



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 02:50 AM UTC

PDB ID : 6UJI / pdb_00006uji
Title : Low resolution crystal structure (5.5 Å) of the anthrax toxin protective antigen heptamer prepore D425A mutant
Authors : Lovell, S.; Mehzabeen, N.; Battaile, K.P.; Bann, J.G.
Deposited on : 2019-10-03
Resolution : 5.50 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

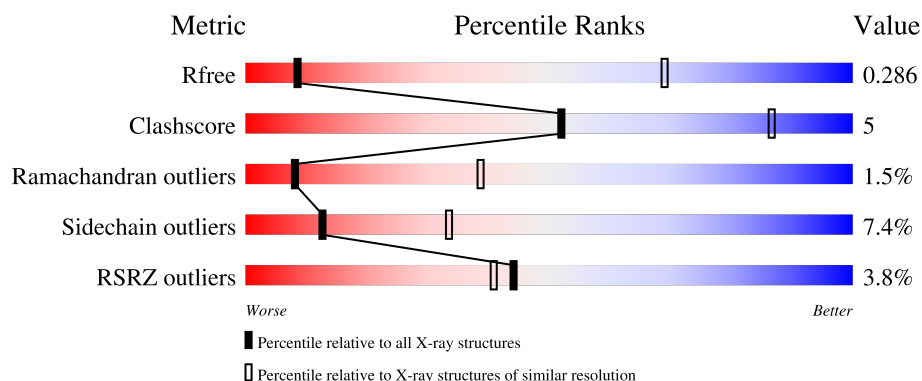
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 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.



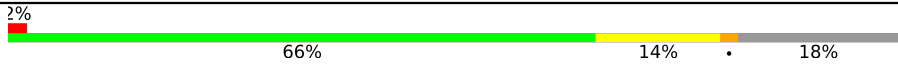
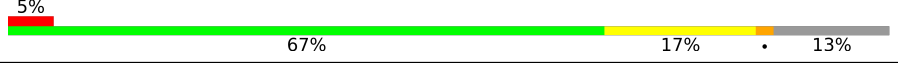
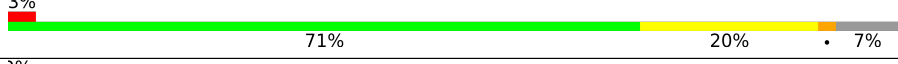
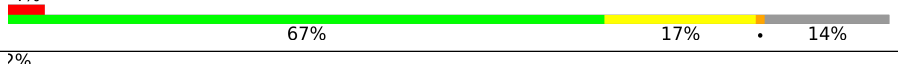
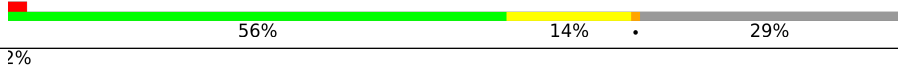
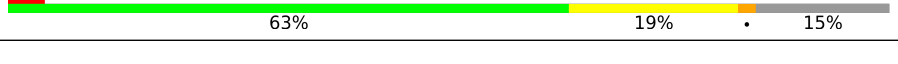
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1088 (7.00-4.00)
Clashscore	190562	1147 (7.00-4.00)
Ramachandran outliers	187476	1012 (7.02-3.98)
Sidechain outliers	187428	1023 (7.04-3.96)
RSRZ outliers	180081	1081 (7.00-4.00)

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	568	2% 65% 16% • 17%
1	B	568	4% 70% 20% • 9%
1	C	568	2% 56% 11% • 32%
1	D	568	7% 75% 18% • 5%
1	E	568	2% 69% 20% • 9%

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Mol	Chain	Length	Quality of chain
1	F	568	
1	G	568	
1	H	568	
1	I	568	
1	J	568	
1	K	568	
1	L	568	
1	M	568	
1	N	568	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 53490 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 Protective antigen PA-63.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3712	2316	650	740	6			
1	B	519	Total	C	N	O	S	0	0	0
			4114	2578	710	820	6			
1	C	388	Total	C	N	O	S	0	0	0
			3083	1929	539	609	6			
1	D	539	Total	C	N	O	S	0	0	0
			4265	2672	735	852	6			
1	E	516	Total	C	N	O	S	0	0	0
			4089	2564	704	815	6			
1	F	467	Total	C	N	O	S	0	0	0
			3688	2316	641	725	6			
1	G	520	Total	C	N	O	S	0	0	0
			4125	2583	710	826	6			
1	H	493	Total	C	N	O	S	0	0	0
			3894	2434	678	776	6			
1	I	529	Total	C	N	O	S	0	0	0
			4189	2622	724	837	6			
1	J	470	Total	C	N	O	S	0	0	0
			3718	2322	649	741	6			
1	K	488	Total	C	N	O	S	0	0	0
			3867	2419	673	769	6			
1	L	404	Total	C	N	O	S	0	0	0
			3189	1992	555	637	5			
1	M	473	Total	C	N	O	S	0	0	0
			3749	2345	656	742	6			
1	N	480	Total	C	N	O	S	0	0	0
			3808	2375	663	764	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	425	ALA	ASP	engineered mutation	UNP P13423

