



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2021 – 12:18 PM EST

PDB ID : 6OAD
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
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)	:	2.16

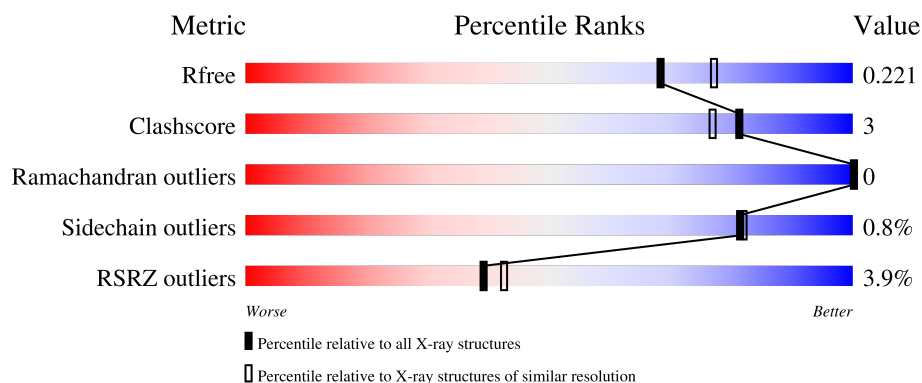
1 Overall quality at a glance

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.



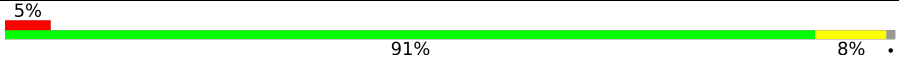
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 ≥ 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	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	B	430	<div> <div>4%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	C	430	<div> <div>6%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
1	D	430	<div> <div>4%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>
1	E	430	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	430	
1	G	430	
1	H	430	
1	I	430	
1	J	430	
1	K	430	
1	L	430	

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
6	EDO	H	506	-	-	-	X

2 Entry composition [i](#)

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 (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	K	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	H	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	I	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	A	2	Total 2	Zn 2	0	0
2	L	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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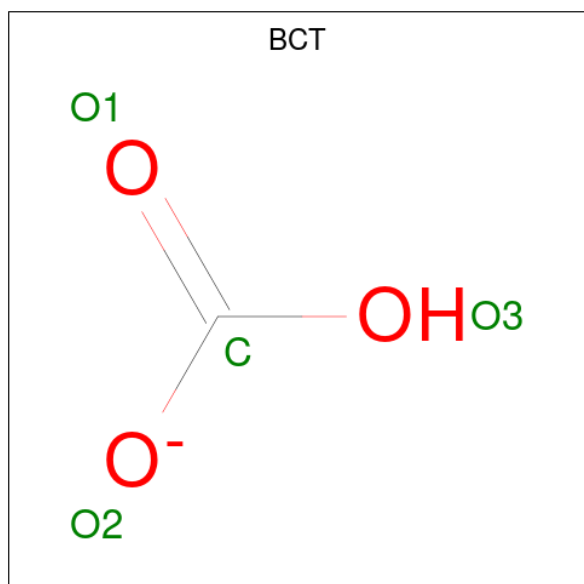
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total	Ca	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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 (three-letter code: EDO) (formula: C₂H₆O₂).



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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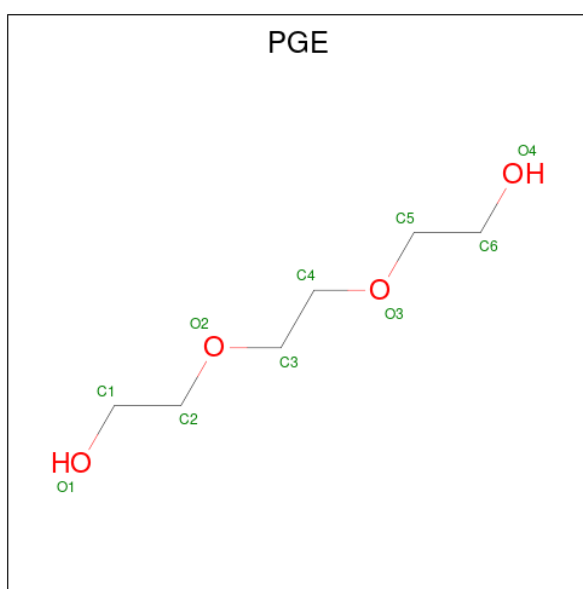
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	F	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	G	1	Total 4	C 2	O 2	0	0
6	H	1	Total 4	C 2	O 2	0	0
6	H	1	Total 4	C 2	O 2	0	0
6	H	1	Total 4	C 2	O 2	0	0
6	H	1	Total 4	C 2	O 2	0	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 (three-letter code: 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 (three-letter code: 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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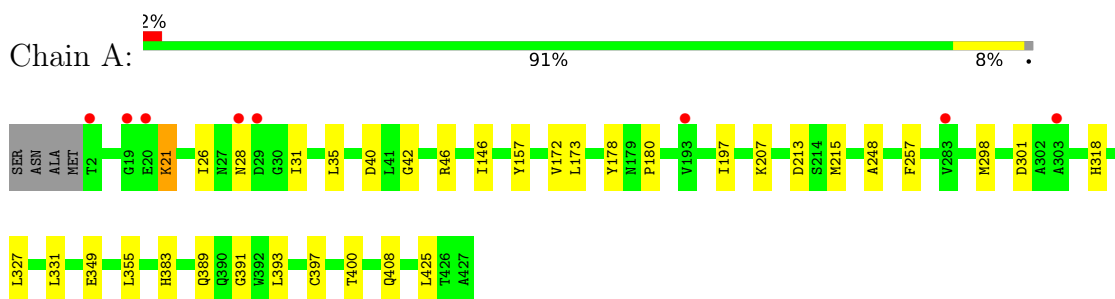
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	324	Total 334	O 334	0	10
9	I	319	Total 350	O 350	0	31
9	J	239	Total 250	O 250	0	11
9	K	338	Total 365	O 365	0	29
9	L	288	Total 301	O 301	0	13

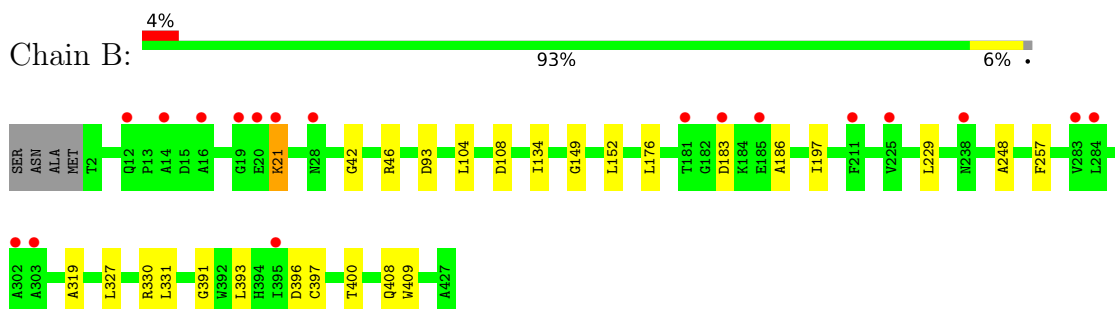
3 Residue-property plots [i](#)

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.

