



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 08:49 pm BST

PDB ID : 5TUO  
Title : Crystal structure of the complex of Helicobacter pylori alpha-carbonic anhydrase with 5-amino-1,3,4-thiadiazole-2-sulfonamide inhibitor.  
Authors : Modak, J.K.; Roujeinikova, A.  
Deposited on : 2016-11-06  
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

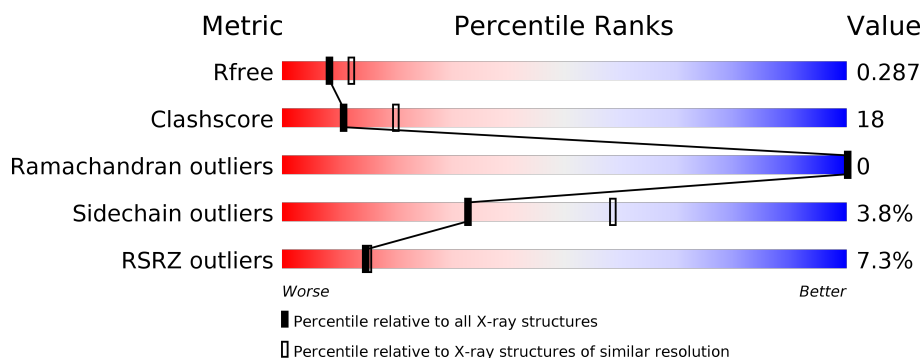
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	234	<div> <div>3%</div> <div>70%</div> <div>24%</div> <div>• •</div> </div>
1	B	234	<div> <div>6%</div> <div>64%</div> <div>28%</div> <div>• 7%</div> </div>
1	C	234	<div> <div>4%</div> <div>68%</div> <div>27%</div> <div>• •</div> </div>
1	D	234	<div> <div>5%</div> <div>59%</div> <div>32%</div> <div>• 7%</div> </div>
1	E	234	<div> <div>6%</div> <div>64%</div> <div>32%</div> <div>• •</div> </div>
1	F	234	<div> <div>19%</div> <div>42%</div> <div>41%</div> <div>• 15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	234	<div><div></div><div>3%</div><div>63%</div><div>31%</div><div></div><div></div></div>
1	H	234	<div><div></div><div>8%</div><div>53%</div><div>38%</div><div></div><div>7%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14560 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	224	Total	C	N	O	S	0	1	0
			1838	1179	322	333	4			
1	B	217	Total	C	N	O	S	0	1	0
			1776	1138	310	324	4			
1	C	226	Total	C	N	O	S	0	1	0
			1853	1188	325	336	4			
1	D	218	Total	C	N	O	S	0	0	0
			1781	1144	311	323	3			
1	E	228	Total	C	N	O	S	0	1	0
			1868	1196	328	340	4			
1	F	199	Total	C	N	O	S	0	0	0
			1619	1046	280	289	4			
1	G	225	Total	C	N	O	S	0	1	0
			1846	1183	323	336	4			
1	H	218	Total	C	N	O	S	0	0	0
			1781	1142	312	323	4			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	H	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

