



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:08 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 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 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

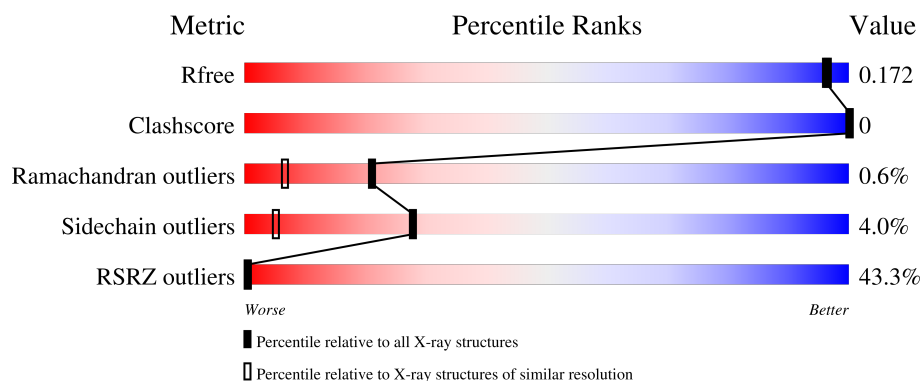
1 Overall quality at a glance

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.



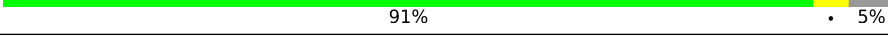
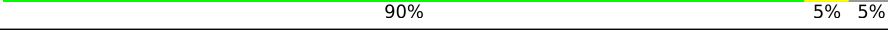
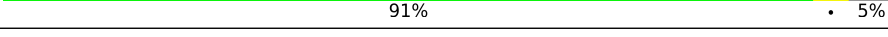
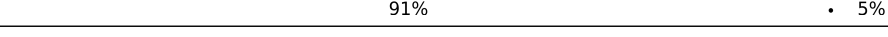
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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%

Continued on next page...

Continued from previous page...

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

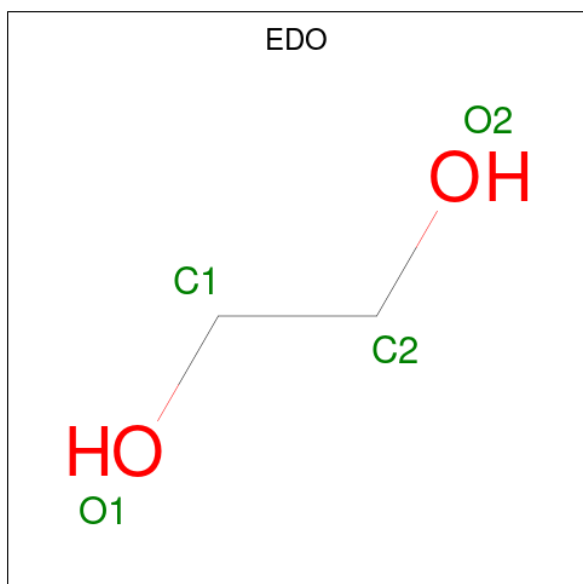
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	1	Total Mg 1 1	0	0
2	2-A	1	Total Mg 1 1	0	0
2	3-A	1	Total Mg 1 1	0	0
2	4-A	1	Total Mg 1 1	0	0
2	5-A	1	Total Mg 1 1	0	0
2	6-A	1	Total Mg 1 1	0	0
2	7-A	1	Total Mg 1 1	0	0
2	8-A	1	Total Mg 1 1	0	0
2	1-B	1	Total Mg 1 1	0	0
2	2-B	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

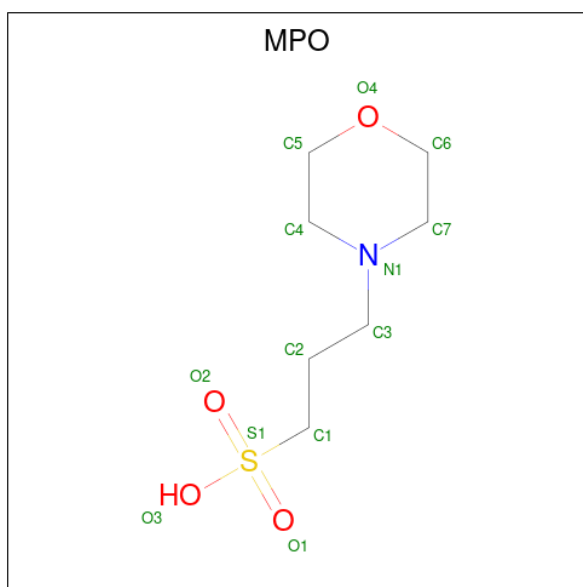
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	5-B	1	Total 4	C 2	O 2	0	0
3	6-B	1	Total 4	C 2	O 2	0	0
3	7-B	1	Total 4	C 2	O 2	0	0
3	8-B	1	Total 4	C 2	O 2	0	0
3	1-B	1	Total 4	C 2	O 2	0	0
3	2-B	1	Total 4	C 2	O 2	0	0
3	3-B	1	Total 4	C 2	O 2	0	0
3	4-B	1	Total 4	C 2	O 2	0	0
3	5-B	1	Total 4	C 2	O 2	0	0
3	6-B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

Continued on next page...

Continued from previous page...

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: $C_7H_{15}NO_4S$).



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		

Continued on next page...