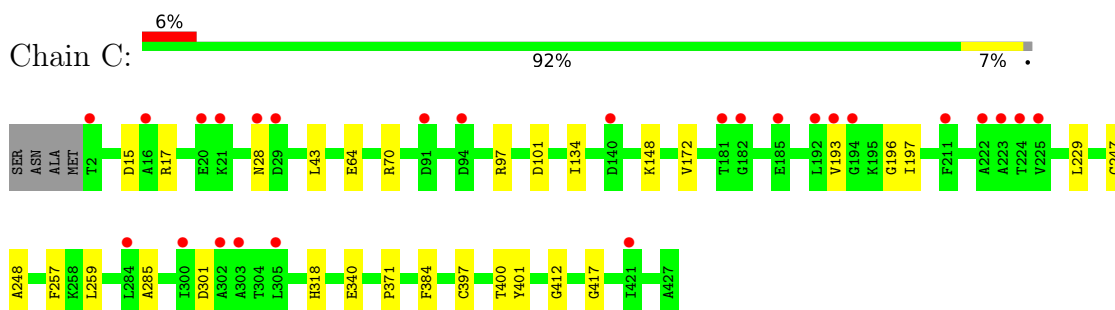
• Molecule 1: Peptidase B



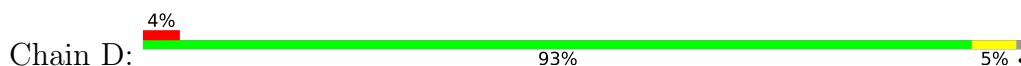
• Molecule 1: Peptidase B

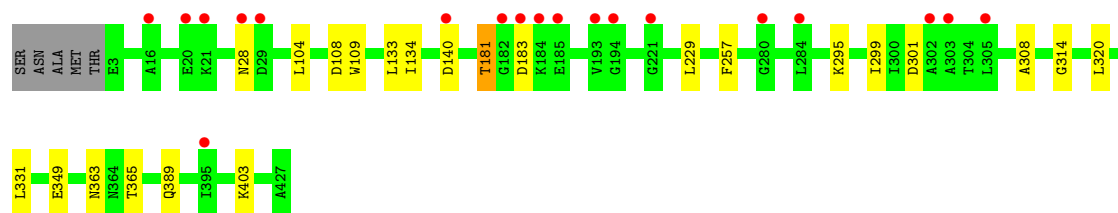


• Molecule 1: Peptidase B

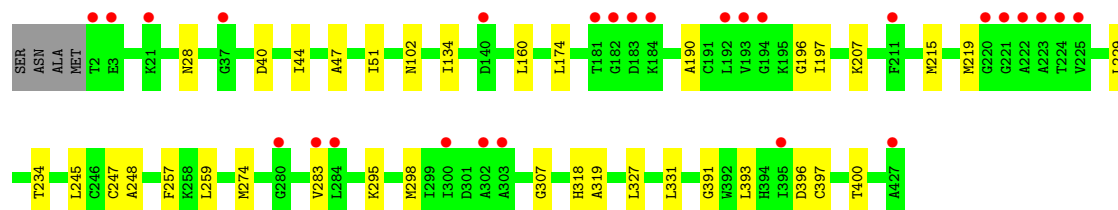
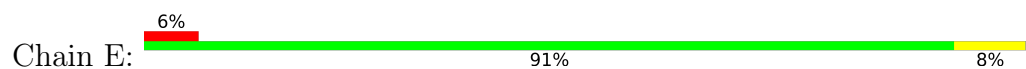


• Molecule 1: Peptidase B

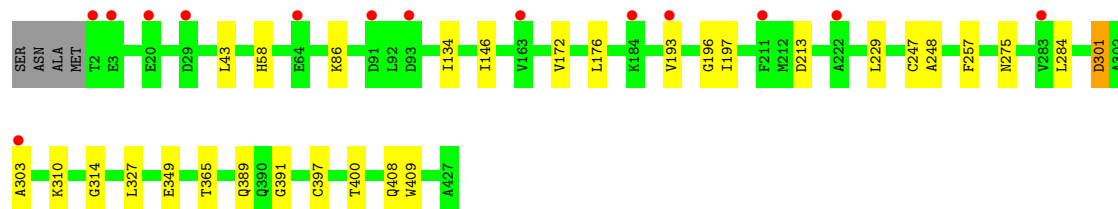
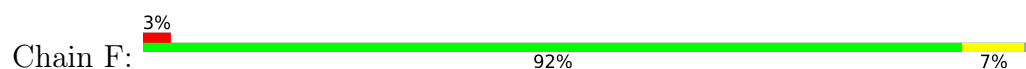




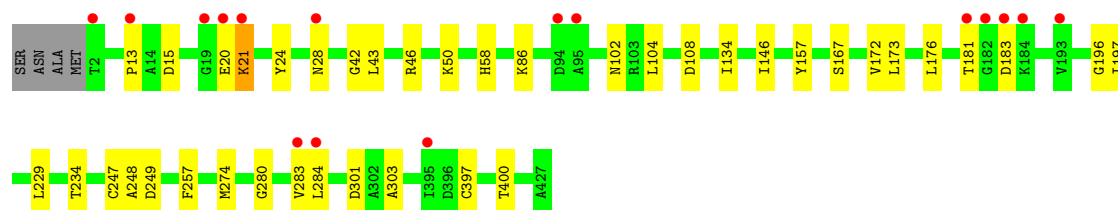
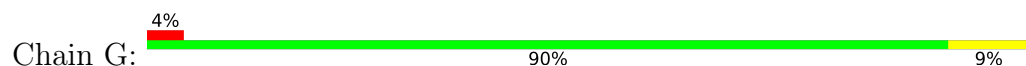
• Molecule 1: Peptidase B



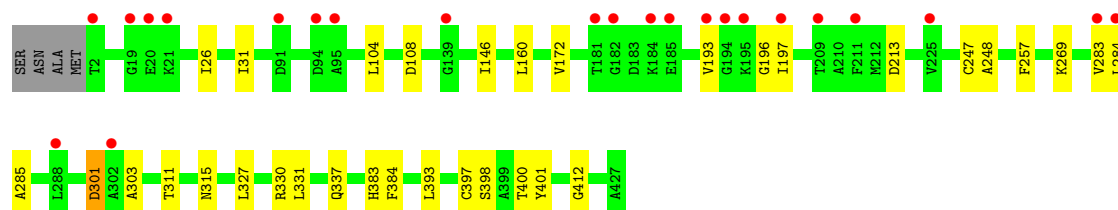
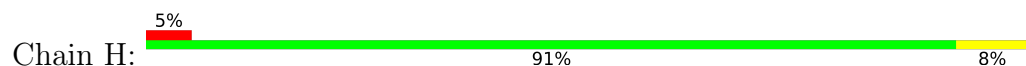
• Molecule 1: Peptidase B



