



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 03:47 pm BST

PDB ID : 2Q42  
Title : Ensemble refinement of the protein crystal structure of glyoxalase II from *Arabidopsis thaliana* gene At2g31350  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-31  
Resolution : 1.74 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

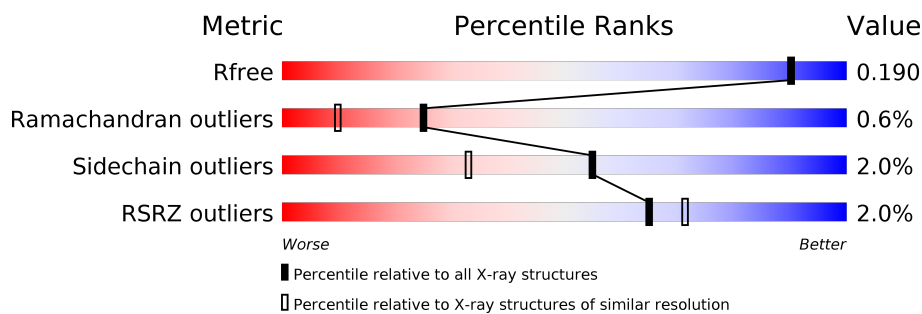
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.74 Å.

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



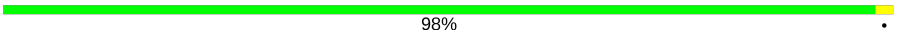
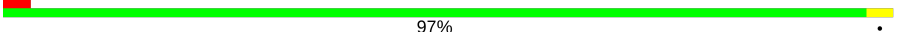
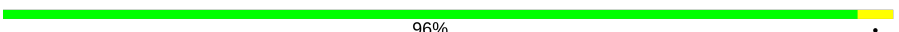











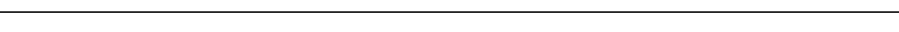
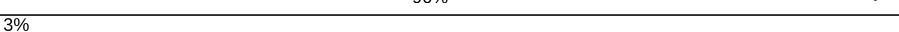
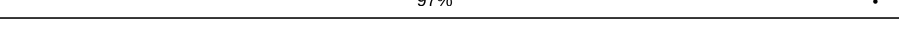
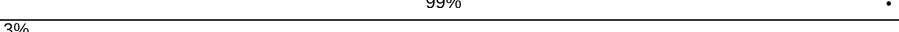
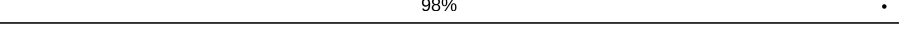
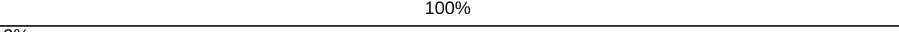
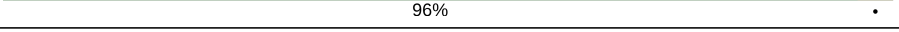
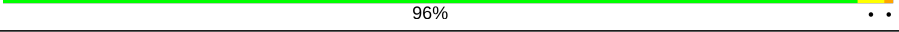
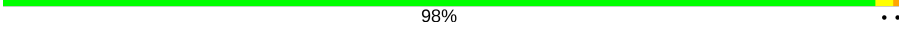
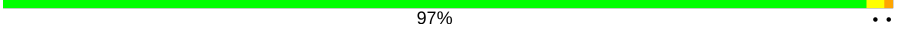
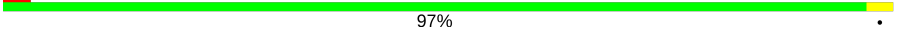
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3764 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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

Mol	Chain	Length	Quality of chain
1	1-A	254	<div> <div>3%</div> <div>97%</div> <div>.</div> </div>
1	1-B	254	<div> <div>96%</div> <div>.</div> </div>
1	10-A	254	<div> <div>3%</div> <div>95%</div> <div>5%</div> </div>
1	10-B	254	<div> <div>98%</div> <div>.</div> </div>
1	11-A	254	<div> <div>3%</div> <div>97%</div> <div>.</div> </div>
1	11-B	254	<div> <div>99%</div> <div>.</div> </div>
1	12-A	254	<div> <div>3%</div> <div>98%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	12-B	254	 98%
1	13-A	254	 97%
1	13-B	254	 96%
1	14-A	254	 96%
1	14-B	254	 95%
1	15-A	254	 96%
1	15-B	254	 93% 6%
1	16-A	254	 99%
1	16-B	254	 92% 7%
1	2-A	254	 98%
1	2-B	254	 98%
1	3-A	254	 96%
1	3-B	254	 96%
1	4-A	254	 98%
1	4-B	254	 96%
1	5-A	254	 97%
1	5-B	254	 99%
1	6-A	254	 98%
1	6-B	254	 100%
1	7-A	254	 96%
1	7-B	254	 96%
1	8-A	254	 98%
1	8-B	254	 97%
1	9-A	254	 97%
1	9-B	254	 96%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 72352 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 Putative hydroxyacylglutathione hydrolase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	2-A	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	3-A	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	4-A	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	5-A	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	6-A	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	7-A	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	8-A	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	9-A	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	10-A	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	11-A	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	12-A	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	13-A	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	14-A	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	15-A	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	16-A	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-B	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	2-B	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	3-B	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	4-B	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	5-B	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	6-B	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	7-B	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	8-B	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	9-B	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	10-B	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	11-B	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	12-B	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	13-B	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	14-B	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	15-B	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			
1	16-B	254	Total	C	N	O	S	0	0	0
			1978	1243	341	382	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP Q9SID3
B	1	MET	-	INITIATING METHIONINE	UNP Q9SID3

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	16-A	1	Total 1 Zn 1	0	0
2	1-B	1	Total 1 Zn 1	0	0
2	5-A	1	Total 1 Zn 1	0	0
2	13-A	1	Total 1 Zn 1	0	0
2	8-A	1	Total 1 Zn 1	0	0
2	2-B	1	Total 1 Zn 1	0	0
2	15-B	1	Total 1 Zn 1	0	0
2	7-B	1	Total 1 Zn 1	0	0
2	16-B	1	Total 1 Zn 1	0	0
2	10-B	1	Total 1 Zn 1	0	0
2	4-A	1	Total 1 Zn 1	0	0
2	12-A	1	Total 1 Zn 1	0	0
2	1-A	1	Total 1 Zn 1	0	0
2	11-B	1	Total 1 Zn 1	0	0
2	8-B	1	Total 1 Zn 1	0	0
2	7-A	1	Total 1 Zn 1	0	0
2	15-A	1	Total 1 Zn 1	0	0
2	3-B	1	Total 1 Zn 1	0	0
2	12-B	1	Total 1 Zn 1	0	0
2	4-B	1	Total 1 Zn 1	0	0
2	9-B	1	Total 1 Zn 1	0	0
2	6-A	1	Total 1 Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	14-A	1	Total 1	Zn 1	0	0
2	3-A	1	Total 1	Zn 1	0	0
2	11-A	1	Total 1	Zn 1	0	0
2	5-B	1	Total 1	Zn 1	0	0
2	6-B	1	Total 1	Zn 1	0	0
2	13-B	1	Total 1	Zn 1	0	0
2	2-A	1	Total 1	Zn 1	0	0
2	10-A	1	Total 1	Zn 1	0	0
2	9-A	1	Total 1	Zn 1	0	0
2	14-B	1	Total 1	Zn 1	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	16-A	1	Total 1	Fe 1	0	0
3	1-B	1	Total 1	Fe 1	0	0
3	5-A	1	Total 1	Fe 1	0	0
3	13-A	1	Total 1	Fe 1	0	0
3	8-A	1	Total 1	Fe 1	0	0
3	2-B	1	Total 1	Fe 1	0	0
3	15-B	1	Total 1	Fe 1	0	0
3	7-B	1	Total 1	Fe 1	0	0
3	16-B	1	Total 1	Fe 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	10-B	1	Total 1	Fe 1	0	0
3	4-A	1	Total 1	Fe 1	0	0
3	12-A	1	Total 1	Fe 1	0	0
3	1-A	1	Total 1	Fe 1	0	0
3	11-B	1	Total 1	Fe 1	0	0
3	8-B	1	Total 1	Fe 1	0	0
3	7-A	1	Total 1	Fe 1	0	0
3	15-A	1	Total 1	Fe 1	0	0
3	3-B	1	Total 1	Fe 1	0	0
3	12-B	1	Total 1	Fe 1	0	0
3	4-B	1	Total 1	Fe 1	0	0
3	9-B	1	Total 1	Fe 1	0	0
3	6-A	1	Total 1	Fe 1	0	0
3	14-A	1	Total 1	Fe 1	0	0
3	3-A	1	Total 1	Fe 1	0	0
3	11-A	1	Total 1	Fe 1	0	0
3	5-B	1	Total 1	Fe 1	0	0
3	6-B	1	Total 1	Fe 1	0	0
3	13-B	1	Total 1	Fe 1	0	0
3	2-A	1	Total 1	Fe 1	0	0
3	10-A	1	Total 1	Fe 1	0	0

