



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 09:27 PM GMT

PDB ID : 4YGF  
Title : Crystal structure of the complex of Helicobacter pylori alpha-Carbonic Anhydrase with acetazolamide  
Authors : Roujeinikova, A.; Modak, J.K.  
Deposited on : 2015-02-26  
Resolution : 2.00 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  
<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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : rb-20026982

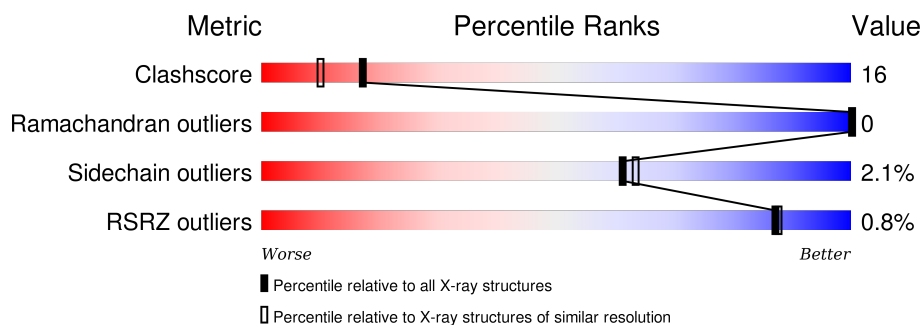
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	234	<div> <div>%</div> <div>64% 32% ..</div> </div>
1	B	234	<div> <div>68% 26% . 5%</div> </div>
1	C	234	<div> <div>%</div> <div>74% 22% ..</div> </div>
1	D	234	<div> <div>2%</div> <div>58% 34% . .</div> </div>
1	E	234	<div> <div>74% 23% .</div> </div>
1	F	234	<div> <div>%</div> <div>63% 33% .</div> </div>
1	G	234	<div> <div>64% 32% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	234	 67% 26% . .

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	B	302	-	-	X	-
3	CL	H	302	-	-	-	X
5	GOL	G	304	-	-	-	X
5	GOL	H	304	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15976 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 Alpha-carbonic anhydrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	4	0
			1866	1201	325	336	4			
1	B	223	Total	C	N	O	S	0	2	0
			1833	1178	320	331	4			
1	C	227	Total	C	N	O	S	0	1	0
			1860	1192	326	338	4			
1	D	224	Total	C	N	O	S	0	1	0
			1836	1180	323	329	4			
1	E	226	Total	C	N	O	S	0	1	0
			1853	1188	325	336	4			
1	F	225	Total	C	N	O	S	0	0	0
			1841	1180	323	334	4			
1	G	228	Total	C	N	O	S	0	3	0
			1877	1205	328	340	4			
1	H	225	Total	C	N	O	S	0	0	0
			1841	1180	323	334	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	GLY	-	expression tag	UNP K4NGD4
A	15	ILE	-	expression tag	UNP K4NGD4
A	16	ASP	-	expression tag	UNP K4NGD4
A	17	PRO	-	expression tag	UNP K4NGD4
A	18	PHE	-	expression tag	UNP K4NGD4
A	19	THR	-	expression tag	UNP K4NGD4
B	14	GLY	-	expression tag	UNP K4NGD4
B	15	ILE	-	expression tag	UNP K4NGD4
B	16	ASP	-	expression tag	UNP K4NGD4
B	17	PRO	-	expression tag	UNP K4NGD4
B	18	PHE	-	expression tag	UNP K4NGD4
B	19	THR	-	expression tag	UNP K4NGD4
C	14	GLY	-	expression tag	UNP K4NGD4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	15	ILE	-	expression tag	UNP K4NGD4
C	16	ASP	-	expression tag	UNP K4NGD4
C	17	PRO	-	expression tag	UNP K4NGD4
C	18	PHE	-	expression tag	UNP K4NGD4
C	19	THR	-	expression tag	UNP K4NGD4
D	14	GLY	-	expression tag	UNP K4NGD4
D	15	ILE	-	expression tag	UNP K4NGD4
D	16	ASP	-	expression tag	UNP K4NGD4
D	17	PRO	-	expression tag	UNP K4NGD4
D	18	PHE	-	expression tag	UNP K4NGD4
D	19	THR	-	expression tag	UNP K4NGD4
E	14	GLY	-	expression tag	UNP K4NGD4
E	15	ILE	-	expression tag	UNP K4NGD4
E	16	ASP	-	expression tag	UNP K4NGD4
E	17	PRO	-	expression tag	UNP K4NGD4
E	18	PHE	-	expression tag	UNP K4NGD4
E	19	THR	-	expression tag	UNP K4NGD4
F	14	GLY	-	expression tag	UNP K4NGD4
F	15	ILE	-	expression tag	UNP K4NGD4
F	16	ASP	-	expression tag	UNP K4NGD4
F	17	PRO	-	expression tag	UNP K4NGD4
F	18	PHE	-	expression tag	UNP K4NGD4
F	19	THR	-	expression tag	UNP K4NGD4
G	14	GLY	-	expression tag	UNP K4NGD4
G	15	ILE	-	expression tag	UNP K4NGD4
G	16	ASP	-	expression tag	UNP K4NGD4
G	17	PRO	-	expression tag	UNP K4NGD4
G	18	PHE	-	expression tag	UNP K4NGD4
G	19	THR	-	expression tag	UNP K4NGD4
H	14	GLY	-	expression tag	UNP K4NGD4
H	15	ILE	-	expression tag	UNP K4NGD4
H	16	ASP	-	expression tag	UNP K4NGD4
H	17	PRO	-	expression tag	UNP K4NGD4
H	18	PHE	-	expression tag	UNP K4NGD4
H	19	THR	-	expression tag	UNP K4NGD4