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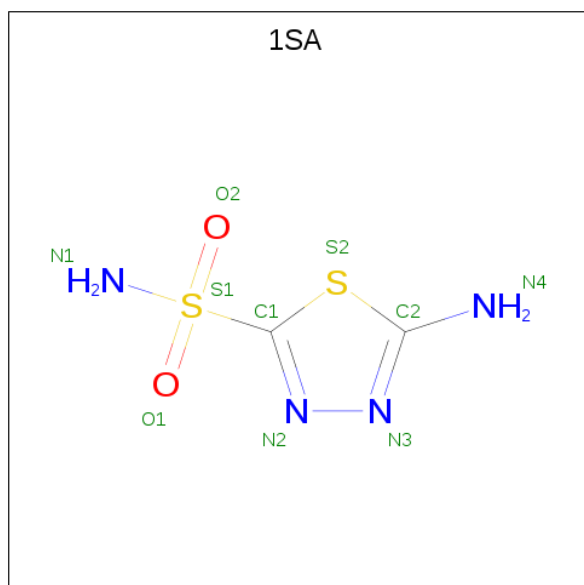
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			10	2	4	2	2		
4	B	1	Total	C	N	O	S	0	0
			10	2	4	2	2		
4	C	1	Total	C	N	O	S	0	0
			10	2	4	2	2		
4	D	1	Total	C	N	O	S	0	0
			10	2	4	2	2		
4	E	1	Total	C	N	O	S	0	0
			10	2	4	2	2		
4	F	1	Total	C	N	O	S	0	0
			10	2	4	2	2		
4	G	1	Total	C	N	O	S	0	0
			10	2	4	2	2		
4	H	1	Total	C	N	O	S	0	0
			10	2	4	2	2		

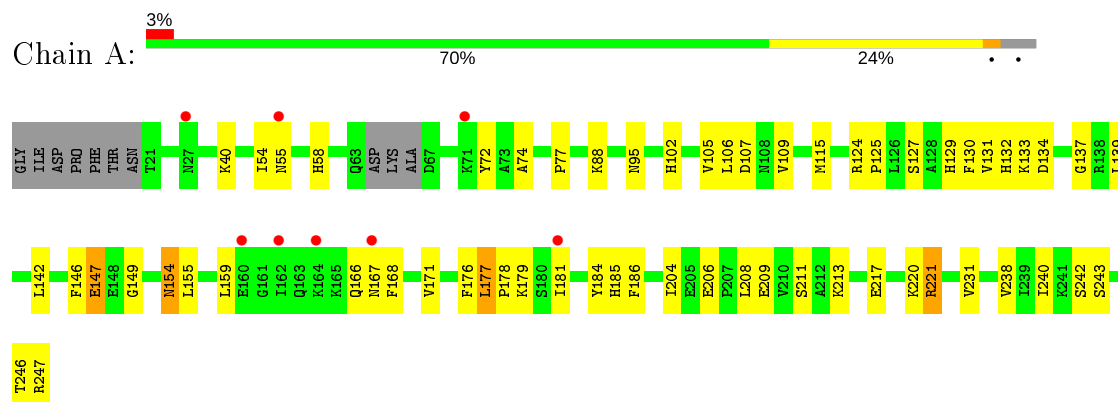
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	O	0	0
			13	13		
5	B	14	Total	O	0	0
			14	14		
5	C	17	Total	O	0	0
			17	17		
5	D	11	Total	O	0	0
			11	11		
5	E	5	Total	O	0	0
			5	5		
5	F	8	Total	O	0	0
			8	8		
5	G	21	Total	O	0	0
			21	21		
5	H	14	Total	O	0	0
			14	14		

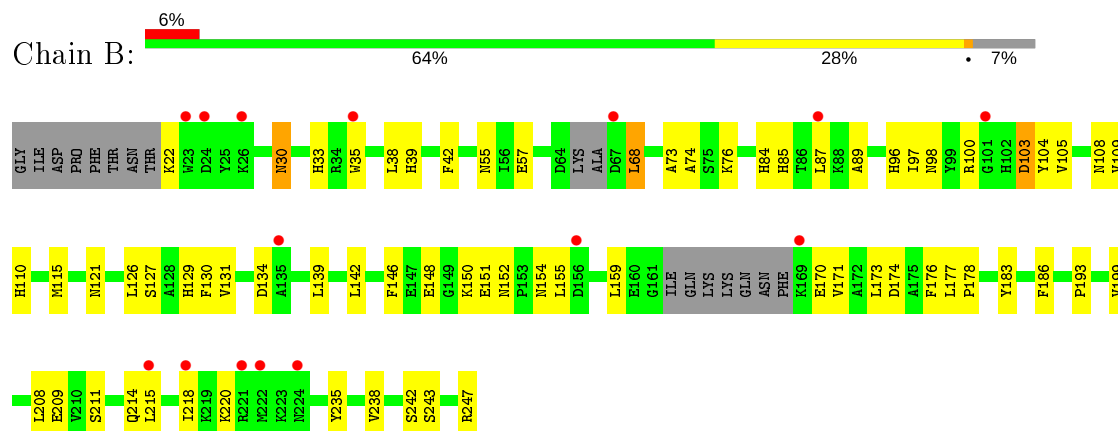
### 3 Residue-property plots [i](#)

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.

