wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2023 – 04:05 PM EDT

PDB ID	:	2IJZ
Title	:	Crystal structure of aminopeptidase
Authors	:	Min, T.; Burley, S.K.; Shapiro, L.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2006-10-02
Resolution	:	3.00 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 (1)) were used in the production of this report:

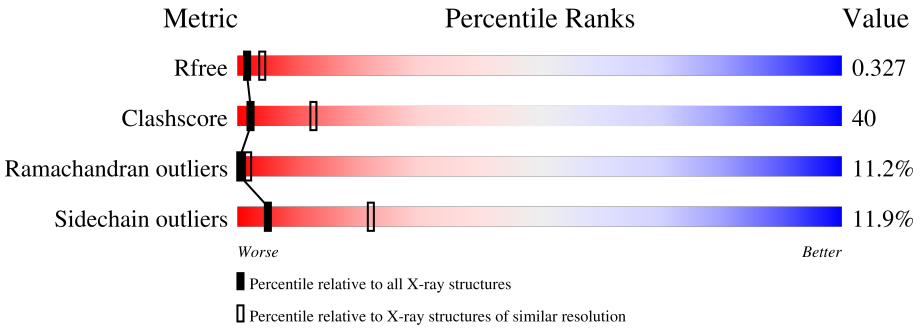
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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%

Mol	Chain	Length	Quality of chain
1	A	428	40% 37% 11% • 11%
1	B	428	36% 42% 9% • 11%
1	C	428	39% 38% 10% • 11%
1	D	428	40% 37% 11% • 11%
1	E	428	39% 37% 11% • 11%
1	F	428	40% 38% 9% • 11%
1	G	428	41% 37% 9% • 11%

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Mol	Chain	Length	Quality of chain
1	H	428	39% 39% 10% • 11%
1	I	428	39% 36% 12% • 11%
1	J	428	42% 36% 10% • 11%
1	K	428	36% 41% 10% • 11%
1	L	428	39% 38% 10% • 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 37617 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 Probable M18-family aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	B	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	C	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	D	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	E	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	F	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	G	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	H	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	I	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	J	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	K	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	L	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
B	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
C	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
D	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
E	154	ASN	ALA	engineered mutation	UNP Q9HYZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
G	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
H	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
I	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
J	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
K	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
L	154	ASN	ALA	engineered mutation	UNP Q9HYZ3

- Molecule 2 is water.

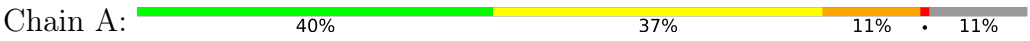
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	262	Total O 262 262	0	0
2	B	271	Total O 271 271	0	0
2	C	298	Total O 298 298	0	0
2	D	247	Total O 247 247	0	0
2	E	268	Total O 268 268	0	0
2	F	247	Total O 247 247	0	0
2	G	255	Total O 255 255	0	0
2	H	252	Total O 252 252	0	0
2	I	274	Total O 274 274	0	0
2	J	258	Total O 258 258	0	0
2	K	276	Total O 276 276	0	0
2	L	269	Total O 269 269	0	0

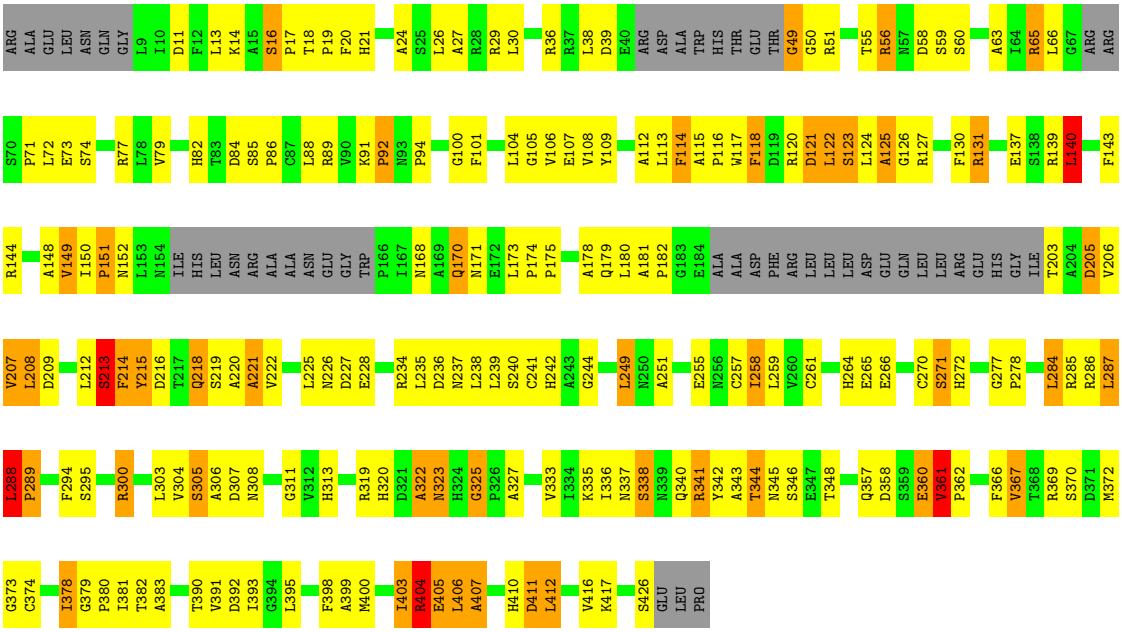
3 Residue-property plots (i)

