



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:53 AM UTC

PDB ID : 1BV3 / pdb_00001bv3
Title : HUMAN CARBONIC ANHYDRASE II COMPLEXED WITH UREA
Authors : Briganti, F.; Mangani, S.; Scozzafava, A.; Vernaglion, G.; Supuran, C.T.
Deposited on : 1998-09-22
Resolution : 1.85 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

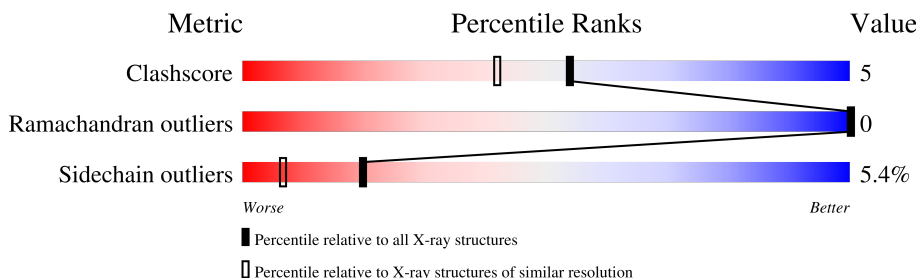
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	259	

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	HGB	A	263	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2191 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.

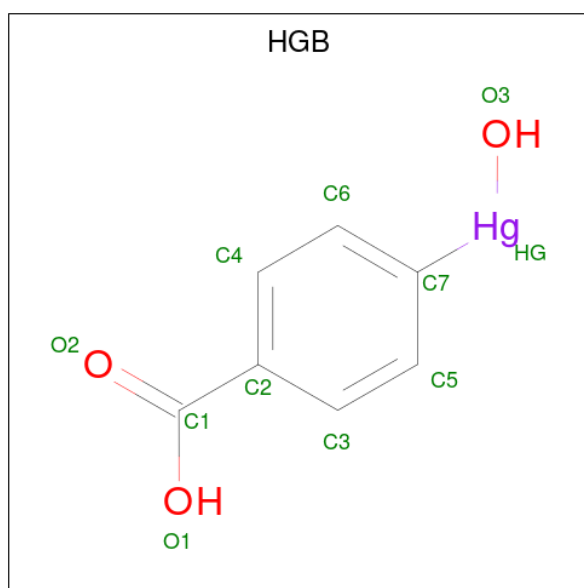
- Molecule 1 is a protein called PROTEIN (CARBONIC ANHYDRASE II).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	1	0
			2043	1312	351	378	2			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

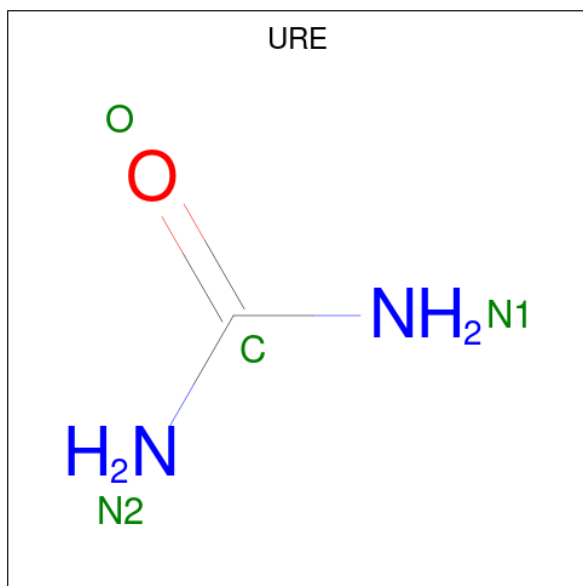
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 4-(HYDROXYMERCURY)BENZOIC ACID (CCD ID: HGB) (formula: C₇H₆HgO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Hg	O	0	0
			9	6	1	2		

- Molecule 4 is UREA (CCD ID: URE) (formula: $\text{CH}_4\text{N}_2\text{O}$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	134	Total	O	0	0
			134	134		

