wwPDB X-ray Structure Validation Summary Report (i)

Apr 28, 2025 – 11:52 PM EDT

PDB ID	:	3CIA / pdb_00003cia
Title	:	Crystal structure of cold-aminopeptidase from Colwellia psychrerythraea
Authors	:	Bauvois, C.; Jacquamet, L.; Borel, F.; Ferrer, J.-L.
Deposited on	:	2008-03-11
Resolution	:	2.70 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 (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 (i)) were used in the production of this report:

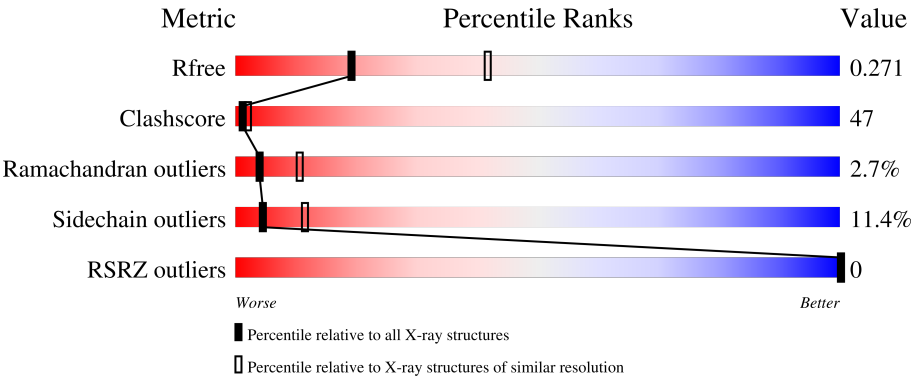
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.70 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	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	A	605	31% 47% 17%
1	B	605	30% 48% 15%
1	C	605	30% 51% 13%
1	D	605	30% 48% 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 19608 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 cold-active aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4708	3023	780	892	13			
1	B	581	Total	C	N	O	S	0	0	0
			4651	2987	770	882	12			
1	C	581	Total	C	N	O	S	0	0	0
			4657	2993	770	882	12			
1	D	582	Total	C	N	O	S	0	0	0
			4669	2999	772	886	12			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

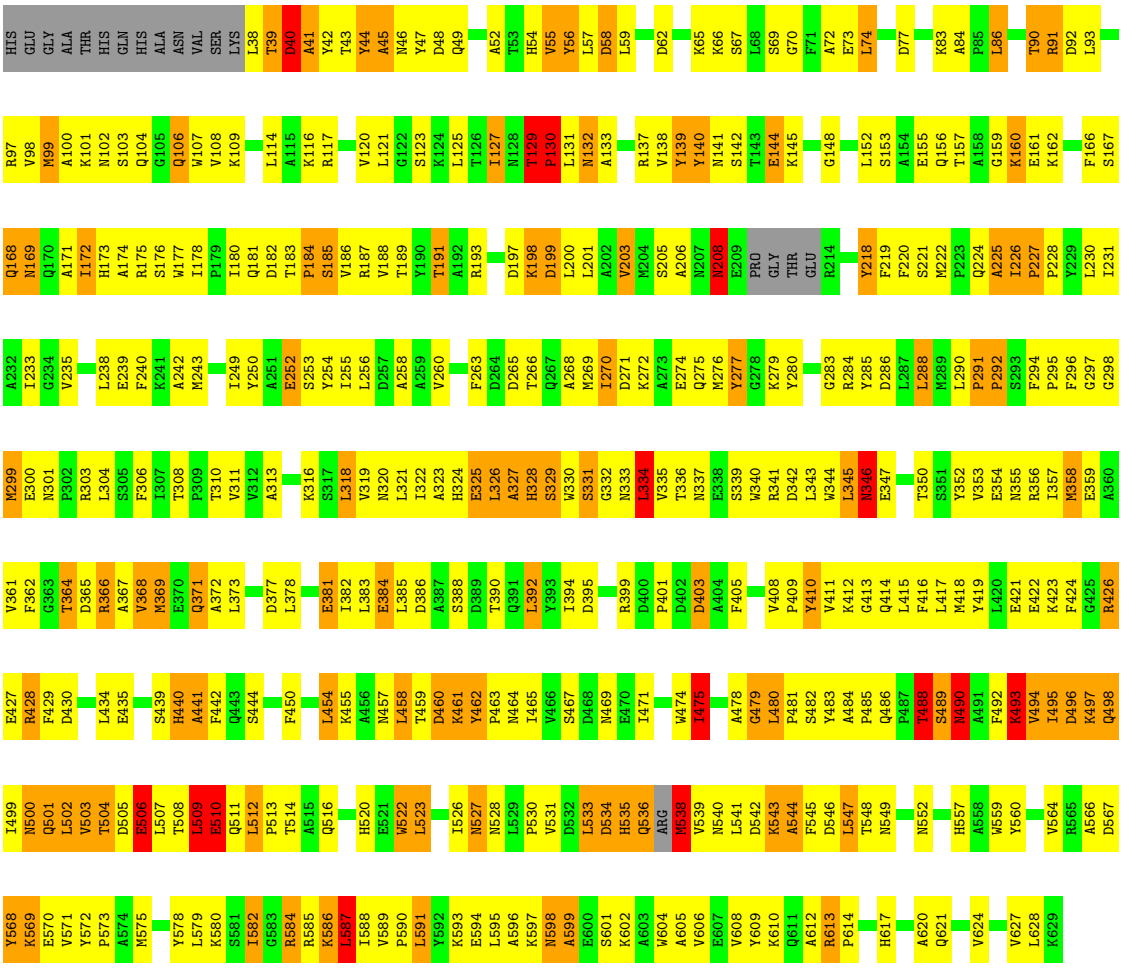
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	331	Total	O	0	0
			331	331		
3	B	154	Total	O	0	0
			154	154		
3	C	156	Total	O	0	0
			156	156		
3	D	278	Total	O	0	0
			278	278		

