



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 12:34 PM UTC

PDB ID : 3RCC / pdb_00003rcc
Title : Crystal Structure of the Streptococcus agalactiae Sortase A
Authors : Khare, B.; Narayana, S.V.L.
Deposited on : 2011-03-30
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
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

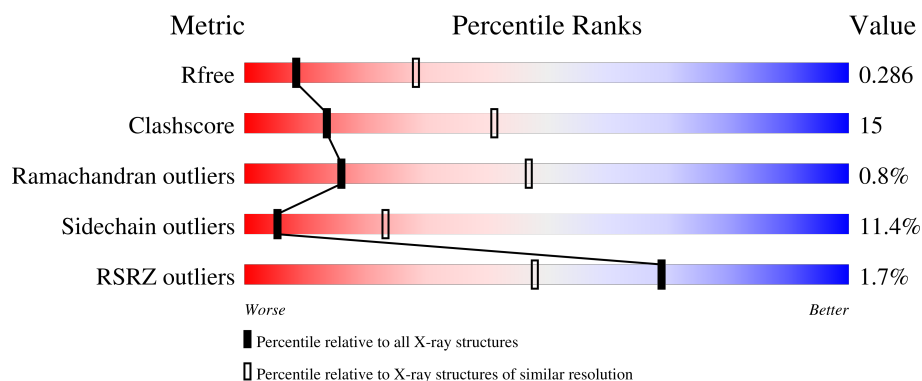
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	160	46% 31% • 19%
1	B	160	2% 48% 27% • 22%
1	C	160	49% 28% • 19%
1	D	160	2% 60% 19% • 19%
1	E	160	54% 22% 8% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	160	
1	G	160	
1	H	160	
1	I	160	
1	J	160	
1	K	160	
1	L	160	
1	M	160	
1	N	160	
1	O	160	
1	P	160	
1	Q	160	
1	R	160	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17807 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 Sortase SrtA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	0
			976	623	161	188	4			
1	B	124	Total	C	N	O	S	0	0	0
			938	601	155	178	4			
1	C	129	Total	C	N	O	S	0	0	0
			973	621	161	187	4			
1	D	129	Total	C	N	O	S	0	0	0
			981	628	161	188	4			
1	E	134	Total	C	N	O	S	0	0	0
			1011	645	166	196	4			
1	F	132	Total	C	N	O	S	0	0	0
			992	632	164	192	4			
1	G	132	Total	C	N	O	S	0	0	0
			992	632	164	192	4			
1	H	130	Total	C	N	O	S	0	0	0
			982	626	162	190	4			
1	I	131	Total	C	N	O	S	0	0	0
			983	627	163	189	4			
1	J	129	Total	C	N	O	S	0	0	0
			980	626	161	189	4			
1	K	129	Total	C	N	O	S	0	0	0
			974	621	161	188	4			
1	L	127	Total	C	N	O	S	0	0	0
			960	613	159	184	4			
1	M	128	Total	C	N	O	S	0	0	0
			964	616	159	185	4			
1	N	137	Total	C	N	O	S	0	0	0
			1031	656	169	202	4			
1	O	131	Total	C	N	O	S	0	0	0
			984	627	163	190	4			
1	P	132	Total	C	N	O	S	0	0	0
			1003	640	164	195	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	133	Total	C	N	O	S	0	0	0
			1009	643	165	197	4			
1	R	125	Total	C	N	O	S	0	0	0
			947	605	157	181	4			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	SER	-	expression tag	UNP Q8DZY1
A	58	ASN	-	expression tag	UNP Q8DZY1
A	59	ALA	-	expression tag	UNP Q8DZY1
B	57	SER	-	expression tag	UNP Q8DZY1
B	58	ASN	-	expression tag	UNP Q8DZY1
B	59	ALA	-	expression tag	UNP Q8DZY1
C	57	SER	-	expression tag	UNP Q8DZY1
C	58	ASN	-	expression tag	UNP Q8DZY1
C	59	ALA	-	expression tag	UNP Q8DZY1
D	57	SER	-	expression tag	UNP Q8DZY1
D	58	ASN	-	expression tag	UNP Q8DZY1
D	59	ALA	-	expression tag	UNP Q8DZY1
E	57	SER	-	expression tag	UNP Q8DZY1
E	58	ASN	-	expression tag	UNP Q8DZY1
E	59	ALA	-	expression tag	UNP Q8DZY1
F	57	SER	-	expression tag	UNP Q8DZY1
F	58	ASN	-	expression tag	UNP Q8DZY1
F	59	ALA	-	expression tag	UNP Q8DZY1
G	57	SER	-	expression tag	UNP Q8DZY1
G	58	ASN	-	expression tag	UNP Q8DZY1
G	59	ALA	-	expression tag	UNP Q8DZY1
H	57	SER	-	expression tag	UNP Q8DZY1
H	58	ASN	-	expression tag	UNP Q8DZY1
H	59	ALA	-	expression tag	UNP Q8DZY1
I	57	SER	-	expression tag	UNP Q8DZY1
I	58	ASN	-	expression tag	UNP Q8DZY1
I	59	ALA	-	expression tag	UNP Q8DZY1
J	57	SER	-	expression tag	UNP Q8DZY1
J	58	ASN	-	expression tag	UNP Q8DZY1
J	59	ALA	-	expression tag	UNP Q8DZY1
K	57	SER	-	expression tag	UNP Q8DZY1
K	58	ASN	-	expression tag	UNP Q8DZY1
K	59	ALA	-	expression tag	UNP Q8DZY1
L	57	SER	-	expression tag	UNP Q8DZY1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	58	ASN	-	expression tag	UNP Q8DZY1
L	59	ALA	-	expression tag	UNP Q8DZY1
M	57	SER	-	expression tag	UNP Q8DZY1
M	58	ASN	-	expression tag	UNP Q8DZY1
M	59	ALA	-	expression tag	UNP Q8DZY1
N	57	SER	-	expression tag	UNP Q8DZY1
N	58	ASN	-	expression tag	UNP Q8DZY1
N	59	ALA	-	expression tag	UNP Q8DZY1
O	57	SER	-	expression tag	UNP Q8DZY1
O	58	ASN	-	expression tag	UNP Q8DZY1
O	59	ALA	-	expression tag	UNP Q8DZY1
P	57	SER	-	expression tag	UNP Q8DZY1
P	58	ASN	-	expression tag	UNP Q8DZY1
P	59	ALA	-	expression tag	UNP Q8DZY1
Q	57	SER	-	expression tag	UNP Q8DZY1
Q	58	ASN	-	expression tag	UNP Q8DZY1
Q	59	ALA	-	expression tag	UNP Q8DZY1
R	57	SER	-	expression tag	UNP Q8DZY1
R	58	ASN	-	expression tag	UNP Q8DZY1
R	59	ALA	-	expression tag	UNP Q8DZY1