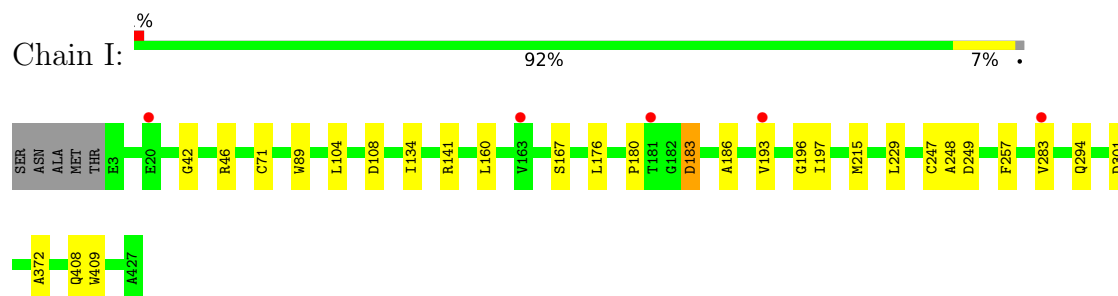
• Molecule 1: Peptidase B



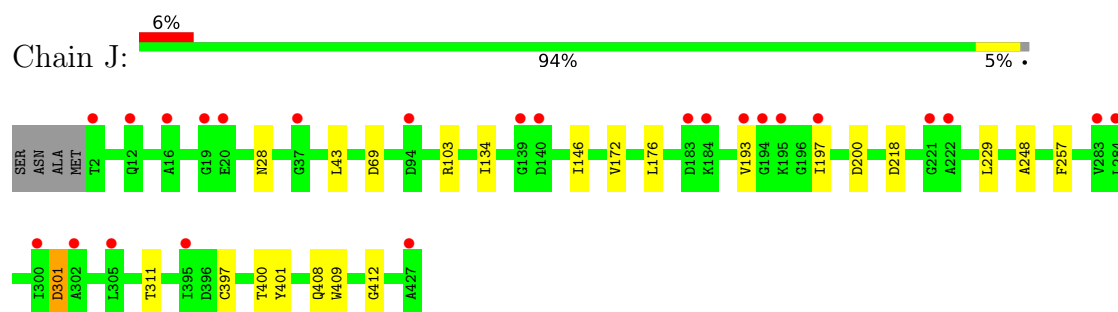
• Molecule 1: Peptidase B



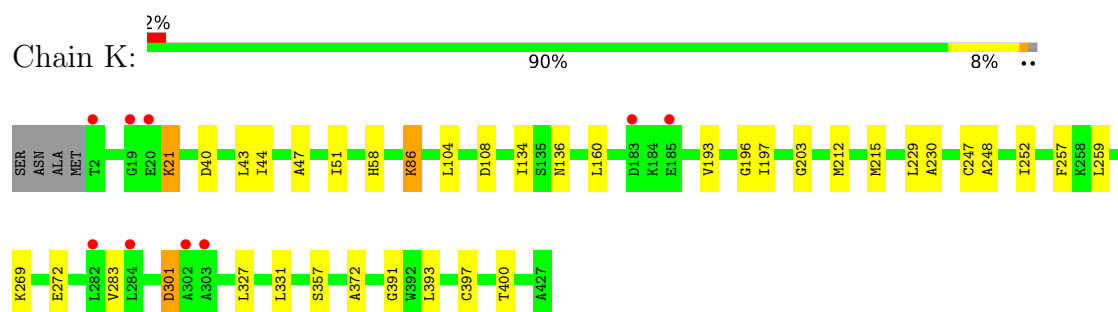
- Molecule 1: Peptidase B



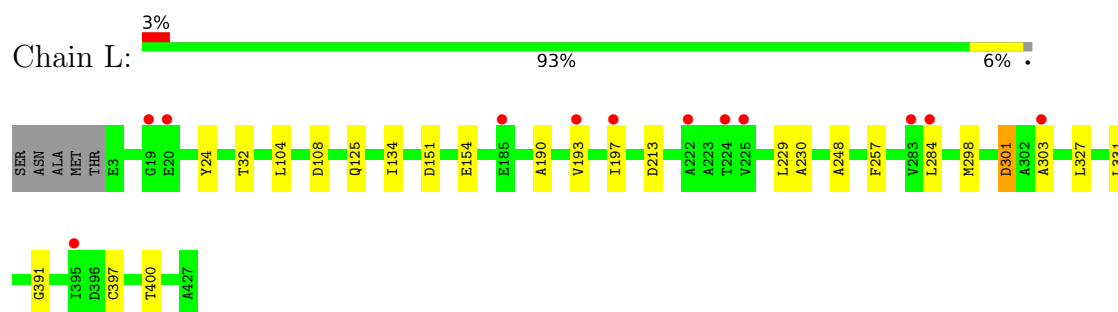
- Molecule 1: Peptidase B



- Molecule 1: Peptidase B



- Molecule 1: Peptidase B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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) 98.7 (29.88-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: ZN, PGE, CL, CA, EDO, BCT, PEG

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	0.69	0/3359	0.81	0/4554
1	B	0.68	0/3339	0.80	0/4526
1	C	0.67	0/3337	0.80	0/4523
1	D	0.68	0/3323	0.81	0/4505
1	E	0.67	0/3341	0.80	0/4529
1	F	0.69	0/3340	0.81	0/4528
1	G	0.68	0/3339	0.80	0/4527
1	H	0.70	0/3322	0.81	0/4504
1	I	0.69	0/3361	0.82	0/4555
1	J	0.67	0/3324	0.79	0/4506
1	K	0.69	0/3416	0.84	0/4628
1	L	0.68	0/3347	0.80	0/4536
All	All	0.68	0/40148	0.81	0/54421

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3296	0	3228	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3276	0	3216	15	0
1	C	3274	0	3210	19	0
1	D	3260	0	3198	13	0
1	E	3278	0	3207	21	0
1	F	3277	0	3214	18	0
1	G	3276	0	3218	24	0
1	H	3259	0	3195	19	0
1	I	3298	0	3233	16	0
1	J	3261	0	3200	13	0
1	K	3344	0	3284	24	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
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	1	0
4	L	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
9	B	268	0	0	1	0
9	C	262	0	0	3	0
9	D	298	0	0	1	0
9	E	243	0	0	1	0
9	F	299	0	0	0	0
9	G	293	0	0	0	0
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	1	0
9	L	301	0	0	0	0
All	All	43282	0	38925	208	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.

