



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 09:37 PM UTC

PDB ID : 6OAD / pdb\_00006oad  
Title : 2.05 Angstrom Resolution Crystal Structure of Aminopeptidase B from Escherichia coli str. K-12 substr. MG1655.  
Authors : Minasov, G.; Shuvalova, L.; Wawrzak, Z.; Kiryukhina, O.; Grimshaw, S.; Kwon, K.; Satchell, K.J.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2019-03-15  
Resolution : 2.05 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

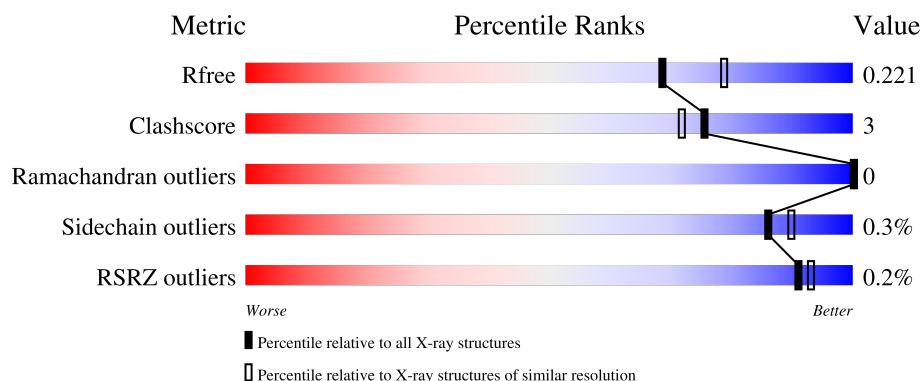
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*




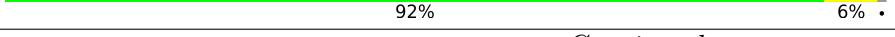
The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	430	
1	B	430	
1	C	430	
1	D	430	

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Mol	Chain	Length	Quality of chain
1	E	430	 90% 9% .
1	F	430	 91% 7% .
1	G	430	 89% 10% .
1	H	430	 90% 10% .
1	I	430	 91% 8% .
1	J	430	 91% 8% .
1	K	430	 89% 10% .
1	L	430	 93% 6% .

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 43282 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 Peptidase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	6	0
			3296	2064	583	636	13			
1	B	426	Total	C	N	O	S	0	4	0
			3276	2053	580	630	13			
1	C	426	Total	C	N	O	S	0	4	0
			3274	2050	580	631	13			
1	D	425	Total	C	N	O	S	0	3	0
			3260	2044	576	627	13			
1	E	426	Total	C	N	O	S	0	4	0
			3278	2053	578	634	13			
1	F	426	Total	C	N	O	S	0	4	0
			3277	2054	579	631	13			
1	G	426	Total	C	N	O	S	0	4	0
			3276	2053	581	629	13			
1	H	426	Total	C	N	O	S	0	2	0
			3259	2042	576	628	13			
1	I	425	Total	C	N	O	S	0	7	0
			3298	2065	586	634	13			
1	J	426	Total	C	N	O	S	0	2	0
			3261	2043	578	627	13			
1	K	426	Total	C	N	O	S	0	12	0
			3344	2093	595	643	13			
1	L	425	Total	C	N	O	S	0	6	0
			3275	2055	578	629	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A0A387CSU7
A	-1	ASN	-	expression tag	UNP A0A387CSU7
A	0	ALA	-	expression tag	UNP A0A387CSU7
B	-2	SER	-	expression tag	UNP A0A387CSU7
B	-1	ASN	-	expression tag	UNP A0A387CSU7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	expression tag	UNP A0A387CSU7
C	-2	SER	-	expression tag	UNP A0A387CSU7
C	-1	ASN	-	expression tag	UNP A0A387CSU7
C	0	ALA	-	expression tag	UNP A0A387CSU7
D	-2	SER	-	expression tag	UNP A0A387CSU7
D	-1	ASN	-	expression tag	UNP A0A387CSU7
D	0	ALA	-	expression tag	UNP A0A387CSU7
E	-2	SER	-	expression tag	UNP A0A387CSU7
E	-1	ASN	-	expression tag	UNP A0A387CSU7
E	0	ALA	-	expression tag	UNP A0A387CSU7
F	-2	SER	-	expression tag	UNP A0A387CSU7
F	-1	ASN	-	expression tag	UNP A0A387CSU7
F	0	ALA	-	expression tag	UNP A0A387CSU7
G	-2	SER	-	expression tag	UNP A0A387CSU7
G	-1	ASN	-	expression tag	UNP A0A387CSU7
G	0	ALA	-	expression tag	UNP A0A387CSU7
H	-2	SER	-	expression tag	UNP A0A387CSU7
H	-1	ASN	-	expression tag	UNP A0A387CSU7
H	0	ALA	-	expression tag	UNP A0A387CSU7
I	-2	SER	-	expression tag	UNP A0A387CSU7
I	-1	ASN	-	expression tag	UNP A0A387CSU7
I	0	ALA	-	expression tag	UNP A0A387CSU7
J	-2	SER	-	expression tag	UNP A0A387CSU7
J	-1	ASN	-	expression tag	UNP A0A387CSU7
J	0	ALA	-	expression tag	UNP A0A387CSU7
K	-2	SER	-	expression tag	UNP A0A387CSU7
K	-1	ASN	-	expression tag	UNP A0A387CSU7
K	0	ALA	-	expression tag	UNP A0A387CSU7
L	-2	SER	-	expression tag	UNP A0A387CSU7
L	-1	ASN	-	expression tag	UNP A0A387CSU7
L	0	ALA	-	expression tag	UNP A0A387CSU7