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total Zn 5 5	0	0
2	B	6	Total Zn 6 6	0	0
2	C	5	Total Zn 5 5	0	0
2	D	4	Total Zn 4 4	0	0
2	E	4	Total Zn 4 4	0	0
2	F	2	Total Zn 2 2	0	0
2	G	7	Total Zn 7 7	0	0
2	H	4	Total Zn 4 4	0	0
2	I	4	Total Zn 4 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	J	3	Total 3	Zn 3	0	0
2	K	3	Total 3	Zn 3	0	0
2	L	2	Total 2	Zn 2	0	0
2	M	6	Total 6	Zn 6	0	0
2	N	4	Total 4	Zn 4	0	0
2	O	4	Total 4	Zn 4	0	0
2	P	4	Total 4	Zn 4	0	0
2	Q	4	Total 4	Zn 4	0	0
2	R	2	Total 2	Zn 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	O 1	0	0
3	B	4	Total 4	O 4	0	0
3	C	3	Total 3	O 3	0	0
3	D	1	Total 1	O 1	0	0
3	E	3	Total 3	O 3	0	0
3	F	5	Total 5	O 5	0	0
3	G	2	Total 2	O 2	0	0
3	H	1	Total 1	O 1	0	0
3	I	5	Total 5	O 5	0	0
3	J	2	Total 2	O 2	0	0

Continued on next page...