All (208) 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:C:70[B]:ARG:NH2	9:C:601:HOH:O	1.89	1.00
1:B:21:LYS:HD3	1:B:21:LYS:H	1.49	0.76
1:A:355[A]:LEU:HD13	9:A:785:HOH:O	1.88	0.73
1:A:21:LYS:HD3	1:A:21:LYS:H	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
1:C:148:LYS:HG2	1:C:172:VAL:HG22	1.78	0.66
1:F:134[A]:ILE:HD12	1:F:176:LEU:HD13	1.78	0.65
1:J:397:CYS:HB3	1:J:400:THR:OG1	2.01	0.61
1:C:97:ARG:NH2	1:C:101:ASP:OD1	2.34	0.60
1:F:327:LEU:HD22	1:F:391:GLY:HA2	1.83	0.60
1:B:21:LYS:CD	1:B:21:LYS:H	2.14	0.60
1:A:28:ASN:OD1	1:D:28:ASN:N	2.31	0.59
1:B:330:ARG:NH1	9:B:601:HOH:O	2.32	0.59
1:B:327:LEU:HD22	1:B:391:GLY:HA2	1.86	0.58
1:E:397:CYS:HB3	1:E:400:THR:OG1	2.03	0.58
1:A:383:HIS:HA	4:A:504:CL:CL	2.41	0.58
1:A:42:GLY:O	1:A:46[A]:ARG:HG3	2.04	0.57
1:G:24:TYR:CE1	1:G:50:LYS:HD3	2.40	0.57
1:C:148:LYS:CG	1:C:172:VAL:HG22	2.34	0.57
1:F:197:ILE:HA	1:F:248:ALA:O	2.05	0.56
1:H:330:ARG:HG2	6:H:506:EDO:H22	1.86	0.56
1:F:58:HIS:CD2	1:F:86:LYS:HB3	2.41	0.56
1:H:104:LEU:O	1:H:108:ASP:HB2	2.06	0.55
1:L:284:LEU:HD11	1:L:303:ALA:HB2	1.87	0.55
1:L:397:CYS:HB3	1:L:400:THR:OG1	2.07	0.55
1:L:134[A]:ILE:HD13	1:L:229:LEU:HD23	1.88	0.55
1:D:308:ALA:H	8:D:511:PEG:H11	1.71	0.54
1:B:42:GLY:O	1:B:46[A]:ARG:HG3	2.07	0.54
1:L:104:LEU:O	1:L:108:ASP:HB2	2.07	0.54
1:D:349[A]:GLU:OE2	1:D:389:GLN:NE2	2.38	0.54
1:B:134[A]:ILE:HD13	1:B:229:LEU:HD23	1.89	0.53
1:K:21:LYS:H	1:K:21:LYS:HD3	1.72	0.53
1:E:134:ILE:HD13	1:E:229:LEU:HD23	1.90	0.53
1:G:21:LYS:H	1:G:21:LYS:HD2	1.74	0.53
1:I:42:GLY:O	1:I:46[A]:ARG:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:160:LEU:HA	1:H:283:VAL:HG12	1.89	0.52
1:K:47:ALA:O	1:K:51:ILE:HG13	2.09	0.52
1:F:349[A]:GLU:OE2	1:F:389:GLN:NE2	2.42	0.52
1:J:69:ASP:HB3	1:J:103:ARG:HH12	1.74	0.52
1:K:134[A]:ILE:HD13	1:K:229:LEU:HD23	1.92	0.52
1:K:58:HIS:CD2	1:K:86:LYS:HB3	2.44	0.52
1:G:58:HIS:CD2	1:G:86:LYS:HB3	2.45	0.52
1:D:181:THR:C	1:D:183:ASP:H	2.13	0.51
1:E:197:ILE:HA	1:E:248:ALA:O	2.11	0.51
1:F:284:LEU:HD11	1:F:303:ALA:HB2	1.92	0.51
1:L:193:VAL:O	1:L:301:ASP:HA	2.11	0.51
1:A:327:LEU:HD22	1:A:391:GLY:HA2	1.92	0.50
1:C:134:ILE:HD13	1:C:229:LEU:HD23	1.93	0.50
1:L:125:GLN:HG3	8:L:509:PEG:H42	1.92	0.50
1:G:196:GLY:O	1:G:247:CYS:HA	2.12	0.50
1:I:408:GLN:HG2	1:I:409:TRP:CD1	2.47	0.50
1:F:134[A]:ILE:HD13	1:F:229:LEU:HD23	1.94	0.50
1:G:43:LEU:C	1:G:43:LEU:HD23	2.32	0.49
1:G:134:ILE:HD13	1:G:229:LEU:HD23	1.94	0.49
1:K:21:LYS:H	1:K:21:LYS:CD	2.24	0.49
1:C:64:GLU:HA	9:C:762:HOH:O	2.12	0.49
1:F:43:LEU:HD23	1:F:43:LEU:C	2.33	0.49
1:I:193:VAL:O	1:I:301:ASP:HA	2.12	0.49
1:C:371:PRO:HG2	1:D:314:GLY:HA2	1.94	0.49
1:G:197:ILE:HA	1:G:248:ALA:O	2.13	0.49
1:H:397:CYS:HB3	1:H:400:THR:OG1	2.12	0.49
1:A:35:LEU:HB3	1:A:40:ASP:OD1	2.12	0.49
1:E:331:LEU:C	1:E:331:LEU:HD23	2.33	0.49
1:I:183:ASP:HB2	1:I:186:ALA:HB2	1.95	0.49
1:J:200:ASP:HB2	1:J:218:ASP:OD2	2.13	0.49
1:L:134[B]:ILE:HD13	1:L:230:ALA:HB2	1.95	0.49
1:G:397:CYS:HB3	1:G:400:THR:OG1	2.13	0.48
1:E:327:LEU:HD22	1:E:391:GLY:HA2	1.95	0.48
1:F:146:ILE:HG23	1:F:172:VAL:HG13	1.95	0.48
1:K:136:ASN:HB2	9:K:881:HOH:O	2.13	0.48
1:E:259:LEU:HB3	1:F:213:ASP:HA	1.95	0.48
1:K:104:LEU:O	1:K:108:ASP:HB2	2.14	0.48
1:L:151:ASP:HA	1:L:154[B]:GLU:HG2	1.95	0.48
1:K:193:VAL:O	1:K:301:ASP:HA	2.13	0.48
1:L:197:ILE:HA	1:L:248:ALA:O	2.13	0.48
1:C:43:LEU:C	1:C:43:LEU:HD23	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:ALA:O	1:E:51:ILE:HG13	2.13	0.47
1:J:134:ILE:HD13	1:J:229:LEU:HD23	1.96	0.47
1:F:196:GLY:O	1:F:247:CYS:HA	2.13	0.47
1:D:104:LEU:O	1:D:108:ASP:HB2	2.15	0.47
1:G:24:TYR:HE1	1:G:50:LYS:HD3	1.79	0.47
1:K:327:LEU:HD22	1:K:391:GLY:HA2	1.97	0.47
1:A:298:MET:CE	1:A:425:LEU:HD23	2.44	0.47
1:H:193:VAL:O	1:H:301:ASP:HA	2.15	0.47
1:H:196:GLY:O	1:H:247:CYS:HA	2.15	0.47
1:K:397:CYS:HB3	1:K:400:THR:OG1	2.14	0.47
1:B:134[A]:ILE:HD12	1:B:176:LEU:HD13	1.97	0.47
1:J:43:LEU:C	1:J:43:LEU:HD23	2.36	0.47
1:H:337:GLN:NE2	9:H:602:HOH:O	2.30	0.46
1:E:207:LYS:HE3	1:E:215:MET:HG3	1.98	0.46
1:E:160:LEU:HA	1:E:283:VAL:HG12	1.97	0.46
1:A:318:HIS:ND1	1:A:397:CYS:HA	2.31	0.46
1:A:207:LYS:HE3	1:A:215:MET:HG3	1.98	0.46
1:I:141[B]:ARG:HH21	1:I:180:PRO:HB3	1.81	0.46
1:L:24:TYR:HA	1:L:32:THR:O	2.15	0.46
1:B:397:CYS:HB3	1:B:400:THR:OG1	2.15	0.46
1:I:215:MET:CE	1:I:215:MET:HA	2.45	0.46
1:C:193:VAL:O	1:C:301:ASP:HA	2.16	0.46
1:D:299:ILE:HD12	8:D:510:PEG:H31	1.96	0.46
1:H:401:TYR:CE1	1:H:412:GLY:HA2	2.51	0.46
1:L:327:LEU:HD22	1:L:391:GLY:HA2	1.97	0.46
1:J:197:ILE:HA	1:J:248:ALA:O	2.16	0.45
1:K:160:LEU:HA	1:K:283:VAL:HG12	1.98	0.45
