



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2018 – 07:08 PM EST

PDB ID : 6AZO  
Title : Structural and biochemical characterization of a non-canonical biuret hydrolase (BiuH) from the cyanuric acid catabolism pathway of *Rhizobium leguminosorum* bv. *viciae* 3841  
Authors : Peat, T.S.; Esquirol, L.; Newman, J.; Scott, C.  
Deposited on : 2017-09-11  
Resolution : 2.46 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030736

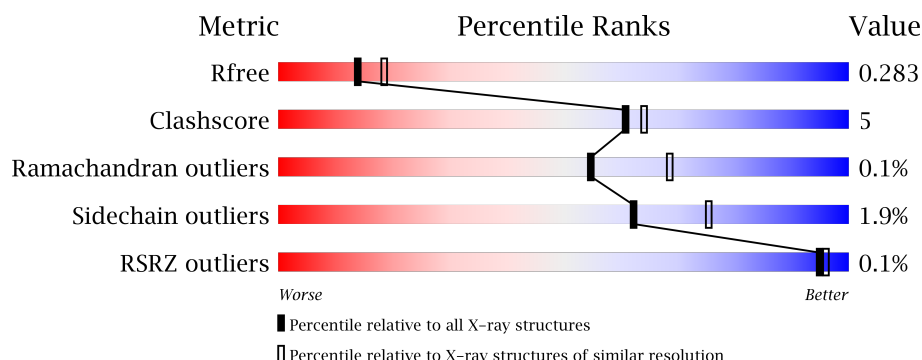
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*





The reported resolution of this entry is 2.46 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))
$R_{free}$	100719	1119 (2.48-2.44)
Clashscore	112137	1193 (2.48-2.44)
Ramachandran outliers	110173	1185 (2.48-2.44)
Sidechain outliers	110143	1185 (2.48-2.44)
RSRZ outliers	101464	1126 (2.48-2.44)

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	262	
1	B	262	
1	C	262	
1	D	262	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7463 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
1	A	230	Total	C	N	O	S	Se	0	0	0
			1759	1107	310	329	7	6			
1	B	230	Total	C	N	O	S	Se	0	0	0
			1758	1108	309	328	7	6			
1	C	231	Total	C	N	O	S	Se	0	1	0
			1773	1117	313	330	7	6			
1	D	230	Total	C	N	O	S	Se	0	0	0
			1758	1108	309	328	7	6			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	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	234	GLY	-	expression tag	UNP Q1M7F4

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Chain	Residue	Modelled	Actual	Comment	Reference
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	MSE	-	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	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	MSE	-	initiating methionine	UNP Q1M7F4
C	-18	GLY	-	expression tag	UNP Q1M7F4
C	-17	SER	-	expression tag	UNP Q1M7F4
C	-16	SER	-	expression tag	UNP Q1M7F4
C	-15	HIS	-	expression tag	UNP Q1M7F4

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	MSE	-	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
D	-4	PRO	-	expression tag	UNP Q1M7F4
D	-3	ARG	-	expression tag	UNP Q1M7F4
D	-2	GLY	-	expression tag	UNP Q1M7F4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	SER	-	expression tag	UNP Q1M7F4
D	0	HIS	-	expression tag	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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0

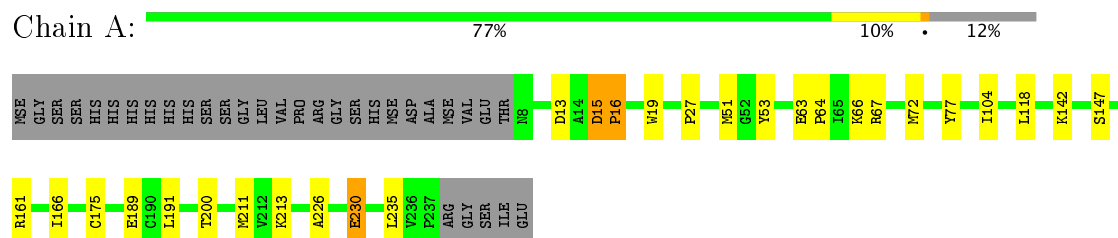
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	106	Total O 106 106	0	0
3	B	96	Total O 96 96	0	0
3	C	97	Total O 97 97	0	0
3	D	114	Total O 114 114	0	0

