

Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 07:12 AM EDT

PDB ID	:	5TZB
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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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.



Matria	Whole archive	Similar resolution		
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution range}({ m \AA}))$		
R_{free}	130704	11647 (2.00-1.96)		
Clashscore	141614	1014 (1.98-1.98)		
Ramachandran outliers	138981	1006 (1.98-1.98)		
Sidechain outliers	138945	1006 (1.98-1.98)		
RSRZ outliers	127900	11410 (2.00-1.96)		

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

Mol	Chain	Length	Quality of chain		
1	А	389	% • 88%		9%
1	В	389	% 86%	•	9%
1	С	389	85%	6%	9%
1	D	389	% 87%	•	9%
1	Е	389	85%	6%	9%



Mol	Chain	Length	Quality of chain		
1	F	389	<mark>6%</mark> 85%	6%	9%
1	G	389	<u>6%</u> 86%	•	9%
1	Н	389	8%	7%	9%



2 Entry composition (i)

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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	254	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	334	2543	1580	469	483	11	0	0	0
1	В	354	Total	С	Ν	0	S	0	0	0
1	D	004	2543	1577	472	483	11	0	0	0
1	С	355	Total	С	Ν	0	S	0	1	0
		000	2558	1588	476	484	10	0	1	0
1	С	353	Total	С	Ν	0	S	0	0	0
1	G	000	2538	1577	471	480	10		0	0
1	F	355	Total	С	Ν	0	S	0	9	0
1	Ľ	000	2571	1596	477	487	11	0	2	0
1	Б	255	Total	С	Ν	0	S	0	0	0
	Г	555	2550	1581	476	482	11	0	0	0
1	П	255	Total	С	Ν	0	S	0	0	0
	D	555	2559	1588	476	484	11	0	0	0
1	ц	252	Total	С	Ν	0	S	0	0	0
	п	ამა	2524	1571	470	473	10	0	0	

• Molecule 1 is a protein called D-aminopeptidase.

There are 160 discrepancies between the modelled and reference sequences:

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



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
А	-3	ARG	-	expression tag	UNP A0A0J6Q6M7
A	-2	GLY	-	expression tag	UNP A0A0J6Q6M7
А	-1	SER	-	expression tag	UNP A0A0J6Q6M7
А	0	HIS	_	expression tag	UNP A0A0J6Q6M7
В	-19	MET	-	initiating methionine	UNP A0A0J6Q6M7
В	-18	GLY	-	expression tag	UNP A0A0J6Q6M7
В	-17	SER	_	expression tag	UNP A0A0J6Q6M7
В	-16	SER	-	expression tag	UNP A0A0J6Q6M7
В	-15	HIS	_	expression tag	UNP A0A0J6Q6M7
В	-14	HIS	-	expression tag	UNP A0A0J6Q6M7
В	-13	HIS	-	expression tag	UNP A0A0J6Q6M7
В	-12	HIS	_	expression tag	UNP A0A0J6Q6M7
В	-11	HIS	-	expression tag	UNP A0A0J6Q6M7
В	-10	HIS	_	expression tag	UNP A0A0J6Q6M7
В	-9	SER	-	expression tag	UNP A0A0J6Q6M7
В	-8	SER	-	expression tag	UNP A0A0J6Q6M7
В	-7	GLY	-	expression tag	UNP A0A0J6Q6M7
В	-6	LEU	-	expression tag	UNP A0A0J6Q6M7
В	-5	VAL	_	expression tag	UNP A0A0J6Q6M7
В	-4	PRO	-	expression tag	UNP A0A0J6Q6M7
В	-3	ARG	_	expression tag	UNP A0A0J6Q6M7
В	-2	GLY	-	expression tag	UNP A0A0J6Q6M7
В	-1	SER	-	expression tag	UNP A0A0J6Q6M7
В	0	HIS	-	expression tag	UNP A0A0J6Q6M7
С	-19	MET	-	initiating methionine	UNP A0A0J6Q6M7
С	-18	GLY	-	expression tag	UNP A0A0J6Q6M7
С	-17	SER	-	expression tag	UNP A0A0J6Q6M7
С	-16	SER	-	expression tag	UNP A0A0J6Q6M7
С	-15	HIS	-	expression tag	UNP A0A0J6Q6M7
С	-14	HIS	-	expression tag	UNP A0A0J6Q6M7
С	-13	HIS	-	expression tag	UNP A0A0J6Q6M7
С	-12	HIS	-	expression tag	UNP A0A0J6Q6M7
С	-11	HIS	-	expression tag	UNP A0A0J6Q6M7
С	-10	HIS	-	expression tag	UNP A0A0J6Q6M7
С	-9	SER	-	expression tag	UNP A0A0J6Q6M7
С	-8	SER	-	expression tag	UNP A0A0J6Q6M7
С	-7	GLY	-	expression tag	UNP A0A0J6Q6M7
С	-6	LEU	-	expression tag	UNP A0A0J6Q6M7
С	-5	VAL	-	expression tag	UNP A0A0J6Q6M7



