wwPDB X-ray Structure Validation Summary Report (i)

Mar 23, 2024 – 02:51 PM EDT

PDB ID	:	1TZN
Title	:	Crystal Structure of the Anthrax Toxin Protective Antigen Heptameric Pre-pore bound to the VWA domain of CMG2, an anthrax toxin receptor
Authors	:	Lacy, D.B.; Wigelsworth, D.J.; Melnyk, R.A.; Collier, R.J.
Deposited on	:	2004-07-10
Resolution	:	4.30 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 (1)) were used in the production of this report:

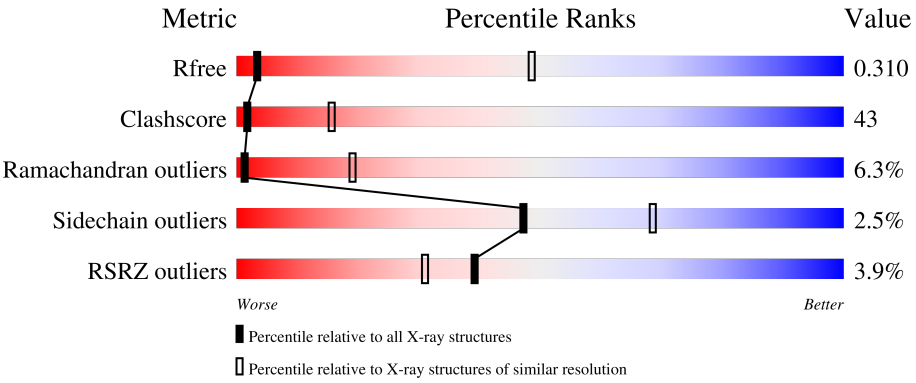
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 4.30 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	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

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	562	% 38% 54% 6%
1	B	562	3% 38% 55%
1	C	562	4% 38% 55% 5%
1	D	562	% 38% 55% 5%
1	E	562	2% 38% 56% 5%

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Mol	Chain	Length	Quality of chain
1	F	562	2% 38% 55% 5%
1	G	562	4% 38% 54% 6%
1	H	562	3% 38% 55% 5%
1	I	562	% 38% 55% 5%
1	J	562	2% 38% 55% 5%
1	K	562	4% 39% 54% 6%
1	L	562	2% 39% 54% 5%
1	M	562	3% 38% 55% 5%
1	O	562	3% 39% 54% 5%
2	a	181	7% 95% 5%
2	b	181	6% 96%
2	c	181	14% 96%
2	d	181	4% 96%
2	e	181	8% 94% 6%
2	f	181	7% 96%
2	g	181	8% 96%
2	h	181	6% 96%
2	i	181	4% 96%
2	j	181	10% 96%
2	k	181	12% 94% 5%
2	l	181	5% 96%
2	m	181	4% 96%
2	o	181	9% 96%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 80570 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4356	2726	752	872	6			
1	B	552	Total	C	N	O	S	0	0	0
			4356	2726	752	872	6			
1	C	552	Total	C	N	O	S	0	0	0
			4356	2726	752	872	6			
1	D	552	Total	C	N	O	S	0	0	0
			4356	2726	752	872	6			
1	E	552	Total	C	N	O	S	0	0	0
			4356	2726	752	872	6			
1	F	552	Total	C	N	O	S	0	0	0
			4356	2726	752	872	6			
1	G	552	Total	C	N	O	S	0	0	0
			4356	2726	752	872	6			
1	H	552	Total	C	N	O	S	0	0	0
			4356	2726	752	872	6			
1	I	552	Total	C	N	O	S	0	0	0
			4356	2726	752	872	6			
1	J	552	Total	C	N	O	S	0	0	0
			4356	2726	752	872	6			
1	K	552	Total	C	N	O	S	0	0	0
			4356	2726	752	872	6			
1	L	552	Total	C	N	O	S	0	0	0
			4356	2726	752	872	6			
1	M	552	Total	C	N	O	S	0	0	0
			4356	2726	752	872	6			
1	O	552	Total	C	N	O	S	0	0	0
			4356	2726	752	872	6			

