



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:53 PM UTC

PDB ID : 1Z7D / pdb_00001z7d
Title : Ornithine aminotransferase PY00104 from Plasmodium Yoelii
Authors : Walker, J.R.; Alam, Z.; Amani, M.; Lew, J.; Wasney, G.; Boulanger, K.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.; Edwards, A.; Bochkarev, A.; Hui, R.; Vedadi, M.; Structural Genomics Consortium (SGC)
Deposited on : 2005-03-24
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

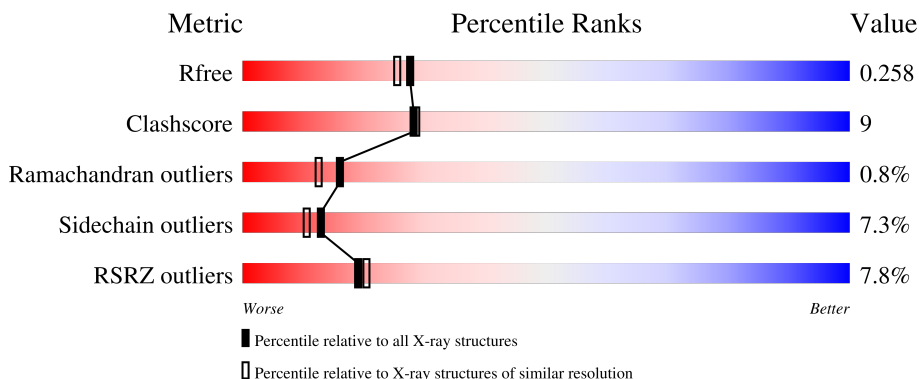
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	433	3% 70% 14% • 13%
1	B	433	7% 68% 16% • 13%
1	C	433	9% 65% 17% • 15%
1	D	433	5% 67% 16% • 13%
1	E	433	9% 70% 15% • 14%

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Mol	Chain	Length	Quality of chain
1	F	433	7% 67% 16% • • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18172 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 ornithine aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2969	1898	497	555	19			
1	B	377	Total	C	N	O	S	0	0	0
			2960	1893	495	553	19			
1	C	369	Total	C	N	O	S	0	0	0
			2895	1851	483	542	19			
1	D	375	Total	C	N	O	S	0	0	0
			2944	1885	491	549	19			
1	E	374	Total	C	N	O	S	0	0	0
			2935	1879	489	548	19			
1	F	375	Total	C	N	O	S	0	0	0
			2944	1885	491	549	19			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	cloning artifact	UNP Q7RT90
A	-18	GLY	-	cloning artifact	UNP Q7RT90
A	-17	SER	-	cloning artifact	UNP Q7RT90
A	-16	SER	-	cloning artifact	UNP Q7RT90
A	-15	HIS	-	cloning artifact	UNP Q7RT90
A	-14	HIS	-	cloning artifact	UNP Q7RT90
A	-13	HIS	-	cloning artifact	UNP Q7RT90
A	-12	HIS	-	cloning artifact	UNP Q7RT90
A	-11	HIS	-	cloning artifact	UNP Q7RT90
A	-10	HIS	-	cloning artifact	UNP Q7RT90
A	-9	SER	-	cloning artifact	UNP Q7RT90
A	-8	SER	-	cloning artifact	UNP Q7RT90
A	-7	GLY	-	cloning artifact	UNP Q7RT90
A	-6	LEU	-	cloning artifact	UNP Q7RT90
A	-5	VAL	-	cloning artifact	UNP Q7RT90
A	-4	PRO	-	cloning artifact	UNP Q7RT90
A	-3	ARG	-	cloning artifact	UNP Q7RT90