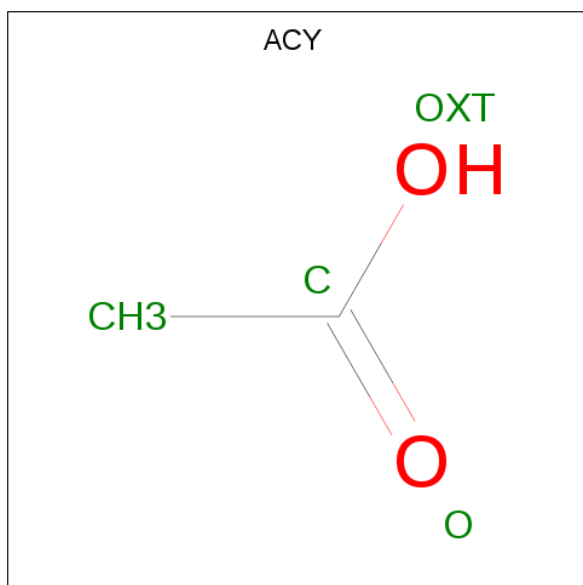
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	9-A	1	Total	Fe	0	0
			1	1		
3	14-B	1	Total	Fe	0	0
			1	1		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	1-A	1	Total	C	O	0	0
			4	2	2		
4	2-A	1	Total	C	O	0	0
			4	2	2		
4	3-A	1	Total	C	O	0	0
			4	2	2		
4	4-A	1	Total	C	O	0	0
			4	2	2		
4	5-A	1	Total	C	O	0	0
			4	2	2		
4	6-A	1	Total	C	O	0	0
			4	2	2		
4	7-A	1	Total	C	O	0	0
			4	2	2		
4	8-A	1	Total	C	O	0	0
			4	2	2		
4	9-A	1	Total	C	O	0	0
			4	2	2		

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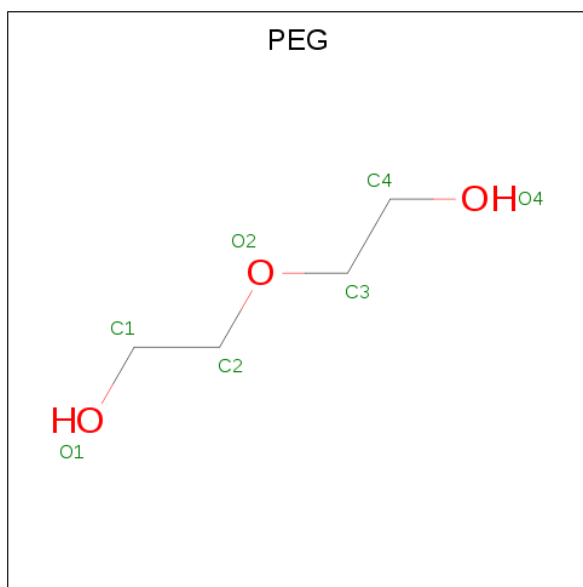
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	10-A	1	Total	C	O	0	0
			4	2	2		
4	11-A	1	Total	C	O	0	0
			4	2	2		
4	12-A	1	Total	C	O	0	0
			4	2	2		
4	13-A	1	Total	C	O	0	0
			4	2	2		
4	14-A	1	Total	C	O	0	0
			4	2	2		
4	15-A	1	Total	C	O	0	0
			4	2	2		
4	16-A	1	Total	C	O	0	0
			4	2	2		
4	1-B	1	Total	C	O	0	0
			4	2	2		
4	2-B	1	Total	C	O	0	0
			4	2	2		
4	3-B	1	Total	C	O	0	0
			4	2	2		
4	4-B	1	Total	C	O	0	0
			4	2	2		
4	5-B	1	Total	C	O	0	0
			4	2	2		
4	6-B	1	Total	C	O	0	0
			4	2	2		
4	7-B	1	Total	C	O	0	0
			4	2	2		
4	8-B	1	Total	C	O	0	0
			4	2	2		
4	9-B	1	Total	C	O	0	0
			4	2	2		
4	10-B	1	Total	C	O	0	0
			4	2	2		
4	11-B	1	Total	C	O	0	0
			4	2	2		
4	12-B	1	Total	C	O	0	0
			4	2	2		
4	13-B	1	Total	C	O	0	0
			4	2	2		
4	14-B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	15-B	1	Total	C	O	0	0
			4	2	2		
4	16-B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	1-A	1	Total	C	O	0	0
			7	4	3		
5	2-A	1	Total	C	O	0	0
			7	4	3		
5	3-A	1	Total	C	O	0	0
			7	4	3		
5	4-A	1	Total	C	O	0	0
			7	4	3		
5	5-A	1	Total	C	O	0	0
			7	4	3		
5	6-A	1	Total	C	O	0	0
			7	4	3		
5	7-A	1	Total	C	O	0	0
			7	4	3		
5	8-A	1	Total	C	O	0	0
			7	4	3		
5	9-A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	10-A	1	Total	C	O	0	0
			7	4	3		
5	11-A	1	Total	C	O	0	0
			7	4	3		
5	12-A	1	Total	C	O	0	0
			7	4	3		
5	13-A	1	Total	C	O	0	0
			7	4	3		
5	14-A	1	Total	C	O	0	0
			7	4	3		
5	15-A	1	Total	C	O	0	0
			7	4	3		
5	16-A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1-A	282	Total	O	0	0
			282	282		
6	2-A	282	Total	O	0	0
			282	282		
6	3-A	282	Total	O	0	0
			282	282		
6	4-A	278	Total	O	0	0
			278	278		
6	5-A	277	Total	O	0	0
			277	277		
6	6-A	278	Total	O	0	0
			278	278		
6	7-A	281	Total	O	0	0
			281	281		
6	8-A	285	Total	O	0	0
			285	285		
6	9-A	281	Total	O	0	0
			281	281		
6	10-A	285	Total	O	0	0
			285	285		
6	11-A	285	Total	O	0	0
			285	285		
6	12-A	283	Total	O	0	0
			283	283		