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0
2	G	2	Total 2	Zn 2	0	0
2	H	2	Total 2	Zn 2	0	0
2	I	2	Total 2	Zn 2	0	0
2	J	2	Total 2	Zn 2	0	0
2	K	2	Total 2	Zn 2	0	0
2	L	2	Total 2	Zn 2	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	D	1	Total 1	Ca 1	0	0
3	E	1	Total 1	Ca 1	0	0
3	F	1	Total 1	Ca 1	0	0
3	G	1	Total 1	Ca 1	0	0
3	H	1	Total 1	Ca 1	0	0
3	I	2	Total 2	Ca 2	0	0
3	J	1	Total 1	Ca 1	0	0
3	K	1	Total 1	Ca 1	0	0

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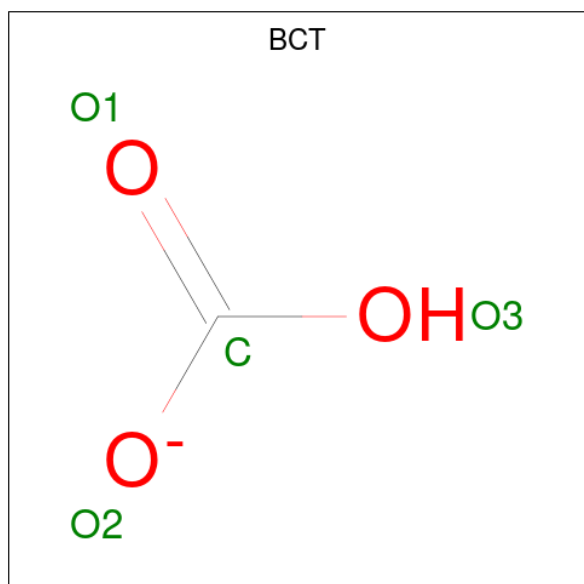
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total	Ca	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	2	Total	Cl	0	0
			2	2		
4	C	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	1
			2	2		
4	K	1	Total	Cl	0	1
			2	2		
4	L	2	Total	Cl	0	0
			2	2		

- Molecule 5 is BICARBONATE ION (CCD ID: BCT) (formula: CHO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	1	3		
5	C	1	Total	C	O	0	0
			4	1	3		
5	C	1	Total	C	O	0	0
			4	1	3		
5	D	1	Total	C	O	0	0
			4	1	3		
5	D	1	Total	C	O	0	0
			4	1	3		
5	D	1	Total	C	O	0	0
			4	1	3		
5	E	1	Total	C	O	0	0
			4	1	3		
5	F	1	Total	C	O	0	0
			4	1	3		
5	F	1	Total	C	O	0	0
			4	1	3		
5	G	1	Total	C	O	0	0
			4	1	3		
5	G	1	Total	C	O	0	0
			4	1	3		
5	H	1	Total	C	O	0	0
			4	1	3		
5	I	1	Total	C	O	0	0
			4	1	3		
5	I	1	Total	C	O	0	0
			4	1	3		
5	J	1	Total	C	O	0	0
			4	1	3		
5	K	1	Total	C	O	0	0
			4	1	3		
5	K	1	Total	C	O	0	0
			4	1	3		
5	L	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		

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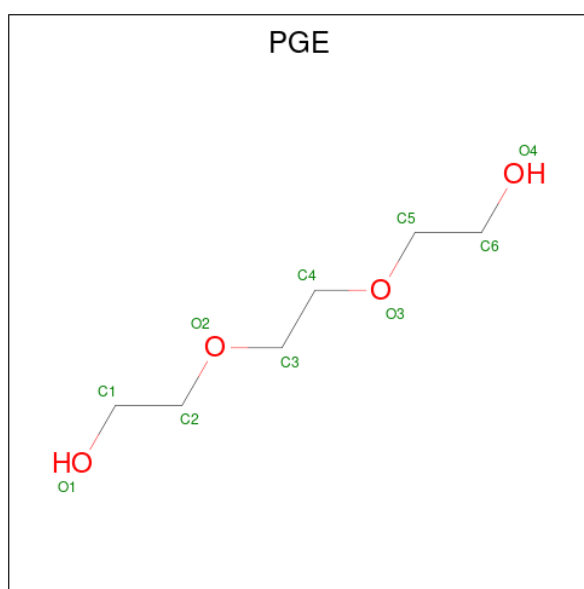
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	H	1	Total 4	C 2	O 2	0	0
6	H	1	Total 4	C 2	O 2	0	0
6	H	1	Total 4	C 2	O 2	0	0
6	H	1	Total 4	C 2	O 2	0	0
6	H	1	Total 4	C 2	O 2	0	0
6	H	1	Total 4	C 2	O 2	0	0
6	H	1	Total 4	C 2	O 2	0	0
6	I	1	Total 4	C 2	O 2	0	0
6	I	1	Total 4	C 2	O 2	0	0
6	I	1	Total 4	C 2	O 2	0	0
6	J	1	Total 4	C 2	O 2	0	0
6	J	1	Total 4	C 2	O 2	0	0
6	J	1	Total 4	C 2	O 2	0	0
6	J	1	Total 4	C 2	O 2	0	0
6	J	1	Total 4	C 2	O 2	0	0
6	K	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	K	1	Total	C	O	0	0
			4	2	2		
6	L	1	Total	C	O	0	0
			4	2	2		
6	L	1	Total	C	O	0	0
			4	2	2		
6	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			7	4	3		
8	D	1	Total	C	O	0	0
			7	4	3		
8	D	1	Total	C	O	0	0
			7	4	3		
8	E	1	Total	C	O	0	0
			7	4	3		
8	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	306	Total	O	0	15
			320	320		
9	B	252	Total	O	0	17
			268	268		
9	C	250	Total	O	0	12
			262	262		
9	D	281	Total	O	0	18
			298	298		
9	E	231	Total	O	0	13
			243	243		
9	F	282	Total	O	0	17
			299	299		
9	G	275	Total	O	0	18
			293	293		