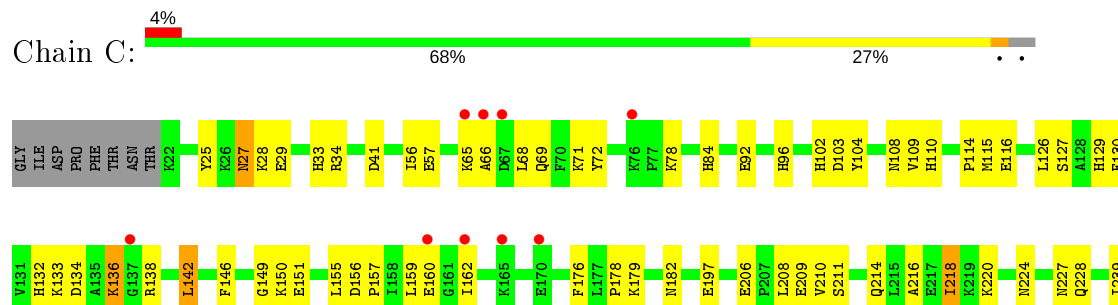
- Molecule 1: Alpha-carbonic anhydrase



- Molecule 1: Alpha-carbonic anhydrase

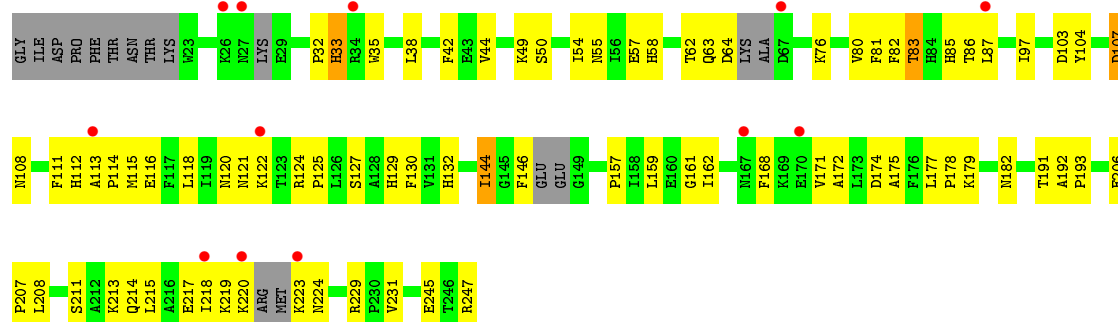


- Molecule 1: Alpha-carbonic anhydrase

