

Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2023 – 05:25 PM EDT

PDB ID	:	2Q42
Title	:	Ensemble refinement of the protein crystal structure of glyoxalase II from Ara-
		bidopsis 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 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 (i) 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 (1)) 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	:	2.35
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)	:	2.35

1 Overall quality at a glance (i)

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.



Matria	Whole archive	Similar resolution		
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
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 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 <=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	3% 97%	•
1	1-B	254	96%	•
1	10-A	254	3% 95%	5%
1	10-B	254	98%	•
1	11-A	254	3% 97%	•
1	11-B	254	99%	•



Mol	Chain	Length	Quality of chain
1	12-A	254	3%
1	12-B	254	98% •
1	13-A	254	^{3%} 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	<u>99%</u> .
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% •



Mol	Chain	Length	Quality of chain
1	9-B	254	96% •



2 Entry composition (i)

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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	1-A	254	Total	C	N	0	S 10	0	0	0
			1978	1243	341	382	12			
1	2-A	254	Total	C	N	0	S	0	0	0
			1978	1243	341	382	12			
1	3-A	254	Total	C	N	0	S	0	0	0
			1978	1243	341	382	12			
1	4-A	254	Total	C	N	0	S	0	0	0
		_	1978	1243	341	382	12	_	_	
1	5-A	254	Total	С	N	0	S	0	0	0
			1978	1243	341	382	12	-		
1	6-A	254	Total	С	Ν	0	\mathbf{S}	0	0	0
	011	201	1978	1243	341	382	12	· · · · · · · · · · · · · · · · · · ·	0	
1	7-A	254	Total	\mathbf{C}	Ν	0	\mathbf{S}	0	0	0
	1 11	201	1978	1243	341	382	12	0	0	0
1	8- A	254	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	0 11	204	1978	1243	341	382	12			
1	Ο_Δ	254	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
1	<i>J</i> -71	204	1978	1243	341	382	12			
1	10.4	254	Total	С	Ν	0	\mathbf{S}	0	0	0
	10-7	204	1978	1243	341	382	12	0	0	U
1	11 A	254	Total	С	Ν	0	\mathbf{S}	0	0	0
1	11-7	204	1978	1243	341	382	12	0	0	0
1	19 A	254	Total	С	Ν	0	S	0	0	0
	12-A	204	1978	1243	341	382	12	0	0	0
1	19 /	254	Total	С	Ν	0	S	0	0	0
	15-A	204	1978	1243	341	382	12	0	0	0
1	14 4	254	Total	С	Ν	0	S	0	0	0
1	14-A	204	1978	1243	341	382	12	0	0	U
1	1 F A	07.4	Total	С	Ν	0	S	0	0	0
	10-A	204	1978	1243	341	382	12	U	U	U
1	10 4	۵۲.4	Total	С	Ν	0	S	0	0	0
	10-A	254	1978	1243	341	382	12	U	U	

• Molecule 1 is a protein called Putative hydroxyacylglutathione hydrolase 2.



Mol

Atoms

Ν

0

С

Total

	ZeroOcc	AltConf
S 12	0	0
S 12	0	0
\sim		1

Conti	nued from	n previous page
Mol	Chain	Residues

1	1 B	254	Total	С	Ν	0	\mathbf{S}	0	0	0
1	1-D	204	1978	1243	341	382	12	0	0	0
1	2 B	254	Total	С	Ν	0	\mathbf{S}	0	0	0
T	2-D	204	1978	1243	341	382	12	0	0	0
1	ЗB	254	Total	\mathbf{C}	Ν	0	\mathbf{S}	0	0	0
T	0-D	204	1978	1243	341	382	12	0	0	0
1	4 B	254	Total	\mathbf{C}	Ν	0	\mathbf{S}	0	0	0
T	4-D	204	1978	1243	341	382	12	0	0	0
1	5 B	254	Total	\mathbf{C}	Ν	0	\mathbf{S}	0	0	0
T	0-D	204	1978	1243	341	382	12	0	0	0
1	6 B	254	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
L	0-D	204	1978	1243	341	382	12	0	0	
1	7 B	254	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
1	1-D	204	1978	1243	341	382	12	0	0	0
1	8 B	254	Total	С	Ν	0	S	0	0	0
T	0-D	204	1978	1243	341	382	12		0	0
1	0 B	254	Total	С	Ν	Ο	\mathbf{S}	0	0	0
T	J-D	204	1978	1243	341	382	12	0	0	
1	10 B	254	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
1	10-D	204	1978	1243	341	382	12	0		
1	11 R	254	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
1	11 - D	204	1978	1243	341	382	12	0		
1	19 B	254	Total	С	Ν	0	\mathbf{S}	0	0	0
1	12-D	204	1978	1243	341	382	12	0	0	0
1	13 B	254	Total	С	Ν	0	\mathbf{S}	0	0	0
1	10-D	204	1978	1243	341	382	12	0	0	0
1	14 P	254	Total	С	Ν	0	S	0	0	0
1	14-В	204	1978	1243	341	382	12	U	0	0
1	15 P	254	Total	С	Ν	0	S	0	0	0
	10-D	204	1978	1243	341	382	12		U	
1	16 P	254	Total	С	Ν	Ο	S	0	0	0
1	1 16-B	ю-в 254	1978	1243	341	382	12	0		U

There are 2 discrepancies between the modelled and reference sequences:

Chain	nain Residue Modelled		Actual	Comment	Reference
А	1	MET	-	initiating methionine	UNP Q9SID3
В	1	MET	-	initiating methionine	UNP Q9SID3

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

Trace



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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	7-B	1	Total Zn 1 1	0	0
2	8-B	1	Total Zn 1 1	0	0
2	9-B	1	Total Zn 1 1	0	0
2	10-B	1	Total Zn 1 1	0	0
2	11-B	1	Total Zn 1 1	0	0
2	12-B	1	Total Zn 1 1	0	0
2	13-B	1	Total Zn 1 1	0	0
2	14-B	1	Total Zn 1 1	0	0
2	15-B	1	Total Zn 1 1	0	0
2	16-B	1	Total Zn 1 1	0	0