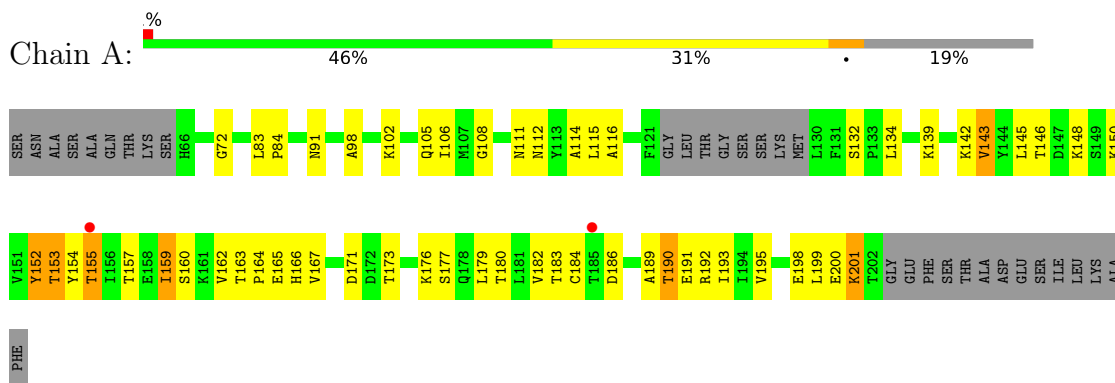
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	5	Total 5	O 5	0	0
3	L	4	Total 4	O 4	0	0
3	M	3	Total 3	O 3	0	0
3	N	4	Total 4	O 4	0	0
3	O	1	Total 1	O 1	0	0
3	P	4	Total 4	O 4	0	0
3	Q	3	Total 3	O 3	0	0
3	R	3	Total 3	O 3	0	0

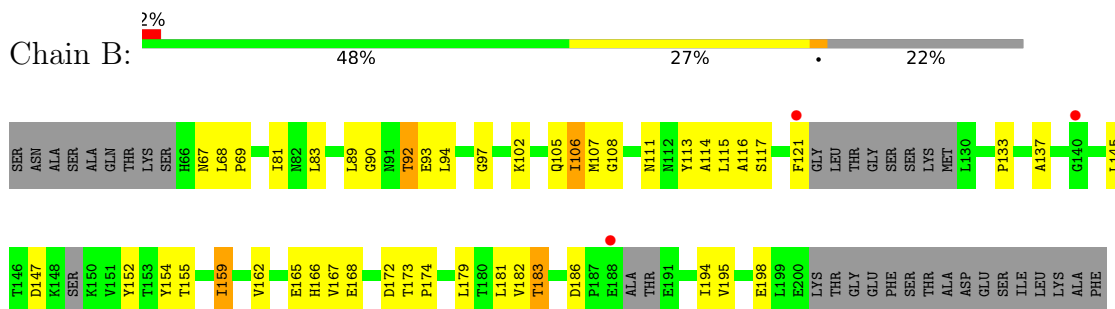
3 Residue-property plots [i](#)

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.