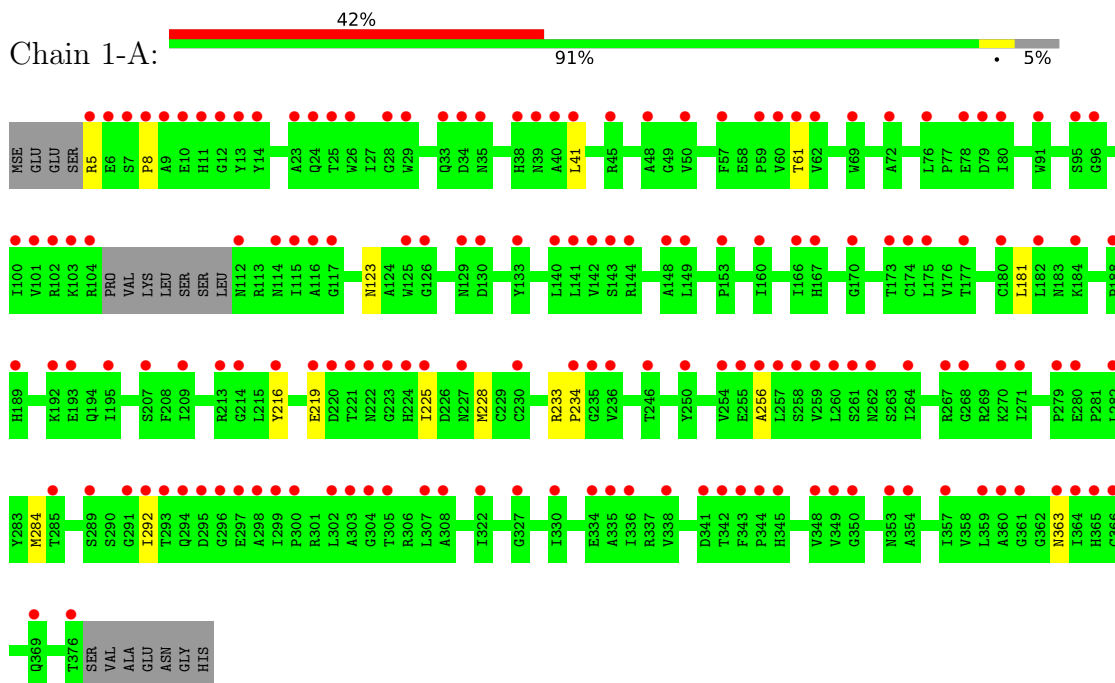
Continued from previous page...

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

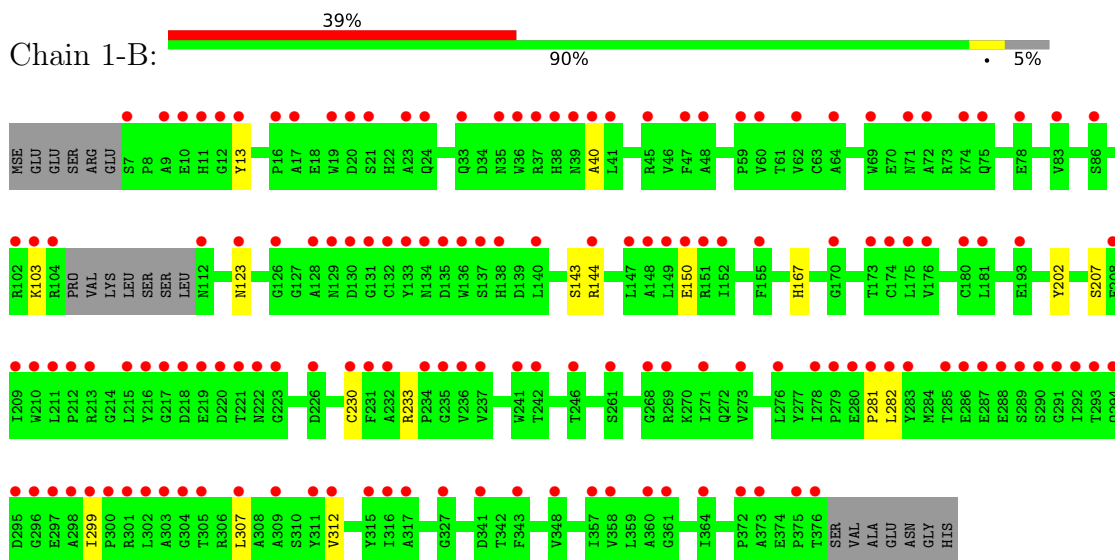
3 Residue-property plots [i](#)

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



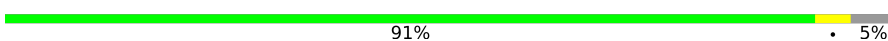
• Molecule 1: Agmatine deiminase

Chain 2-A:  92% • 5%

• Molecule 1: Agmatine deiminase

Chain 2-B:  91% • 5%

• Molecule 1: Agmatine deiminase

Chain 3-A:  91% • 5%

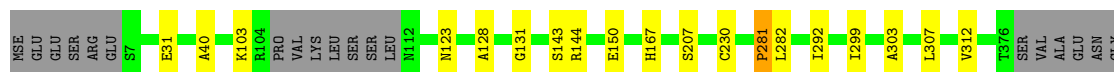
• Molecule 1: Agmatine deiminase

Chain 3-B:  90% • 5%

• Molecule 1: Agmatine deiminase

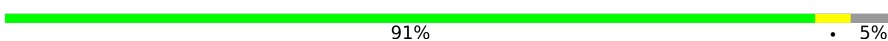
Chain 4-A:  91% • 5%

• 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	SER	LEU	N112	N123	S143	R144	E150	H167	Y202	S207	C230	P281	L282	I299	L307	V312	T376	SER	VAL	ALA	GLU	ASN	GLY	HIS
-----	-----	-----	-----	-----	-----	----	-----	-----	------	------	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----

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

Continued on next page...

Continued from previous page...

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

All (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
1	6-A	256	ALA	CA-CB	5.52	1.62	1.53
1	7-A	256	ALA	CA-CB	5.52	1.62	1.53
1	8-A	256	ALA	CA-CB	5.52	1.62	1.53
1	1-B	40	ALA	CA-CB	5.21	1.61	1.53
1	2-B	40	ALA	CA-CB	5.21	1.61	1.53
1	3-B	40	ALA	CA-CB	5.21	1.61	1.53
1	4-B	40	ALA	CA-CB	5.21	1.61	1.53
1	5-B	40	ALA	CA-CB	5.21	1.61	1.53
1	6-B	40	ALA	CA-CB	5.21	1.61	1.53
1	7-B	40	ALA	CA-CB	5.21	1.61	1.53
1	8-B	40	ALA	CA-CB	5.21	1.61	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (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
1	4-A	122	PHE	Sidechain
1	4-A	133	TYR	Sidechain
1	5-A	155	PHE	Sidechain
1	5-A	315	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	5-B	133	TYR	Sidechain
1	5-B	250	TYR	Sidechain
1	6-B	202	TYR	Sidechain
1	7-A	277	TYR	Sidechain
1	7-A	283	TYR	Sidechain
1	7-B	13	TYR	Sidechain
1	7-B	138	HIS	Sidechain
1	8-A	202	TYR	Sidechain
1	8-A	277	TYR	Sidechain
1	8-B	202	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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 [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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
1	5-A	318	ASN
1	5-B	128	ALA
1	6-B	31	GLU
1	8-B	19	TRP
1	1-A	363	ASN
1	4-B	128	ALA
1	4-B	303	ALA
1	5-B	222	ASN
1	6-A	135	ASP
1	6-B	123	ASN
1	7-A	37	ARG
1	7-A	295	ASP
1	7-A	318	ASN
1	7-B	11	HIS
1	7-B	318	ASN
1	8-A	369	GLN
1	3-A	313	ASN
1	4-B	281	PRO
1	7-A	31	GLU
1	7-B	10	GLU
1	1-A	233	ARG
1	1-B	233	ARG
1	2-B	31	GLU
1	3-A	31	GLU
1	3-B	328	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-A	31	GLU
1	4-B	31	GLU
1	6-A	249	GLN
1	6-B	77	PRO
1	4-B	131	GLY

