



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:06 am GMT

PDB ID : 4Q3S  
Title : Crystal structure of Schistosoma mansoni arginase in complex with inhibitor ABHPE  
Authors : Hai, Y.; Edwards, J.E.; Van Zandt, M.C.; Hoffmann, K.F.; Christianson, D.W.  
Deposited on : 2014-04-12  
Resolution : 2.11 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

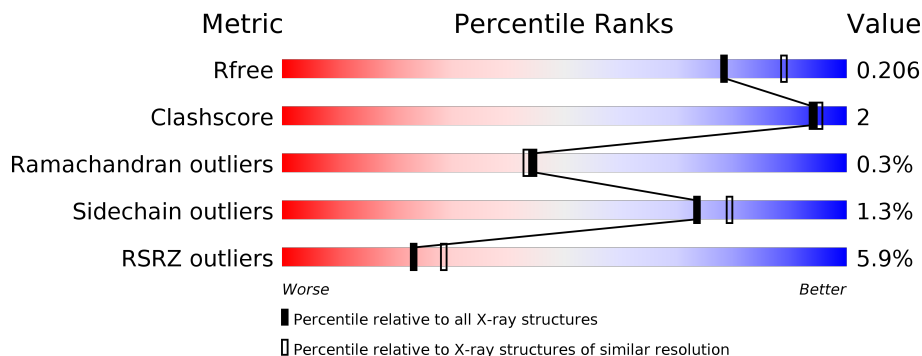
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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))
$R_{free}$	100719	4988 (2.14-2.10)
Clashscore	112137	5557 (2.14-2.10)
Ramachandran outliers	110173	5504 (2.14-2.10)
Sidechain outliers	110143	5505 (2.14-2.10)
RSRZ outliers	101464	5021 (2.14-2.10)