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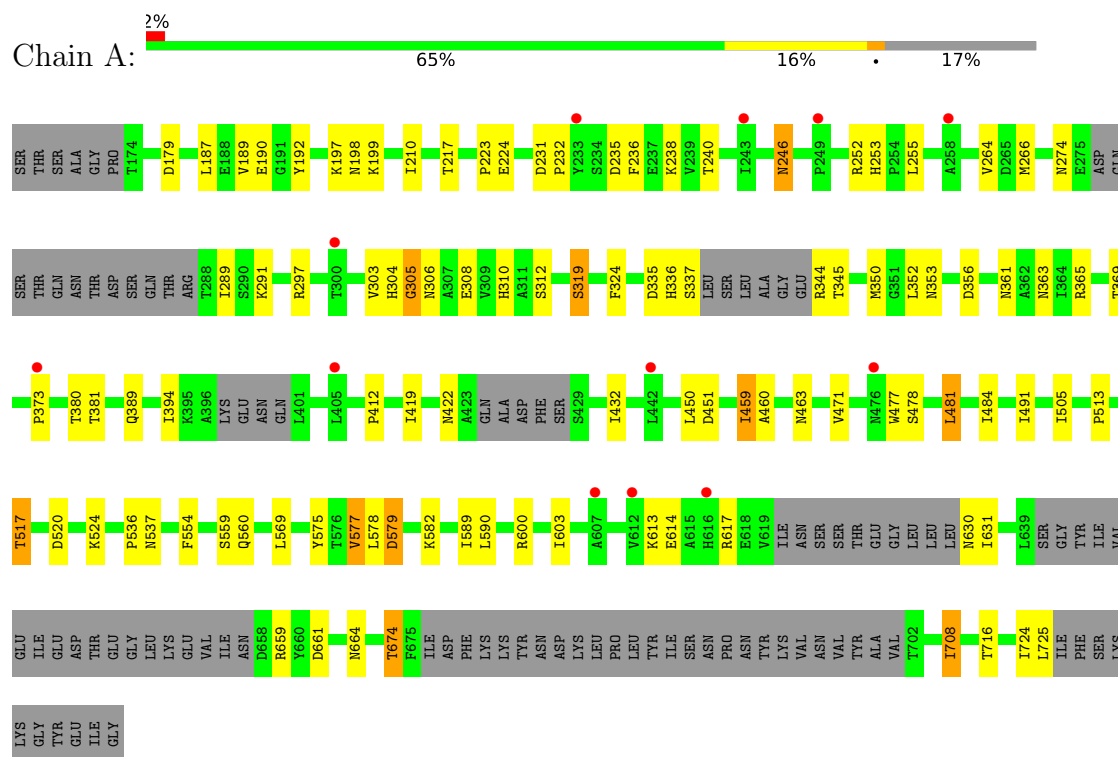
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Chain	Residue	Modelled	Actual	Comment	Reference
B	425	ALA	ASP	engineered mutation	UNP P13423
C	425	ALA	ASP	engineered mutation	UNP P13423
D	425	ALA	ASP	engineered mutation	UNP P13423
E	425	ALA	ASP	engineered mutation	UNP P13423
F	425	ALA	ASP	engineered mutation	UNP P13423
G	425	ALA	ASP	engineered mutation	UNP P13423
H	425	ALA	ASP	engineered mutation	UNP P13423
I	425	ALA	ASP	engineered mutation	UNP P13423
J	425	ALA	ASP	engineered mutation	UNP P13423
K	425	ALA	ASP	engineered mutation	UNP P13423
L	425	ALA	ASP	engineered mutation	UNP P13423
M	425	ALA	ASP	engineered mutation	UNP P13423
N	425	ALA	ASP	engineered mutation	UNP P13423

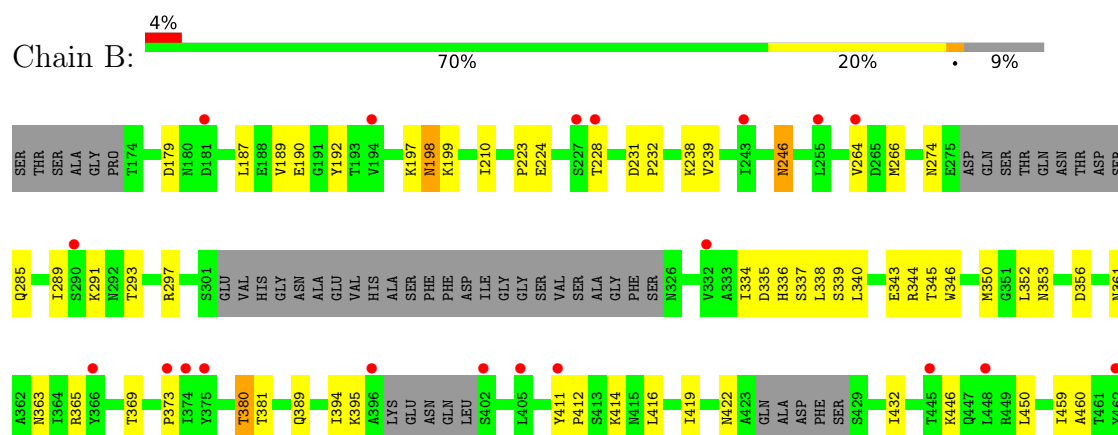
3 Residue-property plots [i](#)

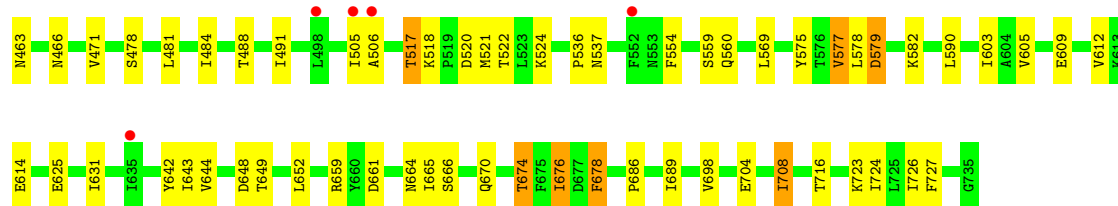
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Protective antigen PA-63

