



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:37 PM UTC

PDB ID : 2Q3U / pdb_00002q3u
Title : Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At5g08170, agmatine iminohydrolase
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-30
Resolution : 1.53 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	:	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

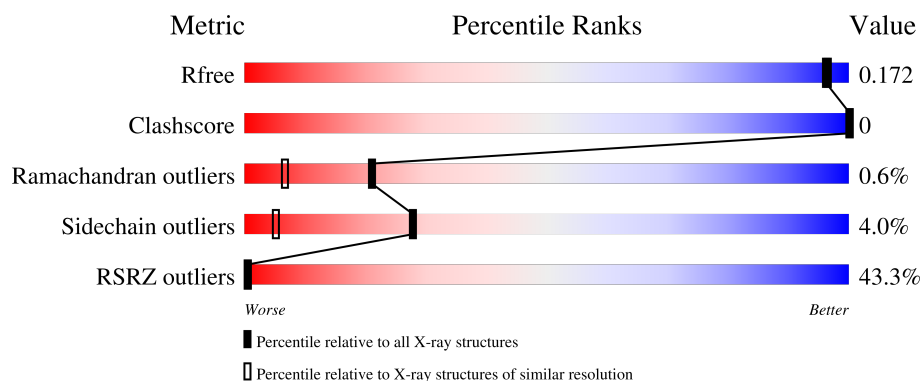
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 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.



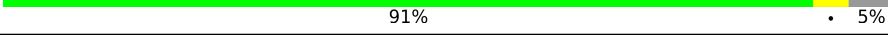
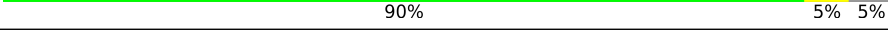
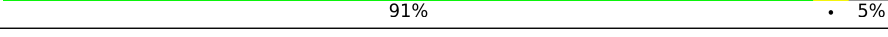
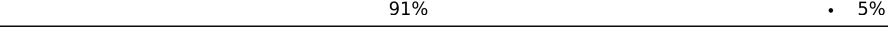
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	1-A	383	42% 91% 5%
1	1-B	383	39% 90% 5%
1	2-A	383	92% 5%
1	2-B	383	91% 5%
1	3-A	383	91% 5%

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Mol	Chain	Length	Quality of chain
1	3-B	383	 90% • 5%
1	4-A	383	 91% • 5%
1	4-B	383	 90% 5% 5%
1	5-A	383	 91% • 5%
1	5-B	383	 90% 5% 5%
1	6-A	383	 91% • 5%
1	6-B	383	 90% • 5%
1	7-A	383	 90% 5% 5%
1	7-B	383	 90% 5% 5%
1	8-A	383	 91% • 5%
1	8-B	383	 91% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 53040 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 Agmatine deiminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	365	Total	C	N	O	S	Se	0	0	0
			2902	1822	517	549	7	7			
1	2-A	365	Total	C	N	O	S	Se	0	0	0
			2902	1822	517	549	7	7			
1	3-A	365	Total	C	N	O	S	Se	0	0	0
			2902	1822	517	549	7	7			
1	4-A	365	Total	C	N	O	S	Se	0	0	0
			2902	1822	517	549	7	7			
1	5-A	365	Total	C	N	O	S	Se	0	0	0
			2902	1822	517	549	7	7			
1	6-A	365	Total	C	N	O	S	Se	0	0	0
			2902	1822	517	549	7	7			
1	7-A	365	Total	C	N	O	S	Se	0	0	0
			2902	1822	517	549	7	7			
1	8-A	365	Total	C	N	O	S	Se	0	0	0
			2902	1822	517	549	7	7			
1	1-B	363	Total	C	N	O	S	Se	0	0	0
			2882	1811	512	545	7	7			
1	2-B	363	Total	C	N	O	S	Se	0	0	0
			2882	1811	512	545	7	7			
1	3-B	363	Total	C	N	O	S	Se	0	0	0
			2882	1811	512	545	7	7			
1	4-B	363	Total	C	N	O	S	Se	0	0	0
			2882	1811	512	545	7	7			
1	5-B	363	Total	C	N	O	S	Se	0	0	0
			2882	1811	512	545	7	7			
1	6-B	363	Total	C	N	O	S	Se	0	0	0
			2882	1811	512	545	7	7			
1	7-B	363	Total	C	N	O	S	Se	0	0	0
			2882	1811	512	545	7	7			
1	8-B	363	Total	C	N	O	S	Se	0	0	0
			2882	1811	512	545	7	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q8GWW7
A	15	MSE	MET	modified residue	UNP Q8GWW7
A	49	GLY	ASP	variant	UNP Q8GWW7
A	85	MSE	MET	modified residue	UNP Q8GWW7
A	87	MSE	MET	modified residue	UNP Q8GWW7
A	159	MSE	MET	modified residue	UNP Q8GWW7
A	190	MSE	MET	modified residue	UNP Q8GWW7
A	228	MSE	MET	modified residue	UNP Q8GWW7
A	284	MSE	MET	modified residue	UNP Q8GWW7
B	1	MSE	MET	modified residue	UNP Q8GWW7
B	15	MSE	MET	modified residue	UNP Q8GWW7
B	49	GLY	ASP	variant	UNP Q8GWW7
B	85	MSE	MET	modified residue	UNP Q8GWW7
B	87	MSE	MET	modified residue	UNP Q8GWW7
B	159	MSE	MET	modified residue	UNP Q8GWW7
B	190	MSE	MET	modified residue	UNP Q8GWW7
B	228	MSE	MET	modified residue	UNP Q8GWW7
B	284	MSE	MET	modified residue	UNP Q8GWW7