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. 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	A	385	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="width: 84%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">84%</span> </div> <div style="width: 13%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">13%</span> </div> </div>
1	B	385	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">2%</span> </div> <div style="width: 83%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">83%</span> </div> <div style="width: 13%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">13%</span> </div> </div>
1	C	385	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="width: 80%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">80%</span> </div> <div style="width: 6%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">6%</span> </div> <div style="width: 14%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">14%</span> </div> </div>
1	D	385	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">17%</span> </div> <div style="width: 80%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">80%</span> </div> <div style="width: 6%; height: 10px; background-color: yellow; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">6%</span> </div> <div style="width: 14%; height: 10px; background-color: grey; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">14%</span> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MN	C	401	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11259 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 Arginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	4	0
			2590	1632	452	490	16			
1	B	335	Total	C	N	O	S	0	1	0
			2579	1624	453	487	15			
1	C	332	Total	C	N	O	S	0	3	0
			2565	1617	448	484	16			
1	D	331	Total	C	N	O	S	0	0	0
			2536	1598	442	481	15			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q6WVP6
A	-19	GLY	-	EXPRESSION TAG	UNP Q6WVP6
A	-18	SER	-	EXPRESSION TAG	UNP Q6WVP6
A	-17	SER	-	EXPRESSION TAG	UNP Q6WVP6
A	-16	HIS	-	EXPRESSION TAG	UNP Q6WVP6
A	-15	HIS	-	EXPRESSION TAG	UNP Q6WVP6
A	-14	HIS	-	EXPRESSION TAG	UNP Q6WVP6
A	-13	HIS	-	EXPRESSION TAG	UNP Q6WVP6
A	-12	HIS	-	EXPRESSION TAG	UNP Q6WVP6
A	-11	HIS	-	EXPRESSION TAG	UNP Q6WVP6
A	-10	SER	-	EXPRESSION TAG	UNP Q6WVP6
A	-9	SER	-	EXPRESSION TAG	UNP Q6WVP6
A	-8	GLY	-	EXPRESSION TAG	UNP Q6WVP6
A	-7	LEU	-	EXPRESSION TAG	UNP Q6WVP6
A	-6	VAL	-	EXPRESSION TAG	UNP Q6WVP6
A	-5	PRO	-	EXPRESSION TAG	UNP Q6WVP6
A	-4	ARG	-	EXPRESSION TAG	UNP Q6WVP6
A	-3	GLY	-	EXPRESSION TAG	UNP Q6WVP6
A	-2	SER	-	EXPRESSION TAG	UNP Q6WVP6
A	-1	HIS	-	EXPRESSION TAG	UNP Q6WVP6
A	0	MET	-	EXPRESSION TAG	UNP Q6WVP6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	EXPRESSION TAG	UNP Q6WVP6
B	-19	GLY	-	EXPRESSION TAG	UNP Q6WVP6
B	-18	SER	-	EXPRESSION TAG	UNP Q6WVP6
B	-17	SER	-	EXPRESSION TAG	UNP Q6WVP6
B	-16	HIS	-	EXPRESSION TAG	UNP Q6WVP6
B	-15	HIS	-	EXPRESSION TAG	UNP Q6WVP6
B	-14	HIS	-	EXPRESSION TAG	UNP Q6WVP6
B	-13	HIS	-	EXPRESSION TAG	UNP Q6WVP6
B	-12	HIS	-	EXPRESSION TAG	UNP Q6WVP6
B	-11	HIS	-	EXPRESSION TAG	UNP Q6WVP6
B	-10	SER	-	EXPRESSION TAG	UNP Q6WVP6
B	-9	SER	-	EXPRESSION TAG	UNP Q6WVP6
B	-8	GLY	-	EXPRESSION TAG	UNP Q6WVP6
B	-7	LEU	-	EXPRESSION TAG	UNP Q6WVP6
B	-6	VAL	-	EXPRESSION TAG	UNP Q6WVP6
B	-5	PRO	-	EXPRESSION TAG	UNP Q6WVP6
B	-4	ARG	-	EXPRESSION TAG	UNP Q6WVP6
B	-3	GLY	-	EXPRESSION TAG	UNP Q6WVP6
B	-2	SER	-	EXPRESSION TAG	UNP Q6WVP6
B	-1	HIS	-	EXPRESSION TAG	UNP Q6WVP6
B	0	MET	-	EXPRESSION TAG	UNP Q6WVP6
C	-20	MET	-	EXPRESSION TAG	UNP Q6WVP6
C	-19	GLY	-	EXPRESSION TAG	UNP Q6WVP6
C	-18	SER	-	EXPRESSION TAG	UNP Q6WVP6
C	-17	SER	-	EXPRESSION TAG	UNP Q6WVP6
C	-16	HIS	-	EXPRESSION TAG	UNP Q6WVP6
C	-15	HIS	-	EXPRESSION TAG	UNP Q6WVP6
C	-14	HIS	-	EXPRESSION TAG	UNP Q6WVP6
C	-13	HIS	-	EXPRESSION TAG	UNP Q6WVP6
C	-12	HIS	-	EXPRESSION TAG	UNP Q6WVP6
C	-11	HIS	-	EXPRESSION TAG	UNP Q6WVP6
C	-10	SER	-	EXPRESSION TAG	UNP Q6WVP6
C	-9	SER	-	EXPRESSION TAG	UNP Q6WVP6
C	-8	GLY	-	EXPRESSION TAG	UNP Q6WVP6
C	-7	LEU	-	EXPRESSION TAG	UNP Q6WVP6
C	-6	VAL	-	EXPRESSION TAG	UNP Q6WVP6
C	-5	PRO	-	EXPRESSION TAG	UNP Q6WVP6
C	-4	ARG	-	EXPRESSION TAG	UNP Q6WVP6
C	-3	GLY	-	EXPRESSION TAG	UNP Q6WVP6
C	-2	SER	-	EXPRESSION TAG	UNP Q6WVP6
C	-1	HIS	-	EXPRESSION TAG	UNP Q6WVP6
C	0	MET	-	EXPRESSION TAG	UNP Q6WVP6

