



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:27 am BST

PDB ID : 4ZG5  
Title : Structural and functional insights into Survival endonuclease, an important virulence factor of Brucella abortus  
Authors : Tarique, K.F.; Abdul Rehman, S.A.; Devi, S.; Gourinath, S.  
Deposited on : 2015-04-22  
Resolution : 1.90 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.

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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)	:	1.13
EDS	:	2.11
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)	:	2.11

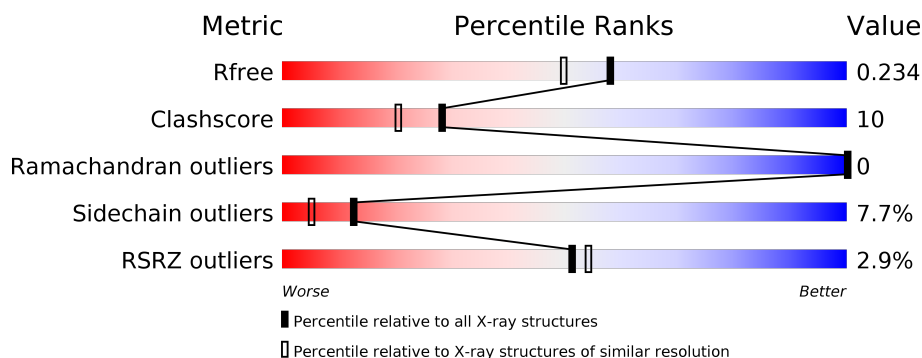
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	263	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>• 6%</div> </div> </div>
1	C	263	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>• • 5%</div> </div> </div>
1	D	263	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• •</div> </div> </div>
1	G	263	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>• 6%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7696 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 5'-nucleotidase SurE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	252	Total	C	N	O	S	0	0	0
			1894	1186	342	357	9			
1	A	247	Total	C	N	O	S	0	0	0
			1861	1167	337	348	9			
1	C	249	Total	C	N	O	S	0	0	0
			1869	1172	334	354	9			
1	G	247	Total	C	N	O	S	0	0	0
			1853	1160	337	347	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	256	LEU	-	expression tag	UNP B2S5B9
D	257	GLU	-	expression tag	UNP B2S5B9
D	258	HIS	-	expression tag	UNP B2S5B9
D	259	HIS	-	expression tag	UNP B2S5B9
D	260	HIS	-	expression tag	UNP B2S5B9
D	261	HIS	-	expression tag	UNP B2S5B9
D	262	HIS	-	expression tag	UNP B2S5B9
D	263	HIS	-	expression tag	UNP B2S5B9
A	256	LEU	-	expression tag	UNP B2S5B9
A	257	GLU	-	expression tag	UNP B2S5B9
A	258	HIS	-	expression tag	UNP B2S5B9
A	259	HIS	-	expression tag	UNP B2S5B9
A	260	HIS	-	expression tag	UNP B2S5B9
A	261	HIS	-	expression tag	UNP B2S5B9
A	262	HIS	-	expression tag	UNP B2S5B9
A	263	HIS	-	expression tag	UNP B2S5B9
C	256	LEU	-	expression tag	UNP B2S5B9
C	257	GLU	-	expression tag	UNP B2S5B9
C	258	HIS	-	expression tag	UNP B2S5B9
C	259	HIS	-	expression tag	UNP B2S5B9
C	260	HIS	-	expression tag	UNP B2S5B9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	261	HIS	-	expression tag	UNP B2S5B9
C	262	HIS	-	expression tag	UNP B2S5B9
C	263	HIS	-	expression tag	UNP B2S5B9
G	256	LEU	-	expression tag	UNP B2S5B9
G	257	GLU	-	expression tag	UNP B2S5B9
G	258	HIS	-	expression tag	UNP B2S5B9
G	259	HIS	-	expression tag	UNP B2S5B9
G	260	HIS	-	expression tag	UNP B2S5B9
G	261	HIS	-	expression tag	UNP B2S5B9
G	262	HIS	-	expression tag	UNP B2S5B9
G	263	HIS	-	expression tag	UNP B2S5B9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

