



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2017 – 02:47 PM EST

PDB ID : 5L6K  
Title : CRYSTAL STRUCTURE OF HUMAN CARBONIC ANHYDRASE II IN  
COMPLEX WITH A QUINOLINE OLIGOAMIDE FOLDAMER  
Authors : JEWGINSKI, M.; LANGLOIS D'ESTAINOT, B.; GRANIER, T.; HUC, Y.  
Deposited on : 2016-05-30  
Resolution : 1.70 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

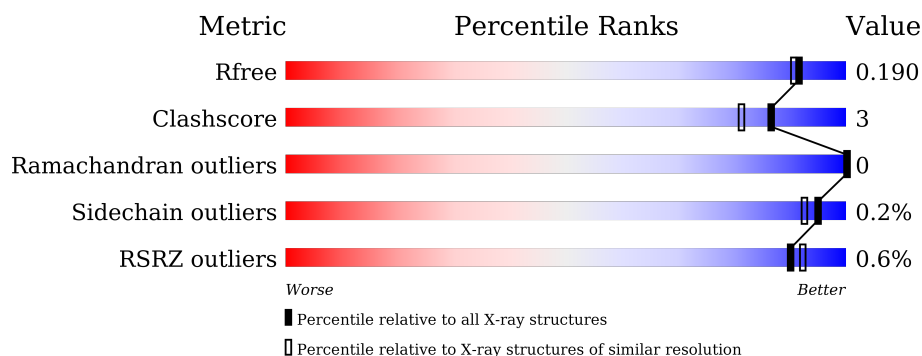
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

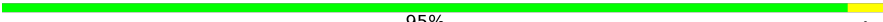
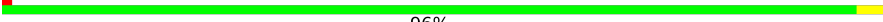
The reported resolution of this entry is 1.70 Å.

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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	 95% .
1	B	260	 96% .

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	312	-	-	X	-
6	QVE	A	307	-	-	X	-
7	GOL	A	308	-	-	-	X
7	GOL	A	309	-	-	-	X
7	GOL	B	312	-	-	-	X
7	GOL	B	313	-	-	-	X

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 4929 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.

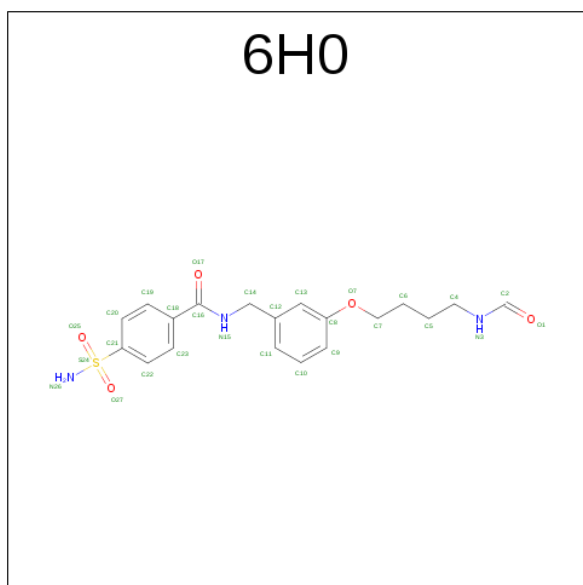
- Molecule 1 is a protein called Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	8	0
			2094	1351	358	383	2			
1	B	259	Total	C	N	O	S	0	6	0
			2081	1342	355	382	2			

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

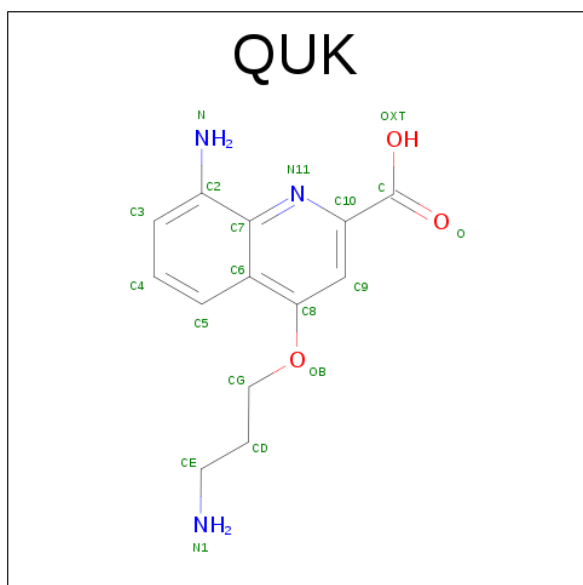
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- 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).