1:B:319:ALA:HB3	1:B:396:ASP:HB3	1.99	0.45
9:C:751:HOH:O	1:E:28:ASN:HB2	2.16	0.45
1:K:196:GLY:O	1:K:247:CYS:HA	2.17	0.45
1:K:43:LEU:HD23	1:K:43:LEU:C	2.36	0.45
1:G:157:TYR:CE2	1:G:173:LEU:HD22	2.52	0.45
1:H:284:LEU:HD11	1:H:303:ALA:HB2	1.97	0.45
1:L:331:LEU:C	1:L:331:LEU:HD23	2.37	0.45
1:F:275:ASN:HB3	1:F:365:THR:HG21	1.97	0.45
1:G:181:THR:C	1:G:183:ASP:H	2.20	0.45
1:D:134[A]:ILE:HD13	1:D:229:LEU:HD23	1.98	0.45
1:G:13:PRO:HB2	1:G:20:GLU:HG3	1.99	0.45
1:K:269:LYS:NZ	4:K:504[A]:CL:CL	2.86	0.45
1:B:197:ILE:HA	1:B:248:ALA:O	2.17	0.44
1:G:15:ASP:OD1	1:G:15:ASP:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:134[A]:ILE:HD12	1:I:176:LEU:HD13	1.99	0.44
1:C:196:GLY:O	1:C:247:CYS:HA	2.18	0.44
1:G:28:ASN:N	1:J:28:ASN:OD1	2.48	0.44
1:I:160:LEU:HA	1:I:283:VAL:HG12	2.00	0.44
1:K:331:LEU:CD1	1:K:393:LEU:HD13	2.48	0.44
1:B:104:LEU:O	1:B:108:ASP:HB2	2.18	0.44
1:G:58:HIS:HD2	1:G:86:LYS:HB3	1.82	0.44
1:I:294:GLN:NE2	9:I:601:HOH:O	2.28	0.44
1:H:146:ILE:HG23	1:H:172:VAL:HG13	2.00	0.43
1:A:197:ILE:HA	1:A:248:ALA:O	2.19	0.43
1:C:397:CYS:HB3	1:C:400:THR:OG1	2.18	0.43
1:H:327:LEU:HG	1:H:393:LEU:HD21	2.01	0.43
1:A:146:ILE:HG23	1:A:172:VAL:HG13	2.00	0.43
1:E:331:LEU:HD13	1:E:393:LEU:HD13	1.99	0.43
1:D:403:LYS:HE2	9:D:767[A]:HOH:O	2.17	0.43
1:E:40:ASP:O	1:E:44:ILE:HG13	2.18	0.43
1:G:274:MET:CE	1:H:213:ASP:HB2	2.49	0.43
1:J:401:TYR:CE1	1:J:412:GLY:HA2	2.54	0.43
1:C:285:ALA:HB1	1:C:384:PHE:CD1	2.53	0.43
1:G:167:SER:HB2	1:G:249:ASP:HB2	2.01	0.43
1:I:71:CYS:HB3	1:I:89:TRP:CZ3	2.54	0.43
1:G:104:LEU:O	1:G:108:ASP:HB2	2.19	0.43
1:H:331:LEU:HD13	1:H:393:LEU:HD13	2.01	0.43
1:L:190:ALA:HA	1:L:298:MET:O	2.19	0.43
1:A:157:TYR:CE2	1:A:173:LEU:HD22	2.53	0.43
1:A:331:LEU:HD13	1:A:393:LEU:HD13	2.01	0.43
1:F:134[A]:ILE:HD12	1:F:176:LEU:CD1	2.46	0.42
1:I:104:LEU:O	1:I:108:ASP:HB2	2.19	0.42
1:K:197:ILE:HA	1:K:248:ALA:O	2.19	0.42
1:K:272:GLU:OE2	1:K:357:SER:OG	2.27	0.42
1:K:259:LEU:HB3	1:L:213:ASP:HA	2.00	0.42
1:C:318:HIS:ND1	1:C:397:CYS:HA	2.34	0.42
1:E:318:HIS:ND1	1:E:397:CYS:HA	2.34	0.42
1:G:146:ILE:HG23	1:G:172:VAL:HG13	2.01	0.42
1:K:331:LEU:HD23	1:K:331:LEU:C	2.40	0.42
1:L:284:LEU:HD11	1:L:303:ALA:CB	2.48	0.42
1:B:183:ASP:HB3	1:B:186:ALA:HB2	2.00	0.42
1:F:397:CYS:HB3	1:F:400:THR:OG1	2.18	0.42
1:H:26:ILE:HG12	1:H:31:ILE:HG12	2.00	0.42
1:H:269:LYS:HE3	1:H:383:HIS:HB3	2.00	0.42
1:E:190:ALA:HA	1:E:298:MET:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:197:ILE:HA	1:H:248:ALA:O	2.18	0.42
1:B:149:GLY:O	1:B:152:LEU:HB2	2.19	0.42
1:C:197:ILE:HA	1:C:248:ALA:O	2.19	0.42
1:G:280:GLY:O	1:G:283:VAL:HG22	2.19	0.42
1:J:193:VAL:O	1:J:301:ASP:HA	2.18	0.42
1:D:140:ASP:N	1:D:140:ASP:OD1	2.53	0.42
1:E:274:MET:CE	1:F:213:ASP:HB2	2.50	0.42
1:C:28:ASN:HB2	9:E:758:HOH:O	2.20	0.42
1:F:193:VAL:O	1:F:301:ASP:HA	2.19	0.42
1:H:311:THR:O	1:K:372:ALA:HA	2.19	0.42
1:D:320:LEU:HD22	1:D:331:LEU:HD22	2.01	0.42
1:I:197:ILE:HA	1:I:248:ALA:O	2.20	0.42
1:C:340:GLU:CD	1:C:417:GLY:H	2.23	0.42
1:A:178:TYR:CE2	1:A:180:PRO:HG3	2.55	0.41
1:G:284:LEU:HD11	1:G:303:ALA:HB2	2.02	0.41
1:H:315:ASN:HA	1:H:398:SER:O	2.20	0.41
1:I:372:ALA:HA	1:J:311:THR:O	2.20	0.41
1:D:363:ASN:OD1	1:D:365:THR:HG22	2.21	0.41
1:E:174:LEU:HB3	1:E:245:LEU:HB2	2.03	0.41
1:K:134[B]:ILE:HD13	1:K:230:ALA:HB2	2.02	0.41
1:A:349[A]:GLU:OE2	1:A:389:GLN:NE2	2.46	0.41
1:E:102:ASN:ND2	1:E:234:THR:HB	2.35	0.41
1:A:21:LYS:N	1:A:21:LYS:HD3	2.29	0.41
1:D:109:TRP:CD2	1:D:133:LEU:HD22	2.56	0.41
1:I:134[A]:ILE:HD13	1:I:229:LEU:HD23	2.03	0.41
1:A:408:GLN:OE1	1:A:408:GLN:N	2.47	0.41
1:B:408:GLN:HG2	1:B:409:TRP:CD1	2.56	0.41
1:J:146:ILE:HG23	1:J:172:VAL:HG13	2.02	0.41
1:K:40:ASP:O	1:K:44:ILE:HG13	2.21	0.41
1:G:102:ASN:ND2	1:G:234:THR:HB	2.35	0.41
1:A:26:ILE:HG12	1:A:31:ILE:HG12	2.02	0.41
1:E:295:LYS:HB3	1:E:295:LYS:HE2	1.90	0.41
1:J:408:GLN:HG2	1:J:409:TRP:CD1	2.56	0.41
1:A:213:ASP:HA	1:C:259:LEU:HB3	2.03	0.40
1:B:331:LEU:CD1	1:B:393:LEU:HD13	2.51	0.40
1:F:310:LYS:O	1:F:314:GLY:N	2.50	0.40
1:I:167:SER:HB2	1:I:249:ASP:HB2	2.03	0.40
1:H:285:ALA:HB1	1:H:384:PHE:CD1	2.55	0.40
1:F:408:GLN:HG2	1:F:409:TRP:CD1	2.56	0.40
1:I:196:GLY:O	1:I:247:CYS:HA	2.20	0.40
1:K:212:MET:HA	1:K:215:MET:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:CYS:HB3	1:A:400:THR:OG1	2.21	0.40
1:C:401:TYR:CE1	1:C:412:GLY:HA2	2.57	0.40
1:E:196:GLY:O	1:E:247:CYS:HA	2.22	0.40
1:E:319:ALA:HB3	1:E:396:ASP:HB3	2.04	0.40
1:G:176:LEU:C	1:G:176:LEU:HD23	2.42	0.40
1:J:176:LEU:HD23	1:J:176:LEU:C	2.42	0.40
1:K:203:GLY:O	1:K:252:ILE:HD11	2.21	0.40