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

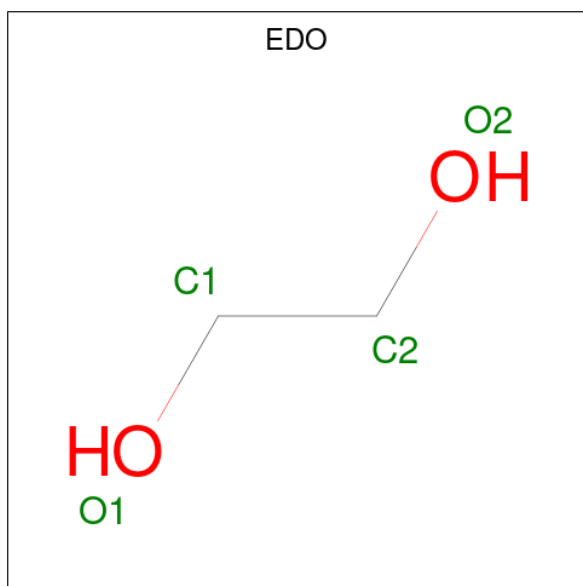
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	1	Total Mg 1 1	0	0
2	2-A	1	Total Mg 1 1	0	0
2	3-A	1	Total Mg 1 1	0	0
2	4-A	1	Total Mg 1 1	0	0
2	5-A	1	Total Mg 1 1	0	0
2	6-A	1	Total Mg 1 1	0	0
2	7-A	1	Total Mg 1 1	0	0
2	8-A	1	Total Mg 1 1	0	0
2	1-B	1	Total Mg 1 1	0	0
2	2-B	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	3-B	1	Total	Mg	0	0
			1	1		
2	4-B	1	Total	Mg	0	0
			1	1		
2	5-B	1	Total	Mg	0	0
			1	1		
2	6-B	1	Total	Mg	0	0
			1	1		
2	7-B	1	Total	Mg	0	0
			1	1		
2	8-B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1-A	1	Total	C	O	0	0
			4	2	2		
3	2-A	1	Total	C	O	0	0
			4	2	2		
3	3-A	1	Total	C	O	0	0
			4	2	2		
3	4-A	1	Total	C	O	0	0
			4	2	2		
3	5-A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	6-A	1	Total 4	C 2	O 2	0	0
3	7-A	1	Total 4	C 2	O 2	0	0
3	8-A	1	Total 4	C 2	O 2	0	0
3	1-A	1	Total 4	C 2	O 2	0	0
3	2-A	1	Total 4	C 2	O 2	0	0
3	3-A	1	Total 4	C 2	O 2	0	0
3	4-A	1	Total 4	C 2	O 2	0	0
3	5-A	1	Total 4	C 2	O 2	0	0
3	6-A	1	Total 4	C 2	O 2	0	0
3	7-A	1	Total 4	C 2	O 2	0	0
3	8-A	1	Total 4	C 2	O 2	0	0
3	1-A	1	Total 4	C 2	O 2	0	0
3	2-A	1	Total 4	C 2	O 2	0	0
3	3-A	1	Total 4	C 2	O 2	0	0
3	4-A	1	Total 4	C 2	O 2	0	0
3	5-A	1	Total 4	C 2	O 2	0	0
3	6-A	1	Total 4	C 2	O 2	0	0
3	7-A	1	Total 4	C 2	O 2	0	0
3	8-A	1	Total 4	C 2	O 2	0	0
3	1-A	1	Total 4	C 2	O 2	0	0
3	2-A	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	3-A	1	Total 4	C 2	O 2	0	0
3	4-A	1	Total 4	C 2	O 2	0	0
3	5-A	1	Total 4	C 2	O 2	0	0
3	6-A	1	Total 4	C 2	O 2	0	0
3	7-A	1	Total 4	C 2	O 2	0	0
3	8-A	1	Total 4	C 2	O 2	0	0
3	1-A	1	Total 4	C 2	O 2	0	0
3	2-A	1	Total 4	C 2	O 2	0	0
3	3-A	1	Total 4	C 2	O 2	0	0
3	4-A	1	Total 4	C 2	O 2	0	0
3	5-A	1	Total 4	C 2	O 2	0	0
3	6-A	1	Total 4	C 2	O 2	0	0
3	7-A	1	Total 4	C 2	O 2	0	0
3	8-A	1	Total 4	C 2	O 2	0	0
3	1-A	1	Total 4	C 2	O 2	0	0
3	2-A	1	Total 4	C 2	O 2	0	0
3	3-A	1	Total 4	C 2	O 2	0	0
3	4-A	1	Total 4	C 2	O 2	0	0
3	5-A	1	Total 4	C 2	O 2	0	0
3	6-A	1	Total 4	C 2	O 2	0	0
3	7-A	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	8-A	1	Total 4	C 2	O 2	0	0
3	1-A	1	Total 4	C 2	O 2	0	0
3	2-A	1	Total 4	C 2	O 2	0	0
3	3-A	1	Total 4	C 2	O 2	0	0
3	4-A	1	Total 4	C 2	O 2	0	0
3	5-A	1	Total 4	C 2	O 2	0	0
3	6-A	1	Total 4	C 2	O 2	0	0
3	7-A	1	Total 4	C 2	O 2	0	0
3	8-A	1	Total 4	C 2	O 2	0	0
3	1-B	1	Total 4	C 2	O 2	0	0
3	2-B	1	Total 4	C 2	O 2	0	0
3	3-B	1	Total 4	C 2	O 2	0	0
3	4-B	1	Total 4	C 2	O 2	0	0
3	5-B	1	Total 4	C 2	O 2	0	0
3	6-B	1	Total 4	C 2	O 2	0	0
3	7-B	1	Total 4	C 2	O 2	0	0
3	8-B	1	Total 4	C 2	O 2	0	0
3	1-B	1	Total 4	C 2	O 2	0	0
3	2-B	1	Total 4	C 2	O 2	0	0
3	3-B	1	Total 4	C 2	O 2	0	0
3	4-B	1	Total 4	C 2	O 2	0	0

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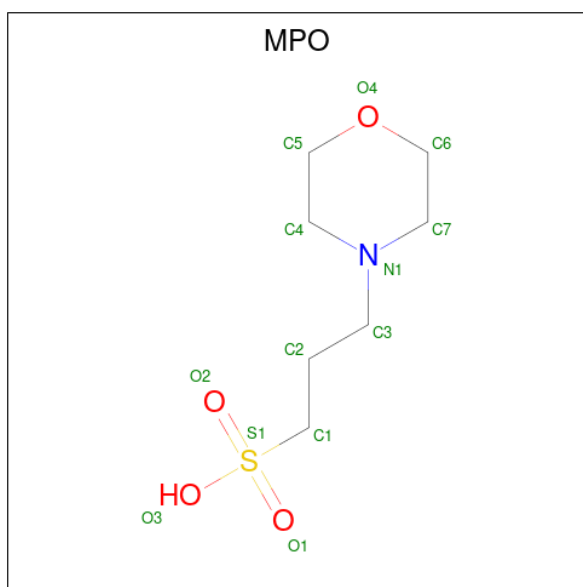
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	5-B	1	Total 4	C 2	O 2	0	0
3	6-B	1	Total 4	C 2	O 2	0	0
3	7-B	1	Total 4	C 2	O 2	0	0
3	8-B	1	Total 4	C 2	O 2	0	0
3	1-B	1	Total 4	C 2	O 2	0	0
3	2-B	1	Total 4	C 2	O 2	0	0
3	3-B	1	Total 4	C 2	O 2	0	0
3	4-B	1	Total 4	C 2	O 2	0	0
3	5-B	1	Total 4	C 2	O 2	0	0
3	6-B	1	Total 4	C 2	O 2	0	0
3	7-B	1	Total 4	C 2	O 2	0	0
3	8-B	1	Total 4	C 2	O 2	0	0
3	1-B	1	Total 4	C 2	O 2	0	0
3	2-B	1	Total 4	C 2	O 2	0	0
3	3-B	1	Total 4	C 2	O 2	0	0
3	4-B	1	Total 4	C 2	O 2	0	0
3	5-B	1	Total 4	C 2	O 2	0	0
3	6-B	1	Total 4	C 2	O 2	0	0
3	7-B	1	Total 4	C 2	O 2	0	0
3	8-B	1	Total 4	C 2	O 2	0	0
3	1-B	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	2-B	1	Total	C	O	0	0
			4	2	2		
3	3-B	1	Total	C	O	0	0
			4	2	2		
3	4-B	1	Total	C	O	0	0
			4	2	2		
3	5-B	1	Total	C	O	0	0
			4	2	2		
3	6-B	1	Total	C	O	0	0
			4	2	2		
3	7-B	1	Total	C	O	0	0
			4	2	2		
3	8-B	1	Total	C	O	0	0
			4	2	2		
3	1-B	1	Total	C	O	0	0
			4	2	2		
3	2-B	1	Total	C	O	0	0
			4	2	2		
3	3-B	1	Total	C	O	0	0
			4	2	2		
3	4-B	1	Total	C	O	0	0
			4	2	2		
3	5-B	1	Total	C	O	0	0
			4	2	2		
3	6-B	1	Total	C	O	0	0
			4	2	2		
3	7-B	1	Total	C	O	0	0
			4	2	2		
3	8-B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: C₇H₁₅NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	1-A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	2-A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	3-A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	4-A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	5-A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	6-A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	7-A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	8-A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-A	404	Total	O	0	0
			404	404		
5	2-A	409	Total	O	0	0
			409	409		
5	3-A	404	Total	O	0	0
			404	404		
5	4-A	410	Total	O	0	0
			410	410		

