



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:25 PM UTC

PDB ID : 5TZB / pdb_00005tzb
Title : Burkholderia sp. beta-aminopeptidase
Authors : McGowan, S.; Drinkwater, N.; John, M.; Dumsday, G.
Deposited on : 2016-11-21
Resolution : 1.98 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	:	4-5-2 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

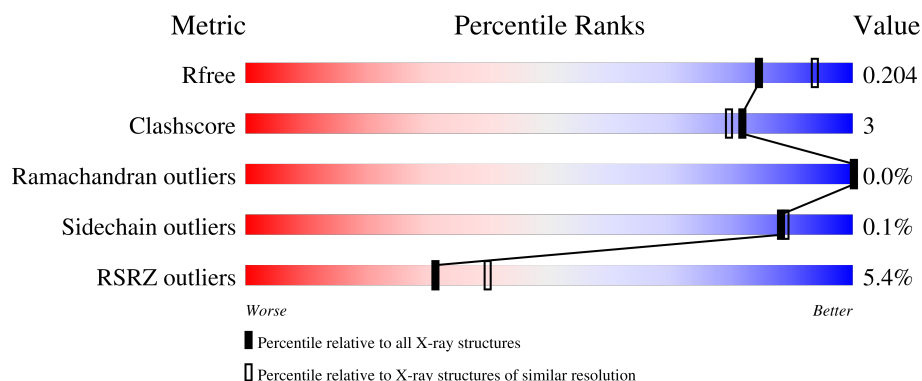
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	389	0% 88% 9%
1	B	389	3% 86% 5% 9%
1	C	389	3% 85% 6% 9%
1	D	389	3% 87% 9%
1	E	389	6% 85% 7% 9%