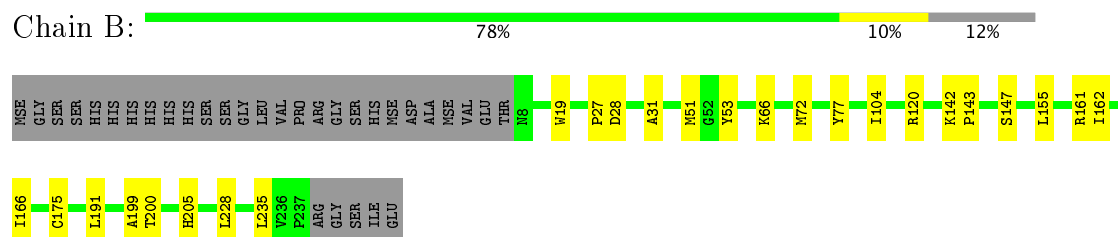
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

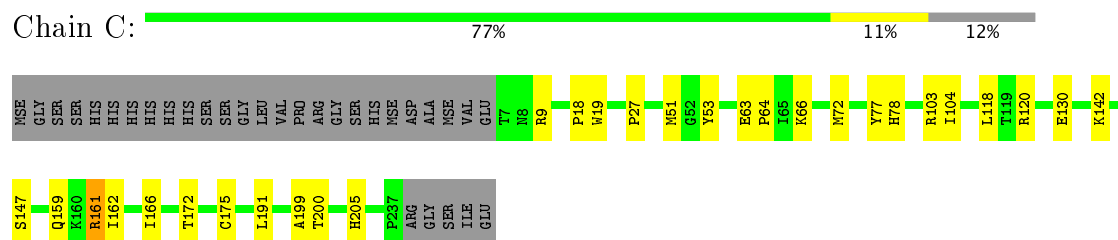
#### • Molecule 1: Putative amidase



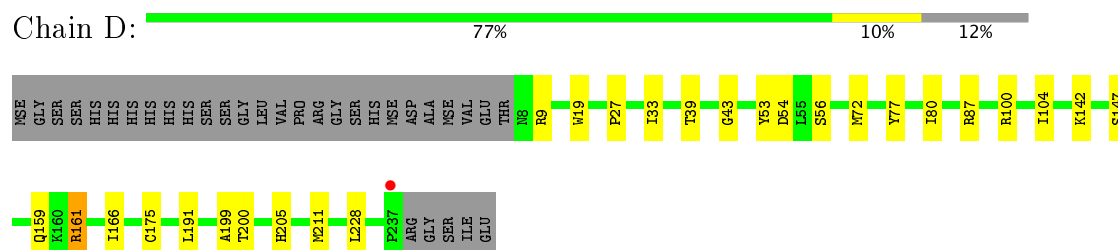
#### • Molecule 1: Putative amidase



#### • Molecule 1: Putative amidase



#### • Molecule 1: Putative amidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.69Å 100.96Å 65.61Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	44.99 – 2.46 40.49 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.99-2.46) 99.8 (40.49-2.46)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.225 , 0.276 0.236 , 0.283	Depositor DCC
$R_{free}$ test set	1647 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.3	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , -7.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.176 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7463	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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:  
CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.66	0/1791	0.98	6/2422 (0.2%)
1	B	0.60	0/1791	0.88	4/2423 (0.2%)
1	C	0.61	0/1807	0.87	2/2445 (0.1%)
1	D	0.63	0/1791	0.89	4/2423 (0.2%)
All	All	0.63	0/7180	0.91	16/9713 (0.2%)

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	1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	ASP	C-N-CD	-16.68	83.90	120.60
1	A	67	ARG	NE-CZ-NH2	9.48	125.04	120.30
1	A	67	ARG	NE-CZ-NH1	-8.29	116.16	120.30
1	B	161	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	161	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	B	28	ASP	CB-CG-OD1	6.27	123.95	118.30
1	C	103	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	B	161	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	D	161	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	D	54	ASP	CB-CG-OD1	5.68	123.42	118.30
1	C	120	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	230	GLU	CA-CB-CG	5.58	125.67	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	72	MSE	CA-CB-CG	-5.35	104.21	113.30
1	D	9	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	120	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	13	ASP	CB-CG-OD1	5.05	122.85	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	ASP	Peptide

## 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	1759	0	1741	20	0
1	B	1758	0	1743	15	0
1	C	1773	0	1751	20	0
1	D	1758	0	1743	21	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	106	0	0	0	0
3	B	96	0	0	2	0
3	C	97	0	0	3	0
3	D	114	0	0	3	1
All	All	7463	0	6978	73	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 5.