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

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



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



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	15-B	1	Total Fe 1 1	0	0
3	16-B	1	Total Fe 1 1	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	2-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	3-A	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	4-A	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	5-A	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	6-A	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	7-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	8-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	9-A	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	10-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	11-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	12-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	13-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	14-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	15-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	16-A	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	1-B	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	2-B	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	3-B	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	4-B	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	5-B	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	6-B	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	7-B	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	8-B	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	9-B	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	10-B	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	11-B	1	$\begin{array}{c cc} \hline \text{Total} & \text{C} & \text{O} \\ \hline 4 & 2 & 2 \end{array}$	0	0
4	12-B	1	$\begin{array}{c cc} \hline \text{Total} & \text{C} & \text{O} \\ \hline 4 & 2 & 2 \end{array}$	0	0
4	13-B	1	$\begin{array}{c ccc} \hline \text{Total} & \text{C} & \text{O} \\ \hline 4 & 2 & 2 \end{array}$	0	0
4	14-B	1	$\begin{array}{c ccc} \hline \text{Total} & \text{C} & \text{O} \\ \hline 4 & 2 & 2 \end{array}$	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	15-B	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	16-B	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
5	2-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
5	3-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
5	4-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
5	5-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
5	6-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
5	7-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
5	8-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
5	9-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	10-A	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
5	11-A	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
5	12-A	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
5	13-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
5	14-A	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
5	15-A	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
5	16-A	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0

• Molecule 6 is water.

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



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	13-A	282	Total O 282 282	0	0
6	14-A	279	Total O 279 279	0	0
6	15-A	285	Total O 285 285	0	0
6	16-A	278	Total O 278 278	0	0
6	1-B	265	Total O 265 265	0	0
6	2-B	265	Total O 265 265	0	0
6	3-B	265	Total O 265 265	0	0
6	4-B	269	Total O 269 269	0	0
6	5-B	270	Total O 270 270	0	0
6	6-B	269	Total O 269 269	0	0
6	7-B	266	Total O 266 266	0	0
6	8-B	262	Total O 262 262	0	0
6	9-B	266	Total O 266 266	0	0
6	10-B	262	Total O 262 262	0	0
6	11-B	262	Total O 262 262	0	0
6	12-B	264	Total O 264 264	0	0
6	13-B	265	Total O 265 265	0	0
6	14-B	268	Total O 268 268	0	0
6	15-B	262	Total O 262 262	0	0
6	16-B	269	Total O 269 269	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: 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% R4 84 64 84 • 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 hydroxyacyl
glutathione hydrolase 2



20	10
2Q	4Z

Chain 13-B:	96%	·
M1 L5 K41 R42 N63 K96 K114 K114	C167 K177 E183 C217 C217 F264	
• Molecule 1: Puta	tive hydroxyacylglutathione hydrolase 2	
Chain 14-A:	96%	•
M1 21 22 23 23 83 843 644 644 644 644 644	B82 K92 S118 S118 C167 Y171 P208 F264	
• Molecule 1: Puta	tive hydroxyacylglutathione hydrolase 2	
Chain 14-B:	95%	• •
M1 L5 K10 D21 T24 D38 B38 R41 K41	R45 M149 K177 S191 R200 F254	
• Molecule 1: Puta	tive hydroxyacylglutathione hydrolase 2	
Chain 15-A:	96%	•
M1 L5 D21 B21 843 843 644 644 644 843 843	G61 B80 K81 M81 M82 M107 M108 M218 M218 M218 M218	
• Molecule 1: Puta	tive hydroxyacylglutathione hydrolase 2	
Chain 15-B:	93%	6%
M1 C8 C8 C8 C8 C9 C9 C9 C9 C9 C9 C9 C9 C9 C9 C9 C9 C9	D95 K96 M107 K114 M149 D161 E183 E183 E183 E214 C217 C217	
• Molecule 1: Puta	tive hydroxyacylglutathione hydrolase 2	
Chain 16-A:	99%	·
M1 21 21 21 21 23 243 643 643 643 643 643 680 881		
• Molecule 1: Puta	tive hydroxyacylglutathione hydrolase 2	
Chain 16-B:	92%	7% •
M1 L5 121 821 821 842 842 842 842 842 842	K114 R125 F134 C138 M149 M149 D161 L182 H169 H169 H169 H169 H169 H169 H169 H169	

ww

PDB

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	68.49Å 58.78 Å 69.05 Å	D
a, b, c, α , β , γ	90.00° 109.22° 90.00°	Depositor
D ecolution $(\hat{\lambda})$	32.97 - 1.74	Depositor
Resolution (A)	32.97 - 1.74	EDS
% Data completeness	97.5 (32.97-1.74)	Depositor
(in resolution range)	97.7 (32.97-1.74)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.00 (at 1.74 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
D D	0.147 , 0.193	Depositor
n, n_{free}	0.148 , 0.190	DCC
R_{free} test set	2630 reflections $(5.06%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	14.4	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31, 51.8	EDS
L-test for $twinning^2$	$< L >=0.50, < L^2>=0.33$	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 $(Å^2)$	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.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

Mal	Chain	Bo	ond lengths	B	ond angles
MOI	Chain	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	$4/\overline{2020}~(0.2\%)$	1.04	$5/\overline{2730}~(0.2\%)$
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%)



Mal	Chain	Bo	Bond lengths		Bond angles	
IVIOI		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

All (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
1	9-B	167	CYS	CB-SG	12.40	2.03	1.82
1	11-B	167	CYS	CB-SG	-12.22	1.61	1.82
1	16-B	167	CYS	CB-SG	-12.15	1.61	1.82
1	12-B	167	CYS	CB-SG	-11.74	1.62	1.82
1	13-A	167	CYS	CB-SG	11.53	2.01	1.82
1	8-A	167	CYS	CA-CB	11.28	1.78	1.53
1	3-A	167	CYS	CA-CB	10.80	1.77	1.53
1	3-A	167	CYS	CB-SG	10.42	2.00	1.82
1	4-B	49	TYR	CD1-CE1	10.18	1.54	1.39
1	10-A	167	CYS	CA-CB	9.90	1.75	1.53
1	13-A	138	CYS	CB-SG	-9.86	1.65	1.82
1	5-A	167	CYS	CA-CB	9.68	1.75	1.53
1	15-B	217	CYS	CB-SG	9.20	1.97	1.82
1	16-B	79	MET	SD-CE	8.74	2.26	1.77
1	4-B	167	CYS	CB-SG	-8.59	1.67	1.82
1	7-B	167	CYS	CB-SG	-8.03	1.68	1.82
1	9-A	167	CYS	CB-SG	-8.02	1.68	1.82
1	1-B	138	CYS	CB-SG	-7.82	1.69	1.82
1	14-B	149	MET	CG-SD	7.40	2.00	1.81
1	4-A	167	CYS	CB-SG	7.29	1.94	1.82
1	2-B	167	CYS	CB-SG	-7.29	1.69	1.82



