



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:10 PM UTC

PDB ID : 2W7U / pdb_00002w7u
Title : SplA serine protease of *Staphylococcus aureus* (2.4A)
Authors : Stec-Niemczyka, J.; Pustelny, K.; Kisielewska, M.; Bista, M.; Boulware, K.T.; Stennicke, H.R.; Thogersen, I.B.; Daugherty, P.S.; Enghild, J.J.; Popowicz, G.M.; Dubin, A.; Potempa, J.; Dubin, G.
Deposited on : 2008-12-30
Resolution : 2.43 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

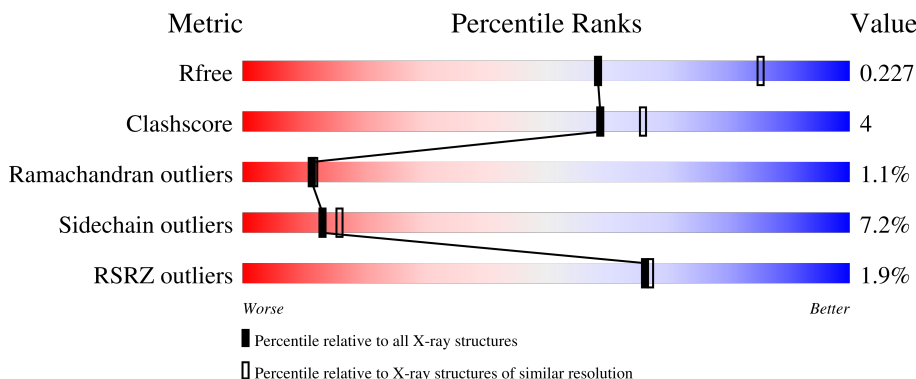
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	200	 2% 84% 14% ..
1	B	200	 2% 82% 14% . .
1	C	200	 % 86% 14% .
1	D	200	 3% 82% 16% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5995 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 SERINE PROTEASE SPLA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1487	938	250	297	2			
1	B	200	Total	C	N	O	S	0	0	0
			1500	946	250	302	2			
1	C	200	Total	C	N	O	S	0	0	0
			1482	934	247	299	2			
1	D	200	Total	C	N	O	S	0	0	0
			1491	940	249	300	2			

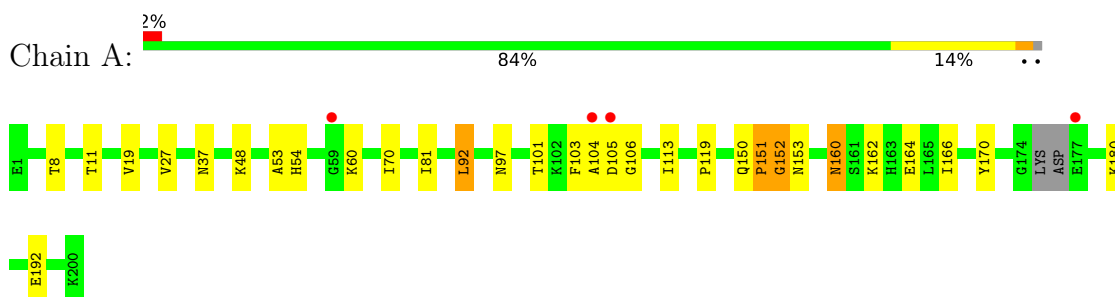
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	B	17	Total	O	0	0
			17	17		
2	C	5	Total	O	0	0
			5	5		
2	D	4	Total	O	0	0
			4	4		

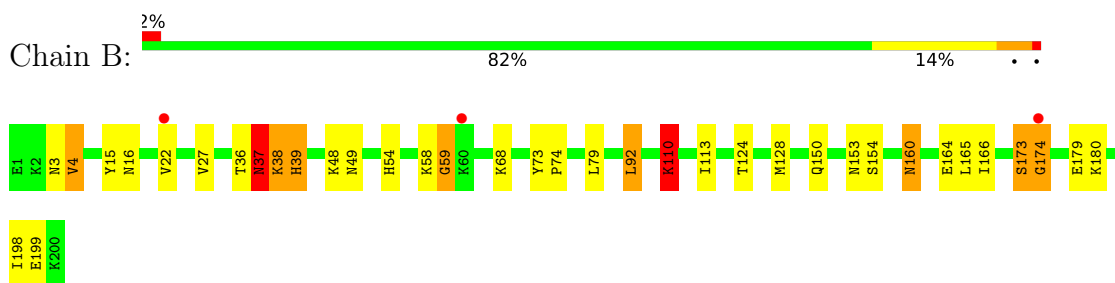
3 Residue-property plots [i](#)

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.