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
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%)	332 (99%)	3 (1%)	78	79
1	B	333/332 (100%)	330 (99%)	3 (1%)	78	79
1	C	333/332 (100%)	332 (100%)	1 (0%)	92	93
1	D	331/332 (100%)	327 (99%)	4 (1%)	71	70
1	E	333/332 (100%)	331 (99%)	2 (1%)	86	87
1	F	333/332 (100%)	331 (99%)	2 (1%)	86	87
1	G	333/332 (100%)	330 (99%)	3 (1%)	78	79
1	H	331/332 (100%)	329 (99%)	2 (1%)	86	87
1	I	335/332 (101%)	333 (99%)	2 (1%)	86	87
1	J	331/332 (100%)	329 (99%)	2 (1%)	86	87
1	K	341/332 (103%)	337 (99%)	4 (1%)	71	70
1	L	334/332 (101%)	332 (99%)	2 (1%)	86	87
All	All	4003/3984 (100%)	3973 (99%)	30 (1%)	81	84

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	257	PHE
1	A	301	ASP
1	B	21	LYS
1	B	93	ASP
1	B	257	PHE
1	C	257	PHE
1	D	181	THR
1	D	257	PHE
1	D	295	LYS
1	D	301	ASP
1	E	219	MET
1	E	257	PHE
1	F	257	PHE

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Mol	Chain	Res	Type
1	F	301	ASP
1	G	21	LYS
1	G	257	PHE
1	G	301	ASP
1	H	257	PHE
1	H	301	ASP
1	I	183	ASP
1	I	257	PHE
1	J	257	PHE
1	J	301	ASP
1	K	21	LYS
1	K	86	LYS
1	K	257	PHE
1	K	301	ASP
1	L	257	PHE
1	L	301	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	58	HIS
1	E	76	GLN
1	G	390	GLN
1	H	102	ASN
1	K	58	HIS
1	L	58	HIS

