Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 06:09 pm GMT

PDB ID	:	7PQ2
Title	:	Crystal Structure of the Ring Nuclease 0811 from Sulfolobus islandicus (Sis0811) in its apo form
Authors	:	Molina, R.; Jensen, A.L.G.; Marchena-Hurtado, J.; Lopez-Mendez, B.; Stella, S.; Montoya, G.
Deposited on	:	2021-09-16
Resolution	:	2.38 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:

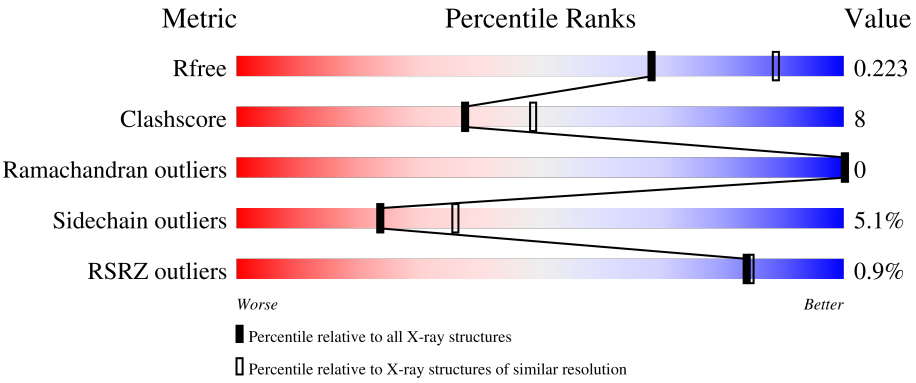
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 <=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	AAA	275	84% 15%
1	BBB	275	2% 79% 19%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4696 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 CRISPR-associated protein, APE2256 family, CRISPR Ring Nuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	275	Total	C	N	O	S	0	0	0
			2234	1443	358	431	2			
1	BBB	272	Total	C	N	O	S	0	0	0
			2208	1427	355	424	2			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	269	GLY	-	expression tag	UNP F0NH89
AAA	270	SER	-	expression tag	UNP F0NH89
AAA	271	GLU	-	expression tag	UNP F0NH89
AAA	272	PHE	-	expression tag	UNP F0NH89
AAA	273	GLU	-	expression tag	UNP F0NH89
AAA	274	LEU	-	expression tag	UNP F0NH89
AAA	275	GLU	-	expression tag	UNP F0NH89
BBB	269	GLY	-	expression tag	UNP F0NH89
BBB	270	SER	-	expression tag	UNP F0NH89
BBB	271	GLU	-	expression tag	UNP F0NH89
BBB	272	PHE	-	expression tag	UNP F0NH89
BBB	273	GLU	-	expression tag	UNP F0NH89
BBB	274	LEU	-	expression tag	UNP F0NH89
BBB	275	GLU	-	expression tag	UNP F0NH89

- Molecule 2 is water.

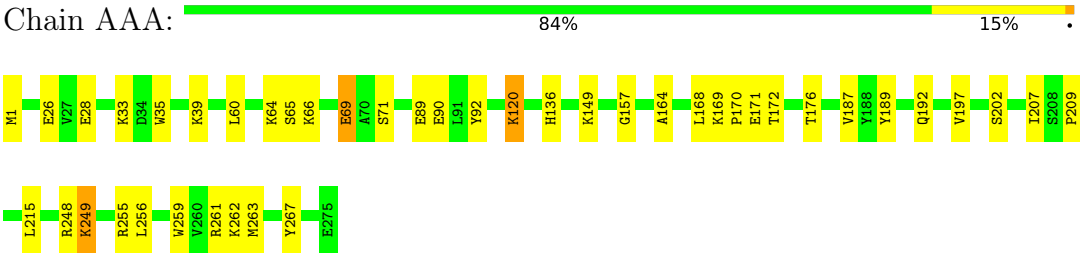
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	132	Total	O	0	0
			132	132		
2	BBB	122	Total	O	0	0
			122	122		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

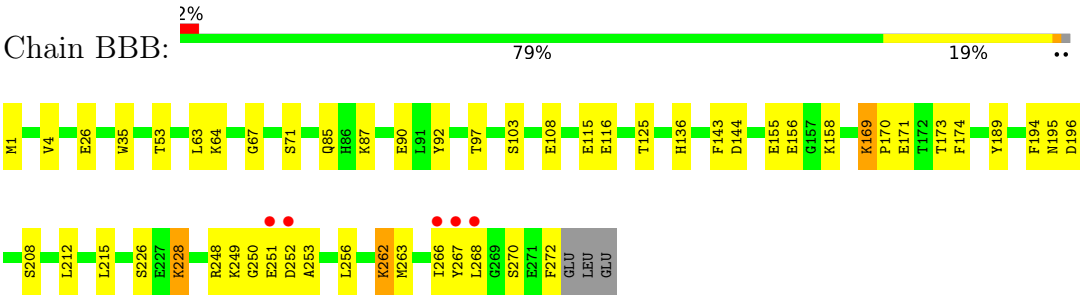
• Molecule 1: CRISPR-associated protein, APE2256 family, CRISPR Ring Nuclease

