



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 04:40 PM EDT

PDB ID : 5BK6  
Title : Structural and biochemical characterization of a non-canonical biuret hydro-  
lase (BiuH) from the cyanuric acid catabolism pathway of *Rhizobium legumi-  
natorum* bv. *viciae* 3841  
Authors : Peat, T.S.; Esquirol, L.; Newman, J.; Scott, C.  
Deposited on : 2017-09-12  
Resolution : 1.59 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

<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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

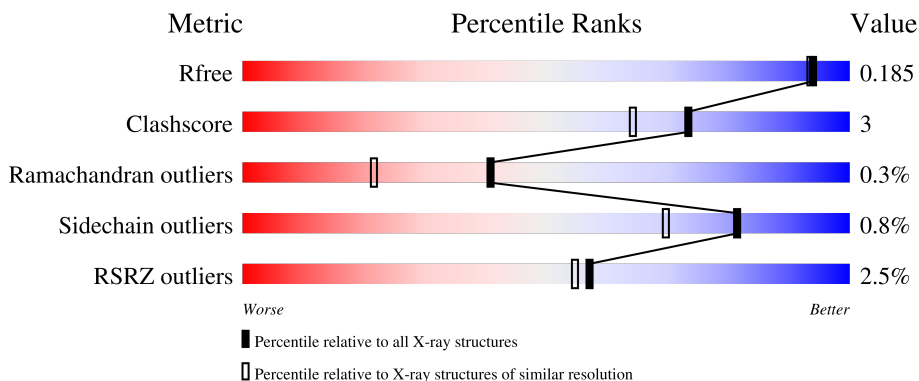
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.59 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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  $\geq 3$ , 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	262	
1	B	262	
1	C	262	
1	D	262	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 8285 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 Putative amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	230	Total 1857	C 1164	N 325	O 352	S 16	0	12	0
1	B	226	Total 1790	C 1123	N 317	O 335	S 15	0	7	0
1	C	230	Total 1818	C 1141	N 318	O 344	S 15	0	7	0
1	D	226	Total 1787	C 1120	N 317	O 335	S 15	0	7	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q1M7F4
A	-18	GLY	-	expression tag	UNP Q1M7F4
A	-17	SER	-	expression tag	UNP Q1M7F4
A	-16	SER	-	expression tag	UNP Q1M7F4
A	-15	HIS	-	expression tag	UNP Q1M7F4
A	-14	HIS	-	expression tag	UNP Q1M7F4
A	-13	HIS	-	expression tag	UNP Q1M7F4
A	-12	HIS	-	expression tag	UNP Q1M7F4
A	-11	HIS	-	expression tag	UNP Q1M7F4
A	-10	HIS	-	expression tag	UNP Q1M7F4
A	-9	SER	-	expression tag	UNP Q1M7F4
A	-8	SER	-	expression tag	UNP Q1M7F4
A	-7	GLY	-	expression tag	UNP Q1M7F4
A	-6	LEU	-	expression tag	UNP Q1M7F4
A	-5	VAL	-	expression tag	UNP Q1M7F4
A	-4	PRO	-	expression tag	UNP Q1M7F4