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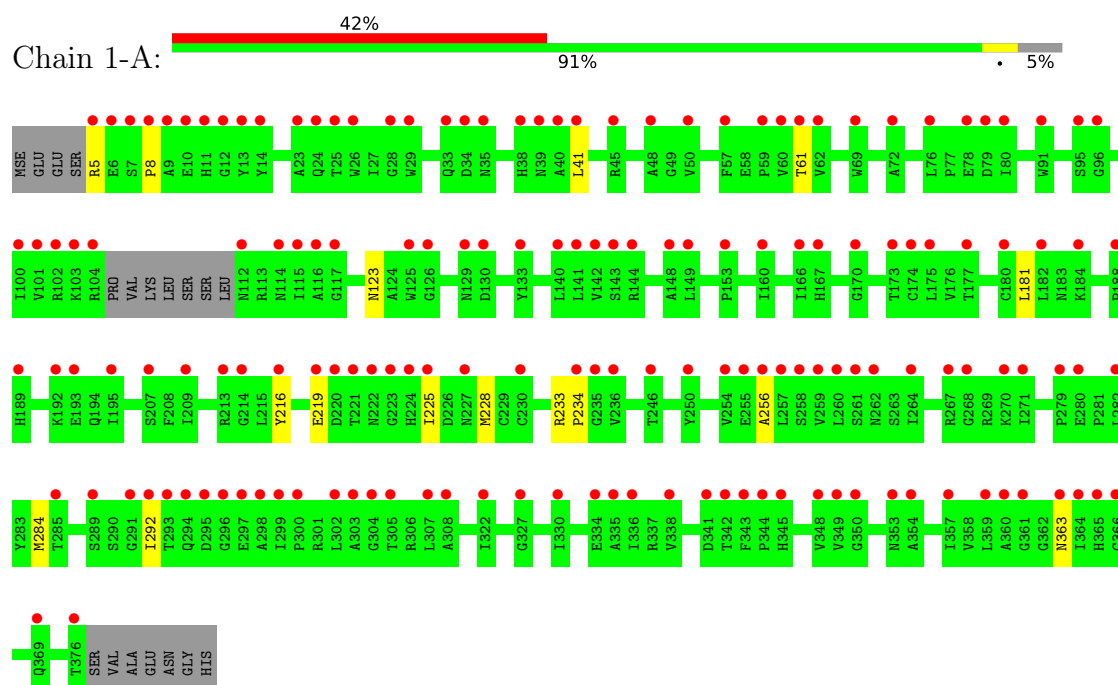
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	5-A	407	Total 407	O 407	0	0
5	6-A	403	Total 403	O 403	0	0
5	7-A	405	Total 405	O 405	0	0
5	8-A	409	Total 409	O 409	0	0
5	1-B	375	Total 375	O 375	0	0
5	2-B	370	Total 370	O 370	0	0
5	3-B	375	Total 375	O 375	0	0
5	4-B	369	Total 369	O 369	0	0
5	5-B	372	Total 372	O 372	0	0
5	6-B	376	Total 376	O 376	0	0
5	7-B	374	Total 374	O 374	0	0
5	8-B	370	Total 370	O 370	0	0

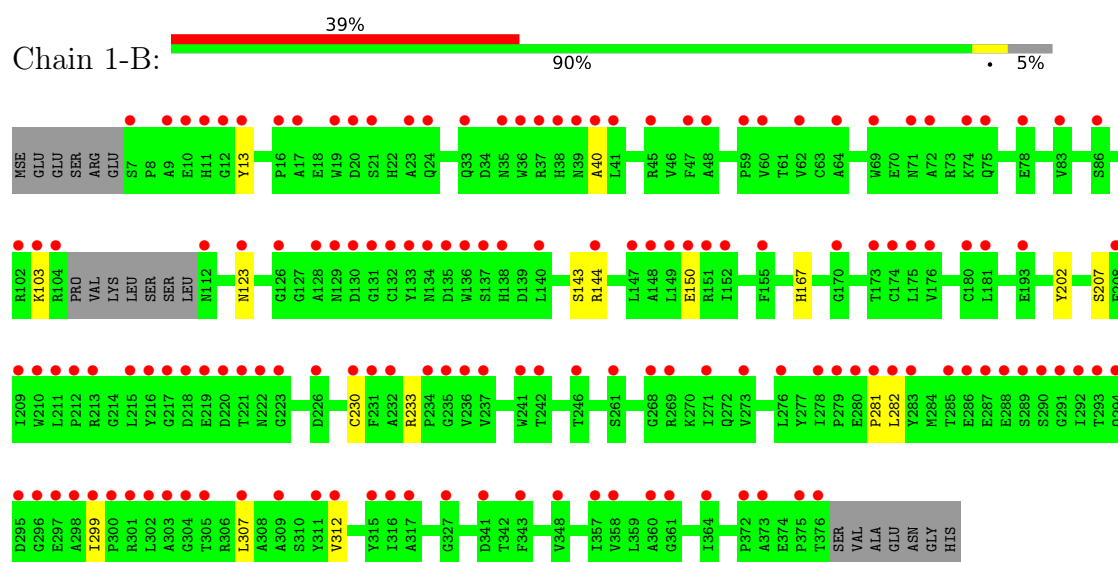
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Agmatine deiminase



• Molecule 1: Agmatine deiminase



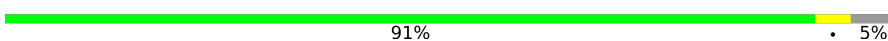
• Molecule 1: Agmatine deiminase

Chain 2-A:  92% • 5%

• Molecule 1: Agmatine deiminase

Chain 2-B:  91% • 5%

• Molecule 1: Agmatine deiminase

Chain 3-A:  91% • 5%

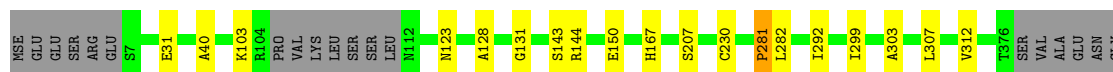
• Molecule 1: Agmatine deiminase

Chain 3-B:  90% • 5%

• Molecule 1: Agmatine deiminase

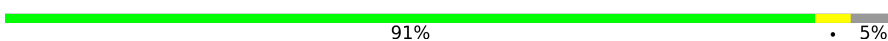
Chain 4-A:  91% • 5%

• Molecule 1: Agmatine deiminase

Chain 4-B:  90% 5% 5%

HIS

• Molecule 1: Agmatine deiminase

Chain 5-A:  91% • 5%



- Molecule 1: Agmatine deiminase

Chain 5-B: 90% 5% 5%



- Molecule 1: Agmatine deiminase

Chain 6-A: 91% 5% 5%



- Molecule 1: Agmatine deiminase

Chain 6-B: 90% 5% 5%



- Molecule 1: Agmatine deiminase

Chain 7-A: 90% 5% 5%



- Molecule 1: Agmatine deiminase

Chain 7-B: 90% 5% 5%



- Molecule 1: Agmatine deiminase

Chain 8-A: 91% 5% 5%



- Molecule 1: Agmatine deiminase

Chain 8-B: 91% 5% 5%

MSE	GLU	GLU	SER	ARG	GLU	S7	W19	A40	K103	R104	PRO	VAL	LYS	LEU	SER	SER	LEU	N112	N123	S143	R144	E150	H167	Y202	S207	C230	P281	L282	I299	L307	V312	T376	SER	VAL	ALA	GLU	ASN	GLY	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.02Å 115.81Å 66.63Å 90.00° 97.10° 90.00°	Depositor
Resolution (Å)	19.87 – 1.53 19.87 – 1.53	Depositor EDS
% Data completeness (in resolution range)	91.8 (19.87-1.53) 91.9 (19.87-1.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 1.53Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.135 , 0.171 0.139 , 0.172	Depositor DCC
R_{free} test set	6038 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.05 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	53040	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, MPO, MG