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

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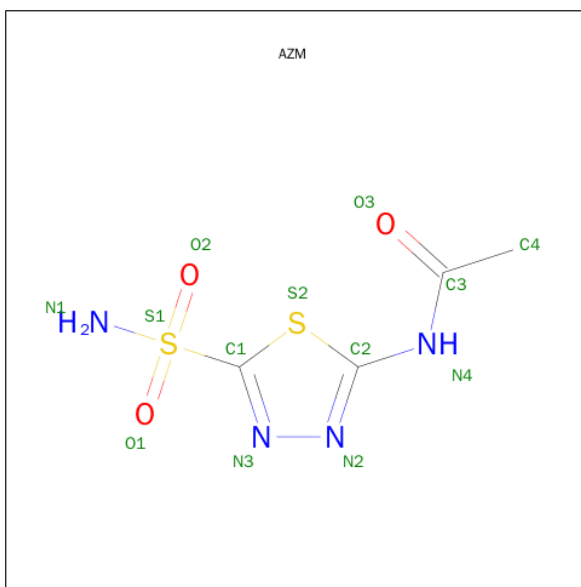
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total 1	Zn 1	0	0
2	H	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	A	1	Total 1	Zn 1	0	0
2	F	1	Total 1	Zn 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

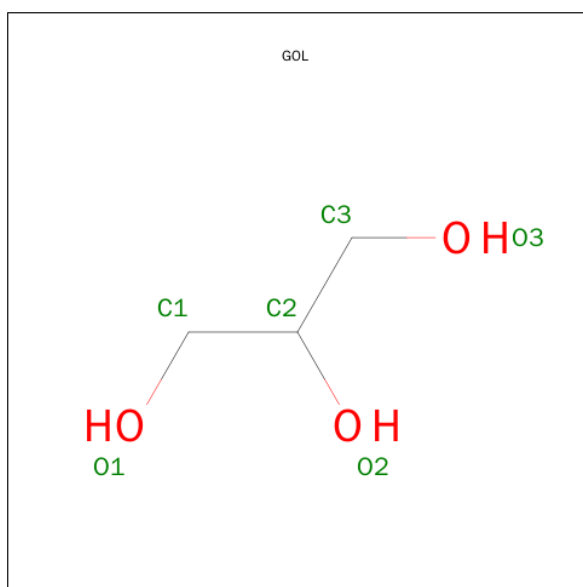
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Cl 1	0	0
3	D	1	Total 1	Cl 1	0	0
3	E	1	Total 1	Cl 1	0	0
3	H	1	Total 1	Cl 1	0	0
3	B	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0
3	A	1	Total 1	Cl 1	0	0
3	F	1	Total 1	Cl 1	0	0