Chain AAA:



• Molecule 1: CRISPR-associated protein, APE2256 family, CRISPR Ring Nuclease

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	77.37Å 106.44Å 78.44Å 90.00° 102.92° 90.00°	Depositor
Resolution (Å)	61.61 – 2.38 61.53 – 2.38	Depositor EDS
% Data completeness (in resolution range)	95.1 (61.61-2.38) 95.1 (61.53-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.163 , 0.223 0.163 , 0.223	Depositor DCC
R_{free} test set	1176 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4696	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	AAA	0.55	2/2275 (0.1%)	0.88	1/3067 (0.0%)
1	BBB	0.60	4/2249 (0.2%)	0.88	0/3032
All	All	0.58	6/4524 (0.1%)	0.88	1/6099 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	156	GLU	CD-OE2	6.41	1.32	1.25
1	BBB	155	GLU	CD-OE2	6.03	1.32	1.25
1	AAA	90	GLU	CD-OE1	5.58	1.31	1.25
1	BBB	90	GLU	CD-OE1	5.36	1.31	1.25
1	BBB	108	GLU	CD-OE1	5.25	1.31	1.25
1	AAA	171	GLU	CD-OE2	5.09	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	261	ARG	NE-CZ-NH2	-5.55	117.53	120.30

There are no chirality outliers.

There are no planarity outliers.

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	AAA	2234	0	2263	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BBB	2208	0	2240	47	0
2	AAA	132	0	0	6	0
2	BBB	122	0	0	8	0
All	All	4696	0	4503	69	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 8.