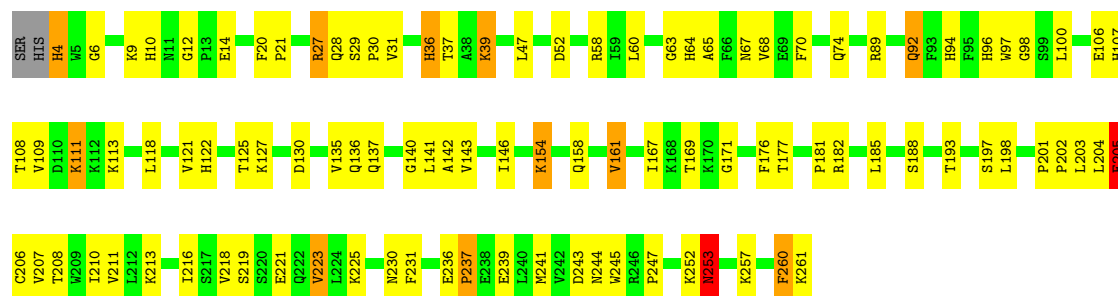
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

Note EDS was not executed.

• Molecule 1: PROTEIN (CARBONIC ANHYDRASE II)

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.82Å 42.02Å 73.03Å 90.00° 104.26° 90.00°	Depositor
Resolution (Å)	10.00 – 1.85	Depositor
% Data completeness (in resolution range)	91.8 (10.00-1.85)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CCP4	Depositor
R, R_{free}	0.171 , 0.213	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2191	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HGB, ZN, URE

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	1.33	6/2103 (0.3%)	2.35	119/2850 (4.2%)

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	A	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	THR	C-N	8.40	1.45	1.33
1	A	205	GLU	C-O	8.39	1.34	1.24
1	A	122	HIS	C-N	5.84	1.42	1.33
1	A	137	GLN	C-O	5.67	1.31	1.24
1	A	140	GLY	C-N	5.45	1.41	1.33
1	A	140	GLY	C-O	-5.14	1.17	1.24