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP Q7RT90
A	-1	SER	-	cloning artifact	UNP Q7RT90
B	-19	MET	-	cloning artifact	UNP Q7RT90
B	-18	GLY	-	cloning artifact	UNP Q7RT90
B	-17	SER	-	cloning artifact	UNP Q7RT90
B	-16	SER	-	cloning artifact	UNP Q7RT90
B	-15	HIS	-	cloning artifact	UNP Q7RT90
B	-14	HIS	-	cloning artifact	UNP Q7RT90
B	-13	HIS	-	cloning artifact	UNP Q7RT90
B	-12	HIS	-	cloning artifact	UNP Q7RT90
B	-11	HIS	-	cloning artifact	UNP Q7RT90
B	-10	HIS	-	cloning artifact	UNP Q7RT90
B	-9	SER	-	cloning artifact	UNP Q7RT90
B	-8	SER	-	cloning artifact	UNP Q7RT90
B	-7	GLY	-	cloning artifact	UNP Q7RT90
B	-6	LEU	-	cloning artifact	UNP Q7RT90
B	-5	VAL	-	cloning artifact	UNP Q7RT90
B	-4	PRO	-	cloning artifact	UNP Q7RT90
B	-3	ARG	-	cloning artifact	UNP Q7RT90
B	-2	GLY	-	cloning artifact	UNP Q7RT90
B	-1	SER	-	cloning artifact	UNP Q7RT90
C	-19	MET	-	cloning artifact	UNP Q7RT90
C	-18	GLY	-	cloning artifact	UNP Q7RT90
C	-17	SER	-	cloning artifact	UNP Q7RT90
C	-16	SER	-	cloning artifact	UNP Q7RT90
C	-15	HIS	-	cloning artifact	UNP Q7RT90
C	-14	HIS	-	cloning artifact	UNP Q7RT90
C	-13	HIS	-	cloning artifact	UNP Q7RT90
C	-12	HIS	-	cloning artifact	UNP Q7RT90
C	-11	HIS	-	cloning artifact	UNP Q7RT90
C	-10	HIS	-	cloning artifact	UNP Q7RT90
C	-9	SER	-	cloning artifact	UNP Q7RT90
C	-8	SER	-	cloning artifact	UNP Q7RT90
C	-7	GLY	-	cloning artifact	UNP Q7RT90
C	-6	LEU	-	cloning artifact	UNP Q7RT90
C	-5	VAL	-	cloning artifact	UNP Q7RT90
C	-4	PRO	-	cloning artifact	UNP Q7RT90
C	-3	ARG	-	cloning artifact	UNP Q7RT90
C	-2	GLY	-	cloning artifact	UNP Q7RT90
C	-1	SER	-	cloning artifact	UNP Q7RT90
D	-19	MET	-	cloning artifact	UNP Q7RT90
D	-18	GLY	-	cloning artifact	UNP Q7RT90

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	cloning artifact	UNP Q7RT90
D	-16	SER	-	cloning artifact	UNP Q7RT90
D	-15	HIS	-	cloning artifact	UNP Q7RT90
D	-14	HIS	-	cloning artifact	UNP Q7RT90
D	-13	HIS	-	cloning artifact	UNP Q7RT90
D	-12	HIS	-	cloning artifact	UNP Q7RT90
D	-11	HIS	-	cloning artifact	UNP Q7RT90
D	-10	HIS	-	cloning artifact	UNP Q7RT90
D	-9	SER	-	cloning artifact	UNP Q7RT90
D	-8	SER	-	cloning artifact	UNP Q7RT90
D	-7	GLY	-	cloning artifact	UNP Q7RT90
D	-6	LEU	-	cloning artifact	UNP Q7RT90
D	-5	VAL	-	cloning artifact	UNP Q7RT90
D	-4	PRO	-	cloning artifact	UNP Q7RT90
D	-3	ARG	-	cloning artifact	UNP Q7RT90
D	-2	GLY	-	cloning artifact	UNP Q7RT90
D	-1	SER	-	cloning artifact	UNP Q7RT90
E	-19	MET	-	cloning artifact	UNP Q7RT90
E	-18	GLY	-	cloning artifact	UNP Q7RT90
E	-17	SER	-	cloning artifact	UNP Q7RT90
E	-16	SER	-	cloning artifact	UNP Q7RT90
E	-15	HIS	-	cloning artifact	UNP Q7RT90
E	-14	HIS	-	cloning artifact	UNP Q7RT90
E	-13	HIS	-	cloning artifact	UNP Q7RT90
E	-12	HIS	-	cloning artifact	UNP Q7RT90
E	-11	HIS	-	cloning artifact	UNP Q7RT90
E	-10	HIS	-	cloning artifact	UNP Q7RT90
E	-9	SER	-	cloning artifact	UNP Q7RT90
E	-8	SER	-	cloning artifact	UNP Q7RT90
E	-7	GLY	-	cloning artifact	UNP Q7RT90
E	-6	LEU	-	cloning artifact	UNP Q7RT90
E	-5	VAL	-	cloning artifact	UNP Q7RT90
E	-4	PRO	-	cloning artifact	UNP Q7RT90
E	-3	ARG	-	cloning artifact	UNP Q7RT90
E	-2	GLY	-	cloning artifact	UNP Q7RT90
E	-1	SER	-	cloning artifact	UNP Q7RT90
F	-19	MET	-	cloning artifact	UNP Q7RT90
F	-18	GLY	-	cloning artifact	UNP Q7RT90
F	-17	SER	-	cloning artifact	UNP Q7RT90
F	-16	SER	-	cloning artifact	UNP Q7RT90
F	-15	HIS	-	cloning artifact	UNP Q7RT90
F	-14	HIS	-	cloning artifact	UNP Q7RT90