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. 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. 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: Probable M18-family aminopeptidase 2

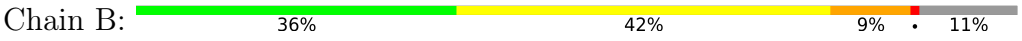
Chain A:

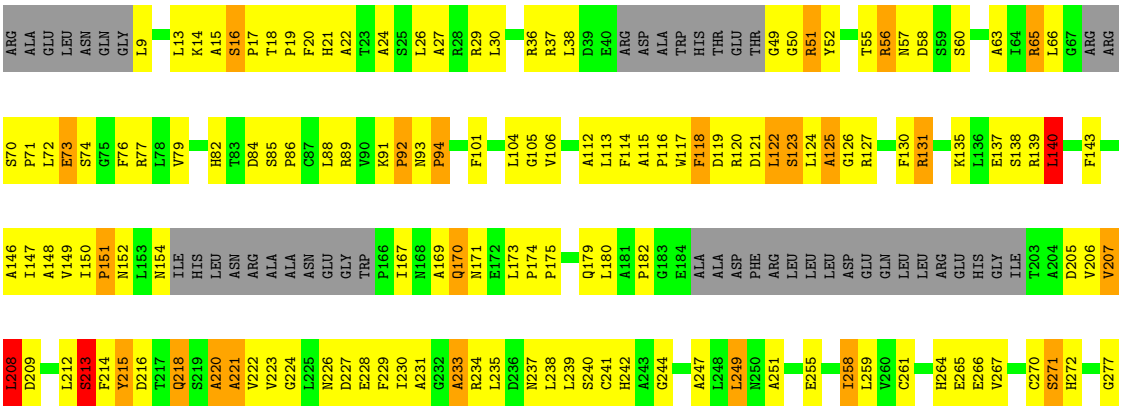


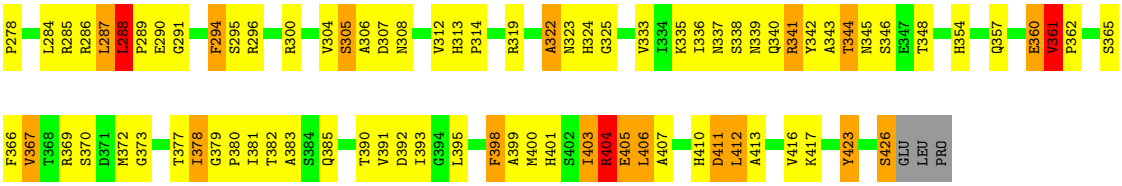


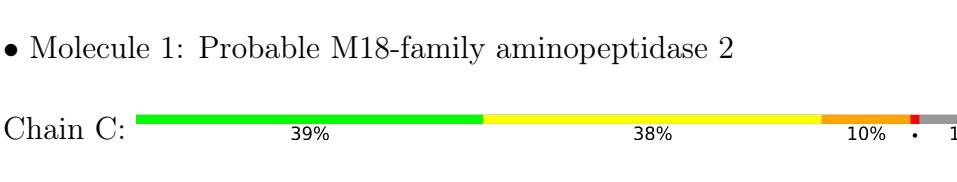
• Molecule 1: Probable M18-family aminopeptidase 2

Chain B:



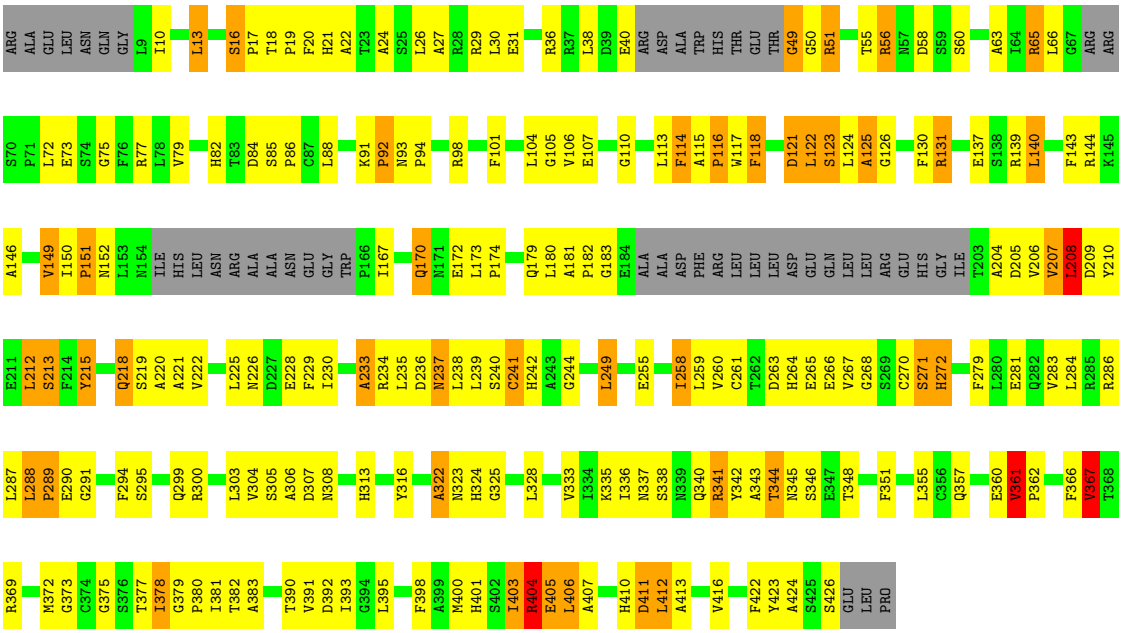






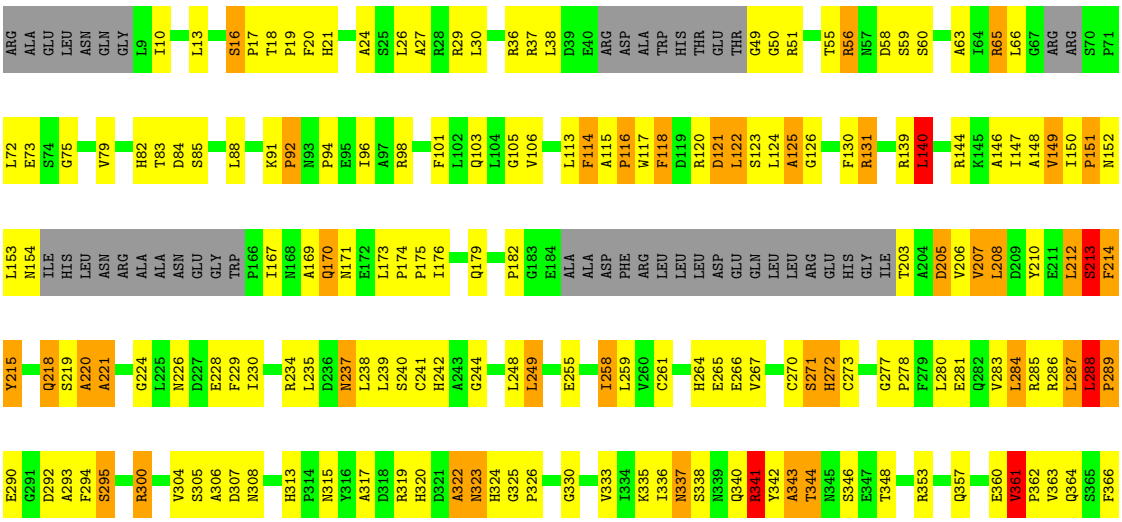
• Molecule 1: Probable M18-family aminopeptidase 2

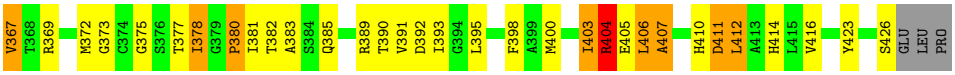
Chain C:



• Molecule 1: Probable M18-family aminopeptidase 2

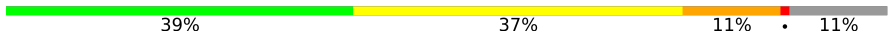
Chain D:

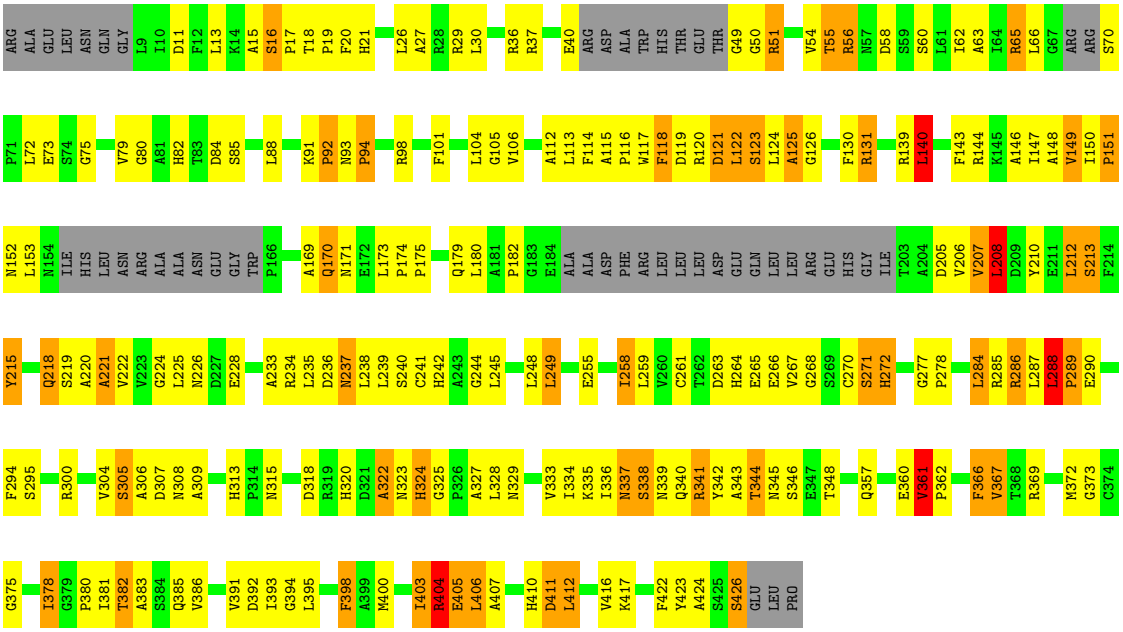




• Molecule 1: Probable M18-family aminopeptidase 2

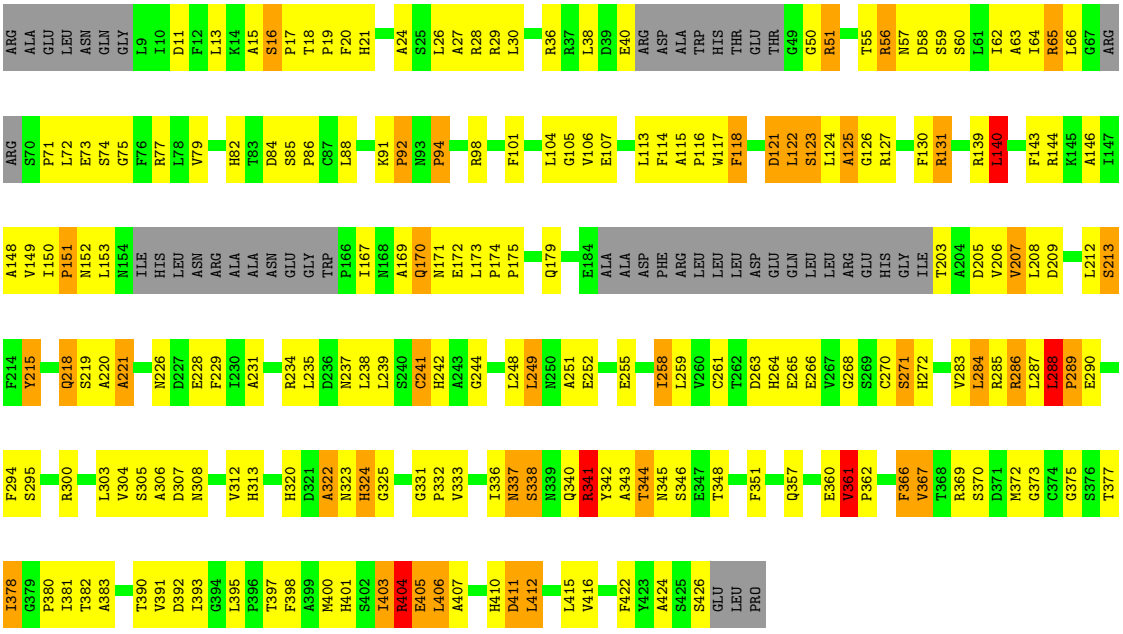
Chain E:





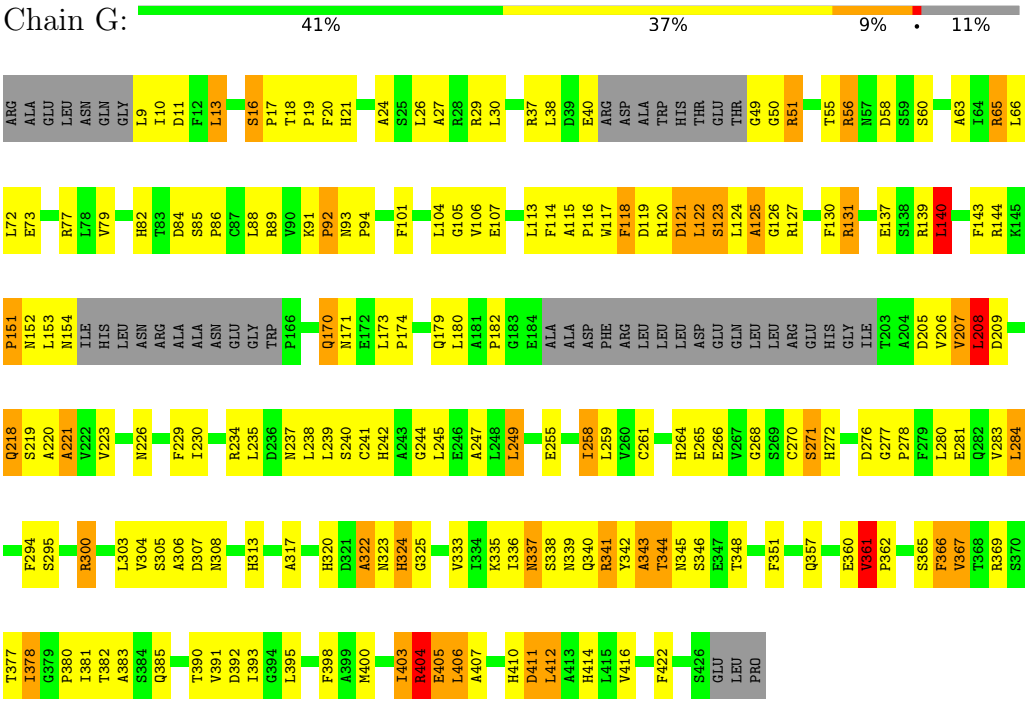
• Molecule 1: Probable M18-family aminopeptidase 2