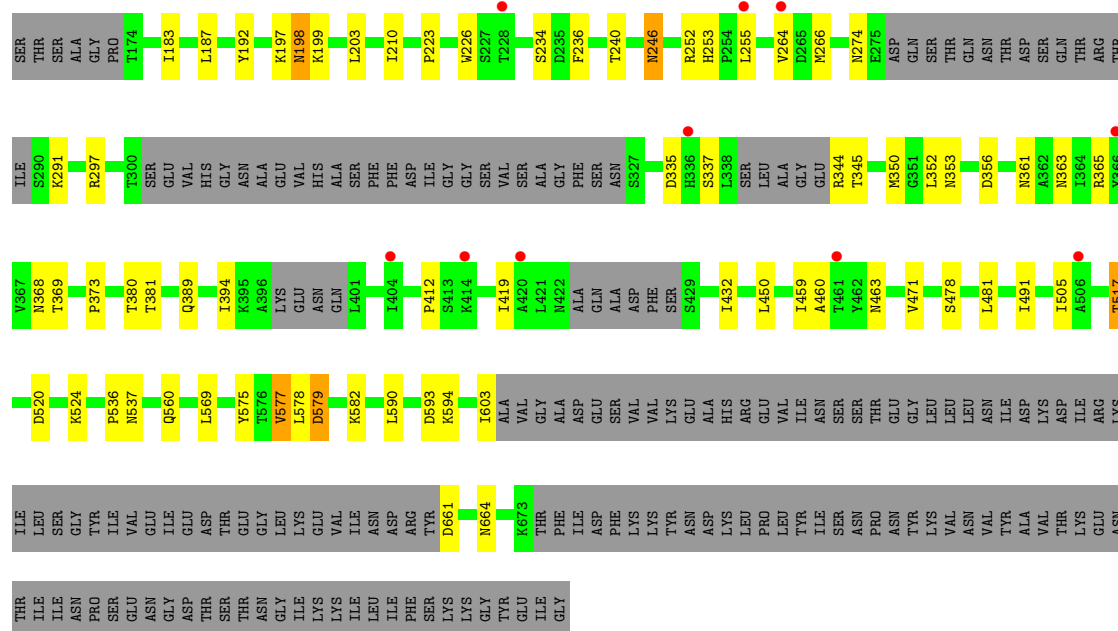


• Molecule 1: Protective antigen PA-63

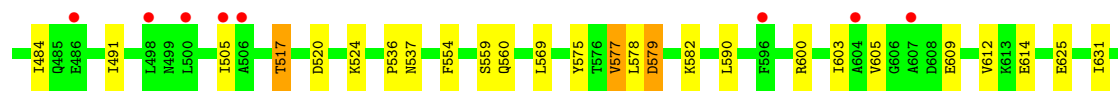
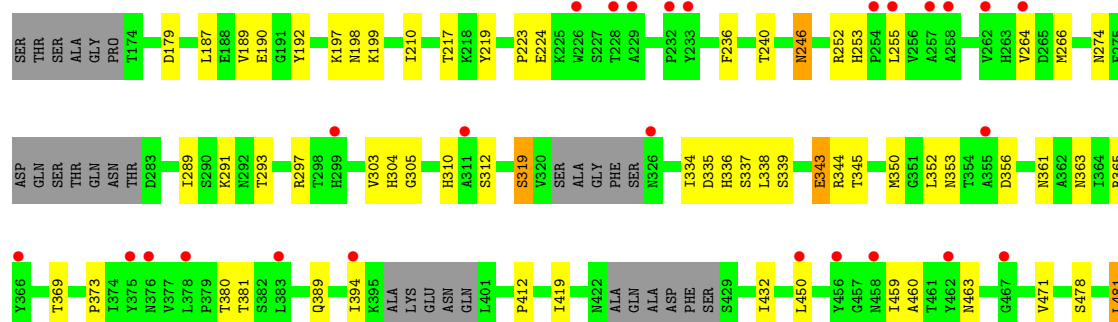
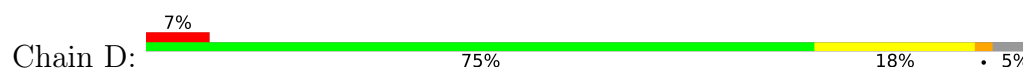