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64[A]	HIS	N-CA-CB	22.79	149.24	110.50
1	A	64[A]	HIS	CA-CB-CG	-13.05	100.75	113.80
1	A	109	VAL	CA-C-O	-12.31	106.93	120.48
1	A	158	GLN	OE1-CD-NE2	-10.29	112.31	122.60
1	A	219	SER	CA-C-O	9.80	133.21	121.94
1	A	29	SER	O-C-N	9.64	129.54	121.35
1	A	64[A]	HIS	CB-CA-C	-9.06	92.89	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	GLY	CA-C-O	8.99	128.99	119.01
1	A	121	VAL	O-C-N	8.92	132.93	123.03
1	A	68	VAL	CA-C-O	-8.86	110.93	120.59
1	A	211	VAL	CA-C-O	-8.77	111.15	120.53
1	A	36	HIS	CA-CB-CG	-8.73	105.07	113.80
1	A	207	VAL	N-CA-C	8.68	120.32	108.17
1	A	4	HIS	CA-CB-CG	-8.53	105.28	113.80
1	A	109	VAL	O-C-N	8.32	131.89	122.99
1	A	31	VAL	CA-C-N	-8.13	110.06	122.09
1	A	31	VAL	C-N-CA	-8.13	110.06	122.09
1	A	231	PHE	CA-CB-CG	8.02	121.82	113.80
1	A	207	VAL	O-C-N	7.99	131.57	123.18
1	A	10	HIS	CA-CB-CG	-7.84	105.96	113.80
1	A	94	HIS	CG-CD2-NE2	7.84	115.04	107.20
1	A	107	HIS	O-C-N	7.76	131.63	122.79
1	A	97	TRP	CA-C-N	-7.71	114.19	122.67
1	A	97	TRP	C-N-CA	-7.71	114.19	122.67
1	A	39	LYS	CA-CB-CG	7.48	129.06	114.10
1	A	245	TRP	O-C-N	-7.32	113.30	123.11
1	A	94	HIS	CE1-NE2-CD2	-7.30	101.70	109.00
1	A	140	GLY	CA-C-O	7.27	127.87	120.09
1	A	122	HIS	CA-CB-CG	7.13	120.93	113.80
1	A	161	VAL	O-C-N	7.10	128.76	121.87
1	A	206	CYS	CA-C-O	7.07	127.82	119.48
1	A	169	THR	CA-C-O	-7.03	113.38	121.68
1	A	108	THR	CA-C-N	-6.99	113.77	123.13
1	A	108	THR	C-N-CA	-6.99	113.77	123.13
1	A	29	SER	CA-C-O	-6.97	113.48	120.66
1	A	253	ASN	CA-CB-CG	-6.88	105.72	112.60
1	A	141	LEU	O-C-N	6.87	132.08	123.15
1	A	143	VAL	O-C-N	6.81	130.62	123.26
1	A	205	GLU	CB-CA-C	6.79	123.94	110.42
1	A	207	VAL	CA-C-N	-6.78	113.76	122.77
1	A	207	VAL	C-N-CA	-6.78	113.76	122.77
1	A	205	GLU	CA-C-O	-6.75	110.86	120.51
1	A	130	ASP	CA-CB-CG	6.67	119.27	112.60
1	A	219	SER	O-C-N	-6.66	114.45	122.65
1	A	142	ALA	CA-C-N	-6.60	114.50	123.14
1	A	142	ALA	C-N-CA	-6.60	114.50	123.14
1	A	121	VAL	CA-C-O	-6.59	113.52	120.57
1	A	125	THR	CA-C-O	-6.55	110.54	119.05
1	A	244	ASN	OD1-CG-ND2	-6.55	116.05	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	LYS	CB-CA-C	-6.54	109.02	116.54
1	A	96	HIS	CG-CD2-NE2	-6.46	100.75	107.20
1	A	181	PRO	N-CA-CB	6.43	109.45	103.41
1	A	154	LYS	CA-C-N	6.37	126.58	119.32
1	A	154	LYS	C-N-CA	6.37	126.58	119.32
1	A	107	HIS	CA-C-O	-6.34	114.51	121.87
1	A	167	ILE	CA-C-O	6.33	128.69	120.78
1	A	140	GLY	N-CA-C	6.31	123.33	113.86
1	A	216	ILE	CA-C-N	-6.26	113.32	122.65
1	A	216	ILE	C-N-CA	-6.26	113.32	122.65
1	A	241	MET	O-C-N	6.26	130.57	122.43
1	A	27	ARG	CA-CB-CG	6.22	126.55	114.10
1	A	20	PHE	CA-C-N	6.21	125.90	119.56
1	A	20	PHE	C-N-CA	6.21	125.90	119.56
1	A	206	CYS	O-C-N	-6.20	114.69	122.19
1	A	70	PHE	CA-CB-CG	-6.16	107.64	113.80
1	A	113	LYS	O-C-N	-6.15	115.99	123.19
1	A	221	GLU	O-C-N	6.15	129.16	122.15
1	A	58	ARG	N-CA-CB	-6.07	101.53	111.66
1	A	92	GLN	O-C-N	6.05	129.46	123.46
1	A	67	ASN	OD1-CG-ND2	-5.89	116.71	122.60
1	A	96	HIS	CE1-NE2-CD2	5.84	114.84	109.00
1	A	74	GLN	CA-C-O	-5.80	115.25	121.45
1	A	237	PRO	N-CA-CB	5.77	108.33	103.25
1	A	21	PRO	N-CA-CB	5.66	109.14	103.48
1	A	136	GLN	CA-CB-CG	-5.65	102.79	114.10
1	A	4	HIS	N-CA-CB	5.64	120.09	110.50
1	A	92	GLN	CA-C-N	-5.63	113.75	122.59
1	A	92	GLN	C-N-CA	-5.63	113.75	122.59
1	A	58	ARG	CA-C-N	-5.61	115.32	123.06
1	A	58	ARG	C-N-CA	-5.61	115.32	123.06
1	A	37	THR	CA-CB-OG1	-5.61	101.19	109.60
1	A	176	PHE	CA-CB-CG	-5.59	108.20	113.80
1	A	223	VAL	CB-CA-C	-5.55	103.26	112.26
1	A	100	LEU	CA-C-O	-5.51	115.00	121.44
1	A	197	SER	N-CA-CB	-5.51	102.68	111.43
1	A	111	LYS	O-C-N	-5.48	116.12	121.87
1	A	171	GLY	O-C-N	-5.46	116.47	122.65
1	A	161	VAL	CA-C-O	-5.45	115.28	120.95
1	A	98	GLY	CA-C-N	-5.43	111.63	121.14
1	A	98	GLY	C-N-CA	-5.43	111.63	121.14
1	A	216	ILE	O-C-N	5.43	128.87	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	A	247	PRO	N-CA-CB	5.39	108.04	103.35
1	A	198	LEU	N-CA-C	-5.38	103.43	110.53
1	A	260	PHE	CA-CB-CG	-5.34	108.46	113.80
1	A	208	THR	N-CA-C	-5.33	100.04	108.73
1	A	68	VAL	O-C-N	5.31	129.98	122.97
1	A	244	ASN	CB-CG-ND2	5.30	124.36	116.40
1	A	158	GLN	N-CA-C	5.26	117.01	111.28
1	A	253	ASN	CA-C-O	-5.25	113.00	120.51
1	A	193	THR	O-C-N	-5.25	117.19	123.27
1	A	177	THR	CA-C-N	5.23	129.57	122.19
1	A	177	THR	C-N-CA	5.23	129.57	122.19
1	A	218	VAL	CA-CB-CG1	-5.23	101.51	110.40
1	A	118	LEU	N-CA-CB	-5.19	101.82	110.23
1	A	188	SER	CA-C-O	-5.19	115.13	121.36
1	A	230	ASN	CA-CB-CG	5.19	117.79	112.60
1	A	143	VAL	CA-C-O	-5.18	114.95	120.39
1	A	146	ILE	CA-CB-CG2	5.18	119.30	110.50
1	A	96	HIS	ND1-CG-CD2	5.17	111.27	106.10
1	A	60	LEU	N-CA-CB	-5.12	101.97	111.13
1	A	243	ASP	CA-C-N	-5.11	113.52	122.62
1	A	243	ASP	C-N-CA	-5.11	113.52	122.62
1	A	52	ASP	CA-C-N	-5.08	115.00	122.83
1	A	52	ASP	C-N-CA	-5.08	115.00	122.83
1	A	96	HIS	N-CA-CB	5.05	119.55	110.80
1	A	52	ASP	CA-C-O	-5.04	114.40	120.10
1	A	182	ARG	CA-CB-CG	-5.03	104.04	114.10
1	A	135	VAL	O-C-N	-5.03	116.29	122.57