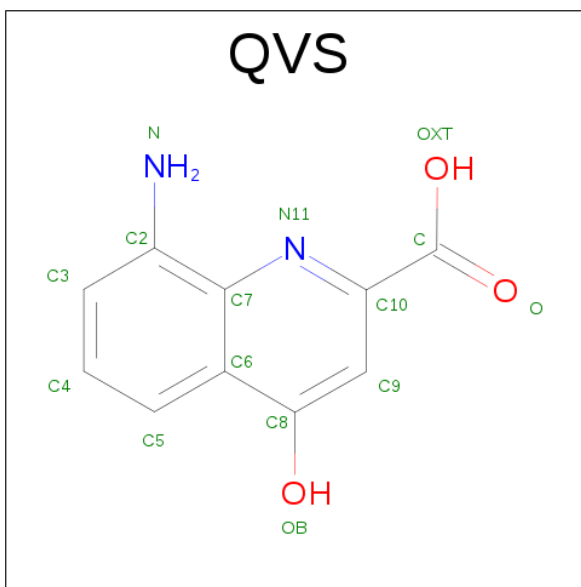
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 19	N 3	O 5	S 1	0	0
3	B	1	Total 28	C 19	N 3	O 5	S 1	0	0

- Molecule 4 is 8-azanyl-4-(3-azanylpropoxy)quinoline-2-carboxylic acid (three-letter code: QUK) (formula:  $\text{C}_{13}\text{H}_{15}\text{N}_3\text{O}_3$ ).



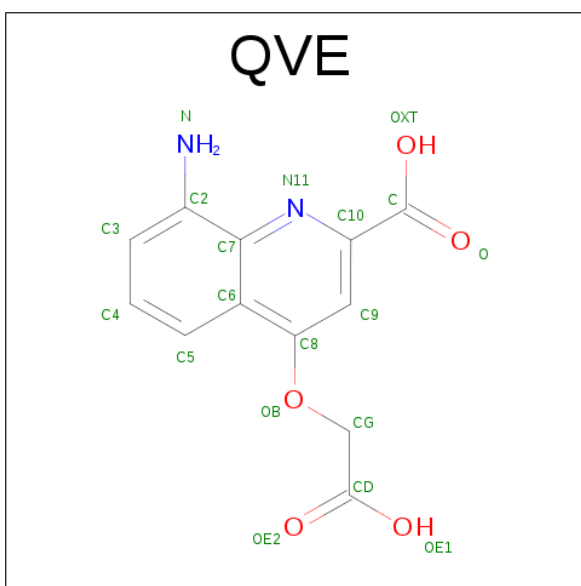
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 17	C 13	N 2	O 2	0	0
4	A	1	Total 14	C 10	N 2	O 2	0	0
4	B	1	Total 17	C 13	N 2	O 2	0	0
4	B	1	Total 14	C 10	N 2	O 2	0	0

- Molecule 5 is 8-azanyl-4-oxidanyl-quinoline-2-carboxylic acid (three-letter code: QVS) (formula:  $\text{C}_{10}\text{H}_8\text{N}_2\text{O}_3$ ).