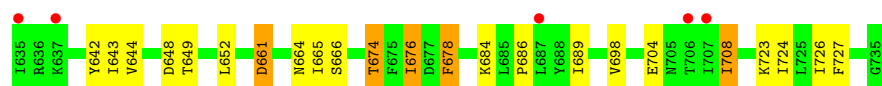


• Molecule 1: Protective antigen PA-63

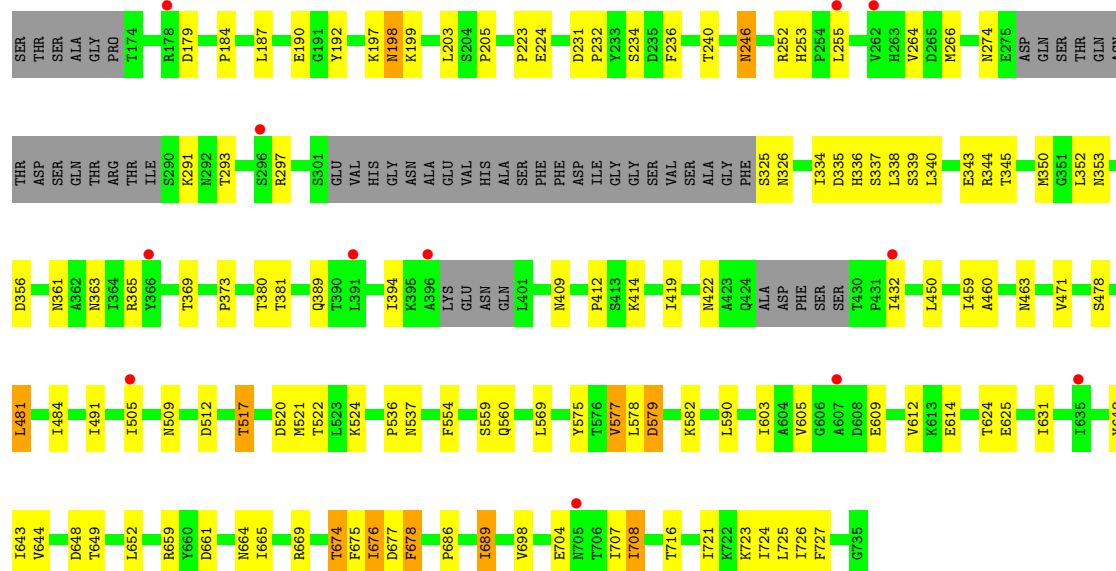


• Molecule 1: Protective antigen PA-63

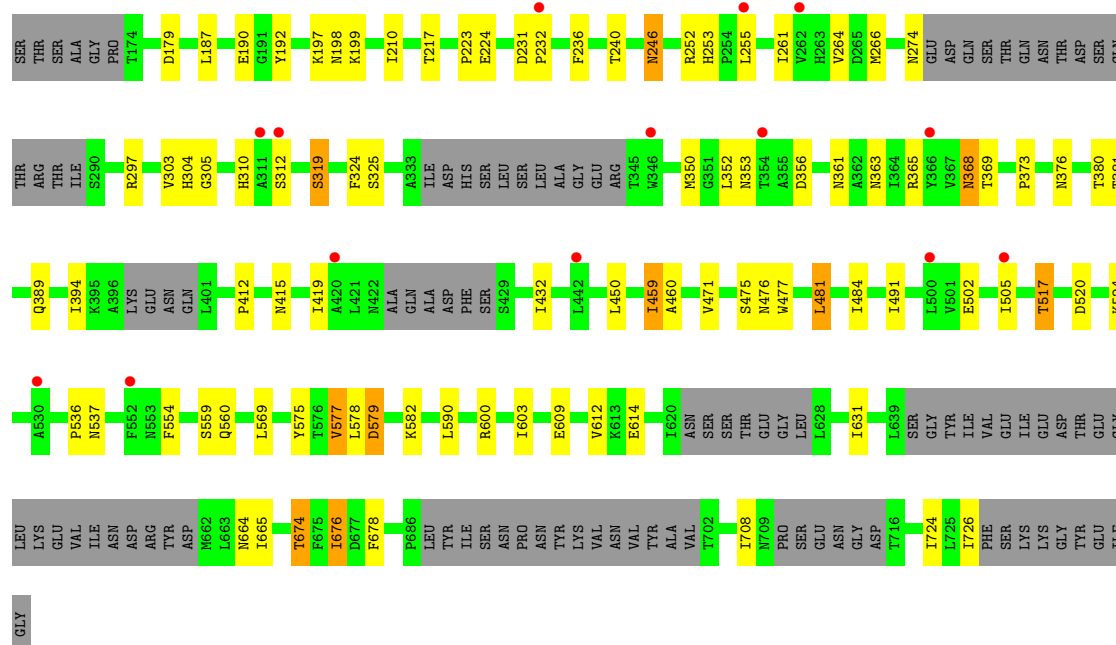




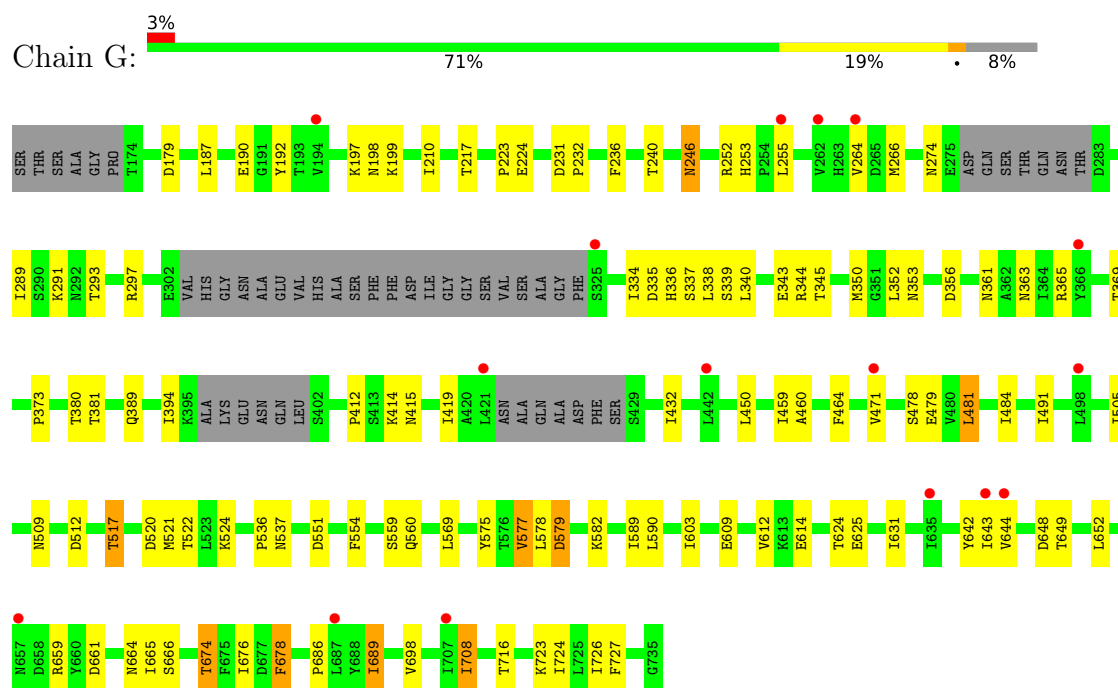