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

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	5	ARG
1	1-A	8	PRO
1	1-A	41	LEU
1	1-A	61	THR
1	1-A	123	ASN
1	1-A	181	LEU
1	1-A	219	GLU
1	1-A	225	ILE
1	1-A	228	MSE
1	1-A	234	PRO
1	1-A	284	MSE
1	1-A	292	ILE
1	1-B	103	LYS
1	1-B	123	ASN
1	1-B	143	SER
1	1-B	144	ARG
1	1-B	150	GLU
1	1-B	167	HIS
1	1-B	207	SER
1	1-B	230	CYS
1	1-B	281	PRO
1	1-B	282	LEU
1	1-B	299	ILE
1	1-B	307	LEU
1	1-B	312	VAL
1	2-A	5	ARG
1	2-A	8	PRO
1	2-A	41	LEU
1	2-A	61	THR
1	2-A	123	ASN
1	2-A	181	LEU
1	2-A	219	GLU
1	2-A	225	ILE
1	2-A	228	MSE
1	2-A	234	PRO
1	2-A	284	MSE
1	2-A	292	ILE
1	2-B	103	LYS
1	2-B	123	ASN
1	2-B	143	SER
1	2-B	144	ARG
1	2-B	150	GLU
1	2-B	167	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-B	207	SER
1	2-B	230	CYS
1	2-B	281	PRO
1	2-B	282	LEU
1	2-B	299	ILE
1	2-B	307	LEU
1	2-B	312	VAL
1	3-A	5	ARG
1	3-A	8	PRO
1	3-A	41	LEU
1	3-A	61	THR
1	3-A	123	ASN
1	3-A	181	LEU
1	3-A	219	GLU
1	3-A	225	ILE
1	3-A	228	MSE
1	3-A	234	PRO
1	3-A	284	MSE
1	3-A	292	ILE
1	3-B	103	LYS
1	3-B	123	ASN
1	3-B	143	SER
1	3-B	144	ARG
1	3-B	150	GLU
1	3-B	167	HIS
1	3-B	207	SER
1	3-B	230	CYS
1	3-B	281	PRO
1	3-B	282	LEU
1	3-B	299	ILE
1	3-B	307	LEU
1	3-B	312	VAL
1	4-A	5	ARG
1	4-A	8	PRO
1	4-A	41	LEU
1	4-A	61	THR
1	4-A	123	ASN
1	4-A	181	LEU
1	4-A	219	GLU
1	4-A	225	ILE
1	4-A	228	MSE
1	4-A	234	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-A	284	MSE
1	4-A	292	ILE
1	4-B	103	LYS
1	4-B	123	ASN
1	4-B	143	SER
1	4-B	144	ARG
1	4-B	150	GLU
1	4-B	167	HIS
1	4-B	207	SER
1	4-B	230	CYS
1	4-B	281	PRO
1	4-B	282	LEU
1	4-B	299	ILE
1	4-B	307	LEU
1	4-B	312	VAL
1	5-A	5	ARG
1	5-A	8	PRO
1	5-A	41	LEU
1	5-A	61	THR
1	5-A	123	ASN
1	5-A	181	LEU
1	5-A	219	GLU
1	5-A	225	ILE
1	5-A	228	MSE
1	5-A	234	PRO
1	5-A	284	MSE
1	5-A	292	ILE
1	5-B	103	LYS
1	5-B	123	ASN
1	5-B	143	SER
1	5-B	144	ARG
1	5-B	150	GLU
1	5-B	167	HIS
1	5-B	207	SER
1	5-B	230	CYS
1	5-B	281	PRO
1	5-B	282	LEU
1	5-B	299	ILE
1	5-B	307	LEU
1	5-B	312	VAL
1	6-A	5	ARG
1	6-A	8	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-A	41	LEU
1	6-A	61	THR
1	6-A	123	ASN
1	6-A	181	LEU
1	6-A	219	GLU
1	6-A	225	ILE
1	6-A	228	MSE
1	6-A	234	PRO
1	6-A	284	MSE
1	6-A	292	ILE
1	6-B	103	LYS
1	6-B	123	ASN
1	6-B	143	SER
1	6-B	144	ARG
1	6-B	150	GLU
1	6-B	167	HIS
1	6-B	207	SER
1	6-B	230	CYS
1	6-B	281	PRO
1	6-B	282	LEU
1	6-B	299	ILE
1	6-B	307	LEU
1	6-B	312	VAL
1	7-A	5	ARG
1	7-A	8	PRO
1	7-A	41	LEU
1	7-A	61	THR
1	7-A	123	ASN
1	7-A	181	LEU
1	7-A	219	GLU
1	7-A	225	ILE
1	7-A	228	MSE
1	7-A	234	PRO
1	7-A	284	MSE
1	7-A	292	ILE
1	7-B	103	LYS
1	7-B	123	ASN
1	7-B	143	SER
1	7-B	144	ARG
1	7-B	150	GLU
1	7-B	167	HIS
1	7-B	207	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-B	230	CYS
1	7-B	281	PRO
1	7-B	282	LEU
1	7-B	299	ILE
1	7-B	307	LEU
1	7-B	312	VAL
1	8-A	5	ARG
1	8-A	8	PRO
1	8-A	41	LEU
1	8-A	61	THR
1	8-A	123	ASN
1	8-A	181	LEU
1	8-A	219	GLU
1	8-A	225	ILE
1	8-A	228	MSE
1	8-A	234	PRO
1	8-A	284	MSE
1	8-A	292	ILE
1	8-B	103	LYS
1	8-B	123	ASN
1	8-B	143	SER
1	8-B	144	ARG
1	8-B	150	GLU
1	8-B	167	HIS
1	8-B	207	SER
1	8-B	230	CYS
1	8-B	281	PRO
1	8-B	282	LEU
1	8-B	299	ILE
1	8-B	307	LEU
1	8-B	312	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (303) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	22	HIS
1	1-A	24	GLN
1	1-A	35	ASN
1	1-A	38	HIS
1	1-A	39	ASN
1	1-A	44	GLN
1	1-A	68	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-A	75	GLN
1	1-A	112	ASN
1	1-A	121	ASN
1	1-A	123	ASN
1	1-A	187	ASN
1	1-A	194	GLN
1	1-A	206	GLN
1	1-A	222	ASN
1	1-A	227	ASN
1	1-A	249	GLN
1	1-A	313	ASN
1	1-A	346	HIS
1	1-A	353	ASN
1	1-A	365	HIS
1	1-A	371	GLN
1	1-B	39	ASN
1	1-B	68	GLN
1	1-B	75	GLN
1	1-B	88	ASN
1	1-B	114	ASN
1	1-B	121	ASN
1	1-B	123	ASN
1	1-B	129	ASN
1	1-B	134	ASN
1	1-B	156	GLN
1	1-B	187	ASN
1	1-B	194	GLN
1	1-B	222	ASN
1	1-B	224	HIS
1	1-B	294	GLN
1	1-B	318	ASN
1	1-B	325	GLN
1	1-B	363	ASN
1	1-B	369	GLN
1	2-A	24	GLN
1	2-A	35	ASN
1	2-A	39	ASN
1	2-A	44	GLN
1	2-A	68	GLN
1	2-A	75	GLN