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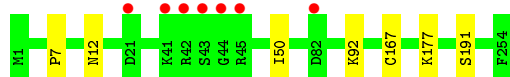
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	13-A	282	Total 282	O 282	0	0
6	14-A	279	Total 279	O 279	0	0
6	15-A	285	Total 285	O 285	0	0
6	16-A	278	Total 278	O 278	0	0
6	1-B	265	Total 265	O 265	0	0
6	2-B	265	Total 265	O 265	0	0
6	3-B	265	Total 265	O 265	0	0
6	4-B	269	Total 269	O 269	0	0
6	5-B	270	Total 270	O 270	0	0
6	6-B	269	Total 269	O 269	0	0
6	7-B	266	Total 266	O 266	0	0
6	8-B	262	Total 262	O 262	0	0
6	9-B	266	Total 266	O 266	0	0
6	10-B	262	Total 262	O 262	0	0
6	11-B	262	Total 262	O 262	0	0
6	12-B	264	Total 264	O 264	0	0
6	13-B	265	Total 265	O 265	0	0
6	14-B	268	Total 268	O 268	0	0
6	15-B	262	Total 262	O 262	0	0
6	16-B	269	Total 269	O 269	0	0

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

These plots are drawn for all protein, RNA and DNA 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.

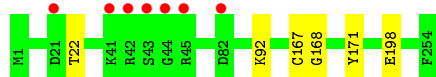
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2



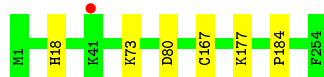
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2



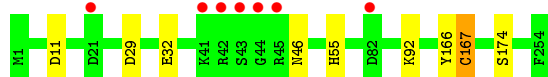
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2



- Molecule 1: Putative hydroxyacylglutathione hydrolase 2



- Molecule 1: Putative hydroxyacylglutathione hydrolase 2



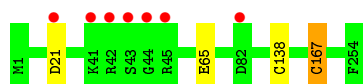
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 3-B:  96% .



- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 4-A:  98% .



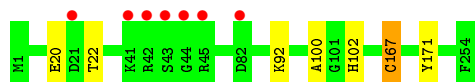
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 4-B:  96% .



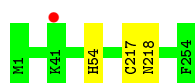
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 5-A:  97% .



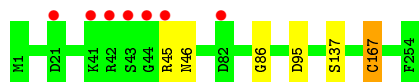
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 5-B:  99% .



- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 6-A:  98% .

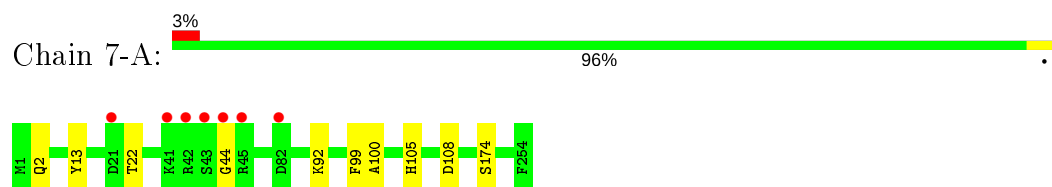


- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

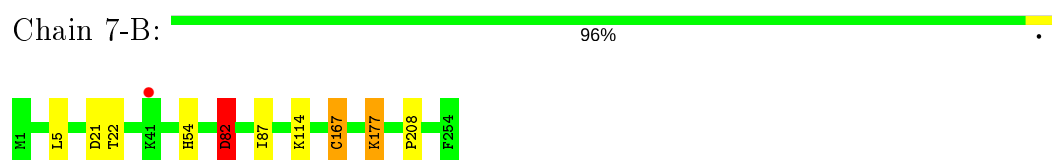
Chain 6-B:  100% .



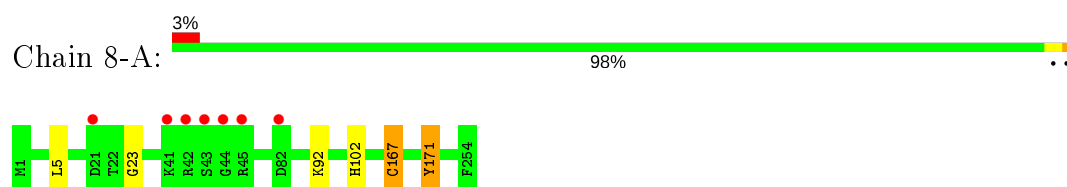
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2



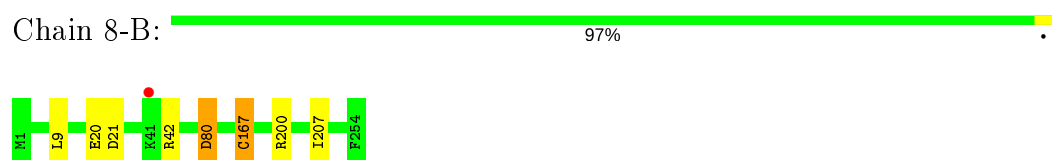
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2



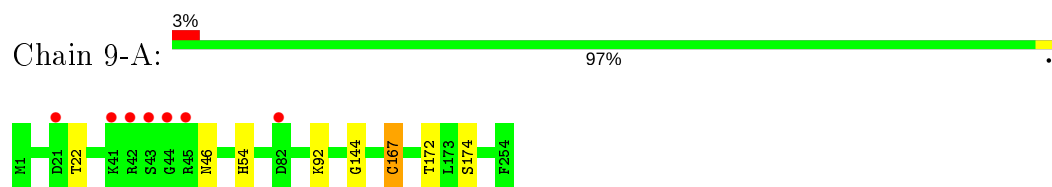
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2



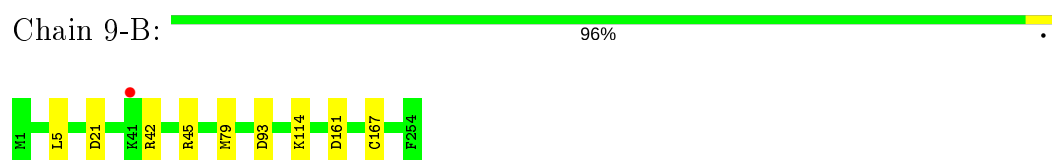
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2



- Molecule 1: Putative hydroxyacylglutathione hydrolase 2



- Molecule 1: Putative hydroxyacylglutathione hydrolase 2



- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

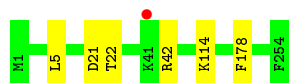






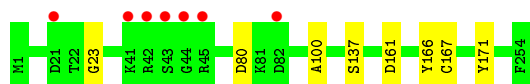
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 10-B:  98%



- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 11-A:  97%



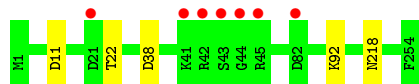
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 11-B:  99%



- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 12-A:  98%



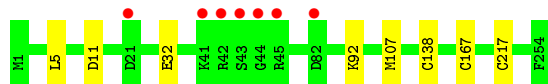
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 12-B:  98%



- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 13-A:  97%



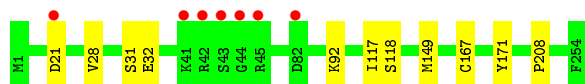
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 13-B:  96%



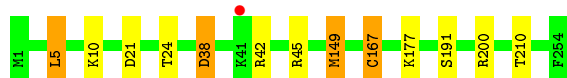
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 14-A:  96%