- Molecule 4 is 5-ACETAMIDO-1,3,4-THIADIAZOLE-2-SULFONAMIDE (three-letter code: AZM) (formula: C<sub>4</sub>H<sub>6</sub>N<sub>4</sub>O<sub>3</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	4	4	3	2		
4	B	1	Total	C	N	O	S	0	0
			13	4	4	3	2		
4	C	1	Total	C	N	O	S	0	0
			13	4	4	3	2		
4	D	1	Total	C	N	O	S	0	0
			13	4	4	3	2		
4	E	1	Total	C	N	O	S	0	0
			13	4	4	3	2		
4	F	1	Total	C	N	O	S	0	0
			13	4	4	3	2		
4	G	1	Total	C	N	O	S	0	0
			13	4	4	3	2		
4	H	1	Total	C	N	O	S	0	0
			13	4	4	3	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

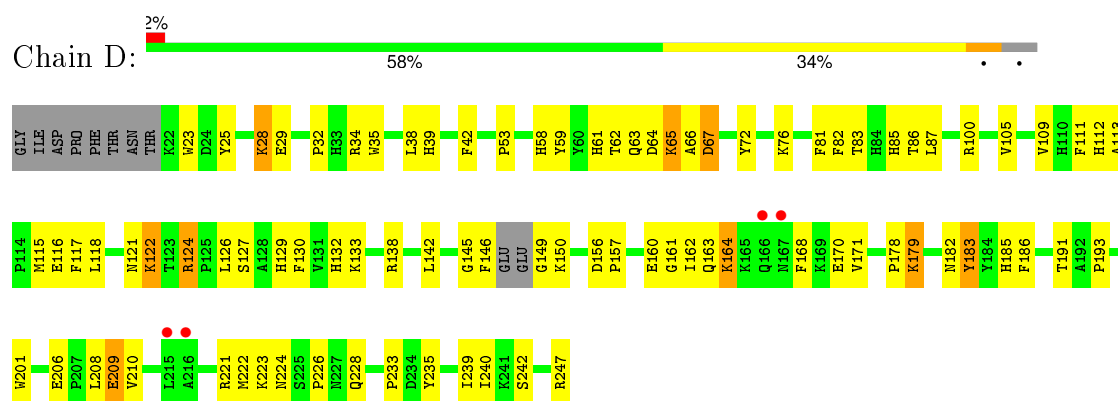
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	90	Total O 90 90	0	0
6	B	134	Total O 134 134	0	0
6	C	210	Total O 210 210	0	0
6	D	68	Total O 68 68	0	0
6	E	237	Total O 237 237	0	0
6	F	69	Total O 69 69	0	0
6	G	92	Total O 92 92	0	0

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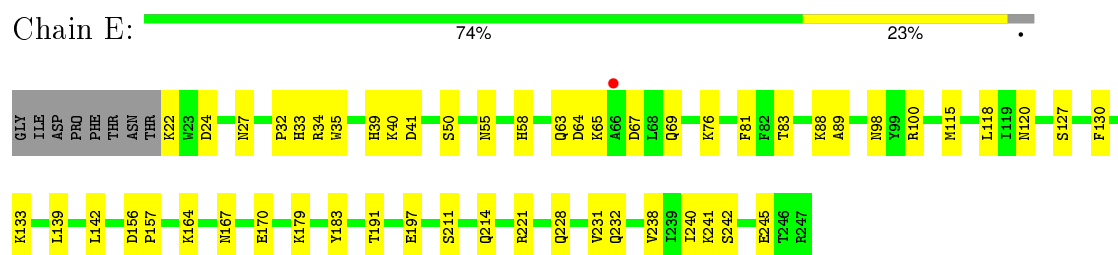
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	119	Total	O	0	0
			119	119		

