



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2017 – 05:05 PM EST

PDB ID : 5L3O  
Title : CRYSTAL STRUCTURE OF HUMAN CARBONIC ANHYDRASE II IN  
COMPLEX WITH A QUINOLINE OLIGOAMIDE FOLDAMER  
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Deposited on : 2016-05-24  
Resolution : 1.98 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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-20028442

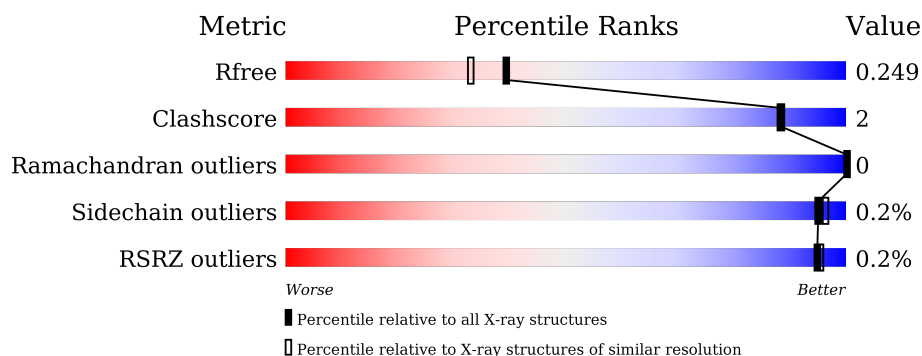
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

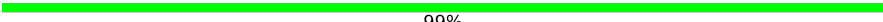
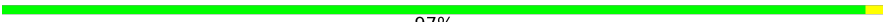
The reported resolution of this entry is 1.98 Å.

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))
$R_{free}$	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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	260	 99%
1	B	260	 97%

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
5	QVS	A	319	-	-	X	-
6	QVE	B	320	-	-	X	-
7	GOL	A	302	-	-	-	X
7	GOL	A	304	-	-	-	X
7	GOL	B	302[A]	-	-	-	X
7	GOL	B	302[B]	-	-	-	X
7	GOL	B	304	-	-	-	X
7	GOL	B	305	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4761 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.

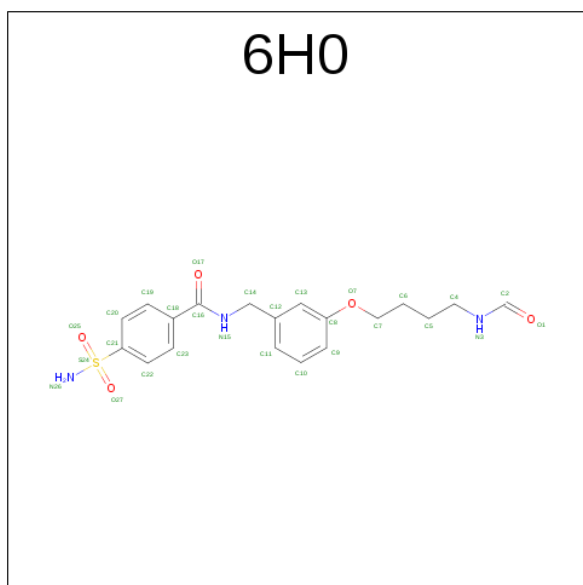
- Molecule 1 is a protein called Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	1	0
			2061	1323	353	383	2			
1	B	259	Total	C	N	O	S	0	1	0
			2070	1327	356	385	2			

