



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:58 am GMT

PDB ID : 2GRE  
Title : Crystal structure of Deblocking aminopeptidase from *Bacillus cereus*  
Authors : Chang, C.; Wu, R.; Abdullah, J.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2006-04-24  
Resolution : 2.65 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

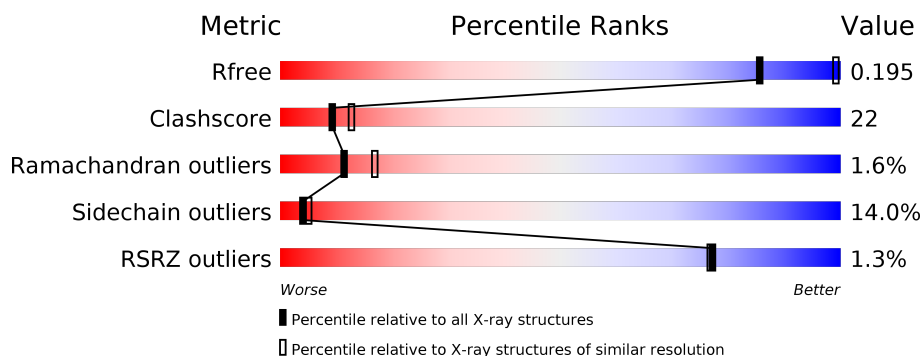
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	349	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>27%</div> <div>9%</div> <div>10%</div> </div> </div>
1	B	349	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>27%</div> <div>8%</div> <div>11%</div> </div> </div>
1	C	349	<div> <div></div> <div> <div>60%</div> <div>23%</div> <div>6%</div> <div>12%</div> </div> </div>
1	D	349	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>28%</div> <div>6%</div> <div>12%</div> </div> </div>
1	E	349	<div> <div>%</div> <div> <div></div> <div>52%</div> <div>29%</div> <div>5%</div> <div>12%</div> </div> </div>
1	F	349	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>25%</div> <div>7%</div> <div>11%</div> </div> </div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	349	
1	H	349	
1	I	349	
1	J	349	
1	K	349	
1	L	349	
1	M	349	
1	N	349	
1	O	349	
1	P	349	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	G	350	-	-	-	X
2	SO4	J	350	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39559 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 Deblocking aminopeptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	Se	0	0	0
			2441	1541	414	478	2	6			
1	B	312	Total	C	N	O	S	Se	0	0	0
			2431	1535	411	477	2	6			
1	C	308	Total	C	N	O	S	Se	0	0	0
			2413	1526	406	473	2	6			
1	D	306	Total	C	N	O	S	Se	0	0	0
			2398	1517	403	470	2	6			
1	E	306	Total	C	N	O	S	Se	0	0	0
			2393	1516	401	468	2	6			
1	F	310	Total	C	N	O	S	Se	0	0	0
			2426	1533	409	476	2	6			
1	G	309	Total	C	N	O	S	Se	0	0	0
			2413	1526	404	475	2	6			
1	H	305	Total	C	N	O	S	Se	0	0	0
			2394	1516	405	465	2	6			
1	I	299	Total	C	N	O	S	Se	0	0	0
			2364	1500	396	460	2	6			
1	J	307	Total	C	N	O	S	Se	0	0	0
			2399	1518	402	471	2	6			
1	K	304	Total	C	N	O	S	Se	0	0	0
			2389	1513	404	464	2	6			
1	L	310	Total	C	N	O	S	Se	0	0	0
			2421	1530	407	476	2	6			
1	M	309	Total	C	N	O	S	Se	0	0	0
			2422	1531	407	476	2	6			
1	N	307	Total	C	N	O	S	Se	0	0	0
			2407	1524	407	468	2	6			
1	O	308	Total	C	N	O	S	Se	0	0	0
			2404	1521	403	473	2	5			
1	P	305	Total	C	N	O	S	Se	0	0	0
			2382	1508	400	466	2	6			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
A	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
A	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
A	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
A	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
A	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
A	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
B	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
B	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
B	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
B	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
B	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
B	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
B	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
C	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
C	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
C	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
C	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
C	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
C	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
C	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
D	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
D	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
D	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
D	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
D	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
D	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
D	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
E	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
E	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
E	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
E	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
E	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
E	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
E	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
F	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
F	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
F	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
F	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
F	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
F	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
F	343	MSE	MET	MODIFIED RESIDUE	GB 29894598

*Continued on next page...*

*Continued from previous page...*

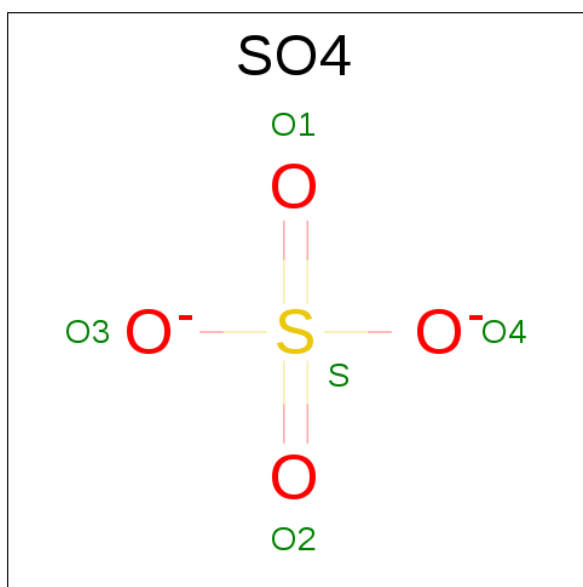
Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
G	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
G	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
G	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
G	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
G	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
G	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
H	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
H	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
H	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
H	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
H	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
H	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
H	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
I	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
I	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
I	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
I	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
I	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
I	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
I	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
J	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
J	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
J	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
J	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
J	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
J	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
J	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
K	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
K	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
K	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
K	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
K	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
K	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
K	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
L	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
L	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
L	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
L	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
L	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
L	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
L	343	MSE	MET	MODIFIED RESIDUE	GB 29894598