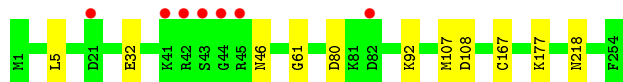
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 14-B:  95%



- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 15-A:  96%



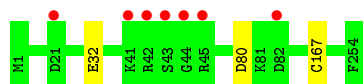
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 15-B:  93%



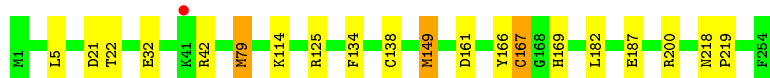
- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 16-A:  99%



- Molecule 1: Putative hydroxyacylglutathione hydrolase 2

Chain 16-B:  92%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.49 Å   58.78 Å   69.05 Å 90.00°   109.22°   90.00°	Depositor
Resolution (Å)	32.97 – 1.74 32.97 – 1.74	Depositor EDS
% Data completeness (in resolution range)	97.5 (32.97-1.74) 97.7 (32.97-1.74)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 1.74 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.147 , 0.193 0.148 , 0.190	Depositor DCC
$R_{free}$ test set	2630 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.4	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 51.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	72352	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, PEG, ZN, FE

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	1.03	1/2020 (0.0%)	0.86	0/2730
1	1-B	0.94	1/2020 (0.0%)	0.92	1/2730 (0.0%)
1	2-A	0.91	2/2020 (0.1%)	0.88	1/2730 (0.0%)
1	2-B	0.92	1/2020 (0.0%)	0.89	2/2730 (0.1%)
1	3-A	0.97	3/2020 (0.1%)	0.92	2/2730 (0.1%)
1	3-B	0.90	1/2020 (0.0%)	0.86	1/2730 (0.0%)
1	4-A	0.89	2/2020 (0.1%)	0.86	0/2730
1	4-B	0.95	5/2020 (0.2%)	0.89	3/2730 (0.1%)
1	5-A	0.96	3/2020 (0.1%)	0.89	2/2730 (0.1%)
1	5-B	0.88	1/2020 (0.0%)	0.86	0/2730
1	6-A	0.88	1/2020 (0.0%)	0.87	1/2730 (0.0%)
1	6-B	0.87	0/2020	0.85	1/2730 (0.0%)
1	7-A	0.89	2/2020 (0.1%)	0.87	1/2730 (0.0%)
1	7-B	0.92	3/2020 (0.1%)	0.92	5/2730 (0.2%)
1	8-A	0.94	2/2020 (0.1%)	0.96	1/2730 (0.0%)
1	8-B	0.98	1/2020 (0.0%)	0.88	2/2730 (0.1%)
1	9-A	0.91	2/2020 (0.1%)	0.89	2/2730 (0.1%)
1	9-B	0.95	2/2020 (0.1%)	0.87	0/2730
1	10-A	1.10	3/2020 (0.1%)	0.91	2/2730 (0.1%)
1	10-B	0.88	1/2020 (0.0%)	0.88	1/2730 (0.0%)
1	11-A	1.11	3/2020 (0.1%)	0.90	2/2730 (0.1%)
1	11-B	0.92	1/2020 (0.0%)	0.87	1/2730 (0.0%)
1	12-A	0.88	0/2020	0.86	1/2730 (0.0%)
1	12-B	0.91	1/2020 (0.0%)	0.88	3/2730 (0.1%)
1	13-A	1.04	3/2020 (0.1%)	0.97	3/2730 (0.1%)
1	13-B	1.02	1/2020 (0.0%)	0.98	1/2730 (0.0%)
1	14-A	1.05	6/2020 (0.3%)	1.01	2/2730 (0.1%)
1	14-B	1.05	1/2020 (0.0%)	1.02	5/2730 (0.2%)
1	15-A	1.03	3/2020 (0.1%)	0.98	0/2730
1	15-B	1.09	4/2020 (0.2%)	1.04	5/2730 (0.2%)
1	16-A	1.03	1/2020 (0.0%)	0.97	0/2730
1	16-B	1.12	4/2020 (0.2%)	1.06	7/2730 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.97	65/64640 (0.1%)	0.92	58/87360 (0.1%)

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	5-A	0	1
1	11-A	0	1
1	14-A	0	1
All	All	0	3

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	11-A	167	CYS	CB-SG	28.60	2.30	1.82
1	10-A	167	CYS	CB-SG	26.97	2.28	1.82
1	1-A	167	CYS	CB-SG	23.37	2.21	1.82
1	8-B	167	CYS	CB-SG	17.77	2.12	1.82
1	5-A	167	CYS	CB-SG	13.22	2.04	1.82