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	138	CYS	CB-SG	-7.23	1.70	1.82
1	11-A	167	CYS	CA-CB	7.03	1.69	1.53
1	15-B	149	MET	CG-SD	-6.94	1.63	1.81
1	15-A	167	CYS	CB-SG	-6.94	1.70	1.82
1	2-A	198	GLU	CG-CD	6.81	1.62	1.51
1	9-A	174	SER	CB-OG	-6.66	1.33	1.42
1	15-B	107	MET	SD-CE	-6.65	1.40	1.77
1	5-A	100	ALA	CA-CB	6.61	1.66	1.52
1	4-B	49	TYR	CZ-OH	6.31	1.48	1.37
1	14-A	167	CYS	CB-SG	-6.24	1.71	1.82
1	14-A	149	MET	CG-SD	6.08	1.97	1.81
1	6-A	167	CYS	CB-SG	6.05	1.92	1.82
1	15-A	107	MET	SD-CE	-6.03	1.44	1.77
1	3-A	174	SER	CB-OG	-6.01	1.34	1.42
1	16-B	166	TYR	CD2-CE2	6.01	1.48	1.39
1	15-B	8	CYS	CB-SG	-6.00	1.72	1.82
1	10-A	126	ALA	CA-CB	-5.90	1.40	1.52
1	8-A	171	TYR	CD2-CE2	5.83	1.48	1.39
1	7-A	174	SER	CB-OG	-5.73	1.34	1.42
1	9-B	167	CYS	CA-CB	5.71	1.66	1.53
1	7-A	99	PHE	CD1-CE1	5.66	1.50	1.39
1	14-A	32	GLU	CG-CD	5.59	1.60	1.51
1	11-A	100	ALA	CA-CB	5.43	1.63	1.52
1	16-B	149	MET	CG-SD	5.43	1.95	1.81
1	14-A	149	MET	CB-CG	5.42	1.68	1.51
1	4-B	167	CYS	CA-CB	5.40	1.65	1.53
1	13-A	32	GLU	CG-CD	5.37	1.60	1.51
1	13-B	167	CYS	CB-SG	-5.31	1.73	1.81
1	15-A	32	GLU	CG-CD	5.29	1.59	1.51
1	14-A	28	VAL	CB-CG1	5.28	1.64	1.52
1	16-A	32	GLU	CG-CD	5.28	1.59	1.51
1	10-B	178	PHE	CE2-CZ	5.27	1.47	1.37
1	4-B	49	TYR	CD2-CE2	5.23	1.47	1.39
1	7-B	82	ASP	CB-CG	5.21	1.62	1.51
1	2-A	198	GLU	CB-CG	5.20	1.62	1.52
1	7-B	87	ILE	CA-CB	5.17	1.66	1.54
1	3-B	89	MET	CG-SD	5.13	1.94	1.81
1	14-A	149	MET	SD-CE	-5.06	1.49	1.77
1	5-B	217	CYS	CB-SG	5.04	1.90	1.82

All (58) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	7.	Observed ⁽⁰⁾	Ideal(°)
1	8-A	167	CVS	CA-CR-SC	-21 42	75.44	114.00
1	7-R	167	CVS	CA-CB-SG	-13 35	89.97	114.00
1	-D 5-Δ	167	CVS	CA-CB-SG	-19.00	92.06	114.00
1	3_Δ	167	CVS	CA-CB-SG	-12.15	94.12	114.00
1	16-R	79	MET	CG-SD-CE	-0.78	84.55	100.20
1	10-D	167	CVS	CA-CB-SG	9.70	131 50	11/ 00
1	16-R	200	ARG	NF-CZ-NH1	8.65	124.63	120.30
1	10-D	$\frac{200}{167}$	CVS	CA-CB-SG	-8 50	08.53	11/ 00
1	4-D 1/ι_Δ	1/10	MET	CG-SD-CE	-0.00	113 78	100.20
1	2 B	145	CVS	CA CB SC	7 70	00.07	11/ 00
1	2-D	166	TVB	$C N C \Lambda$	-1.19		114.00 121.70
1	11 A	167	CVS	$\frac{\text{CACRSC}}{\text{CACRSC}}$	6.82	101.73	11/ 00
1	11-A 11 R	200	APC	NE C7 NH1	6.76	101.73	120.20
1	11-D 10 A	200 166	TVD	$\frac{\text{NE}-\text{OZ}-\text{NH}}{\text{CNCA}}$	6.75	123.00	120.30
1	6 A	167	CVC	$\frac{\text{OPACA}}{\text{OPAC}}$	6 50	130.39	121.70
1	0-A 19 P	107	CVS	N CA C	-0.09 6.46	91.22	110.40
1	12-D	107	ТИР	C N CA	6.40	128.43	111.00
1	9-A 5 A	22	THD	C-N-CA	-0.40 6.27	108.00	122.30 122.30
1	0-A	22		C-N-CA	-0.37	108.92	122.00
	12-A	107	IIR	C-N-CA	-0.50	108.90	122.30
1	13-A	107	ME I CVC	CG-SD-CE	-0.29	90.13	100.20
	10-A	107		CA-UD-5G	-0.27	102.71	114.00
 	2-A	22 166	TVD	C-N-CA	-0.23	109.21	122.30 191.70
1	0 D	100		CP.CC.OD1	0.10	107.11	121.70
1	8-D	80	ASP	CB-CG-ODI	0.10	123.83	118.30
1	10-B	138	CYS	CA-CB-SG	-0.12	102.98	114.00
1	9-A	107		CA-CB-SG	-0.12	102.99	114.00
1	14-B	C OF		CB-CG-CD2	-0.00	100.70	111.00
1	10-B	95	ASP	CB-CG-OD2	5.95	123.00	118.30
1	10-B	<u>22</u> 45	ADC	U-N-UA	-0.80	110.01	122.30
1	10-D	40	ANG	$\frac{\text{NE-U2-N\Pi I}}{\text{CD CE M7}}$	0.01 E 70	123.20	120.30
1	10-D	10		N CA C	0.12 5.71	124.87	111.70
1	10-B	109		NE CZ NII1	0.71 5.61	120.45	111.00
1	14-B	200	AKG		0.01 5.61		120.30
1	(-A 7 D	22 177		CD CE MZ	-0.01	110.05	122.30 111.70
1	(-D	111		C N CA	0.0U	124.37	111.70
1	10-B	22	IHK	U-N-UA	-0.03	110.09	122.30
1	14-B	<u> </u>	ASP	CB-CG-OD1	5.52 5.40	123.27	118.30
1	4-B	82	ASP	OD OF MZ	5.49	123.24	118.30
1	2-B		LYS	CD-CE-NZ	5.40	124.20	111.70
1	12-B	107	UYS MET	UB-UA-U	-5.42	99.50	110.40
1	3-B	149	MET	UB-UG-SD	-5.41	90.10	112.40
1	4-B	5		UA-UB-UG	5.38	127.07	115.30
1	7-B	208	PRO	N-CA-C	5.37	126.07	112.10