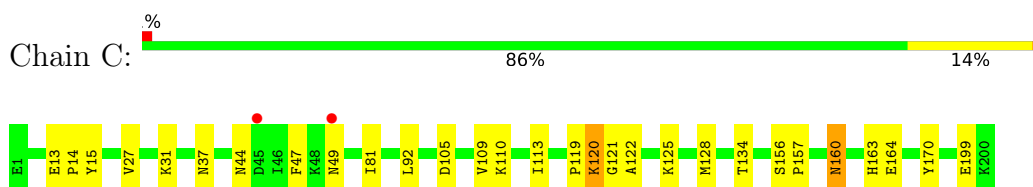
• Molecule 1: SERINE PROTEASE SPLA



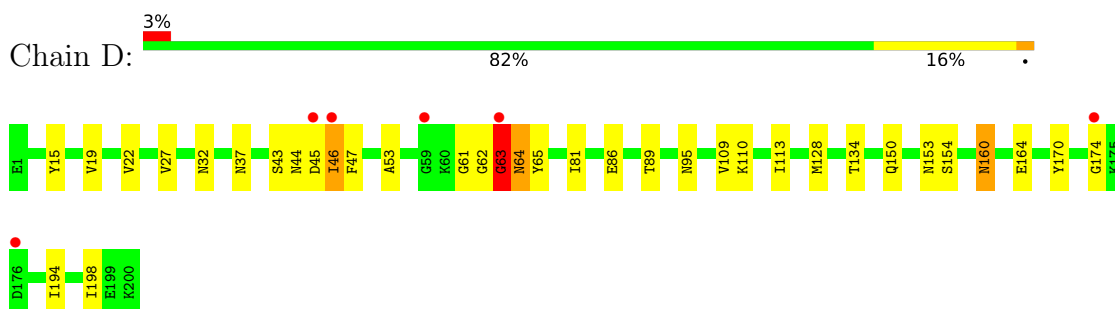
• Molecule 1: SERINE PROTEASE SPLA



• Molecule 1: SERINE PROTEASE SPLA



• Molecule 1: SERINE PROTEASE SPLA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.99Å 82.22Å 134.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 2.43 19.87 – 2.43	Depositor EDS
% Data completeness (in resolution range)	97.9 (19.87-2.43) 97.7 (19.87-2.43)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.44Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.209 , 0.248 (Not available) , 0.227	Depositor DCC
R_{free} test set	1559 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 28.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5995	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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 ⓘ

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	0.88	5/1517 (0.3%)	0.75	4/2052 (0.2%)
1	B	1.03	7/1531 (0.5%)	0.78	4/2073 (0.2%)
1	C	0.45	2/1513 (0.1%)	0.68	3/2053 (0.1%)
1	D	0.29	0/1522	0.62	0/2062
All	All	0.73	14/6083 (0.2%)	0.71	11/8240 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	7
1	C	0	1
1	D	0	8
All	All	0	20

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	110	LYS	C-O	31.30	1.68	1.23
1	A	151	PRO	C-O	18.63	1.43	1.23
1	A	151	PRO	C-N	17.79	1.59	1.33
1	A	152	GLY	CA-C	-16.68	1.28	1.51
1	B	110	LYS	C-N	-12.49	1.16	1.33
1	B	39	HIS	C-O	10.93	1.37	1.24
1	C	120	LYS	CA-CB	9.79	1.70	1.53
1	B	39	HIS	N-CA	8.44	1.57	1.46
1	A	101	THR	CB-OG1	7.30	1.55	1.43
1	A	152	GLY	N-CA	-7.28	1.34	1.45
1	B	37	ASN	CA-C	7.02	1.62	1.52
1	B	38	LYS	C-O	5.64	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	37	ASN	CG-ND2	5.53	1.44	1.33
1	C	119	PRO	CA-CB	5.10	1.59	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	THR	OG1-CB-CG2	-14.79	79.72	109.30
1	B	110	LYS	CA-C-O	-11.99	106.10	121.08
1	B	37	ASN	CB-CA-C	11.55	128.87	109.80
1	C	120	LYS	N-CA-C	9.05	130.08	110.80
1	C	119	PRO	O-C-N	6.57	127.39	122.73
1	A	151	PRO	CA-C-O	6.50	128.58	120.97
1	C	120	LYS	CA-CB-CG	-6.25	101.60	114.10
1	A	151	PRO	CA-C-N	-5.68	110.28	121.41
1	A	151	PRO	C-N-CA	-5.68	110.28	121.41
1	B	39	HIS	N-CA-C	5.37	122.24	110.80
1	B	37	ASN	N-CA-C	-5.00	102.67	110.42