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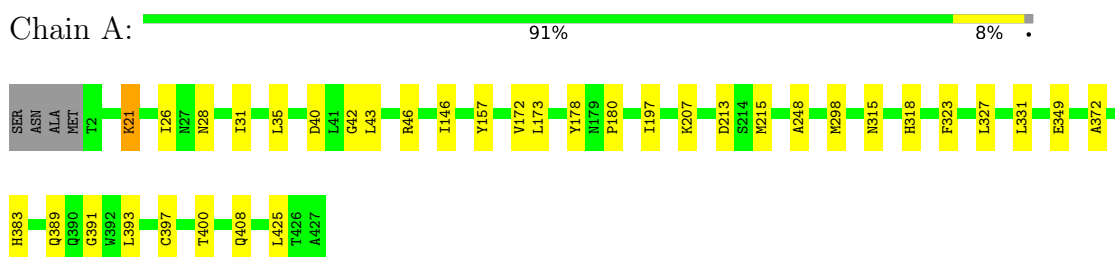
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	324	Total 334	O 334	0	10
9	I	319	Total 350	O 350	0	31
9	J	239	Total 250	O 250	0	11
9	K	338	Total 365	O 365	0	29
9	L	288	Total 301	O 301	0	13

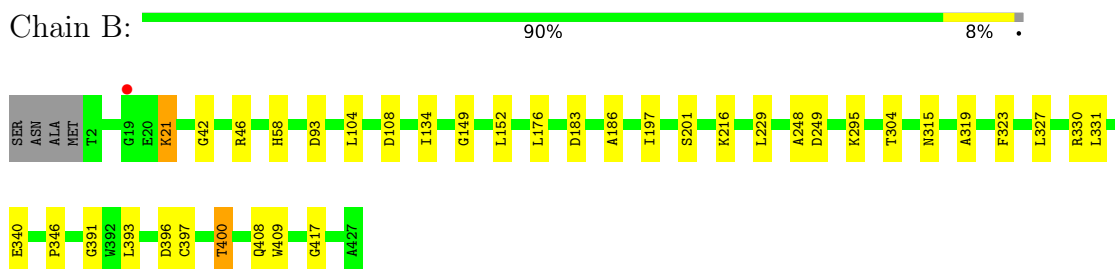
### 3 Residue-property plots [i](#)

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.

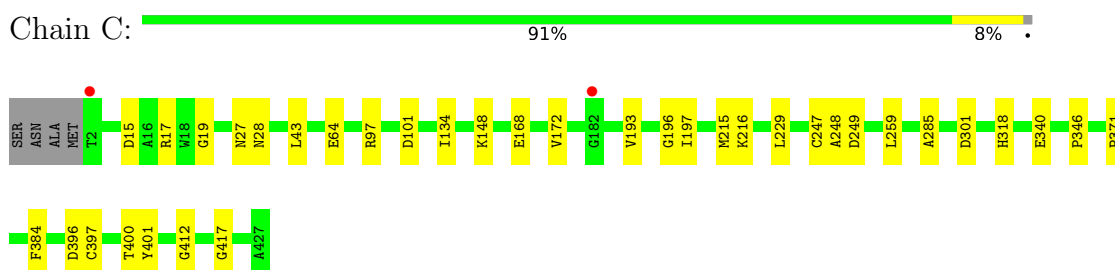
#### • Molecule 1: Peptidase B



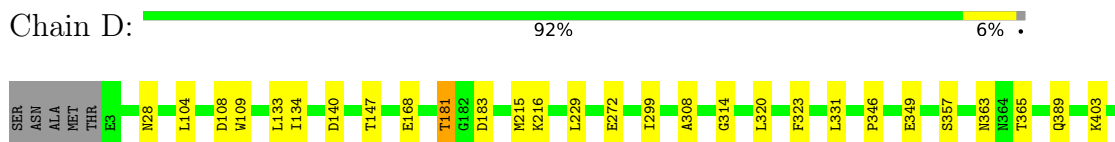
#### • Molecule 1: Peptidase B



#### • Molecule 1: Peptidase B


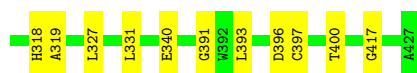


#### • Molecule 1: Peptidase B



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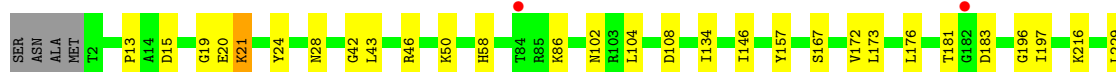
- Molecule 1: Peptidase B

Chain E:  90% 9%


- Molecule 1: Peptidase B

Chain F:  91% 7%


- Molecule 1: Peptidase B

Chain G:  89% 10%

- Molecule 1: Peptidase B

Chain H:  90% 10%

- Molecule 1: Peptidase B

Chain I:  91% 8%



• Molecule 1: Peptidase B

Chain J: 91% 8% .