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
M	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
M	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
M	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
M	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
M	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
M	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
N	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
N	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
N	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
N	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
N	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
N	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
N	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
O	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
O	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
O	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
O	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
O	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
O	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
O	343	MSE	MET	MODIFIED RESIDUE	GB 29894598
P	1	MSE	MET	MODIFIED RESIDUE	GB 29894598
P	9	MSE	MET	MODIFIED RESIDUE	GB 29894598
P	76	MSE	MET	MODIFIED RESIDUE	GB 29894598
P	90	MSE	MET	MODIFIED RESIDUE	GB 29894598
P	120	MSE	MET	MODIFIED RESIDUE	GB 29894598
P	242	MSE	MET	MODIFIED RESIDUE	GB 29894598
P	343	MSE	MET	MODIFIED RESIDUE	GB 29894598

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	P	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

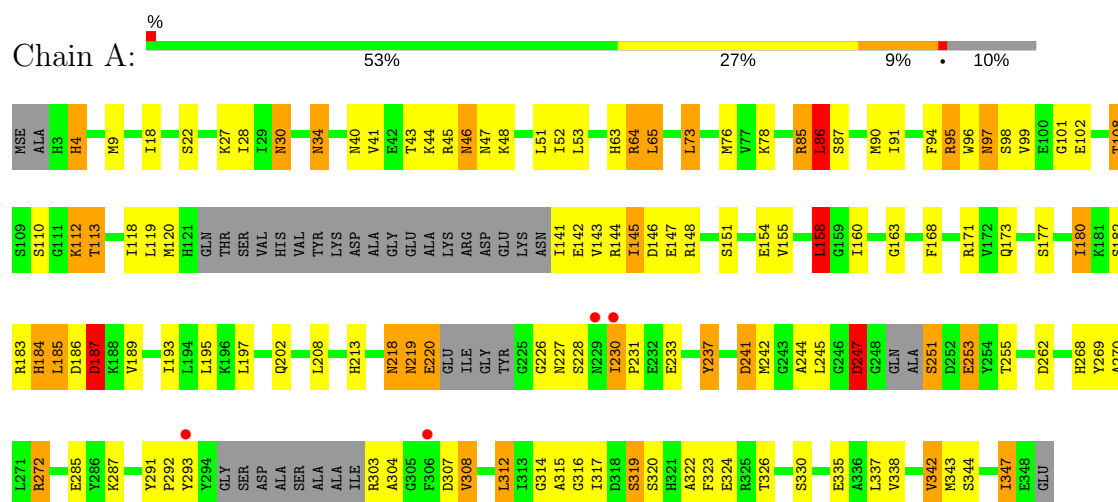
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total	O	0	0
			73	73		
3	B	71	Total	O	0	0
			71	71		
3	C	68	Total	O	0	0
			68	68		
3	D	57	Total	O	0	0
			57	57		
3	E	69	Total	O	0	0
			69	69		
3	F	57	Total	O	0	0
			57	57		
3	G	69	Total	O	0	0
			69	69		
3	H	61	Total	O	0	0
			61	61		
3	I	61	Total	O	0	0
			61	61		
3	J	57	Total	O	0	0
			57	57		
3	K	66	Total	O	0	0
			66	66		
3	L	54	Total	O	0	0
			54	54		
3	M	58	Total	O	0	0
			58	58		
3	N	67	Total	O	0	0
			67	67		
3	O	40	Total	O	0	0
			40	40		
3	P	54	Total	O	0	0
			54	54		

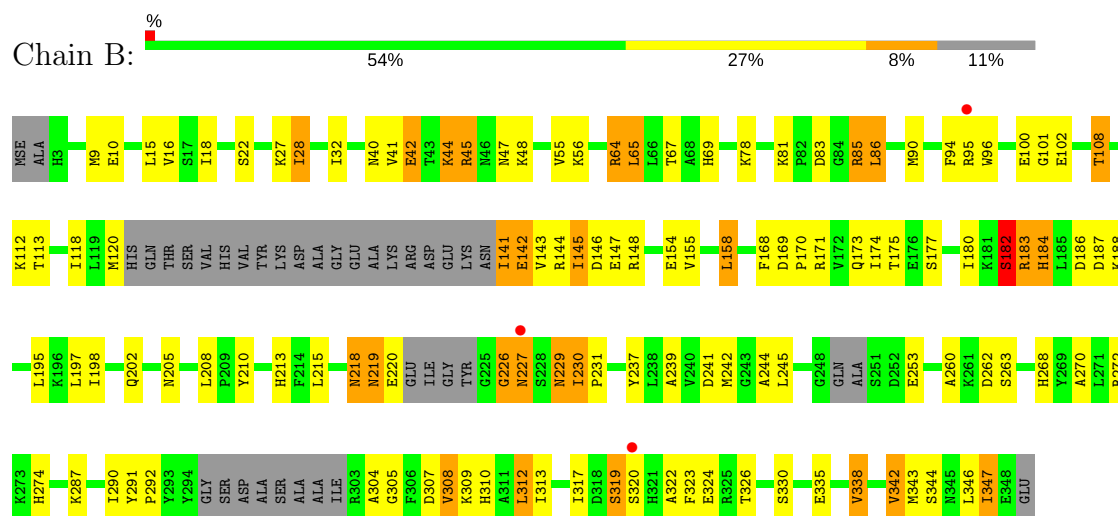
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Deblocking aminopeptidase