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	167	CYS	CA-CB-SG	-21.42	75.44	114.00
1	7-B	167	CYS	CA-CB-SG	-13.35	89.97	114.00
1	5-A	167	CYS	CA-CB-SG	-12.19	92.06	114.00
1	3-A	167	CYS	CA-CB-SG	-11.04	94.12	114.00
1	16-B	79	MET	CG-SD-CE	-9.78	84.55	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	11-A	171	TYR	Sidechain
1	14-A	171	TYR	Sidechain
1	5-A	171	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	1978	0	1957	0	0
1	1-B	1978	0	1957	0	0
1	2-A	1978	0	1957	0	0
1	2-B	1978	0	1957	0	0
1	3-A	1978	0	1957	0	0
1	3-B	1978	0	1957	0	0
1	4-A	1978	0	1957	0	0
1	4-B	1978	0	1957	0	0
1	5-A	1978	0	1957	0	0
1	5-B	1978	0	1957	0	0
1	6-A	1978	0	1957	0	0
1	6-B	1978	0	1957	0	0
1	7-A	1978	0	1957	0	0
1	7-B	1978	0	1957	0	0
1	8-A	1978	0	1957	0	0
1	8-B	1978	0	1957	0	0
1	9-A	1978	0	1957	0	0
1	9-B	1978	0	1957	0	0
1	10-A	1978	0	1957	0	0
1	10-B	1978	0	1957	0	0
1	11-A	1978	0	1957	0	0
1	11-B	1978	0	1957	0	0
1	12-A	1978	0	1957	0	0
1	12-B	1978	0	1957	0	0
1	13-A	1978	0	1957	0	0
1	13-B	1978	0	1957	0	0
1	14-A	1978	0	1957	0	0
1	14-B	1978	0	1957	0	0
1	15-A	1978	0	1957	0	0
1	15-B	1978	0	1957	0	0
1	16-A	1978	0	1957	0	0
1	16-B	1978	0	1957	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
2	9-A	1	0	0	0	0
2	9-B	1	0	0	0	0
2	10-A	1	0	0	0	0
2	10-B	1	0	0	0	0
2	11-A	1	0	0	0	0
2	11-B	1	0	0	0	0
2	12-A	1	0	0	0	0
2	12-B	1	0	0	0	0
2	13-A	1	0	0	0	0
2	13-B	1	0	0	0	0
2	14-A	1	0	0	0	0
2	14-B	1	0	0	0	0
2	15-A	1	0	0	0	0
2	15-B	1	0	0	0	0
2	16-A	1	0	0	0	0
2	16-B	1	0	0	0	0
3	1-A	1	0	0	0	0
3	1-B	1	0	0	0	0
3	2-A	1	0	0	0	0
3	2-B	1	0	0	0	0
3	3-A	1	0	0	0	0
3	3-B	1	0	0	0	0
3	4-A	1	0	0	0	0
3	4-B	1	0	0	0	0
3	5-A	1	0	0	0	0
3	5-B	1	0	0	0	0
3	6-A	1	0	0	0	0
3	6-B	1	0	0	0	0
3	7-A	1	0	0	0	0
3	7-B	1	0	0	0	0
3	8-A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	8-B	1	0	0	0	0
3	9-A	1	0	0	0	0
3	9-B	1	0	0	0	0
3	10-A	1	0	0	0	0
3	10-B	1	0	0	0	0
3	11-A	1	0	0	0	0
3	11-B	1	0	0	0	0
3	12-A	1	0	0	0	0
3	12-B	1	0	0	0	0
3	13-A	1	0	0	0	0
3	13-B	1	0	0	0	0
3	14-A	1	0	0	0	0
3	14-B	1	0	0	0	0
3	15-A	1	0	0	0	0
3	15-B	1	0	0	0	0
3	16-A	1	0	0	0	0
3	16-B	1	0	0	0	0
4	1-A	4	0	3	0	0
4	1-B	4	0	3	0	0
4	2-A	4	0	3	0	0
4	2-B	4	0	3	0	0
4	3-A	4	0	3	0	0
4	3-B	4	0	4	0	0
4	4-A	4	0	4	0	0
4	4-B	4	0	3	0	0
4	5-A	4	0	3	0	0
4	5-B	4	0	3	0	0
4	6-A	4	0	4	0	0
4	6-B	4	0	3	0	0
4	7-A	4	0	3	0	0
4	7-B	4	0	3	0	0
4	8-A	4	0	4	0	0
4	8-B	4	0	3	0	0
4	9-A	4	0	3	0	0
4	9-B	4	0	3	0	0
4	10-A	4	0	3	0	0
4	10-B	4	0	3	0	0
4	11-A	4	0	3	0	0
4	11-B	4	0	3	0	0
4	12-A	4	0	3	0	0
4	12-B	4	0	4	0	0
4	13-A	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	13-B	4	0	3	0	0
4	14-A	4	0	3	0	0
4	14-B	4	0	3	0	0
4	15-A	4	0	3	0	0
4	15-B	4	0	3	0	0
4	16-A	4	0	3	0	0
4	16-B	4	0	3	0	0
5	1-A	7	0	10	0	0
5	2-A	7	0	10	0	0
5	3-A	7	0	10	0	0
5	4-A	7	0	10	0	0
5	5-A	7	0	10	0	0
5	6-A	7	0	10	0	0
5	7-A	7	0	10	0	0
5	8-A	7	0	10	0	0
5	9-A	7	0	10	0	0
5	10-A	7	0	10	0	0
5	11-A	7	0	10	0	0
5	12-A	7	0	10	0	0
5	13-A	7	0	10	0	0
5	14-A	7	0	10	0	0
5	15-A	7	0	10	0	0
5	16-A	7	0	10	0	0
6	1-A	282	0	0	0	0
6	1-B	265	0	0	0	0
6	2-A	282	0	0	0	0
6	2-B	265	0	0	0	0
6	3-A	282	0	0	0	0
6	3-B	265	0	0	0	0
6	4-A	278	0	0	0	0
6	4-B	269	0	0	0	0
6	5-A	277	0	0	0	0
6	5-B	270	0	0	0	0
6	6-A	278	0	0	0	0
6	6-B	269	0	0	0	0
6	7-A	281	0	0	0	0
6	7-B	266	0	0	0	0
6	8-A	285	0	0	0	0
6	8-B	262	0	0	0	0
6	9-A	281	0	0	0	0
6	9-B	266	0	0	0	0
6	10-A	285	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	10-B	262	0	0	0	0
6	11-A	285	0	0	0	0
6	11-B	262	0	0	0	0
6	12-A	283	0	0	0	0
6	12-B	264	0	0	0	0
6	13-A	282	0	0	0	0
6	13-B	265	0	0	0	0
6	14-A	279	0	0	0	0
6	14-B	268	0	0	0	0
6	15-A	285	0	0	0	0
6	15-B	262	0	0	0	0
6	16-A	278	0	0	0	0
6	16-B	269	0	0	0	0
All	All	72352	0	62885	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

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	252/254 (99%)	234 (93%)	16 (6%)	2 (1%)	19	6
1	1-B	252/254 (99%)	219 (87%)	30 (12%)	3 (1%)	13	3
1	2-A	252/254 (99%)	238 (94%)	13 (5%)	1 (0%)	34	17
1	2-B	252/254 (99%)	237 (94%)	14 (6%)	1 (0%)	34	17
1	3-A	252/254 (99%)	240 (95%)	9 (4%)	3 (1%)	13	3
1	3-B	252/254 (99%)	240 (95%)	10 (4%)	2 (1%)	19	6
1	4-A	252/254 (99%)	232 (92%)	19 (8%)	1 (0%)	34	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4-B	252/254 (99%)	243 (96%)	6 (2%)	3 (1%)	13	3
1	5-A	252/254 (99%)	242 (96%)	9 (4%)	1 (0%)	34	17
1	5-B	252/254 (99%)	243 (96%)	9 (4%)	0	100	100
1	6-A	252/254 (99%)	236 (94%)	13 (5%)	3 (1%)	13	3
1	6-B	252/254 (99%)	247 (98%)	5 (2%)	0	100	100
1	7-A	252/254 (99%)	241 (96%)	9 (4%)	2 (1%)	19	6
1	7-B	252/254 (99%)	241 (96%)	10 (4%)	1 (0%)	34	17
1	8-A	252/254 (99%)	243 (96%)	8 (3%)	1 (0%)	34	17
1	8-B	252/254 (99%)	237 (94%)	12 (5%)	3 (1%)	13	3
1	9-A	252/254 (99%)	238 (94%)	12 (5%)	2 (1%)	19	6
1	9-B	252/254 (99%)	239 (95%)	11 (4%)	2 (1%)	19	6
1	10-A	252/254 (99%)	231 (92%)	18 (7%)	3 (1%)	13	3
1	10-B	252/254 (99%)	242 (96%)	10 (4%)	0	100	100
1	11-A	252/254 (99%)	234 (93%)	17 (7%)	1 (0%)	34	17
1	11-B	252/254 (99%)	242 (96%)	10 (4%)	0	100	100
1	12-A	252/254 (99%)	240 (95%)	11 (4%)	1 (0%)	34	17
1	12-B	252/254 (99%)	241 (96%)	10 (4%)	1 (0%)	34	17
1	13-A	252/254 (99%)	238 (94%)	13 (5%)	1 (0%)	34	17
1	13-B	252/254 (99%)	238 (94%)	12 (5%)	2 (1%)	19	6
1	14-A	252/254 (99%)	232 (92%)	18 (7%)	2 (1%)	19	6
1	14-B	252/254 (99%)	237 (94%)	14 (6%)	1 (0%)	34	17
1	15-A	252/254 (99%)	241 (96%)	10 (4%)	1 (0%)	34	17
1	15-B	252/254 (99%)	238 (94%)	11 (4%)	3 (1%)	13	3
1	16-A	252/254 (99%)	239 (95%)	13 (5%)	0	100	100
1	16-B	252/254 (99%)	231 (92%)	18 (7%)	3 (1%)	13	3
All	All	8064/8128 (99%)	7614 (94%)	400 (5%)	50 (1%)	25	10

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-B	46	ASN
1	3-A	55	HIS
1	9-B	93	ASP

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Mol	Chain	Res	Type
1	12-A	11	ASP
1	12-B	63	ASN