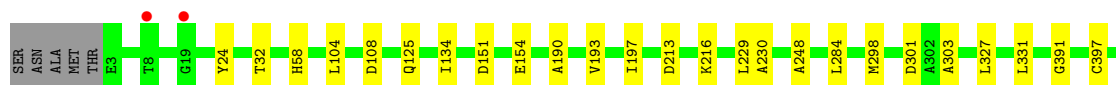
• Molecule 1: Peptidase B

Chain K: 89% 10% .



• Molecule 1: Peptidase B

Chain L: 93% 6% .





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.67Å 114.76Å 161.17Å 90.00° 92.02° 90.00°	Depositor
Resolution (Å)	29.88 – 2.05 29.88 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.88-2.05) 98.6 (29.88-2.05)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.172 , 0.215 0.180 , 0.221	Depositor DCC
$R_{free}$ test set	16698 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	43282	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CL, PEG, BCT, ZN, EDO, PGE

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	1.03	0/3359	1.28	4/4554 (0.1%)
1	B	1.03	1/3339 (0.0%)	1.30	8/4526 (0.2%)
1	C	1.01	0/3337	1.29	7/4523 (0.2%)
1	D	1.01	0/3323	1.30	5/4505 (0.1%)
1	E	1.02	0/3341	1.31	1/4529 (0.0%)
1	F	1.03	0/3340	1.30	3/4528 (0.1%)
1	G	1.03	0/3339	1.29	6/4527 (0.1%)
1	H	1.05	0/3322	1.30	8/4504 (0.2%)
1	I	1.02	0/3361	1.27	4/4555 (0.1%)
1	J	1.02	0/3324	1.30	8/4506 (0.2%)
1	K	1.03	0/3416	1.30	5/4628 (0.1%)
1	L	1.02	0/3347	1.30	2/4536 (0.0%)
All	All	1.02	1/40148 (0.0%)	1.29	61/54421 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	295	LYS	N-CA	5.31	1.50	1.46

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	19	GLY	CA-C-O	-6.77	117.82	122.22
1	C	19	GLY	CA-C-O	-6.76	117.43	122.37
1	G	216	LYS	N-CA-C	-6.70	105.08	113.18
1	K	19	GLY	CA-C-O	-6.46	117.80	122.45
1	K	249	ASP	CA-CB-CG	6.43	119.03	112.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3296	0	3228	22	0
1	B	3276	0	3216	16	0
1	C	3274	0	3210	20	0
1	D	3260	0	3198	16	0
1	E	3278	0	3207	27	0
1	F	3277	0	3214	19	0
1	G	3276	0	3218	24	0
1	H	3259	0	3195	19	0
1	I	3298	0	3233	19	0
1	J	3261	0	3200	18	0
1	K	3344	0	3284	27	0
1	L	3275	0	3224	15	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	2	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	8	0	0	0	0
5	D	12	0	0	0	0
5	E	4	0	0	0	0
5	F	8	0	0	0	0
5	G	8	0	0	0	0
5	H	4	0	0	0	0
5	I	8	0	0	0	0
5	J	4	0	0	0	0
5	K	8	0	0	0	0
5	L	4	0	0	0	0
6	A	12	0	18	0	0
6	B	8	0	12	0	0
6	C	12	0	18	0	0
6	D	12	0	18	0	0
6	E	12	0	18	0	0
6	F	12	0	18	0	0
6	G	12	0	18	0	0
6	H	24	0	36	1	0
6	I	12	0	18	0	0
6	J	20	0	30	0	0
6	K	8	0	12	0	0
6	L	12	0	18	0	0
7	A	10	0	14	0	0
8	C	7	0	10	0	0
8	D	14	0	20	2	0
8	E	7	0	10	1	0
8	L	7	0	10	1	0
9	A	320	0	0	0	0
9	B	268	0	0	1	0
9	C	262	0	0	2	0
9	D	298	0	0	1	0
9	E	243	0	0	2	0
9	F	299	0	0	0	0
9	G	293	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	H	334	0	0	1	0
9	I	350	0	0	1	0
9	J	250	0	0	0	0
9	K	365	0	0	3	0
9	L	301	0	0	0	0
All	All	43282	0	38925	232	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 3.

The worst 5 of 232 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:B:21:LYS:H	1:B:21:LYS:HD3	1.49	0.76
1:A:21:LYS:H	1:A:21:LYS:HD3	1.54	0.72
1:C:15:ASP:OD2	1:C:17:ARG:HD3	1.91	0.71
1:E:307:GLY:H	8:E:509:PEG:H21	1.56	0.70
1:G:42:GLY:O	1:G:46[A]:ARG:HG3	1.92	0.68