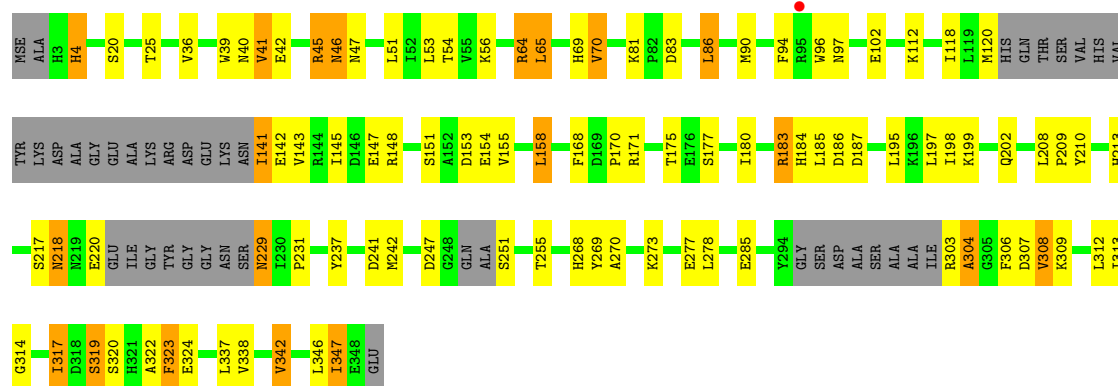


#### • Molecule 1: Deblocking aminopeptidase

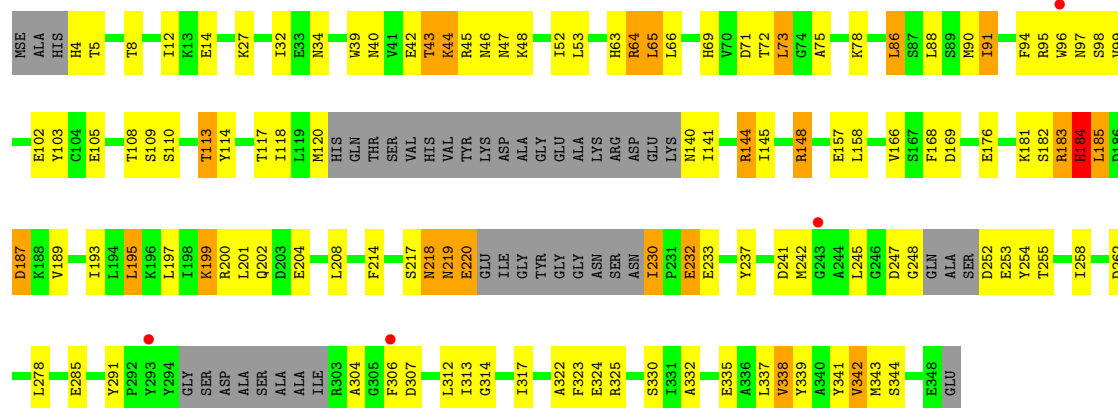


#### • Molecule 1: Deblocking aminopeptidase

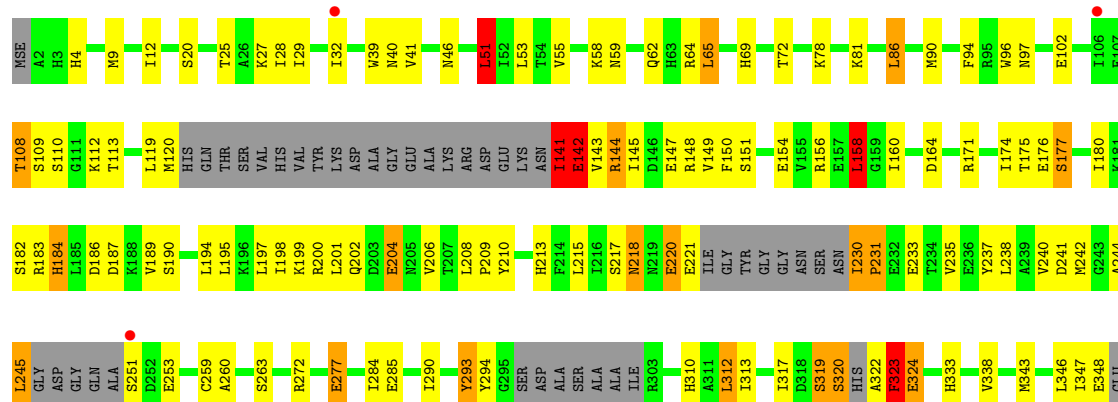




• Molecule 1: Deblocking aminopeptidase



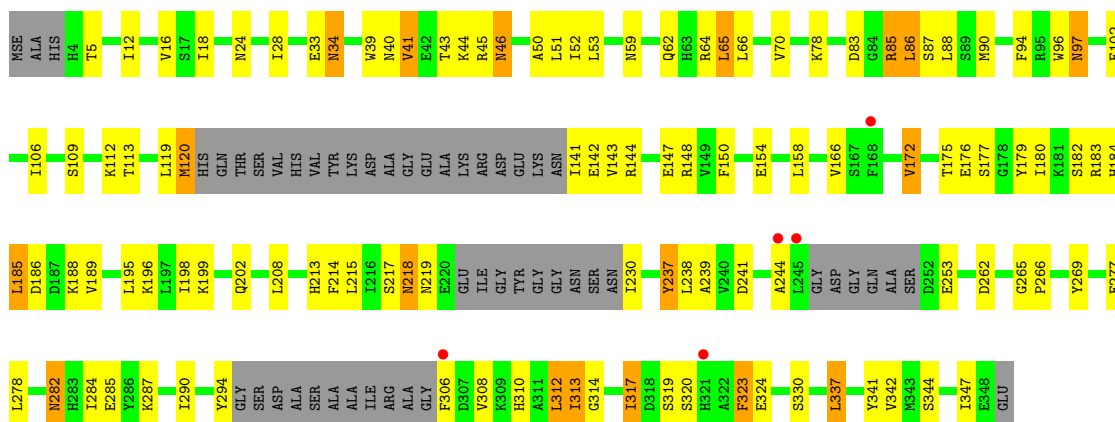
• Molecule 1: Deblocking aminopeptidase



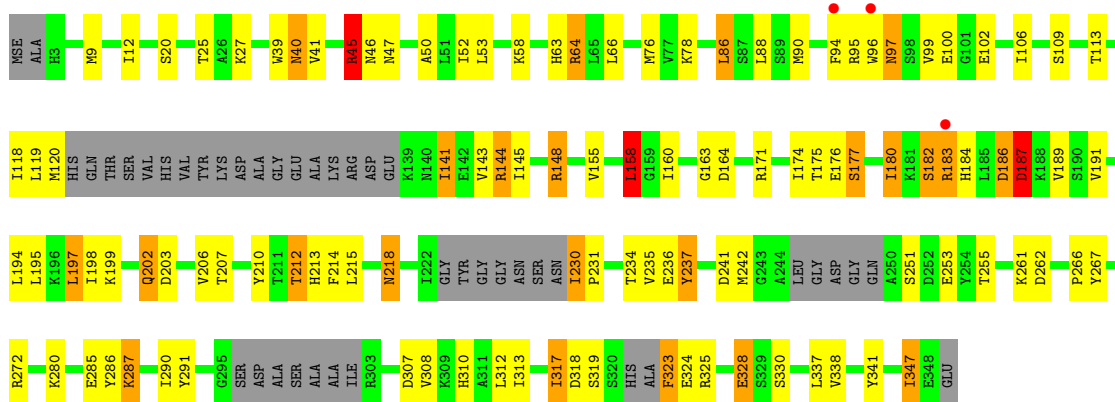
• Molecule 1: Deblocking aminopeptidase



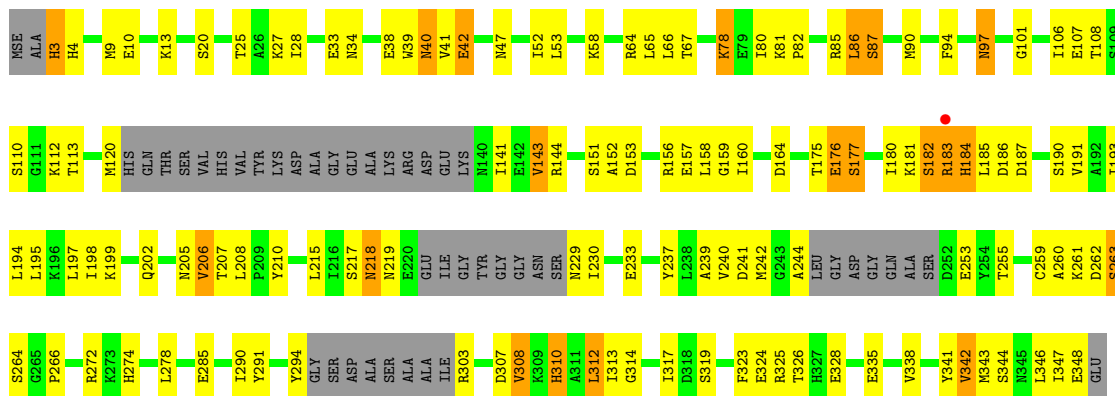




- Molecule 1: Deblocking aminopeptidase

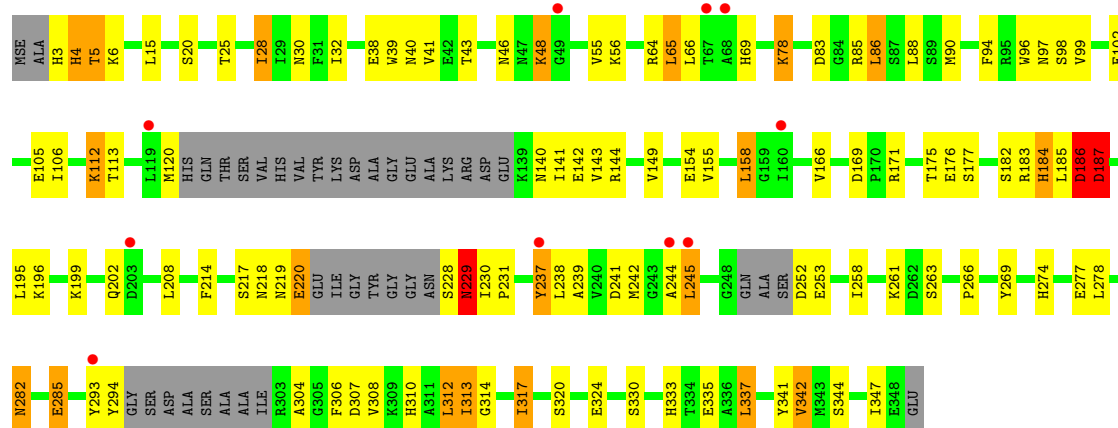


- Molecule 1: Deblocking aminopeptidase

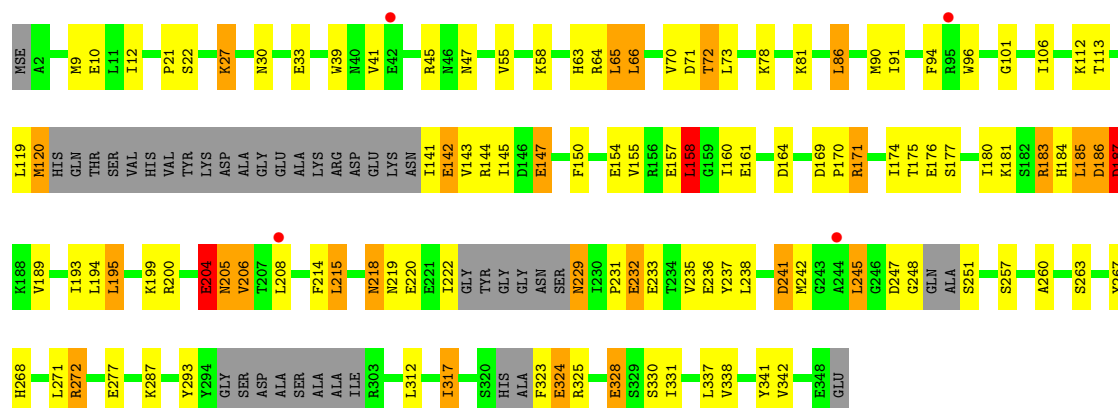


- Molecule 1: Deblocking aminopeptidase

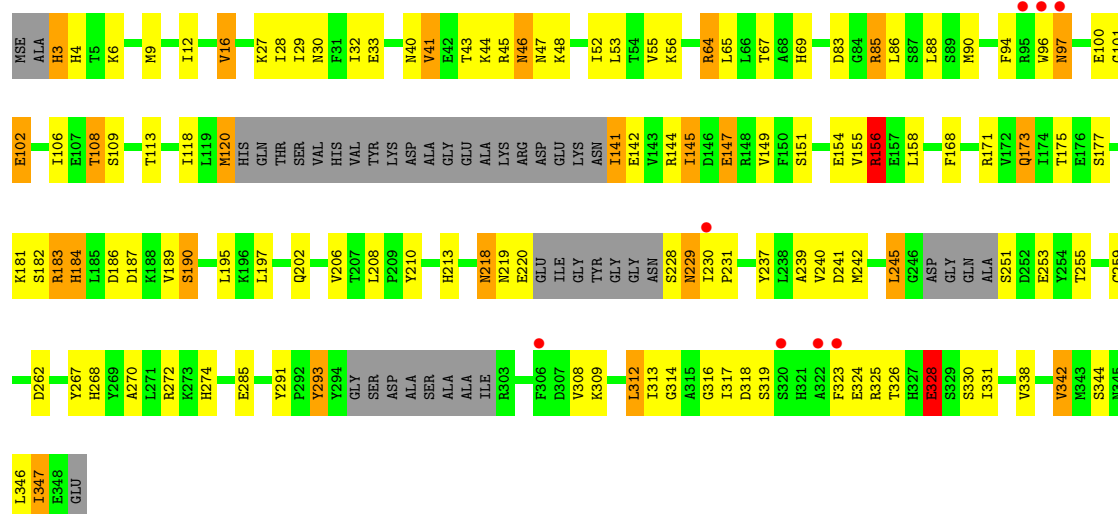




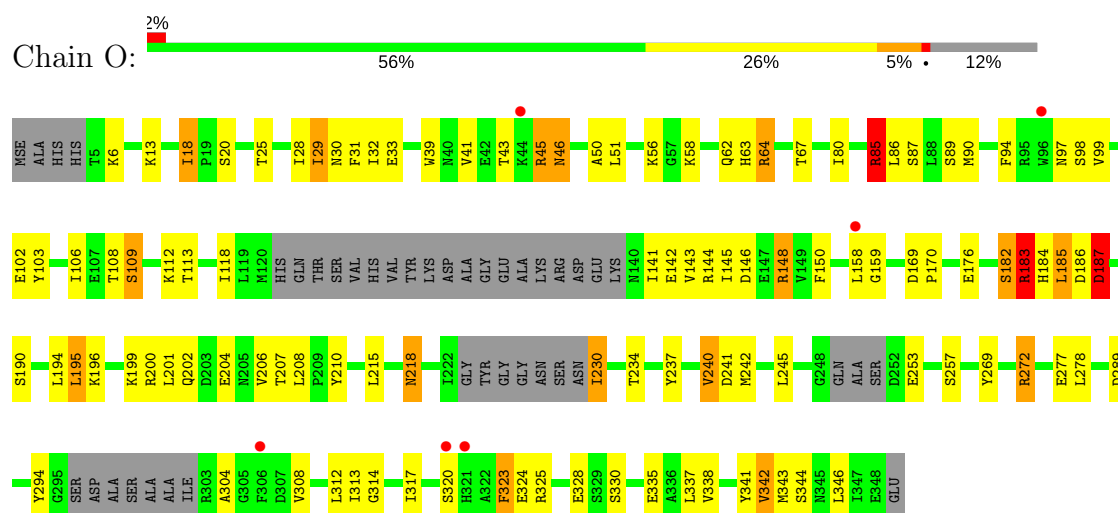
• Molecule 1: Deblocking aminopeptidase



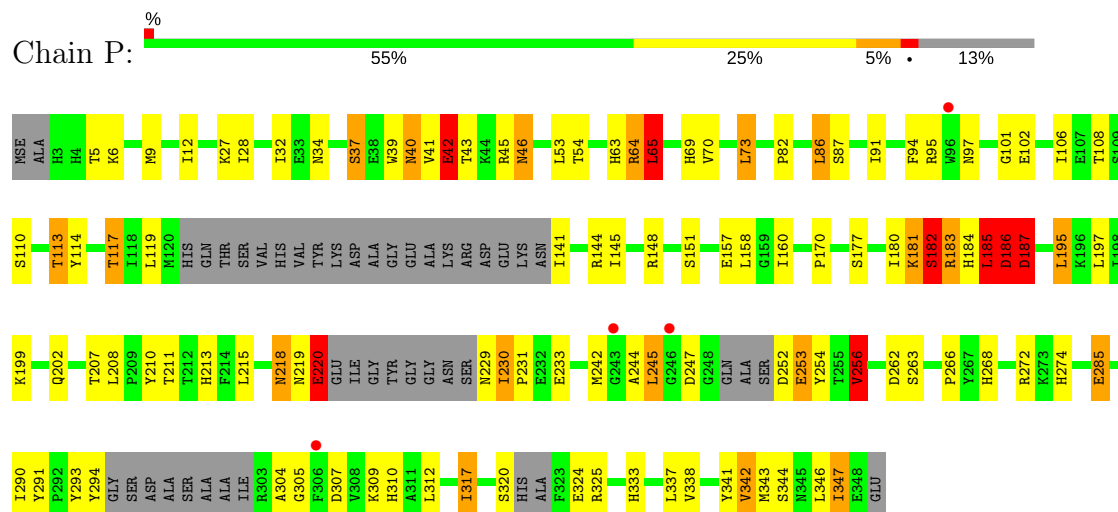