All (73) 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:B:51:MSE:SE	1:B:104:ILE:HD11	2.11	1.00
1:C:51:MSE:SE	1:C:104:ILE:HD11	2.27	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:MSE:SE	1:A:104:ILE:HD11	2.29	0.82
1:A:16:PRO:HD3	1:A:213:LYS:HG2	1.62	0.82
1:A:27:PRO:HG2	1:A:235:LEU:HD23	1.64	0.80
1:B:51:MSE:SE	1:B:104:ILE:CD1	2.84	0.76
1:A:51:MSE:SE	1:A:104:ILE:CD1	2.84	0.75
1:C:51:MSE:SE	1:C:104:ILE:CD1	2.85	0.75
1:B:19:TRP:CE2	1:B:191:LEU:HB2	2.38	0.59
1:C:19:TRP:CE2	1:C:191:LEU:HB2	2.39	0.58
1:C:172:THR:OG1	1:C:205[B]:HIS:HD2	1.87	0.58
1:D:19:TRP:CE2	1:D:191:LEU:HB2	2.40	0.57
1:A:19:TRP:CE2	1:A:191:LEU:HB2	2.40	0.57
1:B:166:ILE:HD13	1:B:228:LEU:HD11	1.88	0.56
1:B:31:ALA:HB2	1:B:162:ILE:HD13	1.90	0.54
1:D:33:ILE:HD12	1:D:80:ILE:HG22	1.91	0.52
1:B:51:MSE:HG2	1:B:104:ILE:HD12	1.91	0.52
1:D:33:ILE:CD1	1:D:80:ILE:CG2	2.88	0.51
1:D:33:ILE:HD12	1:D:80:ILE:CG2	2.41	0.51
1:D:200:THR:HA	3:D:450:HOH:O	2.12	0.50
1:B:143:PRO:HD3	3:B:310:HOH:O	2.13	0.49
1:A:226:ALA:O	1:A:230:GLU:HG2	2.13	0.49
1:D:33:ILE:CD1	1:D:80:ILE:HG22	2.42	0.49
1:C:9:ARG:NH2	3:C:404:HOH:O	2.46	0.48
1:B:142:LYS:HD3	1:B:147:SER:HA	1.94	0.48
1:C:130:GLU:O	3:C:401:HOH:O	2.20	0.47
1:C:142:LYS:HD3	1:C:147:SER:HA	1.95	0.47
1:D:56:SER:HB2	3:D:420:HOH:O	2.14	0.47
1:A:189:GLU:OE1	1:D:100:ARG:NH2	2.48	0.47
1:A:142:LYS:HD3	1:A:147:SER:HA	1.96	0.47
1:D:142:LYS:HD3	1:D:147:SER:HA	1.96	0.47
1:C:51:MSE:SE	1:C:104:ILE:HD12	2.64	0.46
1:C:72:MSE:HE1	1:C:166:ILE:HD12	1.98	0.46
1:D:27:PRO:HA	1:D:77:TYR:CD2	2.51	0.46
1:D:87:ARG:HD3	3:D:422:HOH:O	2.15	0.46
1:C:199:ALA:HB3	1:C:205[B]:HIS:HB2	1.98	0.46
1:A:27:PRO:HA	1:A:77:TYR:CD2	2.51	0.46
1:C:27:PRO:HA	1:C:77:TYR:CD2	2.51	0.45
1:B:27:PRO:HA	1:B:77:TYR:CD2	2.51	0.45
1:A:51:MSE:SE	1:A:104:ILE:HD12	2.64	0.44
1:D:166:ILE:HD13	1:D:228:LEU:HD21	2.00	0.44
1:C:118:LEU:HD23	1:C:118:LEU:HA	1.86	0.44
1:D:33:ILE:HD12	1:D:80:ILE:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:TRP:CD2	1:A:191:LEU:HB2	2.53	0.43
1:C:19:TRP:CD2	1:C:191:LEU:HB2	2.53	0.43
1:A:63:GLU:HB2	1:A:64:PRO:HD3	1.99	0.43
1:D:19:TRP:CD2	1:D:191:LEU:HB2	2.53	0.43
1:A:51:MSE:HG2	1:A:104:ILE:HD12	2.00	0.43
1:B:72:MSE:HE1	1:B:166:ILE:HD12	2.01	0.43
1:C:18:PRO:HG2	3:C:497:HOH:O	2.17	0.43
1:B:19:TRP:CE3	1:B:191:LEU:HD22	2.55	0.42
1:C:53:TYR:CD1	1:C:200:THR:HB	2.54	0.42
1:B:199:ALA:HB3	1:B:205:HIS:HB2	2.00	0.42
1:A:211:MSE:HE1	1:D:211:MSE:CE	2.49	0.42
1:D:199:ALA:HB3	1:D:205:HIS:HB2	2.01	0.41
1:D:39:THR:HG23	1:D:43:GLY:HA3	2.02	0.41
1:A:19:TRP:CE3	1:A:191:LEU:HD22	2.56	0.41
1:C:19:TRP:CE3	1:C:191:LEU:HD22	2.56	0.41
1:D:33:ILE:HD12	1:D:80:ILE:CB	2.50	0.41
1:B:53:TYR:CD1	1:B:200:THR:HB	2.56	0.41
1:A:72:MSE:HE1	1:A:166:ILE:HD12	2.02	0.41
1:A:211:MSE:CE	1:D:211:MSE:HE1	2.50	0.41
1:B:19:TRP:CD2	1:B:191:LEU:HB2	2.54	0.41
1:C:161:ARG:HH21	1:C:161:ARG:HA	1.85	0.41
1:B:142:LYS:HB2	3:B:306:HOH:O	2.21	0.41
1:C:63:GLU:HB2	1:C:64:PRO:HD3	2.02	0.41
1:A:27:PRO:CG	1:A:235:LEU:HD23	2.44	0.41
1:D:53:TYR:CD1	1:D:200:THR:HB	2.56	0.41
1:C:199:ALA:HB3	1:C:205[A]:HIS:HB2	2.03	0.41
1:A:53:TYR:CD1	1:A:200:THR:HB	2.55	0.41
1:C:78:HIS:CG	1:C:162:ILE:HD11	2.56	0.40
1:D:19:TRP:CE3	1:D:191:LEU:HD22	2.56	0.40
1:A:118:LEU:HA	1:A:118:LEU:HD23	1.88	0.40