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Mol	Chain	Length	Quality of chain
1	F	389	7% 85% 6% 9%
1	G	389	5% 86% 5% 9%
1	H	389	11% 83% 8% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22172 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 D-aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2543	1580	469	483	11			
1	B	354	Total	C	N	O	S	0	0	0
			2543	1577	472	483	11			
1	C	355	Total	C	N	O	S	0	1	0
			2558	1588	476	484	10			
1	G	353	Total	C	N	O	S	0	0	0
			2538	1577	471	480	10			
1	E	355	Total	C	N	O	S	0	2	0
			2571	1596	477	487	11			
1	F	355	Total	C	N	O	S	0	0	0
			2550	1581	476	482	11			
1	D	355	Total	C	N	O	S	0	0	0
			2559	1588	476	484	11			
1	H	353	Total	C	N	O	S	0	0	0
			2524	1571	470	473	10			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A0J6Q6M7
A	-18	GLY	-	expression tag	UNP A0A0J6Q6M7
A	-17	SER	-	expression tag	UNP A0A0J6Q6M7
A	-16	SER	-	expression tag	UNP A0A0J6Q6M7
A	-15	HIS	-	expression tag	UNP A0A0J6Q6M7
A	-14	HIS	-	expression tag	UNP A0A0J6Q6M7
A	-13	HIS	-	expression tag	UNP A0A0J6Q6M7
A	-12	HIS	-	expression tag	UNP A0A0J6Q6M7
A	-11	HIS	-	expression tag	UNP A0A0J6Q6M7
A	-10	HIS	-	expression tag	UNP A0A0J6Q6M7
A	-9	SER	-	expression tag	UNP A0A0J6Q6M7
A	-8	SER	-	expression tag	UNP A0A0J6Q6M7
A	-7	GLY	-	expression tag	UNP A0A0J6Q6M7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP A0A0J6Q6M7
A	-5	VAL	-	expression tag	UNP A0A0J6Q6M7
A	-4	PRO	-	expression tag	UNP A0A0J6Q6M7
A	-3	ARG	-	expression tag	UNP A0A0J6Q6M7
A	-2	GLY	-	expression tag	UNP A0A0J6Q6M7
A	-1	SER	-	expression tag	UNP A0A0J6Q6M7
A	0	HIS	-	expression tag	UNP A0A0J6Q6M7
B	-19	MET	-	initiating methionine	UNP A0A0J6Q6M7
B	-18	GLY	-	expression tag	UNP A0A0J6Q6M7
B	-17	SER	-	expression tag	UNP A0A0J6Q6M7
B	-16	SER	-	expression tag	UNP A0A0J6Q6M7
B	-15	HIS	-	expression tag	UNP A0A0J6Q6M7
B	-14	HIS	-	expression tag	UNP A0A0J6Q6M7
B	-13	HIS	-	expression tag	UNP A0A0J6Q6M7
B	-12	HIS	-	expression tag	UNP A0A0J6Q6M7
B	-11	HIS	-	expression tag	UNP A0A0J6Q6M7
B	-10	HIS	-	expression tag	UNP A0A0J6Q6M7
B	-9	SER	-	expression tag	UNP A0A0J6Q6M7
B	-8	SER	-	expression tag	UNP A0A0J6Q6M7
B	-7	GLY	-	expression tag	UNP A0A0J6Q6M7
B	-6	LEU	-	expression tag	UNP A0A0J6Q6M7
B	-5	VAL	-	expression tag	UNP A0A0J6Q6M7
B	-4	PRO	-	expression tag	UNP A0A0J6Q6M7
B	-3	ARG	-	expression tag	UNP A0A0J6Q6M7
B	-2	GLY	-	expression tag	UNP A0A0J6Q6M7
B	-1	SER	-	expression tag	UNP A0A0J6Q6M7
B	0	HIS	-	expression tag	UNP A0A0J6Q6M7
C	-19	MET	-	initiating methionine	UNP A0A0J6Q6M7
C	-18	GLY	-	expression tag	UNP A0A0J6Q6M7
C	-17	SER	-	expression tag	UNP A0A0J6Q6M7
C	-16	SER	-	expression tag	UNP A0A0J6Q6M7
C	-15	HIS	-	expression tag	UNP A0A0J6Q6M7
C	-14	HIS	-	expression tag	UNP A0A0J6Q6M7
C	-13	HIS	-	expression tag	UNP A0A0J6Q6M7
C	-12	HIS	-	expression tag	UNP A0A0J6Q6M7
C	-11	HIS	-	expression tag	UNP A0A0J6Q6M7
C	-10	HIS	-	expression tag	UNP A0A0J6Q6M7
C	-9	SER	-	expression tag	UNP A0A0J6Q6M7
C	-8	SER	-	expression tag	UNP A0A0J6Q6M7
C	-7	GLY	-	expression tag	UNP A0A0J6Q6M7
C	-6	LEU	-	expression tag	UNP A0A0J6Q6M7
C	-5	VAL	-	expression tag	UNP A0A0J6Q6M7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP A0A0J6Q6M7
C	-3	ARG	-	expression tag	UNP A0A0J6Q6M7
C	-2	GLY	-	expression tag	UNP A0A0J6Q6M7
C	-1	SER	-	expression tag	UNP A0A0J6Q6M7
C	0	HIS	-	expression tag	UNP A0A0J6Q6M7
G	-19	MET	-	initiating methionine	UNP A0A0J6Q6M7
G	-18	GLY	-	expression tag	UNP A0A0J6Q6M7
G	-17	SER	-	expression tag	UNP A0A0J6Q6M7
G	-16	SER	-	expression tag	UNP A0A0J6Q6M7
G	-15	HIS	-	expression tag	UNP A0A0J6Q6M7
G	-14	HIS	-	expression tag	UNP A0A0J6Q6M7
G	-13	HIS	-	expression tag	UNP A0A0J6Q6M7
G	-12	HIS	-	expression tag	UNP A0A0J6Q6M7
G	-11	HIS	-	expression tag	UNP A0A0J6Q6M7
G	-10	HIS	-	expression tag	UNP A0A0J6Q6M7
G	-9	SER	-	expression tag	UNP A0A0J6Q6M7
G	-8	SER	-	expression tag	UNP A0A0J6Q6M7
G	-7	GLY	-	expression tag	UNP A0A0J6Q6M7
G	-6	LEU	-	expression tag	UNP A0A0J6Q6M7
G	-5	VAL	-	expression tag	UNP A0A0J6Q6M7
G	-4	PRO	-	expression tag	UNP A0A0J6Q6M7
G	-3	ARG	-	expression tag	UNP A0A0J6Q6M7
G	-2	GLY	-	expression tag	UNP A0A0J6Q6M7
G	-1	SER	-	expression tag	UNP A0A0J6Q6M7
G	0	HIS	-	expression tag	UNP A0A0J6Q6M7
E	-19	MET	-	initiating methionine	UNP A0A0J6Q6M7
E	-18	GLY	-	expression tag	UNP A0A0J6Q6M7
E	-17	SER	-	expression tag	UNP A0A0J6Q6M7
E	-16	SER	-	expression tag	UNP A0A0J6Q6M7
E	-15	HIS	-	expression tag	UNP A0A0J6Q6M7
E	-14	HIS	-	expression tag	UNP A0A0J6Q6M7
E	-13	HIS	-	expression tag	UNP A0A0J6Q6M7
E	-12	HIS	-	expression tag	UNP A0A0J6Q6M7
E	-11	HIS	-	expression tag	UNP A0A0J6Q6M7
E	-10	HIS	-	expression tag	UNP A0A0J6Q6M7
E	-9	SER	-	expression tag	UNP A0A0J6Q6M7
E	-8	SER	-	expression tag	UNP A0A0J6Q6M7
E	-7	GLY	-	expression tag	UNP A0A0J6Q6M7
E	-6	LEU	-	expression tag	UNP A0A0J6Q6M7
E	-5	VAL	-	expression tag	UNP A0A0J6Q6M7
E	-4	PRO	-	expression tag	UNP A0A0J6Q6M7
E	-3	ARG	-	expression tag	UNP A0A0J6Q6M7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP A0A0J6Q6M7
E	-1	SER	-	expression tag	UNP A0A0J6Q6M7
E	0	HIS	-	expression tag	UNP A0A0J6Q6M7
F	-19	MET	-	initiating methionine	UNP A0A0J6Q6M7
F	-18	GLY	-	expression tag	UNP A0A0J6Q6M7
F	-17	SER	-	expression tag	UNP A0A0J6Q6M7
F	-16	SER	-	expression tag	UNP A0A0J6Q6M7
F	-15	HIS	-	expression tag	UNP A0A0J6Q6M7
F	-14	HIS	-	expression tag	UNP A0A0J6Q6M7
F	-13	HIS	-	expression tag	UNP A0A0J6Q6M7
F	-12	HIS	-	expression tag	UNP A0A0J6Q6M7
F	-11	HIS	-	expression tag	UNP A0A0J6Q6M7
F	-10	HIS	-	expression tag	UNP A0A0J6Q6M7
F	-9	SER	-	expression tag	UNP A0A0J6Q6M7
F	-8	SER	-	expression tag	UNP A0A0J6Q6M7
F	-7	GLY	-	expression tag	UNP A0A0J6Q6M7
F	-6	LEU	-	expression tag	UNP A0A0J6Q6M7
F	-5	VAL	-	expression tag	UNP A0A0J6Q6M7
F	-4	PRO	-	expression tag	UNP A0A0J6Q6M7
F	-3	ARG	-	expression tag	UNP A0A0J6Q6M7
F	-2	GLY	-	expression tag	UNP A0A0J6Q6M7
F	-1	SER	-	expression tag	UNP A0A0J6Q6M7
F	0	HIS	-	expression tag	UNP A0A0J6Q6M7
D	-19	MET	-	initiating methionine	UNP A0A0J6Q6M7
D	-18	GLY	-	expression tag	UNP A0A0J6Q6M7
D	-17	SER	-	expression tag	UNP A0A0J6Q6M7
D	-16	SER	-	expression tag	UNP A0A0J6Q6M7
D	-15	HIS	-	expression tag	UNP A0A0J6Q6M7
D	-14	HIS	-	expression tag	UNP A0A0J6Q6M7
D	-13	HIS	-	expression tag	UNP A0A0J6Q6M7
D	-12	HIS	-	expression tag	UNP A0A0J6Q6M7
D	-11	HIS	-	expression tag	UNP A0A0J6Q6M7
D	-10	HIS	-	expression tag	UNP A0A0J6Q6M7
D	-9	SER	-	expression tag	UNP A0A0J6Q6M7
D	-8	SER	-	expression tag	UNP A0A0J6Q6M7
D	-7	GLY	-	expression tag	UNP A0A0J6Q6M7
D	-6	LEU	-	expression tag	UNP A0A0J6Q6M7
D	-5	VAL	-	expression tag	UNP A0A0J6Q6M7
D	-4	PRO	-	expression tag	UNP A0A0J6Q6M7
D	-3	ARG	-	expression tag	UNP A0A0J6Q6M7
D	-2	GLY	-	expression tag	UNP A0A0J6Q6M7
D	-1	SER	-	expression tag	UNP A0A0J6Q6M7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP A0A0J6Q6M7
H	-19	MET	-	initiating methionine	UNP A0A0J6Q6M7
H	-18	GLY	-	expression tag	UNP A0A0J6Q6M7
H	-17	SER	-	expression tag	UNP A0A0J6Q6M7
H	-16	SER	-	expression tag	UNP A0A0J6Q6M7
H	-15	HIS	-	expression tag	UNP A0A0J6Q6M7
H	-14	HIS	-	expression tag	UNP A0A0J6Q6M7
H	-13	HIS	-	expression tag	UNP A0A0J6Q6M7
H	-12	HIS	-	expression tag	UNP A0A0J6Q6M7
H	-11	HIS	-	expression tag	UNP A0A0J6Q6M7
H	-10	HIS	-	expression tag	UNP A0A0J6Q6M7
H	-9	SER	-	expression tag	UNP A0A0J6Q6M7
H	-8	SER	-	expression tag	UNP A0A0J6Q6M7
H	-7	GLY	-	expression tag	UNP A0A0J6Q6M7
H	-6	LEU	-	expression tag	UNP A0A0J6Q6M7
H	-5	VAL	-	expression tag	UNP A0A0J6Q6M7
H	-4	PRO	-	expression tag	UNP A0A0J6Q6M7
H	-3	ARG	-	expression tag	UNP A0A0J6Q6M7
H	-2	GLY	-	expression tag	UNP A0A0J6Q6M7
H	-1	SER	-	expression tag	UNP A0A0J6Q6M7
H	0	HIS	-	expression tag	UNP A0A0J6Q6M7

