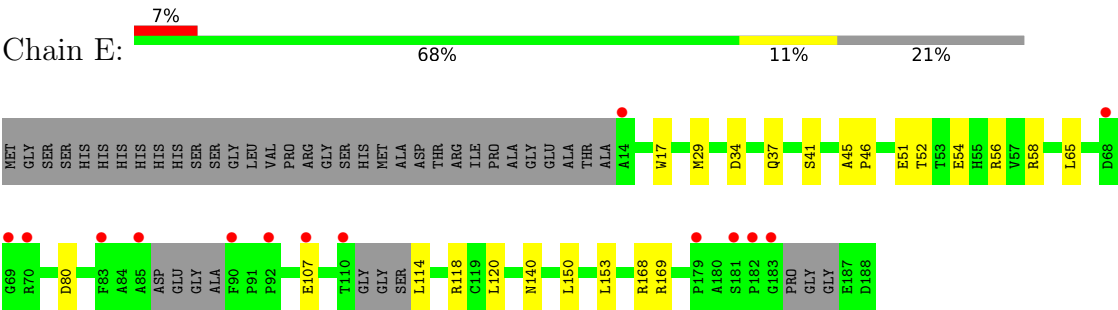


- | | |
|------|------|
| MET | GLY |
| SER | SER |
| SER | SER |
| HIS | HIS |
| HIS | HIS |
| HIS | HIS |
| HIS | HIS |
| HIS | HIS |
| SER | SER |
| SER | SER |
| GLY | LEU |
| VAL | PRO |
| ARG | ARG |
| GLY | GLY |
| SER | SER |
| HIS | HIS |
| MET | MET |
| ALA | ASP |
| THR | THR |
| ARG | ARG |
| ILE | ILE |
| PRO | PRO |
| ALA | GLY |
| GLU | GLU |
| ALA | ALA |
| THR | THR |
| ALA | ALA |
| A14 | F90 |
| A105 | A105 |
| W108 | G111 |
| G112 | G112 |
| I124 | I124 |
| R136 | R136 |
| D142 | D142 |
| F155 | F155 |
| R169 | R169 |
| H172 | L173 |
| H174 | K175 |
| S176 | L177 |

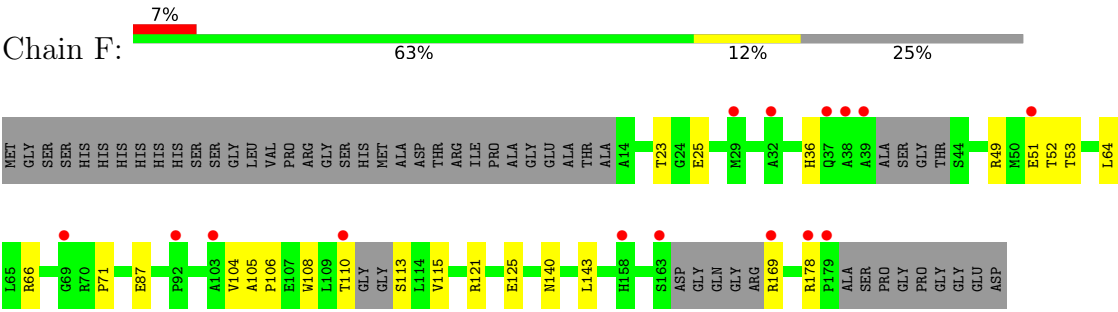
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- Sequence logo for the 100th position. The y-axis represents information content in bits (0 to 1.5). The x-axis lists amino acids. The most abundant residues are MET, GLY, SER, and HIS.

● Molecule 1: GNAT family transferase



● Molecule 1: GNAT family transferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.76Å 64.40Å 93.12Å 108.54° 90.80° 90.01°	Depositor
Resolution (Å)	44.28 – 2.50 44.28 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.1 (44.28-2.50) 98.2 (44.28-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.201 , 0.251 0.201 , 0.250	Depositor DCC
R_{free} test set	36688 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l 0.065 for -h,k,-k-l 0.010 for -h,-k,k+l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7743	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.25	0/1277	0.53	0/1735
1	B	0.25	0/1288	0.53	0/1749
1	C	0.25	0/1288	0.55	0/1749
1	D	0.26	0/1365	0.54	0/1856
1	E	0.25	0/1294	0.53	0/1754
1	F	0.25	0/1224	0.54	0/1662
All	All	0.25	0/7736	0.54	0/10505