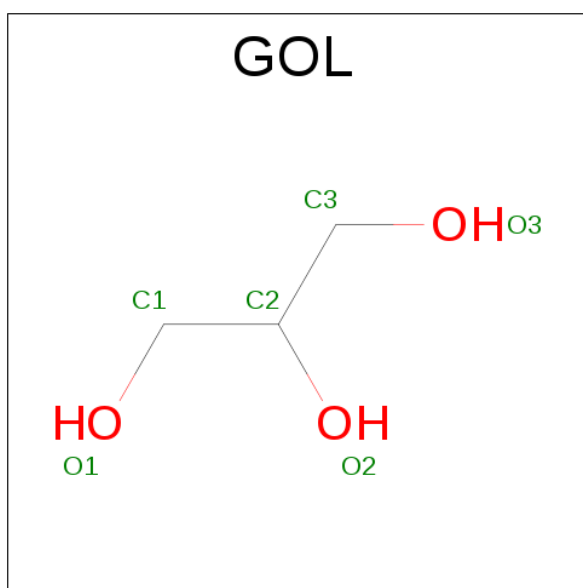
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	10	2	2		
5	A	1	Total	C	N	O	0	0
			14	10	2	2		
5	B	1	Total	C	N	O	0	0
			14	10	2	2		
5	B	1	Total	C	N	O	0	0
			14	10	2	2		

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



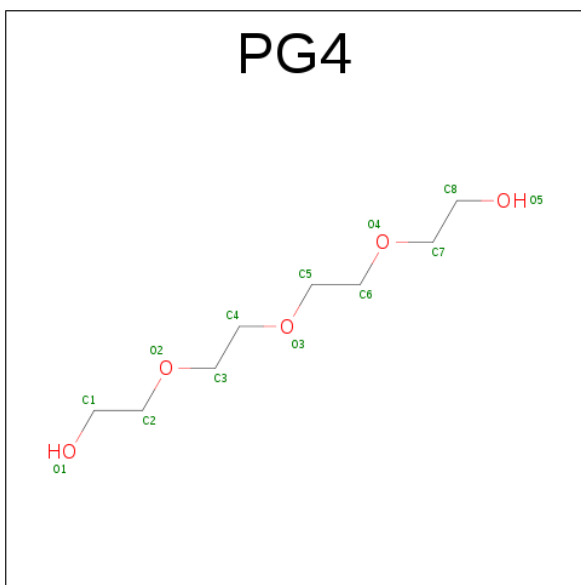
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			19	12	2	5		
6	A	1	Total	C	N	O	0	0
			19	12	2	5		
6	B	1	Total	C	N	O	0	0
			19	12	2	5		
6	B	1	Total	C	N	O	0	0
			15	10	2	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



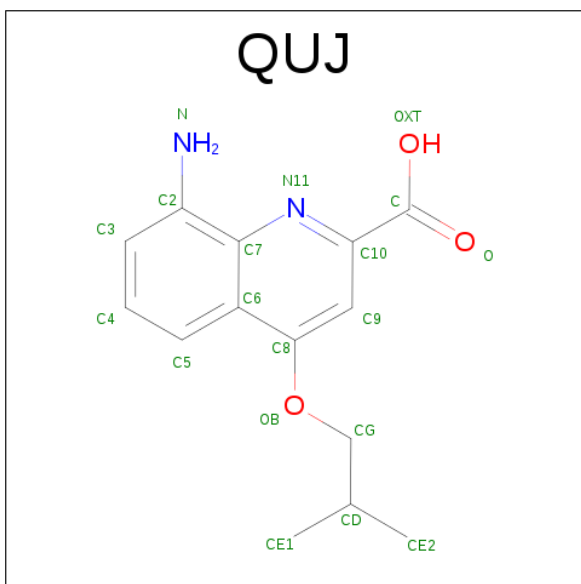
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is 8-azanyl-4-(2-methylpropoxy)quinoline-2-carboxylic acid (three-letter code: QUJ) (formula:  $C_{14}H_{16}N_2O_3$ ).



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

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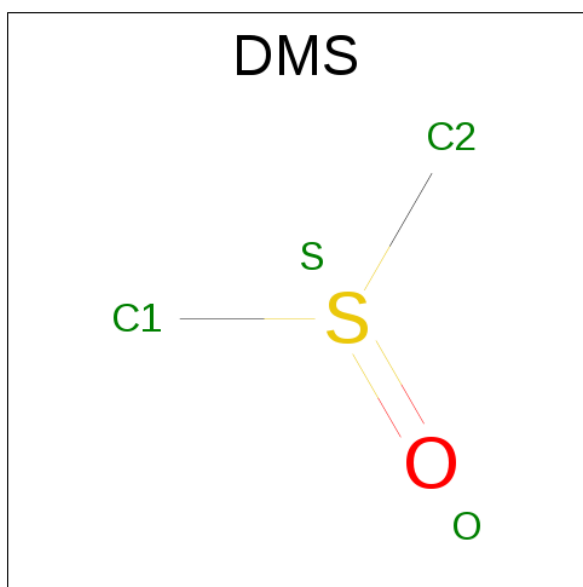
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			17	13	2	2		
9	B	1	Total	C	N	O	0	0
			17	13	2	2		
9	B	1	Total	C	N	O	0	0
			18	14	2	2		