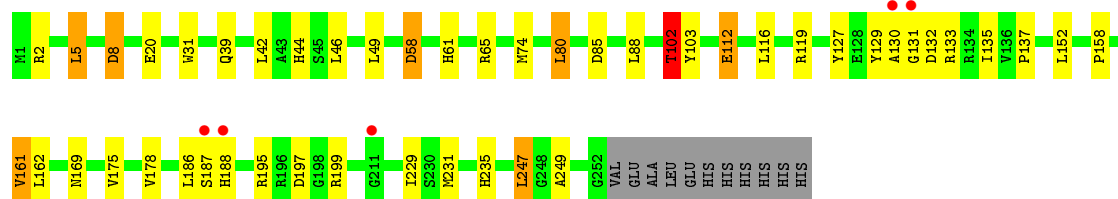
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	64	Total O 64 64	0	0
3	A	51	Total O 51 51	0	0
3	C	56	Total O 56 56	0	0
3	G	44	Total O 44 44	0	0

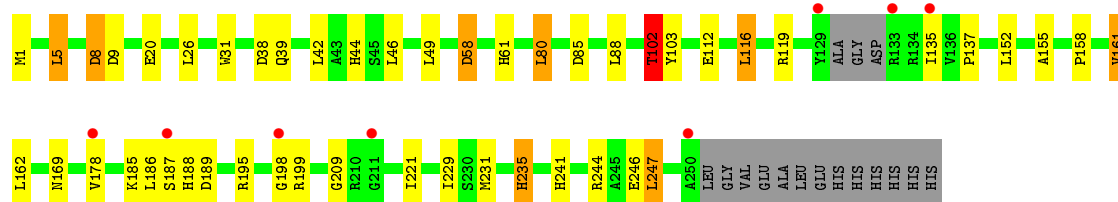
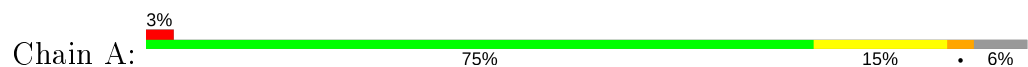
### 3 Residue-property plots [i](#)

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.

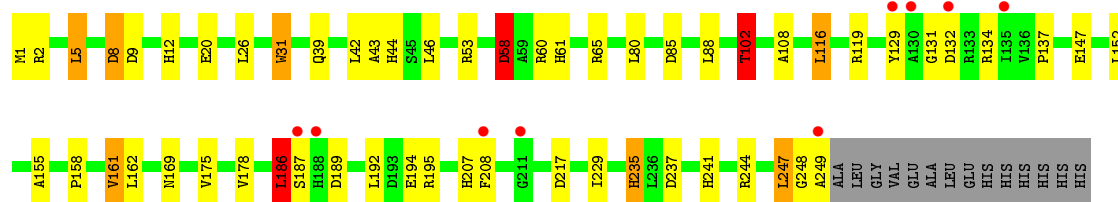
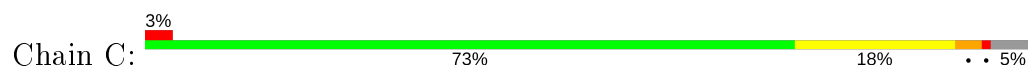
#### • Molecule 1: 5'-nucleotidase SurE



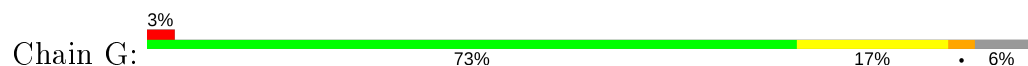
#### • Molecule 1: 5'-nucleotidase SurE

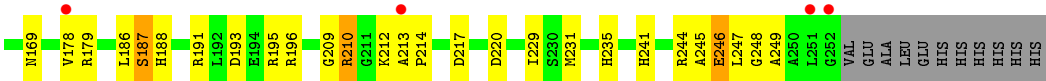


#### • Molecule 1: 5'-nucleotidase SurE



#### • Molecule 1: 5'-nucleotidase SurE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.18 Å 121.07 Å 82.43 Å 90.00° 93.58° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 41.37 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-1.90) 97.7 (41.37-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 1.89 Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.198 , 0.227 0.207 , 0.234	Depositor DCC
$R_{free}$ test set	3807 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7696	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: MG