Chain	Residue	Modelled	Actual	Comment	Reference
С	-4	PRO	-	expression tag	UNP A0A0J6Q6M7
С	-3	ARG	-	expression tag	UNP A0A0J6Q6M7
С	-2	GLY	-	expression tag	UNP A0A0J6Q6M7
С	-1	SER	-	expression tag	UNP A0A0J6Q6M7
С	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
Е	-19	MET	-	initiating methionine	UNP A0A0J6Q6M7
E	-18	GLY	-	expression tag	UNP A0A0J6Q6M7
Е	-17	SER	-	expression tag	UNP A0A0J6Q6M7
E	-16	SER	-	expression tag	UNP A0A0J6Q6M7
Е	-15	HIS	-	expression tag	UNP A0A0J6Q6M7
E	-14	HIS	-	expression tag	UNP A0A0J6Q6M7
Е	-13	HIS	-	expression tag	UNP A0A0J6Q6M7
Е	-12	HIS	-	expression tag	UNP A0A0J6Q6M7
Е	-11	HIS	-	expression tag	UNP A0A0J6Q6M7
Е	-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 A0A0J $\overline{6}$ Q $\overline{6}$ M7
Е	-3	ARG	-	expression tag	UNP A0A0J6Q6M7



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

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Ca 1 1	0	0
2	В	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	Е	1	Total Ca 1 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	265	Total O 265 265	0	0
3	В	239	Total O 239 239	0	0
3	С	261	Total O 261 261	0	0



Continued from previous page...

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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	91.45Å 133.26Å 117.07Å	Deperitor
a, b, c, α , β , γ	90.00° 91.61° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	45.71 - 1.98	Depositor
Resolution (A)	45.71 - 1.98	EDS
% Data completeness	94.9 (45.71-1.98)	Depositor
(in resolution range)	95.9 (45.71-1.98)	EDS
R _{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.68 (at 1.98 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
P.P.	0.198 , 0.238	Depositor
n, n_{free}	0.201 , 0.204	DCC
R_{free} test set	9305 reflections (4.96%)	wwPDB-VP
Wilson B-factor $(Å^2)$	16.9	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , 46.8	EDS
L-test for $twinning^2$	$< L > = 0.50, < L^2 > = 0.33$	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.

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.



¹Intensities estimated from amplitudes.

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: 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).

Mal	Chain	Bond	lengths	Bond	angles
IVIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.42	0/2589	0.56	0/3529
1	В	0.40	0/2588	0.54	0/3527
1	С	0.40	0/2607	0.55	0/3552
1	D	0.39	0/2605	0.55	0/3548
1	Е	0.36	0/2620	0.53	0/3568
1	F	0.37	0/2595	0.56	0/3535
1	G	0.35	0/2584	0.53	0/3522
1	Н	0.35	0/2570	0.53	0/3504
All	All	0.38	0/20758	0.54	0/28285