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	265	Total O 265 265	0	0
3	B	239	Total O 239 239	0	0
3	C	261	Total O 261 261	0	0

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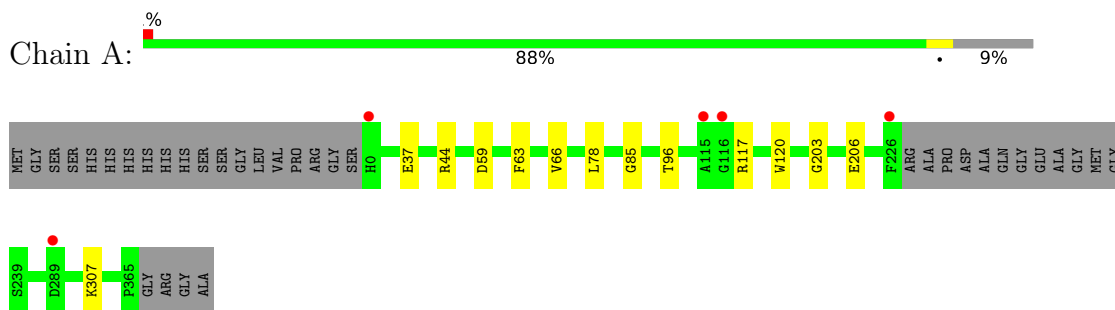
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	192	Total 192	O 192	0	0
3	E	202	Total 202	O 202	0	0
3	F	190	Total 190	O 190	0	0
3	D	263	Total 263	O 263	0	0
3	H	170	Total 170	O 170	0	0