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	0.96	1/1898 (0.1%)	1.14	8/2582 (0.3%)
1	C	1.02	4/1906 (0.2%)	1.17	15/2595 (0.6%)
1	D	0.99	3/1932 (0.2%)	1.10	11/2629 (0.4%)
1	G	0.91	0/1889	1.07	13/2569 (0.5%)
All	All	0.97	8/7625 (0.1%)	1.12	47/10375 (0.5%)

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
1	C	0	1
1	D	0	1
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	THR	CB-CG2	-6.97	1.29	1.52
1	C	58	ASP	CB-CG	-6.65	1.37	1.51
1	C	31	TRP	CB-CG	-6.57	1.38	1.50
1	D	102	THR	CB-CG2	-6.38	1.31	1.52
1	C	102	THR	CB-CG2	-6.07	1.32	1.52
1	C	248	GLY	N-CA	5.82	1.54	1.46
1	D	127	TYR	CE2-CZ	-5.45	1.31	1.38
1	D	112	GLU	CD-OE1	-5.07	1.20	1.25

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ASP	CB-CG-OD1	15.76	132.48	118.30
1	A	8	ASP	OD1-CG-OD2	-8.36	107.43	123.30
1	C	195	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	D	195	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	A	9	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	G	193	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	C	58	ASP	CB-CA-C	-7.21	95.99	110.40
1	D	195	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	C	8	ASP	CB-CG-OD2	7.09	124.68	118.30
1	C	195	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	G	195	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	C	217	ASP	CB-CG-OD1	-6.82	112.16	118.30
1	C	9	ASP	CB-CG-OD1	6.70	124.33	118.30
1	G	38	ASP	N-CA-CB	6.57	122.42	110.60
1	D	133	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	C	58	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	C	9	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	D	8	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	D	8	ASP	CB-CG-OD2	6.20	123.88	118.30
1	G	9	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	247	LEU	N-CA-C	6.02	127.25	111.00
1	A	80	LEU	CB-CG-CD2	6.00	121.20	111.00
1	D	2	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	58	ASP	CB-CG-OD1	5.82	123.54	118.30
1	G	38	ASP	CB-CA-C	-5.80	98.81	110.40
1	C	207	HIS	CB-CA-C	-5.72	98.96	110.40
1	D	80	LEU	CB-CG-CD2	5.66	120.62	111.00
1	A	195	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	G	195	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	G	193	ASP	CB-CG-OD1	5.61	123.35	118.30
1	G	60	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	G	9	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	186	LEU	CA-CB-CG	5.37	127.64	115.30
1	D	65	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	G	39	GLN	N-CA-C	5.32	125.35	111.00
1	D	197	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	195	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	D	133	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	G	8	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	G	220	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	65	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	C	53	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	2	ARG	NE-CZ-NH1	5.06	122.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	MET	CA-CB-CG	-5.04	104.73	113.30
1	C	237	ASP	CB-CG-OD1	5.02	122.82	118.30
1	G	42	LEU	CB-CG-CD1	5.01	119.52	111.00
1	D	58	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	GLY	Peptide
1	A	246	GLU	Peptide
1	A	247	LEU	Peptide
1	C	58	ASP	Mainchain
1	D	130	ALA	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	1861	0	1833	57	0
1	C	1869	0	1838	33	0
1	D	1894	0	1864	46	0
1	G	1853	0	1827	47	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	G	1	0	0	0	0
3	A	51	0	0	2	0
3	C	56	0	0	2	0
3	D	64	0	0	1	0
3	G	44	0	0	3	0
All	All	7696	0	7362	146	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 10.