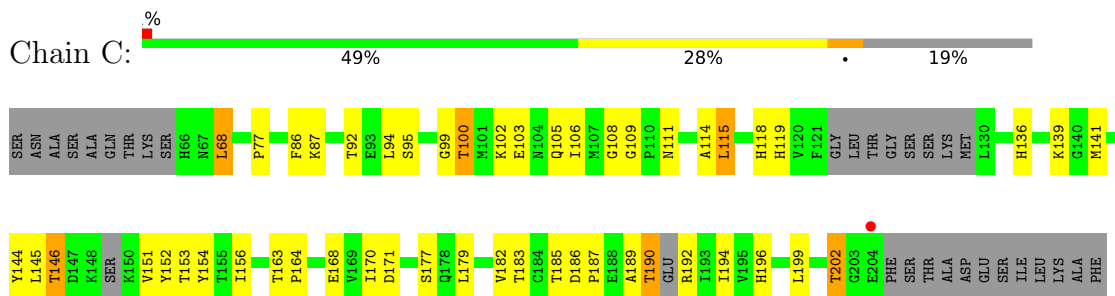
• Molecule 1: Sortase SrtA



• Molecule 1: Sortase SrtA

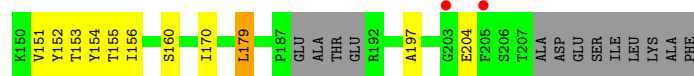


• Molecule 1: Sortase SrtA

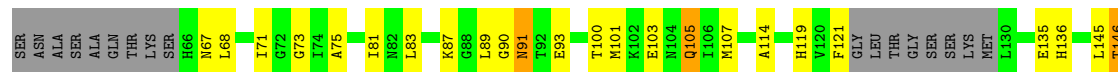


• Molecule 1: Sortase SrtA

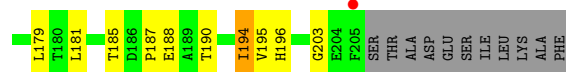




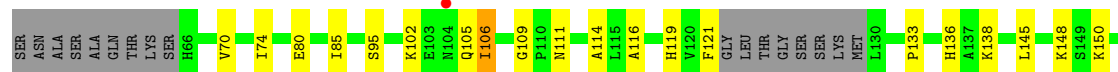
● Molecule 1: Sortase SrtA



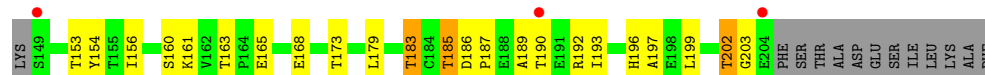
● Molecule 1: Sortase SrtA



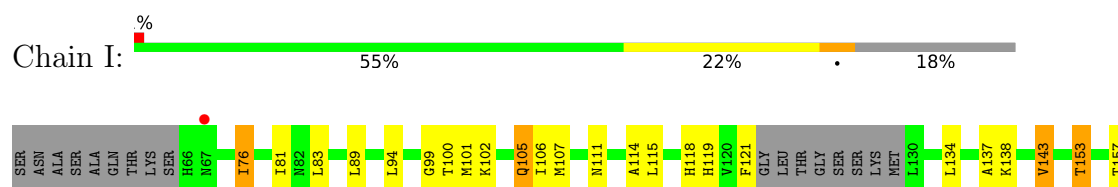
● Molecule 1: Sortase SrtA



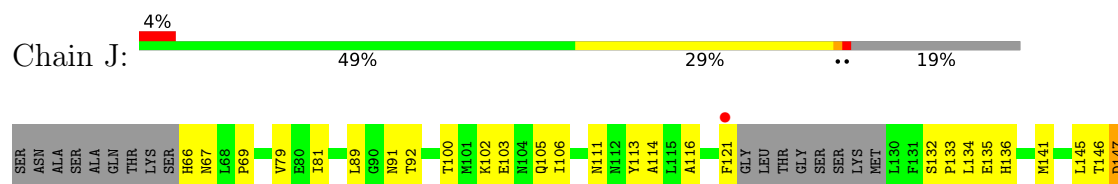
● Molecule 1: Sortase SrtA



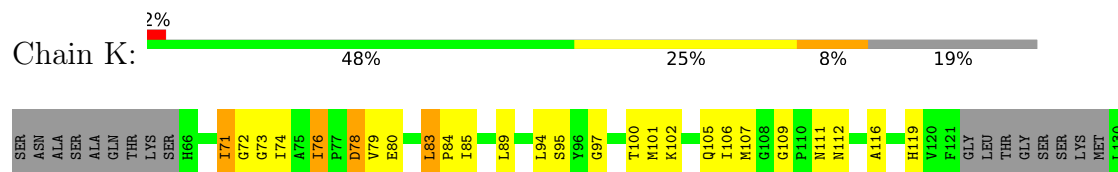
● Molecule 1: Sortase SrtA



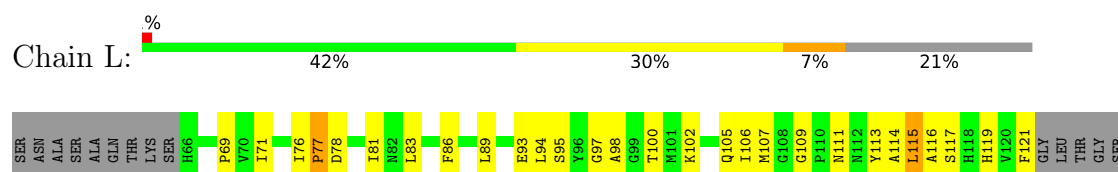
• Molecule 1: Sortase SrtA



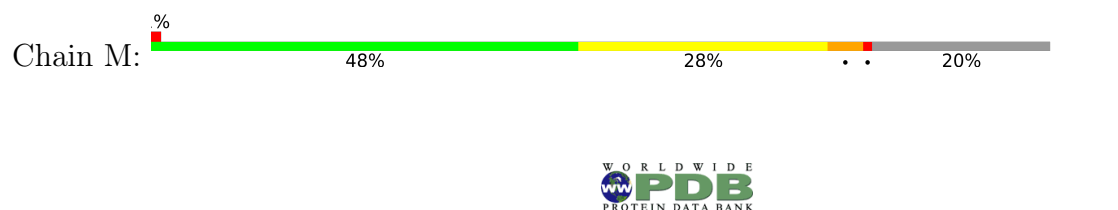
• Molecule 1: Sortase SrtA

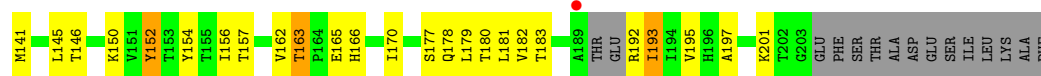


• Molecule 1: Sortase SrtA

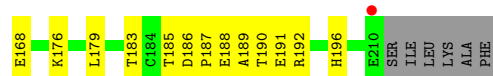


• Molecule 1: Sortase SrtA

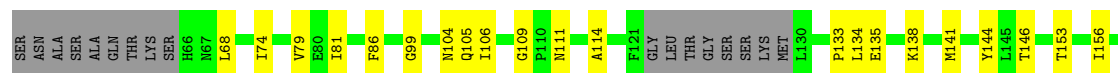




• Molecule 1: Sortase SrtA



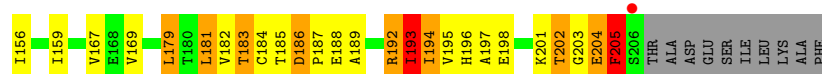
• Molecule 1: Sortase SrtA



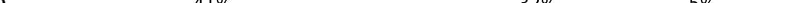
• Molecule 1: Sortase SrtA

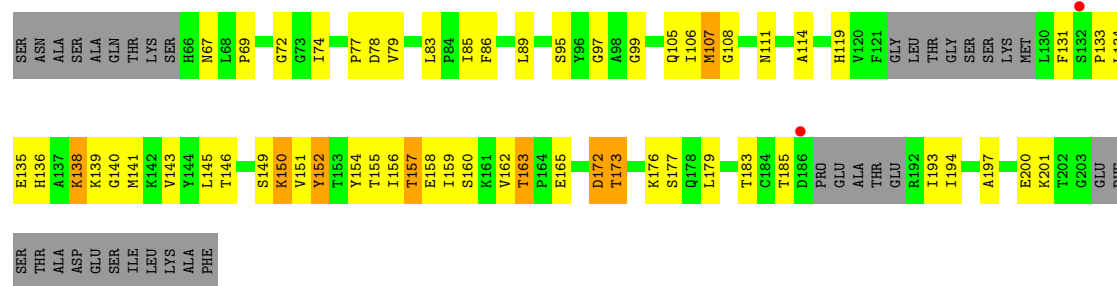


• Molecule 1: Sortase SrtA



• Molecule 1: Sortase SrtA

Chain R: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	237.67Å 167.76Å 97.54Å 90.00° 93.55° 90.00°	Depositor