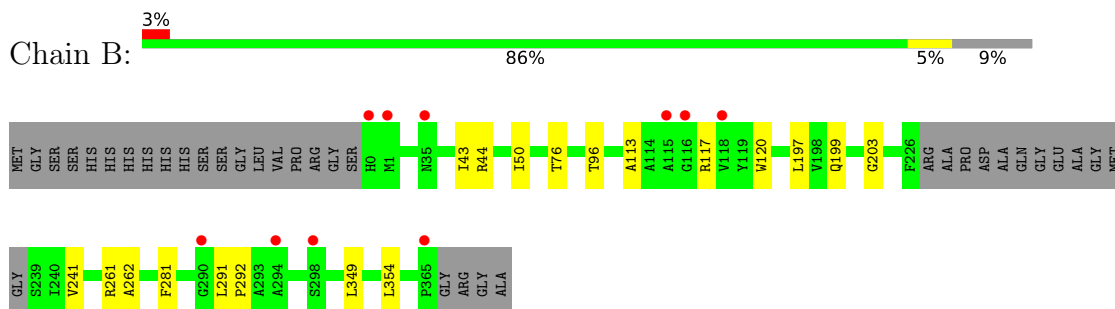
3 Residue-property plots [i](#)

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.

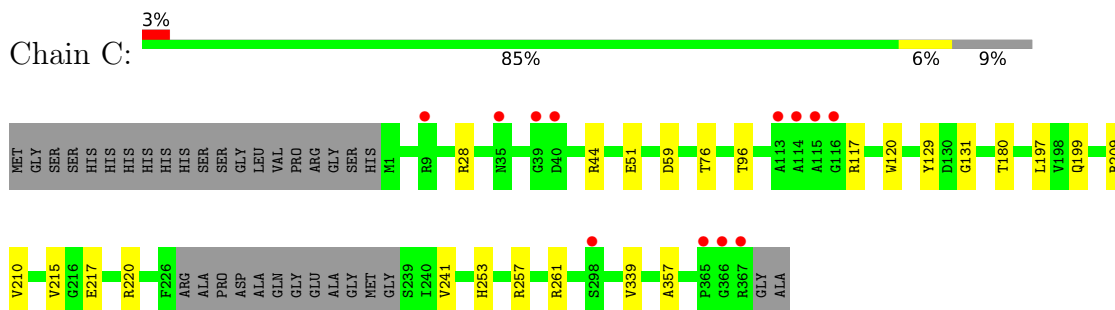
- Molecule 1: D-aminopeptidase



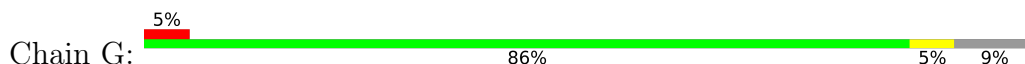
- Molecule 1: D-aminopeptidase

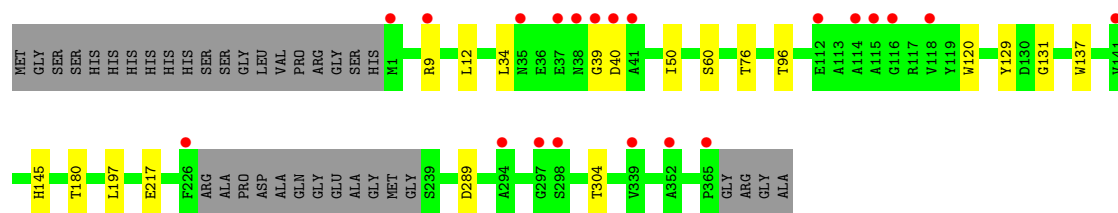


- Molecule 1: D-aminopeptidase

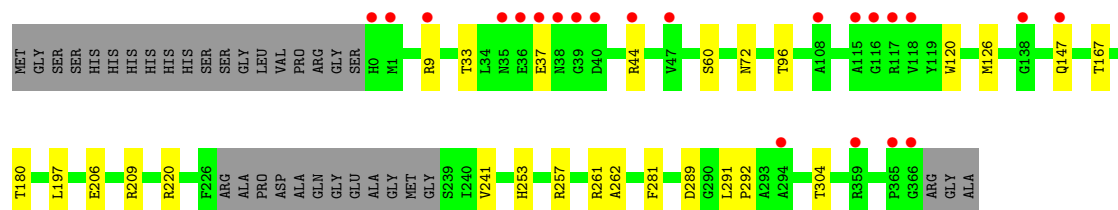
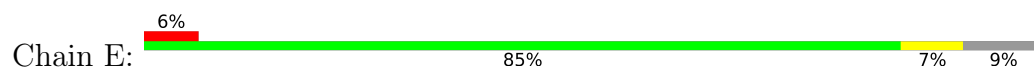


- Molecule 1: D-aminopeptidase

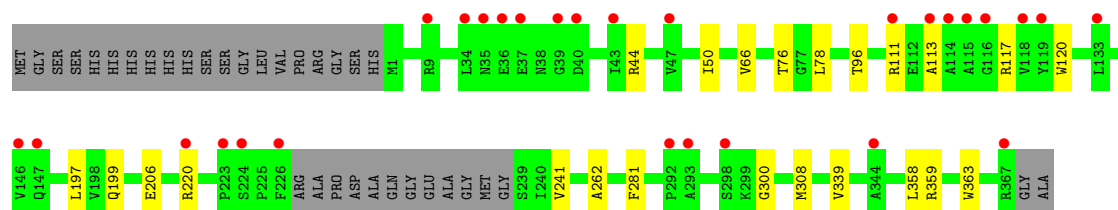
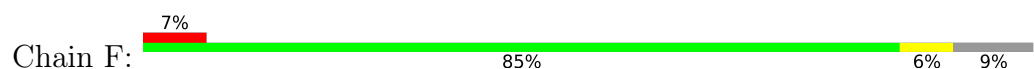