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

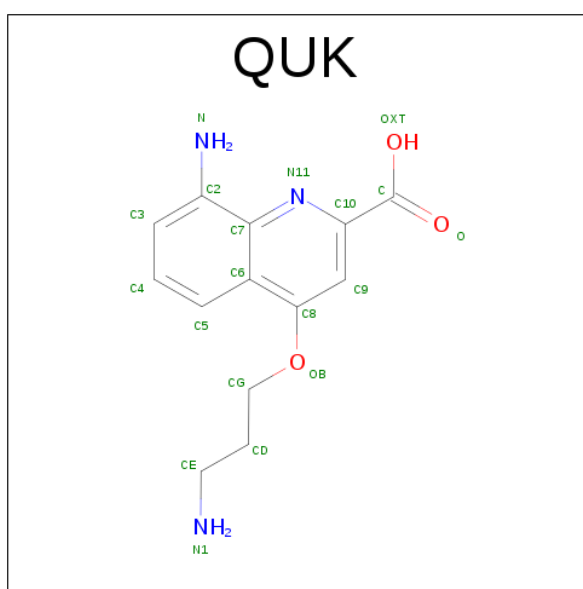
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is {N}-[[3-(4-formamidobutoxy)phenyl]methyl]-4-sulfamoyl-benzamide (three-letter code: 6H0) (formula: C<sub>19</sub>H<sub>23</sub>N<sub>3</sub>O<sub>5</sub>S).



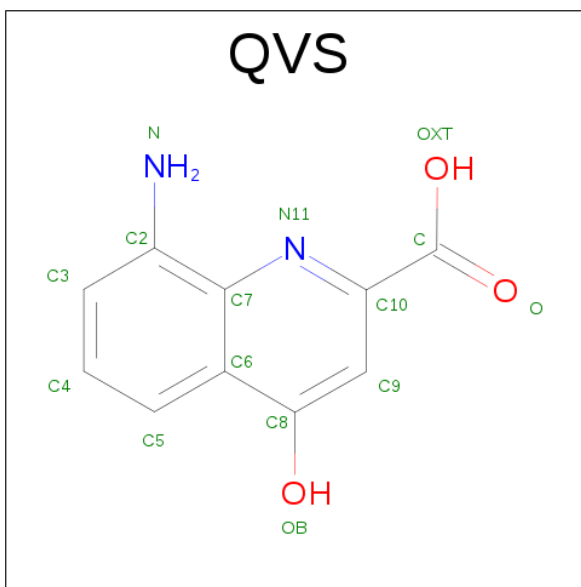
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
3	A	1	Total	C	N	O		0	0
			3	1	1	1			
3	B	1	Total	C	N	O		0	0
			3	1	1	1			
3	B	1	Total	C	N	O	S	0	0
			28	19	3	5	1		

- Molecule 4 is 8-azanyl-4-(3-azanylpropoxy)quinoline-2-carboxylic acid (three-letter code: QUK) (formula:  $C_{13}H_{15}N_3O_3$ ).



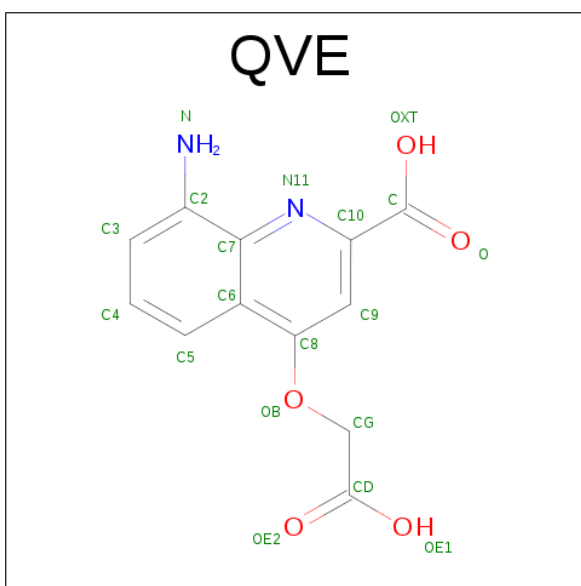
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	13	2	2		
4	A	1	Total	C	N	O	0	0
			14	10	2	2		
4	B	1	Total	C	N	O	0	0
			14	10	2	2		
4	B	1	Total	C	N	O	0	0
			17	13	2	2		

- Molecule 5 is 8-azanyl-4-oxidanyl-quinoline-2-carboxylic acid (three-letter code: QVS) (formula:  $C_{10}H_8N_2O_3$ ).