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	PHE	Peptide
1	A	105	ASP	Peptide
1	A	151	PRO	Peptide,Mainchain
1	B	110	LYS	Mainchain
1	B	173	SER	Peptide
1	B	179	GLU	Peptide
1	B	198	ILE	Peptide
1	B	3	ASN	Peptide
1	B	58	LYS	Peptide
1	B	59	GLY	Peptide
1	C	125	LYS	Peptide
1	D	174	GLY	Peptide
1	D	43	SER	Peptide
1	D	44	ASN	Peptide
1	D	45	ASP	Peptide
1	D	46	ILE	Peptide
1	D	61	GLY	Peptide
1	D	62	GLY	Peptide
1	D	63	GLY	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	1487	0	1403	12	0
1	B	1500	0	1405	17	0
1	C	1482	0	1357	10	0
1	D	1491	0	1381	11	0
2	A	9	0	0	0	0
2	B	17	0	0	0	0
2	C	5	0	0	0	0
2	D	4	0	0	0	0
All	All	5995	0	5546	50	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 4.

All (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LYS:O	1:B:110:LYS:C	1.68	1.36
1:B:173:SER:H	1:B:174:GLY:HA3	1.35	0.91
1:B:173:SER:N	1:B:174:GLY:HA3	1.94	0.81
1:B:15:TYR:HB3	1:B:128:MET:HE1	1.70	0.73
1:D:15:TYR:HB3	1:D:128:MET:HE1	1.73	0.69
1:B:160:ASN:C	1:B:160:ASN:HD22	2.04	0.65
1:B:150:GLN:H	1:B:153:ASN:HD22	1.48	0.59
1:C:15:TYR:HB3	1:C:128:MET:HE1	1.84	0.59
1:A:160:ASN:HD22	1:A:160:ASN:C	2.10	0.58
1:C:31:LYS:O	1:C:199:GLU:HB2	2.04	0.57
1:A:37:ASN:HD21	1:A:170:TYR:HA	1.71	0.56
1:D:150:GLN:H	1:D:153:ASN:HD22	1.54	0.55
1:B:160:ASN:HB3	1:B:166:ILE:HD11	1.87	0.55
1:D:63:GLY:HA2	1:D:65:TYR:CE1	2.41	0.55
1:C:160:ASN:C	1:C:160:ASN:HD22	2.15	0.54
1:A:160:ASN:ND2	1:A:164:GLU:H	2.06	0.54
1:C:109:VAL:O	1:C:110:LYS:HB2	2.08	0.52
1:B:37:ASN:HD21	1:B:154:SER:HB3	1.73	0.52
1:B:37:ASN:ND2	1:B:154:SER:HB3	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ASN:HD21	1:D:86:GLU:HG3	1.76	0.51
1:C:44:ASN:HA	1:C:49:ASN:HD22	1.75	0.51
1:D:19:VAL:HG12	1:D:53:ALA:HA	1.95	0.49
1:B:4:VAL:HG12	1:B:4:VAL:O	2.11	0.48
1:A:119:PRO:HA	1:A:152:GLY:HA3	1.96	0.47
1:A:19:VAL:HG12	1:A:53:ALA:HA	1.95	0.47
1:A:160:ASN:HB3	1:A:166:ILE:HD11	1.96	0.47
1:B:160:ASN:ND2	1:B:164:GLU:H	2.12	0.47
1:B:173:SER:N	1:B:174:GLY:CA	2.71	0.46
1:D:37:ASN:HD21	1:D:170:TYR:HA	1.81	0.46
1:B:36:THR:OG1	1:B:37:ASN:N	2.49	0.44
1:C:37:ASN:HD21	1:C:170:TYR:HA	1.83	0.44
1:A:160:ASN:ND2	1:A:162:LYS:H	2.15	0.43
1:C:160:ASN:ND2	1:C:164:GLU:H	2.16	0.43
1:C:120:LYS:O	1:C:122:ALA:N	2.51	0.43
1:B:173:SER:H	1:B:174:GLY:CA	2.19	0.43
1:D:109:VAL:O	1:D:110:LYS:HB2	2.19	0.42
1:A:150:GLN:H	1:A:153:ASN:HD22	1.68	0.42
1:D:160:ASN:ND2	1:D:164:GLU:H	2.17	0.41
1:B:16:ASN:HA	1:B:54:HIS:HB3	2.01	0.41
1:C:14:PRO:HG3	1:C:163:HIS:CG	2.56	0.41
1:A:92:LEU:HD12	1:A:97:ASN:HD21	1.85	0.41
1:A:104:ALA:O	1:A:106:GLY:HA2	2.20	0.41
1:B:92:LEU:HD12	1:B:92:LEU:HA	1.89	0.41
1:A:160:ASN:C	1:A:160:ASN:ND2	2.75	0.41
1:D:194:ILE:O	1:D:198:ILE:HG13	2.21	0.41
1:B:73:TYR:HA	1:B:74:PRO:HD2	1.95	0.41
1:A:54:HIS:ND1	1:A:54:HIS:O	2.54	0.40
1:D:32:ASN:H	1:D:95:ASN:HD21	1.67	0.40
1:C:156:SER:HA	1:C:157:PRO:HD2	1.91	0.40
1:D:63:GLY:O	1:D:64:ASN:ND2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	194/200 (97%)	182 (94%)	11 (6%)	1 (0%)	24	29
1	B	198/200 (99%)	185 (93%)	9 (4%)	4 (2%)	6	4
1	C	198/200 (99%)	185 (93%)	12 (6%)	1 (0%)	24	29
1	D	198/200 (99%)	181 (91%)	14 (7%)	3 (2%)	8	7
All	All	788/800 (98%)	733 (93%)	46 (6%)	9 (1%)	11	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	46	ILE
1	B	4	VAL
1	B	59	GLY
1	C	121	GLY
1	D	47	PHE
1	B	39	HIS
1	B	174	GLY
1	D	63	GLY
1	A	60	LYS