A	-3	ARG	-	expression tag	UNP Q1M7F4
A	-2	GLY	-	expression tag	UNP Q1M7F4
A	-1	SER	-	expression tag	UNP Q1M7F4
A	0	HIS	-	expression tag	UNP Q1M7F4
A	142	HIS	LYS	conflict	UNP Q1M7F4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	GLY	-	expression tag	UNP Q1M7F4
A	235	LEU	-	expression tag	UNP Q1M7F4
A	236	VAL	-	expression tag	UNP Q1M7F4
A	237	PRO	-	expression tag	UNP Q1M7F4
A	238	ARG	-	expression tag	UNP Q1M7F4
A	239	GLY	-	expression tag	UNP Q1M7F4
A	240	SER	-	expression tag	UNP Q1M7F4
A	241	ILE	-	expression tag	UNP Q1M7F4
A	242	GLU	-	expression tag	UNP Q1M7F4
B	-19	MET	-	initiating methionine	UNP Q1M7F4
B	-18	GLY	-	expression tag	UNP Q1M7F4
B	-17	SER	-	expression tag	UNP Q1M7F4
B	-16	SER	-	expression tag	UNP Q1M7F4
B	-15	HIS	-	expression tag	UNP Q1M7F4
B	-14	HIS	-	expression tag	UNP Q1M7F4
B	-13	HIS	-	expression tag	UNP Q1M7F4
B	-12	HIS	-	expression tag	UNP Q1M7F4
B	-11	HIS	-	expression tag	UNP Q1M7F4
B	-10	HIS	-	expression tag	UNP Q1M7F4
B	-9	SER	-	expression tag	UNP Q1M7F4
B	-8	SER	-	expression tag	UNP Q1M7F4
B	-7	GLY	-	expression tag	UNP Q1M7F4
B	-6	LEU	-	expression tag	UNP Q1M7F4
B	-5	VAL	-	expression tag	UNP Q1M7F4
B	-4	PRO	-	expression tag	UNP Q1M7F4
B	-3	ARG	-	expression tag	UNP Q1M7F4
B	-2	GLY	-	expression tag	UNP Q1M7F4
B	-1	SER	-	expression tag	UNP Q1M7F4
B	0	HIS	-	expression tag	UNP Q1M7F4
B	142	HIS	LYS	conflict	UNP Q1M7F4
B	234	GLY	-	expression tag	UNP Q1M7F4
B	235	LEU	-	expression tag	UNP Q1M7F4
B	236	VAL	-	expression tag	UNP Q1M7F4
B	237	PRO	-	expression tag	UNP Q1M7F4
B	238	ARG	-	expression tag	UNP Q1M7F4
B	239	GLY	-	expression tag	UNP Q1M7F4
B	240	SER	-	expression tag	UNP Q1M7F4
B	241	ILE	-	expression tag	UNP Q1M7F4
B	242	GLU	-	expression tag	UNP Q1M7F4
C	-19	MET	-	initiating methionine	UNP Q1M7F4
C	-18	GLY	-	expression tag	UNP Q1M7F4
C	-17	SER	-	expression tag	UNP Q1M7F4