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	7-B	22	THR	C-N-CA	-5.35	111.06	122.30
1	6-B	22	THR	C-N-CA	-5.31	111.14	122.30
1	16-B	200	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	7-B	5	LEU	CA-CB-CG	5.21	127.27	115.30
1	8-B	200	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	14-A	117	ILE	CG1-CB-CG2	-5.15	100.07	111.40
1	1-B	81	LYS	CD-CE-NZ	5.15	123.54	111.70
1	13-B	177	LYS	CD-CE-NZ	5.13	123.50	111.70
1	14 - B	177	LYS	CD-CE-NZ	5.13	123.49	111.70
1	15-B	177	LYS	CD-CE-NZ	5.11	123.46	111.70
1	16-B	134	PHE	CB-CG-CD1	-5.08	117.25	120.80
1	14-B	167	CYS	CA-CB-SG	-5.07	104.87	114.00
1	13-A	107	MET	CA-CB-CG	5.06	121.91	113.30
1	15-B	95	ASP	CB-CG-OD1	-5.04	113.77	118.30
1	12-B	22	THR	C-N-CA	-5.02	111.76	122.30

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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



Mol

1

1

1

H(added)

1957

1957

1957	0	0
1957	0	0
1957	0	0
1957	0	0
1957	0	0
1957	0	0
1957	0	0
1957	0	0
1957	0	0
1957	0	0
1957	0	0
1957	0	0
1957	0	0
1957	0	0
1957	0	0
1957	0	0
1957	0	0

Clashes

0

0

Symm-Clashes

0

0

Continued from previous page... Chain Non-H

1978

1978

1978

5-B

6-A

6-B

H(model)

0

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
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
					Conting	und an mont mana



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	Chain	Non H	$\mathbf{H}(\mathbf{modol})$	H(addod)	Clashos	Symm Clashes
2	10 R	1				SymmeClashes
	10-D	1	0	0	0	0
	11-A 11 B	1	0	0	0	0
	11-D 12 A	1	0	0	0	0
	12-A 19 P	1	0	0	0	0
	12-D	1	0	0	0	0
	10-A 12 P	1	0	0	0	0
	13-D 14 A	1	0	0	0	0
2	14-A	1	0	0	0	0
	14-D	1	0	0	0	0
	15 P	1	0	0	0	0
	10-D	1	0	0	0	0
2	10-A 16 B	1	0	0	0	0
	10-D	1	0	0	0	0
2 2	1-A 1 P	1	0	0	0	0
<u>り</u>	1-D	1	0	0	0	0
<u>り</u>	2-A	1	0	0	0	0
ວ 	2-D	1	0	0	0	0
<u>う</u>	0-A	1	0	0	0	0
<u> </u>	3-D	1	0	0	0	0
ວ 	4-A	1	0	0	0	0
<u> </u>	4-D	1	0	0	0	0
<u>り</u>	5 D	1	0	0	0	0
3 9	-D 6 Л	1	0	0	0	0
<u>う</u>	0-A 6 P	1	0	0	0	0
<u> </u>	0-D	1	0	0	0	0
<u>り</u>	7-A 7 D	1	0	0	0	0
່ <u>ວ</u>	γ-D	1	0	0	0	0
<u>り</u>	0-A 9 D	1	0	0	0	0
ວ 	0-D	1	0	0	0	0
2 0	0 P	1	0	0	0	0
2 2	9-D 10 A	1	0	0	0	0
2 2	10-A 10 R	1	0	0	0	0
2 2	10-D	1	0	0	0	0
2	11 R	1	0	0	0	0
3	12-D	1	0	0	0	0
3	$12-\Lambda$ 12-R	1	0	0	0	0
3	13-A	1	0	0	0	0
3	13-A	1	0	0	0	0
2	1/ A	1	0	0	0	0
2 2	14-A 1/ R	1	0	0	0	0
ວ 2	14-D 15 A	1	0	0	0	0
<u> </u>	10-A		U	U	0	U

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2Q42	

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	10-A	4	0	ა ე	0	0
4	10-B	4	0	্য 10	0	0
C E	1-A	1	0	10		0
0 F	2-A	1	0	10	0	0
6 5	0-A	1	0	10		0
0 E	4-A	1	0	10	0	0
0 5	6 A	1	0	10	0	0
5	0-A	1	0	10	0	0
О	(-A	1	U	10	U	U



2Q42

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	\mathbf{n} tiles
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

Continued from previous page...