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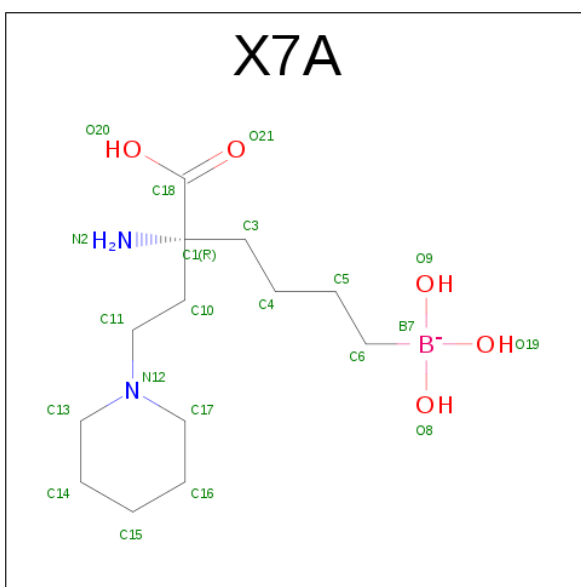
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	EXPRESSION TAG	UNP Q6WVP6
D	-19	GLY	-	EXPRESSION TAG	UNP Q6WVP6
D	-18	SER	-	EXPRESSION TAG	UNP Q6WVP6
D	-17	SER	-	EXPRESSION TAG	UNP Q6WVP6
D	-16	HIS	-	EXPRESSION TAG	UNP Q6WVP6
D	-15	HIS	-	EXPRESSION TAG	UNP Q6WVP6
D	-14	HIS	-	EXPRESSION TAG	UNP Q6WVP6
D	-13	HIS	-	EXPRESSION TAG	UNP Q6WVP6
D	-12	HIS	-	EXPRESSION TAG	UNP Q6WVP6
D	-11	HIS	-	EXPRESSION TAG	UNP Q6WVP6
D	-10	SER	-	EXPRESSION TAG	UNP Q6WVP6
D	-9	SER	-	EXPRESSION TAG	UNP Q6WVP6
D	-8	GLY	-	EXPRESSION TAG	UNP Q6WVP6
D	-7	LEU	-	EXPRESSION TAG	UNP Q6WVP6
D	-6	VAL	-	EXPRESSION TAG	UNP Q6WVP6
D	-5	PRO	-	EXPRESSION TAG	UNP Q6WVP6
D	-4	ARG	-	EXPRESSION TAG	UNP Q6WVP6
D	-3	GLY	-	EXPRESSION TAG	UNP Q6WVP6
D	-2	SER	-	EXPRESSION TAG	UNP Q6WVP6
D	-1	HIS	-	EXPRESSION TAG	UNP Q6WVP6
D	0	MET	-	EXPRESSION TAG	UNP Q6WVP6

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

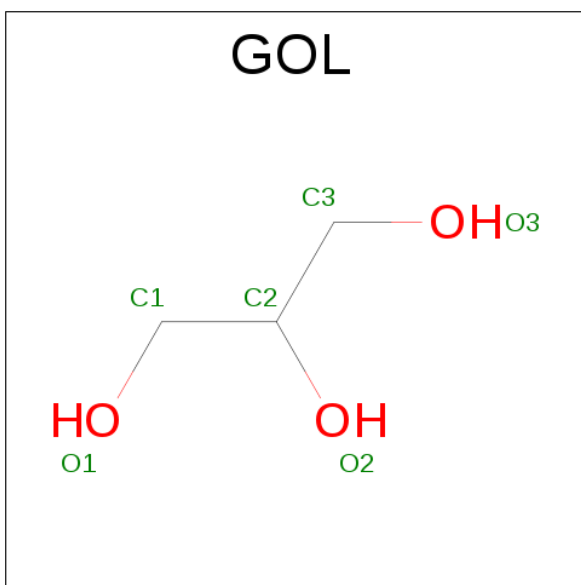
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mn 2 2	0	0
2	A	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0

- Molecule 3 is [(5R)-5-AMINO-5-CARBOXY-7-(PIPERIDIN-1-YL)HEPTYL](TRIHYDROXY)BORATE(1-) (three-letter code: X7A) (formula: C<sub>13</sub>H<sub>28</sub>BN<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	B	C	N	O	0	0
			21	1	13	2	5		
3	B	1	Total	B	C	N	O	0	0
			21	1	13	2	5		
3	C	1	Total	B	C	N	O	0	0
			21	1	13	2	5		
3	D	1	Total	B	C	N	O	0	0
			21	1	13	2	5		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