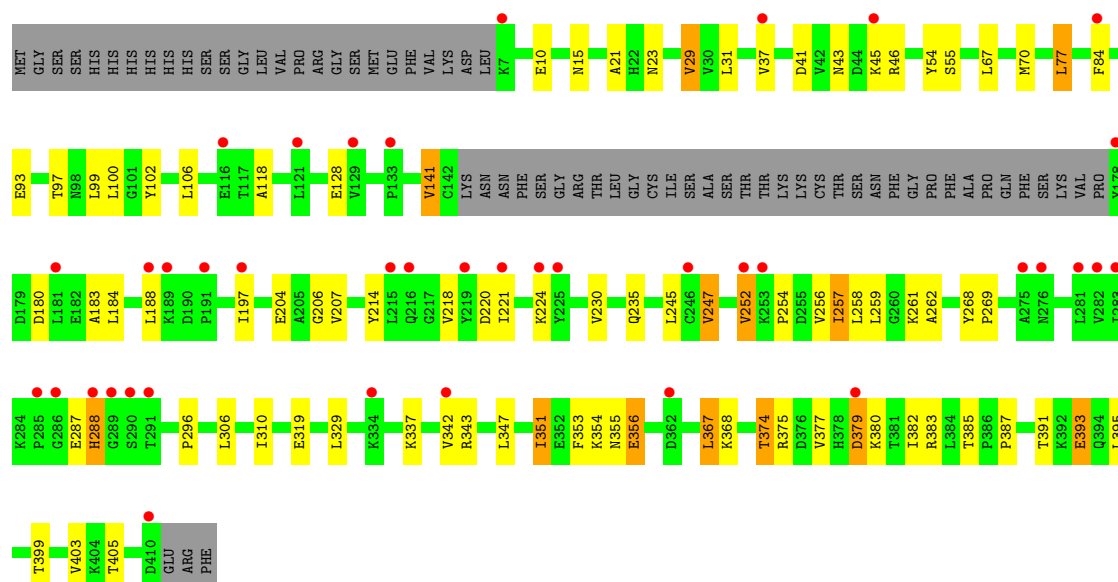
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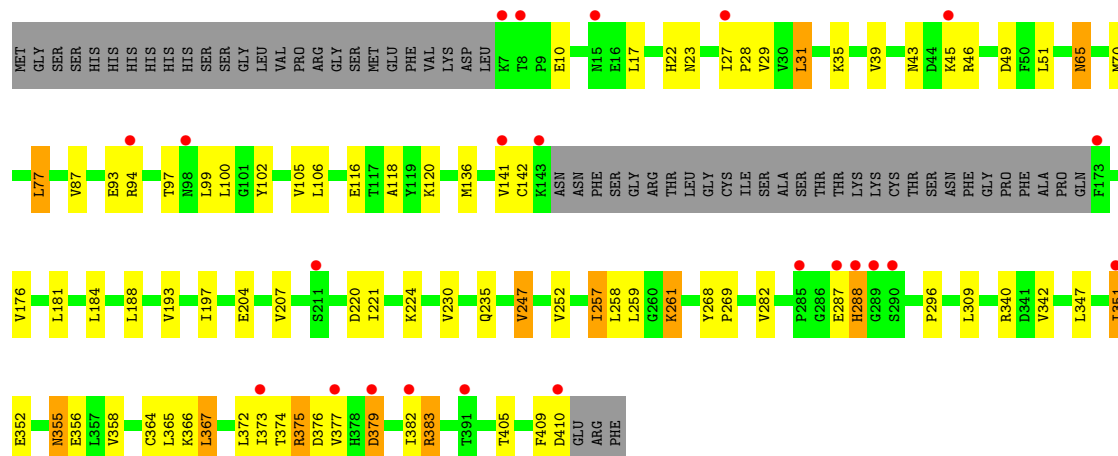
Chain	Residue	Modelled	Actual	Comment	Reference
F	-13	HIS	-	cloning artifact	UNP Q7RT90
F	-12	HIS	-	cloning artifact	UNP Q7RT90
F	-11	HIS	-	cloning artifact	UNP Q7RT90
F	-10	HIS	-	cloning artifact	UNP Q7RT90
F	-9	SER	-	cloning artifact	UNP Q7RT90
F	-8	SER	-	cloning artifact	UNP Q7RT90
F	-7	GLY	-	cloning artifact	UNP Q7RT90
F	-6	LEU	-	cloning artifact	UNP Q7RT90
F	-5	VAL	-	cloning artifact	UNP Q7RT90
F	-4	PRO	-	cloning artifact	UNP Q7RT90
F	-3	ARG	-	cloning artifact	UNP Q7RT90
F	-2	GLY	-	cloning artifact	UNP Q7RT90
F	-1	SER	-	cloning artifact	UNP Q7RT90

- Molecule 2 is water.