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)
3:D:420:HOH:O	3:D:420:HOH:O[2_657]	1.88	0.32

## 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	228/262 (87%)	222 (97%)	5 (2%)	1 (0%)	38	47
1	B	228/262 (87%)	223 (98%)	5 (2%)	0	100	100
1	C	230/262 (88%)	225 (98%)	5 (2%)	0	100	100
1	D	228/262 (87%)	224 (98%)	4 (2%)	0	100	100
All	All	914/1048 (87%)	894 (98%)	19 (2%)	1 (0%)	55	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	PRO

### 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	186/205 (91%)	184 (99%)	2 (1%)	78	86
1	B	186/205 (91%)	182 (98%)	4 (2%)	57	71
1	C	187/205 (91%)	183 (98%)	4 (2%)	59	73
1	D	186/205 (91%)	182 (98%)	4 (2%)	57	71
All	All	745/820 (91%)	731 (98%)	14 (2%)	62	75

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LYS
1	A	175	CYS
1	B	66	LYS
1	B	155	LEU
1	B	175	CYS
1	B	235	LEU
1	C	66	LYS
1	C	159	GLN
1	C	161	ARG
1	C	175	CYS
1	D	104	ILE
1	D	159	GLN
1	D	161	ARG
1	D	175	CYS

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

Mol	Chain	Res	Type
1	B	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	224/262 (85%)	-0.35	0 100 100	7, 14, 25, 47	0
1	B	224/262 (85%)	-0.28	0 100 100	9, 19, 33, 45	0
1	C	225/262 (85%)	-0.30	0 100 100	10, 20, 34, 47	0
1	D	224/262 (85%)	-0.40	1 (0%) 92 93	8, 13, 26, 59	0
All	All	897/1048 (85%)	-0.33	1 (0%) 95 96	7, 16, 32, 59	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	237	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
2	CL	C	301	1/1	0.98	0.10	-	24,24,24,24	0
2	CL	D	301	1/1	0.96	0.08	-	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.