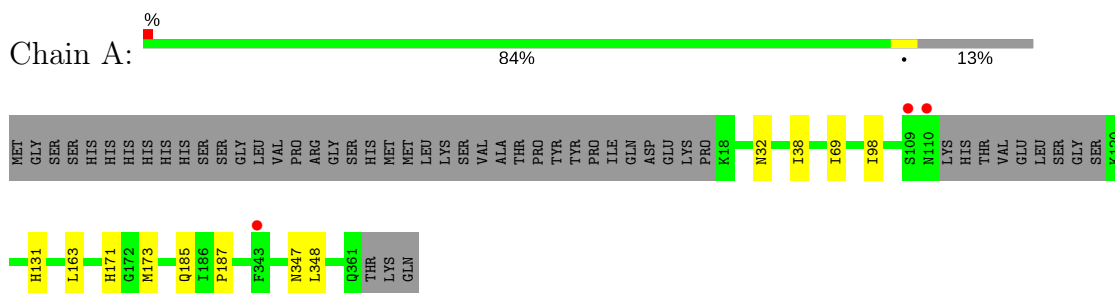
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	289	Total O 289 289	0	0
5	B	294	Total O 294 294	0	0
5	C	207	Total O 207 207	0	0
5	D	59	Total O 59 59	0	0

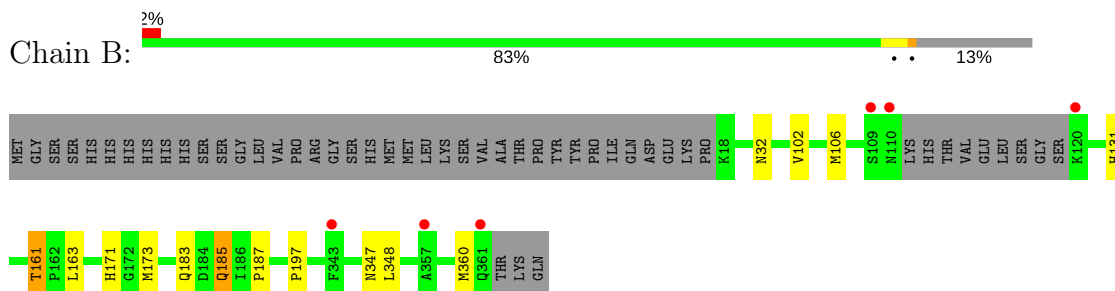
### 3 Residue-property plots [i](#)

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.