All (69) 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:AAA:136:HIS:HD2	2:AAA:420:HOH:O	1.59	0.84
1:BBB:85:GLN:HG2	2:BBB:419:HOH:O	1.76	0.82
1:BBB:143:PHE:HB3	1:BBB:266:ILE:CD1	2.10	0.81
1:BBB:250:GLY:HA3	1:BBB:253:ALA:HB3	1.63	0.80
1:BBB:136:HIS:HD2	2:BBB:408:HOH:O	1.64	0.79
1:BBB:228:LYS:HB2	1:BBB:228:LYS:HZ3	1.55	0.72
1:BBB:228:LYS:HB2	1:BBB:228:LYS:NZ	2.04	0.71
1:BBB:196:ASP:HA	2:BBB:313:HOH:O	1.89	0.71
1:AAA:172:THR:HG22	2:AAA:361:HOH:O	1.92	0.69
1:BBB:1:MET:O	1:BBB:158:LYS:HE3	1.92	0.69
1:BBB:226:SER:HB2	1:BBB:228:LYS:NZ	2.10	0.66
1:AAA:259:TRP:HZ3	1:AAA:263:MET:HE3	1.62	0.65
1:BBB:143:PHE:CZ	1:BBB:263:MET:HG3	2.30	0.65
1:BBB:115:GLU:HB2	2:BBB:333:HOH:O	1.97	0.64
1:BBB:263:MET:HG2	1:BBB:267:TYR:CE2	2.33	0.63
1:AAA:172:THR:HG21	1:BBB:169:LYS:HZ1	1.64	0.61
1:BBB:212:LEU:HD21	1:BBB:268:LEU:HD13	1.83	0.60
1:AAA:69:GLU:HB3	2:AAA:371:HOH:O	2.02	0.59
1:BBB:143:PHE:HB3	1:BBB:266:ILE:HD12	1.85	0.59
1:BBB:204:PRO:HA	2:BBB:357:HOH:O	2.03	0.58
1:BBB:226:SER:HB2	1:BBB:228:LYS:HZ1	1.71	0.56
1:BBB:53:THR:HG23	2:BBB:328:HOH:O	2.07	0.55
1:AAA:189:TYR:CE2	1:BBB:170:PRO:HG3	2.42	0.55
1:AAA:28:GLU:OE1	1:AAA:33:LYS:HD3	2.06	0.55
1:AAA:120:LYS:NZ	2:AAA:304:HOH:O	2.38	0.54
1:AAA:164:ALA:O	1:BBB:169:LYS:NZ	2.41	0.53
1:AAA:172:THR:HG21	1:BBB:169:LYS:NZ	2.24	0.52
1:BBB:251:GLU:HG3	1:BBB:252:ASP:H	1.76	0.51
1:AAA:189:TYR:CD2	1:BBB:170:PRO:HG3	2.47	0.50
1:AAA:169:LYS:HB3	1:AAA:170:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:170:PRO:HG3	1:BBB:189:TYR:CE2	2.48	0.48
1:BBB:262:LYS:HA	1:BBB:262:LYS:HD3	1.71	0.48
1:BBB:263:MET:HG2	1:BBB:267:TYR:CD2	2.48	0.48
1:AAA:157:GLY:HA2	2:AAA:325:HOH:O	2.14	0.47
1:BBB:67:GLY:HA2	2:BBB:392:HOH:O	2.14	0.47
1:BBB:144:ASP:OD1	1:BBB:262:LYS:NZ	2.47	0.47
1:AAA:249:LYS:HG2	1:AAA:255:ARG:HB2	1.97	0.46
1:AAA:168:LEU:O	1:AAA:172:THR:HG23	2.17	0.45
1:BBB:26:GLU:HA	1:BBB:26:GLU:OE1	2.16	0.45
1:AAA:207:ILE:HD12	1:AAA:267:TYR:HE1	1.81	0.45
1:AAA:215:LEU:HD22	1:AAA:256:LEU:HD11	1.99	0.45
1:BBB:143:PHE:CE2	1:BBB:174:PHE:HZ	2.35	0.44
1:AAA:176:THR:HG21	1:BBB:173:THR:CG2	2.48	0.44
1:BBB:136:HIS:CD2	2:BBB:408:HOH:O	2.51	0.44
1:BBB:143:PHE:CE1	1:BBB:263:MET:HG3	2.51	0.44
1:BBB:215:LEU:HD22	1:BBB:256:LEU:HD11	2.00	0.44
1:AAA:136:HIS:CD2	2:AAA:420:HOH:O	2.48	0.43
1:AAA:1:MET:HB3	1:AAA:92:TYR:HB2	2.00	0.43
1:BBB:4:VAL:HA	1:BBB:92:TYR:O	2.19	0.43
1:AAA:60:LEU:O	1:AAA:64:LYS:HG2	2.19	0.43
1:BBB:97:THR:OG1	1:BBB:103:SER:HB3	2.19	0.43
1:AAA:259:TRP:HZ3	1:AAA:263:MET:CE	2.30	0.43
1:AAA:89:GLU:CD	1:AAA:89:GLU:H	2.23	0.42
1:BBB:64:LYS:HE2	1:BBB:116:GLU:OE2	2.19	0.42
1:AAA:26:GLU:OE2	1:AAA:26:GLU:HA	2.20	0.42
1:BBB:263:MET:HG2	1:BBB:267:TYR:HE2	1.82	0.42
1:AAA:169:LYS:N	1:AAA:170:PRO:HD2	2.35	0.42
1:AAA:33:LYS:HD2	1:AAA:33:LYS:HA	1.83	0.41
1:BBB:251:GLU:HG3	1:BBB:252:ASP:N	2.34	0.41
1:BBB:63:LEU:HD12	1:BBB:63:LEU:HA	1.90	0.41
1:BBB:263:MET:CG	1:BBB:267:TYR:HE2	2.33	0.41
1:BBB:228:LYS:NZ	1:BBB:228:LYS:CB	2.75	0.41
1:BBB:262:LYS:HZ2	1:BBB:262:LYS:HG2	1.61	0.41
1:BBB:97:THR:O	1:BBB:125:THR:HA	2.21	0.40
1:BBB:194:PHE:O	1:BBB:195:ASN:C	2.59	0.40
1:AAA:176:THR:HG23	1:AAA:187:VAL:HG21	2.02	0.40
1:AAA:211:TYR:CD2	1:BBB:204:PRO:HG2	2.55	0.40
1:AAA:262:LYS:HA	1:AAA:262:LYS:HD3	1.94	0.40
1:BBB:248:ARG:O	1:BBB:248:ARG:HG3	2.21	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	AAA	273/275 (99%)	270 (99%)	3 (1%)	0	100	100
1	BBB	270/275 (98%)	263 (97%)	7 (3%)	0	100	100
All	All	543/550 (99%)	533 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	245/245 (100%)	231 (94%)	14 (6%)	20	30
1	BBB	242/245 (99%)	231 (96%)	11 (4%)	27	41
All	All	487/490 (99%)	462 (95%)	25 (5%)	24	36

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	35	TRP
1	AAA	39	LYS
1	AAA	65	SER
1	AAA	66	LYS
1	AAA	69	GLU
1	AAA	71	SER
1	AAA	120	LYS
1	AAA	149	LYS

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Mol	Chain	Res	Type
1	AAA	192	GLN
1	AAA	197	VAL
1	AAA	202	SER
1	AAA	209	PRO
1	AAA	248	ARG
1	AAA	249	LYS
1	BBB	35	TRP
1	BBB	71	SER
1	BBB	87	LYS
1	BBB	169	LYS
1	BBB	171	GLU
1	BBB	208	SER
1	BBB	228	LYS
1	BBB	249	LYS
1	BBB	262	LYS
1	BBB	270	SER
1	BBB	272	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

There are no ligands in this entry.

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^{th} 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	AAA	275/275 (100%)	-0.15	0 100 100	24, 37, 71, 95	0
1	BBB	272/275 (98%)	-0.04	5 (1%) 68 70	19, 35, 84, 120	0
All	All	547/550 (99%)	-0.10	5 (0%) 84 84	19, 37, 78, 120	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	266	ILE	3.9
1	BBB	252	ASP	2.8
1	BBB	267	TYR	2.7
1	BBB	268	LEU	2.4
1	BBB	251	GLU	2.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.