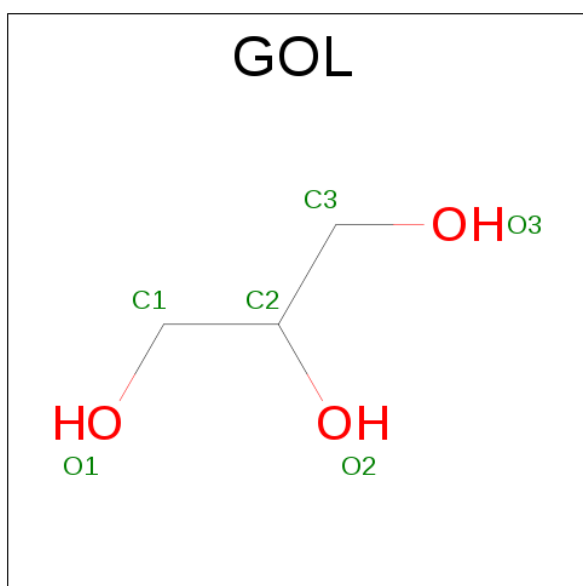
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	10	2	2		
5	A	1	Total	C	N	O	0	0
			14	10	2	2		
5	B	1	Total	C	N	O	0	0
			14	10	2	2		
5	B	1	Total	C	N	O	0	0
			14	10	2	2		

- Molecule 6 is 8-azanyl-4-(2-hydroxy-2-oxoethoxy)quinoline-2-carboxylic acid (three-letter code: QVE) (formula:  $C_{12}H_{10}N_2O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			19	12	2	5		
6	A	1	Total	C	N	O	0	0
			15	10	2	3		
6	B	1	Total	C	N	O	0	0
			19	12	2	5		
6	B	1	Total	C	N	O	0	0
			19	12	2	5		

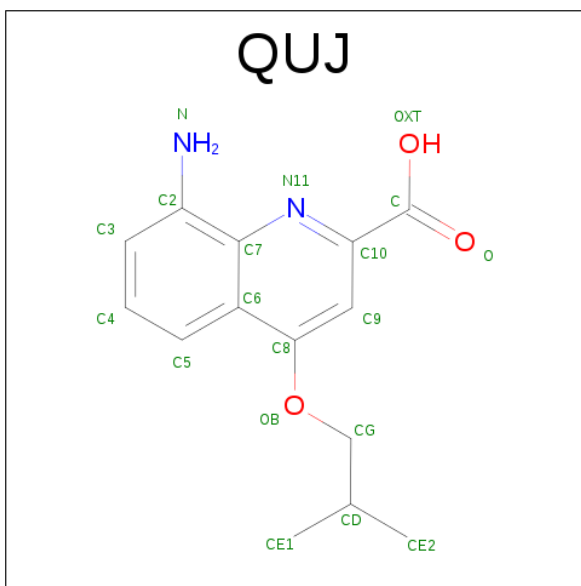
- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	1
			12	6	6		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is 8-azanyl-4-(2-methylpropoxy)quinoline-2-carboxylic acid (three-letter code:

QUJ) (formula: C<sub>14</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	10	2	2		
8	A	1	Total	C	N	O	0	0
			18	14	2	2		
8	B	1	Total	C	N	O	0	0
			18	14	2	2		
8	B	1	Total	C	N	O	0	0
			18	14	2	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	129	Total	O	0	0
			129	129		
9	B	131	Total	O	0	0
			131	131		



### 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 errors 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: Carbonic anhydrase 2

Chain A:  99%



- Molecule 1: Carbonic anhydrase 2

Chain B:  97%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.88Å 54.48Å 84.92Å 90.00° 112.79° 90.00°	Depositor
Resolution (Å)	78.29 – 1.98 51.06 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.3 (78.29-1.98) 98.3 (51.06-1.98)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.207 , 0.236 0.218 , 0.249	Depositor DCC
$R_{free}$ test set	2271 reflections (5.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4761	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% 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, ZN, QVE, 6H0, QUK, QUJ, QVS

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	0.62	0/2126	0.76	1/2885 (0.0%)
1	B	0.64	0/2135	0.76	1/2896 (0.0%)
All	All	0.63	0/4261	0.76	2/5781 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	LYS	CD-CE-NZ	5.48	124.31	111.70
1	A	34	ASP	CB-CG-OD1	5.15	122.94	118.30