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.

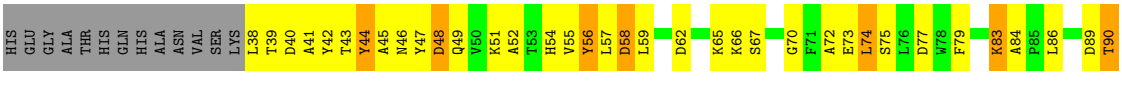
- Molecule 1: cold-active aminopeptidase

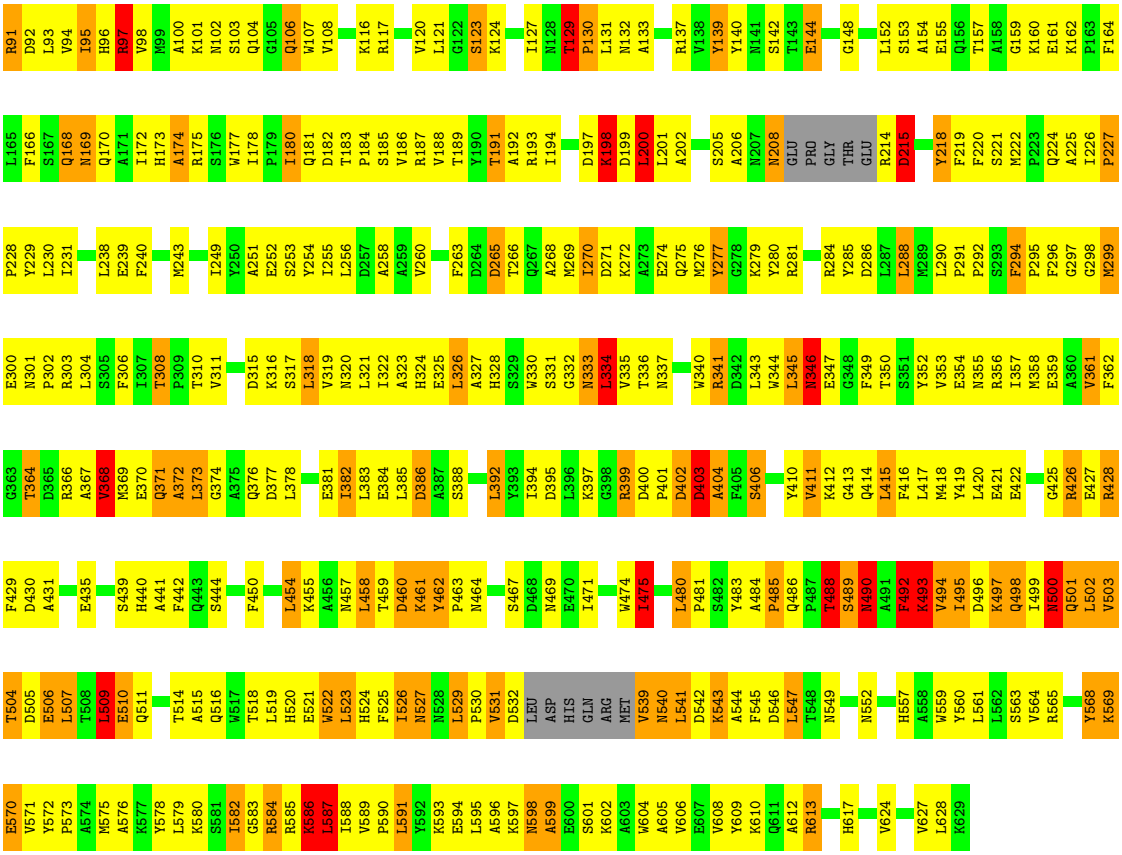
Chain A:



- Molecule 1: cold-active aminopeptidase

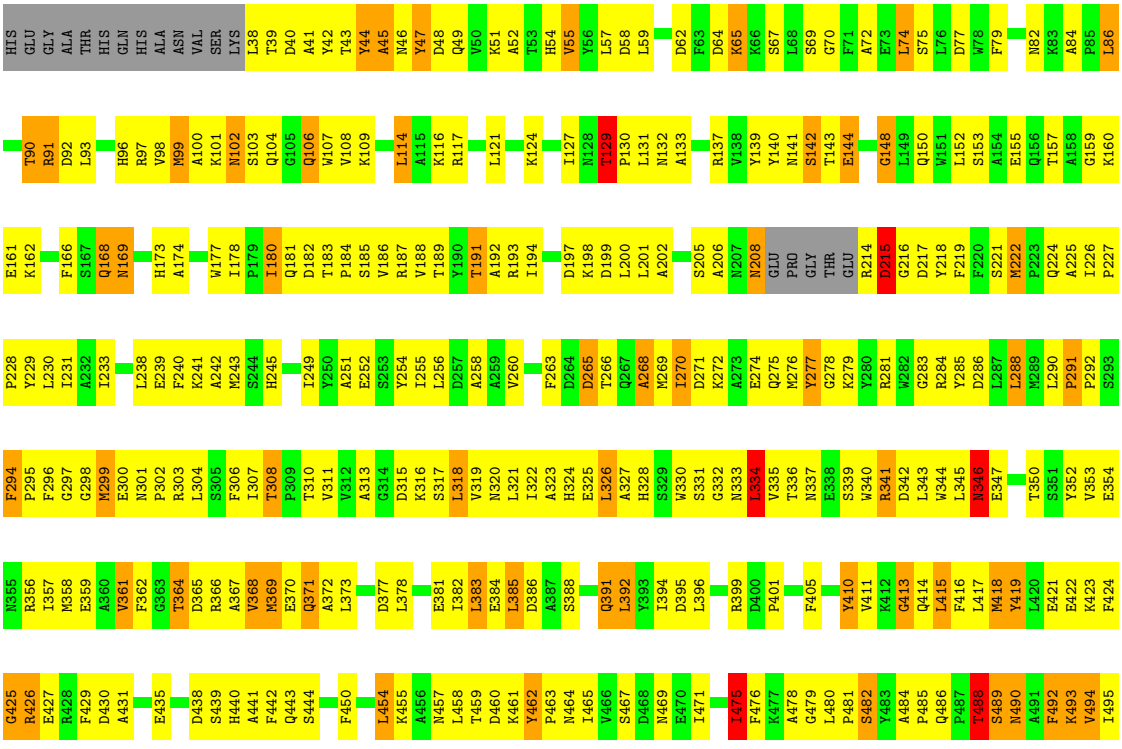
Chain B:

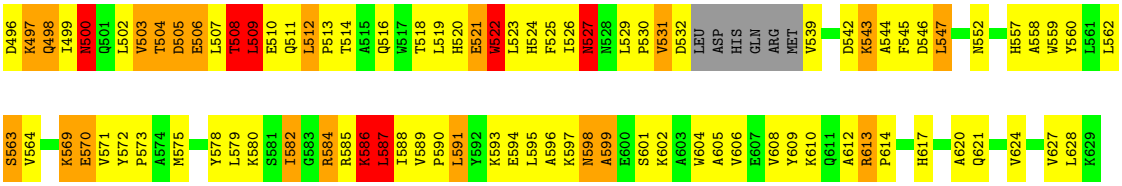


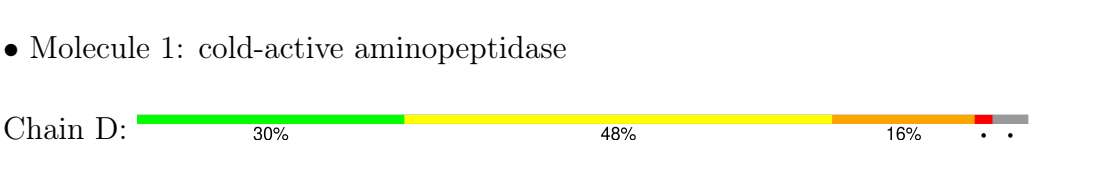


• Molecule 1: cold-active aminopeptidase

Chain C:

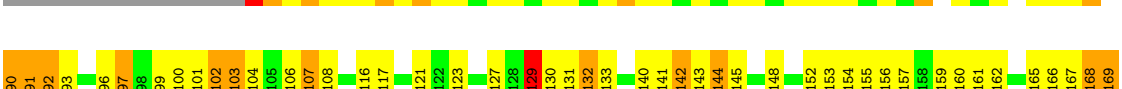


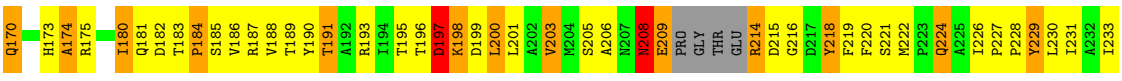


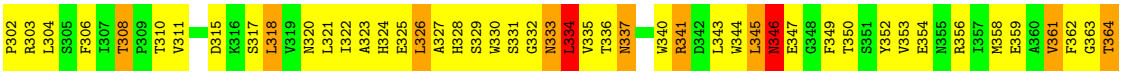


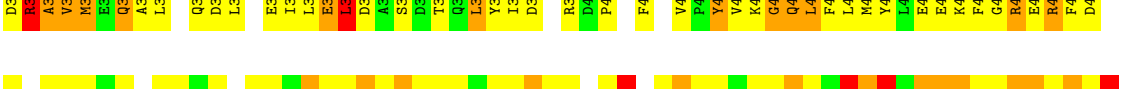
• Molecule 1: cold-active aminopeptidase

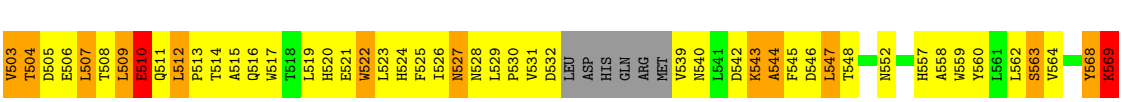
Chain D:

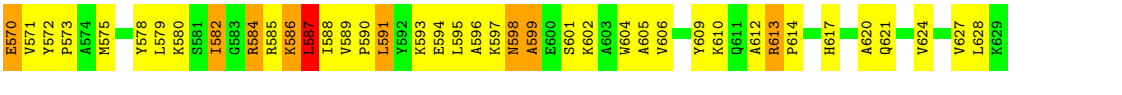












4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	81.37Å 87.10Å 116.36Å 88.83° 70.68° 88.43°	Depositor
Resolution (Å)	46.68 – 2.70 46.68 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (46.68-2.70) 97.3 (46.68-2.70)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.249 , 0.270 0.250 , 0.271	Depositor DCC
R_{free} test set	4034 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.039 for h,-k,h-l 0.186 for -h,k,-l 0.021 for -h,-k,-h+l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	19608	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN

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	1.53	49/4823 (1.0%)	1.46	73/6555 (1.1%)
1	B	1.51	45/4764 (0.9%)	1.45	76/6476 (1.2%)
1	C	1.53	33/4771 (0.7%)	1.43	68/6485 (1.0%)
1	D	1.51	40/4783 (0.8%)	1.49	84/6501 (1.3%)
All	All	1.52	167/19141 (0.9%)	1.46	301/26017 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	3
1	C	0	2
1	D	0	5
All	All	0	17