Resolution (Å)	39.23 – 3.10 39.23 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.23-3.10) 99.3 (39.23-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.232 , 0.299 0.225 , 0.286	Depositor DCC
R_{free} test set	3482 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17807	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: ZN

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	0.93	1/996 (0.1%)	1.13	4/1355 (0.3%)
1	B	0.83	0/956	1.09	3/1298 (0.2%)
1	C	0.81	0/991	0.99	0/1345
1	D	1.01	2/1000 (0.2%)	1.09	2/1356 (0.1%)
1	E	0.91	1/1030 (0.1%)	1.11	8/1398 (0.6%)
1	F	0.99	1/1012 (0.1%)	1.08	2/1377 (0.1%)
1	G	0.83	0/1012	0.98	2/1377 (0.1%)
1	H	0.95	1/1001 (0.1%)	1.09	5/1360 (0.4%)
1	I	0.82	0/1002	0.99	3/1362 (0.2%)
1	J	0.90	0/998	1.14	3/1352 (0.2%)
1	K	0.94	0/993	1.15	7/1349 (0.5%)
1	L	1.02	0/979	1.13	6/1329 (0.5%)
1	M	0.89	0/983	1.07	6/1335 (0.4%)
1	N	0.91	0/1052	1.02	4/1431 (0.3%)
1	O	0.95	0/1004	1.06	4/1366 (0.3%)
1	P	0.96	0/1024	1.07	2/1392 (0.1%)
1	Q	1.26	7/1030 (0.7%)	1.22	10/1400 (0.7%)
1	R	0.91	0/965	1.05	3/1309 (0.2%)
All	All	0.94	13/18028 (0.1%)	1.08	74/24491 (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	D	0	1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	182	VAL	CA-CB	-8.25	1.44	1.54
1	Q	194	ILE	CA-CB	-6.89	1.46	1.54
1	D	90	GLY	C-O	-6.30	1.17	1.23
1	H	190	THR	CA-CB	5.88	1.59	1.52
1	F	151	VAL	CA-CB	-5.64	1.47	1.54

