



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 4, 2023 – 08:08 PM EDT

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

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.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

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

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	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 (three-letter code: 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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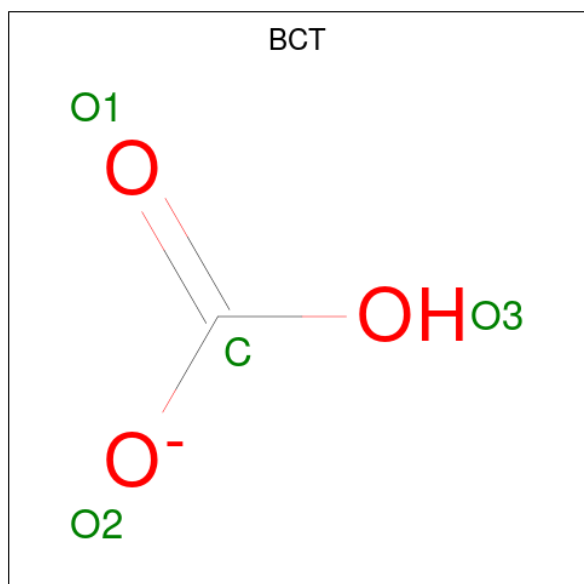
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	1	Total Ca 1 1	0	0

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

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

- Molecule 5 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



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

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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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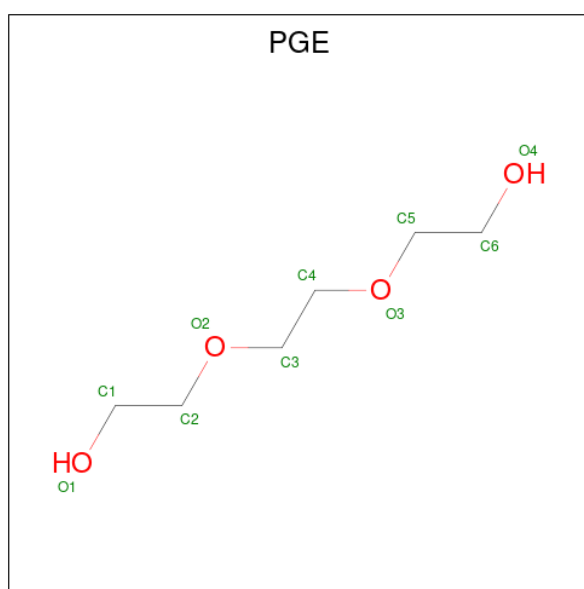
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	G	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total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

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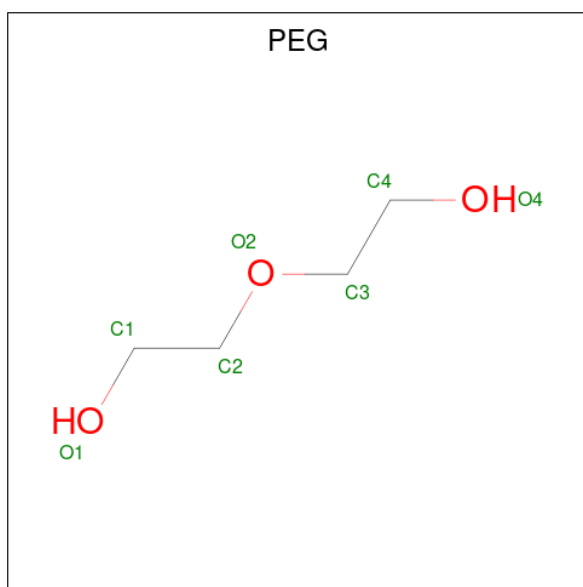
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	K	1	Total	C	O	0	0
			4	2	2		
6	L	1	Total	C	O	0	0
			4	2	2		
6	L	1	Total	C	O	0	0
			4	2	2		
6	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



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: C₄H₁₀O₃).



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

- Molecule 9 is water.

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

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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