1	2-A	112	ASN
1	2-A	121	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-A	123	ASN
1	2-A	187	ASN
1	2-A	194	GLN
1	2-A	206	GLN
1	2-A	249	GLN
1	2-A	272	GLN
1	2-A	353	ASN
1	2-A	365	HIS
1	2-A	369	GLN
1	2-A	371	GLN
1	2-B	11	HIS
1	2-B	24	GLN
1	2-B	33	GLN
1	2-B	68	GLN
1	2-B	88	ASN
1	2-B	112	ASN
1	2-B	121	ASN
1	2-B	123	ASN
1	2-B	134	ASN
1	2-B	138	HIS
1	2-B	187	ASN
1	2-B	194	GLN
1	2-B	222	ASN
1	2-B	318	ASN
1	2-B	325	GLN
1	2-B	345	HIS
1	2-B	346	HIS
1	2-B	363	ASN
1	2-B	365	HIS
1	3-A	24	GLN
1	3-A	35	ASN
1	3-A	38	HIS
1	3-A	39	ASN
1	3-A	44	GLN
1	3-A	68	GLN
1	3-A	75	GLN
1	3-A	112	ASN
1	3-A	121	ASN
1	3-A	123	ASN
1	3-A	187	ASN
1	3-A	194	GLN
1	3-A	249	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-A	313	ASN
1	3-A	353	ASN
1	3-A	365	HIS
1	3-A	369	GLN
1	3-A	371	GLN
1	3-B	24	GLN
1	3-B	33	GLN
1	3-B	39	ASN
1	3-B	68	GLN
1	3-B	75	GLN
1	3-B	88	ASN
1	3-B	112	ASN
1	3-B	114	ASN
1	3-B	121	ASN
1	3-B	123	ASN
1	3-B	156	GLN
1	3-B	187	ASN
1	3-B	194	GLN
1	3-B	222	ASN
1	3-B	224	HIS
1	3-B	318	ASN
1	3-B	353	ASN
1	3-B	363	ASN
1	3-B	365	HIS
1	4-A	24	GLN
1	4-A	35	ASN
1	4-A	38	HIS
1	4-A	39	ASN
1	4-A	44	GLN
1	4-A	68	GLN
1	4-A	75	GLN
1	4-A	121	ASN
1	4-A	123	ASN
1	4-A	187	ASN
1	4-A	194	GLN
1	4-A	206	GLN
1	4-A	249	GLN
1	4-A	346	HIS
1	4-A	353	ASN
1	4-A	365	HIS
1	4-A	369	GLN
1	4-A	371	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-B	24	GLN
1	4-B	33	GLN
1	4-B	39	ASN
1	4-B	68	GLN
1	4-B	75	GLN
1	4-B	88	ASN
1	4-B	112	ASN
1	4-B	114	ASN
1	4-B	121	ASN
1	4-B	129	ASN
1	4-B	134	ASN
1	4-B	156	GLN
1	4-B	189	HIS
1	4-B	194	GLN
1	4-B	222	ASN
1	4-B	224	HIS
1	4-B	272	GLN
1	4-B	294	GLN
1	4-B	318	ASN
1	4-B	325	GLN
1	4-B	363	ASN
1	4-B	365	HIS
1	4-B	369	GLN
1	5-A	24	GLN
1	5-A	35	ASN
1	5-A	39	ASN
1	5-A	68	GLN
1	5-A	75	GLN
1	5-A	112	ASN
1	5-A	121	ASN
1	5-A	123	ASN
1	5-A	134	ASN
1	5-A	187	ASN
1	5-A	194	GLN
1	5-A	206	GLN
1	5-A	249	GLN
1	5-A	313	ASN
1	5-A	369	GLN
1	5-A	371	GLN
1	5-B	24	GLN
1	5-B	39	ASN
1	5-B	44	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-B	71	ASN
1	5-B	88	ASN
1	5-B	112	ASN
1	5-B	121	ASN
1	5-B	123	ASN
1	5-B	134	ASN
1	5-B	167	HIS
1	5-B	187	ASN
1	5-B	194	GLN
1	5-B	227	ASN
1	5-B	318	ASN
1	5-B	325	GLN
1	5-B	363	ASN
1	5-B	365	HIS
1	5-B	369	GLN
1	6-A	11	HIS
1	6-A	24	GLN
1	6-A	35	ASN
1	6-A	44	GLN
1	6-A	68	GLN
1	6-A	112	ASN
1	6-A	121	ASN
1	6-A	123	ASN
1	6-A	134	ASN
1	6-A	167	HIS
1	6-A	187	ASN
1	6-A	194	GLN
1	6-A	206	GLN
1	6-A	224	HIS
1	6-A	249	GLN
1	6-A	313	ASN
1	6-A	346	HIS
1	6-A	365	HIS
1	6-A	371	GLN
1	6-B	24	GLN
1	6-B	39	ASN
1	6-B	68	GLN
1	6-B	75	GLN
1	6-B	88	ASN
1	6-B	112	ASN
1	6-B	114	ASN
1	6-B	121	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-B	156	GLN
1	6-B	194	GLN
1	6-B	222	ASN
1	6-B	224	HIS
1	6-B	318	ASN
1	6-B	325	GLN
1	6-B	353	ASN
1	6-B	363	ASN
1	6-B	365	HIS
1	6-B	369	GLN
1	7-A	11	HIS
1	7-A	24	GLN
1	7-A	35	ASN
1	7-A	39	ASN
1	7-A	44	GLN
1	7-A	68	GLN
1	7-A	75	GLN
1	7-A	121	ASN
1	7-A	123	ASN
1	7-A	187	ASN
1	7-A	194	GLN
1	7-A	206	GLN
1	7-A	224	HIS
1	7-A	249	GLN
1	7-A	272	GLN
1	7-A	313	ASN
1	7-A	365	HIS
1	7-A	369	GLN
1	7-A	371	GLN
1	7-B	24	GLN
1	7-B	39	ASN
1	7-B	68	GLN
1	7-B	88	ASN
1	7-B	114	ASN
1	7-B	121	ASN
1	7-B	123	ASN
1	7-B	134	ASN
1	7-B	167	HIS
1	7-B	187	ASN
1	7-B	194	GLN
1	7-B	222	ASN
1	7-B	224	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-B	318	ASN
1	7-B	325	GLN
1	7-B	363	ASN
1	7-B	365	HIS
1	7-B	370	GLN
1	8-A	24	GLN
1	8-A	35	ASN
1	8-A	39	ASN
1	8-A	44	GLN
1	8-A	68	GLN
1	8-A	75	GLN
1	8-A	121	ASN
1	8-A	123	ASN
1	8-A	134	ASN
1	8-A	194	GLN
1	8-A	222	ASN
1	8-A	249	GLN
1	8-A	272	GLN
1	8-A	313	ASN
1	8-A	346	HIS
1	8-A	365	HIS
1	8-B	11	HIS
1	8-B	24	GLN
1	8-B	39	ASN
1	8-B	68	GLN
1	8-B	75	GLN
1	8-B	88	ASN
1	8-B	112	ASN
1	8-B	114	ASN
1	8-B	121	ASN
1	8-B	123	ASN
1	8-B	134	ASN
1	8-B	156	GLN
1	8-B	187	ASN
1	8-B	194	GLN
1	8-B	222	ASN
1	8-B	224	HIS
1	8-B	294	GLN
1	8-B	318	ASN
1	8-B	325	GLN
1	8-B	346	HIS
1	8-B	363	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-B	365	HIS
1	8-B	369	GLN