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	SER	CA-C-N	-9.49	109.13	119.19
1	A	132	SER	C-N-CA	-9.49	109.13	119.19
1	Q	185	THR	N-CA-C	8.13	119.92	111.14
1	B	186	ASP	CA-C-N	-7.99	109.85	119.84
1	B	186	ASP	C-N-CA	-7.99	109.85	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	204	GLU	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	976	0	957	41	0
1	B	938	0	920	29	0
1	C	973	0	957	28	0
1	D	981	0	966	20	0
1	E	1011	0	989	27	0
1	F	992	0	969	22	0
1	G	992	0	969	18	0
1	H	982	0	964	33	0
1	I	983	0	962	26	0
1	J	980	0	967	35	0
1	K	974	0	961	36	0
1	L	960	0	945	43	0
1	M	964	0	950	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1031	0	1004	18	0
1	O	984	0	966	19	0
1	P	1003	0	983	27	0
1	Q	1009	0	988	37	0
1	R	947	0	938	39	0
2	A	5	0	0	0	0
2	B	6	0	0	0	0
2	C	5	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	2	0	0	0	0
2	G	7	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	2	0	0	0	0
2	M	6	0	0	0	0
2	N	4	0	0	0	0
2	O	4	0	0	0	0
2	P	4	0	0	0	0
2	Q	4	0	0	0	0
2	R	2	0	0	0	0
3	A	1	0	0	0	0
3	B	4	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	1	0
3	E	3	0	0	0	0
3	F	5	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
3	I	5	0	0	0	0
3	J	2	0	0	0	0
3	K	5	0	0	0	0
3	L	4	0	0	0	0
3	M	3	0	0	2	0
3	N	4	0	0	0	0
3	O	1	0	0	0	0
3	P	4	0	0	0	0
3	Q	3	0	0	0	0
3	R	3	0	0	0	0
All	All	17807	0	17355	512	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 15.

The worst 5 of 512 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:Q:159:ILE:HD13	1:Q:195:VAL:HG22	1.26	1.07
1:J:146:THR:HG22	1:J:151:VAL:HG22	1.34	1.05
1:C:106:ILE:H	1:C:111:ASN:HD21	1.02	1.00
1:I:190:THR:O	1:I:192:ARG:N	1.97	0.97
1:M:106:ILE:H	1:M:111:ASN:HD21	1.14	0.95

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	125/160 (78%)	111 (89%)	12 (10%)	2 (2%)	7	30
1	B	116/160 (72%)	106 (91%)	9 (8%)	1 (1%)	14	44
1	C	121/160 (76%)	114 (94%)	6 (5%)	1 (1%)	16	47
1	D	121/160 (76%)	112 (93%)	9 (7%)	0	100	100
1	E	126/160 (79%)	109 (86%)	15 (12%)	2 (2%)	7	30
1	F	128/160 (80%)	120 (94%)	8 (6%)	0	100	100
1	G	128/160 (80%)	116 (91%)	11 (9%)	1 (1%)	16	47
1	H	124/160 (78%)	108 (87%)	14 (11%)	2 (2%)	7	30
1	I	125/160 (78%)	111 (89%)	13 (10%)	1 (1%)	16	47
1	J	121/160 (76%)	112 (93%)	9 (7%)	0	100	100
1	K	123/160 (77%)	110 (89%)	12 (10%)	1 (1%)	16	47
1	L	121/160 (76%)	108 (89%)	9 (7%)	4 (3%)	3	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	122/160 (76%)	101 (83%)	20 (16%)	1 (1%)	16	47
1	N	133/160 (83%)	123 (92%)	10 (8%)	0	100	100
1	O	127/160 (79%)	120 (94%)	7 (6%)	0	100	100
1	P	128/160 (80%)	120 (94%)	8 (6%)	0	100	100
1	Q	129/160 (81%)	120 (93%)	9 (7%)	0	100	100
1	R	119/160 (74%)	102 (86%)	14 (12%)	3 (2%)	4	21
All	All	2237/2880 (78%)	2023 (90%)	195 (9%)	19 (1%)	16	47

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	ASP
1	L	186	ASP
1	L	187	PRO
1	A	148	LYS
1	E	91	ASN