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	LEU	Mainchain
1	A	205	GLU	Mainchain
1	A	36	HIS	Mainchain

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	2043	0	1990	14	0
2	A	1	0	0	0	0
3	A	9	0	2	5	0
4	A	4	0	3	0	0
5	A	134	0	0	5	0
All	All	2191	0	1995	19	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 5.

All (19) 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:A:253:ASN:C	5:A:364:HOH:O	2.03	1.00
3:A:263:HGB:C4	3:A:263:HGB:C3	2.38	0.98
3:A:263:HGB:HC6	5:A:390:HOH:O	1.63	0.96
3:A:263:HGB:C6	5:A:390:HOH:O	2.18	0.90
3:A:263:HGB:C4	3:A:263:HGB:C1	2.53	0.86
3:A:263:HGB:C3	3:A:263:HGB:C1	2.52	0.86
1:A:236:GLU:HB3	1:A:237:PRO:HD2	1.75	0.68
1:A:89:ARG:HG2	5:A:322:HOH:O	1.97	0.65
1:A:161:VAL:CG1	1:A:225:LYS:HD2	2.37	0.54
1:A:14:GLU:CA	5:A:372:HOH:O	2.55	0.53
1:A:213:LYS:HD3	1:A:260:PHE:CZ	2.46	0.51
1:A:27:ARG:CG	1:A:205:GLU:HB3	2.44	0.48
1:A:47:LEU:HD11	1:A:210:ILE:HG21	1.96	0.47
1:A:6:GLY:O	1:A:12:GLY:HA2	2.19	0.43
1:A:201:PRO:HA	1:A:203:LEU:HG	1.99	0.42
1:A:27:ARG:HG3	1:A:205:GLU:HB3	2.02	0.42
1:A:202:PRO:HG2	1:A:204:LEU:HG	2.03	0.41
1:A:30:PRO:HG3	1:A:106:GLU:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	253/259 (98%)	243 (96%)	10 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	221/224 (99%)	209 (95%)	12 (5%)	20	7