• Molecule 1: Deblocking aminopeptidase



• Molecule 1: Deblocking aminopeptidase



• Molecule 1: Deblocking aminopeptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	240.92Å 240.92Å 294.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.65 47.25 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.65) 99.4 (47.25-2.55)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.194 , 0.264 0.197 , 0.195	Depositor DCC
$R_{free}$ test set	9336 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for $-2/3^*h-1/3^*k+2/3^*l, -1/3^*h-2/3^*k-2/3^*l, 2/3^*h-2/3^*k+1/3^*l$ 0.019 for $-h, 1/3^*h-1/3^*k+2/3^*l, 2/3^*h+4/3^*k+1/3^*l$ 0.019 for $-1/3^*h+1/3^*k-2/3^*l, -k, -4/3^*h-2/3^*k+1/3^*l$ 0.477 for $-h, 2/3^*h+1/3^*k-2/3^*l, -2/3^*h-4/3^*k-1/3^*l$ 0.477 for $1/3^*h+2/3^*k+2/3^*l, -k, 4/3^*h+2/3^*k-1/3^*l$ 0.478 for $-1/3^*h-2/3^*k-2/3^*l, -2/3^*h-1/3^*k+2/3^*l, -2/3^*h+2/3^*k-1/3^*l$ 0.020 for $h, -h-k, -l$	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	39559	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SO4

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	0.92	0/2477	1.03	11/3339 (0.3%)
1	B	0.92	0/2466	0.97	3/3324 (0.1%)
1	C	0.91	1/2448 (0.0%)	1.00	5/3300 (0.2%)
1	D	0.75	0/2433	0.85	1/3281 (0.0%)
1	E	0.85	0/2426	0.91	8/3269 (0.2%)
1	F	0.87	2/2461 (0.1%)	0.92	3/3318 (0.1%)
1	G	0.83	0/2446	0.87	4/3295 (0.1%)
1	H	0.85	0/2430	0.91	2/3277 (0.1%)
1	I	0.74	0/2399	0.84	0/3234
1	J	0.85	1/2432 (0.0%)	0.90	4/3277 (0.1%)
1	K	0.89	0/2425	0.91	1/3270 (0.0%)
1	L	0.75	0/2455	0.86	2/3310 (0.1%)
1	M	0.88	2/2456 (0.1%)	0.95	9/3309 (0.3%)
1	N	0.93	2/2443 (0.1%)	0.96	6/3294 (0.2%)
1	O	0.79	1/2438 (0.0%)	0.88	3/3287 (0.1%)
1	P	0.89	3/2415 (0.1%)	0.96	5/3254 (0.2%)
All	All	0.85	12/39050 (0.0%)	0.92	67/52638 (0.1%)

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	1	0
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	2
1	G	0	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	3
1	K	0	1
1	L	1	0
1	N	0	1
1	O	1	0
1	P	0	4
All	All	3	18

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	161	GLU	CG-CD	10.39	1.67	1.51
1	P	253	GLU	CG-CD	7.05	1.62	1.51
1	F	342	VAL	CB-CG1	-6.18	1.39	1.52
1	J	328	GLU	CG-CD	5.99	1.60	1.51
1	M	328	GLU	CG-CD	5.88	1.60	1.51

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	187	ASP	N-CA-C	8.37	133.60	111.00
1	A	148	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	A	272	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	E	144	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	A	272	ARG	NE-CZ-NH2	-7.37	116.61	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	187	ASP	CA
1	L	187	ASP	CA
1	O	187	ASP	CA