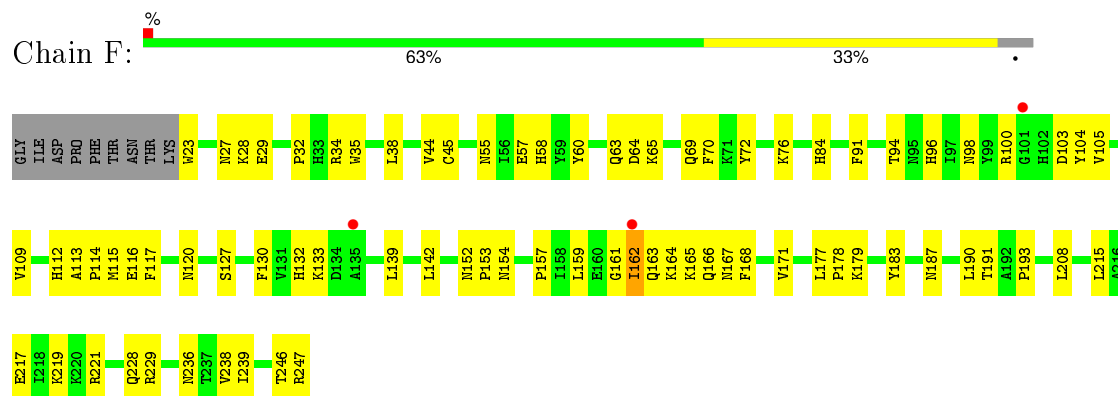




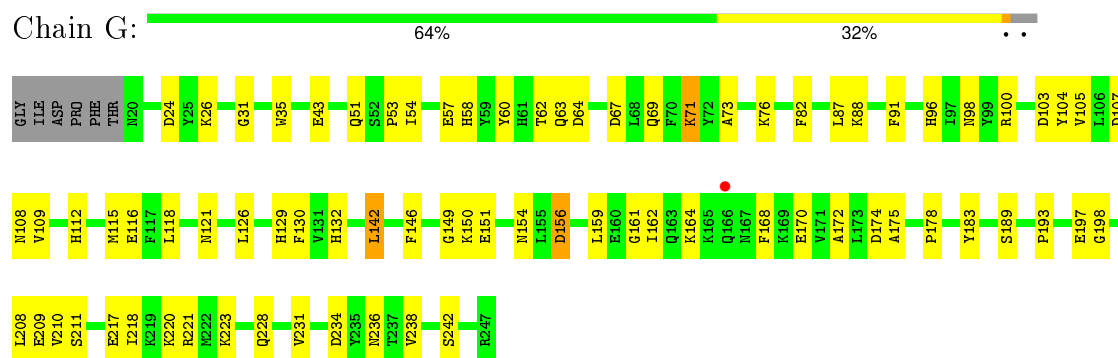
- Molecule 1: Alpha-carbonic anhydrase



- Molecule 1: Alpha-carbonic anhydrase



- Molecule 1: Alpha-carbonic anhydrase

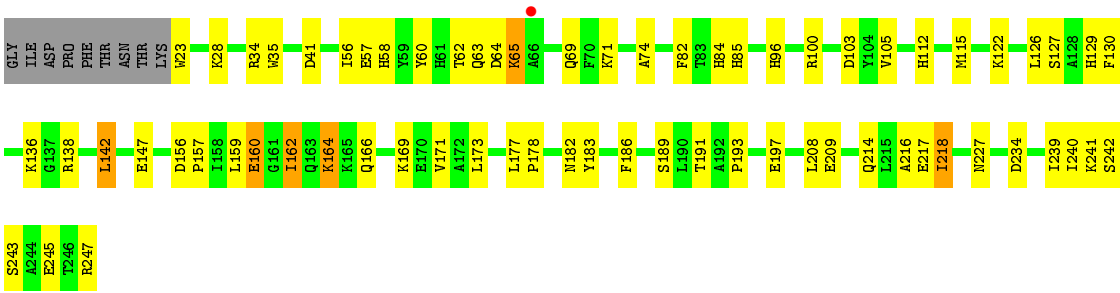


- Molecule 1: Alpha-carbonic anhydrase

Chain H: 