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Na	0	0
			1	1		

- Molecule 11 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	229	Total	O	0	0
			229	229		
12	B	168	Total	O	0	0
			168	168		

### 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 ( $\text{RSRZ} > 2$ ). 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.

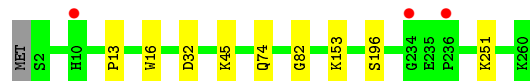
- Molecule 1: Carbonic anhydrase 2

Chain A:  95% .



- Molecule 1: Carbonic anhydrase 2

Chain B:  96% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.07Å 84.87Å 77.22Å 90.00° 97.81° 90.00°	Depositor
Resolution (Å)	76.50 – 1.70 56.82 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (76.50-1.70) 99.7 (56.82-1.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.154 , 0.181 0.163 , 0.190	Depositor DCC
$R_{free}$ test set	3137 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4929	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% 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: GOL, ZN, NA, 6H0, PG4, DMS, QVE, 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	0.89	2/2178 (0.1%)	0.96	3/2956 (0.1%)
1	B	0.82	1/2162 (0.0%)	0.91	0/2934
All	All	0.86	3/4340 (0.1%)	0.94	3/5890 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	196	SER	CA-CB	5.89	1.61	1.52
1	A	219	SER	CB-OG	-5.06	1.35	1.42
1	A	51	TYR	CG-CD1	5.00	1.45	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	51	TYR	CB-CG-CD1	5.19	124.11	121.00
1	A	138	ASP	CB-CG-OD1	5.09	122.88	118.30

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	2094	0	2043	7	0
1	B	2081	0	2042	4	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	0	0	0
3	B	28	0	0	0	0
4	A	31	0	0	0	0
4	B	31	0	0	0	0
5	A	28	0	0	7	0
5	B	28	0	0	2	0
6	A	38	0	0	7	0
6	B	34	0	0	0	0
7	A	12	0	16	0	0
7	B	12	0	16	0	0
8	A	3	0	0	3	0
8	B	7	0	6	2	0
9	A	35	0	0	2	0
9	B	35	0	0	0	0
10	A	1	0	0	0	0
11	A	4	0	6	0	0
12	A	229	0	0	6	0
12	B	168	0	0	1	0
All	All	4929	0	4129	23	1

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 3.

All (23) 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)
6:A:307:QVE:CG	9:A:311:QUJ:C3	2.30	0.86
8:A:310:PG4:C2	5:A:312:QVS:C3	2.60	0.80
8:A:310:PG4:C2	5:A:312:QVS:C2	2.65	0.75
1:A:17[A]:HIS:HE1	12:A:408:HOH:O	1.74	0.71
6:A:307:QVE:C	5:A:312:QVS:C2	2.69	0.70
6:A:307:QVE:OXT	5:A:312:QVS:C2	2.41	0.69
1:A:45:LYS:NZ	12:A:403:HOH:O	2.29	0.66
6:A:307:QVE:C	5:A:312:QVS:C7	2.75	0.64
1:A:135:GLN:NE2	12:A:404:HOH:O	2.32	0.62
8:B:302:PG4:H21	5:B:304:QVS:C3	2.31	0.59
8:A:310:PG4:C2	12:A:465:HOH:O	2.50	0.57
1:B:251:LYS:NZ	12:B:401:HOH:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:307:QVE:OXT	5:A:312:QVS:N	2.44	0.51
8:B:302:PG4:H21	5:B:304:QVS:C2	2.42	0.49
1:A:89:ARG:O	1:A:122:HIS:HA	2.16	0.45
6:A:307:QVE:OE1	9:A:311:QUJ:C4	2.65	0.45
1:A:138:ASP:HA	12:A:468:HOH:O	2.19	0.42
1:A:80:LYS:HE2	12:A:456:HOH:O	2.20	0.41
1:B:13:PRO:HA	1:B:16:TRP:CD2	2.55	0.41
6:A:307:QVE:C10	5:A:312:QVS:C7	2.99	0.41
1:A:239:LEU:HD22	1:A:239:LEU:N	2.36	0.41
1:B:45:LYS:O	1:B:82:GLY:HA2	2.21	0.41

