wwPDB X-ray Structure Validation Summary Report (i)

Feb 15, 2024 – 09:00 PM EST

PDB ID	:	3RCC
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 (i) 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 (i)) were used in the production of this report:

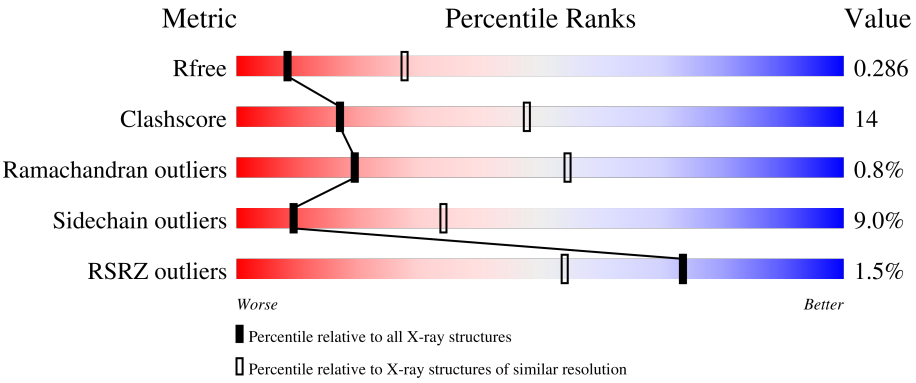
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 <=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	2% 50% 29% • 19%
1	B	160	52% 25% • 22%
1	C	160	% 52% 26% • • 19%
1	D	160	% 62% 18% • 19%
1	E	160	% 58% 21% 5% 16%

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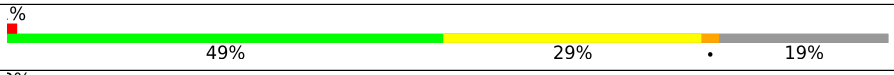
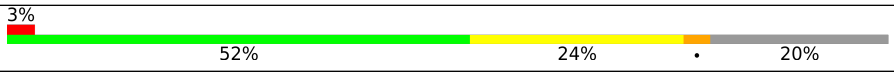
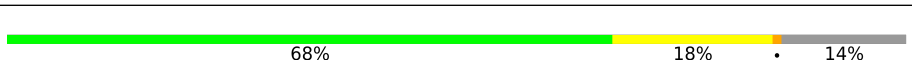
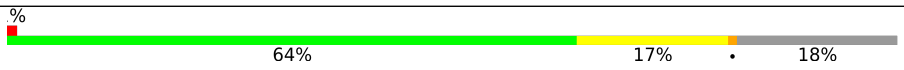
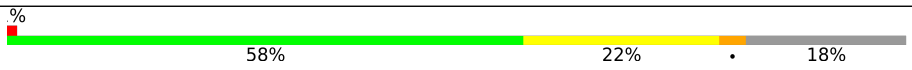
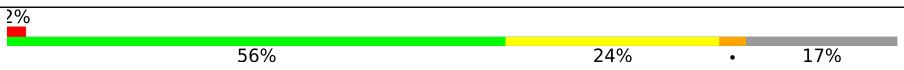
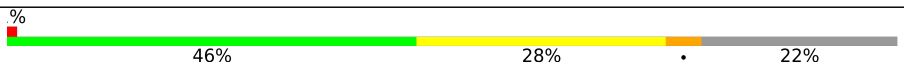
Mol	Chain	Length	Quality of chain
1	F	160	
1	G	160	
1	H	160	
1	I	160	
1	J	160	
1	K	160	
1	L	160	
1	M	160	
1	N	160	
1	O	160	
1	P	160	
1	Q	160	
1	R	160	

2 Entry composition (i)

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			

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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

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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 (three-letter code: 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

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

- Molecule 3 is water.

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

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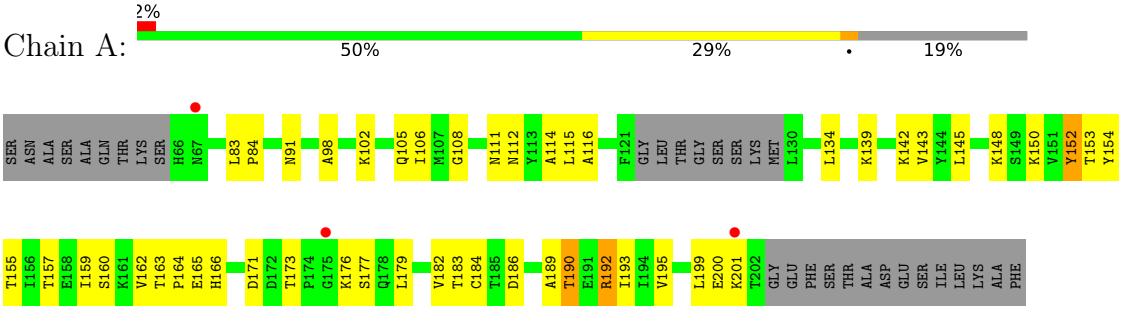
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	K	5	Total O 5 5	0	0
3	L	4	Total O 4 4	0	0
3	M	3	Total O 3 3	0	0
3	N	4	Total O 4 4	0	0
3	O	1	Total O 1 1	0	0
3	P	4	Total O 4 4	0	0
3	Q	3	Total O 3 3	0	0
3	R	3	Total O 3 3	0	0