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	1-A	0.72	1/2968 (0.0%)	0.49	0/4021
1	1-B	0.70	1/2948 (0.0%)	0.51	0/3995
1	2-A	0.72	1/2968 (0.0%)	0.49	0/4021
1	2-B	0.70	1/2948 (0.0%)	0.51	0/3995
1	3-A	0.72	1/2968 (0.0%)	0.49	0/4021
1	3-B	0.70	1/2948 (0.0%)	0.51	0/3995
1	4-A	0.72	1/2968 (0.0%)	0.49	0/4021
1	4-B	0.70	1/2948 (0.0%)	0.51	0/3995
1	5-A	0.72	1/2968 (0.0%)	0.49	0/4021
1	5-B	0.70	1/2948 (0.0%)	0.51	0/3995
1	6-A	0.72	1/2968 (0.0%)	0.49	0/4021
1	6-B	0.70	1/2948 (0.0%)	0.51	0/3995
1	7-A	0.72	1/2968 (0.0%)	0.49	0/4021
1	7-B	0.70	1/2948 (0.0%)	0.51	0/3995
1	8-A	0.72	1/2968 (0.0%)	0.49	0/4021
1	8-B	0.70	1/2948 (0.0%)	0.51	0/3995
All	All	0.71	16/47328 (0.0%)	0.50	0/64128

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	1
1	1-B	0	2
1	2-A	0	1
1	3-B	0	1
1	4-A	0	2
1	5-A	0	2
1	5-B	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	6-B	0	1
1	7-A	0	2
1	7-B	0	2
1	8-A	0	2
1	8-B	0	1
All	All	0	19

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	256	ALA	CA-CB	5.52	1.62	1.53
1	2-A	256	ALA	CA-CB	5.52	1.62	1.53
1	3-A	256	ALA	CA-CB	5.52	1.62	1.53
1	4-A	256	ALA	CA-CB	5.52	1.62	1.53
1	5-A	256	ALA	CA-CB	5.52	1.62	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	216	TYR	Sidechain
1	1-B	13	TYR	Sidechain
1	1-B	202	TYR	Sidechain
1	2-A	311	TYR	Sidechain
1	3-B	315	TYR	Sidechain

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	1-A	2902	0	2786	0	0
1	1-B	2882	0	2767	0	0
1	2-A	2902	0	2786	0	0
1	2-B	2882	0	2767	0	0
1	3-A	2902	0	2786	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3-B	2882	0	2767	0	0
1	4-A	2902	0	2786	0	0
1	4-B	2882	0	2767	0	0
1	5-A	2902	0	2786	0	0
1	5-B	2882	0	2767	0	0
1	6-A	2902	0	2786	0	0
1	6-B	2882	0	2767	0	0
1	7-A	2902	0	2786	0	0
1	7-B	2882	0	2767	0	0
1	8-A	2902	0	2786	0	0
1	8-B	2882	0	2767	0	0
2	1-A	1	0	0	0	0
2	1-B	1	0	0	0	0
2	2-A	1	0	0	0	0
2	2-B	1	0	0	0	0
2	3-A	1	0	0	0	0
2	3-B	1	0	0	0	0
2	4-A	1	0	0	0	0
2	4-B	1	0	0	0	0
2	5-A	1	0	0	0	0
2	5-B	1	0	0	0	0
2	6-A	1	0	0	0	0
2	6-B	1	0	0	0	0
2	7-A	1	0	0	0	0
2	7-B	1	0	0	0	0
2	8-A	1	0	0	0	0
2	8-B	1	0	0	0	0
3	1-A	28	0	42	0	0
3	1-B	24	0	36	0	0
3	2-A	28	0	42	0	0
3	2-B	24	0	36	0	0
3	3-A	28	0	42	0	0
3	3-B	24	0	36	0	0
3	4-A	28	0	42	0	0
3	4-B	24	0	36	0	0
3	5-A	28	0	42	0	0
3	5-B	24	0	36	0	0
3	6-A	28	0	42	0	0
3	6-B	24	0	36	0	0
3	7-A	28	0	42	0	0
3	7-B	24	0	36	0	0
3	8-A	28	0	42	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	8-B	24	0	36	0	0
4	1-A	13	0	15	0	0
4	2-A	13	0	15	0	0
4	3-A	13	0	15	0	0
4	4-A	13	0	15	0	0
4	5-A	13	0	15	0	0
4	6-A	13	0	15	0	0
4	7-A	13	0	15	0	0
4	8-A	13	0	15	0	0
5	1-A	404	0	0	0	0
5	1-B	375	0	0	0	0
5	2-A	409	0	0	0	0
5	2-B	370	0	0	0	0
5	3-A	404	0	0	0	0
5	3-B	375	0	0	0	0
5	4-A	410	0	0	0	0
5	4-B	369	0	0	0	0
5	5-A	407	0	0	0	0
5	5-B	372	0	0	0	0
5	6-A	403	0	0	0	0
5	6-B	376	0	0	0	0
5	7-A	405	0	0	0	0
5	7-B	374	0	0	0	0
5	8-A	409	0	0	0	0
5	8-B	370	0	0	0	0
All	All	53040	0	45168	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	361/383 (94%)	342 (95%)	17 (5%)	2 (1%)	21	7
1	1-B	359/383 (94%)	336 (94%)	22 (6%)	1 (0%)	36	19
1	2-A	361/383 (94%)	346 (96%)	15 (4%)	0	100	100
1	2-B	359/383 (94%)	336 (94%)	21 (6%)	2 (1%)	21	7
1	3-A	361/383 (94%)	342 (95%)	16 (4%)	3 (1%)	16	3
1	3-B	359/383 (94%)	337 (94%)	20 (6%)	2 (1%)	21	7
1	4-A	361/383 (94%)	342 (95%)	18 (5%)	1 (0%)	36	19
1	4-B	359/383 (94%)	335 (93%)	18 (5%)	6 (2%)	7	1
1	5-A	361/383 (94%)	349 (97%)	11 (3%)	1 (0%)	36	19
1	5-B	359/383 (94%)	337 (94%)	20 (6%)	2 (1%)	21	7
1	6-A	361/383 (94%)	329 (91%)	30 (8%)	2 (1%)	21	7
1	6-B	359/383 (94%)	330 (92%)	26 (7%)	3 (1%)	16	3
1	7-A	361/383 (94%)	340 (94%)	17 (5%)	4 (1%)	11	2
1	7-B	359/383 (94%)	332 (92%)	24 (7%)	3 (1%)	16	3
1	8-A	361/383 (94%)	339 (94%)	20 (6%)	2 (1%)	21	7
1	8-B	359/383 (94%)	336 (94%)	22 (6%)	1 (0%)	36	19
All	All	5760/6128 (94%)	5408 (94%)	317 (6%)	35 (1%)	21	7

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3-A	318	ASN
1	8-A	318	ASN
1	2-B	318	ASN
1	3-B	322	ILE
1	4-B	292	ILE

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	1-A	310/318 (98%)	298 (96%)	12 (4%)	28	5
1	1-B	308/318 (97%)	295 (96%)	13 (4%)	26	4
1	2-A	310/318 (98%)	298 (96%)	12 (4%)	28	5
1	2-B	308/318 (97%)	295 (96%)	13 (4%)	26	4
1	3-A	310/318 (98%)	298 (96%)	12 (4%)	28	5
1	3-B	308/318 (97%)	295 (96%)	13 (4%)	26	4
1	4-A	310/318 (98%)	298 (96%)	12 (4%)	28	5
1	4-B	308/318 (97%)	295 (96%)	13 (4%)	26	4
1	5-A	310/318 (98%)	298 (96%)	12 (4%)	28	5
1	5-B	308/318 (97%)	295 (96%)	13 (4%)	26	4
1	6-A	310/318 (98%)	298 (96%)	12 (4%)	28	5
1	6-B	308/318 (97%)	295 (96%)	13 (4%)	26	4
1	7-A	310/318 (98%)	298 (96%)	12 (4%)	28	5
1	7-B	308/318 (97%)	295 (96%)	13 (4%)	26	4
1	8-A	310/318 (98%)	298 (96%)	12 (4%)	28	5
1	8-B	308/318 (97%)	295 (96%)	13 (4%)	26	4
All	All	4944/5088 (97%)	4744 (96%)	200 (4%)	28	5