*Continued on next page...*

*Continued from previous page...*

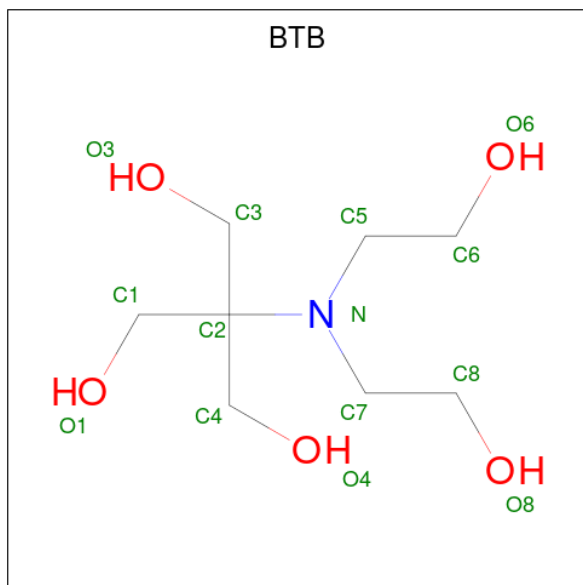
Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	SER	-	expression tag	UNP Q1M7F4
C	-15	HIS	-	expression tag	UNP Q1M7F4
C	-14	HIS	-	expression tag	UNP Q1M7F4
C	-13	HIS	-	expression tag	UNP Q1M7F4
C	-12	HIS	-	expression tag	UNP Q1M7F4
C	-11	HIS	-	expression tag	UNP Q1M7F4
C	-10	HIS	-	expression tag	UNP Q1M7F4
C	-9	SER	-	expression tag	UNP Q1M7F4
C	-8	SER	-	expression tag	UNP Q1M7F4
C	-7	GLY	-	expression tag	UNP Q1M7F4
C	-6	LEU	-	expression tag	UNP Q1M7F4
C	-5	VAL	-	expression tag	UNP Q1M7F4
C	-4	PRO	-	expression tag	UNP Q1M7F4
C	-3	ARG	-	expression tag	UNP Q1M7F4
C	-2	GLY	-	expression tag	UNP Q1M7F4
C	-1	SER	-	expression tag	UNP Q1M7F4
C	0	HIS	-	expression tag	UNP Q1M7F4
C	142	HIS	LYS	conflict	UNP Q1M7F4
C	234	GLY	-	expression tag	UNP Q1M7F4
C	235	LEU	-	expression tag	UNP Q1M7F4
C	236	VAL	-	expression tag	UNP Q1M7F4
C	237	PRO	-	expression tag	UNP Q1M7F4
C	238	ARG	-	expression tag	UNP Q1M7F4
C	239	GLY	-	expression tag	UNP Q1M7F4
C	240	SER	-	expression tag	UNP Q1M7F4
C	241	ILE	-	expression tag	UNP Q1M7F4
C	242	GLU	-	expression tag	UNP Q1M7F4
D	-19	MET	-	initiating methionine	UNP Q1M7F4
D	-18	GLY	-	expression tag	UNP Q1M7F4
D	-17	SER	-	expression tag	UNP Q1M7F4
D	-16	SER	-	expression tag	UNP Q1M7F4
D	-15	HIS	-	expression tag	UNP Q1M7F4
D	-14	HIS	-	expression tag	UNP Q1M7F4
D	-13	HIS	-	expression tag	UNP Q1M7F4
D	-12	HIS	-	expression tag	UNP Q1M7F4
D	-11	HIS	-	expression tag	UNP Q1M7F4
D	-10	HIS	-	expression tag	UNP Q1M7F4
D	-9	SER	-	expression tag	UNP Q1M7F4
D	-8	SER	-	expression tag	UNP Q1M7F4
D	-7	GLY	-	expression tag	UNP Q1M7F4
D	-6	LEU	-	expression tag	UNP Q1M7F4
D	-5	VAL	-	expression tag	UNP Q1M7F4

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	PRO	-	expression tag	UNP Q1M7F4
D	-3	ARG	-	expression tag	UNP Q1M7F4
D	-2	GLY	-	expression tag	UNP Q1M7F4
D	-1	SER	-	expression tag	UNP Q1M7F4
D	0	HIS	-	expression tag	UNP Q1M7F4
D	142	HIS	LYS	conflict	UNP Q1M7F4
D	234	GLY	-	expression tag	UNP Q1M7F4
D	235	LEU	-	expression tag	UNP Q1M7F4
D	236	VAL	-	expression tag	UNP Q1M7F4
D	237	PRO	-	expression tag	UNP Q1M7F4
D	238	ARG	-	expression tag	UNP Q1M7F4
D	239	GLY	-	expression tag	UNP Q1M7F4
D	240	SER	-	expression tag	UNP Q1M7F4
D	241	ILE	-	expression tag	UNP Q1M7F4
D	242	GLU	-	expression tag	UNP Q1M7F4

- Molecule 2 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	D	1	14	8	1	5	0	0

- Molecule 3 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
			Total	C	O		
3	A	1	6	3	3	0	0
3	C	1	6	3	3	0	0
3	D	1	6	3	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	243	243	243	0	0
4	B	265	265	265	0	0
4	C	214	214	214	0	0
4	D	237	237	237	0	0





ARG  
GLY  
SER  
ILE  
GLU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.13Å 122.68Å 135.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.80 – 1.59 45.83 – 1.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.80-1.59) 100.0 (45.83-1.59)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 1.59Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.150 , 0.174 0.163 , 0.185	Depositor DCC
$R_{free}$ test set	6886 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtrriage
Anisotropy	0.027	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8285	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: BTB, GOL