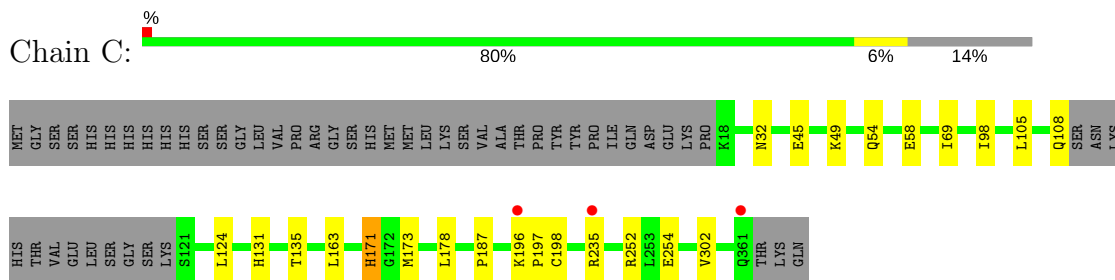
- Molecule 1: Arginase



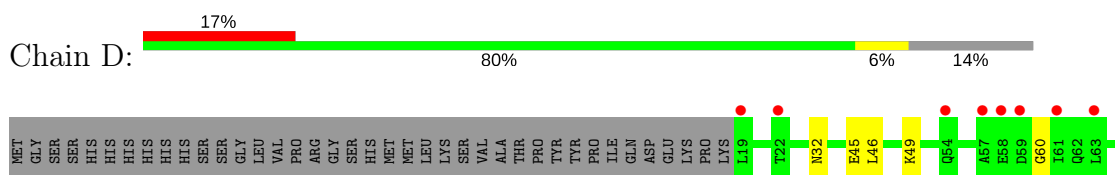
- Molecule 1: Arginase

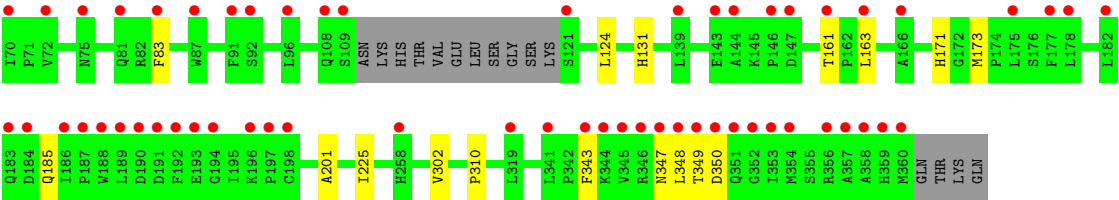


- Molecule 1: Arginase



- Molecule 1: Arginase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.21Å 178.21Å 178.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 2.11 49.43 – 2.11	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.43-2.11) 98.5 (49.43-2.11)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, $R_{free}$	0.173 , 0.206 0.174 , 0.206	Depositor DCC
$R_{free}$ test set	5306 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11259	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MN, X7A

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	A	0.24	0/2649	0.44	0/3588
1	B	0.31	0/2629	0.46	1/3561 (0.0%)
1	C	0.22	0/2621	0.43	0/3551
1	D	0.22	0/2583	0.42	0/3502
All	All	0.25	0/10482	0.44	1/14202 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	THR	C-N-CD	5.31	139.55	128.40

There are no chirality outliers.

There are no planarity outliers.

### 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	A	2590	0	2609	4	0
1	B	2579	0	2598	6	0
1	C	2565	0	2585	12	0
1	D	2536	0	2545	11	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	21	0	25	0	0
3	B	21	0	25	0	0
3	C	21	0	25	1	0
3	D	21	0	26	0	0
4	A	18	0	24	0	0
4	B	18	0	24	0	0
4	C	12	0	16	0	0
5	A	289	0	0	1	0
5	B	294	0	0	0	0
5	C	207	0	0	1	0
5	D	59	0	0	0	0
All	All	11259	0	10502	33	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (33) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:PHE:HB3	1:D:163:LEU:HD11	1.84	0.60
1:D:347:ASN:OD1	1:D:349:THR:N	2.39	0.56
1:C:252:ARG:NH1	1:C:254:GLU:OE1	2.39	0.55