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	2061	0	2005	0	0
1	B	2070	0	2018	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	0	5	0
3	B	31	0	0	0	0
4	A	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	31	0	0	4	0
5	A	28	0	0	6	0
5	B	28	0	0	5	0
6	A	34	0	0	5	0
6	B	38	0	0	7	0
7	A	18	0	24	0	0
7	B	30	0	40	3	0
8	A	32	0	0	1	0
8	B	36	0	0	0	0
9	A	129	0	0	0	0
9	B	131	0	0	0	0
All	All	4761	0	4087	21	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 (21) 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)
8:A:317:QUJ:C4	6:B:320:QVE:CG	1.89	1.17
5:A:319:QVS:C2	6:B:320:QVE:O	2.17	0.93
3:A:316:6H0:N3	5:A:319:QVS:C3	2.37	0.88
6:A:320:QVE:C	5:B:319:QVS:C2	2.70	0.70
3:A:316:6H0:N3	5:A:319:QVS:C2	2.55	0.69
4:B:318:QUK:C10	6:B:320:QVE:O	2.41	0.68
5:A:319:QVS:N	6:B:320:QVE:O	2.27	0.68
6:A:320:QVE:O	5:B:319:QVS:C2	2.54	0.56
3:A:316:6H0:N3	4:B:318:QUK:C8	2.69	0.53
6:A:320:QVE:C	5:B:319:QVS:C3	2.87	0.52
1:B:127:TYR:O	1:B:132:LYS:HE2	2.10	0.52
5:A:319:QVS:C7	6:B:320:QVE:O	2.59	0.51
6:A:320:QVE:OXT	5:B:319:QVS:C4	2.59	0.50
3:A:316:6H0:N3	4:B:318:QUK:C9	2.63	0.49
6:A:320:QVE:C	5:B:319:QVS:C7	2.92	0.47
4:B:318:QUK:N11	6:B:320:QVE:O	2.47	0.46
4:A:318:QUK:C	6:B:320:QVE:O	2.63	0.45
3:A:316:6H0:N3	5:A:319:QVS:C4	2.82	0.43
1:B:96:HIS:CE1	7:B:302[B]:GOL:H32	2.54	0.43
1:B:96:HIS:HE1	7:B:302[B]:GOL:H32	1.84	0.43
1:B:199:THR:HG21	7:B:302[A]:GOL:O3	2.19	0.41