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	0.94	1/1898 (0.1%)	1.06	12/2578 (0.5%)
1	B	0.91	1/1829 (0.1%)	0.98	9/2483 (0.4%)
1	C	0.91	0/1858	0.98	7/2524 (0.3%)
1	D	0.85	0/1826	0.97	7/2479 (0.3%)
All	All	0.90	2/7411 (0.0%)	1.00	35/10064 (0.3%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	GLU	CD-OE2	-6.06	1.19	1.25
1	B	56	SER	CB-OG	-5.25	1.35	1.42

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67[A]	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	A	67[B]	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	B	54	ASP	CB-CG-OD2	-8.71	110.46	118.30
1	D	9	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	A	53[A]	TYR	N-CA-C	7.21	130.47	111.00
1	A	53[B]	TYR	N-CA-C	7.21	130.47	111.00
1	D	67	ARG	NE-CZ-NH2	-6.94	116.83	120.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	B	103[A]	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	B	103[B]	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	A	67[A]	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	A	67[B]	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	B	9	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	A	54[A]	ASP	N-CA-C	6.07	127.38	111.00
1	A	54[B]	ASP	N-CA-C	6.07	127.38	111.00
1	C	161	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	C	126	ASP	CB-CG-OD1	5.80	123.53	118.30
1	B	161	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	C	54	ASP	CB-CG-OD1	5.65	123.39	118.30
1	C	40[A]	ASP	CB-CG-OD1	5.64	123.38	118.30
1	C	40[B]	ASP	CB-CG-OD1	5.64	123.38	118.30
1	D	126	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	36	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	B	13	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	D	181	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	B	126	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	161	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	A	161	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	A	126	ASP	CB-CG-OD1	5.20	122.98	118.30
1	D	9	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	D	89	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	67	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	D	161	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	230	GLU	CA-CB-CG	5.16	124.76	113.40
1	B	161	ARG	NE-CZ-NH1	-5.09	117.75	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	THR	Peptide
1	A	52[A]	GLY	Peptide

## 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	1857	0	1799	9	0
1	B	1790	0	1760	5	0
1	C	1818	0	1773	25	0
1	D	1787	0	1751	4	0
2	A	14	0	19	3	0
2	B	14	0	19	4	0
2	C	14	0	19	3	0
2	D	14	0	19	0	0
3	A	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	A	243	0	0	1	0
4	B	265	0	0	1	0
4	C	214	0	0	0	0
4	D	237	0	0	1	0
All	All	8285	0	7183	48	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 3.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40[B]:ASP:N	1:C:40[B]:ASP:CA	1.68	1.52
1:C:41[A]:PHE:HE1	1:C:47:TYR:HD2	1.04	0.99
1:C:41[A]:PHE:CE1	1:C:47:TYR:HD2	1.88	0.91
1:C:41[A]:PHE:HE1	1:C:47:TYR:CD2	1.91	0.89
1:C:41[A]:PHE:HD1	1:C:48:VAL:HG23	1.44	0.81
1:C:40[A]:ASP:O	1:C:46:GLY:HA3	1.83	0.78
1:A:53[B]:TYR:OH	4:A:401:HOH:O	2.01	0.77
1:C:41[A]:PHE:CD1	1:C:48:VAL:HG23	2.27	0.70
2:C:301:BTB:O4	2:C:301:BTB:H71	2.02	0.59
1:C:40[B]:ASP:N	1:C:40[B]:ASP:HA	2.00	0.58
1:C:41[A]:PHE:CE1	1:C:47:TYR:CD2	2.77	0.58
1:C:41[A]:PHE:CZ	1:C:118:LEU:HD21	2.41	0.56
1:C:51:MET:HG2	1:C:104:ILE:HD12	1.87	0.56
1:D:192[A]:LEU:HD11	1:D:197[A]:CYS:SG	2.46	0.56
1:C:40[A]:ASP:CA	1:C:46:GLY:HA3	2.36	0.55
2:C:301:BTB:O4	2:C:301:BTB:C7	2.54	0.55
1:A:40[A]:ASP:HB3	1:A:47:TYR:CD2	2.41	0.55