1:B:183:GLN:HG3	1:B:197:PRO:HG3	1.89	0.53
1:B:163:LEU:HD23	1:B:187:PRO:HG3	1.91	0.53
1:B:163:LEU:CD2	1:B:187:PRO:HG3	2.39	0.52
1:C:69:ILE:HD13	1:C:98:ILE:HA	1.92	0.52
1:B:347:ASN:OD1	1:B:348:LEU:N	2.43	0.51
1:A:347:ASN:OD1	1:A:348:LEU:N	2.43	0.51
1:D:60:GLY:HA3	1:D:343:PHE:HZ	1.75	0.50
1:C:54:GLN:NE2	1:C:58[A]:GLU:OE2	2.24	0.50
1:D:161:THR:HG21	1:D:185:GLN:HB3	1.94	0.50
1:C:235[B]:ARG:NH1	5:C:670:HOH:O	2.43	0.49
1:A:69:ILE:HD13	1:A:98:ILE:HA	1.95	0.49
1:C:171:HIS:CE1	3:C:403:X7A:H11	2.48	0.48
1:D:347:ASN:O	1:D:350:ASP:HB2	2.14	0.48
1:A:163:LEU:CD2	1:A:187:PRO:HG3	2.44	0.47
1:D:124:LEU:HB3	1:D:302:VAL:HG22	1.96	0.47
1:D:201:ALA:HB1	1:D:225:ILE:HG12	1.98	0.46
1:C:45:GLU:HG3	1:C:49:LYS:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:LEU:HD12	1:D:348:LEU:HA	1.75	0.45
1:B:161:THR:HG21	1:B:185:GLN:HB3	1.99	0.45
1:C:196:LYS:HE2	1:C:198:CYS:HB3	1.98	0.45
1:C:163:LEU:CD2	1:C:187:PRO:HG3	2.47	0.44
1:C:124:LEU:HB3	1:C:302:VAL:HG22	1.99	0.44
1:A:38:ILE:HG22	5:A:766:HOH:O	2.18	0.44
1:B:102:VAL:O	1:B:106:MET:HG2	2.18	0.43
1:D:46:LEU:HD22	1:D:310:PRO:HG3	1.99	0.43
1:C:196:LYS:HA	1:C:197:PRO:HD3	1.89	0.42
1:D:45:GLU:HG3	1:D:49:LYS:HD3	2.02	0.42
1:C:135:THR:HA	1:C:178:LEU:HD11	2.03	0.41
1:C:105:LEU:O	1:C:108:GLN:HG2	2.21	0.41
1:D:347:ASN:HB3	1:D:350:ASP:CG	2.42	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/385 (87%)	328 (98%)	6 (2%)	1 (0%)	44	43
1	B	332/385 (86%)	325 (98%)	6 (2%)	1 (0%)	44	43
1	C	331/385 (86%)	324 (98%)	6 (2%)	1 (0%)	44	43
1	D	327/385 (85%)	321 (98%)	5 (2%)	1 (0%)	44	43
All	All	1325/1540 (86%)	1298 (98%)	23 (2%)	4 (0%)	44	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	173	MET
1	A	173	MET