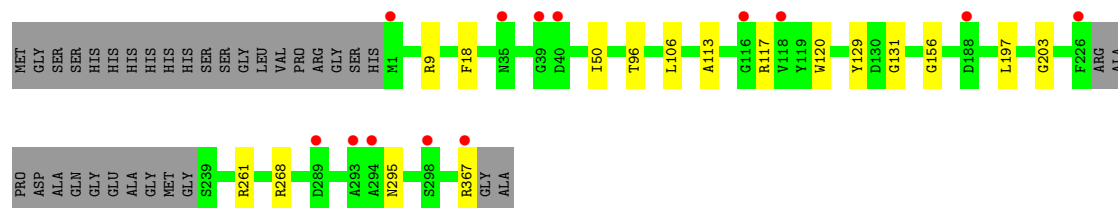
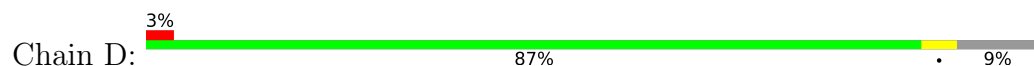
• Molecule 1: D-aminopeptidase



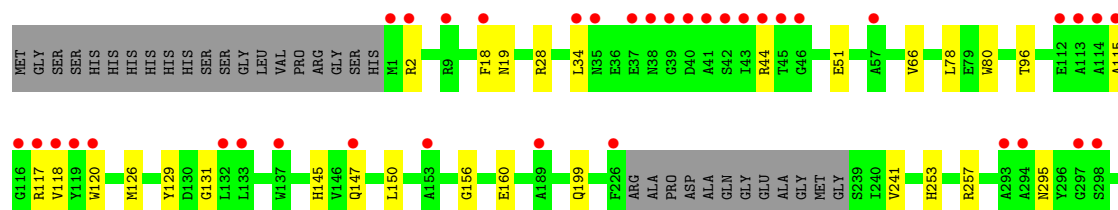
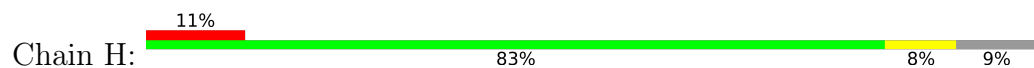
• Molecule 1: D-aminopeptidase

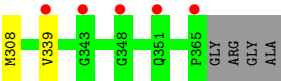


• Molecule 1: D-aminopeptidase



• Molecule 1: D-aminopeptidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.45Å 133.26Å 117.07Å 90.00° 91.61° 90.00°	Depositor
Resolution (Å)	45.71 – 1.98 45.71 – 1.98	Depositor EDS
% Data completeness (in resolution range)	94.9 (45.71-1.98) 95.9 (45.71-1.98)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.198 , 0.238 0.201 , 0.204	Depositor DCC
R_{free} test set	9447 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	22172	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% 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

5.1 Standard geometry

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

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	0.54	0/2589	0.79	1/3529 (0.0%)
1	B	0.51	0/2588	0.79	1/3527 (0.0%)
1	C	0.50	0/2607	0.79	0/3552
1	D	0.49	0/2605	0.81	1/3548 (0.0%)
1	E	0.45	0/2620	0.79	0/3568
1	F	0.47	0/2595	0.79	0/3535
1	G	0.45	0/2584	0.79	1/3522 (0.0%)
1	H	0.46	0/2570	0.79	0/3504
All	All	0.48	0/20758	0.79	4/28285 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	40	ASP	N-CA-C	-5.99	106.22	112.93
1	A	203	GLY	N-CA-C	5.55	119.61	112.18
1	B	203	GLY	N-CA-C	5.31	119.29	112.18
1	D	203	GLY	N-CA-C	5.03	118.91	112.18

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	2543	0	2493	10	0
1	B	2543	0	2497	11	0
1	C	2558	0	2513	19	0
1	D	2559	0	2518	12	0
1	E	2571	0	2527	18	0
1	F	2550	0	2509	16	0
1	G	2538	0	2493	13	0
1	H	2524	0	2479	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
3	A	265	0	0	2	0
3	B	239	0	0	0	1
3	C	261	0	0	2	0
3	D	263	0	0	0	0
3	E	202	0	0	1	0
3	F	190	0	0	1	0
3	G	192	0	0	0	0
3	H	170	0	0	0	1
All	All	22172	0	20029	102	1

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 3.