All (50) Ramachandran outliers are listed below:

\mathbf{Mol}	Chain	\mathbf{Res}	Type
1	1-B	46	ASN
1	3-A	55	HIS
1	9-B	93	ASP
1	12-A	11	ASP
1	12-B	63	ASN
1	2-A	168	GLY
1	4-A	21	ASP
1	8-B	167	CYS
1	10-A	75	ILE
1	14 - B	24	THR
1	15-A	61	GLY
1	3-A	11	ASP
1	3-B	141	LEU
1	5-A	102	HIS
1	6-A	46	ASN
1	8-B	21	ASP
1	9-A	144	GLY
1	10-A	11	ASP
1	14-A	21	ASP
1	15-B	114	LYS
1	1-B	125	ARG



Mol	Chain	Res	Type
1	3-B	77	SER
1	4-B	23	GLY
1	7-A	100	ALA
1	9-B	79	MET
1	13-B	63	ASN
1	15-B	23	GLY
1	16-B	125	ARG
1	1-A	7	PRO
1	1-A	50	ILE
1	3-A	29	ASP
1	6-A	137	SER
1	8-A	23	GLY
1	8-B	9	LEU
1	9-A	172	THR
1	13-A	11	ASP
1	4-B	22	THR
1	6-A	86	GLY
1	7-B	82	ASP
1	11-A	23	GLY
1	14-A	31	SER
1	2-B	184	PRO
1	4-B	130	GLY
1	10-A	44	GLY
1	16-B	218	ASN
1	7-A	44	GLY
1	13-B	183	GLU
1	15-B	183	GLU
1	16-B	219	PRO
1	1-B	111	GLY

5.3.2 Protein sidechains (i)

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



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
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	$\overline{217/217~(100\%)}$	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
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



All	(140)	residues	with	a	non-rotameric	sic	dechain	are	listed	bel	ow:
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Mol	Chain	Res	Type
1	1-A	12	ASN
1	1-A	92	LYS
1	1-A	177	LYS
1	1-A	191	SER
1	1-B	5	LEU
1	1-B	10	LYS
1	1-B	52	ASN
1	1-B	108	ASP
1	1-B	206	THR
1	1-B	236	GLU
1	2-A	92	LYS
1	2-A	167	CYS
1	2-A	171	TYR
1	2-B	18	HIS
1	2-B	73	LYS
1	2-B	80	ASP
1	3-A	32	GLU
1	3-A	46	ASN
1	3-A	92	LYS
1	3-A	167	CYS
1	3-B	18	HIS
1	3-B	21	ASP
1	3-B	42	ARG
1	3-B	114	LYS
1	3-B	161	ASP
1	4-A	65	GLU
1	4-A	167	CYS
1	4-B	21	ASP
1	4-B	42	ARG
1	4-B	80	ASP
1	4-B	227	ASP
1	5-A	20	GLU
1	5-A	92	LYS
1	5-A	167	CYS
1	5-B	54	HIS
1	5-B	218	ASN
1	6-A	45	ARG
1	6-A	95	ASP
1	6-A	167	CYS
1	7-A	2	GLN
1	7-A	13	TYR
1	7-A	92	LYS



Mol	Chain	Res	Type
1	7-A	105	HIS
1	7-A	108	ASP
1	7-B	21	ASP
1	7-B	54	HIS
1	7-B	82	ASP
1	7-B	114	LYS
1	7-B	167	CYS
1	7-B	177	LYS
1	8-A	5	LEU
1	8-A	92	LYS
1	8-A	102	HIS
1	8-A	167	CYS
1	8-A	171	TYR
1	8-B	20	GLU
1	8-B	42	ARG
1	8-B	80	ASP
1	8-B	207	ILE
1	9-A	46	ASN
1	9-A	54	HIS
1	9-A	92	LYS
1	9-A	167	CYS
1	9-B	5	LEU
1	9-B	21	ASP
1	9-B	42	ARG
1	9-B	45	ARG
1	9-B	114	LYS
1	9-B	161	ASP
1	10-A	5	LEU
1	10-A	45	ARG
1	10-A	63	ASN
1	10-A	69	ARG
1	10-A	92	LYS
1	10-A	161	ASP
1	10-A	167	CYS
1	10-A	253	ASP
1	10-B	5	
1	10-B	21	ASP
1	10-B	42	ARG
1	10-B	114	
1	11-A	80	ASP
1	11-A	137	SER
1	11-A	161	ASP



Mol	Chain	Res	Type
1	11-B	42	ARG
1	12-A	38	ASP
1	12-A	92	LYS
1	12-A	218	ASN
1	12-B	21	ASP
1	12-B	42	ARG
1	12-B	114	LYS
1	13-A	5	LEU
1	13-A	92	LYS
1	13-A	217	CYS
1	13-B	5	LEU
1	13-B	42	ARG
1	13-B	96	LYS
1	13-B	114	LYS
1	13-B	161	ASP
1	13-B	217	CYS
1	14-A	92	LYS
1	14-A	118	SER
1	14-A	208	PRO
1	14-B	5	LEU
1	14-B	10	LYS
1	14-B	21	ASP
1	14-B	38	ASP
1	14-B	42	ARG
1	14-B	45	ARG
1	14-B	149	MET
1	14-B	167	CYS
1	14-B	191	SER
1	14-B	210	THR
1	15-A	5	LEU
1	15-A	46	ASN
1	15-A	80	ASP
1	15-A	92	LYS
1	15-A	108	ASP
1	15-A	177	LYS
1	15-A	218	ASN
1	15-B	42	ARG
1	15-B	73	LYS
1	15-B	96	LYS
1	15-B	161	ASP
1	15-B	187	GLU
1	15-B	214	GLU



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Mol	Chain	Res	Type				
1	15-B	217	CYS				
1	16-A	80	ASP				
1	16-A	167	CYS				
1	16-B	5	LEU				
1	16-B	21	ASP				
1	16-B	32	GLU				
1	16-B	42	ARG				
1	16-B	79	MET				
1	16-B	114	LYS				
1	16-B	149	MET				
1	16-B	161	ASP				
1	16-B	167	CYS				
1	16-B	182	LEU				
1	16-B	187	GLU				