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1247	0	1215	7	0
1	B	1258	0	1228	8	0
1	C	1258	0	1228	9	0
1	D	1334	0	1297	5	0
1	E	1265	0	1233	14	0
1	F	1196	0	1168	15	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	52	0	0	0	0
3	B	34	0	0	0	0
3	C	23	0	0	0	0
3	D	46	0	0	0	0
3	E	21	0	0	0	0
3	F	8	0	0	1	0
All	All	7743	0	7369	57	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 (57) 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:F:105:ALA:HB3	1:F:108:TRP:HD1	1.51	0.76
1:F:108:TRP:HB3	1:F:115:VAL:HG21	1.75	0.67
1:C:23:THR:HG21	1:C:54:GLU:HG3	1.78	0.66
1:F:64:LEU:HD21	1:F:71:PRO:HB3	1.81	0.63
1:F:36:HIS:HD2	1:F:106:PRO:HB3	1.67	0.60
1:C:105:ALA:HB3	1:C:108:TRP:HD1	1.69	0.58
1:F:110:THR:O	1:F:113:SER:N	2.37	0.57
1:F:169:ARG:N	3:F:201:HOH:O	2.38	0.57
1:D:95:ARG:HD3	1:E:45:ALA:HB3	1.88	0.56
1:E:120:LEU:HD23	1:E:153:LEU:HD22	1.89	0.55
1:D:125:GLU:O	1:D:129:GLN:HG3	2.07	0.54
1:E:120:LEU:HD21	1:E:150:LEU:HD23	1.90	0.54
1:E:34:ASP:HB3	1:E:45:ALA:HB1	1.90	0.54
1:B:121:ARG:NH2	1:B:125:GLU:OE2	2.41	0.53
1:F:36:HIS:CD2	1:F:106:PRO:HB3	2.45	0.52
1:C:87:GLU:N	1:C:87:GLU:OE1	2.43	0.52
1:F:121:ARG:O	1:F:125:GLU:HG3	2.11	0.50
1:F:178:ARG:NE	1:F:178:ARG:HA	2.26	0.50
1:E:107:GLU:OE2	1:E:107:GLU:N	2.41	0.50
1:C:29:MET:HE1	1:C:105:ALA:HA	1.94	0.50
1:A:136:ARG:HE	1:A:174:HIS:CD2	2.30	0.49
1:B:142:ASP:OD1	1:B:169:ARG:NH1	2.47	0.48
1:E:52:THR:O	1:E:56:ARG:HG2	2.14	0.48
1:A:142:ASP:OD1	1:A:169:ARG:NH1	2.47	0.48
1:E:46:PRO:HA	1:E:168:ARG:HH21	1.79	0.47
1:A:90:PHE:CZ	1:A:172:HIS:HB3	2.50	0.47
1:F:66:ARG:NH1	1:F:71:PRO:HG3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ILE:HD13	1:A:175:LYS:HE2	1.96	0.46
1:B:54:GLU:O	1:B:58:ARG:HG3	2.15	0.46
1:E:140:ASN:ND2	1:E:169:ARG:O	2.43	0.46
1:A:136:ARG:HE	1:A:174:HIS:HD2	1.63	0.46
1:C:52:THR:O	1:C:56:ARG:HG2	2.16	0.46
1:F:49:ARG:HD3	1:F:52:THR:HG23	1.98	0.46
1:E:37:GLN:O	1:E:41:SER:OG	2.27	0.46
1:B:105:ALA:HB3	1:B:108:TRP:HD1	1.81	0.45
1:E:51:GLU:OE1	1:E:51:GLU:N	2.42	0.45
1:F:108:TRP:O	1:F:113:SER:OG	2.23	0.45
1:D:124:ILE:HD13	1:D:175:LYS:HE2	1.99	0.45
1:C:50:MET:O	1:C:50:MET:HE3	2.17	0.45
1:F:23:THR:HG23	1:F:53:THR:HG22	1.99	0.45
1:D:23:THR:OG1	1:D:58:ARG:NH1	2.50	0.44
1:D:155:PHE:HB3	1:D:173:LEU:HB3	1.99	0.44
1:C:105:ALA:HB3	1:C:108:TRP:CD1	2.50	0.44
1:B:34:ASP:HB3	1:B:45:ALA:HB1	2.00	0.44
1:A:105:ALA:HB3	1:A:108:TRP:HD1	1.83	0.43
1:B:124:ILE:HD13	1:B:175:LYS:HE2	1.99	0.43
1:F:51:GLU:OE1	1:F:51:GLU:N	2.48	0.43
1:C:124:ILE:HD13	1:C:175:LYS:HE2	2.00	0.43
1:C:15:TRP:HB3	1:C:65:LEU:HD11	2.01	0.42
1:E:114:LEU:O	1:E:118:ARG:HG3	2.20	0.42
1:F:140:ASN:HB3	1:F:143:LEU:HD13	2.02	0.42
1:A:155:PHE:HB3	1:A:173:LEU:HB3	2.02	0.41