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	430/430 (100%)	419 (97%)	11 (3%)	0	100	100
1	B	428/430 (100%)	419 (98%)	9 (2%)	0	100	100
1	C	428/430 (100%)	418 (98%)	10 (2%)	0	100	100
1	D	426/430 (99%)	412 (97%)	14 (3%)	0	100	100
1	E	428/430 (100%)	415 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	428/430 (100%)	419 (98%)	9 (2%)	0	100	100
1	G	428/430 (100%)	415 (97%)	13 (3%)	0	100	100
1	H	426/430 (99%)	417 (98%)	9 (2%)	0	100	100
1	I	430/430 (100%)	420 (98%)	10 (2%)	0	100	100
1	J	426/430 (99%)	413 (97%)	13 (3%)	0	100	100
1	K	436/430 (101%)	423 (97%)	13 (3%)	0	100	100
1	L	429/430 (100%)	416 (97%)	13 (3%)	0	100	100
All	All	5143/5160 (100%)	5006 (97%)	137 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	335/332 (101%)	334 (100%)	1 (0%)	86	90
1	B	333/332 (100%)	330 (99%)	3 (1%)	70	75
1	C	333/332 (100%)	333 (100%)	0	100	100
1	D	331/332 (100%)	330 (100%)	1 (0%)	86	90
1	E	333/332 (100%)	333 (100%)	0	100	100
1	F	333/332 (100%)	332 (100%)	1 (0%)	86	90
1	G	333/332 (100%)	332 (100%)	1 (0%)	86	90
1	H	331/332 (100%)	331 (100%)	0	100	100
1	I	335/332 (101%)	333 (99%)	2 (1%)	78	83
1	J	331/332 (100%)	331 (100%)	0	100	100
1	K	341/332 (103%)	340 (100%)	1 (0%)	86	90
1	L	334/332 (101%)	334 (100%)	0	100	100
All	All	4003/3984 (100%)	3993 (100%)	10 (0%)	86	91

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	183	ASP
1	I	365	THR
1	K	86	LYS
1	B	400	THR
1	D	181	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	128	GLN
1	K	98	GLN
1	K	60	GLN
1	K	102	ASN
1	D	179	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 112 ligands modelled in this entry, 48 are monoatomic - leaving 64 for Mogul analysis.