All (102) 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:A:307:LYS:HD3	1:F:300:GLY:HA2	1.64	0.80
1:E:120:TRP:HB2	1:H:96:THR:HG21	1.65	0.77
1:A:96:THR:HG21	1:D:120:TRP:HB2	1.70	0.71
1:B:120:TRP:HB2	1:C:96:THR:HG21	1.74	0.69
1:B:113:ALA:O	1:B:117:ARG:NH1	2.24	0.69
1:H:2:ARG:HH22	1:H:19:ASN:HB3	1.57	0.69
1:A:37:GLU:HG2	1:A:44:ARG:HH22	1.58	0.68
1:G:9:ARG:NH2	1:G:12:LEU:HD23	2.10	0.65
1:G:120:TRP:HB2	1:F:96:THR:HG21	1.81	0.62
1:B:96:THR:HG21	1:C:120:TRP:HB2	1.81	0.61
1:A:120:TRP:HB2	1:D:96:THR:HG21	1.82	0.61
1:G:96:THR:HG21	1:F:120:TRP:HB2	1.81	0.61
1:E:96:THR:HG21	1:H:120:TRP:HB2	1.81	0.61
1:D:113:ALA:O	1:D:117:ARG:NH1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209[A]:ARG:NH1	3:E:503:HOH:O	2.35	0.60
1:H:44:ARG:HH12	1:H:339:VAL:HG13	1.69	0.58
1:G:217:GLU:OE1	1:E:9:ARG:NH2	2.38	0.56
1:C:44:ARG:NH1	1:C:339:VAL:HG13	2.21	0.56
1:A:59:ASP:OD1	1:A:117:ARG:NH1	2.34	0.55
1:C:59:ASP:OD1	1:C:117:ARG:NH1	2.40	0.55
1:B:76:THR:HG22	1:C:76:THR:HG22	1.90	0.54
1:G:304:THR:HB	1:H:308:MET:HE2	1.90	0.53
1:F:44:ARG:NH1	1:F:339:VAL:HG13	2.24	0.53
1:C:217:GLU:OE1	1:D:9:ARG:NH2	2.42	0.52
1:E:60:SER:OG	1:E:289:ASP:OD1	2.27	0.52
1:F:66:VAL:HG11	1:F:78:LEU:HD22	1.92	0.52
1:G:9:ARG:HH21	1:G:12:LEU:HD23	1.75	0.52
1:F:113:ALA:O	1:F:117:ARG:NH1	2.43	0.51
1:C:44:ARG:HH12	1:C:339:VAL:HG13	1.74	0.51
1:B:43:ILE:O	1:B:44:ARG:HG2	2.11	0.50
1:C:209[B]:ARG:HH11	1:D:268:ARG:CZ	2.24	0.50
1:C:220:ARG:NH2	3:C:405:HOH:O	2.43	0.50
1:H:66:VAL:HG11	1:H:78:LEU:HD22	1.94	0.50
1:E:37:GLU:OE2	1:E:44:ARG:NH2	2.46	0.49
1:B:50:ILE:HD11	1:B:197:LEU:HD23	1.95	0.49
1:D:117:ARG:HG2	1:D:295:ASN:ND2	2.28	0.49
1:H:115:ALA:HB3	1:H:117:ARG:NH2	2.28	0.48
1:F:358:LEU:HB3	1:F:363:TRP:HB3	1.94	0.48
1:C:215:VAL:HG23	1:C:357:ALA:CB	2.44	0.47
1:G:60:SER:OG	1:G:289:ASP:OD1	2.32	0.47
1:H:44:ARG:NH1	1:H:339:VAL:HG13	2.30	0.47
1:C:129:TYR:CZ	1:C:131:GLY:HA3	2.51	0.46
1:C:215:VAL:HG23	1:C:357:ALA:HB1	1.98	0.46
1:H:2:ARG:NH2	1:H:19:ASN:HB3	2.27	0.46
1:F:199:GLN:HB3	1:F:241:VAL:HG22	1.98	0.46
1:G:34:LEU:HD21	1:G:145:HIS:CD2	2.51	0.46
1:D:129:TYR:CZ	1:D:131:GLY:HA3	2.51	0.46
1:H:2:ARG:HD2	1:H:160:GLU:OE1	2.16	0.46
1:D:9:ARG:NE	1:D:367:ARG:HD2	2.31	0.46
1:H:34:LEU:HD21	1:H:145:HIS:CD2	2.51	0.46
1:A:206:GLU:HG2	3:A:678:HOH:O	2.15	0.45
1:E:206[B]:GLU:HG2	1:E:220:ARG:NH1	2.31	0.45
1:E:72:ASN:HA	1:H:80:TRP:CE3	2.52	0.45
1:F:44:ARG:HH12	1:F:339:VAL:HG13	1.82	0.45
1:F:359:ARG:NH1	3:F:407:HOH:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:GLN:HB3	1:C:241:VAL:HG22	1.97	0.45
1:E:126:MET:HB3	1:E:241:VAL:HG11	1.99	0.44
1:B:199:GLN:HB3	1:B:241:VAL:HG22	1.99	0.44
1:E:9:ARG:HG2	1:E:9:ARG:O	2.16	0.44
1:B:261:ARG:HD2	1:B:261:ARG:HA	1.79	0.44
1:H:118:VAL:H	1:H:295:ASN:ND2	2.15	0.44
1:F:50:ILE:HD11	1:F:197:LEU:HD23	2.00	0.43
1:B:262:ALA:HB3	1:B:281:PHE:CD2	2.54	0.43
1:A:37:GLU:OE2	3:A:501:HOH:O	2.21	0.43
1:F:206:GLU:HB3	1:F:220:ARG:HH11	1.84	0.43
1:E:261:ARG:HA	1:E:261:ARG:HD2	1.82	0.43
1:H:18:PHE:CE2	1:H:156:GLY:HA2	2.53	0.43
1:C:209[B]:ARG:NH2	3:C:419:HOH:O	2.52	0.43
1:D:50:ILE:HD11	1:D:197:LEU:HD23	2.01	0.42
1:H:126:MET:HB3	1:H:241:VAL:HG11	2.01	0.42
1:H:199:GLN:HB3	1:H:241:VAL:HG22	2.01	0.42
1:H:129:TYR:CZ	1:H:131:GLY:HA3	2.54	0.42
1:B:291:LEU:HA	1:B:292:PRO:HD3	1.91	0.42
1:E:33:THR:HG23	1:E:167:THR:OG1	2.19	0.42
1:A:44:ARG:HH11	1:A:44:ARG:HG2	1.84	0.42
1:C:180:THR:HB	1:C:197:LEU:HD12	2.02	0.42
1:C:210:VAL:HG23	1:C:215:VAL:HG11	2.01	0.42
1:G:137:TRP:HB3	1:F:111:ARG:HD2	2.02	0.42
1:G:76:THR:HG22	1:F:76:THR:HG22	2.01	0.42
1:F:262:ALA:HB3	1:F:281:PHE:CD2	2.54	0.42
1:E:304:THR:HB	1:F:308:MET:HE2	2.02	0.41
1:E:180:THR:HB	1:E:197:LEU:HD12	2.03	0.41
1:H:147:GLN:HE21	1:H:150:LEU:HD12	1.85	0.41
1:A:66:VAL:HG11	1:A:78:LEU:HD22	2.02	0.41
1:H:2:ARG:NH2	1:H:19:ASN:HD22	2.18	0.41
1:D:261:ARG:HD2	1:D:261:ARG:HA	1.83	0.41
1:E:206[B]:GLU:CD	1:E:206[B]:GLU:H	2.25	0.41
1:E:253:HIS:O	1:E:257:ARG:HG3	2.20	0.41
1:D:106:LEU:HD23	1:D:106:LEU:HA	1.93	0.41
1:G:129:TYR:CZ	1:G:131:GLY:HA3	2.55	0.41
1:B:349:LEU:HD21	1:B:354:LEU:HD13	2.03	0.41
1:C:28:ARG:HB2	1:C:51:GLU:HB2	2.03	0.41
1:C:253:HIS:O	1:C:257:ARG:HG3	2.21	0.41
1:G:50:ILE:HD11	1:G:197:LEU:HD23	2.02	0.41
1:E:262:ALA:HB3	1:E:281:PHE:CD2	2.55	0.40
1:H:253:HIS:O	1:H:257:ARG:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:ARG:HD2	1:C:261:ARG:HA	1.79	0.40
1:E:291:LEU:HA	1:E:292:PRO:HD3	1.97	0.40
1:D:18:PHE:CZ	1:D:156:GLY:HA2	2.56	0.40
1:H:28:ARG:HB2	1:H:51:GLU:HB2	2.03	0.40
1:A:63:PHE:HA	1:A:85:GLY:O	2.21	0.40
1:G:180:THR:HB	1:G:197:LEU:HD12	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:619:HOH:O	3:H:562:HOH:O[1_556]	2.10	0.10