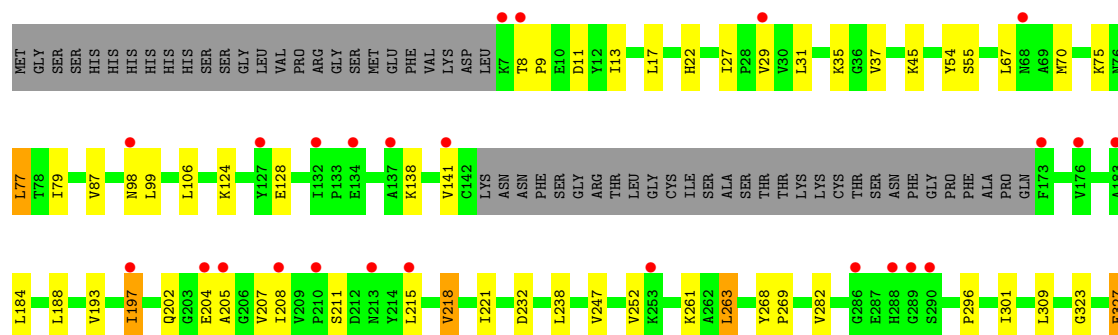
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	127	Total O 127 127	0	0
2	B	87	Total O 87 87	0	0
2	C	56	Total O 56 56	0	0
2	D	82	Total O 82 82	0	0
2	E	67	Total O 67 67	0	0
2	F	106	Total O 106 106	0	0

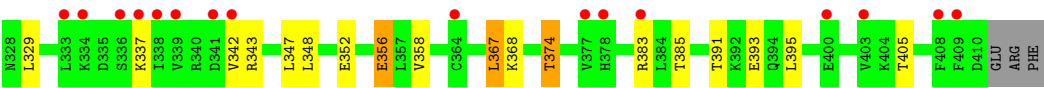


• Molecule 1: ornithine aminotransferase

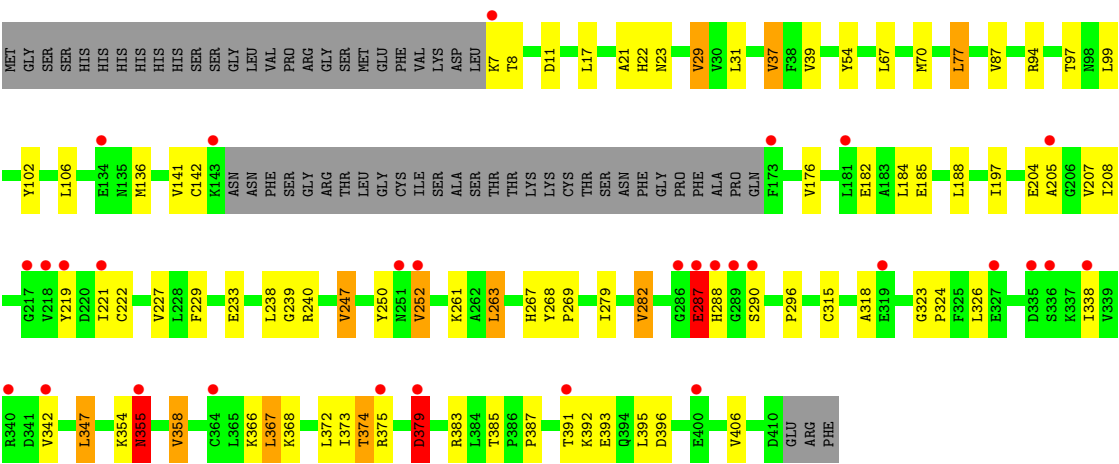


• Molecule 1: ornithine aminotransferase





● Molecule 1: ornithine aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.49Å 221.83Å 114.48Å 90.00° 100.89° 90.00°	Depositor
Resolution (Å)	49.74 – 2.10 49.74 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.74-2.10) 99.8 (49.74-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.259 0.214 , 0.258	Depositor DCC
R_{free} test set	7970 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18172	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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](#)