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	105/136 (77%)	94 (90%)	11 (10%)	6	26
1	B	101/136 (74%)	90 (89%)	11 (11%)	6	24
1	C	105/136 (77%)	93 (89%)	12 (11%)	5	23
1	D	107/136 (79%)	102 (95%)	5 (5%)	23	55
1	E	109/136 (80%)	92 (84%)	17 (16%)	2	12
1	F	106/136 (78%)	100 (94%)	6 (6%)	18	49
1	G	106/136 (78%)	98 (92%)	8 (8%)	12	39
1	H	106/136 (78%)	96 (91%)	10 (9%)	8	31
1	I	105/136 (77%)	93 (89%)	12 (11%)	5	23
1	J	107/136 (79%)	96 (90%)	11 (10%)	7	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	106/136 (78%)	90 (85%)	16 (15%)	3	13
1	L	104/136 (76%)	88 (85%)	16 (15%)	2	12
1	M	104/136 (76%)	88 (85%)	16 (15%)	2	12
1	N	111/136 (82%)	100 (90%)	11 (10%)	7	29
1	O	106/136 (78%)	97 (92%)	9 (8%)	10	35
1	P	109/136 (80%)	96 (88%)	13 (12%)	5	21
1	Q	110/136 (81%)	93 (84%)	17 (16%)	2	12
1	R	103/136 (76%)	86 (84%)	17 (16%)	2	11
All	All	1910/2448 (78%)	1692 (89%)	218 (11%)	5	23

5 of 218 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	185	THR
1	M	150	LYS
1	Q	204	GLU
1	L	71	ILE
1	L	176	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	91	ASN
1	L	66	HIS
1	Q	105	GLN
1	J	105	GLN
1	K	66	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 73 ligands modelled in this entry, 73 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 ⓘ

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, 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	129/160 (80%)	-0.04	2 (1%) 70 49	38, 56, 74, 83	0
1	B	124/160 (77%)	-0.10	3 (2%) 59 38	36, 52, 69, 83	0
1	C	129/160 (80%)	-0.25	1 (0%) 82 65	39, 50, 73, 80	0
1	D	129/160 (80%)	-0.15	3 (2%) 61 39	35, 50, 72, 85	0
1	E	134/160 (83%)	-0.15	1 (0%) 84 68	39, 55, 83, 87	0
1	F	132/160 (82%)	0.06	2 (1%) 72 52	38, 56, 73, 85	0
1	G	132/160 (82%)	-0.09	1 (0%) 82 65	42, 55, 72, 84	0
1	H	130/160 (81%)	-0.04	3 (2%) 61 39	41, 53, 73, 85	0
1	I	131/160 (81%)	-0.23	2 (1%) 72 52	39, 51, 77, 81	0
1	J	129/160 (80%)	-0.24	6 (4%) 36 19	37, 52, 74, 86	0
1	K	129/160 (80%)	0.04	3 (2%) 61 39	41, 57, 75, 86	0
1	L	127/160 (79%)	0.02	2 (1%) 70 49	44, 58, 75, 85	0
1	M	128/160 (80%)	-0.05	2 (1%) 70 49	46, 57, 78, 83	0
1	N	137/160 (85%)	-0.10	1 (0%) 84 68	37, 52, 73, 83	0
1	O	131/160 (81%)	-0.04	2 (1%) 72 52	32, 48, 68, 80	0
1	P	132/160 (82%)	-0.03	3 (2%) 61 39	27, 50, 70, 86	0
1	Q	133/160 (83%)	-0.04	1 (0%) 82 65	39, 54, 75, 85	0
1	R	125/160 (78%)	0.08	2 (1%) 70 49	45, 58, 75, 85	0
All	All	2341/2880 (81%)	-0.08	40 (1%) 69 48	27, 54, 75, 87	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	186	ASP	4.5
1	M	189	ALA	3.7
1	K	203	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	205	PHE	3.3
1	J	186	ASP	3.2