All (146) 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:D:39:GLN:NE2	1:D:42:LEU:CD2	2.23	1.01
1:A:49:LEU:HD13	1:G:39:GLN:OE1	1.69	0.90
1:A:186:LEU:HD11	1:A:221:ILE:CD1	2.04	0.88
1:D:39:GLN:HE21	1:D:42:LEU:CD2	1.90	0.83
1:G:246:GLU:H	1:G:246:GLU:CD	1.81	0.82
1:A:39:GLN:OE1	1:A:42:LEU:CD2	2.30	0.79
1:D:39:GLN:HE21	1:D:42:LEU:HD23	1.48	0.78
1:A:116:LEU:CD1	1:G:188:HIS:CD2	2.67	0.78
1:D:39:GLN:NE2	1:D:42:LEU:HD23	1.99	0.77
1:C:39:GLN:OE1	1:C:42:LEU:CD2	2.34	0.75
1:A:116:LEU:HD12	1:G:188:HIS:CD2	2.22	0.74
1:A:116:LEU:HD11	1:G:188:HIS:NE2	2.03	0.74
1:A:152:LEU:O	1:A:155:ALA:O	2.05	0.73
1:A:186:LEU:HD11	1:A:221:ILE:HD12	1.69	0.73
1:G:152:LEU:O	1:G:155:ALA:O	2.07	0.72
1:C:152:LEU:O	1:C:155:ALA:O	2.06	0.72
1:C:39:GLN:HB3	1:C:42:LEU:HD22	1.71	0.72
1:A:235:HIS:HE1	3:G:430:HOH:O	1.71	0.72
1:G:246:GLU:CD	1:G:246:GLU:N	2.40	0.72
1:A:39:GLN:HB3	1:A:42:LEU:HD22	1.71	0.71
1:D:39:GLN:HB3	1:D:42:LEU:HD22	1.74	0.69
1:D:44:HIS:CD2	1:C:102:THR:HG22	2.28	0.68
1:D:44:HIS:HD2	1:C:102:THR:HG22	1.56	0.68
1:A:112:GLU:OE2	1:G:188:HIS:CE1	2.49	0.66
1:G:246:GLU:OE2	1:G:246:GLU:N	2.29	0.66
1:D:44:HIS:HD2	1:C:102:THR:CG2	2.10	0.64
1:D:44:HIS:CD2	1:C:102:THR:CG2	2.81	0.64
1:A:241:HIS:HD2	1:A:244:ARG:HH11	1.46	0.64
1:A:188:HIS:CD2	1:G:116:LEU:CD1	2.81	0.64
1:A:186:LEU:N	1:A:186:LEU:HD12	2.14	0.63
1:C:241:HIS:HD2	1:C:244:ARG:HH11	1.45	0.63
1:A:186:LEU:CD1	1:A:221:ILE:CD1	2.75	0.62
1:D:49:LEU:HD23	1:A:199:ARG:NH2	2.14	0.62
1:G:245:ALA:O	1:G:247:LEU:N	2.33	0.61
1:A:235:HIS:CE1	3:G:430:HOH:O	2.49	0.61
1:D:58:ASP:OD1	1:D:61:HIS:HD2	1.82	0.61
1:A:116:LEU:CD1	1:G:188:HIS:NE2	2.64	0.60
1:D:158:PRO:O	1:D:161:VAL:HG13	2.00	0.60
1:D:31:TRP:CD2	1:D:80:LEU:HD22	2.36	0.60
1:D:49:LEU:CD2	1:A:199:ARG:HH22	2.15	0.60
1:G:158:PRO:O	1:G:161:VAL:HG13	2.02	0.60
1:A:39:GLN:OE1	1:A:42:LEU:HD23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:TYR:OH	1:D:188:HIS:HE1	1.84	0.60
1:G:38:ASP:C	1:G:39:GLN:HG2	2.22	0.59
1:D:39:GLN:NE2	1:D:42:LEU:HD21	2.14	0.59
1:G:196:ARG:HD3	3:G:421:HOH:O	2.02	0.59
1:A:186:LEU:HD11	1:A:221:ILE:HD13	1.84	0.59
1:A:158:PRO:O	1:A:161:VAL:HG13	2.02	0.58