### 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	217/217 (100%)	213 (98%)	4 (2%)	59	38
1	1-B	217/217 (100%)	211 (97%)	6 (3%)	43	19
1	2-A	217/217 (100%)	214 (99%)	3 (1%)	67	50
1	2-B	217/217 (100%)	214 (99%)	3 (1%)	67	50
1	3-A	217/217 (100%)	213 (98%)	4 (2%)	59	38
1	3-B	217/217 (100%)	212 (98%)	5 (2%)	50	27
1	4-A	217/217 (100%)	215 (99%)	2 (1%)	78	67
1	4-B	217/217 (100%)	213 (98%)	4 (2%)	59	38
1	5-A	217/217 (100%)	214 (99%)	3 (1%)	67	50
1	5-B	217/217 (100%)	215 (99%)	2 (1%)	78	67
1	6-A	217/217 (100%)	214 (99%)	3 (1%)	67	50
1	6-B	217/217 (100%)	217 (100%)	0	100	100
1	7-A	217/217 (100%)	212 (98%)	5 (2%)	50	27
1	7-B	217/217 (100%)	211 (97%)	6 (3%)	43	19
1	8-A	217/217 (100%)	212 (98%)	5 (2%)	50	27
1	8-B	217/217 (100%)	213 (98%)	4 (2%)	59	38
1	9-A	217/217 (100%)	213 (98%)	4 (2%)	59	38
1	9-B	217/217 (100%)	211 (97%)	6 (3%)	43	19
1	10-A	217/217 (100%)	209 (96%)	8 (4%)	34	11
1	10-B	217/217 (100%)	213 (98%)	4 (2%)	59	38
1	11-A	217/217 (100%)	214 (99%)	3 (1%)	67	50
1	11-B	217/217 (100%)	216 (100%)	1 (0%)	88	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	12-A	217/217 (100%)	214 (99%)	3 (1%)	67	50
1	12-B	217/217 (100%)	214 (99%)	3 (1%)	67	50
1	13-A	217/217 (100%)	214 (99%)	3 (1%)	67	50
1	13-B	217/217 (100%)	211 (97%)	6 (3%)	43	19
1	14-A	217/217 (100%)	214 (99%)	3 (1%)	67	50
1	14-B	217/217 (100%)	207 (95%)	10 (5%)	27	7
1	15-A	217/217 (100%)	210 (97%)	7 (3%)	39	15
1	15-B	217/217 (100%)	210 (97%)	7 (3%)	39	15
1	16-A	217/217 (100%)	215 (99%)	2 (1%)	78	67
1	16-B	217/217 (100%)	206 (95%)	11 (5%)	24	5
All	All	6944/6944 (100%)	6804 (98%)	140 (2%)	55	33