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
8	PEG	D	511	-	6,6,6	0.18	0	5,5,5	0.09	0
5	BCT	F	505	-	3,3,3	0.94	0	2,3,3	1.50	0
6	EDO	G	508	-	3,3,3	0.09	0	2,2,2	0.09	0
5	BCT	E	505	-	3,3,3	1.53	0	2,3,3	0.78	0
6	EDO	H	508	-	3,3,3	0.06	0	2,2,2	0.17	0
6	EDO	L	510	-	3,3,3	0.10	0	2,2,2	0.07	0
5	BCT	A	505	-	3,3,3	0.99	0	2,3,3	1.47	0
5	BCT	D	506	-	3,3,3	0.91	0	2,3,3	1.71	1 (50%)
6	EDO	B	507	-	3,3,3	0.14	0	2,2,2	0.29	0
8	PEG	C	509	-	6,6,6	0.16	0	5,5,5	0.09	0
5	BCT	C	506	-	3,3,3	0.99	0	2,3,3	1.65	1 (50%)
6	EDO	E	506	-	3,3,3	0.08	0	2,2,2	0.07	0
6	EDO	J	507	-	3,3,3	0.12	0	2,2,2	0.23	0
5	BCT	L	506	-	3,3,3	1.48	0	2,3,3	0.80	0
6	EDO	C	507	-	3,3,3	0.05	0	2,2,2	0.15	0
6	EDO	K	507	-	3,3,3	0.06	0	2,2,2	0.18	0
6	EDO	H	506	-	3,3,3	0.11	0	2,2,2	0.25	0
5	BCT	B	505	-	3,3,3	1.44	0	2,3,3	0.89	0
6	EDO	F	509	-	3,3,3	0.08	0	2,2,2	0.09	0
6	EDO	D	507	-	3,3,3	0.07	0	2,2,2	0.07	0
6	EDO	A	508	-	3,3,3	0.09	0	2,2,2	0.03	0
5	BCT	C	505	-	3,3,3	1.01	0	2,3,3	1.56	1 (50%)
5	BCT	H	504	-	3,3,3	1.40	0	2,3,3	0.98	0
8	PEG	L	509	-	6,6,6	0.18	0	5,5,5	0.13	0
6	EDO	F	507	-	3,3,3	0.14	0	2,2,2	0.16	0
5	BCT	D	504	-	3,3,3	0.91	0	2,3,3	1.70	1 (50%)
5	BCT	J	504	-	3,3,3	0.96	0	2,3,3	1.47	0
6	EDO	H	509	-	3,3,3	0.08	0	2,2,2	0.15	0
6	EDO	C	508	-	3,3,3	0.06	0	2,2,2	0.12	0
5	BCT	G	505	-	3,3,3	1.47	0	2,3,3	0.85	0
6	EDO	H	505	-	3,3,3	0.12	0	2,2,2	0.17	0
6	EDO	H	510	-	3,3,3	0.08	0	2,2,2	0.10	0
6	EDO	J	509	-	3,3,3	0.07	0	2,2,2	0.06	0
6	EDO	A	506	-	3,3,3	0.08	0	2,2,2	0.21	0
6	EDO	B	506	-	3,3,3	0.08	0	2,2,2	0.16	0
5	BCT	D	505	-	3,3,3	0.88	0	2,3,3	1.73	1 (50%)
6	EDO	L	508	-	3,3,3	0.11	0	2,2,2	0.19	0
5	BCT	K	506	-	3,3,3	1.42	0	2,3,3	0.92	0
6	EDO	G	506	-	3,3,3	0.06	0	2,2,2	0.14	0
6	EDO	K	508	-	3,3,3	0.10	0	2,2,2	0.06	0
6	EDO	J	506	-	3,3,3	0.07	0	2,2,2	0.18	0
6	EDO	J	508	-	3,3,3	0.06	0	2,2,2	0.15	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BCT	K	505	-	3,3,3	1.45	0	2,3,3	0.86	0
6	EDO	F	508	-	3,3,3	0.06	0	2,2,2	0.15	0
7	PGE	A	509	-	9,9,9	0.24	0	8,8,8	0.12	0
6	EDO	I	508	-	3,3,3	0.10	0	2,2,2	0.11	0
5	BCT	I	505	-	3,3,3	1.06	0	2,3,3	1.65	1 (50%)
8	PEG	E	509	-	6,6,6	0.24	0	5,5,5	0.12	0
6	EDO	E	507	-	3,3,3	0.06	0	2,2,2	0.16	0
6	EDO	J	505	-	3,3,3	0.09	0	2,2,2	0.10	0
6	EDO	A	507	-	3,3,3	0.13	0	2,2,2	0.35	0
5	BCT	I	506	-	3,3,3	1.32	0	2,3,3	1.07	0
6	EDO	H	507	-	3,3,3	0.11	0	2,2,2	0.11	0
5	BCT	F	506	-	3,3,3	1.48	0	2,3,3	0.87	0
6	EDO	G	507	-	3,3,3	0.13	0	2,2,2	0.25	0
6	EDO	C	510	-	3,3,3	0.12	0	2,2,2	0.08	0
6	EDO	I	507	-	3,3,3	0.12	0	2,2,2	0.22	0
8	PEG	D	510	-	6,6,6	0.11	0	5,5,5	0.09	0
6	EDO	D	508	-	3,3,3	0.09	0	2,2,2	0.15	0
5	BCT	G	504	-	3,3,3	1.08	0	2,3,3	1.57	1 (50%)
6	EDO	D	509	-	3,3,3	0.09	0	2,2,2	0.07	0
6	EDO	L	507	-	3,3,3	0.10	0	2,2,2	0.23	0
6	EDO	E	508	-	3,3,3	0.07	0	2,2,2	0.17	0
6	EDO	I	509	-	3,3,3	0.09	0	2,2,2	0.16	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
8	PEG	D	511	-	-	2/4/4/4	-
6	EDO	G	508	-	-	1/1/1/1	-
6	EDO	H	508	-	-	0/1/1/1	-
6	EDO	L	510	-	-	1/1/1/1	-
6	EDO	B	507	-	-	1/1/1/1	-
8	PEG	C	509	-	-	2/4/4/4	-
6	EDO	E	506	-	-	0/1/1/1	-
6	EDO	J	507	-	-	1/1/1/1	-
6	EDO	C	507	-	-	0/1/1/1	-
6	EDO	K	507	-	-	0/1/1/1	-
6	EDO	H	506	-	-	1/1/1/1	-
6	EDO	F	509	-	-	0/1/1/1	-
6	EDO	D	507	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	508	-	-	1/1/1/1	-
8	PEG	L	509	-	-	2/4/4/4	-
6	EDO	F	507	-	-	0/1/1/1	-
6	EDO	H	509	-	-	0/1/1/1	-
6	EDO	C	508	-	-	0/1/1/1	-
6	EDO	H	505	-	-	1/1/1/1	-
6	EDO	H	510	-	-	0/1/1/1	-
6	EDO	J	509	-	-	1/1/1/1	-
6	EDO	A	506	-	-	0/1/1/1	-
6	EDO	B	506	-	-	0/1/1/1	-
6	EDO	L	508	-	-	0/1/1/1	-
6	EDO	G	506	-	-	0/1/1/1	-
6	EDO	K	508	-	-	1/1/1/1	-
6	EDO	J	506	-	-	1/1/1/1	-
6	EDO	J	508	-	-	1/1/1/1	-
6	EDO	F	508	-	-	0/1/1/1	-
7	PGE	A	509	-	-	4/7/7/7	-
6	EDO	I	508	-	-	0/1/1/1	-
8	PEG	E	509	-	-	1/4/4/4	-
6	EDO	E	507	-	-	1/1/1/1	-
6	EDO	J	505	-	-	0/1/1/1	-
6	EDO	A	507	-	-	1/1/1/1	-
6	EDO	H	507	-	-	0/1/1/1	-
6	EDO	G	507	-	-	1/1/1/1	-
6	EDO	C	510	-	-	1/1/1/1	-
6	EDO	I	507	-	-	1/1/1/1	-
8	PEG	D	510	-	-	3/4/4/4	-
6	EDO	D	508	-	-	0/1/1/1	-
6	EDO	D	509	-	-	0/1/1/1	-
6	EDO	L	507	-	-	1/1/1/1	-
6	EDO	E	508	-	-	1/1/1/1	-
6	EDO	I	509	-	-	0/1/1/1	-

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	506	BCT	O2-C-O1	2.22	125.36	119.68
5	D	505	BCT	O2-C-O1	2.21	125.33	119.68
5	D	504	BCT	O2-C-O1	2.21	125.32	119.68
5	C	506	BCT	O2-C-O1	2.16	125.20	119.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	505	BCT	O2-C-O1	2.16	125.20	119.68