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

All (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
4	7-A	9000	MPO	C1-S1	4.66	1.84	1.77
4	4-A	9000	MPO	O1-S1	4.50	1.57	1.45
4	5-A	9000	MPO	O3-S1	3.99	1.62	1.47
4	5-A	9000	MPO	O2-S1	3.92	1.56	1.45
4	8-A	9000	MPO	O3-S1	3.77	1.61	1.47
4	6-A	9000	MPO	O3-S1	3.76	1.61	1.47
4	5-A	9000	MPO	O1-S1	3.72	1.55	1.45
4	3-A	9000	MPO	C1-S1	3.54	1.82	1.77
4	2-A	9000	MPO	O3-S1	3.47	1.60	1.47
4	4-A	9000	MPO	O3-S1	3.33	1.59	1.47
4	1-A	9000	MPO	O3-S1	3.32	1.59	1.47
4	6-A	9000	MPO	O2-S1	3.30	1.54	1.45
4	3-A	9000	MPO	O2-S1	3.26	1.54	1.45
4	3-A	9000	MPO	O3-S1	3.02	1.58	1.47
4	8-A	9000	MPO	C2-C1	3.01	1.62	1.52
4	2-A	9000	MPO	O2-S1	2.95	1.53	1.45
4	7-A	9000	MPO	O2-S1	2.87	1.53	1.45
4	1-A	9000	MPO	O2-S1	2.86	1.53	1.45
3	7-B	911	EDO	O1-C1	2.86	1.56	1.42
4	6-A	9000	MPO	O1-S1	2.76	1.52	1.45
4	8-A	9000	MPO	C3-N1	2.66	1.53	1.47
3	6-B	911	EDO	O1-C1	2.66	1.55	1.42
4	1-A	9000	MPO	O1-S1	2.60	1.52	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	8-B	911	EDO	O1-C1	2.59	1.55	1.42
4	8-A	9000	MPO	C2-C3	2.42	1.61	1.51
3	2-B	911	EDO	O1-C1	2.36	1.54	1.42
4	6-A	9000	MPO	C1-S1	2.34	1.80	1.77
4	7-A	9000	MPO	O3-S1	2.34	1.56	1.47
4	1-A	9000	MPO	C2-C1	2.33	1.59	1.52
4	4-A	9000	MPO	O2-S1	2.28	1.51	1.45
3	4-B	911	EDO	O1-C1	2.20	1.53	1.42
4	1-A	9000	MPO	C3-N1	2.15	1.52	1.47
4	8-A	9000	MPO	C7-C6	2.11	1.58	1.50
4	4-A	9000	MPO	C2-C1	2.08	1.58	1.52