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	9-B	5	LEU
1	10-B	21	ASP
1	16-B	5	LEU
1	9-B	42	ARG
1	10-A	63	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
1	8-A	154	GLN
1	9-A	185	ASN
1	15-A	218	ASN
1	8-A	185	ASN
1	8-B	190	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 112 ligands modelled in this entry, 64 are monoatomic - leaving 48 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	$\# Z  > 2$
4	ACY	2-A	800	-	1,3,3	1.22	0	0,3,3	0.00	-
4	ACY	3-B	801	-	1,3,3	1.91	0	0,3,3	0.00	-
4	ACY	3-A	800	-	1,3,3	1.99	0	0,3,3	0.00	-
4	ACY	16-B	801	-	1,3,3	2.03	1 (100%)	0,3,3	0.00	-
5	PEG	7-A	9979	-	6,6,6	1.27	0	5,5,5	0.57	0
5	PEG	3-A	9979	-	6,6,6	1.07	0	5,5,5	0.57	0
5	PEG	10-A	9979	-	6,6,6	0.89	0	5,5,5	0.49	0
4	ACY	1-A	800	-	1,3,3	1.69	0	0,3,3	0.00	-
4	ACY	14-A	800	-	1,3,3	2.14	1 (100%)	0,3,3	0.00	-
4	ACY	15-A	800	-	1,3,3	1.40	0	0,3,3	0.00	-
4	ACY	10-A	800	-	1,3,3	1.98	0	0,3,3	0.00	-
5	PEG	12-A	9979	-	6,6,6	1.14	0	5,5,5	0.60	0
5	PEG	11-A	9979	-	6,6,6	0.97	0	5,5,5	0.52	0
4	ACY	10-B	801	-	1,3,3	0.78	0	0,3,3	0.00	-
5	PEG	9-A	9979	-	6,6,6	0.82	0	5,5,5	0.39	0
4	ACY	5-A	800	-	1,3,3	1.98	0	0,3,3	0.00	-
5	PEG	16-A	9979	-	6,6,6	1.02	0	5,5,5	0.42	0
4	ACY	9-A	800	-	1,3,3	2.03	1 (100%)	0,3,3	0.00	-
4	ACY	13-A	800	-	1,3,3	1.90	0	0,3,3	0.00	-
4	ACY	16-A	800	-	1,3,3	2.23	1 (100%)	0,3,3	0.00	-
4	ACY	7-B	801	-	1,3,3	0.35	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ACY	13-B	801	-	1,3,3	1.88	0	0,3,3	0.00	-
5	PEG	1-A	9979	-	6,6,6	1.02	0	5,5,5	0.55	0
4	ACY	11-B	801	-	1,3,3	0.03	0	0,3,3	0.00	-
5	PEG	6-A	9979	-	6,6,6	0.85	0	5,5,5	0.66	0
5	PEG	5-A	9979	-	6,6,6	1.23	0	5,5,5	0.63	0
4	ACY	9-B	801	-	1,3,3	0.66	0	0,3,3	0.00	-
4	ACY	6-A	800	-	1,3,3	2.56	1 (100%)	0,3,3	0.00	-
4	ACY	11-A	800	-	1,3,3	1.66	0	0,3,3	0.00	-
4	ACY	7-A	800	-	1,3,3	2.06	1 (100%)	0,3,3	0.00	-
5	PEG	8-A	9979	-	6,6,6	0.90	0	5,5,5	0.50	0
4	ACY	2-B	801	-	1,3,3	2.04	1 (100%)	0,3,3	0.00	-
4	ACY	1-B	801	-	1,3,3	1.84	0	0,3,3	0.00	-
4	ACY	8-B	801	-	1,3,3	0.63	0	0,3,3	0.00	-
4	ACY	6-B	801	-	1,3,3	1.60	0	0,3,3	0.00	-
4	ACY	4-A	800	-	1,3,3	3.38	1 (100%)	0,3,3	0.00	-
5	PEG	4-A	9979	-	6,6,6	0.81	0	5,5,5	0.66	0
4	ACY	15-B	801	-	1,3,3	0.63	0	0,3,3	0.00	-
5	PEG	2-A	9979	-	6,6,6	0.69	0	5,5,5	0.46	0
5	PEG	15-A	9979	-	6,6,6	0.92	0	5,5,5	0.44	0
4	ACY	8-A	800	-	1,3,3	0.25	0	0,3,3	0.00	-
4	ACY	14-B	801	-	1,3,3	1.36	0	0,3,3	0.00	-
4	ACY	5-B	801	-	1,3,3	1.65	0	0,3,3	0.00	-
4	ACY	12-A	800	-	1,3,3	1.86	0	0,3,3	0.00	-
4	ACY	4-B	801	-	1,3,3	0.98	0	0,3,3	0.00	-
5	PEG	13-A	9979	-	6,6,6	0.97	0	5,5,5	0.48	0
4	ACY	12-B	801	-	1,3,3	1.92	0	0,3,3	0.00	-
5	PEG	14-A	9979	-	6,6,6	1.02	0	5,5,5	0.48	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
5	PEG	6-A	9979	-	-	1/4/4/4	-
5	PEG	10-A	9979	-	-	0/4/4/4	-
5	PEG	2-A	9979	-	-	1/4/4/4	-
5	PEG	15-A	9979	-	-	0/4/4/4	-
5	PEG	7-A	9979	-	-	0/4/4/4	-
5	PEG	11-A	9979	-	-	0/4/4/4	-
5	PEG	8-A	9979	-	-	0/4/4/4	-
5	PEG	3-A	9979	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	4-A	9979	-	-	1/4/4/4	-
5	PEG	16-A	9979	-	-	0/4/4/4	-
5	PEG	9-A	9979	-	-	1/4/4/4	-
5	PEG	12-A	9979	-	-	0/4/4/4	-
5	PEG	5-A	9979	-	-	1/4/4/4	-
5	PEG	1-A	9979	-	-	0/4/4/4	-
5	PEG	13-A	9979	-	-	0/4/4/4	-
5	PEG	14-A	9979	-	-	0/4/4/4	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4-A	800	ACY	CH3-C	3.38	1.53	1.48
4	6-A	800	ACY	CH3-C	2.56	1.52	1.48
4	16-A	800	ACY	CH3-C	2.23	1.51	1.48
4	14-A	800	ACY	CH3-C	2.14	1.51	1.48
4	7-A	800	ACY	CH3-C	2.06	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	9-A	9979	PEG	O1-C1-C2-O2
5	6-A	9979	PEG	O2-C3-C4-O4
5	4-A	9979	PEG	O2-C3-C4-O4
5	2-A	9979	PEG	O1-C1-C2-O2
5	5-A	9979	PEG	O2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	1-A	254/254 (100%)	-0.30	7 (2%)	53	58	4, 12, 28, 52	254 (100%)
1	1-B	254/254 (100%)	-0.35	1 (0%)	92	94	5, 11, 23, 48	254 (100%)
1	2-A	254/254 (100%)	-0.30	7 (2%)	53	58	4, 12, 28, 52	254 (100%)
1	2-B	254/254 (100%)	-0.35	1 (0%)	92	94	5, 11, 23, 48	254 (100%)
1	3-A	254/254 (100%)	-0.30	7 (2%)	53	58	4, 12, 28, 52	254 (100%)
1	3-B	254/254 (100%)	-0.35	1 (0%)	92	94	5, 11, 23, 48	254 (100%)
1	4-A	254/254 (100%)	-0.30	7 (2%)	53	58	4, 12, 28, 52	254 (100%)
1	4-B	254/254 (100%)	-0.35	1 (0%)	92	94	5, 11, 23, 48	254 (100%)
1	5-A	254/254 (100%)	-0.30	7 (2%)	53	58	4, 12, 28, 52	254 (100%)
1	5-B	254/254 (100%)	-0.35	1 (0%)	92	94	5, 11, 23, 48	254 (100%)
1	6-A	254/254 (100%)	-0.30	7 (2%)	53	58	4, 12, 28, 52	254 (100%)
1	6-B	254/254 (100%)	-0.35	1 (0%)	92	94	5, 11, 23, 48	254 (100%)
1	7-A	254/254 (100%)	-0.30	7 (2%)	53	58	4, 12, 28, 52	254 (100%)
1	7-B	254/254 (100%)	-0.35	1 (0%)	92	94	5, 11, 23, 48	254 (100%)
1	8-A	254/254 (100%)	-0.30	7 (2%)	53	58	4, 12, 28, 52	254 (100%)
1	8-B	254/254 (100%)	-0.35	1 (0%)	92	94	5, 11, 23, 48	254 (100%)
1	9-A	254/254 (100%)	-0.30	7 (2%)	53	58	4, 12, 28, 52	254 (100%)
1	9-B	254/254 (100%)	-0.35	1 (0%)	92	94	5, 11, 23, 48	254 (100%)
1	10-A	254/254 (100%)	-0.30	7 (2%)	53	58	4, 12, 28, 52	254 (100%)
1	10-B	254/254 (100%)	-0.35	1 (0%)	92	94	5, 11, 23, 48	254 (100%)
1	11-A	254/254 (100%)	-0.30	7 (2%)	53	58	4, 12, 28, 52	254 (100%)
1	11-B	254/254 (100%)	-0.35	1 (0%)	92	94	5, 11, 23, 48	254 (100%)
1	12-A	254/254 (100%)	-0.30	7 (2%)	53	58	4, 12, 28, 52	254 (100%)
1	12-B	254/254 (100%)	-0.35	1 (0%)	92	94	5, 11, 23, 48	254 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	13-A	254/254 (100%)	-0.30	7 (2%) 53 58	4, 12, 28, 52	254 (100%)
1	13-B	254/254 (100%)	-0.35	1 (0%) 92 94	5, 11, 23, 48	254 (100%)
1	14-A	254/254 (100%)	-0.30	7 (2%) 53 58	4, 12, 28, 52	254 (100%)
1	14-B	254/254 (100%)	-0.35	1 (0%) 92 94	5, 11, 23, 48	254 (100%)
1	15-A	254/254 (100%)	-0.30	7 (2%) 53 58	4, 12, 28, 52	254 (100%)
1	15-B	254/254 (100%)	-0.35	1 (0%) 92 94	5, 11, 23, 48	254 (100%)
1	16-A	254/254 (100%)	-0.30	7 (2%) 53 58	4, 12, 28, 52	254 (100%)
1	16-B	254/254 (100%)	-0.35	1 (0%) 92 94	5, 11, 23, 48	254 (100%)
All	All	8128/8128 (100%)	-0.32	128 (1%) 65 78	4, 11, 27, 52	8128 (100%)

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	42	ARG	6.5
1	2-A	42	ARG	6.5
1	3-A	42	ARG	6.5
1	4-A	42	ARG	6.5
1	5-A	42	ARG	6.5