5 of 200 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	5-B	144	ARG
1	6-B	207	SER
1	8-B	312	VAL
1	5-B	230	CYS
1	6-A	181	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 303 such sidechains are listed below:

Mol	Chain	Res	Type
1	7-A	44	GLN
1	8-B	112	ASN
1	7-A	206	GLN
1	7-B	325	GLN
1	8-B	363	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 128 ligands modelled in this entry, 16 are monoatomic - leaving 112 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	$\# Z > 2$
3	EDO	6-A	907	-	3,3,3	0.88	0	2,2,2	0.72	0
3	EDO	7-A	906	-	3,3,3	0.67	0	2,2,2	0.27	0
3	EDO	3-A	906	-	3,3,3	0.65	0	2,2,2	0.28	0
3	EDO	2-B	909	-	3,3,3	0.42	0	2,2,2	0.68	0
3	EDO	4-A	902	-	3,3,3	0.84	0	2,2,2	0.30	0
3	EDO	5-A	908	-	3,3,3	1.16	0	2,2,2	0.35	0
3	EDO	3-B	911	-	3,3,3	1.45	0	2,2,2	0.47	0
3	EDO	6-A	902	-	3,3,3	1.14	0	2,2,2	0.44	0
3	EDO	8-A	910	-	3,3,3	0.56	0	2,2,2	0.55	0
3	EDO	8-A	903	-	3,3,3	0.46	0	2,2,2	1.00	0
3	EDO	8-B	911	-	3,3,3	1.82	1 (33%)	2,2,2	0.52	0
3	EDO	4-B	912	-	3,3,3	1.08	0	2,2,2	0.55	0
4	MPO	3-A	9000	-	13,13,13	1.90	3 (23%)	17,17,17	5.71	8 (47%)
3	EDO	7-A	910	-	3,3,3	0.59	0	2,2,2	0.55	0
3	EDO	4-A	910	-	3,3,3	0.57	0	2,2,2	0.51	0
3	EDO	1-B	912	-	3,3,3	0.99	0	2,2,2	0.58	0
3	EDO	4-A	907	-	3,3,3	0.86	0	2,2,2	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	4-B	905	-	3,3,3	0.22	0	2,2,2	0.56	0
3	EDO	5-A	903	-	3,3,3	0.58	0	2,2,2	0.78	0
3	EDO	6-A	906	-	3,3,3	0.67	0	2,2,2	0.23	0
3	EDO	8-A	901	-	3,3,3	0.68	0	2,2,2	0.30	0
3	EDO	6-B	904	-	3,3,3	0.53	0	2,2,2	0.52	0
3	EDO	2-A	903	-	3,3,3	0.46	0	2,2,2	0.91	0
3	EDO	2-B	913	-	3,3,3	0.71	0	2,2,2	0.55	0
3	EDO	6-B	913	-	3,3,3	0.74	0	2,2,2	0.50	0
3	EDO	5-B	911	-	3,3,3	1.35	0	2,2,2	0.27	0
3	EDO	5-A	910	-	3,3,3	0.57	0	2,2,2	0.55	0
3	EDO	3-A	908	-	3,3,3	0.70	0	2,2,2	0.52	0
3	EDO	7-A	903	-	3,3,3	0.55	0	2,2,2	0.89	0
3	EDO	3-A	902	-	3,3,3	0.84	0	2,2,2	0.30	0
3	EDO	7-A	901	-	3,3,3	0.60	0	2,2,2	0.50	0
3	EDO	4-A	903	-	3,3,3	0.58	0	2,2,2	0.76	0
3	EDO	3-B	909	-	3,3,3	0.42	0	2,2,2	0.68	0
3	EDO	5-A	901	-	3,3,3	0.66	0	2,2,2	0.29	0
3	EDO	1-B	909	-	3,3,3	0.41	0	2,2,2	0.68	0
3	EDO	6-B	909	-	3,3,3	0.41	0	2,2,2	0.71	0
3	EDO	2-B	904	-	3,3,3	0.46	0	2,2,2	0.45	0
3	EDO	3-B	913	-	3,3,3	0.75	0	2,2,2	0.56	0
3	EDO	1-B	913	-	3,3,3	0.72	0	2,2,2	0.52	0
3	EDO	3-A	910	-	3,3,3	0.57	0	2,2,2	0.51	0
3	EDO	3-A	903	-	3,3,3	0.59	0	2,2,2	0.83	0
3	EDO	3-A	907	-	3,3,3	0.96	0	2,2,2	0.59	0
3	EDO	1-A	908	-	3,3,3	0.91	0	2,2,2	0.44	0
3	EDO	3-B	905	-	3,3,3	0.22	0	2,2,2	0.56	0
3	EDO	2-A	902	-	3,3,3	0.84	0	2,2,2	0.30	0
3	EDO	8-B	913	-	3,3,3	0.88	0	2,2,2	0.52	0
3	EDO	7-A	908	-	3,3,3	1.29	0	2,2,2	0.34	0
3	EDO	5-B	905	-	3,3,3	0.22	0	2,2,2	0.60	0
3	EDO	8-B	909	-	3,3,3	0.42	0	2,2,2	0.71	0
3	EDO	8-B	904	-	3,3,3	0.54	0	2,2,2	0.47	0
3	EDO	5-A	902	-	3,3,3	1.14	0	2,2,2	0.45	0
3	EDO	3-A	901	-	3,3,3	0.61	0	2,2,2	0.38	0
3	EDO	7-A	907	-	3,3,3	0.92	0	2,2,2	0.86	0
3	EDO	2-A	910	-	3,3,3	0.57	0	2,2,2	0.51	0
3	EDO	7-B	913	-	3,3,3	0.78	0	2,2,2	0.55	0
3	EDO	5-A	907	-	3,3,3	0.90	0	2,2,2	0.74	0
4	MPO	5-A	9000	-	13,13,13	2.56	4 (30%)	17,17,17	5.83	6 (35%)
3	EDO	1-A	910	-	3,3,3	0.57	0	2,2,2	0.51	0
3	EDO	6-A	908	-	3,3,3	1.26	0	2,2,2	0.35	0
3	EDO	1-A	906	-	3,3,3	0.65	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	6-B	912	-	3,3,3	1.10	0	2,2,2	0.61	0
3	EDO	4-B	909	-	3,3,3	0.41	0	2,2,2	0.68	0
3	EDO	1-B	904	-	3,3,3	0.44	0	2,2,2	0.46	0
3	EDO	1-A	902	-	3,3,3	0.84	0	2,2,2	0.30	0
3	EDO	1-A	903	-	3,3,3	0.59	0	2,2,2	0.83	0
3	EDO	8-A	907	-	3,3,3	0.88	0	2,2,2	0.73	0
4	MPO	7-A	9000	-	13,13,13	1.95	3 (23%)	17,17,17	5.81	8 (47%)
4	MPO	4-A	9000	-	13,13,13	3.80	5 (38%)	17,17,17	5.24	6 (35%)
3	EDO	2-A	908	-	3,3,3	0.69	0	2,2,2	0.43	0
3	EDO	8-A	902	-	3,3,3	1.14	0	2,2,2	0.45	0
3	EDO	8-A	906	-	3,3,3	0.66	0	2,2,2	0.23	0
3	EDO	4-A	901	-	3,3,3	0.56	0	2,2,2	0.32	0
3	EDO	1-B	911	-	3,3,3	0.83	0	2,2,2	0.45	0
3	EDO	2-A	907	-	3,3,3	0.85	0	2,2,2	0.80	0
3	EDO	8-B	905	-	3,3,3	0.22	0	2,2,2	0.59	0
3	EDO	5-B	904	-	3,3,3	0.45	0	2,2,2	0.55	0
3	EDO	5-B	913	-	3,3,3	0.87	0	2,2,2	0.63	0
3	EDO	5-A	906	-	3,3,3	0.66	0	2,2,2	0.28	0
3	EDO	1-B	905	-	3,3,3	0.22	0	2,2,2	0.60	0
3	EDO	2-B	905	-	3,3,3	0.22	0	2,2,2	0.58	0
3	EDO	3-B	904	-	3,3,3	0.42	0	2,2,2	0.48	0
3	EDO	2-A	906	-	3,3,3	0.66	0	2,2,2	0.28	0
3	EDO	2-B	911	-	3,3,3	1.51	1 (33%)	2,2,2	0.52	0
3	EDO	6-A	910	-	3,3,3	0.50	0	2,2,2	0.56	0
3	EDO	6-A	903	-	3,3,3	0.50	0	2,2,2	1.02	0
3	EDO	6-B	905	-	3,3,3	0.22	0	2,2,2	0.60	0
3	EDO	7-B	911	-	3,3,3	2.00	1 (33%)	2,2,2	0.64	0
3	EDO	5-B	912	-	3,3,3	1.08	0	2,2,2	0.59	0
3	EDO	4-A	906	-	3,3,3	0.66	0	2,2,2	0.28	0
3	EDO	7-B	904	-	3,3,3	0.43	0	2,2,2	0.47	0