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

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	$\# Z > 2$
6	EDO	C	510	-	3,3,3	0.11	0	2,2,2	0.13	0
6	EDO	E	506	-	3,3,3	0.08	0	2,2,2	0.14	0
6	EDO	J	505	-	3,3,3	0.09	0	2,2,2	0.17	0
6	EDO	B	506	-	3,3,3	0.08	0	2,2,2	0.23	0
6	EDO	H	510	-	3,3,3	0.08	0	2,2,2	0.18	0
5	BCT	L	506	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BCT	K	506	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BCT	F	506	-	0,3,3	0.00	-	0,3,3	0.00	-
6	EDO	H	506	-	3,3,3	0.12	0	2,2,2	0.33	0
6	EDO	F	509	-	3,3,3	0.07	0	2,2,2	0.15	0
6	EDO	I	508	-	3,3,3	0.10	0	2,2,2	0.17	0
6	EDO	C	508	-	3,3,3	0.06	0	2,2,2	0.19	0
6	EDO	J	507	-	3,3,3	0.12	0	2,2,2	0.31	0
6	EDO	E	507	-	3,3,3	0.06	0	2,2,2	0.23	0
6	EDO	A	508	-	3,3,3	0.09	0	2,2,2	0.09	0
6	EDO	H	508	-	3,3,3	0.06	0	2,2,2	0.25	0
6	EDO	J	508	-	3,3,3	0.06	0	2,2,2	0.22	0
6	EDO	G	506	-	3,3,3	0.06	0	2,2,2	0.21	0
6	EDO	J	509	-	3,3,3	0.07	0	2,2,2	0.12	0
6	EDO	I	507	-	3,3,3	0.12	0	2,2,2	0.30	0
6	EDO	H	505	-	3,3,3	0.13	0	2,2,2	0.24	0
6	EDO	I	509	-	3,3,3	0.09	0	2,2,2	0.23	0
8	PEG	L	509	-	6,6,6	0.18	0	5,5,5	0.13	0
6	EDO	H	509	-	3,3,3	0.08	0	2,2,2	0.23	0
6	EDO	D	508	-	3,3,3	0.09	0	2,2,2	0.22	0
5	BCT	D	504	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BCT	J	504	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BCT	I	506	-	0,3,3	0.00	-	0,3,3	0.00	-
8	PEG	D	511	-	6,6,6	0.17	0	5,5,5	0.09	0
6	EDO	G	507	-	3,3,3	0.14	0	2,2,2	0.33	0
6	EDO	K	508	-	3,3,3	0.10	0	2,2,2	0.12	0
6	EDO	C	507	-	3,3,3	0.05	0	2,2,2	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	D	507	-	3,3,3	0.07	0	2,2,2	0.12	0
6	EDO	A	507	-	3,3,3	0.12	0	2,2,2	0.43	0
5	BCT	D	506	-	0,3,3	0.00	-	0,3,3	0.00	-
6	EDO	A	506	-	3,3,3	0.09	0	2,2,2	0.29	0
5	BCT	C	505	-	0,3,3	0.00	-	0,3,3	0.00	-
6	EDO	K	507	-	3,3,3	0.06	0	2,2,2	0.26	0
5	BCT	B	505	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BCT	I	505	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BCT	K	505	-	0,3,3	0.00	-	0,3,3	0.00	-
6	EDO	J	506	-	3,3,3	0.07	0	2,2,2	0.25	0
6	EDO	L	510	-	3,3,3	0.10	0	2,2,2	0.12	0
6	EDO	F	508	-	3,3,3	0.06	0	2,2,2	0.22	0
5	BCT	H	504	-	0,3,3	0.00	-	0,3,3	0.00	-
8	PEG	E	509	-	6,6,6	0.23	0	5,5,5	0.12	0
6	EDO	H	507	-	3,3,3	0.10	0	2,2,2	0.18	0
6	EDO	B	507	-	3,3,3	0.14	0	2,2,2	0.38	0
6	EDO	E	508	-	3,3,3	0.07	0	2,2,2	0.25	0
5	BCT	A	505	-	0,3,3	0.00	-	0,3,3	0.00	-
8	PEG	D	510	-	6,6,6	0.11	0	5,5,5	0.10	0
6	EDO	L	508	-	3,3,3	0.12	0	2,2,2	0.26	0
5	BCT	E	505	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BCT	D	505	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BCT	G	505	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BCT	C	506	-	0,3,3	0.00	-	0,3,3	0.00	-
6	EDO	F	507	-	3,3,3	0.15	0	2,2,2	0.24	0
6	EDO	L	507	-	3,3,3	0.10	0	2,2,2	0.31	0
5	BCT	F	505	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BCT	G	504	-	0,3,3	0.00	-	0,3,3	0.00	-
7	PGE	A	509	-	9,9,9	0.24	0	8,8,8	0.12	0
8	PEG	C	509	-	6,6,6	0.16	0	5,5,5	0.09	0
6	EDO	D	509	-	3,3,3	0.09	0	2,2,2	0.14	0
6	EDO	G	508	-	3,3,3	0.09	0	2,2,2	0.15	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
6	EDO	C	510	-	-	1/1/1/1	-
6	EDO	E	506	-	-	0/1/1/1	-
6	EDO	J	505	-	-	0/1/1/1	-
6	EDO	B	506	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	H	510	-	-	0/1/1/1	-
6	EDO	L	507	-	-	1/1/1/1	-
6	EDO	H	506	-	-	1/1/1/1	-
6	EDO	F	509	-	-	0/1/1/1	-
6	EDO	I	508	-	-	0/1/1/1	-
6	EDO	C	508	-	-	0/1/1/1	-
6	EDO	J	507	-	-	1/1/1/1	-
6	EDO	E	507	-	-	1/1/1/1	-
6	EDO	A	508	-	-	1/1/1/1	-
6	EDO	H	508	-	-	0/1/1/1	-
6	EDO	J	508	-	-	1/1/1/1	-
6	EDO	G	506	-	-	0/1/1/1	-
6	EDO	J	509	-	-	1/1/1/1	-
6	EDO	I	507	-	-	1/1/1/1	-
6	EDO	H	505	-	-	1/1/1/1	-
6	EDO	I	509	-	-	0/1/1/1	-
8	PEG	L	509	-	-	2/4/4/4	-
6	EDO	H	509	-	-	0/1/1/1	-
6	EDO	D	508	-	-	0/1/1/1	-
6	EDO	K	507	-	-	0/1/1/1	-
6	EDO	G	507	-	-	1/1/1/1	-
6	EDO	C	507	-	-	0/1/1/1	-
6	EDO	D	507	-	-	0/1/1/1	-
6	EDO	A	507	-	-	1/1/1/1	-
6	EDO	A	506	-	-	0/1/1/1	-
8	PEG	D	511	-	-	2/4/4/4	-
6	EDO	J	506	-	-	1/1/1/1	-
6	EDO	L	510	-	-	1/1/1/1	-
6	EDO	F	508	-	-	0/1/1/1	-
6	EDO	H	507	-	-	0/1/1/1	-
8	PEG	E	509	-	-	1/4/4/4	-
6	EDO	E	508	-	-	1/1/1/1	-
8	PEG	D	510	-	-	3/4/4/4	-
6	EDO	L	508	-	-	0/1/1/1	-
6	EDO	F	507	-	-	0/1/1/1	-
6	EDO	K	508	-	-	1/1/1/1	-
6	EDO	B	507	-	-	1/1/1/1	-
7	PGE	A	509	-	-	4/7/7/7	-
8	PEG	C	509	-	-	2/4/4/4	-
6	EDO	D	509	-	-	0/1/1/1	-
6	EDO	G	508	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (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	G	508	EDO	O1-C1-C2-O2
6	H	506	EDO	O1-C1-C2-O2
6	J	506	EDO	O1-C1-C2-O2
6	B	507	EDO	O1-C1-C2-O2
6	C	510	EDO	O1-C1-C2-O2
6	G	507	EDO	O1-C1-C2-O2
8	D	510	PEG	O2-C3-C4-O4
6	J	508	EDO	O1-C1-C2-O2
6	J	509	EDO	O1-C1-C2-O2
6	A	507	EDO	O1-C1-C2-O2
8	D	510	PEG	O1-C1-C2-O2
8	D	511	PEG	C4-C3-O2-C2
8	L	509	PEG	C4-C3-O2-C2
8	E	509	PEG	C1-C2-O2-C3
8	C	509	PEG	C4-C3-O2-C2
8	D	510	PEG	C1-C2-O2-C3
6	L	507	EDO	O1-C1-C2-O2
6	E	507	EDO	O1-C1-C2-O2
6	K	508	EDO	O1-C1-C2-O2
8	D	511	PEG	O2-C3-C4-O4
6	H	505	EDO	O1-C1-C2-O2
6	I	507	EDO	O1-C1-C2-O2
7	A	509	PGE	C3-C4-O3-C5
7	A	509	PGE	C6-C5-O3-C4
6	E	508	EDO	O1-C1-C2-O2
6	L	510	EDO	O1-C1-C2-O2
6	J	507	EDO	O1-C1-C2-O2
6	A	508	EDO	O1-C1-C2-O2
7	A	509	PGE	C1-C2-O2-C3
8	L	509	PEG	O2-C3-C4-O4

There are no ring outliers.