• Molecule 1: Protective antigen PA-63



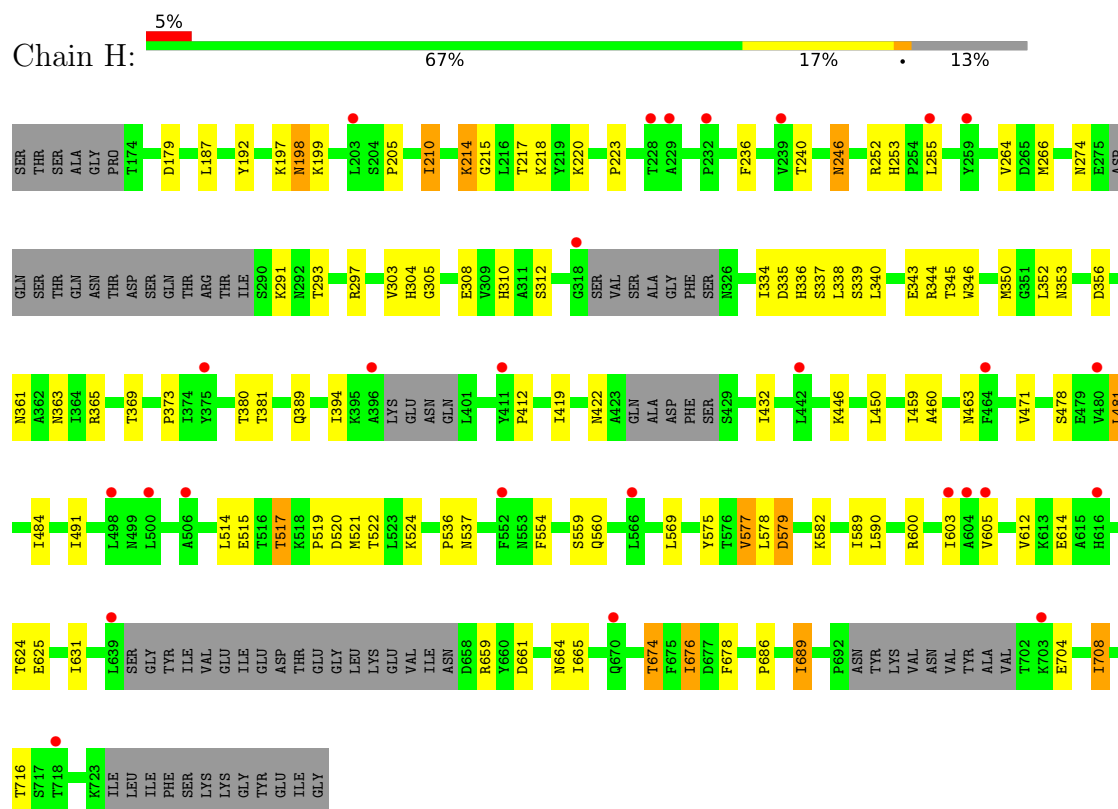
• Molecule 1: Protective antigen PA-63



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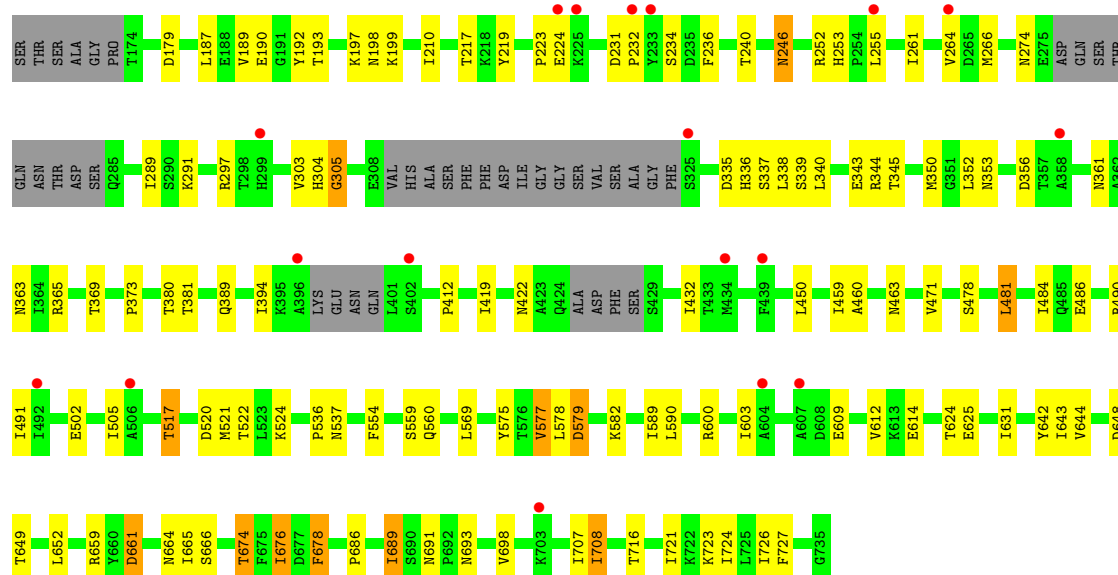