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	350/389 (90%)	341 (97%)	9 (3%)	0	100	100
1	B	350/389 (90%)	342 (98%)	8 (2%)	0	100	100
1	C	352/389 (90%)	343 (97%)	9 (3%)	0	100	100
1	D	351/389 (90%)	344 (98%)	7 (2%)	0	100	100
1	E	353/389 (91%)	346 (98%)	7 (2%)	0	100	100
1	F	351/389 (90%)	341 (97%)	10 (3%)	0	100	100
1	G	349/389 (90%)	340 (97%)	8 (2%)	1 (0%)	36	27
1	H	349/389 (90%)	334 (96%)	15 (4%)	0	100	100
All	All	2805/3112 (90%)	2731 (97%)	73 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	39	GLY

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	249/277 (90%)	249 (100%)	0	100	100
1	B	249/277 (90%)	249 (100%)	0	100	100
1	C	250/277 (90%)	250 (100%)	0	100	100
1	D	251/277 (91%)	251 (100%)	0	100	100
1	E	252/277 (91%)	251 (100%)	1 (0%)	84	82
1	F	249/277 (90%)	249 (100%)	0	100	100
1	G	248/277 (90%)	248 (100%)	0	100	100
1	H	244/277 (88%)	244 (100%)	0	100	100
All	All	1992/2216 (90%)	1991 (100%)	1 (0%)	88	89

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

Mol	Chain	Res	Type
1	E	147	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	HIS
1	A	221	HIS
1	A	253	HIS
1	B	109	ASN
1	B	147	GLN
1	B	221	HIS
1	G	221	HIS
1	G	253	HIS
1	E	147	GLN

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Mol	Chain	Res	Type
1	E	221	HIS
1	E	253	HIS
1	F	253	HIS
1	D	253	HIS
1	H	72	ASN
1	H	147	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are 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 ⓘ