1:A:112:GLU:OE2	1:G:188:HIS:HE1	1.85	0.58
1:D:247:LEU:HD22	1:D:247:LEU:O	2.03	0.58
1:C:158:PRO:O	1:C:161:VAL:HG13	2.02	0.57
1:A:31:TRP:CD2	1:A:80:LEU:HD22	2.40	0.57
1:D:178:VAL:HG12	1:D:229:ILE:HB	1.86	0.57
1:G:38:ASP:OD2	1:G:38:ASP:C	2.44	0.56
1:G:31:TRP:CD2	1:G:80:LEU:HD22	2.40	0.56
1:D:188:HIS:CD2	1:C:116:LEU:CD1	2.89	0.55
1:A:20:GLU:OE1	1:A:61:HIS:HE1	1.90	0.55
1:A:116:LEU:HD11	1:G:188:HIS:CD2	2.37	0.55
1:A:58:ASP:OD1	1:A:61:HIS:HD2	1.88	0.55
1:A:103:TYR:OH	1:A:188:HIS:HE1	1.89	0.55
1:C:39:GLN:OE1	1:C:42:LEU:HD23	2.07	0.54
1:C:147:GLU:HG3	1:C:147:GLU:O	1.96	0.54
1:C:20:GLU:OE1	1:C:61:HIS:HE1	1.91	0.54
1:G:178:VAL:HG12	1:G:229:ILE:HB	1.89	0.54
1:A:186:LEU:CD1	1:A:221:ILE:HD12	2.36	0.53
1:A:116:LEU:HD12	1:G:188:HIS:CG	2.43	0.53
1:C:178:VAL:HG12	1:C:229:ILE:HB	1.89	0.53
1:D:247:LEU:HD22	1:D:247:LEU:C	2.30	0.52
1:C:247:LEU:O	1:C:249:ALA:HB3	2.09	0.52
1:D:20:GLU:OE1	1:D:61:HIS:HE1	1.93	0.52
1:G:158:PRO:O	1:G:161:VAL:CG1	2.58	0.52
1:A:44:HIS:ND1	1:G:102:THR:HG22	2.25	0.52
1:G:213:ALA:HB1	1:G:214:PRO:HD2	1.91	0.51
1:D:39:GLN:NE2	1:D:42:LEU:HD22	2.21	0.51
1:A:185:LYS:C	1:A:186:LEU:HD12	2.31	0.50
1:A:178:VAL:HG12	1:A:229:ILE:HB	1.92	0.50
1:G:20:GLU:OE1	1:G:61:HIS:HE1	1.93	0.50
1:D:44:HIS:HE1	1:D:112:GLU:OE1	1.94	0.50
1:C:31:TRP:CD2	1:C:80:LEU:HD22	2.46	0.50
1:G:241:HIS:HD2	1:G:244:ARG:HH11	1.59	0.50
1:C:158:PRO:O	1:C:161:VAL:CG1	2.60	0.50
1:A:188:HIS:CD2	1:G:116:LEU:HD12	2.47	0.50
1:A:85:ASP:O	1:A:119:ARG:CG	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PRO:O	1:A:161:VAL:CG1	2.60	0.49
1:A:5:LEU:HD12	1:A:88:LEU:HB2	1.92	0.49
1:C:194:GLU:OE1	3:C:401:HOH:O	2.19	0.49
1:D:74:MET:HA	1:C:192:LEU:HD11	1.95	0.49
1:D:158:PRO:O	1:D:161:VAL:CG1	2.60	0.49
1:D:49:LEU:HD23	1:A:199:ARG:HH22	1.75	0.48
1:A:102:THR:CG2	1:G:44:HIS:ND1	2.76	0.48
1:G:246:GLU:OE2	1:G:246:GLU:CA	2.58	0.48
1:G:58:ASP:OD2	1:G:61:HIS:HD2	1.96	0.48
1:D:102:THR:CG2	1:C:44:HIS:ND1	2.77	0.47
1:D:188:HIS:CD2	1:C:116:LEU:HD12	2.49	0.47
1:A:39:GLN:CB	1:A:42:LEU:HD22	2.43	0.47
1:D:102:THR:HG22	1:C:44:HIS:ND1	2.30	0.47
1:D:49:LEU:CD2	1:A:199:ARG:NH2	2.75	0.47