• Molecule 1: Protective antigen PA-63

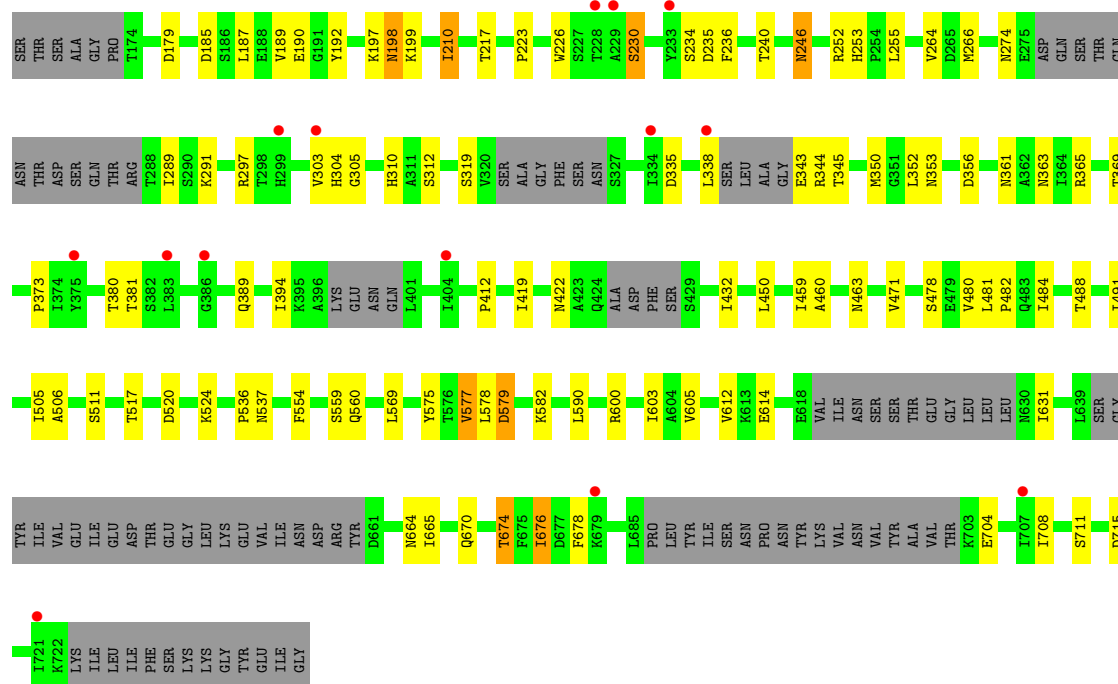


• Molecule 1: Protective antigen PA-63



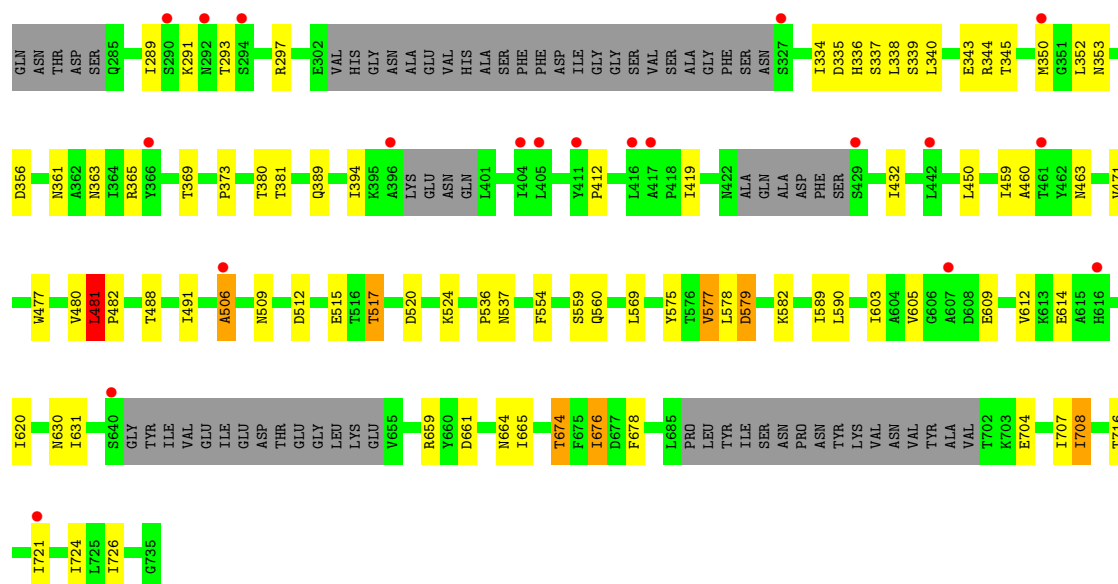


• Molecule 1: Protective antigen PA-63

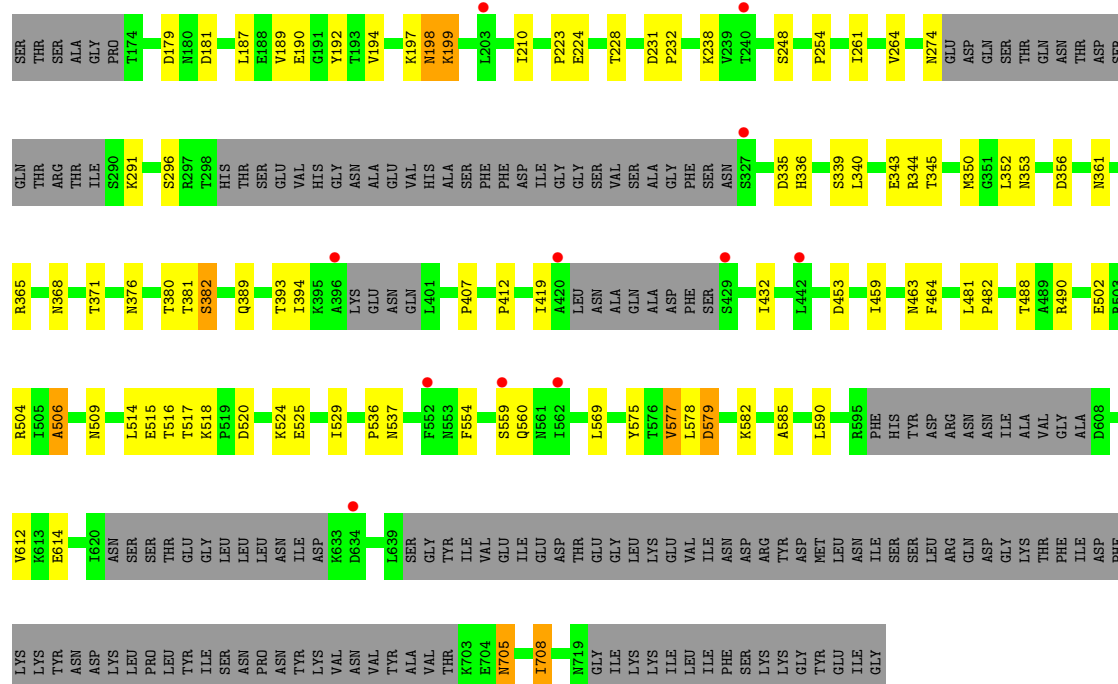


• Molecule 1: Protective antigen PA-63

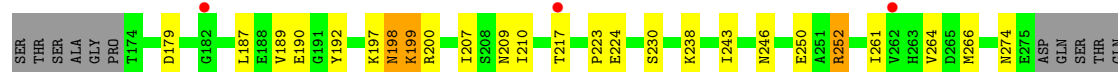


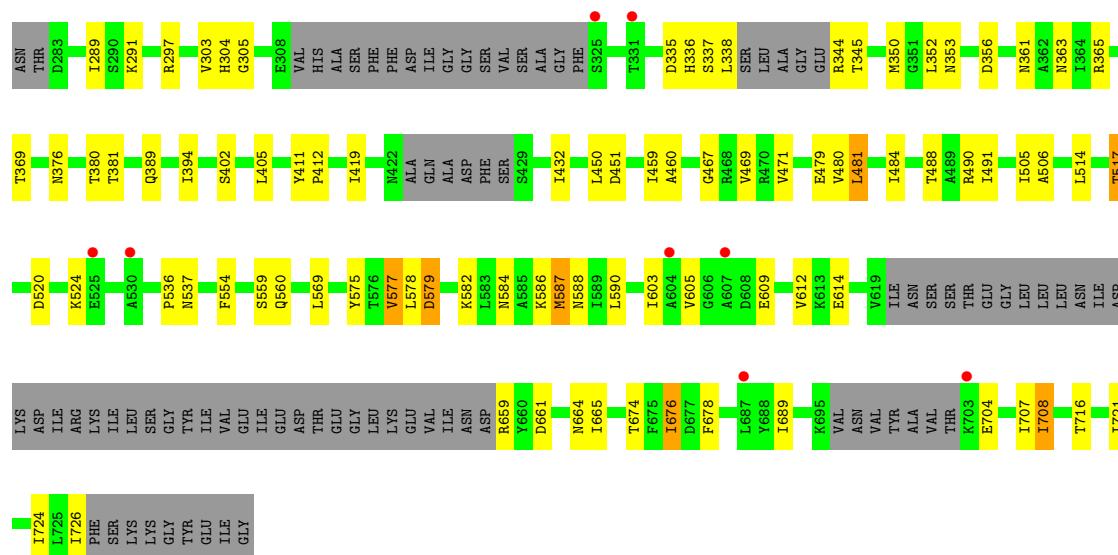


• Molecule 1: Protective antigen PA-63

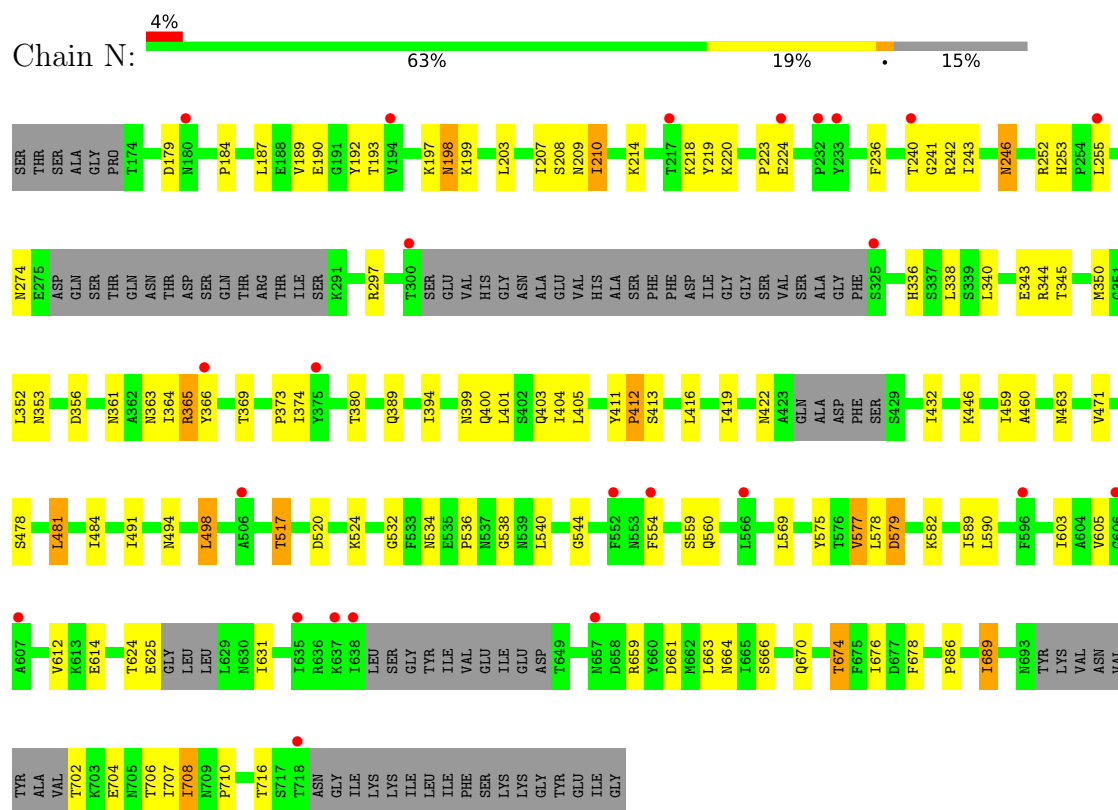


• Molecule 1: Protective antigen PA-63





• Molecule 1: Protective antigen PA-63



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	166.18Å 144.25Å 304.82Å 90.00° 102.41° 90.00°	Depositor
Resolution (Å)	44.83 – 5.50 44.83 – 5.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.83-5.50) 99.1 (44.83-5.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 5.39Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.251 , 0.278 0.266 , 0.286	Depositor DCC
R_{free} test set	2250 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	183.8	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 272.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	53490	wwPDB-VP
Average B, all atoms (Å ²)	257.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% 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	0.71	0/3771	1.22	8/5109 (0.2%)
1	B	0.70	0/4181	1.20	11/5667 (0.2%)
1	C	0.69	0/3134	1.20	9/4250 (0.2%)
1	D	0.67	0/4336	1.20	10/5877 (0.2%)
1	E	0.68	0/4156	1.20	11/5633 (0.2%)
1	F	0.70	0/3746	1.21	7/5072 (0.1%)
1	G	0.68	0/4192	1.18	9/5681 (0.2%)
1	H	0.68	0/3958	1.21	9/5364 (0.2%)
1	I	0.68	0/4257	1.21	12/5770 (0.2%)
1	J	0.72	0/3776	1.25	11/5112 (0.2%)
1	K	0.72	0/3926	1.22	10/5314 (0.2%)
1	L	0.77	0/3237	1.24	12/4388 (0.3%)
1	M	0.74	0/3811	1.23	8/5166 (0.2%)
1	N	0.74	0/3868	1.22	10/5243 (0.2%)
All	All	0.70	0/54349	1.21	137/73646 (0.2%)

There are no bond length outliers.