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($\text{\AA}^2$)	Q<0.9
2	ZN	B	305	1/1	0.93	0.12	47,47,47,47	0
2	ZN	I	301	1/1	0.93	0.05	82,82,82,82	0
2	ZN	B	304	1/1	0.94	0.09	97,97,97,97	0
2	ZN	M	304	1/1	0.94	0.07	88,88,88,88	0
2	ZN	B	306	1/1	0.95	0.07	77,77,77,77	0
2	ZN	C	305	1/1	0.95	0.09	88,88,88,88	0
2	ZN	H	304	1/1	0.96	0.05	71,71,71,71	0
2	ZN	N	304	1/1	0.96	0.08	77,77,77,77	0
2	ZN	Q	304	1/1	0.96	0.07	75,75,75,75	0
2	ZN	O	304	1/1	0.97	0.03	64,64,64,64	0
2	ZN	P	304	1/1	0.97	0.04	78,78,78,78	0
2	ZN	K	301	1/1	0.97	0.04	88,88,88,88	0
2	ZN	R	302	1/1	0.97	0.07	83,83,83,83	0
2	ZN	H	301	1/1	0.98	0.03	63,63,63,63	0
2	ZN	A	304	1/1	0.98	0.03	76,76,76,76	0
2	ZN	C	304	1/1	0.98	0.04	59,59,59,59	0
2	ZN	J	301	1/1	0.98	0.04	114,114,114,114	0
2	ZN	A	305	1/1	0.98	0.04	95,95,95,95	0
2	ZN	L	301	1/1	0.98	0.03	65,65,65,65	0
2	ZN	D	301	1/1	0.98	0.04	73,73,73,73	0
2	ZN	D	304	1/1	0.98	0.03	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	E	304	1/1	0.98	0.03	74,74,74,74	0
2	ZN	F	301	1/1	0.98	0.04	71,71,71,71	0
2	ZN	Q	301	1/1	0.98	0.02	76,76,76,76	0
2	ZN	G	302	1/1	0.98	0.07	74,74,74,74	0
2	ZN	G	306	1/1	0.98	0.04	71,71,71,71	0
2	ZN	J	302	1/1	0.99	0.04	53,53,53,53	0
2	ZN	B	302	1/1	0.99	0.02	36,36,36,36	0
2	ZN	K	302	1/1	0.99	0.04	53,53,53,53	0
2	ZN	K	303	1/1	0.99	0.02	59,59,59,59	0
2	ZN	G	303	1/1	0.99	0.02	65,65,65,65	0
2	ZN	L	302	1/1	0.99	0.04	67,67,67,67	0
2	ZN	G	304	1/1	0.99	0.03	48,48,48,48	0
2	ZN	M	306	1/1	0.99	0.04	66,66,66,66	0
2	ZN	N	301	1/1	0.99	0.02	65,65,65,65	0
2	ZN	C	301	1/1	0.99	0.02	61,61,61,61	0
2	ZN	O	301	1/1	0.99	0.02	39,39,39,39	0
2	ZN	E	301	1/1	0.99	0.02	70,70,70,70	0
2	ZN	P	301	1/1	0.99	0.03	65,65,65,65	0
2	ZN	P	302	1/1	0.99	0.05	33,33,33,33	0
2	ZN	E	303	1/1	0.99	0.02	46,46,46,46	0
2	ZN	A	301	1/1	0.99	0.02	48,48,48,48	0
2	ZN	Q	303	1/1	0.99	0.02	41,41,41,41	0
2	ZN	I	302	1/1	0.99	0.02	71,71,71,71	0
2	ZN	B	301	1/1	0.99	0.04	68,68,68,68	0
2	ZN	D	303	1/1	1.00	0.01	41,41,41,41	0
2	ZN	C	302	1/1	1.00	0.03	40,40,40,40	0
2	ZN	G	305	1/1	1.00	0.02	39,39,39,39	0
2	ZN	C	303	1/1	1.00	0.02	46,46,46,46	0
2	ZN	M	301	1/1	1.00	0.01	80,80,80,80	0
2	ZN	M	302	1/1	1.00	0.02	53,53,53,53	0
2	ZN	M	303	1/1	1.00	0.02	59,59,59,59	0
2	ZN	G	307	1/1	1.00	0.03	51,51,51,51	0
2	ZN	M	305	1/1	1.00	0.03	76,76,76,76	0
2	ZN	E	302	1/1	1.00	0.03	45,45,45,45	0
2	ZN	H	302	1/1	1.00	0.04	42,42,42,42	0
2	ZN	N	302	1/1	1.00	0.03	34,34,34,34	0
2	ZN	N	303	1/1	1.00	0.01	36,36,36,36	0
2	ZN	H	303	1/1	1.00	0.01	56,56,56,56	0
2	ZN	A	303	1/1	1.00	0.02	58,58,58,58	0
2	ZN	O	302	1/1	1.00	0.04	37,37,37,37	0
2	ZN	O	303	1/1	1.00	0.01	38,38,38,38	0
2	ZN	B	303	1/1	1.00	0.01	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	302	1/1	1.00	0.03	49,49,49,49	0
2	ZN	I	303	1/1	1.00	0.04	48,48,48,48	0
2	ZN	P	303	1/1	1.00	0.04	38,38,38,38	0
2	ZN	I	304	1/1	1.00	0.02	57,57,57,57	0
2	ZN	F	302	1/1	1.00	0.02	48,48,48,48	0
2	ZN	Q	302	1/1	1.00	0.03	53,53,53,53	0
2	ZN	G	301	1/1	1.00	0.01	45,45,45,45	0
2	ZN	J	303	1/1	1.00	0.01	40,40,40,40	0
2	ZN	R	301	1/1	1.00	0.01	69,69,69,69	0
2	ZN	D	302	1/1	1.00	0.05	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.