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Mol	Chain	Res	Type
1	B	173	MET
1	C	173	MET

### 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	A	285/327 (87%)	281 (99%)	4 (1%)	71	77
1	B	283/327 (86%)	278 (98%)	5 (2%)	64	69
1	C	282/327 (86%)	279 (99%)	3 (1%)	78	82
1	D	278/327 (85%)	275 (99%)	3 (1%)	78	82
All	All	1128/1308 (86%)	1113 (99%)	15 (1%)	73	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	131	HIS
1	A	171	HIS
1	A	185	GLN
1	B	32	ASN
1	B	131	HIS
1	B	171	HIS
1	B	185	GLN
1	B	360	MET
1	C	32	ASN
1	C	131	HIS
1	C	171	HIS
1	D	32	ASN
1	D	131	HIS
1	D	171	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	203	ASN
1	D	359	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	X7A	A	403	2	14,21,21	3.17	5 (35%)	16,29,29	1.53	3 (18%)
4	GOL	A	404	-	5,5,5	0.36	0	5,5,5	0.27	0
4	GOL	A	405	-	5,5,5	0.35	0	5,5,5	0.25	0
4	GOL	A	406	-	5,5,5	0.35	0	5,5,5	0.14	0
3	X7A	B	403	2	14,21,21	3.20	5 (35%)	16,29,29	1.61	5 (31%)
4	GOL	B	404	-	5,5,5	0.33	0	5,5,5	0.27	0
4	GOL	B	405	-	5,5,5	0.38	0	5,5,5	0.25	0
4	GOL	B	406	-	5,5,5	0.31	0	5,5,5	0.32	0
3	X7A	C	403	2	14,21,21	3.18	5 (35%)	16,29,29	1.65	5 (31%)
4	GOL	C	404	-	5,5,5	0.35	0	5,5,5	0.30	0
4	GOL	C	405	-	5,5,5	0.36	0	5,5,5	0.23	0
3	X7A	D	403	2	14,21,21	3.20	5 (35%)	16,29,29	1.29	2 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	X7A	A	403	2	-	0/11/29/29	0/1/1/1
4	GOL	A	404	-	-	0/4/4/4	0/0/0/0
4	GOL	A	405	-	-	0/4/4/4	0/0/0/0
4	GOL	A	406	-	-	0/4/4/4	0/0/0/0
3	X7A	B	403	2	-	0/11/29/29	0/1/1/1
4	GOL	B	404	-	-	0/4/4/4	0/0/0/0
4	GOL	B	405	-	-	0/4/4/4	0/0/0/0
4	GOL	B	406	-	-	0/4/4/4	0/0/0/0
3	X7A	C	403	2	-	0/11/29/29	0/1/1/1
4	GOL	C	404	-	-	0/4/4/4	0/0/0/0
4	GOL	C	405	-	-	0/4/4/4	0/0/0/0
3	X7A	D	403	2	-	0/11/29/29	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	403	X7A	C11-N12	-9.84	1.24	1.47
3	B	403	X7A	C11-N12	-9.74	1.24	1.47
3	C	403	X7A	C11-N12	-9.65	1.25	1.47
3	A	403	X7A	C11-N12	-9.56	1.25	1.47
3	D	403	X7A	C14-C15	-2.59	1.41	1.51
3	A	403	X7A	C3-C1	-2.38	1.52	1.55
3	A	403	X7A	C14-C15	-2.35	1.42	1.51
3	B	403	X7A	C14-C15	-2.34	1.42	1.51
3	C	403	X7A	C14-C15	-2.32	1.42	1.51
3	C	403	X7A	C3-C1	-2.26	1.52	1.55
3	D	403	X7A	C3-C1	-2.25	1.52	1.55
3	B	403	X7A	C3-C1	-2.13	1.52	1.55
3	D	403	X7A	C10-C11	3.33	1.58	1.53
3	B	403	X7A	C10-C11	3.54	1.58	1.53
3	C	403	X7A	C10-C11	3.56	1.58	1.53
3	C	403	X7A	B7-C6	3.60	1.67	1.57
3	A	403	X7A	C10-C11	3.60	1.58	1.53
3	D	403	X7A	B7-C6	3.67	1.67	1.57
3	B	403	X7A	B7-C6	3.76	1.67	1.57
3	A	403	X7A	B7-C6	3.76	1.67	1.57