1:C:5:LEU:HD12	1:C:88:LEU:HB2	1.97	0.47
1:A:38:ASP:OD1	3:A:401:HOH:O	2.21	0.47
1:D:5:LEU:HD12	1:D:88:LEU:HB2	1.96	0.47
1:C:186:LEU:O	1:C:186:LEU:HD12	2.15	0.47
1:C:137:PRO:HG3	1:C:169:ASN:HD22	1.79	0.46
1:G:137:PRO:HG3	1:G:169:ASN:HD22	1.79	0.46
1:A:137:PRO:HG3	1:A:169:ASN:HD22	1.79	0.46
1:D:137:PRO:HG3	1:D:169:ASN:HD22	1.81	0.46
1:D:199:ARG:NH2	1:A:49:LEU:HD23	2.30	0.46
1:G:248:GLY:HA2	1:G:249:ALA:HA	1.80	0.46
1:A:1:MET:N	3:A:405:HOH:O	2.48	0.46
1:G:5:LEU:HD12	1:G:88:LEU:HB2	1.98	0.46
1:C:58:ASP:HB3	1:C:60:ARG:H	1.80	0.46
1:D:186:LEU:O	1:D:186:LEU:HD12	2.16	0.45
1:G:187:SER:CB	1:G:212:LYS:H	2.29	0.45
1:G:152:LEU:HD21	1:G:231:MET:SD	2.56	0.45
1:G:186:LEU:HD12	1:G:186:LEU:O	2.16	0.45
1:D:85:ASP:O	1:D:119:ARG:CG	2.64	0.45
1:D:152:LEU:HD21	1:D:231:MET:SD	2.56	0.45
1:D:44:HIS:CE1	1:D:112:GLU:OE1	2.70	0.44
1:A:116:LEU:CD1	1:G:188:HIS:CE1	3.01	0.43
3:D:427:HOH:O	1:C:235:HIS:HE1	2.00	0.43
1:G:186:LEU:HD12	1:G:186:LEU:C	2.39	0.43
1:A:152:LEU:HD21	1:A:231:MET:SD	2.59	0.43
1:D:103:TYR:CE1	1:C:44:HIS:CE1	3.06	0.43
1:G:210:ARG:HD2	1:G:210:ARG:HA	1.85	0.43
1:D:129:TYR:HB3	1:D:131:GLY:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:TYR:HB3	1:C:131:GLY:O	2.19	0.42
1:A:49:LEU:CD1	1:G:39:GLN:OE1	2.54	0.42
1:A:44:HIS:ND1	1:G:102:THR:CG2	2.82	0.42
1:D:49:LEU:HD21	1:A:199:ARG:HH22	1.82	0.42
1:A:186:LEU:N	1:A:186:LEU:CD1	2.80	0.42
1:D:74:MET:HA	1:C:192:LEU:CD1	2.50	0.42
1:C:43:ALA:O	1:C:108:ALA:CB	2.68	0.42
1:G:191:ARG:CZ	1:G:209:GLY:HA3	2.50	0.42
1:D:103:TYR:OH	1:D:188:HIS:CE1	2.71	0.41
1:D:58:ASP:OD1	1:D:61:HIS:CD2	2.67	0.41
1:A:188:HIS:HD2	1:G:116:LEU:HD12	1.83	0.41
1:A:102:THR:HG22	1:G:44:HIS:ND1	2.34	0.41
1:C:85:ASP:O	1:C:119:ARG:CG	2.68	0.41
1:G:85:ASP:O	1:G:119:ARG:CG	2.69	0.41
1:G:213:ALA:HB1	1:G:214:PRO:CD	2.51	0.41
1:C:12:HIS:CE1	3:C:429:HOH:O	2.74	0.41
1:A:189:ASP:HB3	1:A:209:GLY:O	2.20	0.41
1:D:199:ARG:HH22	1:A:49:LEU:HD23	1.86	0.41
1:D:247:LEU:HD23	1:D:249:ALA:H	1.86	0.41
1:A:188:HIS:HD2	1:G:116:LEU:CD1	2.34	0.40
1:A:31:TRP:CG	1:A:80:LEU:HD22	2.56	0.40
1:D:31:TRP:CG	1:D:80:LEU:HD22	2.56	0.40