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.

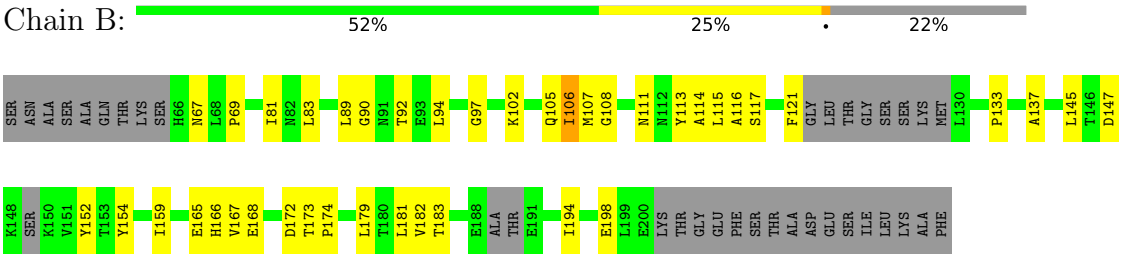
• Molecule 1: Sortase SrtA

Chain A:



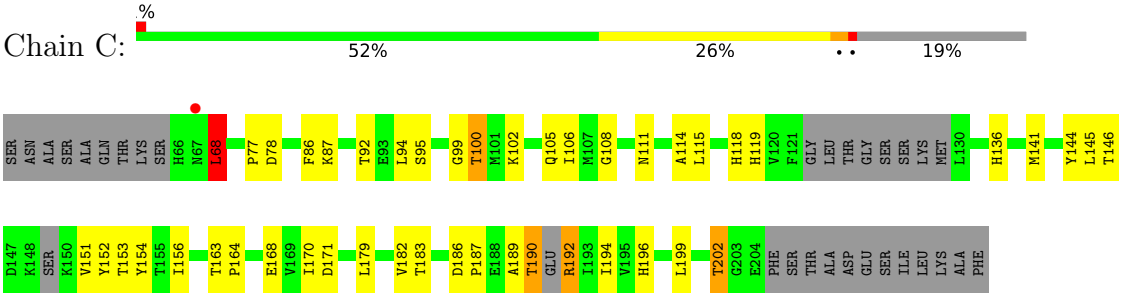
• Molecule 1: Sortase SrtA

Chain B:



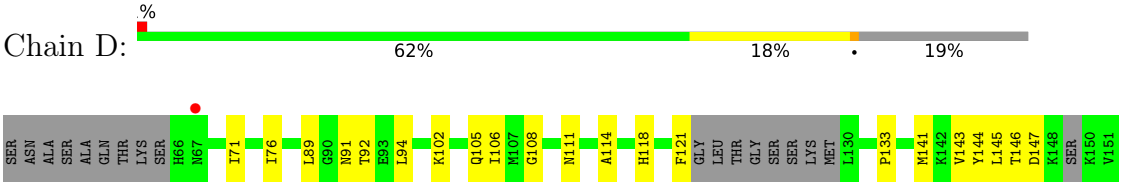
• Molecule 1: Sortase SrtA

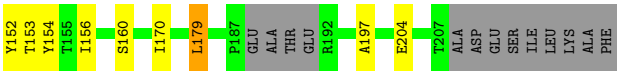
Chain C:



• Molecule 1: Sortase SrtA

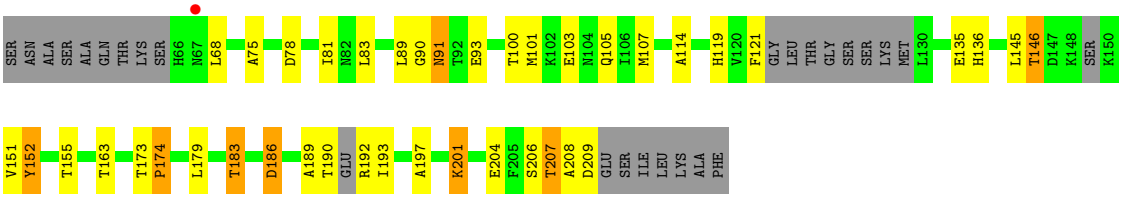
Chain D:





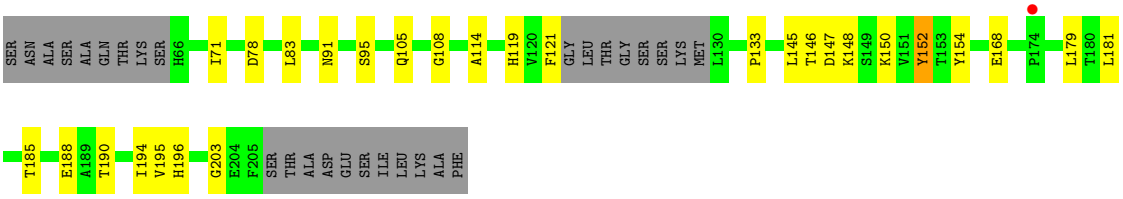
• Molecule 1: Sortase SrtA

Chain E:



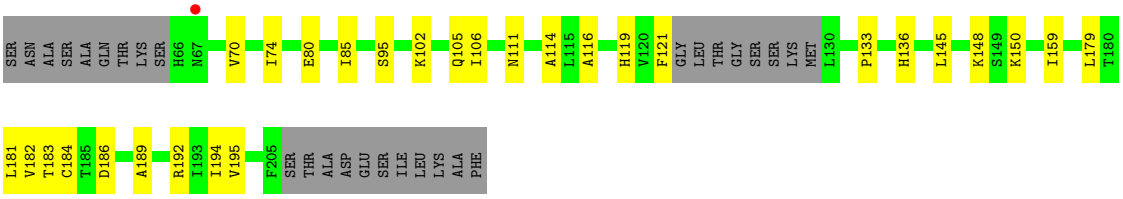
• Molecule 1: Sortase SrtA

Chain F:



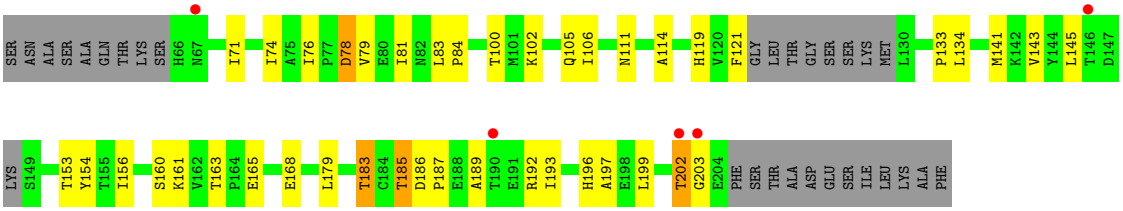
• Molecule 1: Sortase SrtA

Chain G:



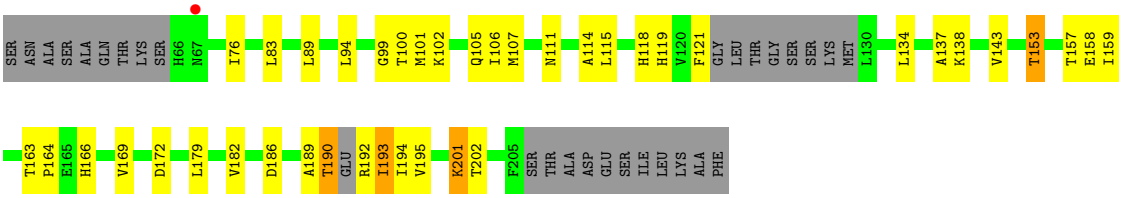
• Molecule 1: Sortase SrtA

Chain H:



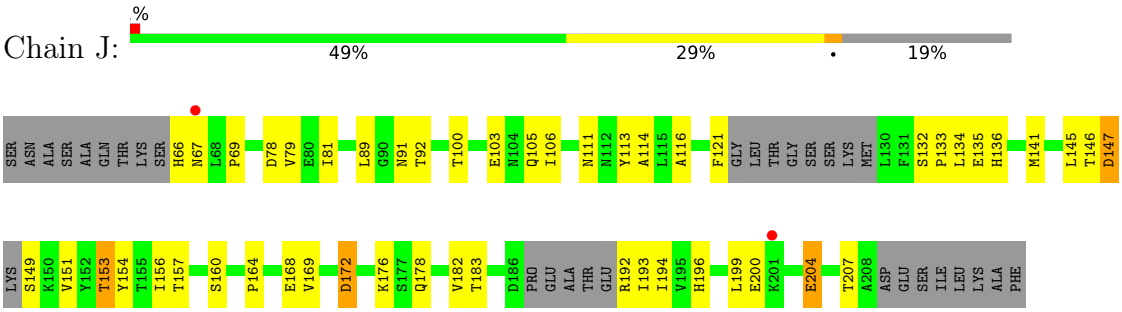
• Molecule 1: Sortase SrtA

Chain I:



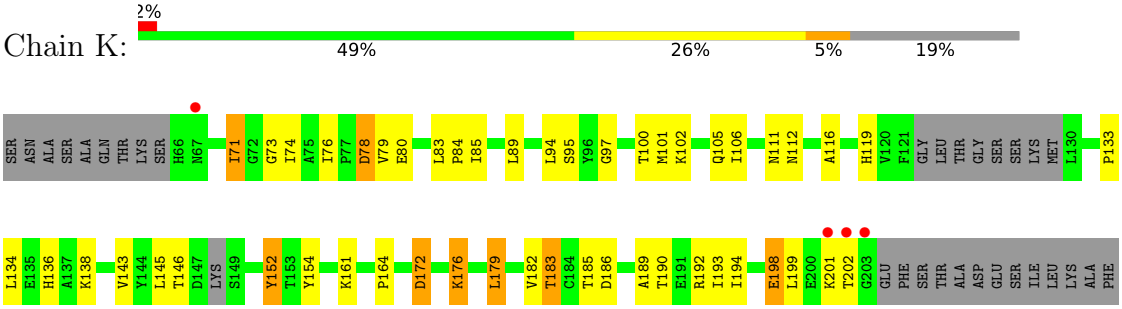
• Molecule 1: Sortase SrtA

Chain J:



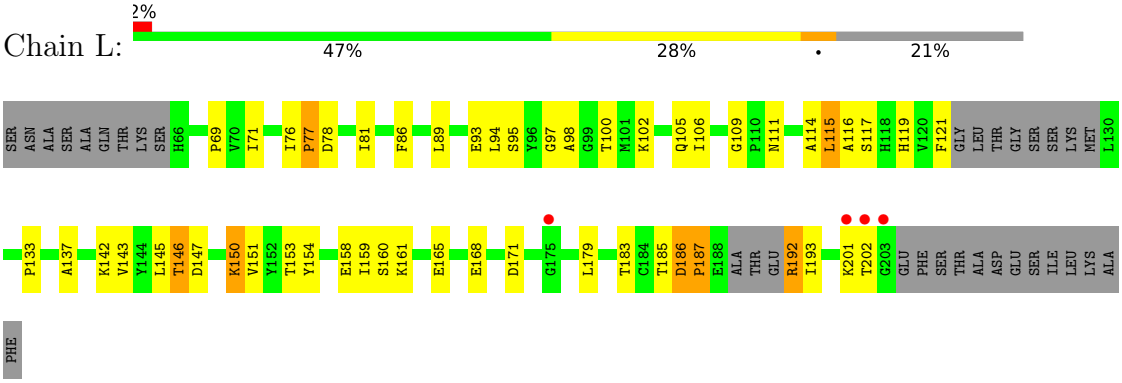
• Molecule 1: Sortase SrtA

Chain K:



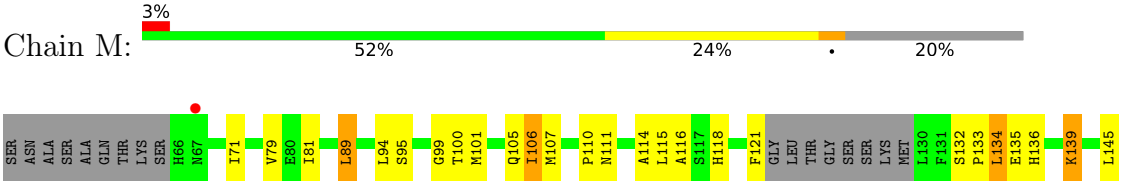
• Molecule 1: Sortase SrtA

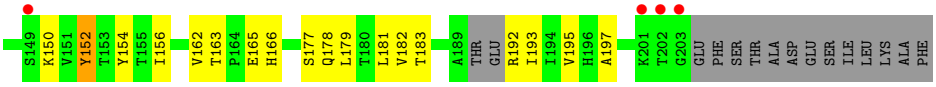
Chain L:



• Molecule 1: Sortase SrtA

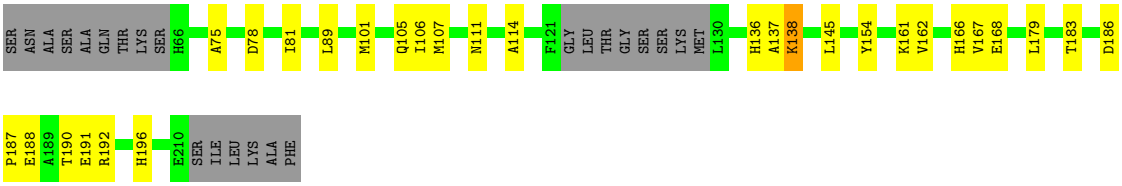
Chain M:





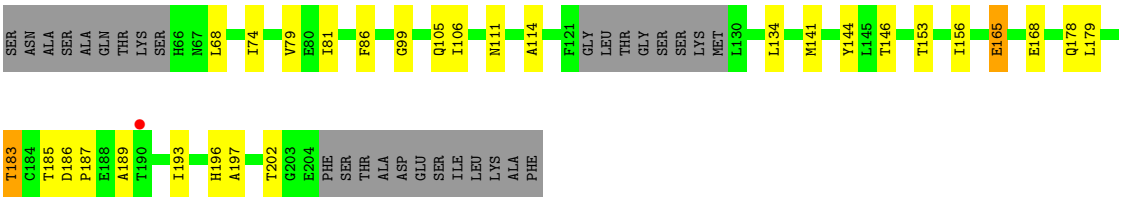
• Molecule 1: Sortase SrtA

Chain N:



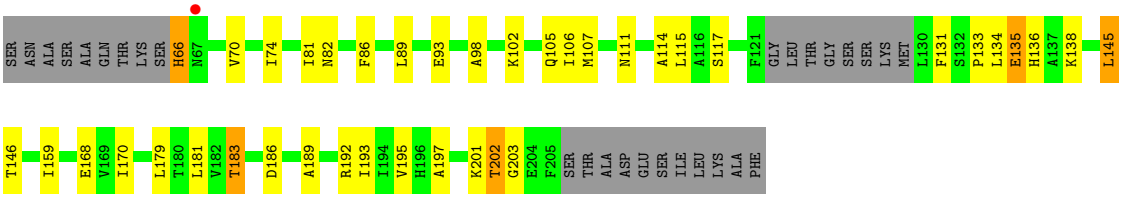
• Molecule 1: Sortase SrtA

Chain O:



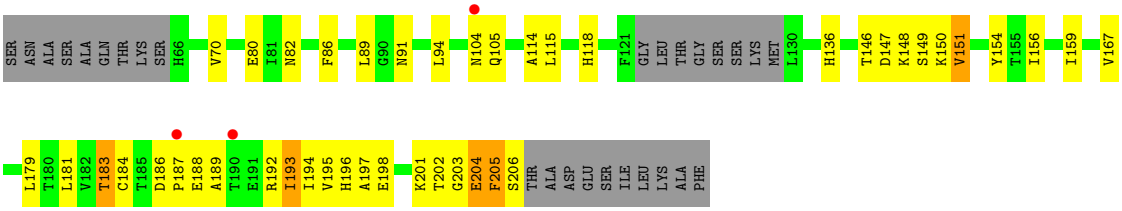
• Molecule 1: Sortase SrtA

Chain P:



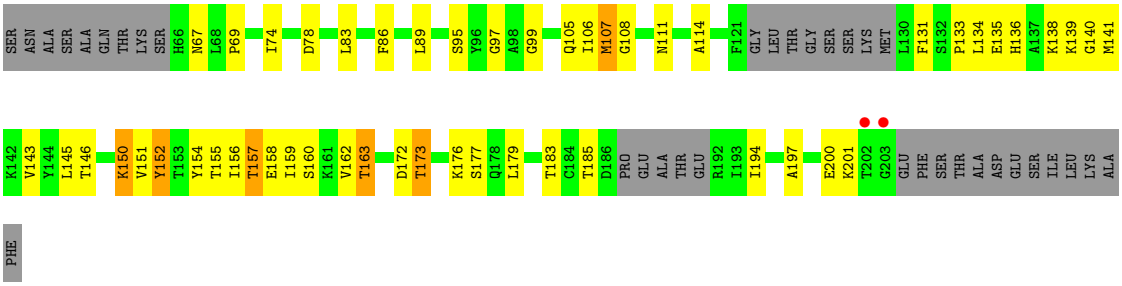
• Molecule 1: Sortase SrtA

Chain Q:



• Molecule 1: Sortase SrtA

Chain R:


SER ASN ALA SER ALA GLN THR LYS SER H66 N67 L68 P69 I74 D78 L83 F86 L89 S95 Y96 G97 A98 G99 Q105 I106 M107 G108 N111 A114 P121 GLY LEU THR GLY SER SER LYS MET L130 F131 S132 P133 L134 E135 H136 A137 K138 K139 G140 M141
K142 V143 Y144 L145 T146 K150 V151 Y152 T153 Y154 T155 I156 T157 E158 I159 S160 K161 V162 T163 D172 T173 K176 S177 Q178 L179 T183 C184 T185 D186 PRO GLU ALA THR GLU R192 I193 I194 A197 E200 K201 T202 G203 GLU PHE SER THR ALA ASP GLU SER ILE LEU LYS ALA
PHE

4 Data and refinement statistics (i)

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) 99.2 (39.23-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	3479 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)	0.31 , 56.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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

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	0.77	0/996	0.76	0/1355
1	B	0.70	1/956 (0.1%)	0.76	0/1298
1	C	0.67	0/991	0.74	1/1345 (0.1%)
1	D	0.79	0/1000	0.77	0/1356
1	E	0.72	0/1030	0.76	0/1398
1	F	0.77	0/1012	0.74	0/1377
1	G	0.66	0/1012	0.73	0/1377
1	H	0.74	0/1001	0.77	0/1360
1	I	0.63	0/1002	0.67	0/1362
1	J	0.71	0/998	0.79	0/1352
1	K	0.79	0/993	0.74	0/1349
1	L	0.80	0/979	0.74	0/1329
1	M	0.73	0/983	0.74	0/1335
1	N	0.72	0/1052	0.74	0/1431
1	O	0.74	0/1004	0.77	0/1366
1	P	0.77	0/1024	0.80	0/1392
1	Q	0.97	0/1030	0.86	1/1400 (0.1%)
1	R	0.73	0/965	0.77	0/1309
All	All	0.75	1/18028 (0.0%)	0.76	2/24491 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	PHE	CE2-CZ	5.09	1.47	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	68	LEU	CA-CB-CG	6.59	130.45	115.30
1	Q	206	SER	N-CA-C	-5.17	97.05	111.00

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 (i)

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	27	0
1	C	973	0	957	27	0
1	D	981	0	966	19	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	30	0
1	I	983	0	962	26	0
1	J	980	0	967	35	0
1	K	974	0	961	34	0
1	L	960	0	945	40	0
1	M	964	0	950	35	0
1	N	1031	0	1004	17	0
1	O	984	0	966	18	0
1	P	1003	0	983	27	0
1	Q	1009	0	988	36	0
1	R	947	0	938	35	0
2	A	5	0	0	0	0
2	B	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	491	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 14.

The worst 5 of 491 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%)	9 37
1	B	116/160 (72%)	106 (91%)	9 (8%)	1 (1%)	17 52
1	C	121/160 (76%)	114 (94%)	6 (5%)	1 (1%)	19 54
1	D	121/160 (76%)	112 (93%)	9 (7%)	0	100 100
1	E	126/160 (79%)	109 (86%)	15 (12%)	2 (2%)	9 37
1	F	128/160 (80%)	120 (94%)	8 (6%)	0	100 100
1	G	128/160 (80%)	116 (91%)	11 (9%)	1 (1%)	19 54
1	H	124/160 (78%)	108 (87%)	14 (11%)	2 (2%)	9 37
1	I	125/160 (78%)	111 (89%)	13 (10%)	1 (1%)	19 54
1	J	121/160 (76%)	112 (93%)	9 (7%)	0	100 100
1	K	123/160 (77%)	110 (89%)	12 (10%)	1 (1%)	19 54
1	L	121/160 (76%)	108 (89%)	9 (7%)	4 (3%)	4 21
1	M	122/160 (76%)	101 (83%)	20 (16%)	1 (1%)	19 54
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Q	129/160 (81%)	120 (93%)	9 (7%)	0	100 100
1	R	119/160 (74%)	102 (86%)	14 (12%)	3 (2%)	5 27
All	All	2237/2880 (78%)	2023 (90%)	195 (9%)	19 (1%)	19 54