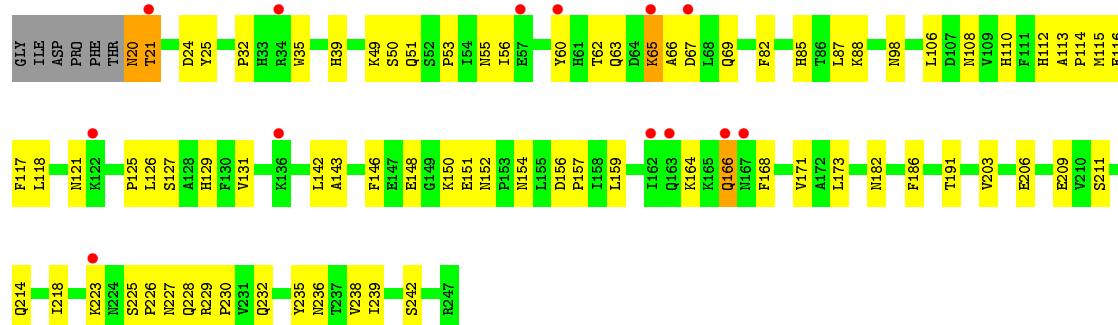




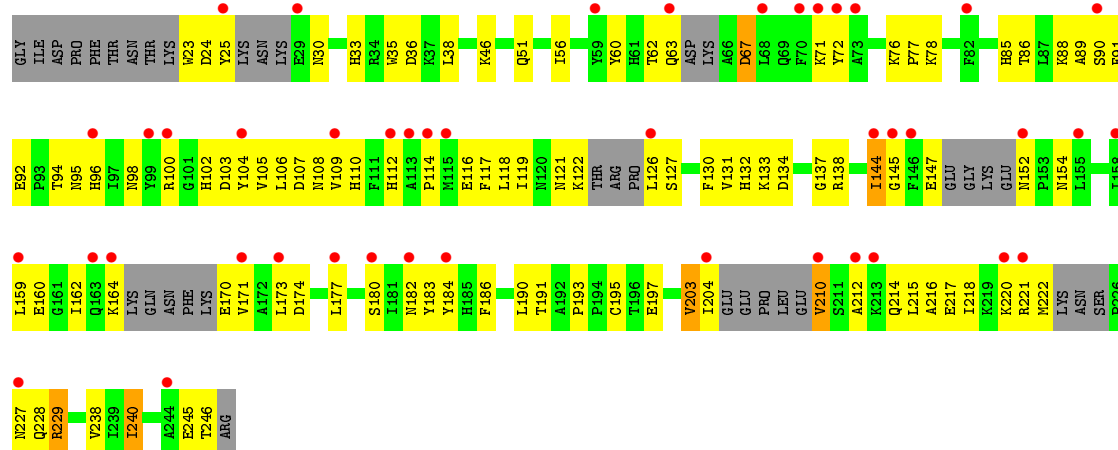
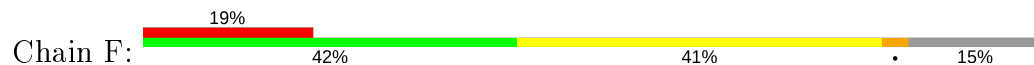
• Molecule 1: Alpha-carbonic anhydrase