67%

26%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.78Å 133.61Å 166.54Å 90.00° 90.16° 90.00°	Depositor
Resolution (Å)	32.57 – 2.00 32.57 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (32.57-2.00) 96.6 (32.57-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.187 , 0.215 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.0	EDS
Estimated twinning fraction	0.500 for h,-k,-l 0.457 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 119815 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15976	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, ZN, AZM, CL

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	0.46	0/1933	0.65	0/2615
1	B	0.47	0/1893	0.69	1/2560 (0.0%)
1	C	0.52	0/1918	0.66	0/2594
1	D	0.44	0/1893	0.65	0/2559
1	E	0.51	0/1911	0.64	0/2584
1	F	0.46	0/1896	0.65	0/2565
1	G	0.43	0/1941	0.70	1/2626 (0.0%)
1	H	0.49	0/1896	0.73	2/2565 (0.1%)
All	All	0.47	0/15281	0.67	4/20668 (0.0%)

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	C	0	2
1	D	0	3
All	All	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	H	142	LEU	CA-CB-CG	6.41	130.05	115.30
1	G	142	LEU	CA-CB-CG	5.24	127.35	115.30
1	H	65	LYS	CA-CB-CG	5.03	124.47	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	63	GLN	Peptide
1	C	65	LYS	Peptide
1	D	64	ASP	Peptide
1	D	65	LYS	Peptide
1	D	66	ALA	Peptide

## 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	A	1866	0	1845	65	0
1	B	1833	0	1801	58	1
1	C	1860	0	1823	62	1
1	D	1836	0	1807	71	0
1	E	1853	0	1816	64	0
1	F	1841	0	1798	67	1
1	G	1877	0	1849	64	2
1	H	1841	0	1798	66	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	2	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	1	0
4	A	13	0	6	0	0
4	B	13	0	6	0	0
4	C	13	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	13	0	6	1	0
4	E	13	0	6	1	0
4	F	13	0	6	1	0
4	G	13	0	6	0	0
4	H	13	0	6	2	0
5	A	6	0	8	2	0
5	C	6	0	8	1	0
5	E	6	0	8	1	0
5	G	6	0	8	0	0
5	H	6	0	8	1	0
6	A	90	0	0	10	0
6	B	134	0	0	19	3
6	C	210	0	0	11	5
6	D	68	0	0	16	1
6	E	237	0	0	31	4
6	F	69	0	0	17	0
6	G	92	0	0	8	0
6	H	119	0	0	17	2
All	All	15976	0	14625	478	11

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 16.

The worst 5 of 478 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:C:64:ASP:HB2	1:H:64:ASP:OD2	1.54	1.05
1:E:58:HIS:CD2	1:F:65:LYS:HZ2	1.76	1.03
1:B:164:LYS:HE3	1:B:166:GLN:HG3	1.39	1.02
1:A:195:CYS:SG	6:A:470:HOH:O	2.14	1.01
1:A:166:GLN:HG2	1:A:167:ASN:H	1.27	0.97

The worst 5 of 11 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:499:HOH:O	6:E:530:HOH:O[2_444]	2.08	0.12
6:E:587:HOH:O	6:E:600:HOH:O[1_455]	2.12	0.08
1:B:150:LYS:NZ	1:C:163:GLN:O[2_454]	2.14	0.06
6:E:597:HOH:O	6:H:419:HOH:O[2_554]	2.16	0.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:508:HOH:O	6:D:460:HOH:O[1_655]	2.16	0.04