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

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	Depositor
% Data completeness (in resolution range)	98.6 (29.88-2.05)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.04Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.172 , 0.215	Depositor
Wilson B-factor (Å ²)	30.9	Xtrriage
Anisotropy	0.070	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.016 for h,-k,-l	Xtrriage
Total number of atoms	43282	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage'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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 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
5	BCT	J	504	-	2,3,3	1.00	0	2,3,3	1.47	0
6	EDO	D	507	-	3,3,3	0.07	0	2,2,2	0.12	0
5	BCT	H	504	-	2,3,3	1.26	0	2,3,3	0.91	0
6	EDO	J	507	-	3,3,3	0.12	0	2,2,2	0.31	0
6	EDO	F	508	-	3,3,3	0.06	0	2,2,2	0.22	0
5	BCT	C	506	-	2,3,3	0.96	0	2,3,3	1.65	1 (50%)
5	BCT	D	505	-	2,3,3	0.85	0	2,3,3	1.73	1 (50%)
5	BCT	G	504	-	2,3,3	1.03	0	2,3,3	1.57	1 (50%)
6	EDO	C	507	-	3,3,3	0.05	0	2,2,2	0.22	0
6	EDO	I	507	-	3,3,3	0.12	0	2,2,2	0.30	0
6	EDO	B	507	-	3,3,3	0.14	0	2,2,2	0.38	0
6	EDO	L	508	-	3,3,3	0.12	0	2,2,2	0.26	0
5	BCT	C	505	-	2,3,3	1.02	0	2,3,3	1.56	1 (50%)
5	BCT	F	506	-	2,3,3	1.34	0	2,3,3	0.81	0
6	EDO	H	507	-	3,3,3	0.10	0	2,2,2	0.18	0
6	EDO	G	507	-	3,3,3	0.14	0	2,2,2	0.33	0
6	EDO	A	507	-	3,3,3	0.12	0	2,2,2	0.43	0
5	BCT	F	505	-	2,3,3	0.94	0	2,3,3	1.50	1 (50%)
8	PEG	L	509	-	6,6,6	0.18	0	5,5,5	0.13	0
6	EDO	K	508	-	3,3,3	0.10	0	2,2,2	0.12	0
6	EDO	H	506	-	3,3,3	0.12	0	2,2,2	0.33	0
8	PEG	D	510	-	6,6,6	0.11	0	5,5,5	0.10	0
5	BCT	K	505	-	2,3,3	1.21	0	2,3,3	0.80	0
6	EDO	I	508	-	3,3,3	0.10	0	2,2,2	0.17	0
6	EDO	J	509	-	3,3,3	0.07	0	2,2,2	0.12	0
6	EDO	E	506	-	3,3,3	0.08	0	2,2,2	0.14	0
8	PEG	C	509	-	6,6,6	0.16	0	5,5,5	0.09	0
6	EDO	H	508	-	3,3,3	0.06	0	2,2,2	0.25	0
6	EDO	J	506	-	3,3,3	0.07	0	2,2,2	0.25	0
6	EDO	I	509	-	3,3,3	0.09	0	2,2,2	0.23	0
6	EDO	E	508	-	3,3,3	0.07	0	2,2,2	0.25	0
6	EDO	G	508	-	3,3,3	0.09	0	2,2,2	0.15	0
8	PEG	D	511	-	6,6,6	0.17	0	5,5,5	0.09	0
6	EDO	K	507	-	3,3,3	0.06	0	2,2,2	0.26	0
6	EDO	L	507	-	3,3,3	0.10	0	2,2,2	0.31	0
5	BCT	D	506	-	2,3,3	0.93	0	2,3,3	1.70	1 (50%)
5	BCT	L	506	-	2,3,3	1.40	0	2,3,3	0.74	0
6	EDO	D	508	-	3,3,3	0.09	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	G	506	-	3,3,3	0.06	0	2,2,2	0.21	0
6	EDO	H	509	-	3,3,3	0.08	0	2,2,2	0.23	0
6	EDO	J	505	-	3,3,3	0.09	0	2,2,2	0.17	0
6	EDO	D	509	-	3,3,3	0.09	0	2,2,2	0.14	0
7	PGE	A	509	-	9,9,9	0.24	0	8,8,8	0.12	0
6	EDO	F	507	-	3,3,3	0.15	0	2,2,2	0.24	0
6	EDO	L	510	-	3,3,3	0.10	0	2,2,2	0.12	0
6	EDO	F	509	-	3,3,3	0.07	0	2,2,2	0.15	0
5	BCT	B	505	-	2,3,3	1.33	0	2,3,3	0.83	0
6	EDO	A	506	-	3,3,3	0.09	0	2,2,2	0.29	0
5	BCT	I	506	-	2,3,3	1.22	0	2,3,3	1.00	0
6	EDO	C	508	-	3,3,3	0.06	0	2,2,2	0.19	0
6	EDO	E	507	-	3,3,3	0.06	0	2,2,2	0.23	0
6	EDO	J	508	-	3,3,3	0.06	0	2,2,2	0.22	0
5	BCT	A	505	-	2,3,3	0.88	0	2,3,3	1.47	0
5	BCT	E	505	-	2,3,3	1.34	0	2,3,3	0.72	0
6	EDO	C	510	-	3,3,3	0.11	0	2,2,2	0.13	0
6	EDO	H	505	-	3,3,3	0.13	0	2,2,2	0.24	0
8	PEG	E	509	-	6,6,6	0.23	0	5,5,5	0.12	0
5	BCT	K	506	-	2,3,3	1.28	0	2,3,3	0.85	0
5	BCT	D	504	-	2,3,3	0.89	0	2,3,3	1.69	1 (50%)
5	BCT	G	505	-	2,3,3	1.29	0	2,3,3	0.79	0
6	EDO	A	508	-	3,3,3	0.09	0	2,2,2	0.09	0
5	BCT	I	505	-	2,3,3	1.04	0	2,3,3	1.64	1 (50%)
6	EDO	H	510	-	3,3,3	0.08	0	2,2,2	0.18	0
6	EDO	B	506	-	3,3,3	0.08	0	2,2,2	0.23	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	D	507	-	-	0/1/1/1	-
6	EDO	J	507	-	-	1/1/1/1	-
6	EDO	F	508	-	-	0/1/1/1	-
6	EDO	L	508	-	-	0/1/1/1	-
6	EDO	C	507	-	-	0/1/1/1	-
6	EDO	I	507	-	-	1/1/1/1	-
6	EDO	B	507	-	-	1/1/1/1	-
6	EDO	H	507	-	-	0/1/1/1	-
6	EDO	G	507	-	-	1/1/1/1	-

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

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	506	BCT	O2-C-O1	2.24	125.36	119.55
5	D	505	BCT	O2-C-O1	2.23	125.33	119.55
5	D	504	BCT	O2-C-O1	2.23	125.32	119.55
5	C	506	BCT	O2-C-O1	2.18	125.20	119.55
5	I	505	BCT	O2-C-O1	2.18	125.20	119.55

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	B	507	EDO	O1-C1-C2-O2
6	C	510	EDO	O1-C1-C2-O2
6	G	507	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.