• Molecule 1: Alpha-carbonic anhydrase

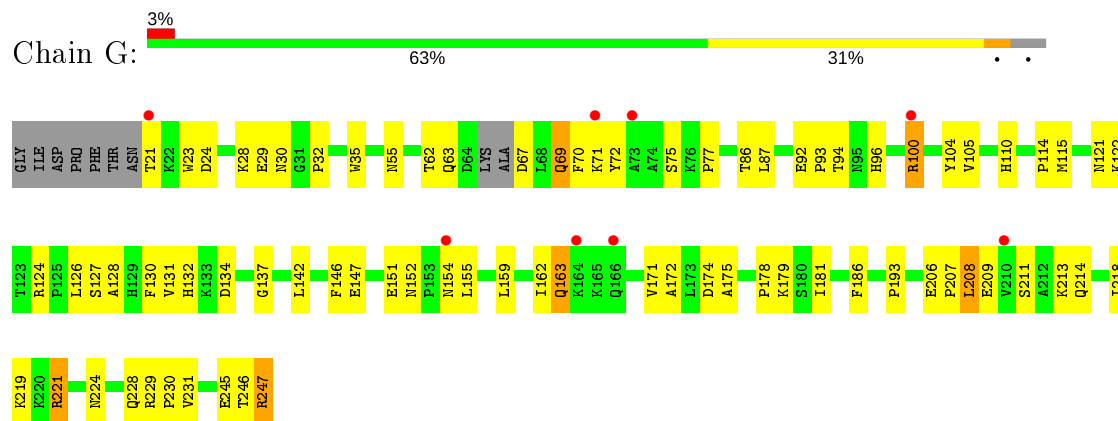


• Molecule 1: Alpha-carbonic anhydrase

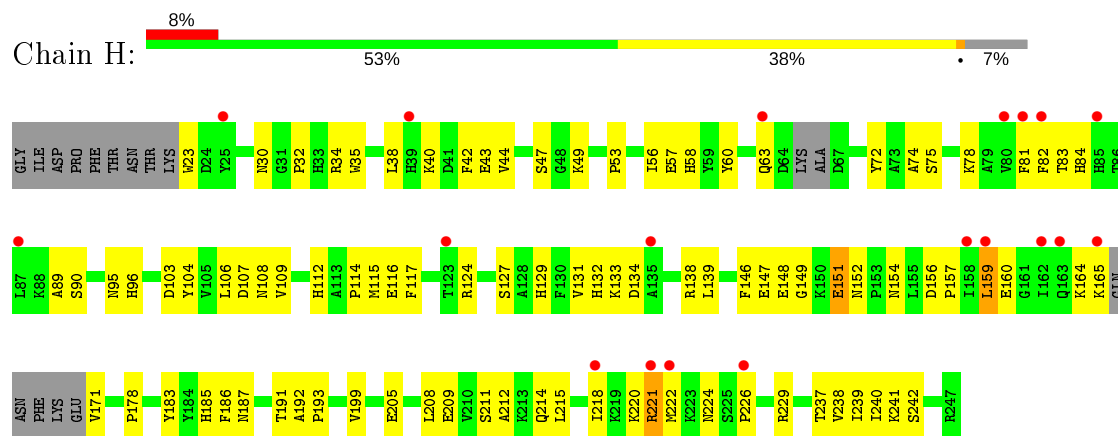




- Molecule 1: Alpha-carbonic anhydrase



- Molecule 1: Alpha-carbonic anhydrase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.84Å 136.92Å 166.27Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	29.91 – 2.50 29.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.91-2.50) 99.6 (29.91-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.28 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.227 , 0.272 0.246 , 0.287	Depositor DCC
$R_{free}$ test set	3273 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.120 for h,-k,-l	Xtriage
Reported twinning fraction	0.150 for h,-k,-l	Depositor
Outliers	1 of 64589 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14560	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1SA, ZN, 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	0.48	0/1895	0.62	0/2562
1	B	0.50	0/1831	0.63	0/2476
1	C	0.49	0/1911	0.63	1/2584 (0.0%)
1	D	0.43	0/1832	0.58	0/2476
1	E	0.49	0/1926	0.62	1/2605 (0.0%)
1	F	0.45	0/1664	0.63	0/2248
1	G	0.53	0/1903	0.62	1/2573 (0.0%)
1	H	0.52	0/1833	0.66	1/2479 (0.0%)
All	All	0.49	0/14795	0.62	4/20003 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	142	LEU	CA-CB-CG	5.91	128.89	115.30
1	G	100	ARG	N-CA-C	5.61	126.14	111.00
1	E	142	LEU	CA-CB-CG	5.24	127.35	115.30
1	H	159	LEU	CA-CB-CG	5.13	127.11	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	1838	0	1800	46	0
1	B	1776	0	1728	57	0
1	C	1853	0	1816	49	0
1	D	1781	0	1729	66	0
1	E	1868	0	1829	81	0
1	F	1619	0	1566	109	0
1	G	1846	0	1804	57	0
1	H	1781	0	1736	70	0
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	0	0
3	C	1	0	0	0	0
3	D	1	0	0	1	0
3	E	1	0	0	1	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	10	0	4	0	0
4	B	10	0	3	3	0
4	C	10	0	4	1	0
4	D	10	0	4	2	0
4	E	10	0	3	1	0
4	F	10	0	3	0	0
4	G	10	0	3	0	0
4	H	10	0	4	3	0
5	A	13	0	0	1	0
5	B	14	0	0	2	0
5	C	17	0	0	1	0
5	D	11	0	0	2	0
5	E	5	0	0	0	0
5	F	8	0	0	0	0
5	G	21	0	0	0	0
5	H	14	0	0	1	0
All	All	14560	0	14036	518	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 18.