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(Å ²)	Q < 0.9
1	A	354/389 (91%)	-0.00	5 (1%)	73	81	12, 20, 35, 66	0
1	B	354/389 (91%)	0.09	10 (2%)	55	65	11, 21, 40, 67	0
1	C	355/389 (91%)	0.18	12 (3%)	48	58	12, 22, 43, 73	1 (0%)
1	D	355/389 (91%)	0.18	13 (3%)	45	55	12, 22, 41, 65	0
1	E	355/389 (91%)	0.51	22 (6%)	26	35	14, 29, 50, 90	2 (0%)
1	F	355/389 (91%)	0.60	28 (7%)	18	25	14, 30, 55, 73	0
1	G	353/389 (90%)	0.55	21 (5%)	28	37	15, 28, 51, 76	0
1	H	353/389 (90%)	0.87	42 (11%)	9	12	21, 34, 56, 70	0
All	All	2834/3112 (91%)	0.37	153 (5%)	31	40	11, 26, 49, 90	3 (0%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	37	GLU	5.8
1	H	114	ALA	5.6
1	H	115	ALA	4.9
1	E	39	GLY	4.6
1	H	41	ALA	4.6
1	B	0	HIS	4.3
1	G	39	GLY	4.3
1	H	34	LEU	4.3
1	C	114	ALA	4.2
1	C	367	ARG	4.1
1	E	366	GLY	4.1
1	C	115	ALA	3.9
1	G	115	ALA	3.9
1	G	118	VAL	3.9
1	H	1	MET	3.8
1	F	115	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	116	GLY	3.7
1	H	113	ALA	3.7
1	H	35	ASN	3.6
1	H	37	GLU	3.6
1	F	39	GLY	3.6
1	D	188	ASP	3.6
1	G	116	GLY	3.6
1	E	116	GLY	3.6
1	F	226	PHE	3.6
1	E	40	ASP	3.5
1	H	43	ILE	3.5
1	H	116	GLY	3.5
1	H	40	ASP	3.5
1	E	36	GLU	3.5
1	D	226	PHE	3.5
1	F	147	GLN	3.4
1	E	38	ASN	3.4
1	E	0	HIS	3.4
1	G	38	ASN	3.4
1	H	147	GLN	3.3
1	F	116	GLY	3.3
1	H	294	ALA	3.2
1	H	2	ARG	3.2
1	H	132	LEU	3.1
1	G	9	ARG	3.1
1	B	1	MET	3.1
1	F	367	ARG	3.1
1	D	367	ARG	3.1
1	H	117	ARG	3.1
1	G	114	ALA	3.1
1	B	116	GLY	3.1
1	H	39	GLY	3.1
1	G	37	GLU	3.1
1	G	294	ALA	3.1
1	F	113	ALA	3.0
1	A	115	ALA	3.0
1	F	40	ASP	3.0
1	A	0	HIS	2.9
1	D	39	GLY	2.9
1	D	118	VAL	2.9
1	C	113	ALA	2.9
1	H	46	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	117	ARG	2.8
1	B	365	PRO	2.8
1	B	115	ALA	2.7
1	G	40	ASP	2.7
1	E	44	ARG	2.7
1	F	35	ASN	2.7
1	D	116	GLY	2.6
1	C	35	ASN	2.6
1	H	18	PHE	2.6
1	C	366	GLY	2.6
1	D	294	ALA	2.6
1	B	298	SER	2.6
1	H	133	LEU	2.6
1	H	348	GLY	2.6
1	E	118	VAL	2.6
1	H	293	ALA	2.6
1	D	35	ASN	2.6
1	H	38	ASN	2.6
1	G	226	PHE	2.5
1	H	42	SER	2.5
1	H	9	ARG	2.5
1	F	37	GLU	2.5
1	H	45	THR	2.5
1	D	1	MET	2.5
1	G	298	SER	2.5
1	D	293	ALA	2.5
1	A	289	ASP	2.5
1	H	112	GLU	2.4
1	D	298	SER	2.4
1	F	114	ALA	2.4
1	H	137	TRP	2.4
1	F	9	ARG	2.4
1	C	116	GLY	2.4
1	G	35	ASN	2.4
1	F	34	LEU	2.4
1	E	108	ALA	2.4
1	H	298	SER	2.4
1	D	40	ASP	2.3
1	F	119	TYR	2.3
1	F	36	GLU	2.3
1	E	115	ALA	2.3
1	E	294	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	290	GLY	2.3
1	G	297	GLY	2.3
1	E	138	GLY	2.3
1	E	359	ARG	2.3
1	H	297	GLY	2.3
1	C	298	SER	2.3
1	G	112	GLU	2.3
1	H	339	VAL	2.3
1	F	111	ARG	2.2
1	F	220	ARG	2.2
1	E	35	ASN	2.2
1	C	40	ASP	2.2
1	H	351	GLN	2.2
1	G	352	ALA	2.2
1	A	226	PHE	2.2
1	F	43	ILE	2.2
1	E	147	GLN	2.2
1	C	39	GLY	2.2
1	F	224	SER	2.2
1	F	293	ALA	2.2
1	H	226	PHE	2.2
1	E	365	PRO	2.2
1	F	344	ALA	2.2
1	E	9	ARG	2.2
1	H	120	TRP	2.1
1	G	141	VAL	2.1
1	G	339	VAL	2.1
1	C	9	ARG	2.1
1	H	189	ALA	2.1
1	F	146	VAL	2.1
1	H	118	VAL	2.1
1	H	365	PRO	2.1
1	G	41	ALA	2.1
1	H	57	ALA	2.1
1	H	153	ALA	2.1
1	B	35	ASN	2.1
1	F	47	VAL	2.1
1	F	118	VAL	2.1
1	F	133	LEU	2.1
1	D	289	ASP	2.1
1	F	298	SER	2.0
1	H	119	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	1	MET	2.0
1	H	343	GLY	2.0
1	B	118	VAL	2.0
1	E	47	VAL	2.0
1	F	223	PRO	2.0
1	B	294	ALA	2.0
1	E	1	MET	2.0
1	C	365	PRO	2.0
1	G	365	PRO	2.0
1	F	292	PRO	2.0
1	H	44	ARG	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	CA	A	401	1/1	0.98	0.08	18,18,18,18	0
2	CA	G	401	1/1	0.98	0.09	29,29,29,29	0
2	CA	B	401	1/1	0.99	0.08	18,18,18,18	0
2	CA	E	401	1/1	0.99	0.07	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.