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	155/168 (92%)	144 (93%)	11 (7%)	13	16
1	B	155/168 (92%)	140 (90%)	15 (10%)	8	8
1	C	149/168 (89%)	140 (94%)	9 (6%)	17	23
1	D	151/168 (90%)	142 (94%)	9 (6%)	17	23
All	All	610/672 (91%)	566 (93%)	44 (7%)	13	16

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	11	THR
1	A	27	VAL
1	A	48	LYS
1	A	70	ILE
1	A	81	ILE
1	A	92	LEU
1	A	113	ILE
1	A	160	ASN
1	A	180	LYS
1	A	192	GLU
1	B	22	VAL
1	B	27	VAL
1	B	37	ASN
1	B	38	LYS
1	B	48	LYS
1	B	49	ASN
1	B	68	LYS
1	B	79	LEU
1	B	92	LEU
1	B	113	ILE
1	B	124	THR
1	B	160	ASN
1	B	165	LEU
1	B	180	LYS
1	B	199	GLU
1	C	13	GLU
1	C	27	VAL
1	C	47	PHE
1	C	81	ILE
1	C	92	LEU
1	C	105	ASP
1	C	113	ILE
1	C	134	THR
1	C	160	ASN
1	D	22	VAL
1	D	27	VAL
1	D	64	ASN
1	D	81	ILE
1	D	89	THR
1	D	113	ILE
1	D	134	THR
1	D	154	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	160	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	37	ASN
1	A	44	ASN
1	A	64	ASN
1	A	85	HIS
1	A	93	ASN
1	A	95	ASN
1	A	97	ASN
1	A	123	GLN
1	A	153	ASN
1	A	160	ASN
1	A	196	ASN
1	B	3	ASN
1	B	32	ASN
1	B	37	ASN
1	B	39	HIS
1	B	49	ASN
1	B	95	ASN
1	B	153	ASN
1	B	160	ASN
1	B	163	HIS
1	B	196	ASN
1	C	37	ASN
1	C	39	HIS
1	C	49	ASN
1	C	55	HIS
1	C	136	ASN
1	C	153	ASN
1	C	160	ASN
1	C	196	ASN
1	C	197	ASN
1	D	32	ASN
1	D	37	ASN
1	D	64	ASN
1	D	85	HIS
1	D	93	ASN
1	D	95	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	153	ASN
1	D	160	ASN
1	D	196	ASN
1	D	197	ASN

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](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	110:LYS	C	111:ASP	N	1.16

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	198/200 (99%)	-0.23	4 (2%) 65 66	14, 28, 44, 52	0
1	B	200/200 (100%)	-0.17	3 (1%) 72 73	14, 27, 45, 55	0
1	C	200/200 (100%)	-0.09	2 (1%) 79 81	19, 31, 54, 68	0
1	D	200/200 (100%)	0.10	6 (3%) 52 52	20, 36, 55, 60	0
All	All	798/800 (99%)	-0.10	15 (1%) 66 67	14, 30, 51, 68	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	ALA	4.8
1	A	59	GLY	3.1
1	B	174	GLY	3.1
1	D	174	GLY	3.1
1	D	63	GLY	2.9
1	A	105	ASP	2.8
1	D	46	ILE	2.5
1	D	45	ASP	2.5
1	C	49	ASN	2.3
1	A	177	GLU	2.3
1	C	45	ASP	2.2
1	B	22	VAL	2.2
1	B	60	LYS	2.1
1	D	59	GLY	2.1
1	D	176	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.