Chain F:



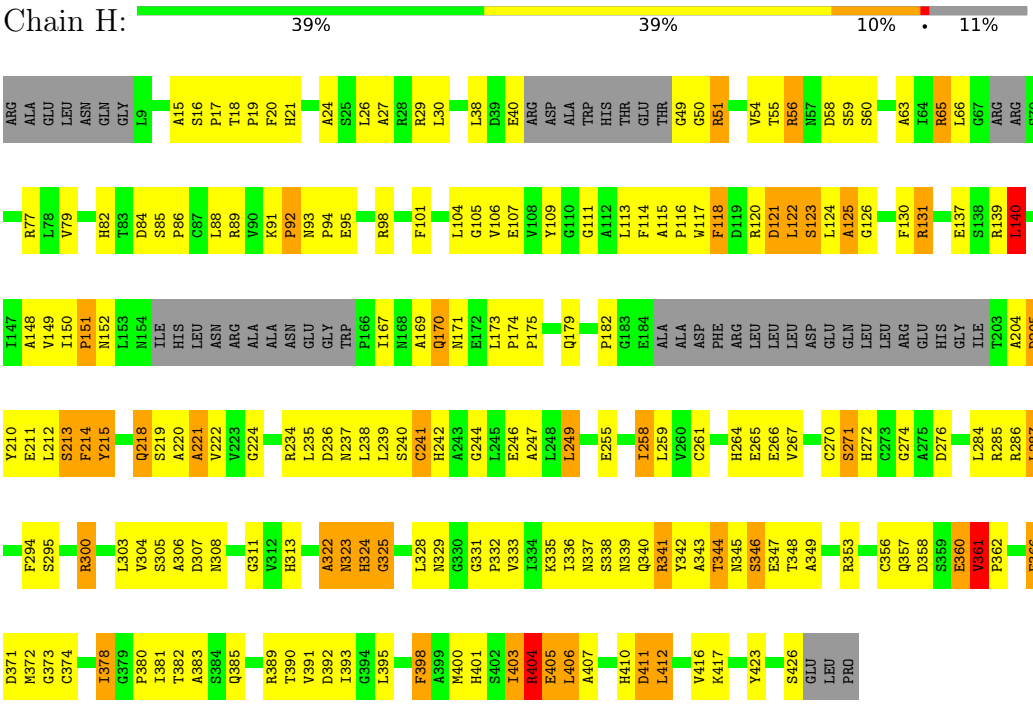
• Molecule 1: Probable M18-family aminopeptidase 2

Chain G:



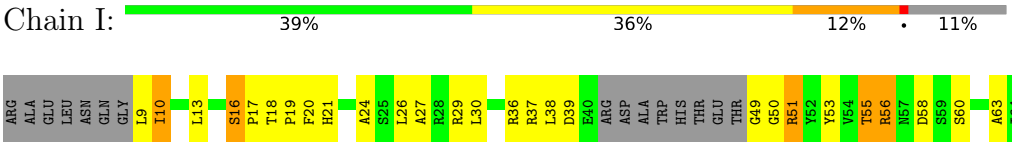
• Molecule 1: Probable M18-family aminopeptidase 2

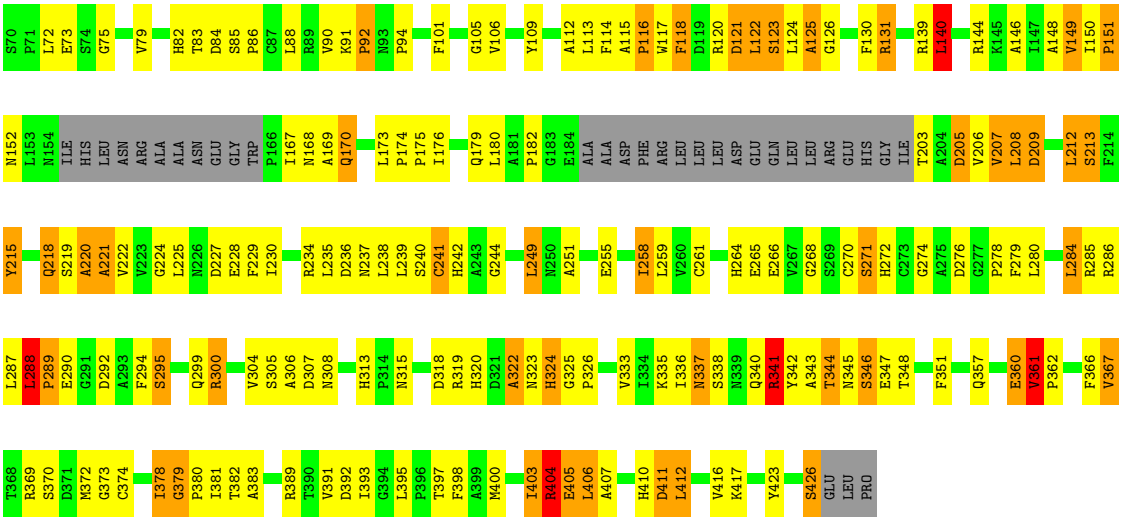
Chain H:



• Molecule 1: Probable M18-family aminopeptidase 2

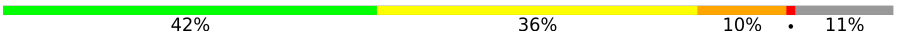
Chain I:

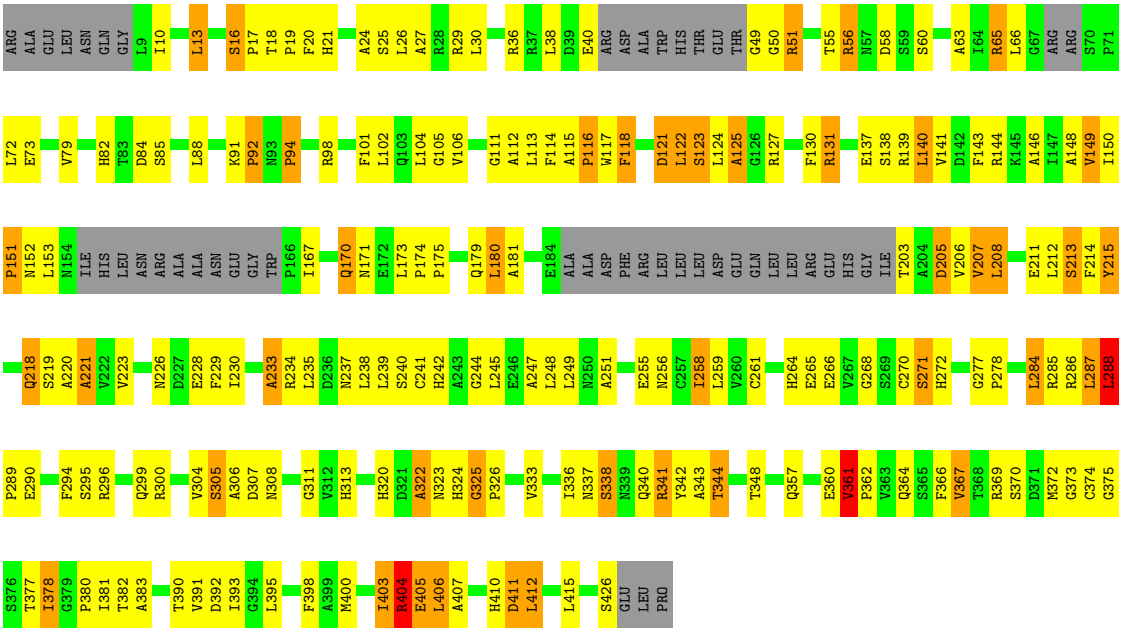




• Molecule 1: Probable M18-family aminopeptidase 2

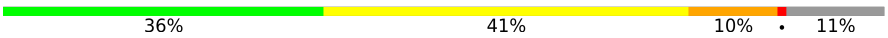
Chain J:

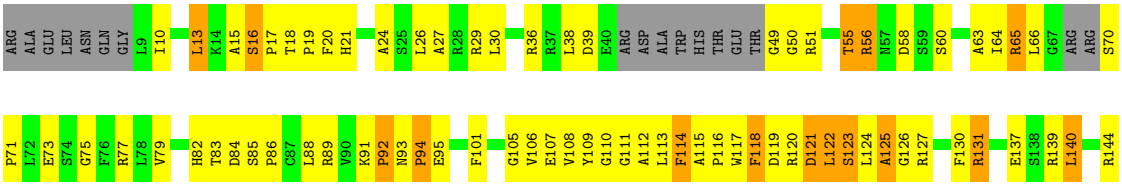


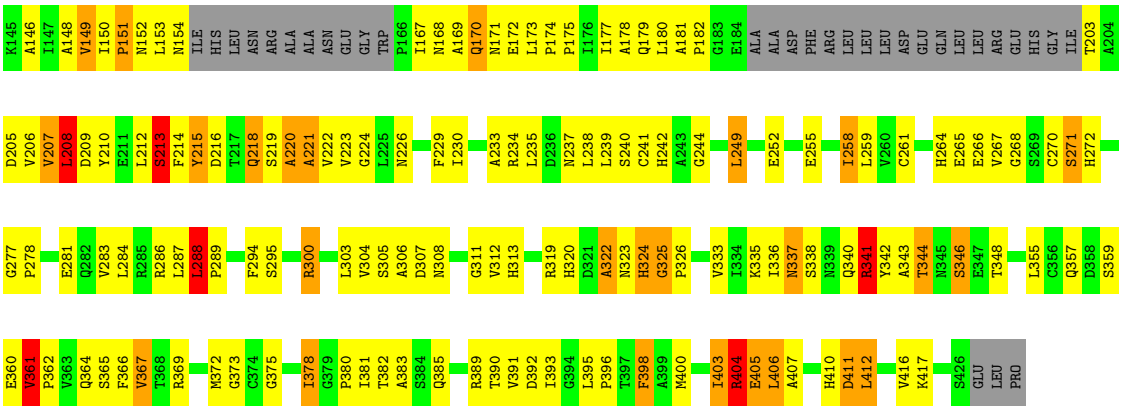


• Molecule 1: Probable M18-family aminopeptidase 2

Chain K:

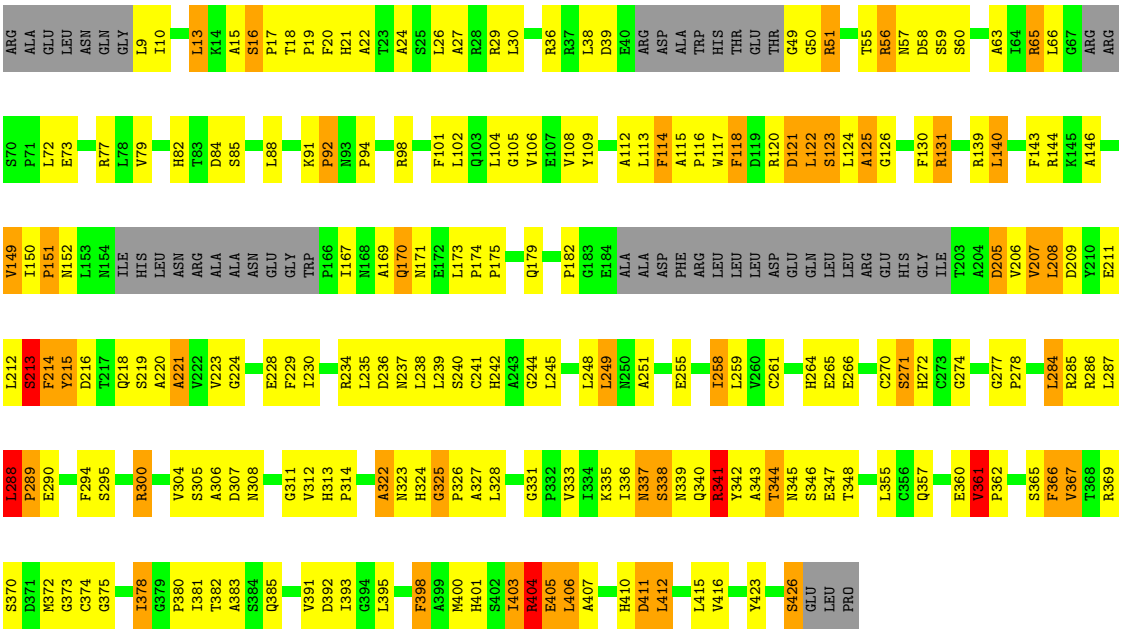






• Molecule 1: Probable M18-family aminopeptidase 2

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	134.68Å 134.55Å 134.60Å 60.12° 60.10° 60.16°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	52.9 (20.00-3.00) 73.0 (20.00-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.30Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.255 , 0.291 0.317 , 0.327	Depositor DCC
R_{free} test set	9838 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 33.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage

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[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.

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Property	Value	Source
Estimated twinning fraction	0.033 for h-l,h,h-k 0.033 for k,k-l,-h+k 0.030 for l,-h+l,-k+l 0.030 for h-k,h-l,h 0.031 for -k+l,l,-h+l 0.031 for k-l,-h+k,k 0.408 for k,l,h 0.408 for l,h,k 0.417 for h-k,-k+l,-k 0.417 for h-l,-l,k-l 0.409 for -k,h-k,-k+l 0.409 for -h+k,-h,-h+l 0.407 for -h+l,-h+k,-h 0.407 for -l,k-l,h-l 0.032 for -h+k,k,k-l 0.033 for -h+l,-k+l,l 0.029 for h,h-k,h-l 0.032 for -h,-l,-k 0.033 for -k,-h,-l 0.033 for -l,-k,-h 0.427 for k-l,h-l,-l 0.427 for -k+l,-k,h-k 0.419 for -h,-h+l,-h+k	Xtriage
F_o,F_c correlation	0.63	EDS
Total number of atoms	37617	wwPDB-VP
Average B, all atoms (Å^2)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.41	2/2926 (0.1%)	0.57	0/3970
1	B	0.64	1/2926 (0.0%)	0.59	1/3970 (0.0%)
1	C	0.37	2/2926 (0.1%)	0.58	0/3970
1	D	0.35	0/2926	0.63	2/3970 (0.1%)
1	E	0.75	1/2926 (0.0%)	0.59	1/3970 (0.0%)
1	F	0.39	1/2926 (0.0%)	0.57	1/3970 (0.0%)
1	G	0.35	0/2926	0.58	0/3970
1	H	0.42	1/2926 (0.0%)	0.58	1/3970 (0.0%)
1	I	0.58	1/2926 (0.0%)	0.58	0/3970
1	J	0.44	1/2926 (0.0%)	0.59	1/3970 (0.0%)
1	K	0.37	1/2926 (0.0%)	0.57	0/3970
1	L	0.61	1/2926 (0.0%)	0.58	1/3970 (0.0%)
All	All	0.49	12/35112 (0.0%)	0.58	8/47640 (0.0%)