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	258/260 (99%)	246 (95%)	12 (5%)	0	100	100
1	B	258/260 (99%)	245 (95%)	13 (5%)	0	100	100
All	All	516/520 (99%)	491 (95%)	25 (5%)	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	223/225 (99%)	223 (100%)	0	100	100
1	B	225/225 (100%)	224 (100%)	1 (0%)	93	95
All	All	448/450 (100%)	447 (100%)	1 (0%)	95	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	238	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 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$
7	GOL	A	302	-	5,5,5	0.46	0	5,5,5	0.40	0
7	GOL	A	303	-	5,5,5	0.30	0	5,5,5	0.35	0
7	GOL	A	304	-	5,5,5	0.26	0	5,5,5	0.28	0
3	6H0	A	311	8,2	29,29,29	2.46	5 (17%)	37,38,38	2.70	3 (8%)
8	QUJ	A	312	3,4	19,19,20	1.71	2 (10%)	21,26,28	2.56	4 (19%)
4	QUK	A	313	8,5	18,18,20	1.60	2 (11%)	19,24,27	2.74	6 (31%)
5	QVS	A	314	4,6	15,15,16	1.93	1 (6%)	17,21,23	3.12	4 (23%)
6	QVE	A	315	5	14,20,20	0.82	0	18,28,28	2.15	5 (27%)
3	6H0	A	316	8,6	2,2,29	0.49	0	1,1,38	0.72	0
8	QUJ	A	317	3,5,4,6	15,15,20	1.97	3 (20%)	17,21,28	2.07	2 (11%)
4	QUK	A	318	8,5,4	15,15,20	2.16	3 (20%)	17,21,27	2.37	5 (29%)
5	QVS	A	319	8,4,6	15,15,16	2.01	2 (13%)	17,21,23	1.98	4 (23%)
6	QVE	A	320	8,3,5,4	13,16,20	1.14	1 (7%)	16,23,28	2.01	3 (18%)
7	GOL	B	302[A]	-	5,5,5	0.48	0	5,5,5	0.88	0
7	GOL	B	302[B]	-	5,5,5	0.27	0	5,5,5	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	B	303	-	5,5,5	0.19	0	5,5,5	0.33	0
7	GOL	B	304	-	5,5,5	0.21	0	5,5,5	0.18	0
7	GOL	B	305	-	5,5,5	0.40	0	5,5,5	0.56	0
3	6H0	B	311	8,2	29,29,29	2.66	5 (17%)	37,38,38	2.09	7 (18%)
8	QUJ	B	312	3,4	19,19,20	1.68	2 (10%)	21,26,28	2.76	6 (28%)
4	QUK	B	313	8,5	18,18,20	2.04	2 (11%)	19,24,27	2.24	4 (21%)
5	QVS	B	314	4,6	15,15,16	1.84	3 (20%)	17,21,23	2.99	5 (29%)
6	QVE	B	315	5	14,20,20	0.88	1 (7%)	18,28,28	2.61	5 (27%)
3	6H0	B	316	8,6	2,2,29	0.56	0	1,1,38	0.64	0
8	QUJ	B	317	3,5,4,6	19,19,20	1.84	2 (10%)	21,26,28	1.61	3 (14%)
4	QUK	B	318	8,5,4,6	15,15,20	2.09	1 (6%)	17,21,27	2.77	4 (23%)
5	QVS	B	319	8,4,6	15,15,16	2.06	3 (20%)	17,21,23	2.01	2 (11%)
6	QVE	B	320	8,3,5	14,20,20	1.03	1 (7%)	18,28,28	1.97	7 (38%)