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	0.76	1/3023 (0.0%)	0.94	2/4092 (0.0%)
1	B	0.69	2/3014 (0.1%)	0.93	1/4080 (0.0%)
1	C	0.62	0/2947	0.89	0/3990
1	D	0.68	1/2998 (0.0%)	0.91	0/4058
1	E	0.67	1/2989 (0.0%)	0.90	0/4047
1	F	0.71	1/2998 (0.0%)	0.93	0/4058
All	All	0.69	6/17969 (0.0%)	0.92	3/24325 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	385	THR	CA-CB	7.93	1.63	1.53
1	E	87	VAL	CA-CB	5.54	1.56	1.54
1	B	87	VAL	CA-CB	5.52	1.56	1.54
1	B	197	ILE	CA-CB	5.46	1.61	1.54
1	F	87	VAL	CA-CB	5.46	1.57	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	PRO	CA-C-N	-5.50	114.11	119.78
1	A	386	PRO	C-N-CA	-5.50	114.11	119.78
1	B	374	THR	CB-CA-C	-5.26	100.97	113.02

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	2969	0	3015	59	0
1	B	2960	0	3007	58	0
1	C	2895	0	2939	67	0
1	D	2944	0	2995	63	0
1	E	2935	0	2982	41	0
1	F	2944	0	2995	60	0
2	A	127	0	0	4	0
2	B	87	0	0	2	0
2	C	56	0	0	4	0
2	D	82	0	0	1	0
2	E	67	0	0	2	0
2	F	106	0	0	4	0
All	All	18172	0	17933	316	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 9.

The worst 5 of 316 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:366:LYS:HD2	2:F:514:HOH:O	1.49	1.10
1:C:374:THR:HG21	1:C:383:ARG:O	1.52	1.09
1:A:21:ALA:HB3	1:B:106:LEU:HD23	1.34	1.07
1:E:98:ASN:HB3	2:E:459:HOH:O	1.58	1.03
1:A:374:THR:HG21	1:A:383:ARG:O	1.60	1.02

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	374/433 (86%)	356 (95%)	14 (4%)	4 (1%)	11	8
1	B	373/433 (86%)	353 (95%)	18 (5%)	2 (0%)	24	22
1	C	365/433 (84%)	350 (96%)	13 (4%)	2 (0%)	24	22
1	D	371/433 (86%)	352 (95%)	16 (4%)	3 (1%)	16	12
1	E	370/433 (86%)	350 (95%)	19 (5%)	1 (0%)	36	36
1	F	371/433 (86%)	348 (94%)	18 (5%)	5 (1%)	9	6
All	All	2224/2598 (86%)	2109 (95%)	98 (4%)	17 (1%)	16	12

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	SER
1	C	288	HIS
1	C	379	ASP
1	D	288	HIS
1	D	379	ASP

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	331/378 (88%)	305 (92%)	26 (8%)	11	9
1	B	330/378 (87%)	307 (93%)	23 (7%)	14	11
1	C	322/378 (85%)	300 (93%)	22 (7%)	14	12
1	D	328/378 (87%)	305 (93%)	23 (7%)	14	11
1	E	327/378 (86%)	301 (92%)	26 (8%)	11	8
1	F	328/378 (87%)	304 (93%)	24 (7%)	13	10
All	All	1966/2268 (87%)	1822 (93%)	144 (7%)	13	10

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	356	GLU

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Mol	Chain	Res	Type
1	F	395	LEU
1	E	395	LEU
1	F	204	GLU
1	B	391	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	288	HIS
1	F	370	ASN
1	E	307	ASN
1	F	22	HIS
1	B	378	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](#)

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 [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, 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	378/433 (87%)	0.26	13 (3%)	48 50	16, 34, 57, 71	0
1	B	377/433 (87%)	0.63	30 (7%)	18 19	20, 38, 63, 71	0
1	C	369/433 (85%)	0.84	39 (10%)	11 12	27, 43, 72, 81	0
1	D	375/433 (86%)	0.64	23 (6%)	27 29	23, 40, 57, 83	0
1	E	374/433 (86%)	0.76	41 (10%)	10 11	23, 43, 68, 81	0
1	F	375/433 (86%)	0.47	30 (8%)	18 19	20, 36, 58, 71	0
All	All	2248/2598 (86%)	0.60	176 (7%)	19 20	16, 39, 64, 83	0

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	289	GLY	6.9
1	B	181	LEU	6.8
1	D	289	GLY	5.8
1	D	288	HIS	5.4
1	B	289	GLY	4.9

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 oligosaccharides 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.