All (1) 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)
1:B:32:ASP:OD2	1:B:74:GLN:NE2[1_655]	2.18	0.02

## 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	265/260 (102%)	260 (98%)	5 (2%)	0	100	100
1	B	263/260 (101%)	257 (98%)	6 (2%)	0	100	100
All	All	528/520 (102%)	517 (98%)	11 (2%)	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	225/225 (100%)	224 (100%)	1 (0%)	93	90
1	B	227/225 (101%)	227 (100%)	0	100	100
All	All	452/450 (100%)	451 (100%)	1 (0%)	95	92

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

Mol	Chain	Res	Type
1	A	21	PRO

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 28 ligands modelled in this entry, 3 are monoatomic - leaving 25 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	6H0	A	302	9,2	29,29,29	1.80	4 (13%)	37,38,38	2.12	6 (16%)
4	QUK	A	303	9,5	18,18,20	1.53	2 (11%)	19,24,27	2.25	4 (21%)
5	QVS	A	304	4,6	15,15,16	1.90	1 (6%)	17,21,23	2.43	3 (17%)
6	QVE	A	305	5	14,20,20	0.89	0	18,28,28	2.85	4 (22%)
4	QUK	A	306	9,5,4,6	15,15,20	1.84	2 (13%)	17,21,27	2.56	4 (23%)
6	QVE	A	307	9,8,5,4	14,20,20	1.05	0	18,28,28	1.62	5 (27%)
7	GOL	A	308	-	5,5,5	0.23	0	5,5,5	0.29	0
7	GOL	A	309	-	5,5,5	0.53	0	5,5,5	0.83	0
8	PG4	A	310	9,6	2,2,12	1.49	0	1,1,11	0.65	0
9	QUJ	A	311	8,5,4,6	19,19,20	1.94	1 (5%)	21,26,28	1.88	6 (28%)
5	QVS	A	312	9,4,6	15,15,16	1.99	1 (6%)	17,21,23	1.80	2 (11%)
11	DMS	A	314	-	3,3,3	0.45	0	3,3,3	0.79	0
9	QUJ	A	315	3,4	18,18,20	1.69	2 (11%)	19,24,28	2.97	5 (26%)
9	QUJ	B	301	3,4	18,18,20	1.65	2 (11%)	19,24,28	2.22	3 (15%)
8	PG4	B	302	9,6	6,6,12	1.44	1 (16%)	5,5,11	1.30	0
9	QUJ	B	303	8,5,4,6	19,19,20	1.83	2 (10%)	21,26,28	2.07	3 (14%)
5	QVS	B	304	9,4,6	15,15,16	1.88	1 (6%)	17,21,23	1.95	4 (23%)
3	6H0	B	306	9,2	29,29,29	1.61	6 (20%)	37,38,38	1.26	3 (8%)
4	QUK	B	307	9,5	18,18,20	1.41	1 (5%)	19,24,27	2.48	4 (21%)
5	QVS	B	308	4,6	15,15,16	1.62	1 (6%)	17,21,23	2.22	4 (23%)
6	QVE	B	309	5	14,20,20	0.89	0	18,28,28	2.35	5 (27%)
4	QUK	B	310	9,5,4,6	15,15,20	2.12	1 (6%)	17,21,27	2.38	3 (17%)
6	QVE	B	311	9,8,5,4	13,16,20	1.05	0	16,23,28	1.90	3 (18%)
7	GOL	B	312	-	5,5,5	0.17	0	5,5,5	0.94	0