3	EDO	2-A	901	-	3,3,3	0.63	0	2,2,2	0.33	0
4	MPO	8-A	9000	-	13,13,13	4.80	7 (53%)	17,17,17	5.25	6 (35%)
3	EDO	1-A	907	-	3,3,3	0.93	0	2,2,2	0.60	0
3	EDO	6-B	911	-	3,3,3	1.70	1 (33%)	2,2,2	0.53	0
3	EDO	4-B	913	-	3,3,3	0.74	0	2,2,2	0.55	0
4	MPO	6-A	9000	-	13,13,13	1.89	4 (30%)	17,17,17	5.85	9 (52%)
3	EDO	7-B	905	-	3,3,3	0.22	0	2,2,2	0.60	0
3	EDO	3-B	912	-	3,3,3	1.04	0	2,2,2	0.56	0
3	EDO	7-B	909	-	3,3,3	0.41	0	2,2,2	0.71	0
3	EDO	6-A	901	-	3,3,3	0.67	0	2,2,2	0.31	0
3	EDO	4-B	904	-	3,3,3	0.44	0	2,2,2	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	8-A	908	-	3,3,3	0.97	0	2,2,2	0.49	0
3	EDO	8-B	912	-	3,3,3	1.12	0	2,2,2	0.60	0
3	EDO	7-A	902	-	3,3,3	1.31	0	2,2,2	0.56	0
4	MPO	2-A	9000	-	13,13,13	1.64	2 (15%)	17,17,17	5.65	10 (58%)
3	EDO	4-B	911	-	3,3,3	1.56	1 (33%)	2,2,2	0.46	0
3	EDO	2-B	912	-	3,3,3	0.99	0	2,2,2	0.57	0
3	EDO	5-B	909	-	3,3,3	0.41	0	2,2,2	0.71	0
3	EDO	7-B	912	-	3,3,3	1.13	0	2,2,2	0.58	0
4	MPO	1-A	9000	-	13,13,13	3.79	6 (46%)	17,17,17	5.24	5 (29%)
3	EDO	1-A	901	-	3,3,3	0.61	0	2,2,2	0.34	0
3	EDO	4-A	908	-	3,3,3	1.16	0	2,2,2	0.28	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
3	EDO	6-A	907	-	-	0/1/1/1	-
3	EDO	7-A	906	-	-	1/1/1/1	-
3	EDO	3-A	906	-	-	1/1/1/1	-
3	EDO	2-B	909	-	-	1/1/1/1	-
3	EDO	4-A	902	-	-	0/1/1/1	-
3	EDO	5-A	908	-	-	0/1/1/1	-
3	EDO	3-B	911	-	-	1/1/1/1	-
3	EDO	6-A	902	-	-	0/1/1/1	-
3	EDO	8-A	910	-	-	1/1/1/1	-
3	EDO	8-A	903	-	-	1/1/1/1	-
3	EDO	8-B	911	-	-	1/1/1/1	-
3	EDO	4-B	912	-	-	1/1/1/1	-
4	MPO	3-A	9000	-	-	2/7/15/15	0/1/1/1
3	EDO	7-A	910	-	-	1/1/1/1	-
3	EDO	4-A	910	-	-	1/1/1/1	-
3	EDO	1-B	912	-	-	1/1/1/1	-
3	EDO	4-A	907	-	-	1/1/1/1	-
3	EDO	4-B	905	-	-	0/1/1/1	-
3	EDO	5-A	903	-	-	1/1/1/1	-
3	EDO	6-A	906	-	-	1/1/1/1	-
3	EDO	8-A	901	-	-	1/1/1/1	-
3	EDO	6-B	904	-	-	1/1/1/1	-
3	EDO	2-A	903	-	-	1/1/1/1	-
3	EDO	2-B	913	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	6-B	913	-	-	1/1/1/1	-
3	EDO	5-B	911	-	-	1/1/1/1	-
3	EDO	5-A	910	-	-	1/1/1/1	-
3	EDO	3-A	908	-	-	1/1/1/1	-
3	EDO	7-A	903	-	-	1/1/1/1	-
3	EDO	3-A	902	-	-	0/1/1/1	-
3	EDO	7-A	901	-	-	0/1/1/1	-
3	EDO	4-A	903	-	-	1/1/1/1	-
3	EDO	3-B	909	-	-	1/1/1/1	-
3	EDO	5-A	901	-	-	1/1/1/1	-
3	EDO	1-B	909	-	-	1/1/1/1	-
3	EDO	6-B	909	-	-	1/1/1/1	-
3	EDO	2-B	904	-	-	1/1/1/1	-
3	EDO	3-B	913	-	-	0/1/1/1	-
3	EDO	1-B	913	-	-	1/1/1/1	-
3	EDO	3-A	910	-	-	1/1/1/1	-
3	EDO	3-A	903	-	-	1/1/1/1	-
3	EDO	3-A	907	-	-	0/1/1/1	-
3	EDO	1-A	908	-	-	1/1/1/1	-
3	EDO	3-B	905	-	-	0/1/1/1	-
3	EDO	2-A	902	-	-	0/1/1/1	-
3	EDO	8-B	913	-	-	1/1/1/1	-
3	EDO	7-A	908	-	-	1/1/1/1	-
3	EDO	5-B	905	-	-	0/1/1/1	-
3	EDO	8-B	909	-	-	1/1/1/1	-
3	EDO	8-B	904	-	-	1/1/1/1	-
3	EDO	5-A	902	-	-	0/1/1/1	-
3	EDO	3-A	901	-	-	1/1/1/1	-
3	EDO	7-A	907	-	-	1/1/1/1	-
3	EDO	2-A	910	-	-	1/1/1/1	-
3	EDO	7-B	913	-	-	0/1/1/1	-
3	EDO	5-A	907	-	-	0/1/1/1	-
4	MPO	5-A	9000	-	-	2/7/15/15	0/1/1/1
3	EDO	1-A	910	-	-	1/1/1/1	-
3	EDO	6-A	908	-	-	0/1/1/1	-
3	EDO	1-A	906	-	-	1/1/1/1	-
3	EDO	6-B	912	-	-	1/1/1/1	-
3	EDO	4-B	909	-	-	1/1/1/1	-
3	EDO	1-B	904	-	-	1/1/1/1	-
3	EDO	1-A	902	-	-	0/1/1/1	-
3	EDO	1-A	903	-	-	1/1/1/1	-
3	EDO	8-A	907	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPO	7-A	9000	-	-	2/7/15/15	0/1/1/1
4	MPO	4-A	9000	-	-	2/7/15/15	0/1/1/1
3	EDO	2-A	908	-	-	0/1/1/1	-
3	EDO	8-A	902	-	-	0/1/1/1	-
3	EDO	8-A	906	-	-	1/1/1/1	-
3	EDO	4-A	901	-	-	1/1/1/1	-
3	EDO	1-B	911	-	-	1/1/1/1	-
3	EDO	2-A	907	-	-	0/1/1/1	-
3	EDO	8-B	905	-	-	0/1/1/1	-
3	EDO	5-B	904	-	-	1/1/1/1	-
3	EDO	5-B	913	-	-	1/1/1/1	-
3	EDO	5-A	906	-	-	1/1/1/1	-
3	EDO	1-B	905	-	-	0/1/1/1	-
3	EDO	2-B	905	-	-	0/1/1/1	-
3	EDO	3-B	904	-	-	1/1/1/1	-
3	EDO	2-A	906	-	-	1/1/1/1	-
3	EDO	2-B	911	-	-	1/1/1/1	-
3	EDO	6-A	910	-	-	1/1/1/1	-
3	EDO	6-A	903	-	-	1/1/1/1	-
3	EDO	6-B	905	-	-	0/1/1/1	-
3	EDO	7-B	911	-	-	1/1/1/1	-
3	EDO	5-B	912	-	-	1/1/1/1	-
3	EDO	4-A	906	-	-	1/1/1/1	-
3	EDO	7-B	904	-	-	1/1/1/1	-
3	EDO	2-A	901	-	-	1/1/1/1	-
4	MPO	8-A	9000	-	-	2/7/15/15	0/1/1/1
3	EDO	1-A	907	-	-	0/1/1/1	-
3	EDO	6-B	911	-	-	1/1/1/1	-
3	EDO	4-B	913	-	-	0/1/1/1	-
4	MPO	6-A	9000	-	-	2/7/15/15	0/1/1/1
3	EDO	7-B	905	-	-	0/1/1/1	-
3	EDO	3-B	912	-	-	1/1/1/1	-
3	EDO	7-B	909	-	-	1/1/1/1	-
3	EDO	6-A	901	-	-	1/1/1/1	-
3	EDO	4-B	904	-	-	1/1/1/1	-
3	EDO	8-A	908	-	-	1/1/1/1	-
3	EDO	8-B	912	-	-	1/1/1/1	-
3	EDO	7-A	902	-	-	0/1/1/1	-
4	MPO	2-A	9000	-	-	2/7/15/15	0/1/1/1
3	EDO	4-B	911	-	-	1/1/1/1	-
3	EDO	2-B	912	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	5-B	909	-	-	1/1/1/1	-
3	EDO	7-B	912	-	-	1/1/1/1	-
4	MPO	1-A	9000	-	-	2/7/15/15	0/1/1/1
3	EDO	1-A	901	-	-	1/1/1/1	-
3	EDO	4-A	908	-	-	0/1/1/1	-