There are no symmetry-related clashes.

## 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	243/263 (92%)	236 (97%)	7 (3%)	0	100	100
1	C	247/263 (94%)	242 (98%)	5 (2%)	0	100	100
1	D	250/263 (95%)	241 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	243/263 (92%)	236 (97%)	7 (3%)	0	100	100
All	All	983/1052 (93%)	955 (97%)	28 (3%)	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	190/207 (92%)	179 (94%)	11 (6%)	20	10
1	C	191/207 (92%)	173 (91%)	18 (9%)	8	3
1	D	193/207 (93%)	180 (93%)	13 (7%)	16	7
1	G	189/207 (91%)	172 (91%)	17 (9%)	9	3
All	All	763/828 (92%)	704 (92%)	59 (8%)	13	5

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	5	LEU
1	D	8	ASP
1	D	46	LEU
1	D	102	THR
1	D	116	LEU
1	D	132	ASP
1	D	135	ILE
1	D	161	VAL
1	D	162	LEU
1	D	175	VAL
1	D	187	SER
1	D	235	HIS
1	D	247	LEU
1	A	5	LEU
1	A	8	ASP
1	A	26	LEU

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Mol	Chain	Res	Type
1	A	46	LEU
1	A	102	THR
1	A	116	LEU
1	A	135	ILE
1	A	161	VAL
1	A	162	LEU
1	A	187	SER
1	A	235	HIS
1	C	5	LEU
1	C	8	ASP
1	C	26	LEU
1	C	46	LEU
1	C	58	ASP
1	C	102	THR
1	C	116	LEU
1	C	132	ASP
1	C	134	ARG
1	C	161	VAL
1	C	162	LEU
1	C	175	VAL
1	C	186	LEU
1	C	187	SER
1	C	189	ASP
1	C	208	PHE
1	C	235	HIS
1	C	247	LEU
1	G	5	LEU
1	G	8	ASP
1	G	26	LEU
1	G	38	ASP
1	G	46	LEU
1	G	102	THR
1	G	116	LEU
1	G	134	ARG
1	G	135	ILE
1	G	161	VAL
1	G	162	LEU
1	G	179	ARG
1	G	187	SER
1	G	210	ARG
1	G	217	ASP
1	G	235	HIS

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Mol	Chain	Res	Type
1	G	246	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	39	GLN
1	D	44	HIS
1	D	61	HIS
1	D	96	ASN
1	D	125	GLN
1	D	169	ASN
1	D	188	HIS
1	D	241	HIS
1	A	61	HIS
1	A	125	GLN
1	A	169	ASN
1	A	188	HIS
1	A	241	HIS
1	C	61	HIS
1	C	96	ASN
1	C	125	GLN
1	C	169	ASN
1	C	241	HIS
1	G	61	HIS
1	G	125	GLN
1	G	169	ASN
1	G	188	HIS
1	G	241	HIS

### 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 4 ligands modelled in this entry, 4 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 ⓘ

### 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	247/263 (93%)	0.15	8 (3%) 47 50	24, 38, 67, 94	0
1	C	249/263 (94%)	0.08	9 (3%) 42 45	24, 36, 68, 83	0
1	D	252/263 (95%)	-0.04	5 (1%) 65 68	24, 35, 66, 84	0
1	G	247/263 (93%)	0.13	7 (2%) 53 56	26, 41, 71, 79	0
All	All	995/1052 (94%)	0.08	29 (2%) 51 54	24, 37, 68, 94	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	GLY	4.8
1	C	129	TYR	4.7
1	G	135	ILE	4.1
1	A	135	ILE	4.0
1	G	28	ASP	3.6
1	G	251	LEU	3.6
1	A	211	GLY	3.4
1	G	213	ALA	3.3
1	C	249	ALA	3.3
1	G	178	VAL	3.3
1	C	130	ALA	3.3
1	C	208	PHE	3.2
1	C	211	GLY	3.1
1	C	135	ILE	3.0
1	A	187	SER	3.0
1	A	133	ARG	2.9
1	C	132	ASP	2.8
1	G	252	GLY	2.6
1	D	188	HIS	2.4
1	C	188	HIS	2.4
1	G	134	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	131	GLY	2.4
1	A	250	ALA	2.3
1	A	129	TYR	2.2
1	C	187	SER	2.2
1	D	130	ALA	2.2
1	D	187	SER	2.1
1	D	211	GLY	2.1
1	A	178	VAL	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 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. 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	MG	A	301	1/1	0.85	0.06	31,31,31,31	0
2	MG	D	301	1/1	0.98	0.04	28,28,28,28	0
2	MG	C	301	1/1	0.98	0.05	26,26,26,26	0
2	MG	G	301	1/1	0.99	0.07	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.