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	179	ASP	CA-CB-CG	6.87	119.47	112.60
1	L	179	ASP	CA-CB-CG	6.69	119.29	112.60
1	I	179	ASP	CA-CB-CG	6.55	119.15	112.60
1	L	705	ASN	CA-CB-CG	6.51	119.11	112.60
1	E	179	ASP	CA-CB-CG	6.45	119.05	112.60

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	A	3712	0	3666	41	0
1	B	4114	0	4098	51	0
1	C	3083	0	3058	22	0
1	D	4265	0	4229	42	0
1	E	4089	0	4071	49	0
1	F	3688	0	3679	31	0
1	G	4125	0	4102	45	0
1	H	3894	0	3852	40	0
1	I	4189	0	4164	49	0
1	J	3718	0	3673	33	0
1	K	3867	0	3860	41	0
1	L	3189	0	3177	34	0
1	M	3749	0	3697	42	0
1	N	3808	0	3769	48	0
All	All	53490	0	53095	541	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 5.

The worst 5 of 541 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:G:642:TYR:HB2	1:G:665:ILE:HD11	1.57	0.87
1:I:642:TYR:HB2	1:I:665:ILE:HD11	1.58	0.83
1:B:642:TYR:HB2	1:B:665:ILE:HD11	1.60	0.81
1:N:297:ARG:HD3	1:N:369:THR:HG21	1.68	0.75
1:K:481:LEU:H	1:K:482:PRO:HD2	1.56	0.71

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	455/568 (80%)	407 (90%)	39 (9%)	9 (2%)	6	30
1	B	509/568 (90%)	454 (89%)	49 (10%)	6 (1%)	10	43
1	C	374/568 (66%)	335 (90%)	35 (9%)	4 (1%)	11	45
1	D	529/568 (93%)	473 (89%)	49 (9%)	7 (1%)	9	41
1	E	506/568 (89%)	457 (90%)	43 (8%)	6 (1%)	10	43
1	F	449/568 (79%)	402 (90%)	41 (9%)	6 (1%)	9	41
1	G	510/568 (90%)	460 (90%)	45 (9%)	5 (1%)	12	48
1	H	479/568 (84%)	424 (88%)	46 (10%)	9 (2%)	6	31
1	I	519/568 (91%)	460 (89%)	52 (10%)	7 (1%)	9	41
1	J	452/568 (80%)	401 (89%)	39 (9%)	12 (3%)	4	25
1	K	474/568 (84%)	424 (90%)	44 (9%)	6 (1%)	9	41
1	L	388/568 (68%)	347 (89%)	36 (9%)	5 (1%)	9	41
1	M	459/568 (81%)	403 (88%)	48 (10%)	8 (2%)	7	35
1	N	466/568 (82%)	415 (89%)	40 (9%)	11 (2%)	4	26
All	All	6569/7952 (83%)	5862 (89%)	606 (9%)	101 (2%)	8	39

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	587	MET
1	N	413	SER
1	B	422	ASN
1	I	304	HIS
1	J	715	ASP

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	418/504 (83%)	387 (93%)	31 (7%)	13	33
1	B	465/504 (92%)	435 (94%)	30 (6%)	15	37
1	C	349/504 (69%)	326 (93%)	23 (7%)	15	37
1	D	482/504 (96%)	448 (93%)	34 (7%)	13	35
1	E	462/504 (92%)	429 (93%)	33 (7%)	13	35
1	F	416/504 (82%)	383 (92%)	33 (8%)	11	32
1	G	468/504 (93%)	436 (93%)	32 (7%)	14	36
1	H	439/504 (87%)	407 (93%)	32 (7%)	13	34
1	I	473/504 (94%)	440 (93%)	33 (7%)	14	36
1	J	419/504 (83%)	388 (93%)	31 (7%)	13	33
1	K	438/504 (87%)	406 (93%)	32 (7%)	13	34
1	L	362/504 (72%)	336 (93%)	26 (7%)	13	35
1	M	419/504 (83%)	380 (91%)	39 (9%)	8	26
1	N	432/504 (86%)	393 (91%)	39 (9%)	9	27
All	All	6042/7056 (86%)	5594 (93%)	448 (7%)	13	33

5 of 448 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	481	LEU
1	N	689	ILE
1	J	252	ARG
1	N	614	GLU
1	M	603	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 209 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	485	GLN

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Mol	Chain	Res	Type
1	J	463	ASN
1	N	485	GLN
1	H	621	ASN
1	I	543	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 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](#)

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	471/568 (82%)	0.22	12 (2%) 58 49	257, 257, 257, 257	0
1	B	519/568 (91%)	0.38	25 (4%) 35 35	257, 257, 257, 257	0
1	C	388/568 (68%)	0.13	10 (2%) 57 48	257, 257, 257, 257	0
1	D	539/568 (94%)	0.43	39 (7%) 21 26	257, 257, 257, 257	0
1	E	516/568 (90%)	0.27	12 (2%) 61 52	257, 257, 257, 257	0
1	F	467/568 (82%)	0.34	14 (2%) 52 45	257, 257, 257, 257	0
1	G	520/568 (91%)	0.24	16 (3%) 51 44	257, 257, 257, 257	0
1	H	493/568 (86%)	0.46	27 (5%) 30 32	257, 257, 257, 257	0
1	I	529/568 (93%)	0.24	18 (3%) 48 43	257, 257, 257, 257	0
1	J	470/568 (82%)	0.21	14 (2%) 52 45	257, 257, 257, 257	0
1	K	488/568 (85%)	0.32	25 (5%) 33 34	257, 257, 257, 257	0
1	L	404/568 (71%)	0.11	11 (2%) 56 47	257, 257, 257, 257	0
1	M	473/568 (83%)	0.22	11 (2%) 61 52	257, 257, 257, 257	0
1	N	480/568 (84%)	0.31	24 (5%) 34 34	257, 257, 257, 257	0
All	All	6757/7952 (84%)	0.28	258 (3%) 44 41	257, 257, 257, 257	0

The worst 5 of 258 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	604	ALA	7.3
1	N	607	ALA	6.8
1	D	229	ALA	4.9
1	B	255	LEU	4.9
1	F	346	TRP	4.7

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.