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	2	GLN
1	1-A	52	ASN
1	1-A	185	ASN
1	1-A	190	GLN
1	1-B	52	ASN
1	1-B	55	HIS
1	1-B	190	GLN
1	2-A	2	GLN
1	2-A	18	HIS
1	2-A	59	HIS
1	2-A	169	HIS
1	2-A	195	HIS
1	2-B	190	GLN
1	3-A	2	GLN
1	3-A	46	ASN
1	3-A	55	HIS
1	3-A	185	ASN
1	3-B	46	ASN
1	3-B	190	GLN
1	4-A	2	GLN
1	4-A	46	ASN
1	4-B	46	ASN
1	4-B	190	GLN
1	5-A	2	GLN



Mol	Chain	Res	Type
1	5-A	18	HIS
1	5-B	46	ASN
1	5-B	54	HIS
1	5-B	55	HIS
1	5-B	190	GLN
1	5-B	218	ASN
1	6-A	175	ASN
1	6-B	46	ASN
1	6-B	148	GLN
1	6-B	190	GLN
1	7-A	2	GLN
1	7-A	18	HIS
1	7-A	46	ASN
1	7-A	105	HIS
1	7-A	185	ASN
1	7-B	12	ASN
1	7-B	46	ASN
1	7-B	55	HIS
1	7-B	190	GLN
1	8-A	2	GLN
1	8-A	18	HIS
1	8-A	154	GLN
1	8-A	185	ASN
1	8-B	2	GLN
1	8-B	12	ASN
1	8-B	46	ASN
1	8-B	190	GLN
1	9-A	2	GLN
1	9-A	18	HIS
1	9-A	46	ASN
1	9-A	102	HIS
1	9-A	185	ASN
1	9-A	218	ASN
1	9-B	46	ASN
1	9-B	190	GLN
1	10-A	102	HIS
1	10-A	185	ASN
1	10-B	46	ASN
1	10-B	190	GLN
1	11-A	2	GLN
1	11-A	18	HIS
1	11-A	46	ASN



Mol	Chain	Res	Type
1	11-A	102	HIS
1	11-B	46	ASN
1	11-B	148	GLN
1	11-B	190	GLN
1	12-A	2	GLN
1	12-A	18	HIS
1	12-A	46	ASN
1	12-A	218	ASN
1	12-B	46	ASN
1	12-B	190	GLN
1	13-A	18	HIS
1	13-B	46	ASN
1	13-B	105	HIS
1	13-B	154	GLN
1	13-B	190	GLN
1	14-A	2	GLN
1	14-A	18	HIS
1	14-A	102	HIS
1	14-B	46	ASN
1	14-B	102	HIS
1	14 - B	190	GLN
1	15-A	2	GLN
1	15-A	18	HIS
1	15-A	46	ASN
1	15-A	102	HIS
1	15-A	105	HIS
1	15-A	218	ASN
1	15-B	46	ASN
1	15-B	190	GLN
1	16-A	2	GLN
1	16-A	18	HIS
1	16-A	102	HIS
1	16-B	46	ASN
1	16-B	190	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (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).

Mal	Trune	Chain	Dec	Timle	Bond lengths		Bond angles			
IVIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	ACY	7-B	801	-	$3,\!3,\!3$	0.31	0	$3,\!3,\!3$	0.52	0
4	ACY	14 - B	801	-	$3,\!3,\!3$	0.35	0	$3,\!3,\!3$	0.49	0
4	ACY	4-B	801	-	$3,\!3,\!3$	0.33	0	$3,\!3,\!3$	0.49	0
4	ACY	15-A	800	-	$3,\!3,\!3$	0.57	0	$3,\!3,\!3$	0.63	0
4	ACY	12-A	800	-	$3,\!3,\!3$	0.39	0	$3,\!3,\!3$	0.56	0
4	ACY	11 - B	801	-	$3,\!3,\!3$	0.29	0	$3,\!3,\!3$	0.64	0
4	ACY	13-B	801	-	$3,\!3,\!3$	0.40	0	$3,\!3,\!3$	0.86	0
5	PEG	7-A	9979	-	$6,\!6,\!6$	1.27	0	$5,\!5,\!5$	0.57	0
5	PEG	12-A	9979	-	$6,\!6,\!6$	1.14	0	$5,\!5,\!5$	0.60	0
4	ACY	1-B	801	-	$3,\!3,\!3$	0.42	0	$3,\!3,\!3$	0.86	0
5	PEG	1-A	9979	-	$6,\!6,\!6$	1.02	0	$5,\!5,\!5$	0.55	0
4	ACY	14-A	800	-	$3,\!3,\!3$	0.39	0	$3,\!3,\!3$	0.58	0
4	ACY	6-A	800	-	$3,\!3,\!3$	0.84	0	$3,\!3,\!3$	0.99	0
4	ACY	3-A	800	-	$3,\!3,\!3$	0.38	0	$3,\!3,\!3$	0.59	0
5	PEG	14-A	9979	-	$6,\!6,\!6$	1.02	0	$5,\!5,\!5$	0.48	0
4	ACY	7-A	800	-	$3,\!3,\!3$	0.39	0	$3,\!3,\!3$	0.60	0
5	PEG	5-A	9979	-	$6,\!6,\!6$	1.23	0	$5,\!5,\!5$	0.63	0
4	ACY	5-B	801	-	$3,\!3,\!3$	0.38	0	$3,\!3,\!3$	0.52	0
5	PEG	16-A	9979	-	$6,\!6,\!6$	1.02	0	$5,\!5,\!5$	0.42	0
4	ACY	5-A	800	-	$3,\!3,\!3$	0.40	0	$3,\!3,\!3$	0.59	0
4	ACY	11-A	800	-	$3,\!3,\!3$	0.41	0	$3,\!3,\!3$	0.59	0
4	ACY	8-A	800	-	$3,\!3,\!3$	0.74	0	$3,\!3,\!3$	0.79	0
5	PEG	15-A	9979	-	$6,\!6,\!6$	0.92	0	$5,\!5,\!5$	0.44	0
4	ACY	2-B	801	-	3,3,3	0.71	0	3,3,3	0.92	0
4	ACY	9-A	800	-	$\overline{3,3,3}$	0.38	0	$\overline{3,3,3}$	0.60	0
5	PEG	8-A	9979	-	$\overline{6,\!6,\!6}$	0.90	0	$\overline{5,5,5}$	0.50	0
5	PEG	9-A	9979	-	$6,\!6,\!6$	0.82	0	$5,\!5,\!5$	0.39	0



