



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:13 PM UTC

PDB ID : 6AZO / pdb_00006azo
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

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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

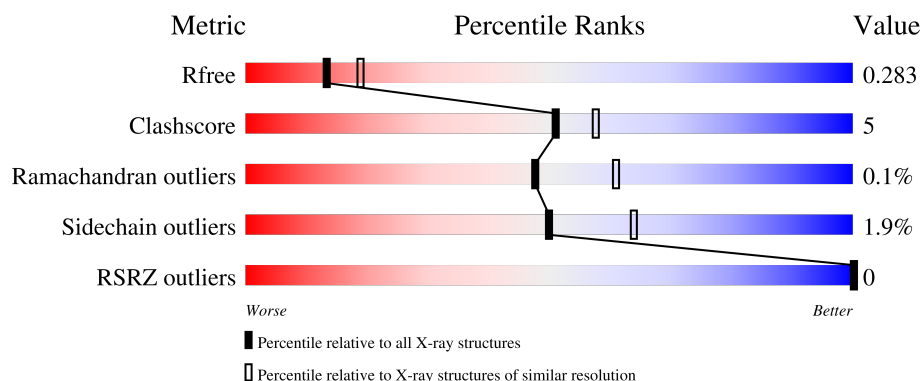
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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 $\leq 5\%$. 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	 77% 9% 12%
1	B	262	 79% 8% 12%
1	C	262	 77% 10% 12%
1	D	262	 78% 10% 12%

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 (CCD ID: CL) (formula: Cl).

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

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- Molecule 1: Putative amidase

L166	L167	C175	E189	C190	L191	T200	M211	V212	K213	A226	E230	L235	V236	P237	ARG	GLY	SER	ILE	GLU	NSE	GLY	SER	ARG	PRO	VAL	LEU	GLY	SER	SER	SER	HIS	HIS	HIS	HIS	HIS	SER	GLY	H8	D15	P16	W19	P27	M51	G52	Y53	E63	P64	I66	K66	R67	M72	Y77	I104	L118	K142	S147	Q159
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- Molecule 1: Putative amidase

C176	MSE
L191	GLY
A199	SER
T200	HIS
H205	HIS
L228	HIS
P237	SER
ARG	GLY
GLY	LEU
SER	VAL
ILE	PRO
GLU	ARG
	GLY
	SER
	HIS
	MSE
	ASP
	ALA
	MLE
	VAL
	GLU
	THR
	H8
	H19
	P27
	A31
	I35
	M51
	G52
	Y53
	H72
	Y77
	I104
	K142
	P143
	S147
	L155
	M158
	I162
	I166

- Molecule 1: Putative amidase

Q159	Q160	R161	I162	I166	T172	C175	L191	A199	T200	H205	P237	ARG	GLY	SER	ILE	GLU	MSE	GLY	SER	HIS	HIS	HIS	HIS	HIS	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	MSE	ASP	ALA	MSE	VAL	GLU	T7	H8	R9	P18	W19	P27	M51	G52	Y53	E63	P64	G65	A66	M72	Y77	H78	I104	L118	E130	K142	S147	H159
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- Molecule 1: Putative amidase

MSE	GLY	SER	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	GLY	HIS	HIS	MSE	ASP	ALA	ALA	MSE	VAL	GLU	THR	N8	N9	W19	P27	I33	I33	I34	I35	I39	G43	Y53	S56	Y77	I80	R87	R100	I104	K142	S147	Q150
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K160	R161	I166	I170	C175	L191	A199	T200	H205	M211	L228	P237	ARG	GLY	SER	ILE	GLU
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.69Å 100.96Å 65.61Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	44.99 – 2.46 44.99 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.99-2.46) 99.8 (44.99-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	14.3	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.176 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7463	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.90	1/1791 (0.1%)	1.10	4/2422 (0.2%)
1	B	0.85	1/1791 (0.1%)	1.01	1/2423 (0.0%)
1	C	0.86	1/1807 (0.1%)	1.02	0/2445
1	D	0.88	0/1791	1.02	1/2423 (0.0%)
All	All	0.87	3/7180 (0.0%)	1.04	6/9713 (0.1%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	158	ASN	C-O	-5.82	1.17	1.24
1	A	235	LEU	C-O	-5.26	1.17	1.24
1	B	158	ASN	C-O	-5.12	1.18	1.24

All (6) 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	6.49	125.04	119.20
1	A	230	GLU	CA-CB-CG	5.78	125.67	114.10
1	A	67	ARG	NE-CZ-NH1	-5.34	116.16	121.50
1	B	35	ILE	N-CA-C	5.07	115.06	107.51
1	D	35	ILE	N-CA-C	5.02	114.99	107.51

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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:39:THR:HG23	1:D:43:GLY:HA3	2.02	0.41
1:D:199:ALA:HB3	1:D:205:HIS:HB2	2.01	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:C:199:ALA:HB3	1:C:205[A]:HIS:HB2	2.03	0.41
1:D:53:TYR:CD1	1:D:200:THR:HB	2.56	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 [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	228/262 (87%)	222 (97%)	5 (2%)	1 (0%)	30	37
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%)	48	61

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%)	183 (98%)	3 (2%)	55	69
1	B	186/205 (91%)	184 (99%)	2 (1%)	65	76
1	C	187/205 (91%)	183 (98%)	4 (2%)	47	62
1	D	186/205 (91%)	181 (97%)	5 (3%)	39	54
All	All	745/820 (91%)	731 (98%)	14 (2%)	50	64

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

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

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Mol	Chain	Res	Type
1	D	159	GLN
1	D	161	ARG
1	D	170	ILE
1	D	175	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	A	224	ASN
1	B	10	HIS
1	B	215	GLN
1	B	224	ASN
1	C	159	GLN
1	C	215	GLN
1	C	224	ASN
1	D	50	HIS
1	D	224	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	A	224/262 (85%)	-1.64	0 100 100	7, 14, 25, 47	0
1	B	224/262 (85%)	-1.60	0 100 100	9, 19, 33, 45	0
1	C	225/262 (85%)	-1.57	0 100 100	10, 20, 34, 47	1 (0%)
1	D	224/262 (85%)	-1.64	0 100 100	8, 13, 26, 59	0
All	All	897/1048 (85%)	-1.61	0 100 100	7, 16, 32, 59	1 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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, 95th 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 ²)	Q<0.9
2	CL	C	301	1/1	0.99	0.04	24,24,24,24	0
2	CL	D	301	1/1	0.99	0.04	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.