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	C	0	1
1	D	0	2
1	E	0	1
1	G	0	1
1	I	0	1
1	L	0	1
All	All	0	7

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	426	SER	C-O	35.87	1.91	1.23
1	B	426	SER	C-O	29.30	1.79	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	426	SER	C-O	27.37	1.75	1.23
1	I	426	SER	C-O	25.28	1.71	1.23
1	J	426	SER	C-O	15.10	1.52	1.23

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	426	SER	CA-C-O	15.91	153.50	120.10
1	B	426	SER	CA-C-O	-8.93	101.35	120.10
1	J	426	SER	CA-C-O	-8.68	101.87	120.10
1	L	426	SER	CA-C-O	-7.23	104.91	120.10
1	E	426	SER	CA-C-O	-6.53	106.38	120.10

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	212	LEU	Peptide
1	D	212	LEU	Peptide
1	D	213	SER	Peptide
1	E	212	LEU	Peptide
1	G	212	LEU	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	2870	0	2800	237	0
1	B	2870	0	2800	242	0
1	C	2870	0	2800	225	0
1	D	2870	0	2800	228	0
1	E	2870	0	2800	240	0
1	F	2870	0	2800	225	0
1	G	2870	0	2800	206	0
1	H	2870	0	2800	232	0
1	I	2870	0	2800	259	0
1	J	2870	0	2800	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2870	0	2800	236	0
1	L	2870	0	2800	235	0
2	A	262	0	0	132	0
2	B	271	0	0	117	0
2	C	298	0	0	136	0
2	D	247	0	0	105	0
2	E	268	0	0	124	0
2	F	247	0	0	111	0
2	G	255	0	0	93	0
2	H	252	0	0	117	0
2	I	274	0	0	152	0
2	J	258	0	0	129	0
2	K	276	0	0	123	0
2	L	269	0	0	118	0
All	All	37617	0	33600	2700	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 40.

The worst 5 of 2700 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:L:230:ILE:CD1	2:L:582:HOH:O	1.71	1.33
1:L:230:ILE:HD13	2:L:582:HOH:O	1.23	1.33
1:F:13:LEU:HD22	2:F:655:HOH:O	1.29	1.32
1:I:361:VAL:HG23	2:I:581:HOH:O	1.26	1.32
1:K:181:ALA:HB3	2:K:550:HOH:O	1.13	1.30

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	369/428 (86%)	246 (67%)	82 (22%)	41 (11%)	0 2
1	B	369/428 (86%)	241 (65%)	84 (23%)	44 (12%)	0 1
1	C	369/428 (86%)	245 (66%)	81 (22%)	43 (12%)	0 1
1	D	369/428 (86%)	240 (65%)	86 (23%)	43 (12%)	0 1
1	E	369/428 (86%)	243 (66%)	84 (23%)	42 (11%)	0 2
1	F	369/428 (86%)	243 (66%)	85 (23%)	41 (11%)	0 2
1	G	369/428 (86%)	242 (66%)	90 (24%)	37 (10%)	0 2
1	H	369/428 (86%)	245 (66%)	86 (23%)	38 (10%)	0 2
1	I	369/428 (86%)	240 (65%)	88 (24%)	41 (11%)	0 2
1	J	369/428 (86%)	241 (65%)	85 (23%)	43 (12%)	0 1
1	K	369/428 (86%)	244 (66%)	83 (22%)	42 (11%)	0 2
1	L	369/428 (86%)	244 (66%)	83 (22%)	42 (11%)	0 2
All	All	4428/5136 (86%)	2914 (66%)	1017 (23%)	497 (11%)	0 2

5 of 497 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	PRO
1	A	125	ALA
1	A	131	ARG
1	A	207	VAL
1	A	214	PHE

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	303/344 (88%)	268 (88%)	35 (12%)	5 23
1	B	303/344 (88%)	266 (88%)	37 (12%)	5 21
1	C	303/344 (88%)	266 (88%)	37 (12%)	5 21
1	D	303/344 (88%)	269 (89%)	34 (11%)	6 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	303/344 (88%)	266 (88%)	37 (12%)	5	21
1	F	303/344 (88%)	268 (88%)	35 (12%)	5	23
1	G	303/344 (88%)	267 (88%)	36 (12%)	5	22
1	H	303/344 (88%)	268 (88%)	35 (12%)	5	23
1	I	303/344 (88%)	264 (87%)	39 (13%)	4	19
1	J	303/344 (88%)	269 (89%)	34 (11%)	6	24
1	K	303/344 (88%)	266 (88%)	37 (12%)	5	21
1	L	303/344 (88%)	268 (88%)	35 (12%)	5	23
All	All	3636/4128 (88%)	3205 (88%)	431 (12%)	5	22

5 of 431 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	286	ARG
1	I	10	ILE
1	L	73	GLU
1	G	341	ARG
1	H	215	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 141 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	385	GLN
1	K	170	GLN
1	L	152	ASN
1	D	315	ASN
1	D	308	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 monosaccharides 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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.