1:E:54:GLU:OE1	1:E:58:ARG:HD3	2.20	0.41
1:B:95:ARG:H	1:B:133:ASP:HB2	1.86	0.41
1:B:155:PHE:HB3	1:B:173:LEU:HB3	2.03	0.40
1:E:80:ASP:OD1	1:E:80:ASP:N	2.49	0.40
1:E:17:TRP:CZ2	1:E:65:LEU:HB2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	162/208 (78%)	162 (100%)	0	0	100	100
1	B	163/208 (78%)	161 (99%)	2 (1%)	0	100	100
1	C	163/208 (78%)	161 (99%)	2 (1%)	0	100	100
1	D	175/208 (84%)	169 (97%)	6 (3%)	0	100	100
1	E	157/208 (76%)	157 (100%)	0	0	100	100
1	F	147/208 (71%)	147 (100%)	0	0	100	100
All	All	967/1248 (78%)	957 (99%)	10 (1%)	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	126/158 (80%)	126 (100%)	0	100	100
1	B	127/158 (80%)	127 (100%)	0	100	100
1	C	127/158 (80%)	127 (100%)	0	100	100
1	D	134/158 (85%)	134 (100%)	0	100	100
1	E	129/158 (82%)	128 (99%)	1 (1%)	79	91
1	F	122/158 (77%)	119 (98%)	3 (2%)	42	69
All	All	765/948 (81%)	761 (100%)	4 (0%)	86	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	29	MET
1	F	25	GLU
1	F	87	GLU
1	F	104	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	HIS
1	C	55	HIS
1	C	129	GLN
1	C	158	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	164/208 (78%)	-0.05	2 (1%) 76 73	25, 38, 56, 67	0
1	B	165/208 (79%)	0.11	7 (4%) 41 38	28, 41, 74, 122	0
1	C	165/208 (79%)	0.40	10 (6%) 28 26	29, 46, 76, 116	0
1	D	175/208 (84%)	-0.00	3 (1%) 69 65	25, 37, 61, 78	2 (1%)
1	E	165/208 (79%)	0.53	14 (8%) 18 17	32, 53, 84, 91	0
1	F	155/208 (74%)	0.90	15 (9%) 15 14	43, 63, 99, 114	0
All	All	989/1248 (79%)	0.31	51 (5%) 34 31	25, 46, 84, 122	2 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	131	GLY	5.4
1	F	32	ALA	3.5
1	E	68	ASP	3.5
1	E	110	THR	3.3
1	F	39	ALA	3.3
1	E	85	ALA	3.2
1	F	163	SER	3.2
1	C	130	ALA	3.1
1	F	158	HIS	3.1
1	F	179	PRO	3.0
1	D	89	ALA	3.0
1	C	165	GLY	3.0
1	D	21	ARG	2.9
1	E	183	GLY	2.8
1	F	103	ALA	2.8
1	E	83	PHE	2.8
1	E	107	GLU	2.7
1	F	37	GLN	2.7
1	F	51	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	111	GLY	2.6
1	F	38	ALA	2.6
1	E	182	PRO	2.6
1	A	112	GLY	2.6
1	B	111	GLY	2.5
1	F	29	MET	2.5
1	B	113	SER	2.4
1	F	110	THR	2.4
1	B	14	ALA	2.4
1	C	50	MET	2.4
1	E	179	PRO	2.4
1	F	69	GLY	2.3
1	F	169	ARG	2.3
1	B	50	MET	2.3
1	D	8	ALA	2.2
1	C	112	GLY	2.2
1	C	132	GLY	2.2
1	C	167	GLY	2.2
1	B	166	GLN	2.2
1	C	89	ALA	2.2
1	E	14	ALA	2.2
1	B	167	GLY	2.2
1	E	69	GLY	2.2
1	F	178	ARG	2.2
1	E	92	PRO	2.2
1	E	70	ARG	2.1
1	B	165	GLY	2.1
1	F	92	PRO	2.1
1	E	181	SER	2.1
1	C	133	ASP	2.1
1	C	47	ALA	2.0
1	E	90	PHE	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](#)

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
2	CL	B	201	1/1	0.94	0.10	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.