Mal	Tune	Chain	Dec	Box Link Bond lengths Bond angles				gles		
MOI	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	ACY	13-A	800	-	3,3,3	0.38	0	$3,\!3,\!3$	0.55	0
5	PEG	11-A	9979	-	$6,\!6,\!6$	0.97	0	$5,\!5,\!5$	0.52	0
5	PEG	13-A	9979	-	$6,\!6,\!6$	0.97	0	$5,\!5,\!5$	0.48	0
5	PEG	3-A	9979	-	$6,\!6,\!6$	1.07	0	$5,\!5,\!5$	0.57	0
5	PEG	6-A	9979	-	$6,\!6,\!6$	0.85	0	$5,\!5,\!5$	0.66	0
4	ACY	6-B	801	-	3,3,3	0.38	0	$3,\!3,\!3$	0.52	0
5	PEG	10-A	9979	-	6,6,6	0.89	0	$5,\!5,\!5$	0.49	0
4	ACY	16-B	801	-	3,3,3	0.74	0	$3,\!3,\!3$	0.96	0
5	PEG	2-A	9979	-	6,6,6	0.69	0	$5,\!5,\!5$	0.46	0
5	PEG	4-A	9979	-	$6,\!6,\!6$	0.81	0	$5,\!5,\!5$	0.66	0
4	ACY	8-B	801	-	3,3,3	0.43	0	$3,\!3,\!3$	0.55	0
4	ACY	9-B	801	-	3,3,3	0.29	0	$3,\!3,\!3$	0.51	0
4	ACY	1-A	800	-	3,3,3	0.66	0	$3,\!3,\!3$	0.95	0
4	ACY	10-A	800	-	3,3,3	0.41	0	$3,\!3,\!3$	0.58	0
4	ACY	10-B	801	-	3,3,3	0.25	0	$3,\!3,\!3$	0.52	0
4	ACY	12-B	801	-	3,3,3	0.87	0	$3,\!3,\!3$	1.01	0
4	ACY	15-B	801	-	3,3,3	0.71	0	$3,\!3,\!3$	0.79	0
4	ACY	16-A	800	-	3,3,3	0.54	0	$3,\!3,\!3$	0.63	0
4	ACY	4-A	800	-	3,3,3	1.11	0	$3,\!3,\!3$	0.88	0
4	ACY	2-A	800	-	3,3,3	0.56	0	$3,\!3,\!3$	0.77	0
4	ACY	3-B	801	-	3,3,3	0.81	0	3,3,3	1.01	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	8-A	9979	-	-	0/4/4/4	-
5	PEG	14-A	9979	-	-	0/4/4/4	-
5	PEG	9-A	9979	-	-	1/4/4/4	-
5	PEG	5-A	9979	-	-	1/4/4/4	-
5	PEG	4-A	9979	-	-	1/4/4/4	-
5	PEG	2-A	9979	-	-	1/4/4/4	-
5	PEG	16-A	9979	-	-	0/4/4/4	-
5	PEG	11-A	9979	-	-	0/4/4/4	-
5	PEG	13-A	9979	-	-	0/4/4/4	-
5	PEG	3-A	9979	-	-	0/4/4/4	-
5	PEG	6-A	9979	-	-	1/4/4/4	-
5	PEG	12-A	9979	-	-	0/4/4/4	-
5	PEG	7-A	9979	-	-	0/4/4/4	-
5	PEG	1-A	9979	-	-	0/4/4/4	-
5	PEG	10-A	9979	-	-	0/4/4/4	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	15-A	9979	-	-	0/4/4/4	-

There are no bond length outliers.

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ	5>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	$\mathbf{Q}{<}0.9$
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	$4, 12, \overline{28}, 52$	$254 \ (100\%)$
1	12-B	254/254~(100%)	-0.35	1 (0%) 92	94	5, 11, 23, 48	254 (100%)



20	10
ZQ^{2}	±Ζ

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	$Q{<}0.9$
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%)

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All (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
1	6-A	42	ARG	6.5
1	7-A	42	ARG	6.5
1	8-A	42	ARG	6.5
1	9-A	42	ARG	6.5
1	10-A	42	ARG	6.5
1	11-A	42	ARG	6.5
1	12-A	42	ARG	6.5
1	13-A	42	ARG	6.5
1	14-A	42	ARG	6.5
1	15-A	42	ARG	6.5
1	16-A	42	ARG	6.5
1	1-A	41	LYS	2.7
1	2-A	41	LYS	2.7
1	3-A	41	LYS	2.7
1	4-A	41	LYS	2.7
1	5-A	41	LYS	2.7
1	6-A	41	LYS	2.7
1	7-A	41	LYS	2.7
1	8-A	41	LYS	2.7
1	9-A	41	LYS	2.7
1	10-A	41	LYS	2.7



Mol	Chain	Res	Type	RSRZ
1	11-A	41	LYS	2.7
1	12-A	41	LYS	2.7
1	13-A	41	LYS	2.7
1	14-A	41	LYS	2.7
1	15-A	41	LYS	2.7
1	16-A	41	LYS	2.7
1	1-A	43	SER	2.6
1	2-A	43	SER	2.6
1	3-A	43	SER	2.6
1	4-A	43	SER	2.6
1	5-A	43	SER	2.6
1	6-A	43	SER	2.6
1	7-A	43	SER	2.6
1	8-A	43	SER	2.6
1	9-A	43	SER	2.6
1	10-A	43	SER	2.6
1	11-A	43	SER	2.6
1	12-A	43	SER	2.6
1	13-A	43	SER	2.6
1	14-A	43	SER	2.6
1	15-A	43	SER	2.6
1	16-A	43	SER	2.6
1	1-A	45	ARG	2.4
1	2-A	45	ARG	2.4
1	3-A	45	ARG	2.4
1	4-A	45	ARG	2.4
1	5-A	45	ARG	2.4
1	6-A	45	ARG	2.4
1	7-A	45	ARG	2.4
1	8-A	45	ARG	2.4
1	9-A	45	ARG	2.4
1	10-A	45	ARG	2.4
1	11-A	45	ARG	2.4
1	12-A	45	ARG	2.4
1	13-A	45	ARG	2.4
1	14-A	45	ARG	2.4
1	15-A	45	ARG	2.4
1	16-A	45	ARG	2.4
1	1-A	21	ASP	2.2
1	2-A	21	ASP	2.2
1	3-A	21	ASP	2.2
1	4-A	21	ASP	2.2