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	А	2543	0	2493	10	0
1	В	2543	0	2497	11	0
1	С	2558	0	2513	19	0
1	D	2559	0	2518	12	0
1	Е	2571	0	2527	16	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2550	0	2509	16	0
1	G	2538	0	2493	12	0
1	Н	2524	0	2479	20	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	Е	1	0	0	0	0
2	G	1	0	0	0	0
3	А	265	0	0	2	0
3	В	239	0	0	0	1
3	С	261	0	0	2	0
3	D	263	0	0	0	0
3	Е	202	0	0	1	0
3	F	190	0	0	2	0
3	G	192	0	0	0	0
3	Н	170	0	0	0	1
All	All	22172	0	20029	100	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 2.

All (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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
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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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: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
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



	t i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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: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: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
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:F:169:MET:HE2	3:F:406:HOH: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	$\begin{array}{l} \text{Interatomic} \\ \text{distance} \ (\text{\AA}) \end{array}$	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	Perce	ntiles
1	А	350/389~(90%)	341 (97%)	9~(3%)	0	100	100
1	В	350/389~(90%)	342~(98%)	8 (2%)	0	100	100
1	С	352/389~(90%)	343~(97%)	9~(3%)	0	100	100
1	D	351/389~(90%)	344 (98%)	7 (2%)	0	100	100
1	Е	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%)	41	29
1	Н	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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	249/277~(90%)	248 (100%)	1 (0%)	91	90
1	В	249/277~(90%)	248 (100%)	1 (0%)	91	90
1	С	250/277~(90%)	250 (100%)	0	100	100
1	D	251/277~(91%)	251 (100%)	0	100	100
1	Ε	252/277~(91%)	252 (100%)	0	100	100
1	F	249/277~(90%)	249 (100%)	0	100	100
1	G	248/277~(90%)	248 (100%)	0	100	100
1	Н	244/277~(88%)	244 (100%)	0	100	100
All	All	1992/2216~(90%)	1990 (100%)	2(0%)	93	94

analysed, and the total number of residues.

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	37	GLU
1	В	261	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	Н	147	GLN

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 monosaccharides in this entry.



5.6 Ligand geometry (i)

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 (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^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	OWAB(Å ²)	Q < 0.9
1	А	354/389~(91%)	0.02	4 (1%) 80 82	12, 20, 35, 66	0
1	В	354/389~(91%)	0.13	5 (1%) 75 77	11, 21, 40, 67	0
1	С	355/389~(91%)	0.26	18 (5%) 28 30	12, 22, 43, 73	0
1	D	355/389~(91%)	0.15	5 (1%) 75 77	12, 22, 41, 65	0
1	Ε	355/389~(91%)	0.36	13 (3%) 41 44	14, 29, 50, 90	0
1	F	355/389~(91%)	0.47	22 (6%) 20 22	14, 30, 55, 73	0
1	G	353/389~(90%)	0.48	23 (6%) 18 20	15, 28, 51, 76	0
1	Η	353/389~(90%)	0.71	32 (9%) 9 10	21, 34, 56, 70	0
All	All	2834/3112 (91%)	0.32	122 (4%) 35 37	11, 26, 49, 90	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Н	18	PHE	4.2
1	В	0	HIS	4.2
1	Н	34	LEU	4.0
1	Н	68	VAL	4.0
1	Н	114	ALA	3.9
1	Н	115	ALA	3.8
1	Е	37	GLU	3.8
1	Н	69	LEU	3.7
1	G	39	GLY	3.6
1	С	115	ALA	3.5
1	Н	35	ASN	3.5
1	С	69	LEU	3.4
1	F	36	GLU	3.4
1	F	35	ASN	3.4
1	G	43	ILE	3.3
1	F	147	GLN	3.3