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	X7A	C16-C17-N12	2.03	114.79	111.40
3	C	403	X7A	C14-C13-N12	2.13	114.96	111.40
3	A	403	X7A	C13-N12-C17	2.21	113.87	108.87
3	C	403	X7A	C14-C15-C16	2.23	118.21	111.21
3	B	403	X7A	C14-C15-C16	2.28	118.34	111.21
3	D	403	X7A	C16-C17-N12	2.40	115.40	111.40
3	C	403	X7A	C16-C17-N12	2.43	115.46	111.40
3	B	403	X7A	C14-C13-N12	2.46	115.50	111.40
3	A	403	X7A	C16-C17-N12	2.94	116.31	111.40
3	C	403	X7A	C15-C16-C17	2.95	117.08	111.21
3	B	403	X7A	C15-C16-C17	2.98	117.14	111.21
3	B	403	X7A	C15-C14-C13	3.11	117.40	111.21
3	A	403	X7A	C15-C16-C17	3.19	117.56	111.21
3	C	403	X7A	C15-C14-C13	3.27	117.73	111.21
3	D	403	X7A	C13-N12-C17	3.29	116.33	108.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	403	X7A	1	0

## 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	A	335/385 (87%)	-0.41	3 (0%) 84 86	13, 21, 42, 63	0
1	B	335/385 (87%)	-0.17	6 (1%) 69 73	14, 22, 47, 71	0
1	C	332/385 (86%)	-0.33	3 (0%) 84 86	20, 28, 45, 70	0
1	D	331/385 (85%)	0.98	66 (19%) 1 1	34, 46, 62, 72	0
All	All	1333/1540 (86%)	0.01	78 (5%) 23 28	13, 27, 55, 72	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	343	PHE	6.6
1	D	345	VAL	6.3
1	D	357	ALA	6.2
1	D	358	ALA	5.9
1	D	346	ARG	5.7
1	D	350	ASP	5.6
1	D	351	GLN	5.6
1	D	353	ILE	5.4
1	D	360	MET	5.1
1	D	349	THR	5.1
1	D	189	LEU	4.9
1	D	109	SER	4.7
1	D	352	GLY	4.5
1	B	109	SER	4.5
1	B	343	PHE	4.5
1	D	188	TRP	4.3
1	D	166	ALA	4.1
1	D	344	LYS	4.1
1	D	19	LEU	4.1
1	D	192	PHE	4.0
1	D	147	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	190	ASP	3.7
1	D	177	PHE	3.7
1	D	359	HIS	3.6
1	D	354	MET	3.6
1	D	348	LEU	3.6
1	B	110	ASN	3.5
1	D	70	ILE	3.5
1	D	22	THR	3.5
1	D	81	GLN	3.4
1	D	347	ASN	3.3
1	A	343	PHE	3.3
1	D	175	LEU	3.3
1	B	361	GLN	3.3
1	D	96	LEU	3.2
1	D	184	ASP	3.1
1	D	187	PRO	3.1
1	D	197	PRO	3.0
1	A	110	ASN	3.0
1	D	72	VAL	2.9
1	D	146	PRO	2.9
1	D	92	SER	2.9
1	C	361	GLN	2.8
1	D	108	GLN	2.7
1	C	235[A]	ARG	2.7
1	D	91	PHE	2.6
1	B	357	ALA	2.6
1	B	120	LYS	2.5
1	D	57	ALA	2.5
1	D	193	GLU	2.5
1	D	61	ILE	2.5
1	D	161	THR	2.5
1	D	356	ARG	2.5
1	D	121	SER	2.5
1	D	163	LEU	2.4
1	D	191	ASP	2.4
1	D	139	LEU	2.4
1	D	63	LEU	2.4
1	D	196	LYS	2.4
1	D	144	ALA	2.2
1	D	83	PHE	2.2
1	D	186	ILE	2.2
1	D	319	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	58	GLU	2.2
1	D	54	GLN	2.2
1	D	341	LEU	2.2
1	A	109	SER	2.2
1	D	183	GLN	2.1
1	D	87	TRP	2.1
1	D	258	HIS	2.1
1	D	194	GLY	2.1
1	D	182	LEU	2.1
1	D	198	CYS	2.1
1	D	75	ASN	2.1
1	D	59	ASP	2.1
1	C	196	LYS	2.1
1	D	143	GLU	2.0
1	D	178	LEU	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q < 0.9
2	MN	C	401	1/1	1.00	0.12	2.01	22,22,22,22	0
2	MN	A	402	1/1	1.00	0.12	1.84	15,15,15,15	0
2	MN	B	402	1/1	1.00	0.14	1.60	16,16,16,16	0
2	MN	B	401	1/1	1.00	0.13	1.60	15,15,15,15	0
3	X7A	B	403	21/21	0.95	0.12	0.82	18,22,29,33	0
4	GOL	A	404	6/6	0.92	0.12	0.76	24,32,44,48	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	A	401	1/1	1.00	0.10	0.73	14,14,14,14	0
4	GOL	B	404	6/6	0.93	0.13	0.71	28,37,42,53	1
3	X7A	C	403	21/21	0.93	0.11	0.56	22,27,38,38	0
3	X7A	D	403	21/21	0.90	0.17	0.46	37,49,54,57	0
4	GOL	C	404	6/6	0.93	0.12	0.29	28,39,45,56	1
2	MN	C	402	1/1	1.00	0.11	0.16	22,22,22,22	0
3	X7A	A	403	21/21	0.96	0.10	-0.03	14,21,29,33	0
2	MN	D	402	1/1	0.97	0.04	-2.59	38,38,38,38	0
2	MN	D	401	1/1	0.99	0.05	-3.56	39,39,39,39	0
4	GOL	B	406	6/6	0.72	0.22	-	38,45,50,54	1
4	GOL	A	406	6/6	0.77	0.20	-	37,43,47,52	1
4	GOL	C	405	6/6	0.96	0.10	-	39,40,42,44	1
4	GOL	A	405	6/6	0.96	0.10	-	28,33,34,43	0
4	GOL	B	405	6/6	0.94	0.13	-	29,37,40,42	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.