2Q42

Mol	Chain	Res	Type	RSRZ
1	5-A	21	ASP	2.2
1	6-A	21	ASP	2.2
1	7-A	21	ASP	2.2
1	8-A	21	ASP	2.2
1	9-A	21	ASP	2.2
1	10-A	21	ASP	2.2
1	11-A	21	ASP	2.2
1	12-A	21	ASP	2.2
1	13-A	21	ASP	2.2
1	14-A	21	ASP	2.2
1	15-A	21	ASP	2.2
1	16-A	21	ASP	2.2
1	1-A	44	GLY	2.2
1	2-A	44	GLY	2.2
1	3-A	44	GLY	2.2
1	4-A	44	GLY	2.2
1	5-A	44	GLY	2.2
1	6-A	44	GLY	2.2
1	7-A	44	GLY	2.2
1	8-A	44	GLY	2.2
1	9-A	44	GLY	2.2
1	10-A	44	GLY	2.2
1	11-A	44	GLY	2.2
1	12-A	44	GLY	2.2
1	13-A	44	GLY	2.2
1	14-A	44	GLY	2.2
1	15-A	44	GLY	2.2
1	16-A	44	GLY	2.2
1	1-B	41	LYS	2.1
1	2-B	41	LYS	2.1
1	3-B	41	LYS	2.1
1	4-B	41	LYS	2.1
1	5-B	41	LYS	2.1
1	6-B	41	LYS	2.1
1	7-B	41	LYS	2.1
1	8-B	41	LYS	2.1
1	9-B	41	LYS	2.1
1	10-B	41	LYS	2.1
1	11-B	41	LYS	2.1
1	12-B	41	LYS	2.1
1	13-B	41	LYS	2.1
1	14-B	41	LYS	2.1



Mol	Chain	Res	Type	RSRZ
1	15-B	41	LYS	2.1
1	16-B	41	LYS	2.1
1	1-A	82	ASP	2.0
1	2-A	82	ASP	2.0
1	3-A	82	ASP	2.0
1	4-A	82	ASP	2.0
1	5-A	82	ASP	2.0
1	6-A	82	ASP	2.0
1	7-A	82	ASP	2.0
1	8-A	82	ASP	2.0
1	9-A	82	ASP	2.0
1	10-A	82	ASP	2.0
1	11-A	82	ASP	2.0
1	12-A	82	ASP	2.0
1	13-A	82	ASP	2.0
1	14-A	82	ASP	2.0
1	15-A	82	ASP	2.0
1	16-A	82	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
5	PEG	1-A	9979	7/7	0.92	0.09	18,19,23,23	7
5	PEG	2-A	9979	7/7	0.92	0.09	17,20,23,24	7
5	PEG	3-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	5-A	9979	7/7	0.92	0.09	18,19,23,24	7



2Q	42
^{2}Q	42

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



2Q	42
^{2}Q	42

Continued from previous page									
Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	\mathbf{RSR}	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9	
4	ACY	16-B	801	4/4	0.99	0.10	$15,\!17,\!18,\!19$	4	
3	FE	1-A	701	1/1	0.99	0.04	3,3,3,3	1	
3	FE	2-A	701	1/1	0.99	0.04	6, 6, 6, 6	1	
3	FE	3-A	701	1/1	0.99	0.04	3,3,3,3	1	
3	FE	4-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	
3	FE	6-A	701	1/1	0.99	0.04	2,2,2,2	1	
3	FE	7-A	701	1/1	0.99	0.04	3,3,3,3	1	
3	FE	8-A	701	1/1	0.99	0.04	3,3,3,3	1	
3	FE	9-A	701	1/1	0.99	0.04	1,1,1,1	1	
3	FE	10-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	12-A	701	1/1	0.99	0.04	3,3,3,3	1	
3	FE	13-A	701	1/1	0.99	0.04	3,3,3,3	1	
3	FE	14-A	701	1/1	0.99	0.04	2,2,2,2	1	
3	FE	15-A	701	1/1	0.99	0.04	3,3,3,3	1	
3	FE	16-A	701	1/1	0.99	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	2-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	
2	ZN	4-B	703	1/1	1.00	0.04	8,8,8,8	1	
2	ZN	5-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	
2	ZN	7-B	703	1/1	1.00	0.04	6,6,6,6	1	
2	ZN	8-B	703	1/1	1.00	0.04	6,6,6,6	1	
2	ZN	9-B	703	1/1	1.00	0.04	6,6,6,6	1	
2	ZN	10-B	703	1/1	1.00	0.04	8,8,8,8	1	
2	ZN	11-B	703	1/1	1.00	0.04	6,6,6,6	1	
2	ZN	12-B	703	1/1	1.00	0.04	6,6,6,6	1	
2	ZN	13-B	703	1/1	1.00	0.04	5,5,5,5	1	
2	ZN	14-B	703	1/1	1.00	0.04	5,5,5,5	1	
2	ZN	15-B	703	1/1	1.00	0.04	5,5,5,5	1	
2	ZN	16-B	703	1/1	1.00	0.04	6,6,6,6	1	
2	ZN	1-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	
2	ZN	3-A	700	1/1	1.00	0.03	8,8,8,8	1	
2	ZN	4-A	700	1/1	1.00	0.03	7,7,7,7	1	
2	ZN	5-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	7-A	700	1/1	1.00	0.03	7,7.7.7	1	
2	ZN	8-A	700	1/1	1.00	0.03	8,8.8.8	1	
2	ZN	9-A	700	1/1	1.00	0.03	7,7,7,7	1	



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

6.5 Other polymers (i)

There are no such residues in this entry.