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	8-A	9000	MPO	C1-S1	14.89	1.98	1.77
4	1-A	9000	MPO	C1-S1	11.62	1.93	1.77
4	4-A	9000	MPO	C1-S1	11.38	1.93	1.77
4	5-A	9000	MPO	C1-S1	5.57	1.85	1.77
4	8-A	9000	MPO	O1-S1	5.12	1.59	1.45

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5-A	9000	MPO	O3-S1-C1	-15.60	75.50	106.00
4	7-A	9000	MPO	O3-S1-O1	-15.46	72.72	111.40
4	6-A	9000	MPO	O3-S1-C1	-14.38	77.86	106.00
4	1-A	9000	MPO	O3-S1-O1	-14.01	76.36	111.40
4	3-A	9000	MPO	O3-S1-O1	-13.47	77.70	111.40

There are no chirality outliers.

5 of 89 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	2-A	9000	MPO	C2-C1-S1-O1
4	4-A	9000	MPO	C2-C1-S1-O1
4	8-A	9000	MPO	C2-C1-S1-O1
3	1-B	911	EDO	O1-C1-C2-O2
3	3-B	912	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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, 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	1-A	358/383 (93%)	2.14	160 (44%) 0 0	1, 2, 4, 7	358 (100%)
1	1-B	356/383 (92%)	2.08	149 (41%) 0 0	1, 2, 6, 9	356 (100%)
1	2-A	0/383	-	-	-	-
1	2-B	0/383	-	-	-	-
1	3-A	0/383	-	-	-	-
1	3-B	0/383	-	-	-	-
1	4-A	0/383	-	-	-	-
1	4-B	0/383	-	-	-	-
1	5-A	0/383	-	-	-	-
1	5-B	0/383	-	-	-	-
1	6-A	0/383	-	-	-	-
1	6-B	0/383	-	-	-	-
1	7-A	0/383	-	-	-	-
1	7-B	0/383	-	-	-	-
1	8-A	0/383	-	-	-	-
1	8-B	0/383	-	-	-	-
All	All	714/6128 (11%)	2.11	309 (43%) 0 0	1, 2, 5, 9	714 (100%)

The worst 5 of 309 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	174	CYS	9.2
1	1-B	299	ILE	9.0
1	1-A	304	GLY	8.1
1	1-B	300	PRO	7.1
1	1-B	71	ASN	7.0