All (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
4	2-A	9000	MPO	O3-S1-C1	-13.20	80.17	106.00
4	8-A	9000	MPO	O3-S1-O1	-12.84	79.28	111.40
4	4-A	9000	MPO	O3-S1-O1	-12.02	81.32	111.40
4	4-A	9000	MPO	O3-S1-C1	-11.86	82.79	106.00
4	3-A	9000	MPO	O3-S1-C1	-11.21	84.07	106.00
4	5-A	9000	MPO	O3-S1-O1	-11.11	83.60	111.40
4	2-A	9000	MPO	O3-S1-O1	-11.09	83.64	111.40
4	6-A	9000	MPO	O3-S1-O1	-10.94	84.02	111.40
4	1-A	9000	MPO	O3-S1-O2	-10.83	84.31	111.40
4	6-A	9000	MPO	O1-S1-C1	10.76	122.98	106.73
4	8-A	9000	MPO	O3-S1-C1	-10.44	85.58	106.00
4	5-A	9000	MPO	O1-S1-C1	10.33	122.34	106.73
4	8-A	9000	MPO	O3-S1-O2	-10.31	85.61	111.40
4	4-A	9000	MPO	O3-S1-O2	-10.27	85.71	111.40
4	7-A	9000	MPO	O3-S1-C1	-9.98	86.47	106.00
4	3-A	9000	MPO	O3-S1-O2	-9.48	87.67	111.40
4	2-A	9000	MPO	O3-S1-O2	-9.42	87.84	111.40
4	1-A	9000	MPO	O3-S1-C1	-8.88	88.63	106.00
4	7-A	9000	MPO	O3-S1-O2	-8.74	89.53	111.40
4	6-A	9000	MPO	O3-S1-O2	-8.67	89.71	111.40
4	5-A	9000	MPO	O3-S1-O2	-8.46	90.23	111.40
4	2-A	9000	MPO	O1-S1-C1	8.41	119.44	106.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	7-A	9000	MPO	O1-S1-C1	8.21	119.13	106.73
4	3-A	9000	MPO	O1-S1-C1	8.07	118.92	106.73
4	3-A	9000	MPO	C2-C1-S1	-7.20	102.21	113.25
4	7-A	9000	MPO	C2-C1-S1	-6.87	102.72	113.25
4	1-A	9000	MPO	O2-S1-O1	6.07	133.55	113.82
4	8-A	9000	MPO	O2-S1-O1	6.04	133.47	113.82
4	2-A	9000	MPO	C2-C1-S1	-5.78	104.38	113.25
4	4-A	9000	MPO	O1-S1-C1	5.66	115.29	106.73
4	4-A	9000	MPO	O2-S1-O1	5.52	131.79	113.82
4	1-A	9000	MPO	O1-S1-C1	5.35	114.81	106.73
4	8-A	9000	MPO	O1-S1-C1	5.14	114.49	106.73
4	2-A	9000	MPO	O2-S1-O1	5.07	130.32	113.82
4	3-A	9000	MPO	O2-S1-O1	4.96	129.96	113.82
4	7-A	9000	MPO	O2-S1-O1	4.94	129.90	113.82
4	6-A	9000	MPO	C2-C1-S1	-4.80	105.89	113.25
4	8-A	9000	MPO	C2-C1-S1	4.37	119.94	113.25
4	6-A	9000	MPO	O2-S1-O1	4.20	127.47	113.82
4	5-A	9000	MPO	O2-S1-O1	3.84	126.33	113.82
4	7-A	9000	MPO	C2-C3-N1	-2.91	105.76	113.93
4	2-A	9000	MPO	C3-C2-C1	-2.60	104.24	113.02
4	2-A	9000	MPO	C6-C7-N1	-2.40	106.48	110.12
4	6-A	9000	MPO	O4-C6-C7	-2.33	106.75	111.77
4	3-A	9000	MPO	C2-C3-N1	-2.23	107.67	113.93
4	5-A	9000	MPO	C2-C3-N1	-2.14	107.92	113.93
4	6-A	9000	MPO	C3-C2-C1	-2.13	105.82	113.02
4	2-A	9000	MPO	C3-N1-C4	-2.13	105.57	111.24
4	3-A	9000	MPO	O4-C6-C7	-2.08	107.28	111.77
4	6-A	9000	MPO	C6-C7-N1	-2.06	106.98	110.12
4	4-A	9000	MPO	C2-C1-S1	2.05	116.39	113.25
4	7-A	9000	MPO	O4-C6-C7	-2.05	107.36	111.77
4	2-A	9000	MPO	O4-C6-C7	-2.03	107.41	111.77

There are no chirality outliers.

All (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
3	4-B	912	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	8-B	912	EDO	O1-C1-C2-O2
3	1-A	910	EDO	O1-C1-C2-O2
3	2-A	910	EDO	O1-C1-C2-O2
3	3-A	910	EDO	O1-C1-C2-O2
3	4-A	910	EDO	O1-C1-C2-O2
3	5-A	910	EDO	O1-C1-C2-O2
3	7-A	910	EDO	O1-C1-C2-O2
3	8-A	910	EDO	O1-C1-C2-O2
3	3-B	911	EDO	O1-C1-C2-O2
3	7-B	911	EDO	O1-C1-C2-O2
3	8-B	911	EDO	O1-C1-C2-O2
3	1-B	912	EDO	O1-C1-C2-O2
3	2-B	912	EDO	O1-C1-C2-O2
3	6-B	912	EDO	O1-C1-C2-O2
4	1-A	9000	MPO	C2-C1-S1-O1
4	1-A	9000	MPO	C2-C1-S1-O2
4	2-A	9000	MPO	C2-C1-S1-O2
4	3-A	9000	MPO	C2-C1-S1-O1
4	4-A	9000	MPO	C2-C1-S1-O2
4	5-A	9000	MPO	C2-C1-S1-O1
4	6-A	9000	MPO	C2-C1-S1-O1
4	7-A	9000	MPO	C2-C1-S1-O1
4	8-A	9000	MPO	C2-C1-S1-O2
3	8-A	906	EDO	O1-C1-C2-O2
3	1-B	909	EDO	O1-C1-C2-O2
3	2-B	909	EDO	O1-C1-C2-O2
3	3-B	909	EDO	O1-C1-C2-O2
3	4-B	909	EDO	O1-C1-C2-O2
3	5-B	909	EDO	O1-C1-C2-O2
3	6-B	909	EDO	O1-C1-C2-O2
3	7-B	909	EDO	O1-C1-C2-O2
3	8-B	909	EDO	O1-C1-C2-O2
3	2-B	911	EDO	O1-C1-C2-O2
3	4-B	911	EDO	O1-C1-C2-O2
3	6-B	911	EDO	O1-C1-C2-O2
3	5-B	912	EDO	O1-C1-C2-O2
3	7-B	912	EDO	O1-C1-C2-O2
3	5-B	911	EDO	O1-C1-C2-O2
3	3-A	903	EDO	O1-C1-C2-O2
3	8-A	903	EDO	O1-C1-C2-O2
4	3-A	9000	MPO	C2-C1-S1-O2
4	5-A	9000	MPO	C2-C1-S1-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	6-A	9000	MPO	C2-C1-S1-O2
3	6-A	903	EDO	O1-C1-C2-O2
3	6-A	910	EDO	O1-C1-C2-O2
3	5-B	904	EDO	O1-C1-C2-O2
3	7-B	904	EDO	O1-C1-C2-O2
3	8-B	913	EDO	O1-C1-C2-O2
3	8-A	901	EDO	O1-C1-C2-O2
3	1-A	903	EDO	O1-C1-C2-O2
3	5-A	903	EDO	O1-C1-C2-O2
3	6-A	906	EDO	O1-C1-C2-O2
3	2-B	904	EDO	O1-C1-C2-O2
3	4-B	904	EDO	O1-C1-C2-O2
3	5-A	901	EDO	O1-C1-C2-O2
3	2-A	903	EDO	O1-C1-C2-O2
3	4-A	903	EDO	O1-C1-C2-O2
3	7-A	903	EDO	O1-C1-C2-O2
3	2-A	906	EDO	O1-C1-C2-O2
3	7-A	906	EDO	O1-C1-C2-O2
3	3-A	908	EDO	O1-C1-C2-O2
3	7-A	908	EDO	O1-C1-C2-O2
3	1-B	904	EDO	O1-C1-C2-O2
3	3-B	904	EDO	O1-C1-C2-O2
3	8-B	904	EDO	O1-C1-C2-O2
3	1-B	913	EDO	O1-C1-C2-O2
3	5-B	913	EDO	O1-C1-C2-O2
3	6-B	913	EDO	O1-C1-C2-O2
4	7-A	9000	MPO	C2-C1-S1-O2
3	1-A	901	EDO	O1-C1-C2-O2
3	2-A	901	EDO	O1-C1-C2-O2
3	3-A	901	EDO	O1-C1-C2-O2
3	4-A	901	EDO	O1-C1-C2-O2
3	1-A	906	EDO	O1-C1-C2-O2
3	3-A	906	EDO	O1-C1-C2-O2
3	5-A	906	EDO	O1-C1-C2-O2
3	4-A	907	EDO	O1-C1-C2-O2
3	7-A	907	EDO	O1-C1-C2-O2
3	1-A	908	EDO	O1-C1-C2-O2
3	6-A	901	EDO	O1-C1-C2-O2
3	8-A	908	EDO	O1-C1-C2-O2
3	4-A	906	EDO	O1-C1-C2-O2
3	6-B	904	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 ⓘ