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
7	GOL	A	302	-	-	0/4/4/4	0/0/0/0
7	GOL	A	303	-	-	0/4/4/4	0/0/0/0
7	GOL	A	304	-	-	0/4/4/4	0/0/0/0
3	6H0	A	311	8,2	-	0/23/23/23	0/2/2/2
8	QUJ	A	312	3,4	-	0/7/7/9	0/2/2/2
4	QUK	A	313	8,5	-	0/6/6/9	0/2/2/2
5	QVS	A	314	4,6	-	0/2/2/4	0/2/2/2
6	QVE	A	315	5	-	0/3/9/9	0/2/2/2
3	6H0	A	316	8,6	-	0/0/0/23	0/0/0/2
8	QUJ	A	317	3,5,4,6	-	0/2/2/9	0/2/2/2
4	QUK	A	318	8,5,4	-	0/2/2/9	0/2/2/2
5	QVS	A	319	8,4,6	-	0/2/2/4	0/2/2/2
6	QVE	A	320	8,3,5,4	-	0/0/4/9	0/2/2/2
7	GOL	B	302[A]	-	-	0/4/4/4	0/0/0/0
7	GOL	B	302[B]	-	-	0/4/4/4	0/0/0/0
7	GOL	B	303	-	-	0/4/4/4	0/0/0/0
7	GOL	B	304	-	-	0/4/4/4	0/0/0/0
7	GOL	B	305	-	-	0/4/4/4	0/0/0/0
3	6H0	B	311	8,2	-	0/23/23/23	0/2/2/2
8	QUJ	B	312	3,4	-	0/7/7/9	0/2/2/2
4	QUK	B	313	8,5	-	0/6/6/9	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	QVS	B	314	4,6	-	0/2/2/4	0/2/2/2
6	QVE	B	315	5	-	0/3/9/9	0/2/2/2
3	6H0	B	316	8,6	-	0/0/0/23	0/0/0/2
8	QUJ	B	317	3,5,4,6	-	0/7/7/9	0/2/2/2
4	QUK	B	318	8,5,4,6	-	0/2/2/9	0/2/2/2
5	QVS	B	319	8,4,6	-	0/2/2/4	0/2/2/2
6	QVE	B	320	8,3,5	-	0/3/9/9	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	313	QUK	C10-C	-7.41	1.39	1.48
4	A	318	QUK	C10-C	-7.06	1.39	1.48
4	B	318	QUK	C10-C	-6.80	1.39	1.48
8	B	317	QUJ	C10-C	-6.78	1.39	1.48
5	A	314	QVS	C10-C	-6.61	1.40	1.48
5	A	319	QVS	C10-C	-6.42	1.40	1.48
5	B	319	QVS	C10-C	-6.36	1.40	1.48
8	A	312	QUJ	C10-C	-6.28	1.40	1.48
8	A	317	QUJ	C10-C	-6.06	1.40	1.48
8	B	312	QUJ	C10-C	-6.03	1.40	1.48
5	B	314	QVS	C10-C	-5.90	1.41	1.48
4	A	313	QUK	C10-C	-5.48	1.41	1.48
3	B	311	6H0	C14-C12	-4.57	1.41	1.51
3	A	311	6H0	C14-C12	-4.23	1.41	1.51
3	A	311	6H0	C21-S24	-4.23	1.70	1.77
3	A	311	6H0	C18-C16	-3.29	1.43	1.50
3	B	311	6H0	C18-C16	-3.10	1.43	1.50
6	B	320	QVE	C2-C7	-2.30	1.37	1.42
5	B	319	QVS	C8-C6	-2.28	1.38	1.43
5	A	319	QVS	C8-C6	-2.20	1.38	1.43
6	A	320	QVE	C2-C7	-2.09	1.38	1.42
4	A	318	QUK	C2-C7	-2.07	1.38	1.42
8	A	317	QUJ	C8-C6	-2.01	1.39	1.43
6	B	315	QVE	C10-N11	2.00	1.36	1.33
5	B	314	QVS	C4-C5	2.00	1.41	1.36
4	A	318	QUK	C10-N11	2.04	1.35	1.33
3	B	311	6H0	C14-N15	2.10	1.50	1.46
8	B	317	QUJ	C10-N11	2.14	1.35	1.33
8	A	312	QUJ	C10-N11	2.55	1.36	1.33
4	A	313	QUK	C10-N11	2.55	1.36	1.33
5	B	314	QVS	C10-N11	2.68	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	317	QUJ	C10-N11	2.72	1.36	1.33
5	B	319	QVS	C10-N11	2.75	1.36	1.33
8	B	312	QUJ	C10-N11	3.20	1.36	1.33
4	B	313	QUK	C10-N11	3.57	1.37	1.33
3	A	311	6H0	O27-S24	6.72	1.52	1.43
3	A	311	6H0	O25-S24	8.62	1.54	1.43
3	B	311	6H0	O27-S24	8.81	1.54	1.43
3	B	311	6H0	O25-S24	8.83	1.54	1.43