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	182	SER	Peptide
1	C	229	ASN	Peptide
1	D	182	SER	Peptide
1	D	185	LEU	Peptide
1	E	141	ILE	Peptide

## 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	2441	0	2395	134	0
1	B	2431	0	2388	137	0
1	C	2413	0	2375	102	0
1	D	2398	0	2357	91	0
1	E	2393	0	2361	132	0
1	F	2426	0	2383	102	0
1	G	2413	0	2369	108	0
1	H	2394	0	2354	105	0
1	I	2364	0	2342	94	0
1	J	2399	0	2355	123	0
1	K	2389	0	2352	121	0
1	L	2421	0	2378	113	0
1	M	2422	0	2380	109	0
1	N	2407	0	2371	108	0
1	O	2404	0	2361	78	0
1	P	2382	0	2340	117	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
2	M	5	0	0	0	0
2	N	5	0	0	0	0
2	O	5	0	0	0	0
2	P	5	0	0	0	0
3	A	73	0	0	23	0
3	B	71	0	0	23	0
3	C	68	0	0	19	0
3	D	57	0	0	9	0
3	E	69	0	0	20	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	57	0	0	28	0
3	G	69	0	0	6	0
3	H	61	0	0	16	0
3	I	61	0	0	12	0
3	J	57	0	0	12	0
3	K	66	0	0	18	0
3	L	54	0	0	23	0
3	M	58	0	0	21	0
3	N	67	0	0	14	0
3	O	40	0	0	8	0
3	P	54	0	0	24	0
All	All	39559	0	37861	1685	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 22.

The worst 5 of 1685 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:102:GLU:HG3	1:D:183:ARG:NH2	1.25	1.46
1:J:45:ARG:HB2	1:J:45:ARG:NH1	1.18	1.42
1:P:208:LEU:HD23	1:P:343:MSE:CE	1.50	1.39
1:L:102:GLU:HG3	1:L:183:ARG:NH1	1.31	1.37
1:J:102:GLU:HG3	1:J:183:ARG:NH2	1.39	1.35

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	303/349 (87%)	278 (92%)	21 (7%)	4 (1%)	14 22

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	302/349 (86%)	278 (92%)	19 (6%)	5 (2%)	11	16
1	C	298/349 (85%)	274 (92%)	20 (7%)	4 (1%)	14	22
1	D	296/349 (85%)	268 (90%)	25 (8%)	3 (1%)	18	28
1	E	294/349 (84%)	273 (93%)	15 (5%)	6 (2%)	9	13
1	F	300/349 (86%)	271 (90%)	20 (7%)	9 (3%)	5	7
1	G	297/349 (85%)	276 (93%)	17 (6%)	4 (1%)	14	22
1	H	295/349 (84%)	276 (94%)	13 (4%)	6 (2%)	9	13
1	I	289/349 (83%)	268 (93%)	18 (6%)	3 (1%)	18	28
1	J	295/349 (84%)	273 (92%)	20 (7%)	2 (1%)	25	39
1	K	294/349 (84%)	267 (91%)	25 (8%)	2 (1%)	25	39
1	L	300/349 (86%)	269 (90%)	24 (8%)	7 (2%)	7	10
1	M	297/349 (85%)	271 (91%)	21 (7%)	5 (2%)	11	16
1	N	297/349 (85%)	276 (93%)	17 (6%)	4 (1%)	14	22
1	O	298/349 (85%)	270 (91%)	21 (7%)	7 (2%)	7	10
1	P	293/349 (84%)	269 (92%)	19 (6%)	5 (2%)	11	16
All	All	4748/5584 (85%)	4357 (92%)	315 (7%)	76 (2%)	11	17

5 of 76 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	SER
1	A	247	ASP
1	C	41	VAL
1	D	184	HIS
1	D	304	ALA

### 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	267/291 (92%)	225 (84%)	42 (16%)	3	3

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	266/291 (91%)	223 (84%)	43 (16%)	3	3
1	C	265/291 (91%)	233 (88%)	32 (12%)	6	8
1	D	263/291 (90%)	225 (86%)	38 (14%)	4	4
1	E	262/291 (90%)	227 (87%)	35 (13%)	4	6
1	F	266/291 (91%)	227 (85%)	39 (15%)	3	4
1	G	264/291 (91%)	231 (88%)	33 (12%)	5	7
1	H	262/291 (90%)	225 (86%)	37 (14%)	4	5
1	I	262/291 (90%)	231 (88%)	31 (12%)	6	8
1	J	262/291 (90%)	228 (87%)	34 (13%)	5	7
1	K	262/291 (90%)	226 (86%)	36 (14%)	4	5
1	L	265/291 (91%)	231 (87%)	34 (13%)	5	7
1	M	266/291 (91%)	229 (86%)	37 (14%)	4	5
1	N	264/291 (91%)	224 (85%)	40 (15%)	3	4
1	O	262/291 (90%)	223 (85%)	39 (15%)	3	4
1	P	260/291 (89%)	218 (84%)	42 (16%)	3	3
All	All	4218/4656 (91%)	3626 (86%)	592 (14%)	4	5