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	9	LYS
1	A	39	LYS
1	A	92	GLN
1	A	111	LYS
1	A	127	LYS
1	A	154	LYS
1	A	223	VAL
1	A	239	GLU
1	A	253	ASN
1	A	257	LYS
1	A	261	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64[A]	HIS
1	A	67	ASN
1	A	137	GLN
1	A	253	ASN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	URE	A	264	2	3,3,3	0.29	0	3,3,3	2.30	1 (33%)
3	HGB	A	263	1,5	5,7,11	1.61	1 (20%)	2,6,14	1.90	1 (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
3	HGB	A	263	1,5	-	0/0/0/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	263	HGB	C4-C6	-2.93	1.38	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	264	URE	O-C-N2	-3.13	114.18	121.04
3	A	263	HGB	C4-C6-C7	-2.65	119.62	126.12

There are no chirality outliers.

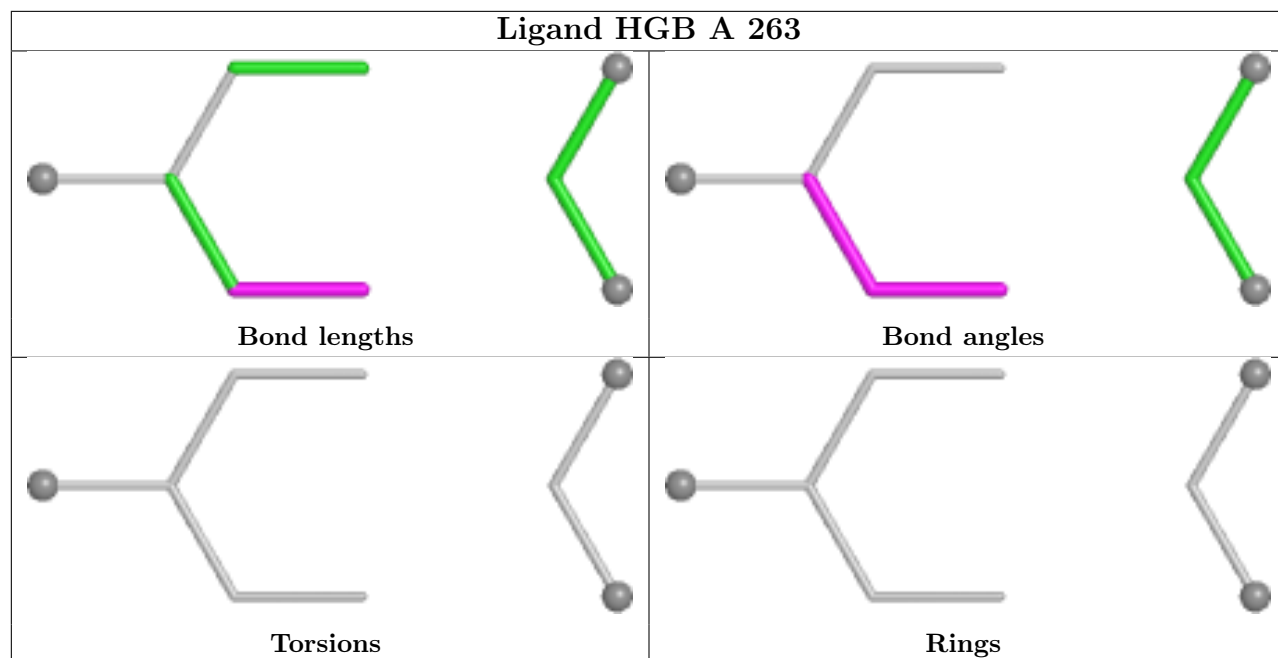
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	263	HGB	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.