- Molecule 2 is a protein called Anthrax toxin receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	181	Total	C	N	O	S	0	0	0
			1396	891	236	265	4			
2	b	181	Total	C	N	O	S	0	0	0
			1396	891	236	265	4			
2	c	181	Total	C	N	O	S	0	0	0
			1396	891	236	265	4			
2	d	181	Total	C	N	O	S	0	0	0
			1396	891	236	265	4			
2	e	181	Total	C	N	O	S	0	0	0
			1396	891	236	265	4			
2	f	181	Total	C	N	O	S	0	0	0
			1396	891	236	265	4			
2	g	181	Total	C	N	O	S	0	0	0
			1396	891	236	265	4			
2	h	181	Total	C	N	O	S	0	0	0
			1396	891	236	265	4			
2	i	181	Total	C	N	O	S	0	0	0
			1396	891	236	265	4			
2	j	181	Total	C	N	O	S	0	0	0
			1396	891	236	265	4			
2	k	181	Total	C	N	O	S	0	0	0
			1396	891	236	265	4			
2	l	181	Total	C	N	O	S	0	0	0
			1396	891	236	265	4			
2	m	181	Total	C	N	O	S	0	0	0
			1396	891	236	265	4			
2	o	181	Total	C	N	O	S	0	0	0
			1396	891	236	265	4			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		
3	C	2	Total	Ca	0	0
			2	2		
3	D	2	Total	Ca	0	0
			2	2		
3	E	2	Total	Ca	0	0
			2	2		
3	F	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total Ca 2 2	0	0
3	H	2	Total Ca 2 2	0	0
3	I	2	Total Ca 2 2	0	0
3	J	2	Total Ca 2 2	0	0
3	K	2	Total Ca 2 2	0	0
3	L	2	Total Ca 2 2	0	0
3	M	2	Total Ca 2 2	0	0
3	O	2	Total Ca 2 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0
4	I	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0
4	K	1	Total Mg 1 1	0	0

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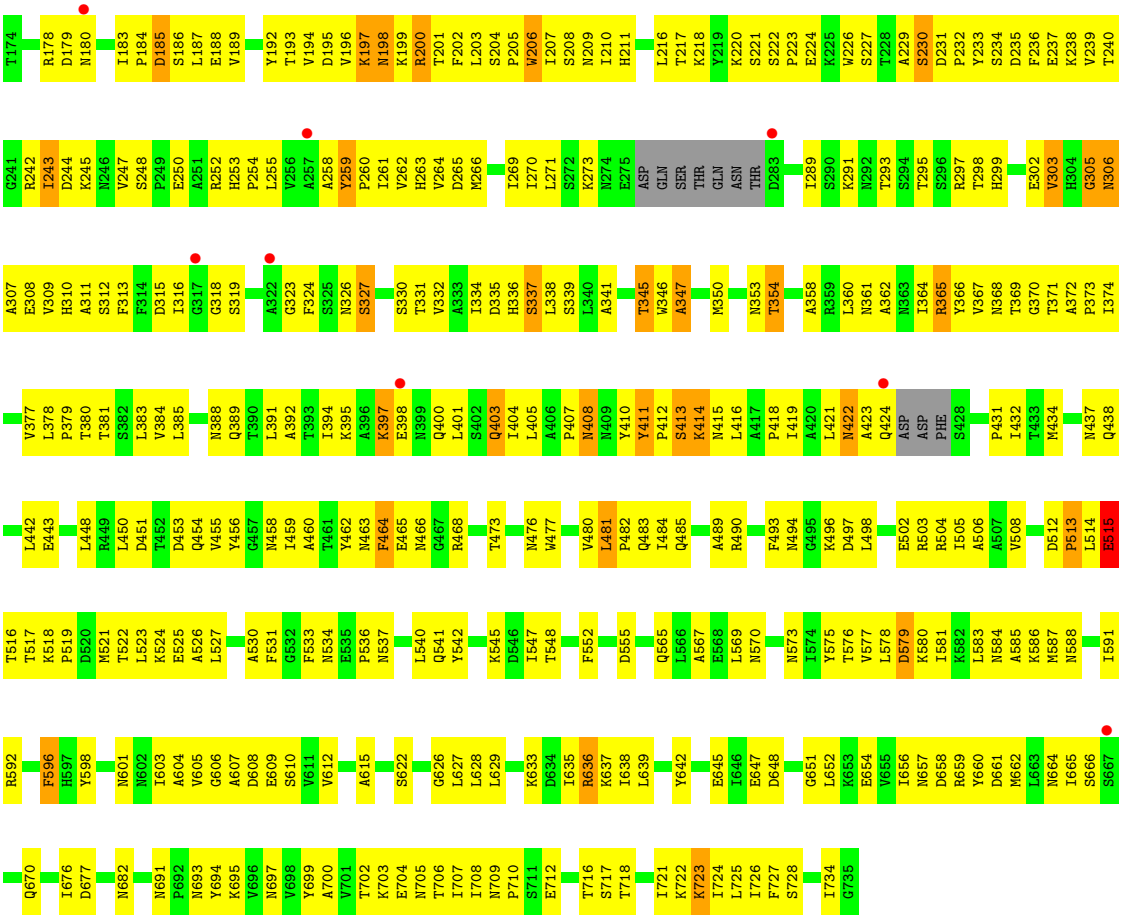
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total Mg 1 1	0	0
4	M	1	Total Mg 1 1	0	0
4	O	1	Total Mg 1 1	0	0