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
3	EDO	1-A	908	4/4	0.57	0.32	27,31,31,43	4
2	MG	2-A	802	1/1	-	-	15,15,15,15	1
2	MG	3-A	802	1/1	-	-	12,12,12,12	1
2	MG	4-A	802	1/1	-	-	12,12,12,12	1
2	MG	5-A	802	1/1	-	-	15,15,15,15	1
2	MG	6-A	802	1/1	-	-	20,20,20,20	1
2	MG	7-A	802	1/1	-	-	15,15,15,15	1
2	MG	8-A	802	1/1	-	-	17,17,17,17	1
4	MPO	1-A	9000	13/13	0.59	0.24	38,46,55,55	13
2	MG	2-B	801	1/1	-	-	15,15,15,15	1
2	MG	3-B	801	1/1	-	-	15,15,15,15	1
2	MG	4-B	801	1/1	-	-	15,15,15,15	1
2	MG	5-B	801	1/1	-	-	20,20,20,20	1
2	MG	6-B	801	1/1	-	-	18,18,18,18	1
2	MG	7-B	801	1/1	-	-	19,19,19,19	1
2	MG	8-B	801	1/1	-	-	17,17,17,17	1
3	EDO	1-B	912	4/4	0.64	0.23	31,34,36,38	4
3	EDO	2-A	901	4/4	-	-	32,33,33,35	4
3	EDO	3-A	901	4/4	-	-	32,33,33,35	4
3	EDO	4-A	901	4/4	-	-	32,33,33,35	4
3	EDO	5-A	901	4/4	-	-	32,33,33,35	4
3	EDO	6-A	901	4/4	-	-	32,33,33,35	4
3	EDO	7-A	901	4/4	-	-	32,33,33,35	4
3	EDO	8-A	901	4/4	-	-	32,33,33,35	4
3	EDO	1-B	911	4/4	0.71	0.22	21,28,31,36	4
3	EDO	2-A	902	4/4	-	-	27,27,29,33	4
3	EDO	3-A	902	4/4	-	-	27,27,29,33	4
3	EDO	4-A	902	4/4	-	-	27,27,29,33	4
3	EDO	5-A	902	4/4	-	-	27,28,29,33	4
3	EDO	6-A	902	4/4	-	-	27,28,29,33	4
3	EDO	7-A	902	4/4	-	-	27,27,30,33	4
3	EDO	8-A	902	4/4	-	-	27,28,29,33	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	1-A	906	4/4	0.74	0.22	41,42,43,44	4
3	EDO	2-A	903	4/4	-	-	43,44,48,50	4
3	EDO	3-A	903	4/4	-	-	43,43,48,50	4
3	EDO	4-A	903	4/4	-	-	43,43,48,50	4
3	EDO	5-A	903	4/4	-	-	43,43,48,50	4
3	EDO	6-A	903	4/4	-	-	43,44,48,50	4
3	EDO	7-A	903	4/4	-	-	43,43,48,50	4
3	EDO	8-A	903	4/4	-	-	43,44,48,50	4
3	EDO	1-B	909	4/4	0.76	0.21	41,42,45,47	4
3	EDO	2-A	906	4/4	-	-	41,42,43,44	4
3	EDO	3-A	906	4/4	-	-	41,42,43,44	4
3	EDO	4-A	906	4/4	-	-	41,42,43,44	4
3	EDO	5-A	906	4/4	-	-	41,42,43,44	4
3	EDO	6-A	906	4/4	-	-	41,42,43,44	4
3	EDO	7-A	906	4/4	-	-	41,42,43,44	4
3	EDO	8-A	906	4/4	-	-	41,42,43,44	4
3	EDO	1-A	903	4/4	0.77	0.21	43,43,48,50	4
3	EDO	2-A	907	4/4	-	-	27,31,32,32	4
3	EDO	3-A	907	4/4	-	-	27,30,32,32	4
3	EDO	4-A	907	4/4	-	-	27,31,32,32	4
3	EDO	5-A	907	4/4	-	-	27,31,32,32	4
3	EDO	6-A	907	4/4	-	-	27,31,32,32	4
3	EDO	7-A	907	4/4	-	-	27,31,32,32	4
3	EDO	8-A	907	4/4	-	-	27,30,32,32	4
3	EDO	1-B	904	4/4	0.78	0.21	35,37,38,41	4
3	EDO	2-A	908	4/4	-	-	27,31,31,43	4
3	EDO	3-A	908	4/4	-	-	27,30,31,43	4
3	EDO	4-A	908	4/4	-	-	27,30,31,43	4
3	EDO	5-A	908	4/4	-	-	27,30,31,43	4
3	EDO	6-A	908	4/4	-	-	27,30,31,43	4
3	EDO	7-A	908	4/4	-	-	27,30,31,43	4
3	EDO	8-A	908	4/4	-	-	27,30,31,43	4
3	EDO	1-B	913	4/4	0.78	0.17	29,31,34,37	4
3	EDO	2-A	910	4/4	-	-	42,47,47,48	4
3	EDO	3-A	910	4/4	-	-	42,47,47,48	4
3	EDO	4-A	910	4/4	-	-	42,47,47,48	4
3	EDO	5-A	910	4/4	-	-	42,47,47,48	4
3	EDO	6-A	910	4/4	-	-	42,47,47,48	4
3	EDO	7-A	910	4/4	-	-	42,47,47,48	4
3	EDO	8-A	910	4/4	-	-	42,47,47,48	4
3	EDO	1-B	905	4/4	0.78	0.15	35,36,39,39	4
3	EDO	2-B	904	4/4	-	-	35,37,38,41	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	3-B	904	4/4	-	-	35,37,38,41	4
3	EDO	4-B	904	4/4	-	-	35,37,38,41	4
3	EDO	5-B	904	4/4	-	-	35,37,38,41	4
3	EDO	6-B	904	4/4	-	-	35,37,38,41	4
3	EDO	7-B	904	4/4	-	-	35,37,38,41	4
3	EDO	8-B	904	4/4	-	-	35,37,38,41	4
2	MG	1-B	801	1/1	0.84	0.12	15,15,15,15	1
3	EDO	2-B	905	4/4	-	-	35,36,39,39	4
3	EDO	3-B	905	4/4	-	-	35,36,39,39	4
3	EDO	4-B	905	4/4	-	-	35,36,39,39	4
3	EDO	5-B	905	4/4	-	-	35,36,39,39	4
3	EDO	6-B	905	4/4	-	-	35,36,39,39	4
3	EDO	7-B	905	4/4	-	-	35,36,39,39	4
3	EDO	8-B	905	4/4	-	-	35,36,39,39	4
3	EDO	1-A	901	4/4	0.85	0.15	32,33,33,35	4
3	EDO	2-B	909	4/4	-	-	41,42,45,47	4
3	EDO	3-B	909	4/4	-	-	41,42,45,47	4
3	EDO	4-B	909	4/4	-	-	41,42,45,47	4
3	EDO	5-B	909	4/4	-	-	41,42,45,47	4
3	EDO	6-B	909	4/4	-	-	41,42,45,47	4
3	EDO	7-B	909	4/4	-	-	41,42,45,47	4
3	EDO	8-B	909	4/4	-	-	41,42,45,47	4
3	EDO	1-A	910	4/4	0.85	0.22	42,47,47,48	4
3	EDO	2-B	911	4/4	-	-	21,28,30,36	4
3	EDO	3-B	911	4/4	-	-	22,28,31,36	4
3	EDO	4-B	911	4/4	-	-	21,28,31,36	4
3	EDO	5-B	911	4/4	-	-	20,28,31,36	4
3	EDO	6-B	911	4/4	-	-	21,28,30,36	4
3	EDO	7-B	911	4/4	-	-	22,28,30,36	4
3	EDO	8-B	911	4/4	-	-	21,28,31,36	4
3	EDO	1-A	907	4/4	0.85	0.14	27,31,32,32	4
3	EDO	2-B	912	4/4	-	-	31,34,36,38	4
3	EDO	3-B	912	4/4	-	-	31,34,36,38	4
3	EDO	4-B	912	4/4	-	-	31,34,36,38	4
3	EDO	5-B	912	4/4	-	-	31,34,36,38	4
3	EDO	6-B	912	4/4	-	-	31,34,36,38	4
3	EDO	7-B	912	4/4	-	-	31,34,36,39	4
3	EDO	8-B	912	4/4	-	-	31,34,36,38	4
3	EDO	1-A	902	4/4	0.89	0.12	27,27,29,33	4
3	EDO	2-B	913	4/4	-	-	29,31,34,37	4
3	EDO	3-B	913	4/4	-	-	29,31,34,37	4
3	EDO	4-B	913	4/4	-	-	29,31,34,37	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	5-B	913	4/4	-	-	29,31,34,37	4
3	EDO	6-B	913	4/4	-	-	28,31,34,37	4
3	EDO	7-B	913	4/4	-	-	29,31,34,37	4
3	EDO	8-B	913	4/4	-	-	29,31,34,37	4
2	MG	1-A	802	1/1	0.92	0.08	12,12,12,12	1
4	MPO	2-A	9000	13/13	-	-	38,46,55,55	13
4	MPO	3-A	9000	13/13	-	-	38,46,55,55	13
4	MPO	4-A	9000	13/13	-	-	38,46,55,55	13
4	MPO	5-A	9000	13/13	-	-	38,46,55,55	13
4	MPO	6-A	9000	13/13	-	-	38,46,55,55	13
4	MPO	7-A	9000	13/13	-	-	38,46,55,55	13
4	MPO	8-A	9000	13/13	-	-	37,46,55,55	13

6.5 Other polymers [i](#)

There are no such residues in this entry.