## 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	228/234 (97%)	216 (95%)	12 (5%)	0	100	100
1	B	221/234 (94%)	212 (96%)	9 (4%)	0	100	100
1	C	226/234 (97%)	216 (96%)	10 (4%)	0	100	100
1	D	221/234 (94%)	215 (97%)	6 (3%)	0	100	100
1	E	225/234 (96%)	213 (95%)	12 (5%)	0	100	100
1	F	223/234 (95%)	213 (96%)	10 (4%)	0	100	100
1	G	229/234 (98%)	219 (96%)	10 (4%)	0	100	100
1	H	223/234 (95%)	215 (96%)	8 (4%)	0	100	100
All	All	1796/1872 (96%)	1719 (96%)	77 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	205/208 (99%)	201 (98%)	4 (2%)	63	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	201/208 (97%)	198 (98%)	3 (2%)	72	75
1	C	203/208 (98%)	200 (98%)	3 (2%)	72	75
1	D	200/208 (96%)	190 (95%)	10 (5%)	30	24
1	E	202/208 (97%)	201 (100%)	1 (0%)	92	94
1	F	200/208 (96%)	195 (98%)	5 (2%)	55	55
1	G	206/208 (99%)	203 (98%)	3 (2%)	72	75
1	H	200/208 (96%)	194 (97%)	6 (3%)	48	47
All	All	1617/1664 (97%)	1582 (98%)	35 (2%)	61	62

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	164	LYS
1	D	224	ASN
1	H	162	ILE
1	D	179	LYS
1	D	183	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	163	GLN
1	E	39	HIS
1	H	96	HIS
1	C	112	HIS
1	C	163	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 16 are monoatomic - leaving 13 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	AZM	A	303	2	9,13,13	3.54	6 (66%)	7,19,19	3.12	4 (57%)
5	GOL	A	304	-	5,5,5	0.47	0	5,5,5	0.69	0
4	AZM	B	303	2	9,13,13	3.44	5 (55%)	7,19,19	3.22	4 (57%)
4	AZM	C	303	2	9,13,13	3.36	5 (55%)	7,19,19	2.72	3 (42%)
5	GOL	C	304	-	5,5,5	0.66	0	5,5,5	0.76	0
4	AZM	D	303	2	9,13,13	3.61	5 (55%)	7,19,19	2.99	3 (42%)
4	AZM	E	303	2	9,13,13	3.29	4 (44%)	7,19,19	2.57	5 (71%)
5	GOL	E	304	-	5,5,5	0.79	0	5,5,5	0.73	0
4	AZM	F	303	2	9,13,13	3.64	5 (55%)	7,19,19	2.98	3 (42%)
4	AZM	G	303	2	9,13,13	3.35	5 (55%)	7,19,19	2.46	3 (42%)
5	GOL	G	304	-	5,5,5	0.34	0	5,5,5	0.55	0
4	AZM	H	303	2	9,13,13	3.37	5 (55%)	7,19,19	2.98	3 (42%)
5	GOL	H	304	-	5,5,5	0.48	0	5,5,5	0.41	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
4	AZM	A	303	2	-	0/2/10/10	0/0/1/1
5	GOL	A	304	-	-	0/4/4/4	0/0/0/0
4	AZM	B	303	2	-	0/2/10/10	0/0/1/1
4	AZM	C	303	2	-	0/2/10/10	0/0/1/1
5	GOL	C	304	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AZM	D	303	2	-	0/2/10/10	0/0/1/1
4	AZM	E	303	2	-	0/2/10/10	0/0/1/1
5	GOL	E	304	-	-	0/4/4/4	0/0/0/0
4	AZM	F	303	2	-	0/2/10/10	0/0/1/1
4	AZM	G	303	2	-	0/2/10/10	0/0/1/1
5	GOL	G	304	-	-	0/4/4/4	0/0/0/0
4	AZM	H	303	2	-	0/2/10/10	0/0/1/1
5	GOL	H	304	-	-	0/4/4/4	0/0/0/0

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	303	AZM	C1-S1	-2.60	1.75	1.78
4	G	303	AZM	S1-N1	2.49	1.64	1.60
4	B	303	AZM	S1-N1	2.58	1.65	1.60
4	H	303	AZM	S1-N1	2.58	1.65	1.60
4	C	303	AZM	S1-N1	2.61	1.65	1.60