The worst 5 of 518 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:G:67:ASP:HB3	1:G:100:ARG:CG	1.71	1.19
1:B:159:LEU:HD21	1:B:218:ILE:CG1	1.73	1.17
1:A:181:ILE:HD12	1:A:246:THR:HG21	1.25	1.12
1:F:100:ARG:NH2	1:F:138:ARG:HH12	1.50	1.08
1:E:85:HIS:HA	1:E:223:LYS:HE2	1.33	1.06

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	221/234 (94%)	206 (93%)	15 (7%)	0	100	100
1	B	212/234 (91%)	201 (95%)	11 (5%)	0	100	100
1	C	225/234 (96%)	208 (92%)	17 (8%)	0	100	100
1	D	208/234 (89%)	201 (97%)	7 (3%)	0	100	100
1	E	227/234 (97%)	208 (92%)	19 (8%)	0	100	100
1	F	183/234 (78%)	168 (92%)	15 (8%)	0	100	100
1	G	222/234 (95%)	210 (95%)	12 (5%)	0	100	100
1	H	212/234 (91%)	200 (94%)	12 (6%)	0	100	100
All	All	1710/1872 (91%)	1602 (94%)	108 (6%)	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	201/208 (97%)	193 (96%)	8 (4%)	31	56
1	B	194/208 (93%)	188 (97%)	6 (3%)	40	67
1	C	202/208 (97%)	192 (95%)	10 (5%)	24	46
1	D	194/208 (93%)	185 (95%)	9 (5%)	27	50
1	E	204/208 (98%)	197 (97%)	7 (3%)	37	63
1	F	175/208 (84%)	168 (96%)	7 (4%)	31	56
1	G	202/208 (97%)	194 (96%)	8 (4%)	31	56
1	H	194/208 (93%)	188 (97%)	6 (3%)	40	67
All	All	1566/1664 (94%)	1505 (96%)	61 (4%)	33	57

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	83	THR
1	E	21	THR
1	H	40	LYS
1	D	103	ASP
1	D	144	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	39	HIS
1	E	167	ASN
1	H	112	HIS
1	E	69	GLN
1	E	236	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 15 are monoatomic - leaving 8 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	1SA	H	303	2	5,10,10	2.92	2 (40%)	6,15,15	2.28	3 (50%)
4	1SA	A	303	2	5,10,10	2.93	2 (40%)	6,15,15	2.26	3 (50%)
4	1SA	E	303	2	5,10,10	2.93	2 (40%)	6,15,15	2.26	3 (50%)
4	1SA	C	303	2	5,10,10	2.93	2 (40%)	6,15,15	2.26	3 (50%)
4	1SA	G	303	2	5,10,10	2.93	2 (40%)	6,15,15	2.25	3 (50%)
4	1SA	B	303	2	5,10,10	2.92	2 (40%)	6,15,15	2.26	3 (50%)
4	1SA	F	302	2	5,10,10	2.93	2 (40%)	6,15,15	2.25	3 (50%)
4	1SA	D	303	2	5,10,10	2.93	2 (40%)	6,15,15	2.27	3 (50%)

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	1SA	H	303	2	-	0/0/6/6	0/1/1/1
4	1SA	A	303	2	-	0/0/6/6	0/1/1/1
4	1SA	E	303	2	-	0/0/6/6	0/1/1/1
4	1SA	C	303	2	-	0/0/6/6	0/1/1/1
4	1SA	G	303	2	-	0/0/6/6	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1SA	B	303	2	-	0/0/6/6	0/1/1/1
4	1SA	F	302	2	-	0/0/6/6	0/1/1/1
4	1SA	D	303	2	-	0/0/6/6	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	303	1SA	N3-N2	-5.67	1.26	1.37
4	D	303	1SA	N3-N2	-5.66	1.26	1.37
4	F	302	1SA	N3-N2	-5.65	1.26	1.37
4	A	303	1SA	N3-N2	-5.64	1.26	1.37
4	G	303	1SA	N3-N2	-5.64	1.26	1.37