7	GOL	B	313	-	5,5,5	0.21	0	5,5,5	0.84	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
3	6H0	A	302	9,2	-	0/23/23/23	0/2/2/2
4	QUK	A	303	9,5	-	0/6/6/9	0/2/2/2
5	QVS	A	304	4,6	-	0/2/2/4	0/2/2/2
6	QVE	A	305	5	-	0/3/9/9	0/2/2/2
4	QUK	A	306	9,5,4,6	-	0/2/2/9	0/2/2/2
6	QVE	A	307	9,8,5,4	-	0/3/9/9	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	308	-	-	0/4/4/4	0/0/0/0
7	GOL	A	309	-	-	0/4/4/4	0/0/0/0
8	PG4	A	310	9,6	-	0/0/0/10	0/0/0/0
9	QUJ	A	311	8,5,4,6	-	0/7/7/9	0/2/2/2
5	QVS	A	312	9,4,6	-	0/2/2/4	0/2/2/2
11	DMS	A	314	-	-	0/0/0/0	0/0/0/0
9	QUJ	A	315	3,4	-	0/6/6/9	0/2/2/2
9	QUJ	B	301	3,4	-	0/6/6/9	0/2/2/2
8	PG4	B	302	9,6	-	0/4/4/10	0/0/0/0
9	QUJ	B	303	8,5,4,6	-	0/7/7/9	0/2/2/2
5	QVS	B	304	9,4,6	-	0/2/2/4	0/2/2/2
3	6H0	B	306	9,2	-	0/23/23/23	0/2/2/2
4	QUK	B	307	9,5	-	0/6/6/9	0/2/2/2
5	QVS	B	308	4,6	-	0/2/2/4	0/2/2/2
6	QVE	B	309	5	-	0/3/9/9	0/2/2/2
4	QUK	B	310	9,5,4,6	-	0/2/2/9	0/2/2/2
6	QVE	B	311	9,8,5,4	-	0/0/4/9	0/2/2/2
7	GOL	B	312	-	-	0/4/4/4	0/0/0/0
7	GOL	B	313	-	-	0/4/4/4	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	311	QUJ	C10-C	-7.30	1.39	1.48
4	B	310	QUK	C10-C	-7.04	1.39	1.48
5	A	304	QVS	C10-C	-6.65	1.40	1.48
9	B	303	QUJ	C10-C	-6.60	1.40	1.48
5	A	312	QVS	C10-C	-6.27	1.40	1.48
5	B	304	QVS	C10-C	-6.17	1.40	1.48
9	A	315	QUJ	C10-C	-6.05	1.40	1.48
9	B	301	QUJ	C10-C	-5.97	1.40	1.48
4	A	306	QUK	C10-C	-5.85	1.41	1.48
5	B	308	QVS	C10-C	-5.30	1.41	1.48
4	A	303	QUK	C10-C	-5.27	1.41	1.48
4	B	307	QUK	C10-C	-4.63	1.42	1.48
3	A	302	6H0	C14-C12	-3.61	1.43	1.51
3	B	306	6H0	C14-C12	-3.44	1.43	1.51
8	B	302	PG4	O1-C1	-3.44	1.23	1.42
3	B	306	6H0	C18-C16	-3.16	1.43	1.50
3	A	302	6H0	S24-N26	-2.84	1.55	1.60
3	A	302	6H0	C18-C16	-2.36	1.45	1.50
4	A	306	QUK	C10-N11	2.05	1.35	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	301	QUJ	C10-N11	2.06	1.35	1.33
3	B	306	6H0	O27-S24	2.18	1.46	1.43
9	B	303	QUJ	C10-N11	2.18	1.35	1.33
3	B	306	6H0	C14-N15	2.23	1.50	1.46
3	B	306	6H0	C23-C18	2.39	1.43	1.39
4	A	303	QUK	C10-N11	2.40	1.35	1.33
9	A	315	QUJ	C10-N11	2.73	1.36	1.33
3	B	306	6H0	O25-S24	4.90	1.50	1.43
3	A	302	6H0	O25-S24	6.52	1.52	1.43