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	303	AZM	O2-S1-O1	-6.19	110.55	118.87
4	F	303	AZM	O2-S1-O1	-6.13	110.63	118.87
4	D	303	AZM	O2-S1-O1	-5.96	110.86	118.87
4	A	303	AZM	O2-S1-O1	-5.42	111.59	118.87
4	C	303	AZM	O2-S1-O1	-4.88	112.31	118.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	304	GOL	2	0
5	C	304	GOL	1	0
4	D	303	AZM	1	0
4	E	303	AZM	1	0
5	E	304	GOL	1	0
4	F	303	AZM	1	0
4	H	303	AZM	2	0
5	H	304	GOL	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	226/234 (96%)	-0.39	2 (0%) 85 86	15, 30, 43, 60	0
1	B	223/234 (95%)	-0.43	0 100 100	13, 25, 44, 55	0
1	C	227/234 (97%)	-0.60	2 (0%) 85 86	10, 17, 33, 50	0
1	D	224/234 (95%)	-0.04	4 (1%) 71 72	18, 37, 57, 88	0
1	E	226/234 (96%)	-0.59	1 (0%) 93 93	9, 16, 33, 49	0
1	F	225/234 (96%)	-0.14	3 (1%) 79 80	18, 34, 52, 74	0
1	G	228/234 (97%)	-0.35	1 (0%) 93 93	15, 31, 50, 64	0
1	H	225/234 (96%)	-0.48	1 (0%) 93 93	10, 23, 41, 55	0
All	All	1804/1872 (96%)	-0.38	14 (0%) 87 88	9, 26, 50, 88	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	66	ALA	4.1
1	E	66	ALA	3.8
1	G	166	GLN	3.2
1	A	166	GLN	3.0
1	D	167	ASN	3.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
5	GOL	H	304	6/6	0.97	0.12	3.03	18,22,27,33	0
5	GOL	G	304	6/6	0.94	0.16	2.90	26,32,35,37	0
3	CL	H	302	1/1	0.99	0.11	2.84	18,18,18,18	0
5	GOL	C	304	6/6	0.95	0.10	1.97	15,17,20,30	0
5	GOL	E	304	6/6	0.97	0.10	1.94	14,16,19,19	0
4	AZM	G	303	13/13	0.98	0.11	1.08	16,21,32,35	2
4	AZM	C	303	13/13	0.99	0.09	1.02	11,14,21,23	9
4	AZM	E	303	13/13	0.99	0.10	0.76	9,12,19,20	7
5	GOL	A	304	6/6	0.95	0.10	0.69	18,23,24,30	0
4	AZM	A	303	13/13	0.99	0.10	0.57	15,18,27,30	0
3	CL	C	302	1/1	1.00	0.09	0.29	13,13,13,13	0
3	CL	B	302	1/1	0.98	0.10	0.17	20,20,20,20	0
4	AZM	F	303	13/13	0.98	0.11	-0.03	20,23,31,38	12
4	AZM	B	303	13/13	0.98	0.09	-0.17	12,18,23,24	0
4	AZM	H	303	13/13	0.98	0.09	-0.44	14,18,28,28	2
4	AZM	D	303	13/13	0.98	0.08	-0.84	19,21,27,31	9
3	CL	E	302	1/1	1.00	0.08	-1.37	12,12,12,12	0
3	CL	D	302	1/1	0.97	0.05	-1.56	35,35,35,35	0
3	CL	G	302	1/1	0.99	0.06	-2.59	24,24,24,24	0
3	CL	A	302	1/1	0.99	0.06	-3.36	26,26,26,26	0
3	CL	F	302	1/1	0.97	0.07	-3.99	31,31,31,31	0
2	ZN	G	301	1/1	0.99	0.07	-	24,24,24,24	0
2	ZN	A	301	1/1	0.99	0.07	-	21,21,21,21	0
2	ZN	F	301	1/1	0.99	0.06	-	31,31,31,31	0
2	ZN	B	301	1/1	0.98	0.10	-	19,19,19,19	0
2	ZN	D	301	1/1	0.99	0.07	-	32,32,32,32	0
2	ZN	C	301	1/1	1.00	0.09	-	14,14,14,14	0
2	ZN	H	301	1/1	0.98	0.10	-	24,24,24,24	0
2	ZN	E	301	1/1	1.00	0.09	-	14,14,14,14	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.