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	303	1SA	O2-S1-O1	4.08	125.46	118.76
4	D	303	1SA	O2-S1-O1	4.06	125.43	118.76
4	A	303	1SA	O2-S1-O1	4.05	125.42	118.76
4	C	303	1SA	O2-S1-O1	4.05	125.41	118.76
4	B	303	1SA	O2-S1-O1	4.04	125.40	118.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	303	1SA	3	0
4	E	303	1SA	1	0
4	C	303	1SA	1	0
4	B	303	1SA	3	0
4	D	303	1SA	2	0

## 5.7 Other polymers

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	224/234 (95%)	0.24	8 (3%) 42 46	26, 48, 70, 86	0
1	B	217/234 (92%)	0.37	15 (6%) 16 17	28, 49, 74, 88	0
1	C	226/234 (96%)	0.17	9 (3%) 38 41	27, 41, 64, 78	0
1	D	218/234 (93%)	0.51	12 (5%) 25 26	31, 56, 82, 95	0
1	E	228/234 (97%)	0.34	13 (5%) 23 25	30, 47, 70, 83	0
1	F	199/234 (85%)	1.22	44 (22%) 0 0	46, 71, 87, 94	0
1	G	225/234 (96%)	0.38	8 (3%) 42 46	25, 52, 73, 90	0
1	H	218/234 (93%)	0.55	19 (8%) 10 10	25, 51, 71, 82	0
All	All	1755/1872 (93%)	0.46	128 (7%) 15 15	25, 51, 79, 95	0

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	100	ARG	6.0
1	D	220	LYS	5.0
1	G	73	ALA	5.0
1	B	218	ILE	4.6
1	A	27	ASN	4.5

### 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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	F	301	1/1	0.74	0.12	59,59,59,59	1
4	1SA	D	303	10/10	0.80	0.26	43,55,64,70	0
4	1SA	C	303	10/10	0.81	0.26	28,46,57,59	0
4	1SA	H	303	10/10	0.81	0.26	40,54,60,70	10
4	1SA	A	303	10/10	0.82	0.25	23,41,46,51	10
4	1SA	F	302	10/10	0.87	0.16	54,55,59,61	10
4	1SA	E	303	10/10	0.87	0.24	36,45,54,64	10
4	1SA	B	303	10/10	0.90	0.21	37,43,55,58	10
4	1SA	G	303	10/10	0.93	0.17	32,38,49,53	0
3	CL	D	302	1/1	0.94	0.07	53,53,53,53	0
2	ZN	H	301	1/1	0.96	0.17	46,46,46,46	0
3	CL	E	302	1/1	0.97	0.09	40,40,40,40	0
2	ZN	B	301	1/1	0.98	0.12	32,32,32,32	0
3	CL	H	302	1/1	0.98	0.08	38,38,38,38	0
3	CL	C	302	1/1	0.98	0.09	34,34,34,34	0
3	CL	G	302	1/1	0.99	0.06	35,35,35,35	0
2	ZN	C	301	1/1	0.99	0.16	34,34,34,34	0
2	ZN	D	301	1/1	0.99	0.12	46,46,46,46	0
3	CL	B	302	1/1	0.99	0.09	39,39,39,39	0
2	ZN	A	301	1/1	0.99	0.16	32,32,32,32	0
2	ZN	G	301	1/1	0.99	0.16	30,30,30,30	0
3	CL	A	302	1/1	0.99	0.11	34,34,34,34	0
2	ZN	E	301	1/1	0.99	0.13	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.