5 of 592 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	41	VAL
1	J	40	ASN
1	O	328	GLU
1	H	86	LEU
1	I	41	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 127 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	40	ASN
1	I	274	HIS
1	O	218	ASN
1	H	47	ASN
1	H	218	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	350	-	4,4,4	0.26	0	6,6,6	0.52	0
2	SO4	B	350	-	4,4,4	0.23	0	6,6,6	0.49	0
2	SO4	C	350	-	4,4,4	0.13	0	6,6,6	0.51	0
2	SO4	D	350	-	4,4,4	0.23	0	6,6,6	0.52	0
2	SO4	E	350	-	4,4,4	0.22	0	6,6,6	0.10	0
2	SO4	F	350	-	4,4,4	0.19	0	6,6,6	0.29	0
2	SO4	G	350	-	4,4,4	0.19	0	6,6,6	0.12	0
2	SO4	H	350	-	4,4,4	0.20	0	6,6,6	0.46	0
2	SO4	I	350	-	4,4,4	0.18	0	6,6,6	0.39	0
2	SO4	J	350	-	4,4,4	0.17	0	6,6,6	0.10	0
2	SO4	K	350	-	4,4,4	0.20	0	6,6,6	0.31	0
2	SO4	L	350	-	4,4,4	0.24	0	6,6,6	0.38	0
2	SO4	M	350	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	N	350	-	4,4,4	0.09	0	6,6,6	0.81	0
2	SO4	O	350	-	4,4,4	0.19	0	6,6,6	0.37	0
2	SO4	P	350	-	4,4,4	0.19	0	6,6,6	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	350	-	-	0/0/0/0	0/0/0/0
2	SO4	B	350	-	-	0/0/0/0	0/0/0/0
2	SO4	C	350	-	-	0/0/0/0	0/0/0/0
2	SO4	D	350	-	-	0/0/0/0	0/0/0/0
2	SO4	E	350	-	-	0/0/0/0	0/0/0/0
2	SO4	F	350	-	-	0/0/0/0	0/0/0/0
2	SO4	G	350	-	-	0/0/0/0	0/0/0/0
2	SO4	H	350	-	-	0/0/0/0	0/0/0/0
2	SO4	I	350	-	-	0/0/0/0	0/0/0/0
2	SO4	J	350	-	-	0/0/0/0	0/0/0/0
2	SO4	K	350	-	-	0/0/0/0	0/0/0/0
2	SO4	L	350	-	-	0/0/0/0	0/0/0/0
2	SO4	M	350	-	-	0/0/0/0	0/0/0/0
2	SO4	N	350	-	-	0/0/0/0	0/0/0/0
2	SO4	O	350	-	-	0/0/0/0	0/0/0/0
2	SO4	P	350	-	-	0/0/0/0	0/0/0/0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	307/349 (87%)	0.14	4 (1%) 77 77	47, 57, 85, 106	0
1	B	306/349 (87%)	0.06	3 (0%) 82 82	51, 60, 88, 111	0
1	C	302/349 (86%)	0.04	1 (0%) 93 94	45, 55, 79, 93	0
1	D	300/349 (85%)	0.09	4 (1%) 77 77	39, 53, 71, 91	0
1	E	300/349 (85%)	0.05	3 (1%) 82 82	39, 55, 74, 87	0
1	F	304/349 (87%)	0.11	3 (0%) 82 82	48, 57, 80, 98	0
1	G	303/349 (86%)	0.12	3 (0%) 82 82	40, 54, 72, 98	0
1	H	299/349 (85%)	0.00	3 (1%) 82 82	47, 56, 77, 91	0
1	I	293/349 (83%)	0.12	5 (1%) 70 70	42, 53, 67, 78	0
1	J	301/349 (86%)	0.20	3 (0%) 82 82	43, 59, 75, 86	0
1	K	298/349 (85%)	0.13	1 (0%) 93 94	45, 56, 78, 97	0
1	L	304/349 (87%)	0.28	10 (3%) 47 45	45, 56, 75, 88	0
1	M	303/349 (86%)	0.11	4 (1%) 77 77	27, 41, 63, 83	0
1	N	301/349 (86%)	0.16	8 (2%) 55 53	35, 44, 68, 81	0
1	O	302/349 (86%)	0.18	6 (1%) 65 64	15, 33, 54, 67	0
1	P	299/349 (85%)	0.07	4 (1%) 77 77	27, 38, 61, 75	0
All	All	4822/5584 (86%)	0.12	65 (1%) 77 77	15, 54, 75, 111	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	94	PHE	3.9
1	O	321	HIS	3.9
1	F	317	ILE	3.7
1	O	44	LYS	3.7
1	H	96	TRP	3.5

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	J	350	5/5	0.90	0.52	8.40	145,145,145,146	0
2	SO4	G	350	5/5	0.90	0.30	2.94	124,125,125,126	0
2	SO4	E	350	5/5	0.83	0.24	1.05	128,129,129,129	0
2	SO4	M	350	5/5	0.97	0.20	0.04	130,130,131,131	0
2	SO4	L	350	5/5	0.97	0.14	-	75,76,77,78	0
2	SO4	A	350	5/5	0.96	0.16	-	58,59,60,61	0
2	SO4	C	350	5/5	0.98	0.11	-	50,50,52,54	0
2	SO4	P	350	5/5	0.98	0.24	-	67,68,70,70	0
2	SO4	D	350	5/5	0.96	0.21	-	75,78,80,80	0
2	SO4	N	350	5/5	0.96	0.13	-	53,54,56,57	0
2	SO4	H	350	5/5	0.96	0.19	-	69,69,71,72	0
2	SO4	I	350	5/5	0.96	0.14	-	86,87,89,90	0
2	SO4	K	350	5/5	0.97	0.14	-	63,64,64,65	0
2	SO4	B	350	5/5	0.96	0.15	-	54,56,58,59	0
2	SO4	O	350	5/5	0.94	0.23	-	74,75,77,78	0
2	SO4	F	350	5/5	0.97	0.18	-	69,70,71,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.