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:301:BTB:O6	2:C:301:BTB:H72	2.05	0.55
2:A:301:BTB:H82	1:B:158:ASN:O	2.08	0.54
1:B:44:LYS:HE3	1:B:49:ASP:OD2	2.08	0.54
1:D:192[B]:LEU:HD21	1:D:197[B]:CYS:SG	2.48	0.54
2:A:301:BTB:H81	2:B:301:BTB:H82	1.91	0.51
1:A:163:GLU:OE1	1:B:161:ARG:NH1	2.44	0.50
1:A:40[B]:ASP:OD1	1:A:47:TYR:HD2	1.95	0.50
1:C:41[A]:PHE:HD1	1:C:48:VAL:CG2	2.21	0.50
1:C:40[A]:ASP:C	1:C:46:GLY:HA3	2.31	0.49
1:C:51:MET:SD	1:C:104:ILE:HD12	2.53	0.48
1:C:51:MET:SD	1:C:104:ILE:CD1	3.02	0.48
2:A:301:BTB:H62	2:B:301:BTB:H61	1.96	0.46
1:C:192[A]:LEU:HD11	1:C:197[A]:CYS:SG	2.55	0.46
1:B:19:TRP:CE2	1:B:191:LEU:HB2	2.51	0.45
1:C:19:TRP:CE2	1:C:191:LEU:HB2	2.52	0.45
1:D:19:TRP:CE2	1:D:191:LEU:HB2	2.51	0.45
1:A:19:TRP:CE2	1:A:191:LEU:HB2	2.53	0.44
1:A:49:ASP:HB2	1:A:55:LEU:HD11	1.99	0.44
1:A:192[A]:LEU:HD11	1:A:197[A]:CYS:SG	2.58	0.43
1:C:40[A]:ASP:OD1	1:C:114:CYS:HB2	2.18	0.43
1:C:40[A]:ASP:OD1	1:C:124:GLY:HA3	2.19	0.43
1:D:9:ARG:NH1	4:D:406:HOH:O	2.52	0.42
1:C:192[B]:LEU:C	1:C:192[B]:LEU:HD23	2.39	0.42
2:B:301:BTB:H42	2:B:301:BTB:H71	1.88	0.42
1:C:192[B]:LEU:HD21	1:C:197[B]:CYS:SG	2.60	0.42
1:C:40[A]:ASP:HB3	1:C:47:TYR:H	1.85	0.41
1:A:158:ASN:HB3	2:B:301:BTB:H52	2.02	0.41
1:C:51:MET:CG	1:C:104:ILE:HD12	2.50	0.41
1:A:40[A]:ASP:HB3	1:A:47:TYR:HD2	1.86	0.40
1:B:130:GLU:HG3	4:B:455:HOH:O	2.21	0.40
1:C:118:LEU:HD23	1:C:118:LEU:HA	1.97	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	240/262 (92%)	229 (95%)	9 (4%)	2 (1%)	19	6
1	B	231/262 (88%)	226 (98%)	5 (2%)	0	100	100
1	C	235/262 (90%)	227 (97%)	6 (3%)	2 (1%)	17	4
1	D	231/262 (88%)	227 (98%)	3 (1%)	1 (0%)	34	15
All	All	937/1048 (89%)	909 (97%)	23 (2%)	5 (0%)	41	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	40[A]	ASP
1	C	40[B]	ASP
1	A	40[A]	ASP
1	A	40[B]	ASP
1	D	174	VAL

### 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	197/214 (92%)	195 (99%)	2 (1%)	76	61
1	B	191/214 (89%)	191 (100%)	0	100	100
1	C	194/214 (91%)	192 (99%)	2 (1%)	76	61
1	D	190/214 (89%)	188 (99%)	2 (1%)	73	57
All	All	772/856 (90%)	766 (99%)	6 (1%)	81	70