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	311	6H0	O27-S24-O25	-11.02	104.06	118.87
8	A	312	QUJ	O-C-C10	-6.13	119.34	124.47
3	B	311	6H0	O27-S24-O25	-6.07	110.71	118.87
4	B	313	QUK	O-C-C10	-5.73	119.67	124.47
4	A	313	QUK	O-C-C10	-5.62	119.77	124.47
8	B	312	QUJ	O-C-C10	-5.30	120.03	124.47
5	A	314	QVS	O-C-C10	-5.10	120.20	124.47
5	B	314	QVS	O-C-C10	-5.06	120.23	124.47
6	B	315	QVE	C9-C10-N11	-4.60	118.54	122.24
3	B	311	6H0	O25-S24-N26	-3.75	102.59	107.25
4	A	318	QUK	O-C-C10	-3.47	121.57	124.47
6	A	315	QVE	C9-C10-N11	-3.33	119.56	122.24
6	A	320	QVE	C9-C10-N11	-3.28	119.59	122.24
6	B	320	QVE	CG-OB-C8	-2.99	113.02	117.56
6	B	320	QVE	C9-C10-N11	-2.77	120.01	122.24
8	B	317	QUJ	O-C-C10	-2.74	122.18	124.47
5	A	319	QVS	O-C-C10	-2.69	122.22	124.47
3	B	311	6H0	C23-C18-C19	-2.46	115.25	118.61
3	B	311	6H0	O1-C2-N3	-2.34	122.09	124.90
8	B	312	QUJ	C6-C7-N11	-2.27	117.82	123.03
6	B	320	QVE	OB-C8-C9	-2.18	117.27	124.72
3	A	311	6H0	C23-C18-C19	-2.16	115.66	118.61
4	B	318	QUK	O-C-C10	-2.08	122.73	124.47
5	B	314	QVS	C6-C7-N11	-2.04	118.36	123.03
4	A	313	QUK	C6-C7-N11	-2.00	118.45	123.03
6	A	315	QVE	C3-C2-N	2.02	125.06	120.39
3	B	311	6H0	C20-C19-C18	2.06	123.19	120.76
4	A	313	QUK	C3-C2-N	2.07	125.17	120.39
6	B	315	QVE	OB-C8-C6	2.08	120.69	114.94
5	A	319	QVS	C3-C2-N	2.10	125.25	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	313	QUK	CG-OB-C8	2.13	124.98	117.77
8	B	312	QUJ	C3-C2-N	2.17	125.41	120.39
8	A	312	QUJ	C3-C2-N	2.22	125.53	120.39
4	B	313	QUK	C3-C2-N	2.23	125.55	120.39
5	B	319	QVS	C9-C10-C	2.31	122.82	121.49
6	B	315	QVE	C3-C2-N	2.37	125.87	120.39
6	B	320	QVE	OB-CG-CD	2.38	112.93	108.01
6	B	315	QVE	CG-OB-C8	2.48	121.33	117.56
4	A	318	QUK	C3-C2-N	2.49	126.15	120.39
4	B	318	QUK	OB-C8-C6	2.52	119.79	116.18
4	A	313	QUK	C9-C10-C	2.58	122.97	121.49
5	A	319	QVS	C9-C10-C	2.59	122.98	121.49
6	B	320	QVE	C3-C2-N	2.60	126.40	120.39
8	B	312	QUJ	CG-OB-C8	2.64	127.09	118.25
4	A	318	QUK	OB-C8-C6	2.71	120.06	116.18
6	A	315	QVE	OB-C8-C6	2.71	122.41	114.94
4	A	313	QUK	CG-OB-C8	2.76	127.11	117.77
5	B	314	QVS	C9-C10-C	2.79	123.09	121.49
6	A	315	QVE	CG-OB-C8	3.07	122.24	117.56
3	B	311	6H0	C21-S24-N26	3.12	112.25	108.33
5	B	314	QVS	C3-C2-N	3.16	127.69	120.39
6	B	320	QVE	OB-C8-C6	3.28	123.97	114.94
8	A	312	QUJ	C9-C10-C	3.31	123.39	121.49
6	A	320	QVE	OB-C8-C6	3.38	121.03	116.18
5	A	314	QVS	C3-C2-N	3.51	128.52	120.39
8	B	312	QUJ	C9-C10-C	3.82	123.69	121.49
8	B	317	QUJ	C9-C10-C	3.99	123.79	121.49
8	A	317	QUJ	C9-C10-C	4.17	123.89	121.49
6	B	320	QVE	C10-N11-C7	4.53	120.92	118.26
8	B	317	QUJ	C10-N11-C7	4.57	121.23	118.04
5	A	314	QVS	C9-C10-C	4.96	124.35	121.49
4	A	318	QUK	C10-N11-C7	5.09	121.60	118.04
6	A	320	QVE	C10-N11-C7	5.62	121.56	118.26
4	A	318	QUK	C9-C10-C	6.20	125.06	121.49
6	A	315	QVE	C10-N11-C7	6.40	122.01	118.26
8	A	317	QUJ	C10-N11-C7	6.51	122.58	118.04
4	B	313	QUK	C10-N11-C7	6.57	122.63	118.04
5	A	319	QVS	C10-N11-C7	6.61	122.66	118.04
4	B	318	QUK	C10-N11-C7	6.65	122.68	118.04
5	B	319	QVS	C10-N11-C7	7.17	123.05	118.04
3	B	311	6H0	O27-S24-N26	7.51	116.57	107.25
4	B	318	QUK	C9-C10-C	8.17	126.20	121.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	312	QUJ	C10-N11-C7	8.49	123.97	118.04
6	B	315	QVE	C10-N11-C7	8.68	123.35	118.26
4	A	313	QUK	C10-N11-C7	9.11	124.40	118.04
5	A	314	QVS	C10-N11-C7	9.68	124.80	118.04
8	B	312	QUJ	C10-N11-C7	9.82	124.90	118.04
5	B	314	QVS	C10-N11-C7	9.89	124.95	118.04
3	A	311	6H0	O27-S24-N26	10.46	120.23	107.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	316	6H0	5	0
8	A	317	QUJ	1	0
4	A	318	QUK	1	0
5	A	319	QVS	6	0
6	A	320	QVE	5	0
7	B	302[A]	GOL	1	0
7	B	302[B]	GOL	2	0
4	B	318	QUK	4	0
5	B	319	QVS	5	0
6	B	320	QVE	7	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 [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<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	259/260 (99%)	0.02	0	100   100	27, 42, 67, 89	0
1	B	259/260 (99%)	0.08	1 (0%)	93   94	29, 41, 62, 79	0
All	All	518/520 (99%)	0.05	1 (0%)	95   95	27, 42, 66, 89	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	HIS	2.1