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	315	QUJ	O-C-C10	-6.32	119.18	124.47
3	A	302	6H0	O27-S24-O25	-5.99	110.83	118.87
5	A	304	QVS	O-C-C10	-5.78	119.63	124.47
6	B	309	QVE	C9-C10-N11	-5.00	118.21	122.24
6	A	305	QVE	C9-C10-N11	-4.96	118.24	122.24
9	B	301	QUJ	O-C-C10	-4.83	120.43	124.47
5	B	308	QVS	O-C-C10	-4.79	120.46	124.47
3	A	302	6H0	C23-C22-C21	-4.62	114.56	119.49
9	A	311	QUJ	O-C-C10	-4.21	120.95	124.47
4	B	307	QUK	O-C-C10	-3.99	121.13	124.47
4	A	303	QUK	O-C-C10	-3.39	121.64	124.47
4	A	306	QUK	O-C-C10	-3.31	121.70	124.47
9	B	303	QUJ	O-C-C10	-3.17	121.82	124.47
6	A	307	QVE	C9-C10-N11	-3.16	119.70	122.24
5	B	304	QVS	O-C-C10	-3.01	121.95	124.47
6	B	311	QVE	C9-C10-N11	-2.69	120.07	122.24
3	B	306	6H0	O1-C2-N3	-2.43	121.99	124.90
9	A	315	QUJ	C6-C7-N11	-2.39	117.56	123.03
3	A	302	6H0	C20-C19-C18	-2.24	118.11	120.76
3	B	306	6H0	O27-S24-C21	-2.11	105.03	107.41
9	A	311	QUJ	OB-C8-C9	-2.04	117.74	124.72
6	B	309	QVE	OB-CG-CD	2.04	112.22	108.01
9	A	311	QUJ	C9-C10-C	2.07	122.68	121.49
5	A	312	QVS	C3-C2-N	2.10	125.24	120.39
5	B	304	QVS	OB-C8-C6	2.17	119.29	116.18
5	B	308	QVS	OB-C8-C6	2.18	119.31	116.18
6	A	307	QVE	C3-C2-N	2.20	125.47	120.39
4	A	303	QUK	CG-OB-C8	2.26	125.40	117.77
6	B	309	QVE	CG-OB-C8	2.31	121.08	117.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	311	QUJ	OB-CG-CD	2.31	119.06	108.57
6	A	305	QVE	C3-C2-N	2.36	125.84	120.39
9	A	315	QUJ	C3-C2-N	2.45	126.06	120.39
9	A	315	QUJ	C9-C10-C	2.46	122.91	121.49
6	A	307	QVE	OB-C8-C6	2.49	121.81	114.94
5	B	304	QVS	C3-C2-N	2.53	126.23	120.39
9	B	301	QUJ	C3-C2-N	2.57	126.32	120.39
6	A	307	QVE	CG-OB-C8	2.59	121.50	117.56
4	B	307	QUK	C9-C10-C	2.64	123.01	121.49
4	B	310	QUK	OB-C8-C6	2.73	120.10	116.18
4	B	307	QUK	C3-C2-N	2.78	126.83	120.39
6	B	309	QVE	C3-C2-N	2.83	126.94	120.39
3	A	302	6H0	C19-C20-C21	3.00	122.69	119.49
4	A	303	QUK	C3-C2-N	3.03	127.40	120.39
6	A	307	QVE	C10-N11-C7	3.12	120.09	118.26
4	A	306	QUK	OB-C8-C6	3.44	121.12	116.18
5	B	308	QVS	C3-C2-N	3.48	128.44	120.39
5	A	304	QVS	C3-C2-N	3.55	128.59	120.39
6	B	311	QVE	OB-C8-C6	3.67	121.45	116.18
3	A	302	6H0	C22-C23-C18	3.74	125.17	120.76
9	A	311	QUJ	C10-N11-C7	3.77	120.68	118.04
9	A	311	QUJ	OB-C8-C6	3.84	125.54	114.94
6	A	305	QVE	CG-OB-C8	4.31	124.12	117.56
3	B	306	6H0	O27-S24-N26	4.60	112.96	107.25
5	B	308	QVS	C10-N11-C7	4.99	121.53	118.04
6	B	311	QVE	C10-N11-C7	5.44	121.45	118.26
4	A	306	QUK	C9-C10-C	5.49	124.65	121.49
9	B	303	QUJ	C9-C10-C	5.54	124.68	121.49