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	PEG	3-A	9979	7/7	0.92	0.09	18,19,23,23	7
5	PEG	11-A	9979	7/7	0.92	0.09	18,19,23,23	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PEG	1-A	9979	7/7	0.92	0.09	18,19,23,23	7
5	PEG	15-A	9979	7/7	0.92	0.09	17,19,23,24	7
5	PEG	9-A	9979	7/7	0.92	0.09	17,20,23,24	7
5	PEG	13-A	9979	7/7	0.92	0.09	17,19,23,23	7
5	PEG	10-A	9979	7/7	0.92	0.09	18,19,23,24	7
5	PEG	16-A	9979	7/7	0.92	0.09	17,19,23,24	7
5	PEG	6-A	9979	7/7	0.92	0.09	18,19,24,24	7
5	PEG	5-A	9979	7/7	0.92	0.09	18,19,23,24	7
5	PEG	8-A	9979	7/7	0.92	0.09	18,19,23,24	7
5	PEG	2-A	9979	7/7	0.92	0.09	17,20,23,24	7
5	PEG	7-A	9979	7/7	0.92	0.09	18,19,23,23	7
5	PEG	12-A	9979	7/7	0.92	0.09	18,19,23,23	7
5	PEG	4-A	9979	7/7	0.92	0.09	18,19,24,24	7
5	PEG	14-A	9979	7/7	0.92	0.09	18,19,23,23	7
4	ACY	10-A	800	4/4	0.98	0.16	17,19,19,20	4
4	ACY	12-A	800	4/4	0.98	0.16	17,19,19,20	4
4	ACY	6-A	800	4/4	0.98	0.16	17,19,19,19	4
4	ACY	14-A	800	4/4	0.98	0.16	16,19,19,19	4
4	ACY	4-A	800	4/4	0.98	0.16	16,19,20,20	4
4	ACY	9-A	800	4/4	0.98	0.16	17,19,19,20	4
4	ACY	8-A	800	4/4	0.98	0.16	17,19,19,19	4
4	ACY	3-A	800	4/4	0.98	0.16	17,19,19,20	4
4	ACY	2-A	800	4/4	0.98	0.16	16,19,19,19	4
4	ACY	11-A	800	4/4	0.98	0.16	17,19,20,20	4
4	ACY	1-A	800	4/4	0.98	0.16	17,19,19,19	4
4	ACY	5-A	800	4/4	0.98	0.16	17,19,19,20	4
4	ACY	16-A	800	4/4	0.98	0.16	16,19,19,19	4
4	ACY	7-A	800	4/4	0.98	0.16	17,19,19,20	4
4	ACY	15-A	800	4/4	0.98	0.16	16,19,19,19	4
4	ACY	13-A	800	4/4	0.98	0.16	16,19,19,19	4
4	ACY	10-B	801	4/4	0.99	0.10	15,17,17,19	4
4	ACY	13-B	801	4/4	0.99	0.10	15,17,17,18	4
3	FE	8-A	701	1/1	0.99	0.04	3,3,3,3	1
4	ACY	7-B	801	4/4	0.99	0.10	15,17,17,19	4
4	ACY	15-B	801	4/4	0.99	0.10	15,17,18,19	4
4	ACY	9-B	801	4/4	0.99	0.10	15,17,17,19	4
3	FE	16-A	701	1/1	0.99	0.04	4,4,4,4	1
3	FE	2-A	701	1/1	0.99	0.04	6,6,6,6	1
4	ACY	2-B	801	4/4	0.99	0.10	14,17,18,18	4
4	ACY	6-B	801	4/4	0.99	0.10	15,17,17,19	4
4	ACY	8-B	801	4/4	0.99	0.10	15,17,18,19	4
3	FE	14-A	701	1/1	0.99	0.04	2,2,2,2	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ACY	5-B	801	4/4	0.99	0.10	15,17,17,19	4
4	ACY	11-B	801	4/4	0.99	0.10	15,17,17,19	4
4	ACY	12-B	801	4/4	0.99	0.10	15,18,18,19	4
3	FE	3-A	701	1/1	0.99	0.04	3,3,3,3	1
4	ACY	3-B	801	4/4	0.99	0.10	15,18,18,19	4
3	FE	1-A	701	1/1	0.99	0.04	3,3,3,3	1
4	ACY	14-B	801	4/4	0.99	0.10	15,17,17,19	4
4	ACY	4-B	801	4/4	0.99	0.10	15,17,17,19	4
3	FE	4-A	701	1/1	0.99	0.04	2,2,2,2	1
3	FE	6-A	701	1/1	0.99	0.04	2,2,2,2	1
3	FE	5-A	701	1/1	0.99	0.04	3,3,3,3	1
4	ACY	16-B	801	4/4	0.99	0.10	15,17,18,19	4
3	FE	9-A	701	1/1	0.99	0.04	1,1,1,1	1
3	FE	15-A	701	1/1	0.99	0.04	3,3,3,3	1
4	ACY	1-B	801	4/4	0.99	0.10	15,17,17,18	4
3	FE	13-A	701	1/1	0.99	0.04	3,3,3,3	1
3	FE	7-A	701	1/1	0.99	0.04	3,3,3,3	1
3	FE	12-A	701	1/1	0.99	0.04	3,3,3,3	1
3	FE	11-A	701	1/1	0.99	0.04	3,3,3,3	1
3	FE	10-A	701	1/1	0.99	0.04	3,3,3,3	1
2	ZN	12-A	700	1/1	1.00	0.03	7,7,7,7	1
2	ZN	4-B	703	1/1	1.00	0.04	8,8,8,8	1
2	ZN	10-B	703	1/1	1.00	0.04	8,8,8,8	1
3	FE	16-B	704	1/1	1.00	0.04	4,4,4,4	1
3	FE	1-B	704	1/1	1.00	0.04	3,3,3,3	1
2	ZN	4-A	700	1/1	1.00	0.03	7,7,7,7	1
3	FE	9-B	704	1/1	1.00	0.04	3,3,3,3	1
2	ZN	15-A	700	1/1	1.00	0.03	7,7,7,7	1
2	ZN	15-B	703	1/1	1.00	0.04	5,5,5,5	1
2	ZN	3-B	703	1/1	1.00	0.04	6,6,6,6	1
3	FE	8-B	704	1/1	1.00	0.04	3,3,3,3	1
3	FE	13-B	704	1/1	1.00	0.04	4,4,4,4	1
2	ZN	1-B	703	1/1	1.00	0.04	11,11,11,11	1
2	ZN	1-A	700	1/1	1.00	0.03	7,7,7,7	1
2	ZN	13-A	700	1/1	1.00	0.03	7,7,7,7	1
2	ZN	9-B	703	1/1	1.00	0.04	6,6,6,6	1
3	FE	12-B	704	1/1	1.00	0.04	3,3,3,3	1
2	ZN	16-B	703	1/1	1.00	0.04	6,6,6,6	1
3	FE	6-B	704	1/1	1.00	0.04	3,3,3,3	1
2	ZN	10-A	700	1/1	1.00	0.03	7,7,7,7	1
2	ZN	11-A	700	1/1	1.00	0.03	7,7,7,7	1
2	ZN	2-A	700	1/1	1.00	0.03	10,10,10,10	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	8-A	700	1/1	1.00	0.03	8,8,8,8	1
2	ZN	14-B	703	1/1	1.00	0.04	5,5,5,5	1
2	ZN	13-B	703	1/1	1.00	0.04	5,5,5,5	1
2	ZN	11-B	703	1/1	1.00	0.04	6,6,6,6	1
2	ZN	6-B	703	1/1	1.00	0.04	6,6,6,6	1
3	FE	10-B	704	1/1	1.00	0.04	3,3,3,3	1
3	FE	5-B	704	1/1	1.00	0.04	3,3,3,3	1
2	ZN	8-B	703	1/1	1.00	0.04	6,6,6,6	1
3	FE	3-B	704	1/1	1.00	0.04	3,3,3,3	1
3	FE	15-B	704	1/1	1.00	0.04	4,4,4,4	1
2	ZN	14-A	700	1/1	1.00	0.03	7,7,7,7	1
2	ZN	9-A	700	1/1	1.00	0.03	7,7,7,7	1
2	ZN	7-B	703	1/1	1.00	0.04	6,6,6,6	1
3	FE	11-B	704	1/1	1.00	0.04	3,3,3,3	1
2	ZN	2-B	703	1/1	1.00	0.04	5,5,5,5	1
2	ZN	16-A	700	1/1	1.00	0.03	7,7,7,7	1
3	FE	2-B	704	1/1	1.00	0.04	3,3,3,3	1
3	FE	7-B	704	1/1	1.00	0.04	6,6,6,6	1
2	ZN	7-A	700	1/1	1.00	0.03	7,7,7,7	1
2	ZN	6-A	700	1/1	1.00	0.03	7,7,7,7	1
2	ZN	5-B	703	1/1	1.00	0.04	6,6,6,6	1
2	ZN	5-A	700	1/1	1.00	0.03	7,7,7,7	1
3	FE	14-B	704	1/1	1.00	0.04	4,4,4,4	1
3	FE	4-B	704	1/1	1.00	0.04	3,3,3,3	1
2	ZN	3-A	700	1/1	1.00	0.03	8,8,8,8	1
2	ZN	12-B	703	1/1	1.00	0.04	6,6,6,6	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.