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	509	PEG	O2-C3-C4-O4
7	A	509	PGE	O3-C5-C6-O4
6	C	510	EDO	O1-C1-C2-O2
6	G	507	EDO	O1-C1-C2-O2
6	G	508	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	511	PEG	1	0
6	H	506	EDO	1	0
8	L	509	PEG	1	0
8	E	509	PEG	1	0
8	D	510	PEG	1	0

## 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<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	426/430 (99%)	-0.31	0 100 100	16, 33, 55, 82	6 (1%)
1	B	426/430 (99%)	-0.19	1 (0%) 91 93	20, 38, 69, 104	4 (0%)
1	C	426/430 (99%)	-0.12	2 (0%) 87 89	19, 41, 71, 98	4 (0%)
1	D	425/430 (98%)	-0.23	0 100 100	19, 37, 61, 80	3 (0%)
1	E	426/430 (99%)	-0.10	0 100 100	19, 41, 71, 103	4 (0%)
1	F	426/430 (99%)	-0.21	0 100 100	16, 34, 64, 91	4 (0%)
1	G	426/430 (99%)	-0.18	2 (0%) 87 89	22, 38, 69, 88	4 (0%)
1	H	426/430 (99%)	-0.25	1 (0%) 91 93	19, 34, 57, 81	2 (0%)
1	I	425/430 (98%)	-0.36	0 100 100	14, 32, 46, 76	7 (1%)
1	J	426/430 (99%)	-0.13	0 100 100	23, 42, 68, 97	2 (0%)
1	K	426/430 (99%)	-0.32	0 100 100	16, 32, 49, 93	12 (2%)
1	L	425/430 (98%)	-0.22	2 (0%) 87 89	19, 38, 55, 99	6 (1%)
All	All	5109/5160 (99%)	-0.22	8 (0%) 91 93	14, 36, 65, 104	58 (1%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	2	THR	2.6
1	L	8	THR	2.1
1	B	19	GLY	2.1
1	G	182	GLY	2.1
1	L	19	GLY	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	BCT	C	506	4/4	0.64	0.10	77,81,83,85	0
8	PEG	L	509	7/7	0.74	0.16	71,74,80,81	0
8	PEG	C	509	7/7	0.77	0.13	62,73,79,82	0
6	EDO	H	506	4/4	0.78	0.20	57,62,63,63	0
6	EDO	G	507	4/4	0.80	0.18	65,65,67,68	0
5	BCT	I	505	4/4	0.80	0.22	31,31,32,34	4
8	PEG	D	511	7/7	0.81	0.16	61,64,69,70	0
7	PGE	A	509	10/10	0.82	0.18	43,64,72,78	0
5	BCT	D	505	4/4	0.82	0.18	55,66,67,69	0
4	CL	A	504	1/1	0.83	0.13	58,58,58,58	0
8	PEG	E	509	7/7	0.83	0.15	49,59,62,67	0
6	EDO	H	509	4/4	0.83	0.14	63,65,66,67	0
6	EDO	B	507	4/4	0.84	0.15	49,57,57,59	0
6	EDO	J	508	4/4	0.85	0.12	58,61,69,73	0
6	EDO	D	509	4/4	0.85	0.12	48,51,52,56	0
4	CL	B	504	1/1	0.85	0.19	47,47,47,47	1
6	EDO	J	507	4/4	0.86	0.12	46,51,55,55	0
6	EDO	G	508	4/4	0.87	0.12	58,59,61,61	0
4	CL	E	504	1/1	0.87	0.12	67,67,67,67	0
8	PEG	D	510	7/7	0.87	0.12	56,57,60,62	0
4	CL	K	504[A]	1/1	0.87	0.10	51,51,51,51	1
6	EDO	E	506	4/4	0.87	0.15	52,55,60,60	0
4	CL	K	504[B]	1/1	0.87	0.10	43,43,43,43	1
6	EDO	C	507	4/4	0.88	0.12	50,53,54,55	0
6	EDO	D	508	4/4	0.88	0.13	47,51,52,53	0
6	EDO	A	507	4/4	0.88	0.15	41,44,46,49	0
6	EDO	H	508	4/4	0.88	0.10	49,60,61,68	0
5	BCT	F	506	4/4	0.88	0.12	52,61,63,70	0
6	EDO	J	506	4/4	0.88	0.14	52,56,57,57	0
6	EDO	F	509	4/4	0.88	0.11	54,56,58,62	0
6	EDO	C	508	4/4	0.90	0.10	54,60,60,62	0
6	EDO	L	510	4/4	0.90	0.12	51,51,52,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BCT	K	506	4/4	0.90	0.13	45,62,62,67	0
4	CL	L	505	1/1	0.90	0.10	67,67,67,67	0
6	EDO	J	509	4/4	0.91	0.11	59,59,63,63	0
4	CL	B	508	1/1	0.91	0.13	78,78,78,78	0
5	BCT	D	506	4/4	0.91	0.12	42,46,50,58	0
6	EDO	J	505	4/4	0.91	0.12	46,47,47,48	0
6	EDO	A	508	4/4	0.92	0.11	42,45,47,49	0
6	EDO	C	510	4/4	0.92	0.08	47,50,53,56	0