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	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%)

All (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
1	1-B	230	CYS	6.9
1	1-A	195	ILE	6.8
1	1-B	126	GLY	6.7
1	1-B	298	ALA	6.5
1	1-A	14	TYR	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-B	376	THR	6.4
1	1-A	295	ASP	6.1
1	1-A	214	GLY	5.9
1	1-B	21	SER	5.8
1	1-A	104	ARG	5.8
1	1-A	305	THR	5.8
1	1-B	11	HIS	5.7
1	1-A	13	TYR	5.5
1	1-B	112	ASN	5.4
1	1-A	363	ASN	5.4
1	1-B	296	GLY	5.3
1	1-B	180	CYS	5.3
1	1-A	61	THR	5.3
1	1-B	218	ASP	5.3
1	1-A	376	THR	5.2
1	1-B	72	ALA	5.1
1	1-A	261	SER	5.1
1	1-A	148	ALA	5.1
1	1-A	230	CYS	5.1
1	1-A	296	GLY	5.0
1	1-B	132	CYS	5.0
1	1-A	254	VAL	5.0
1	1-B	302	LEU	5.0
1	1-A	292	ILE	4.9
1	1-A	357	ILE	4.9
1	1-A	300	PRO	4.8
1	1-B	209	ILE	4.8
1	1-B	303	ALA	4.7
1	1-B	130	ASP	4.6
1	1-B	129	ASN	4.6
1	1-B	287	GLU	4.6
1	1-A	114	ASN	4.6
1	1-B	292	ILE	4.5
1	1-B	291	GLY	4.5
1	1-B	285	THR	4.5
1	1-B	293	THR	4.4
1	1-A	6	GLU	4.4
1	1-B	305	THR	4.4
1	1-A	250	TYR	4.4
1	1-B	137	SER	4.4
1	1-B	268	GLY	4.4
1	1-B	297	GLU	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-A	345	HIS	4.4
1	1-A	344	PRO	4.3
1	1-B	60	VAL	4.3
1	1-A	234	PRO	4.3
1	1-A	80	ILE	4.3
1	1-B	152	ILE	4.3
1	1-B	295	ASP	4.3
1	1-B	281	PRO	4.2
1	1-A	79	ASP	4.2
1	1-A	361	GLY	4.2
1	1-B	294	GLN	4.2
1	1-A	343	PHE	4.2
1	1-B	136	TRP	4.2
1	1-B	9	ALA	4.2
1	1-A	130	ASP	4.2
1	1-B	104	ARG	4.2
1	1-B	223	GLY	4.2
1	1-B	220	ASP	4.1
1	1-B	301	ARG	4.1
1	1-A	189	HIS	4.1
1	1-A	294	GLN	4.1
1	1-B	235	GLY	4.1
1	1-A	297	GLU	4.1
1	1-B	232	ALA	4.1
1	1-A	102	ARG	4.0
1	1-A	129	ASN	4.0
1	1-B	38	HIS	4.0
1	1-A	112	ASN	4.0
1	1-B	231	PHE	4.0
1	1-B	269	ARG	4.0
1	1-A	76	LEU	4.0
1	1-A	360	ALA	4.0
1	1-B	309	ALA	4.0
1	1-B	131	GLY	3.9
1	1-B	246	THR	4.0
1	1-A	160	ILE	3.9
1	1-A	216	TYR	3.9
1	1-A	366	CYS	3.9
1	1-B	234	PRO	3.9
1	1-B	219	GLU	3.8
1	1-B	290	SER	3.8
1	1-B	134	ASN	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-A	258	SER	3.8
1	1-A	149	LEU	3.8
1	1-B	286	GLU	3.8
1	1-A	103	LYS	3.8
1	1-B	222	ASN	3.7
1	1-B	242	THR	3.7
1	1-A	170	GLY	3.7
1	1-B	149	LEU	3.6
1	1-B	103	LYS	3.6
1	1-A	166	ILE	3.6
1	1-A	126	GLY	3.6
1	1-A	5	ARG	3.6
1	1-A	41	LEU	3.6
1	1-A	9	ALA	3.6
1	1-B	10	GLU	3.5
1	1-A	262	ASN	3.5
1	1-A	308	ALA	3.5
1	1-A	177	THR	3.5
1	1-A	12	GLY	3.5
1	1-A	291	GLY	3.5
1	1-A	62	VAL	3.5
1	1-B	372	PRO	3.5
1	1-A	307	LEU	3.5
1	1-A	60	VAL	3.4
1	1-B	20	ASP	3.4
1	1-B	304	GLY	3.4
1	1-B	62	VAL	3.4
1	1-B	19	TRP	3.4
1	1-B	361	GLY	3.4
1	1-B	41	LEU	3.4
1	1-A	115	ILE	3.3
1	1-B	144	ARG	3.3
1	1-B	59	PRO	3.3
1	1-A	270	LYS	3.3
1	1-A	23	ALA	3.3
1	1-A	298	ALA	3.3
1	1-B	236	VAL	3.3
1	1-A	140	LEU	3.3
1	1-B	282	LEU	3.3
1	1-A	11	HIS	3.3
1	1-A	174	CYS	3.3
1	1-A	33	GLN	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-B	283	TYR	3.3
1	1-A	182	LEU	3.2
1	1-A	91	TRP	3.2
1	1-A	342	THR	3.2
1	1-A	338	VAL	3.2
1	1-B	279	PRO	3.2
1	1-B	36	TRP	3.2
1	1-A	302	LEU	3.2
1	1-B	215	LEU	3.2
1	1-A	336	ILE	3.2
1	1-A	236	VAL	3.2
1	1-A	303	ALA	3.2
1	1-A	10	GLU	3.1
1	1-B	173	THR	3.1
1	1-B	271	ILE	3.1
1	1-B	348	VAL	3.1
1	1-B	317	ALA	3.1
1	1-A	359	LEU	3.1