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 (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	A	105/136 (77%)	101 (96%)	4 (4%)	33 66
1	B	101/136 (74%)	95 (94%)	6 (6%)	19 50
1	C	105/136 (77%)	96 (91%)	9 (9%)	10 37
1	D	107/136 (79%)	101 (94%)	6 (6%)	21 52
1	E	109/136 (80%)	96 (88%)	13 (12%)	5 20
1	F	106/136 (78%)	101 (95%)	5 (5%)	26 59
1	G	106/136 (78%)	99 (93%)	7 (7%)	16 47
1	H	106/136 (78%)	97 (92%)	9 (8%)	10 37
1	I	105/136 (77%)	95 (90%)	10 (10%)	8 31
1	J	107/136 (79%)	94 (88%)	13 (12%)	5 20
1	K	106/136 (78%)	90 (85%)	16 (15%)	3 12
1	L	104/136 (76%)	92 (88%)	12 (12%)	5 22
1	M	104/136 (76%)	92 (88%)	12 (12%)	5 22
1	N	111/136 (82%)	105 (95%)	6 (5%)	22 53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	106/136 (78%)	98 (92%)	8 (8%)	13 42
1	P	109/136 (80%)	99 (91%)	10 (9%)	9 33
1	Q	110/136 (81%)	97 (88%)	13 (12%)	5 21
1	R	103/136 (76%)	91 (88%)	12 (12%)	5 22
All	All	1910/2448 (78%)	1739 (91%)	171 (9%)	9 34