6	EDO	D	507	4/4	0.92	0.10	39,42,43,44	0
6	EDO	H	505	4/4	0.92	0.10	39,41,41,42	0
6	EDO	E	508	4/4	0.92	0.10	55,57,59,60	0
6	EDO	F	507	4/4	0.92	0.11	48,50,50,52	0
6	EDO	L	508	4/4	0.92	0.11	48,49,50,52	0
6	EDO	G	506	4/4	0.93	0.10	47,51,51,51	0
6	EDO	K	507	4/4	0.93	0.09	41,45,45,49	0
6	EDO	K	508	4/4	0.93	0.10	46,47,48,49	0
5	BCT	G	505	4/4	0.93	0.10	52,65,71,75	0
6	EDO	I	507	4/4	0.93	0.09	36,39,39,41	0
6	EDO	I	508	4/4	0.93	0.07	43,44,44,46	0
6	EDO	I	509	4/4	0.93	0.10	46,48,49,55	0
6	EDO	A	506	4/4	0.93	0.09	41,43,45,45	0
6	EDO	F	508	4/4	0.93	0.10	49,51,52,52	0
6	EDO	E	507	4/4	0.93	0.10	44,47,48,50	0
6	EDO	H	507	4/4	0.93	0.11	40,44,49,54	0
6	EDO	B	506	4/4	0.94	0.09	46,46,48,49	0
5	BCT	L	506	4/4	0.94	0.09	31,33,33,42	0
5	BCT	G	504	4/4	0.94	0.08	32,32,33,42	0
5	BCT	I	506	4/4	0.94	0.10	28,29,30,37	0
5	BCT	E	505	4/4	0.94	0.07	26,30,30,38	0
4	CL	C	504	1/1	0.95	0.09	60,60,60,60	0
6	EDO	H	510	4/4	0.95	0.07	42,43,44,48	0
5	BCT	H	504	4/4	0.95	0.10	25,27,31,36	0
5	BCT	A	505	4/4	0.95	0.08	28,31,32,37	0
4	CL	F	504[A]	1/1	0.96	0.14	43,43,43,43	1
4	CL	F	504[B]	1/1	0.96	0.14	39,39,39,39	1
4	CL	L	504	1/1	0.96	0.06	54,54,54,54	0
6	EDO	L	507	4/4	0.96	0.07	43,44,46,47	0
5	BCT	J	504	4/4	0.96	0.08	34,36,39,44	0
5	BCT	K	505	4/4	0.96	0.08	26,26,34,38	0
5	BCT	F	505	4/4	0.97	0.06	27,29,34,42	0
5	BCT	B	505	4/4	0.97	0.07	30,30,34,35	0
5	BCT	C	505	4/4	0.97	0.08	27,29,29,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	H	503	1/1	0.97	0.07	39,39,39,39	0
3	CA	I	504	1/1	0.98	0.08	45,45,45,45	0
3	CA	J	503	1/1	0.98	0.07	42,42,42,42	0
3	CA	K	503	1/1	0.98	0.09	37,37,37,37	0
3	CA	A	503	1/1	0.98	0.05	33,33,33,33	0
5	BCT	D	504	4/4	0.98	0.08	26,27,31,36	0
3	CA	D	503	1/1	0.98	0.07	36,36,36,36	0
3	CA	E	503	1/1	0.98	0.09	41,41,41,41	0
2	ZN	G	501	1/1	0.98	0.03	30,30,30,30	0
2	ZN	D	501	1/1	0.99	0.03	28,28,28,28	0
2	ZN	D	502	1/1	0.99	0.02	28,28,28,28	0
3	CA	L	503	1/1	0.99	0.08	39,39,39,39	0
2	ZN	E	501	1/1	0.99	0.03	32,32,32,32	0
2	ZN	F	501	1/1	0.99	0.02	29,29,29,29	0
2	ZN	A	501	1/1	0.99	0.02	27,27,27,27	0
2	ZN	G	502	1/1	0.99	0.04	32,32,32,32	0
2	ZN	H	501	1/1	0.99	0.03	30,30,30,30	0
2	ZN	H	502	1/1	0.99	0.03	27,27,27,27	0
2	ZN	I	501	1/1	0.99	0.03	32,32,32,32	0
2	ZN	I	502	1/1	0.99	0.03	29,29,29,29	0
2	ZN	J	501	1/1	0.99	0.03	32,32,32,32	0
2	ZN	J	502	1/1	0.99	0.03	31,31,31,31	0
2	ZN	K	501	1/1	0.99	0.03	28,28,28,28	0
2	ZN	L	501	1/1	0.99	0.02	35,35,35,35	0
2	ZN	L	502	1/1	0.99	0.03	33,33,33,33	0
2	ZN	A	502	1/1	0.99	0.02	27,27,27,27	0
3	CA	B	503	1/1	0.99	0.07	35,35,35,35	0
3	CA	C	503	1/1	0.99	0.06	40,40,40,40	0
2	ZN	B	501	1/1	0.99	0.03	28,28,28,28	0
2	ZN	B	502	1/1	0.99	0.02	28,28,28,28	0
3	CA	F	503	1/1	0.99	0.05	36,36,36,36	0
3	CA	G	503	1/1	0.99	0.07	35,35,35,35	0
2	ZN	C	501	1/1	0.99	0.03	31,31,31,31	0
3	CA	I	503	1/1	0.99	0.10	31,31,31,31	0
2	ZN	C	502	1/1	0.99	0.03	29,29,29,29	0
2	ZN	F	502	1/1	1.00	0.02	28,28,28,28	0
2	ZN	E	502	1/1	1.00	0.02	30,30,30,30	0
2	ZN	K	502	1/1	1.00	0.02	28,28,28,28	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.