Mol	Chain	Res	Type	RSRZ
1	G	68	VAL	3.2
1	Е	116	GLY	3.2
1	Е	297	GLY	3.2
1	G	37	GLU	3.2
1	С	41	ALA	3.1
1	G	116	GLY	3.1
1	F	115	ALA	3.1
1	Н	66	VAL	3.1
1	F	69	LEU	3.1
1	G	9	ARG	3.0
1	G	35	ASN	3.0
1	Н	1	MET	3.0
1	Н	17	ARG	3.0
1	F	281	PHE	3.0
1	G	40	ASP	2.9
1	Е	69	LEU	2.9
1	F	68	VAL	2.9
1	G	115	ALA	2.9
1	С	78	LEU	2.8
1	Е	44	ARG	2.8
1	F	66	VAL	2.8
1	Е	115	ALA	2.7
1	G	44	ARG	2.7
1	Н	281	PHE	2.7
1	G	69	LEU	2.7
1	С	66	VAL	2.7
1	С	367	ARG	2.7
1	Н	186	ALA	2.7
1	С	40	ASP	2.6
1	С	68	VAL	2.6
1	Н	43	ILE	2.6
1	В	66	VAL	2.6
1	Η	2	ARG	2.6
1	Η	44	ARG	2.6
1	F	136	ILE	2.6
1	G	38	ASN	2.6
1	Е	36	GLU	2.6
1	F	43	ILE	2.5
1	С	44	ARG	2.5
1	G	226	PHE	2.5
1	С	43	ILE	2.5
1	С	298	SER	2.5



Mol	Chain	Res	Type	RSRZ
1	С	114	ALA	2.5
1	Н	280	ILE	2.5
1	Н	16	GLY	2.5
1	С	280	ILE	2.5
1	В	115	ALA	2.5
1	Н	147	GLN	2.4
1	Н	117	ARG	2.4
1	С	259	ALA	2.4
1	F	9	ARG	2.4
1	С	35	ASN	2.4
1	Н	294	ALA	2.4
1	Н	163	VAL	2.4
1	D	40	ASP	2.4
1	Е	68	VAL	2.4
1	Н	78	LEU	2.3
1	Е	241	VAL	2.3
1	Е	131	GLY	2.3
1	F	116	GLY	2.3
1	G	118	VAL	2.3
1	Н	256	THR	2.3
1	Н	343	GLY	2.3
1	А	66	VAL	2.3
1	А	68	VAL	2.3
1	С	344	ALA	2.3
1	Н	157	PRO	2.3
1	В	116	GLY	2.2
1	G	344	ALA	2.2
1	В	81	ILE	2.2
1	А	0	HIS	2.2
1	Е	117	ARG	2.2
1	F	133	LEU	2.2
1	F	78	LEU	2.2
1	Н	42	SER	2.2
1	Н	67	HIS	2.2
1	G	294	ALA	2.2
1	Н	39	GLY	2.2
1	F	44	ARG	2.2
1	D	118	VAL	2.2
1	Н	9	ARG	2.1
1	С	42	SER	2.1
1	F	42	SER	2.1
1	G	36	GLU	2.1



5TZB

Mol	Chain	Res	Type	RSRZ
1	Е	138	GLY	2.1
1	Н	156	GLY	2.1
1	А	78	LEU	2.1
1	D	262	ALA	2.1
1	D	367	ARG	2.1
1	Н	351	GLN	2.1
1	G	297	GLY	2.1
1	G	256	THR	2.1
1	F	344	ALA	2.1
1	F	37	GLU	2.1
1	G	82	ARG	2.1
1	С	37	GLU	2.1
1	D	37	GLU	2.1
1	G	66	VAL	2.0
1	Е	226	PHE	2.0
1	G	283	ALA	2.0
1	F	262	ALA	2.0
1	F	339	VAL	2.0
1	Н	158	VAL	2.0
1	F	226	PHE	2.0
1	F	67	HIS	2.0
1	G	111	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 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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	CA	А	401	1/1	0.99	0.04	$18,\!18,\!18,\!18$	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	CA	G	401	1/1	0.99	0.05	29,29,29,29	0
2	CA	Е	401	1/1	0.99	0.07	22,22,22,22	0
2	CA	В	401	1/1	1.00	0.04	18,18,18,18	0

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6.5 Other polymers (i)

There are no such residues in this entry.