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	106	ILE
1	P	192	ARG
1	M	163	THR
1	O	165	GLU
1	Q	151	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	105	GLN
1	O	111	ASN
1	M	105	GLN
1	N	105	GLN
1	P	105	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides 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, 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	A	129/160 (80%)	-0.16	3 (2%) 60 39	38, 56, 74, 83	0
1	B	124/160 (77%)	-0.36	0 100 100	36, 52, 69, 83	0
1	C	129/160 (80%)	-0.18	1 (0%) 86 72	39, 50, 73, 80	0
1	D	129/160 (80%)	-0.19	1 (0%) 86 72	35, 50, 72, 85	0
1	E	134/160 (83%)	-0.20	1 (0%) 87 75	39, 55, 83, 87	0
1	F	132/160 (82%)	-0.19	1 (0%) 86 72	38, 56, 73, 85	0
1	G	132/160 (82%)	-0.15	1 (0%) 86 72	42, 55, 72, 84	0
1	H	130/160 (81%)	-0.04	5 (3%) 40 20	41, 53, 73, 85	0
1	I	131/160 (81%)	-0.04	1 (0%) 86 72	39, 51, 77, 81	0
1	J	129/160 (80%)	-0.18	2 (1%) 72 51	37, 52, 74, 86	0
1	K	129/160 (80%)	0.01	4 (3%) 49 26	41, 57, 75, 86	0
1	L	127/160 (79%)	-0.08	4 (3%) 49 26	44, 58, 75, 85	0
1	M	128/160 (80%)	-0.06	5 (3%) 39 20	46, 57, 78, 83	0
1	N	137/160 (85%)	-0.06	0 100 100	37, 52, 73, 83	0
1	O	131/160 (81%)	-0.15	1 (0%) 86 72	32, 48, 68, 80	0
1	P	132/160 (82%)	-0.10	1 (0%) 86 72	27, 50, 70, 86	0
1	Q	133/160 (83%)	-0.12	3 (2%) 60 39	39, 54, 75, 85	0
1	R	125/160 (78%)	-0.13	2 (1%) 72 51	45, 58, 75, 85	0
All	All	2341/2880 (81%)	-0.13	36 (1%) 73 54	27, 54, 75, 87	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	202	THR	4.9
1	L	201	LYS	4.8
1	I	67	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
1	M	203	GLY	4.5
1	L	202	THR	4.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides 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^{th} 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	ZN	M	304	1/1	0.86	0.12	88,88,88,88	0
2	ZN	N	304	1/1	0.89	0.07	77,77,77,77	0
2	ZN	I	301	1/1	0.92	0.13	82,82,82,82	0
2	ZN	C	305	1/1	0.94	0.16	88,88,88,88	0
2	ZN	L	301	1/1	0.94	0.06	65,65,65,65	0
2	ZN	H	304	1/1	0.95	0.15	71,71,71,71	0
2	ZN	B	305	1/1	0.95	0.27	47,47,47,47	0
2	ZN	B	306	1/1	0.95	0.14	77,77,77,77	0
2	ZN	B	304	1/1	0.95	0.15	97,97,97,97	0
2	ZN	G	302	1/1	0.95	0.18	74,74,74,74	0
2	ZN	P	301	1/1	0.95	0.09	65,65,65,65	0
2	ZN	A	305	1/1	0.96	0.05	95,95,95,95	0
2	ZN	P	304	1/1	0.96	0.16	78,78,78,78	0
2	ZN	Q	304	1/1	0.96	0.04	75,75,75,75	0
2	ZN	K	301	1/1	0.97	0.09	88,88,88,88	0
2	ZN	E	304	1/1	0.97	0.09	74,74,74,74	0
2	ZN	L	302	1/1	0.97	0.14	67,67,67,67	0
2	ZN	C	304	1/1	0.97	0.14	59,59,59,59	0
2	ZN	H	301	1/1	0.97	0.05	63,63,63,63	0
2	ZN	O	301	1/1	0.97	0.11	39,39,39,39	0
2	ZN	B	301	1/1	0.97	0.10	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	D	304	1/1	0.97	0.08	67,67,67,67	0
2	ZN	J	301	1/1	0.97	0.06	114,114,114,114	0
2	ZN	A	304	1/1	0.98	0.12	76,76,76,76	0
2	ZN	C	301	1/1	0.98	0.07	61,61,61,61	0
2	ZN	G	306	1/1	0.98	0.09	71,71,71,71	0
2	ZN	M	303	1/1	0.98	0.13	59,59,59,59	0
2	ZN	D	301	1/1	0.98	0.04	73,73,73,73	0
2	ZN	M	305	1/1	0.98	0.08	76,76,76,76	0
2	ZN	N	301	1/1	0.98	0.07	65,65,65,65	0
2	ZN	C	303	1/1	0.98	0.14	46,46,46,46	0
2	ZN	E	301	1/1	0.98	0.05	70,70,70,70	0
2	ZN	O	304	1/1	0.98	0.13	64,64,64,64	0
2	ZN	I	302	1/1	0.98	0.06	71,71,71,71	0
2	ZN	I	303	1/1	0.98	0.17	48,48,48,48	0
2	ZN	E	302	1/1	0.98	0.15	45,45,45,45	0
2	ZN	R	302	1/1	0.98	0.17	83,83,83,83	0
2	ZN	D	302	1/1	0.99	0.16	51,51,51,51	0
2	ZN	K	302	1/1	0.99	0.17	53,53,53,53	0
2	ZN	K	303	1/1	0.99	0.12	59,59,59,59	0
2	ZN	G	303	1/1	0.99	0.07	65,65,65,65	0
2	ZN	A	303	1/1	0.99	0.10	58,58,58,58	0
2	ZN	M	301	1/1	0.99	0.09	80,80,80,80	0
2	ZN	M	302	1/1	0.99	0.14	53,53,53,53	0
2	ZN	G	307	1/1	0.99	0.14	51,51,51,51	0
2	ZN	A	301	1/1	0.99	0.07	48,48,48,48	0
2	ZN	H	303	1/1	0.99	0.13	56,56,56,56	0
2	ZN	M	306	1/1	0.99	0.14	66,66,66,66	0
2	ZN	B	302	1/1	0.99	0.13	36,36,36,36	0
2	ZN	N	302	1/1	0.99	0.19	34,34,34,34	0
2	ZN	N	303	1/1	0.99	0.13	36,36,36,36	0
2	ZN	E	303	1/1	0.99	0.12	46,46,46,46	0
2	ZN	B	303	1/1	0.99	0.12	55,55,55,55	0
2	ZN	O	302	1/1	0.99	0.17	37,37,37,37	0
2	ZN	O	303	1/1	0.99	0.15	38,38,38,38	0
2	ZN	F	301	1/1	0.99	0.08	71,71,71,71	0
2	ZN	I	304	1/1	0.99	0.11	57,57,57,57	0
2	ZN	F	302	1/1	0.99	0.15	48,48,48,48	0
2	ZN	Q	301	1/1	0.99	0.05	76,76,76,76	0
2	ZN	Q	302	1/1	0.99	0.14	53,53,53,53	0
2	ZN	J	302	1/1	0.99	0.16	53,53,53,53	0
2	ZN	R	301	1/1	0.99	0.13	69,69,69,69	0
2	ZN	J	303	1/1	0.99	0.12	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	D	303	1/1	1.00	0.15	41,41,41,41	0
2	ZN	P	302	1/1	1.00	0.14	33,33,33,33	0
2	ZN	P	303	1/1	1.00	0.18	38,38,38,38	0
2	ZN	G	304	1/1	1.00	0.16	48,48,48,48	0
2	ZN	G	305	1/1	1.00	0.16	39,39,39,39	0
2	ZN	C	302	1/1	1.00	0.15	40,40,40,40	0
2	ZN	Q	303	1/1	1.00	0.15	41,41,41,41	0
2	ZN	G	301	1/1	1.00	0.15	45,45,45,45	0
2	ZN	A	302	1/1	1.00	0.14	49,49,49,49	0
2	ZN	H	302	1/1	1.00	0.15	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.