### 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
7	GOL	A	304	6/6	0.82	0.21	10.02	50,65,70,72	0
7	GOL	B	302[B]	6/6	0.85	0.25	7.64	25,28,31,39	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	GOL	B	302[A]	6/6	0.85	0.25	7.50	18,23,28,28	6
7	GOL	B	304	6/6	0.81	0.23	7.23	44,52,66,68	0
7	GOL	B	305	6/6	0.82	0.24	5.31	50,55,67,72	0
7	GOL	A	302	6/6	0.89	0.17	4.86	22,28,32,53	0
7	GOL	B	303	6/6	0.87	0.21	1.98	53,58,70,73	0
7	GOL	A	303	6/6	0.86	0.14	1.09	50,61,64,66	0
3	6H0	A	311	28/28	0.97	0.12	0.84	25,35,44,44	0
3	6H0	B	311	28/28	0.96	0.12	-0.21	25,37,45,49	0
5	QVS	A	314	14/15	0.90	0.09	-1.27	38,45,49,51	0
5	QVS	B	314	14/15	0.94	0.09	-1.44	29,35,41,41	0
5	QVS	B	319	14/15	0.96	0.10	-	26,36,44,45	14
4	QUK	B	313	17/19	0.92	0.10	-	32,37,50,52	0
6	QVE	B	320	19/19	0.93	0.12	-	27,34,49,50	19
4	QUK	A	313	17/19	0.95	0.10	-	31,40,52,55	0
6	QVE	A	315	19/19	0.95	0.09	-	34,39,68,80	0
4	QUK	B	318	14/19	0.90	0.12	-	29,33,42,44	14
8	QUJ	B	312	18/19	0.97	0.12	-	30,36,76,80	0
6	QVE	B	315	19/19	0.95	0.10	-	31,36,69,89	0
2	ZN	B	301	1/1	1.00	0.12	-	32,32,32,32	0
6	QVE	A	320	15/19	0.92	0.12	-	38,41,47,49	15
8	QUJ	B	317	18/19	0.93	0.14	-	25,30,35,36	18
2	ZN	A	301	1/1	0.99	0.13	-	29,29,29,29	0
8	QUJ	A	312	18/19	0.95	0.11	-	31,35,63,66	0
3	6H0	A	316	3/28	0.99	0.23	-	34,34,36,37	3
5	QVS	A	319	14/15	0.92	0.12	-	39,44,54,55	14
4	QUK	A	318	14/19	0.96	0.10	-	33,39,47,48	14
3	6H0	B	316	3/28	0.86	0.14	-	34,34,37,38	3
8	QUJ	A	317	14/19	0.94	0.09	-	37,42,45,52	14

## 6.5 Other polymers ⓘ

There are no such residues in this entry.