The worst 5 of 167 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	500	ASN	C-N	-30.81	0.90	1.33
1	D	208	ASN	C-N	12.06	1.50	1.33
1	D	97	ARG	C-N	11.42	1.48	1.33
1	B	168	GLN	C-O	-10.97	1.10	1.23
1	A	127	ILE	CA-CB	-10.69	1.41	1.54

The worst 5 of 301 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	97	ARG	O-C-N	13.88	141.24	122.78
1	A	498	GLN	N-CA-C	10.58	124.14	111.33
1	C	523	LEU	N-CA-C	-10.56	100.89	113.88
1	D	208	ASN	CA-C-N	-10.51	102.78	121.70
1	D	208	ASN	C-N-CA	-10.51	102.78	121.70

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	ASP	Peptide
1	A	208	ASN	Mainchain
1	A	40	ASP	Peptide
1	A	506	GLU	Peptide
1	A	535	HIS	Peptide

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	4708	0	4594	433	0
1	B	4651	0	4543	426	1
1	C	4657	0	4549	413	1
1	D	4669	0	4560	453	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	331	0	0	23	0
3	B	154	0	0	8	1
3	C	156	0	0	13	2
3	D	278	0	0	27	1
All	All	19608	0	18246	1718	3

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 47.

The worst 5 of 1718 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:D:502:LEU:HD12	1:D:506:GLU:O	1.34	1.27
1:A:42:TYR:OH	1:A:399:ARG:O	1.53	1.26
1:A:503:VAL:O	1:A:504:THR:HG23	1.39	1.22
1:B:42:TYR:OH	1:B:399:ARG:O	1.59	1.19
1:A:42:TYR:CE2	1:A:401:PRO:HD3	1.80	1.17

All (3) 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)
1:B:97:ARG:NH1	1:C:217:ASP:OD1[1_545]	1.80	0.40
3:C:946:HOH:O	3:D:797:HOH:O[1_565]	2.03	0.17
3:B:712:HOH:O	3:C:856:HOH:O[1_545]	2.19	0.01

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	581/605 (96%)	484 (83%)	81 (14%)	16 (3%)	4 10
1	B	575/605 (95%)	481 (84%)	81 (14%)	13 (2%)	5 14
1	C	575/605 (95%)	478 (83%)	84 (15%)	13 (2%)	5 14
1	D	576/605 (95%)	482 (84%)	74 (13%)	20 (4%)	3 7
All	All	2307/2420 (95%)	1925 (83%)	320 (14%)	62 (3%)	4 10

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	41	ALA
1	A	509	LEU
1	A	511	GLN

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Mol	Chain	Res	Type
1	B	504	THR

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 analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	502/517 (97%)	448 (89%)	54 (11%)	5 13
1	B	495/517 (96%)	433 (88%)	62 (12%)	3 9
1	C	496/517 (96%)	442 (89%)	54 (11%)	5 13
1	D	498/517 (96%)	441 (89%)	57 (11%)	4 11
All	All	1991/2068 (96%)	1764 (89%)	227 (11%)	4 11

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	613	ARG
1	D	543	LYS
1	C	384	GLU
1	D	512	LEU
1	D	383	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	128	ASN
1	D	500	ASN
1	D	168	GLN
1	D	379	ASN
1	B	301	ASN

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 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	508:THR	C	509:LEU	N	1.20
1	C	500:ASN	C	501:GLN	N	0.90

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, 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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	587/605 (97%)	-1.78	0	100	100	7, 25, 67, 83	0
1	B	581/605 (96%)	-1.75	0	100	100	9, 25, 74, 87	0
1	C	581/605 (96%)	-1.75	0	100	100	7, 27, 74, 86	0
1	D	582/605 (96%)	-1.74	0	100	100	8, 27, 76, 89	0
All	All	2331/2420 (96%)	-1.76	0	100	100	7, 26, 73, 89	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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	B-factors(Å^2)	Q<0.9
2	ZN	B	701	1/1	0.98	0.04	24,24,24,24	1
2	ZN	A	701	1/1	0.99	0.03	9,9,9,9	1
2	ZN	C	701	1/1	0.99	0.02	15,15,15,15	1
2	ZN	D	701	1/1	1.00	0.04	28,28,28,28	1

6.5 Other polymers (i)

There are no such residues in this entry.