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	LEU
1	A	125	TRP
1	C	125	TRP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	230	GLU
1	D	47	TYR
1	D	118	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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	$\# Z  > 2$
2	BTB	C	301	-	13,13,13	1.20	2 (15%)	7,16,16	1.60	1 (14%)
3	GOL	A	302	-	5,5,5	0.99	0	5,5,5	0.57	0
3	GOL	C	302	-	5,5,5	0.95	0	5,5,5	0.95	0
2	BTB	B	301	-	13,13,13	1.53	2 (15%)	7,16,16	1.05	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BTB	A	301	-	13,13,13	1.15	1 (7%)	7,16,16	0.87	0
3	GOL	D	302	-	5,5,5	0.65	0	5,5,5	0.87	0
2	BTB	D	301	-	13,13,13	1.38	2 (15%)	7,16,16	1.25	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
2	BTB	C	301	-	-	2/21/21/21	-
3	GOL	A	302	-	-	0/4/4/4	-
3	GOL	C	302	-	-	0/4/4/4	-
2	BTB	B	301	-	-	1/21/21/21	-
2	BTB	A	301	-	-	1/21/21/21	-
3	GOL	D	302	-	-	0/4/4/4	-
2	BTB	D	301	-	-	1/21/21/21	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	BTB	C5-N	3.90	1.53	1.48
2	A	301	BTB	C7-N	3.47	1.53	1.48
2	D	301	BTB	C5-N	3.41	1.52	1.48
2	B	301	BTB	C7-N	2.96	1.52	1.48
2	C	301	BTB	C7-N	2.62	1.51	1.48
2	C	301	BTB	C5-N	2.55	1.51	1.48
2	D	301	BTB	C1-C2	2.53	1.56	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	BTB	C6-C5-N	3.08	123.61	111.59

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	BTB	C6-C5-N-C7
2	B	301	BTB	N-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	C	301	BTB	N-C7-C8-O8
2	D	301	BTB	N-C5-C6-O6
2	A	301	BTB	N-C7-C8-O8

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	BTB	3	0
2	B	301	BTB	4	0
2	A	301	BTB	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	230/262 (87%)	-0.21	7 (3%) 50 48	14, 19, 36, 62	0
1	B	226/262 (86%)	-0.46	1 (0%) 92 92	14, 18, 28, 52	0
1	C	230/262 (87%)	-0.03	13 (5%) 23 21	14, 20, 40, 51	0
1	D	226/262 (86%)	-0.37	2 (0%) 84 84	15, 20, 32, 54	0
All	All	912/1048 (87%)	-0.27	23 (2%) 57 55	14, 19, 36, 62	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	48	VAL	9.1
1	A	53[A]	TYR	8.8
1	C	53	TYR	5.3
1	C	47	TYR	4.9
1	A	52[A]	GLY	3.8
1	C	51	MET	3.7
1	C	50	HIS	3.7
1	C	46	GLY	3.5
1	A	50	HIS	3.4
1	C	4	MET	3.3
1	C	41[A]	PHE	3.3
1	C	52	GLY	3.0
1	A	5	VAL	2.9
1	B	8	ASN	2.8
1	A	4	MET	2.8
1	A	51[A]	MET	2.7
1	C	40[A]	ASP	2.6
1	C	114	CYS	2.6
1	C	44	LYS	2.5
1	C	49	ASP	2.4
1	A	47	TYR	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	8	ASN	2.1
1	D	50	HIS	2.0

## 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 monosaccharides 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	BTB	C	301	14/14	0.86	0.13	21,26,39,39	0
2	BTB	B	301	14/14	0.87	0.11	27,31,36,47	0
2	BTB	A	301	14/14	0.89	0.10	23,28,33,42	0
2	BTB	D	301	14/14	0.92	0.10	25,31,39,45	0
3	GOL	A	302	6/6	0.95	0.15	19,27,30,31	0
3	GOL	C	302	6/6	0.95	0.16	20,29,29,30	0
3	GOL	D	302	6/6	0.96	0.10	22,31,34,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.