5 monomers are involved in 5 short contacts:

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

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, 95th 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	426/430 (99%)	-0.15	8 (1%) 66 71	24, 33, 55, 82	0
1	B	426/430 (99%)	0.00	18 (4%) 36 39	25, 38, 69, 104	0
1	C	426/430 (99%)	0.04	26 (6%) 21 22	25, 41, 71, 98	0
1	D	425/430 (98%)	-0.10	19 (4%) 33 35	25, 37, 61, 80	0
1	E	426/430 (99%)	0.09	27 (6%) 20 21	26, 41, 71, 103	0
1	F	426/430 (99%)	-0.09	14 (3%) 46 50	24, 35, 64, 91	0
1	G	426/430 (99%)	-0.06	16 (3%) 40 44	27, 38, 69, 88	0
1	H	426/430 (99%)	-0.07	23 (5%) 25 28	24, 34, 57, 81	0
1	I	425/430 (98%)	-0.25	5 (1%) 79 81	25, 33, 46, 76	0
1	J	426/430 (99%)	0.03	24 (5%) 24 26	27, 42, 70, 97	0
1	K	426/430 (99%)	-0.22	9 (2%) 63 67	24, 32, 50, 93	0
1	L	425/430 (98%)	-0.14	12 (2%) 53 58	28, 38, 55, 99	0
All	All	5109/5160 (99%)	-0.08	201 (3%) 39 42	24, 37, 65, 104	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	GLU	7.4
1	J	20	GLU	6.4
1	A	2	THR	6.1
1	F	2	THR	6.0
1	L	20	GLU	5.1
1	C	20	GLU	4.9
1	E	21	LYS	4.6
1	A	20	GLU	4.5
1	G	19	GLY	4.5
1	H	2	THR	4.5
1	B	19	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	185	GLU	4.3
1	G	182	GLY	4.2
1	G	20	GLU	4.2
1	E	2	THR	4.1
1	C	225	VAL	4.0
1	K	20	GLU	3.9
1	J	16	ALA	3.9
1	H	193	VAL	3.9
1	B	395	ILE	3.8
1	E	225	VAL	3.6
1	J	140	ASP	3.6
1	J	2	THR	3.6
1	B	181	THR	3.6
1	E	284	LEU	3.5
1	G	284	LEU	3.5
1	C	192	LEU	3.5
1	L	185	GLU	3.4
1	C	300	ILE	3.4
1	H	284	LEU	3.4
1	G	181	THR	3.4
1	J	139	GLY	3.4
1	E	184	LYS	3.4
1	C	222	ALA	3.3
1	L	303	ALA	3.3
1	C	302	ALA	3.3
1	J	302	ALA	3.3
1	F	20	GLU	3.3
1	H	20	GLU	3.3
1	C	182	GLY	3.3
1	D	395	ILE	3.3
1	J	19	GLY	3.2
1	E	181	THR	3.2
1	D	193	VAL	3.2
1	E	302	ALA	3.2
1	D	28	ASN	3.1
1	B	14	ALA	3.1
1	F	283	VAL	3.1
1	L	19	GLY	3.1
1	I	20	GLU	3.1
1	J	94	ASP	3.1
1	D	303	ALA	3.1
1	H	184	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	20	GLU	3.1
1	G	94	ASP	3.0
1	E	193	VAL	3.0
1	H	91[A]	ASP	3.0
1	C	284	LEU	3.0
1	E	223	ALA	3.0
1	J	427	ALA	3.0
1	J	197	ILE	2.9
1	L	225	VAL	2.9
1	H	283	VAL	2.9
1	F	29	ASP	2.9
1	E	222	ALA	2.9
1	E	183	ASP	2.9
1	B	302	ALA	2.8
1	H	181	THR	2.8
1	B	21	LYS	2.8
1	C	303	ALA	2.8
1	D	302	ALA	2.8
1	K	284	LEU	2.8
1	C	193	VAL	2.8
1	A	19	GLY	2.7
1	L	222	ALA	2.7
1	B	284	LEU	2.7
1	G	95	ALA	2.7
1	H	302	ALA	2.7
1	J	183	ASP	2.7
1	C	181	THR	2.6
1	D	184	LYS	2.6
1	E	283	VAL	2.6
1	J	283	VAL	2.6
1	H	94	ASP	2.6
1	E	303	ALA	2.6
1	D	182	GLY	2.6
1	D	284	LEU	2.6
1	D	16	ALA	2.6
1	E	300	ILE	2.6
1	H	225	VAL	2.6
1	K	183	ASP	2.6
1	E	37	GLY	2.6
1	G	28	ASN	2.6
1	E	194	GLY	2.5
1	J	221	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	183	ASP	2.5
1	L	197	ILE	2.5
1	F	211	PHE	2.5
1	G	193	VAL	2.5
1	H	197	ILE	2.5
1	G	183	ASP	2.5
1	D	183	ASP	2.5
1	H	211	PHE	2.5
1	G	2	THR	2.5
1	I	181	THR	2.5
1	J	193	VAL	2.5
1	E	3	GLU	2.5
1	F	91	ASP	2.4
1	H	19	GLY	2.4
1	B	28	ASN	2.4
1	B	238	ASN	2.4
1	H	288	LEU	2.4
1	L	283	VAL	2.4
1	C	224	THR	2.4
1	K	2	THR	2.4
1	L	224	THR	2.4
1	E	395	ILE	2.4
1	C	194	GLY	2.4
1	H	21	LYS	2.4
1	K	282	LEU	2.4
1	D	185	GLU	2.4
1	J	222	ALA	2.4
1	D	29	ASP	2.3
1	A	303	ALA	2.3
1	D	140	ASP	2.3
1	D	280	GLY	2.3
1	C	2	THR	2.3
1	E	220	GLY	2.3
1	J	184	LYS	2.3
1	H	185	GLU	2.3
1	J	395	ILE	2.3
1	C	140	ASP	2.3
1	F	184	LYS	2.3
1	I	283	VAL	2.3
1	G	184	LYS	2.3
1	H	194	GLY	2.3
1	J	284	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	302	ALA	2.2
1	C	29	ASP	2.2
1	C	185	GLU	2.2
1	B	16	ALA	2.2
1	A	28	ASN	2.2
1	C	21	LYS	2.2
1	D	221	GLY	2.2
1	K	19	GLY	2.2
1	F	3	GLU	2.2
1	E	192	LEU	2.2
1	L	284	LEU	2.2
1	B	225	VAL	2.2
1	L	193	VAL	2.2
1	D	21	LYS	2.2
1	E	427	ALA	2.2
1	D	305	LEU	2.2
1	A	283	VAL	2.2
1	C	94	ASP	2.2
1	C	305	LEU	2.2
1	F	222	ALA	2.2
1	J	305	LEU	2.1
1	A	193	VAL	2.1
1	F	163	VAL	2.1
1	I	193	VAL	2.1
1	H	182	GLY	2.1
1	K	185[A]	GLU	2.1
1	C	421	ILE	2.1
1	G	395	ILE	2.1
1	J	195	LYS	2.1
1	B	211	PHE	2.1
1	E	221	GLY	2.1
1	H	139	GLY	2.1
1	B	303	ALA	2.1
1	C	223	ALA	2.1
1	F	303	ALA	2.1
1	H	95	ALA	2.1
1	J	12	GLN	2.1
1	I	163	VAL	2.1
1	K	303	ALA	2.1
1	C	91	ASP	2.1
1	D	194	GLY	2.1
1	F	93	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	194	GLY	2.1
1	A	29	ASP	2.1
1	F	64	GLU	2.1
1	C	211	PHE	2.1
1	G	21	LYS	2.1
1	H	195	LYS	2.1
1	L	395	ILE	2.0
1	B	12	GLN	2.0
1	B	283	VAL	2.0
1	E	224	THR	2.0
1	G	283	VAL	2.0
1	J	300	ILE	2.0
1	C	16	ALA	2.0
1	H	209	THR	2.0
1	F	193	VAL	2.0
1	E	182	GLY	2.0
1	E	211	PHE	2.0
1	C	28	ASN	2.0
1	G	13	PRO	2.0
1	E	140	ASP	2.0
1	E	280	GLY	2.0
1	J	37	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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
8	PEG	L	509	7/7	0.52	0.37	71,74,80,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	PEG	C	509	7/7	0.66	0.32	62,73,79,82	0
8	PEG	D	511	7/7	0.67	0.22	61,64,69,70	0
6	EDO	G	507	4/4	0.68	0.23	65,65,67,68	0
7	PGE	A	509	10/10	0.70	0.20	43,64,72,78	0
8	PEG	E	509	7/7	0.72	0.22	49,59,62,67	0
4	CL	B	504	1/1	0.78	0.14	47,47,47,47	1
5	BCT	D	505	4/4	0.78	0.31	55,66,67,69	0
6	EDO	J	508	4/4	0.78	0.19	58,61,69,73	0
6	EDO	H	509	4/4	0.79	0.26	63,65,66,67	0
4	CL	L	505	1/1	0.80	0.12	67,67,67,67	0
6	EDO	H	506	4/4	0.80	0.51	57,62,63,63	0
5	BCT	C	506	4/4	0.81	0.33	77,81,83,85	0
5	BCT	G	505	4/4	0.83	0.17	52,65,71,75	0
6	EDO	J	507	4/4	0.84	0.18	46,51,55,55	0
5	BCT	K	506	4/4	0.84	0.21	45,62,62,67	0
6	EDO	H	508	4/4	0.85	0.28	49,60,61,68	0
6	EDO	A	507	4/4	0.86	0.28	41,44,46,49	0
5	BCT	I	505	4/4	0.86	0.27	31,31,32,34	4
6	EDO	D	508	4/4	0.86	0.22	47,51,52,53	0
6	EDO	L	508	4/4	0.87	0.14	48,49,50,52	0
5	BCT	F	506	4/4	0.88	0.21	52,61,63,70	0
4	CL	K	504[A]	1/1	0.88	0.26	51,51,51,51	1
6	EDO	B	507	4/4	0.88	0.17	49,57,57,59	0
4	CL	A	504	1/1	0.88	0.07	58,58,58,58	0
4	CL	B	508	1/1	0.88	0.13	78,78,78,78	0
4	CL	K	504[B]	1/1	0.88	0.26	43,43,43,43	1
6	EDO	J	505	4/4	0.89	0.16	46,47,47,48	0
8	PEG	D	510	7/7	0.89	0.22	56,57,60,62	0
6	EDO	G	508	4/4	0.89	0.14	58,59,61,61	0
6	EDO	J	509	4/4	0.90	0.13	59,59,63,63	0
6	EDO	E	506	4/4	0.90	0.18	52,55,60,60	0
4	CL	E	504	1/1	0.90	0.10	67,67,67,67	0
6	EDO	D	509	4/4	0.90	0.13	48,51,52,56	0
6	EDO	A	508	4/4	0.91	0.15	42,45,47,49	0
6	EDO	C	508	4/4	0.91	0.12	54,60,60,62	0
5	BCT	D	506	4/4	0.91	0.21	42,46,50,58	0
6	EDO	C	510	4/4	0.91	0.12	47,50,53,56	0
6	EDO	F	507	4/4	0.92	0.22	48,50,50,52	0
6	EDO	C	507	4/4	0.92	0.13	50,53,54,55	0
6	EDO	I	509	4/4	0.92	0.18	46,48,49,55	0
6	EDO	K	508	4/4	0.92	0.11	46,47,48,49	0
6	EDO	L	510	4/4	0.92	0.15	51,51,52,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EDO	I	508	4/4	0.93	0.12	43,44,44,46	0
6	EDO	H	507	4/4	0.93	0.12	40,44,49,54	0
6	EDO	J	506	4/4	0.93	0.23	52,56,57,57	0
4	CL	C	504	1/1	0.93	0.07	60,60,60,60	0
4	CL	F	504[B]	1/1	0.93	0.17	39,39,39,39	1
4	CL	F	504[A]	1/1	0.93	0.17	43,43,43,43	1
6	EDO	A	506	4/4	0.94	0.15	41,43,45,45	0
6	EDO	D	507	4/4	0.94	0.14	39,42,43,44	0
6	EDO	F	509	4/4	0.94	0.11	54,56,58,62	0
6	EDO	E	508	4/4	0.94	0.17	55,57,59,60	0
6	EDO	E	507	4/4	0.94	0.17	44,47,48,50	0
5	BCT	E	505	4/4	0.95	0.14	26,30,30,38	0
6	EDO	H	505	4/4	0.95	0.12	39,41,41,42	0
6	EDO	K	507	4/4	0.95	0.13	41,45,45,49	0
6	EDO	H	510	4/4	0.95	0.09	42,43,44,48	0
6	EDO	G	506	4/4	0.95	0.12	47,51,51,51	0
6	EDO	F	508	4/4	0.95	0.13	49,51,52,52	0
4	CL	L	504	1/1	0.95	0.06	54,54,54,54	0
5	BCT	A	505	4/4	0.96	0.13	28,31,32,37	0
5	BCT	I	506	4/4	0.96	0.12	28,29,30,37	0
5	BCT	J	504	4/4	0.96	0.14	34,36,39,44	0
6	EDO	I	507	4/4	0.96	0.14	36,39,39,41	0
6	EDO	B	506	4/4	0.96	0.14	46,46,48,49	0
6	EDO	L	507	4/4	0.97	0.14	43,44,46,47	0
5	BCT	K	505	4/4	0.97	0.11	26,26,34,38	0
3	CA	H	503	1/1	0.97	0.06	39,39,39,39	0
5	BCT	G	504	4/4	0.97	0.12	32,32,33,42	0
3	CA	I	504	1/1	0.97	0.08	45,45,45,45	0
5	BCT	B	505	4/4	0.98	0.09	30,30,34,35	0
2	ZN	D	501	1/1	0.98	0.06	28,28,28,28	0
5	BCT	H	504	4/4	0.98	0.07	25,27,31,36	0
3	CA	E	503	1/1	0.98	0.05	41,41,41,41	0
2	ZN	G	501	1/1	0.98	0.06	30,30,30,30	0
5	BCT	L	506	4/4	0.98	0.09	31,33,33,42	0
5	BCT	F	505	4/4	0.98	0.14	27,29,34,42	0
2	ZN	J	501	1/1	0.98	0.06	32,32,32,32	0
5	BCT	C	505	4/4	0.98	0.08	27,29,29,40	0
2	ZN	A	501	1/1	0.99	0.07	27,27,27,27	0
2	ZN	E	502	1/1	0.99	0.06	30,30,30,30	0
2	ZN	A	502	1/1	0.99	0.08	27,27,27,27	0
3	CA	L	503	1/1	0.99	0.04	39,39,39,39	0
3	CA	B	503	1/1	0.99	0.04	35,35,35,35	0

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

6.5 Other polymers [i](#)

There are no such residues in this entry.