1	1-B	47	PHE	3.1
1	1-A	259	VAL	3.1
1	1-B	155	PHE	3.1
1	1-A	223	GLY	3.1
1	1-A	268	GLY	3.1
1	1-A	38	HIS	3.0
1	1-B	289	SER	3.0
1	1-A	188	PRO	3.0
1	1-A	227	ASN	3.0
1	1-B	138	HIS	3.0
1	1-A	293	THR	3.0
1	1-A	209	ILE	2.9
1	1-A	39	ASN	2.9
1	1-B	221	THR	2.9
1	1-B	69	TRP	2.9
1	1-A	369	GLN	2.9
1	1-A	334	GLU	2.9
1	1-A	257	LEU	2.9
1	1-B	7	SER	2.9
1	1-A	225	ILE	2.9
1	1-A	256	ALA	2.8
1	1-A	264	ILE	2.8
1	1-A	221	THR	2.8
1	1-A	271	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-B	86	SER	2.8
1	1-A	125	TRP	2.8
1	1-A	350	GLY	2.8
1	1-B	358	VAL	2.8
1	1-A	48	ALA	2.8
1	1-B	212	PRO	2.8
1	1-A	222	ASN	2.8
1	1-B	35	ASN	2.8
1	1-B	12	GLY	2.8
1	1-B	75	GLN	2.8
1	1-B	216	TYR	2.8
1	1-B	312	VAL	2.7
1	1-A	143	SER	2.7
1	1-A	220	ASP	2.7
1	1-A	173	THR	2.7
1	1-B	39	ASN	2.7
1	1-A	180	CYS	2.7
1	1-B	315	TYR	2.7
1	1-B	276	LEU	2.7
1	1-A	69	TRP	2.7
1	1-A	8	PRO	2.7
1	1-A	59	PRO	2.7
1	1-B	133	TYR	2.7
1	1-A	72	ALA	2.7
1	1-B	128	ALA	2.7
1	1-B	327	GLY	2.7
1	1-A	167	HIS	2.7
1	1-B	33	GLN	2.7
1	1-A	45	ARG	2.7
1	1-A	100	ILE	2.7
1	1-A	364	ILE	2.7
1	1-B	74	LYS	2.6
1	1-A	95	SER	2.6
1	1-A	235	GLY	2.6
1	1-A	116	ALA	2.6
1	1-A	335	ALA	2.6
1	1-A	341	ASP	2.6
1	1-B	357	ILE	2.6
1	1-A	285	THR	2.6
1	1-A	142	VAL	2.6
1	1-B	217	GLY	2.6
1	1-B	48	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-A	330	ILE	2.5
1	1-B	288	GLU	2.5
1	1-B	23	ALA	2.5
1	1-A	299	ILE	2.5
1	1-A	282	LEU	2.5
1	1-A	7	SER	2.5
1	1-A	255	GLU	2.5
1	1-B	45	ARG	2.5
1	1-B	64	ALA	2.5
1	1-A	78	GLU	2.5
1	1-A	327	GLY	2.5
1	1-B	175	LEU	2.5
1	1-B	241	TRP	2.5
1	1-A	101	VAL	2.5
1	1-B	83	VAL	2.5
1	1-B	237	VAL	2.5
1	1-B	360	ALA	2.4
1	1-B	40	ALA	2.4
1	1-A	260	LEU	2.4
1	1-B	211	LEU	2.4
1	1-B	280	GLU	2.4
1	1-A	219	GLU	2.4
1	1-A	175	LEU	2.4
1	1-A	213	ARG	2.4
1	1-B	307	LEU	2.4
1	1-B	13	TYR	2.4
1	1-B	78	GLU	2.4
1	1-B	373	ALA	2.3
1	1-A	348	VAL	2.3
1	1-A	153	PRO	2.3
1	1-A	184	LYS	2.3
1	1-A	193	GLU	2.3
1	1-A	96	GLY	2.3
1	1-A	192	LYS	2.3
1	1-A	246	THR	2.3
1	1-B	226	ASP	2.3
1	1-A	267	ARG	2.3
1	1-B	24	GLN	2.3
1	1-B	17	ALA	2.3
1	1-A	353	ASN	2.3
1	1-A	24	GLN	2.3
1	1-B	151	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-B	147	LEU	2.3
1	1-B	181	LEU	2.3
1	1-B	364	ILE	2.3
1	1-B	261	SER	2.3
1	1-B	148	ALA	2.2
1	1-B	135	ASP	2.2
1	1-B	193	GLU	2.2
1	1-A	289	SER	2.2
1	1-A	354	ALA	2.2
1	1-B	341	ASP	2.2
1	1-B	16	PRO	2.2
1	1-A	224	HIS	2.2
1	1-B	150	GLU	2.2
1	1-B	273	VAL	2.2
1	1-B	37	ARG	2.2
1	1-B	123	ASN	2.2
1	1-B	210	TRP	2.2
1	1-A	28	GLY	2.2
1	1-A	207	SER	2.2
1	1-A	35	ASN	2.2
1	1-A	57	PHE	2.2
1	1-A	365	HIS	2.2
1	1-A	141	LEU	2.1
1	1-A	117	GLY	2.1
1	1-A	322	ILE	2.1
1	1-B	316	ILE	2.1
1	1-B	311	TYR	2.1
1	1-A	144	ARG	2.1
1	1-A	34	ASP	2.1
1	1-A	279	PRO	2.1
1	1-B	375	PRO	2.1
1	1-A	29	TRP	2.1
1	1-A	50	VAL	2.1
1	1-B	102	ARG	2.1
1	1-B	208	PHE	2.0
1	1-A	349	VAL	2.0
1	1-A	40	ALA	2.0
1	1-B	140	LEU	2.0
1	1-B	278	ILE	2.0
1	1-B	170	GLY	2.0
1	1-A	25	THR	2.0
1	1-B	213	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-A	26	TRP	2.0
1	1-A	280	GLU	2.0
1	1-B	176	VAL	2.0
1	1-B	343	PHE	2.0
1	1-A	133	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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.