4	B	310	QUK	C9-C10-C	5.99	124.94	121.49
5	B	304	QVS	C10-N11-C7	6.09	122.29	118.04
9	B	303	QUJ	C10-N11-C7	6.14	122.33	118.04
5	A	312	QVS	C10-N11-C7	6.24	122.40	118.04
4	B	310	QUK	C10-N11-C7	6.49	122.58	118.04
5	A	304	QVS	C10-N11-C7	6.50	122.58	118.04
6	B	309	QVE	C10-N11-C7	6.75	122.22	118.26
4	A	306	QUK	C10-N11-C7	6.89	122.85	118.04
9	B	301	QUJ	C10-N11-C7	7.11	123.00	118.04
3	A	302	6H0	O27-S24-N26	7.33	116.35	107.25
4	A	303	QUK	C10-N11-C7	7.85	123.52	118.04
4	B	307	QUK	C10-N11-C7	9.03	124.34	118.04
6	A	305	QVE	C10-N11-C7	9.25	123.68	118.26
9	A	315	QUJ	C10-N11-C7	10.11	125.10	118.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	307	QVE	7	0
8	A	310	PG4	3	0
9	A	311	QUJ	2	0
5	A	312	QVS	7	0
8	B	302	PG4	2	0
5	B	304	QVS	2	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%)	-0.33	0 100 100	12, 20, 39, 64	0
1	B	259/260 (99%)	-0.25	3 (1%) 81 85	14, 24, 43, 76	0
All	All	518/520 (99%)	-0.29	3 (0%) 90 92	12, 22, 42, 76	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	HIS	3.4
1	B	234	GLY	3.0
1	B	236	PRO	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( $\text{\AA}^2$ )	Q<0.9
7	GOL	B	313	6/6	0.87	0.15	14.20	30,37,54,54	0
7	GOL	B	312	6/6	0.93	0.12	5.79	25,30,31,42	0
7	GOL	A	309	6/6	0.90	0.12	3.21	24,30,37,50	0
7	GOL	A	308	6/6	0.97	0.09	3.12	16,17,19,21	0
11	DMS	A	314	4/4	0.85	0.14	1.12	30,33,54,92	0
3	6H0	B	306	28/28	0.97	0.09	0.90	15,20,33,40	0
3	6H0	A	302	28/28	0.97	0.09	0.53	10,17,24,28	0
6	QVE	B	309	19/19	0.94	0.10	-0.19	18,23,39,44	0
5	QVS	A	304	14/15	0.96	0.07	-0.61	17,19,25,25	0
5	QVS	B	308	14/15	0.97	0.07	-0.74	11,16,22,23	0
2	ZN	A	301	1/1	0.99	0.11	-	12,12,12,12	0
9	QUJ	B	303	18/19	0.91	0.12	-	13,16,23,23	18
5	QVS	B	304	14/15	0.96	0.07	-	12,18,23,26	14
9	QUJ	B	301	17/19	0.96	0.08	-	16,21,37,42	0
4	QUK	B	307	17/19	0.96	0.07	-	20,23,36,40	0
2	ZN	B	305	1/1	0.99	0.09	-	16,16,16,16	0
9	QUJ	A	315	17/19	0.93	0.10	-	19,23,40,41	0
8	PG4	A	310	3/13	0.95	0.10	-	37,37,39,45	3
9	QUJ	A	311	18/19	0.93	0.12	-	17,29,38,45	18
6	QVE	A	307	19/19	0.92	0.10	-	10,17,30,31	19
4	QUK	A	303	17/19	0.95	0.08	-	20,25,42,45	0
4	QUK	B	310	14/19	0.95	0.10	-	22,34,43,51	14
5	QVS	A	312	14/15	0.96	0.14	-	20,36,46,48	14
4	QUK	A	306	14/19	0.92	0.09	-	12,18,22,24	14
8	PG4	B	302	7/13	0.89	0.17	-	24,30,45,49	7
10	NA	A	313	1/1	0.94	0.10	-	44,44,44,44	0
6	QVE	B	311	15/19	0.96	0.10	-	22,30,40,46	15
6	QVE	A	305	19/19	0.93	0.09	-	22,28,62,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.