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.

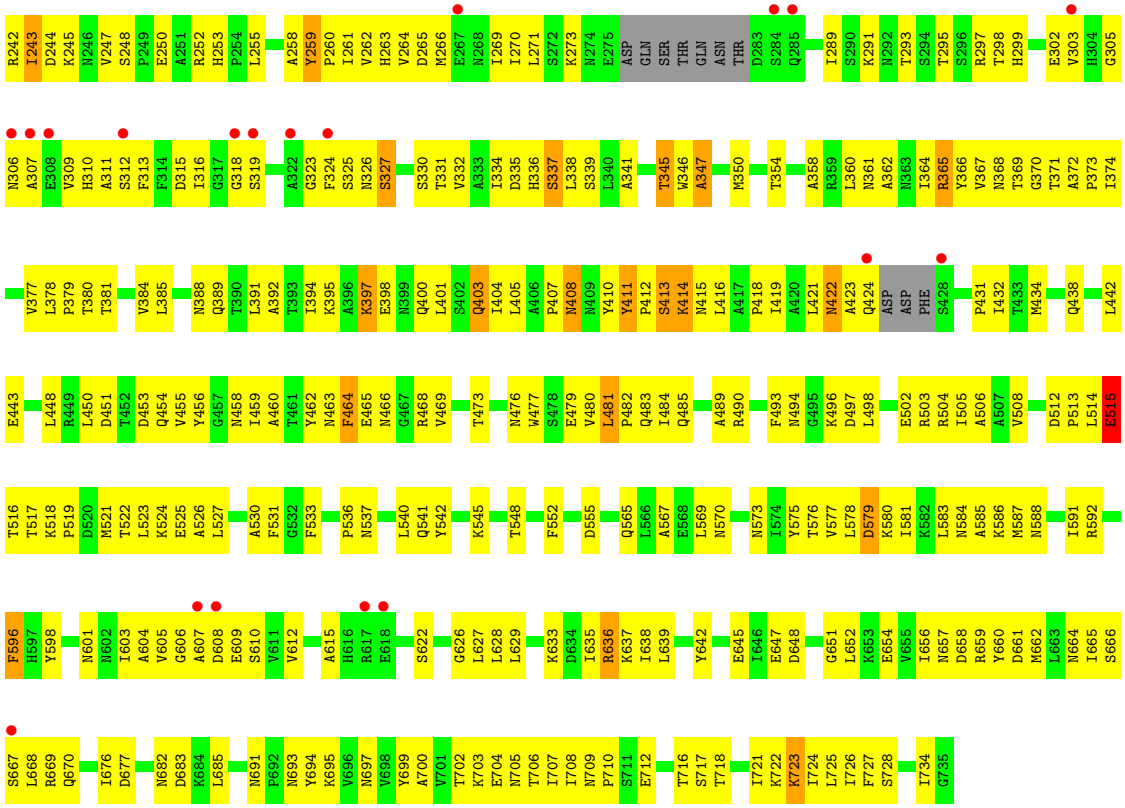
• Molecule 1: Protective antigen

Chain A:



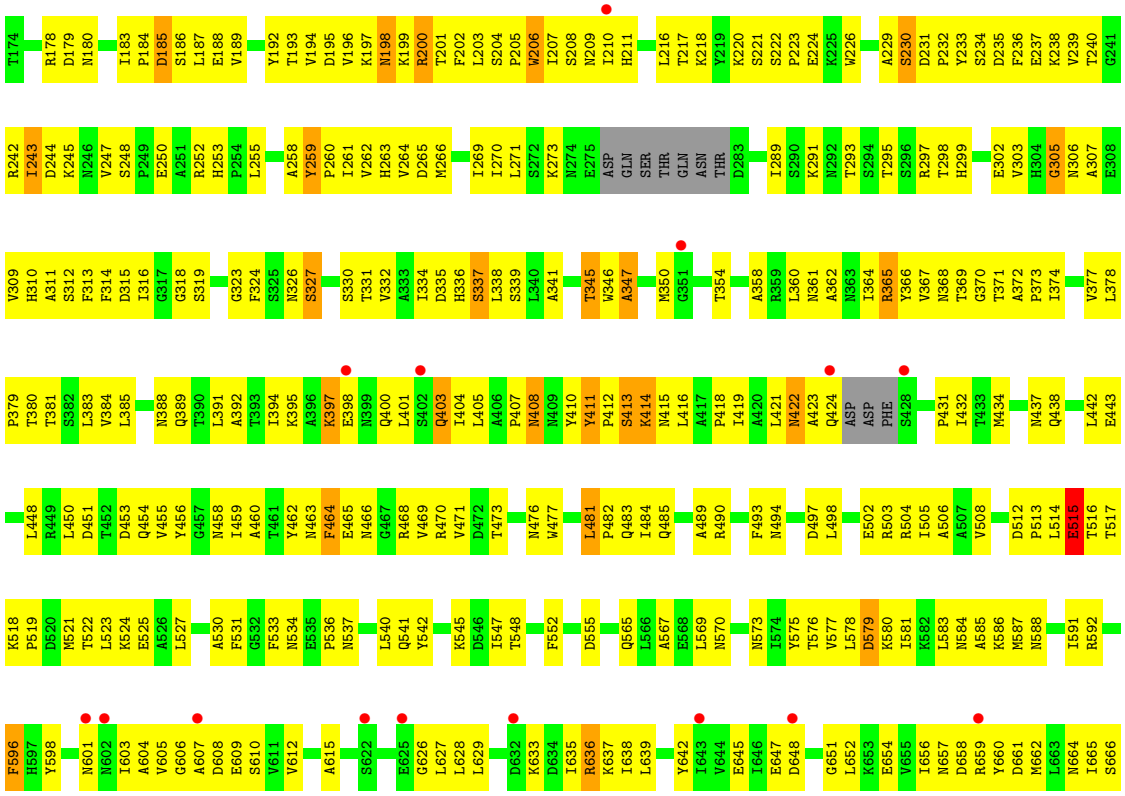
• Molecule 1: Protective antigen

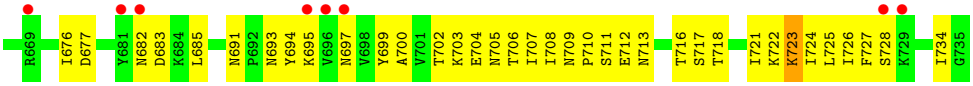
Chain B:



• Molecule 1: Protective antigen

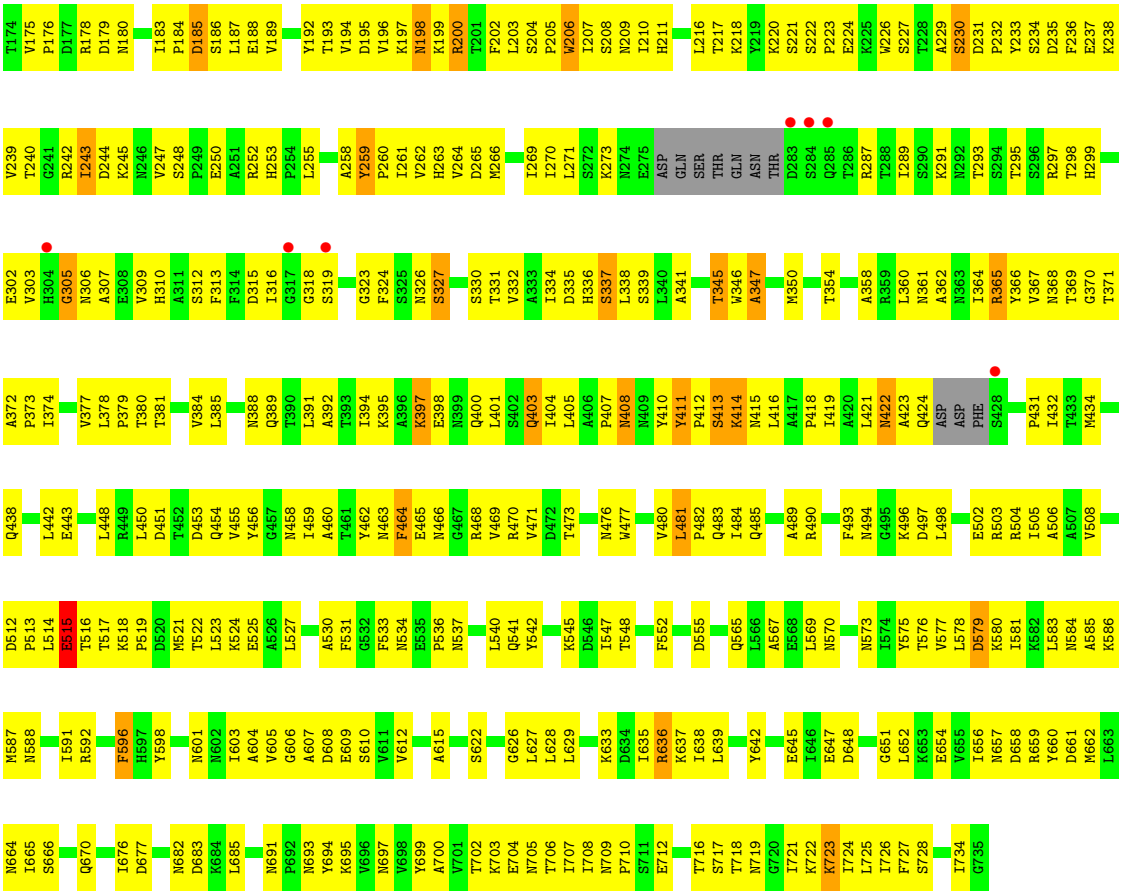
Chain C:





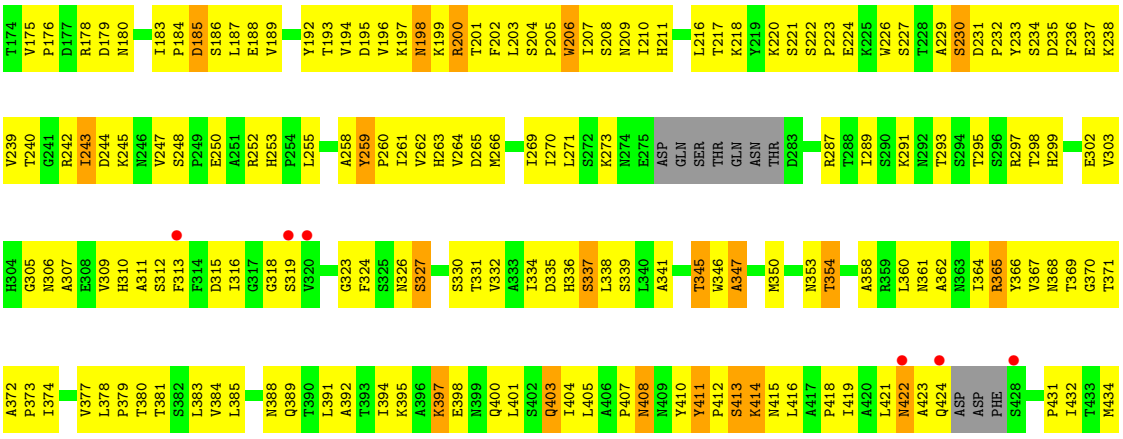
• Molecule 1: Protective antigen

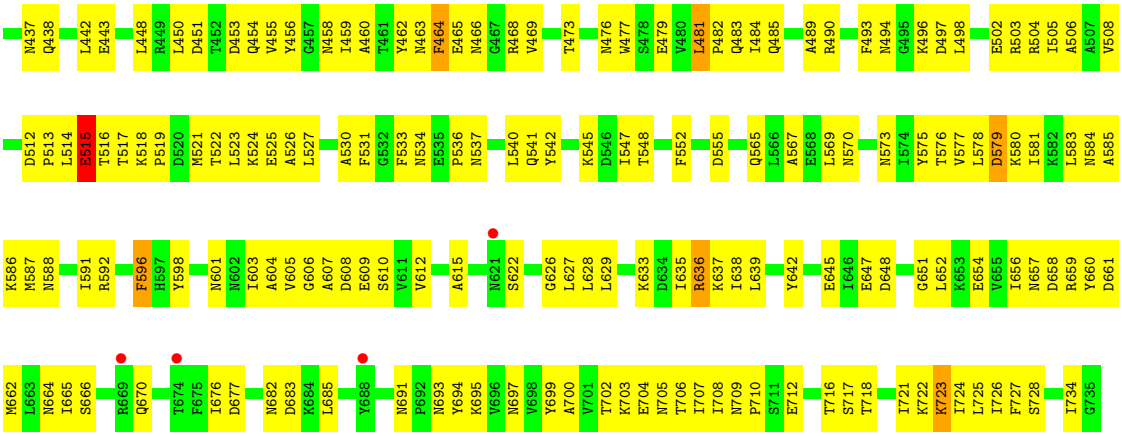
Chain D:



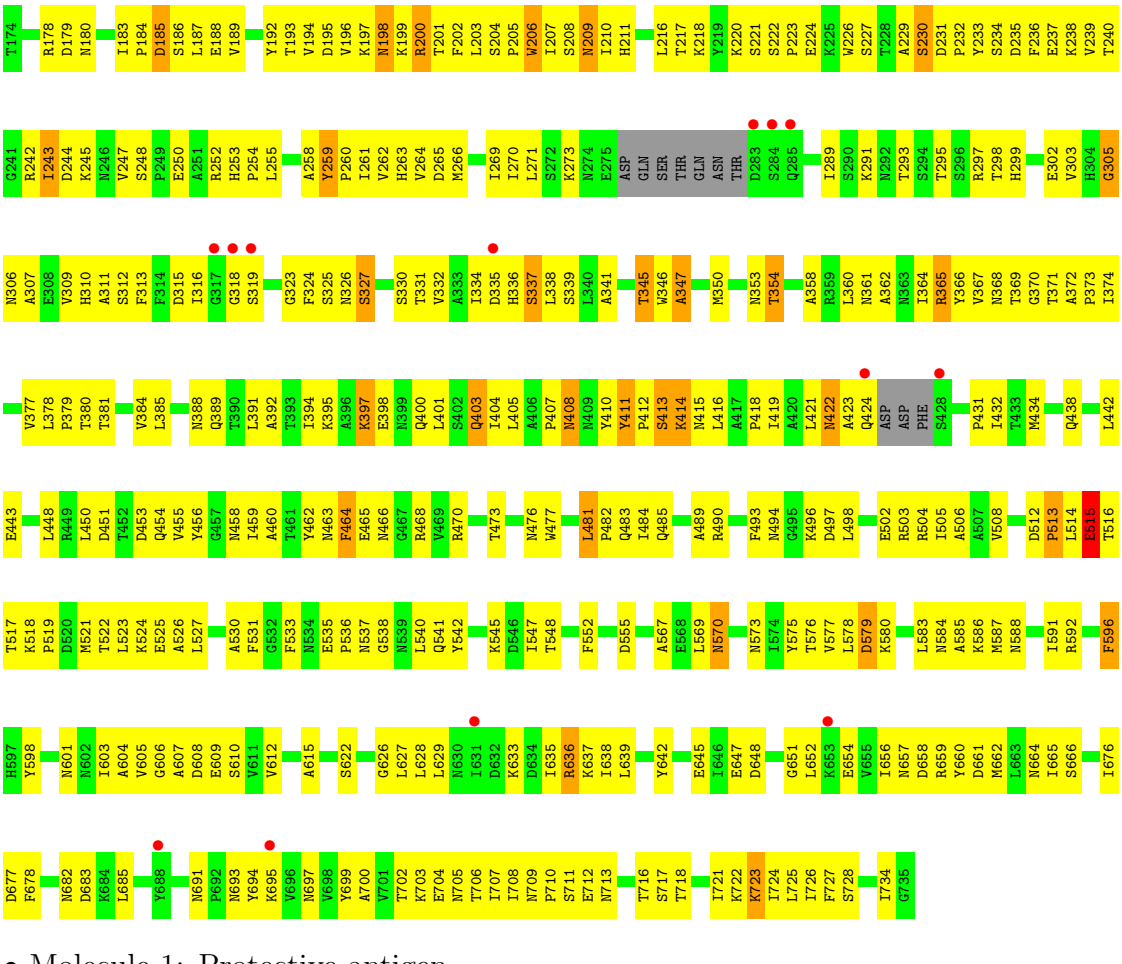
• Molecule 1: Protective antigen

Chain E:

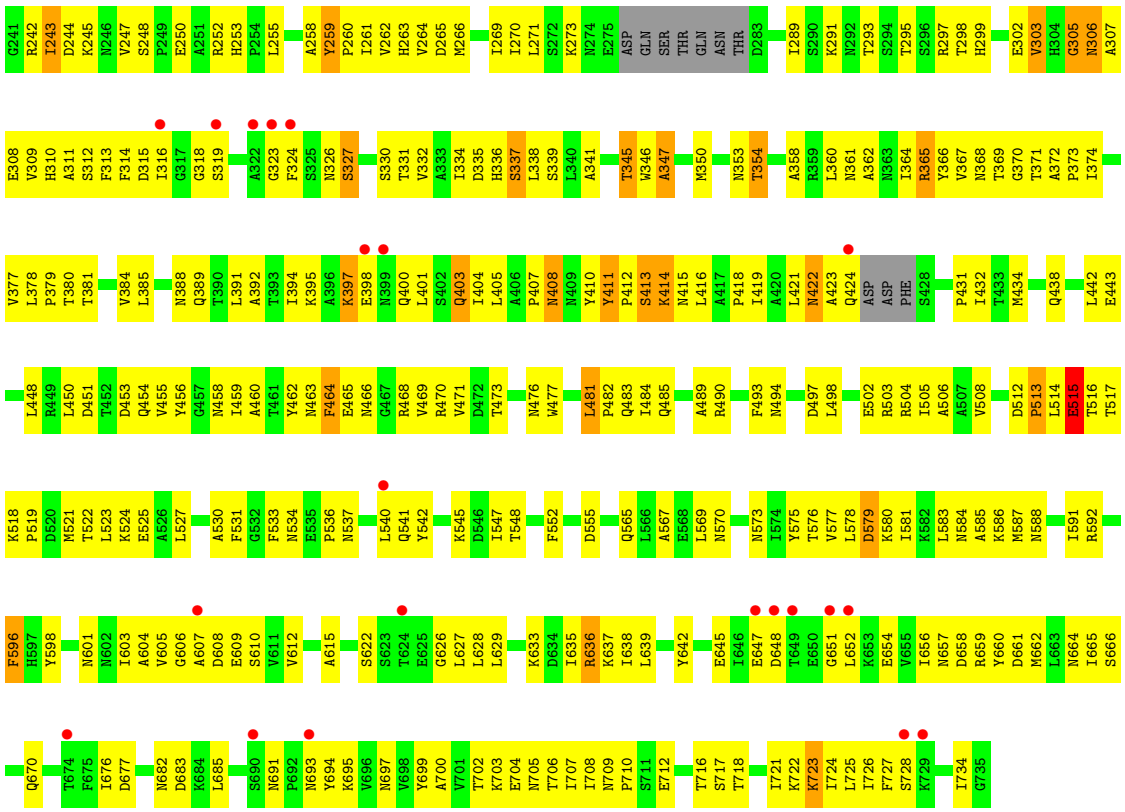




• Molecule 1: Protective antigen

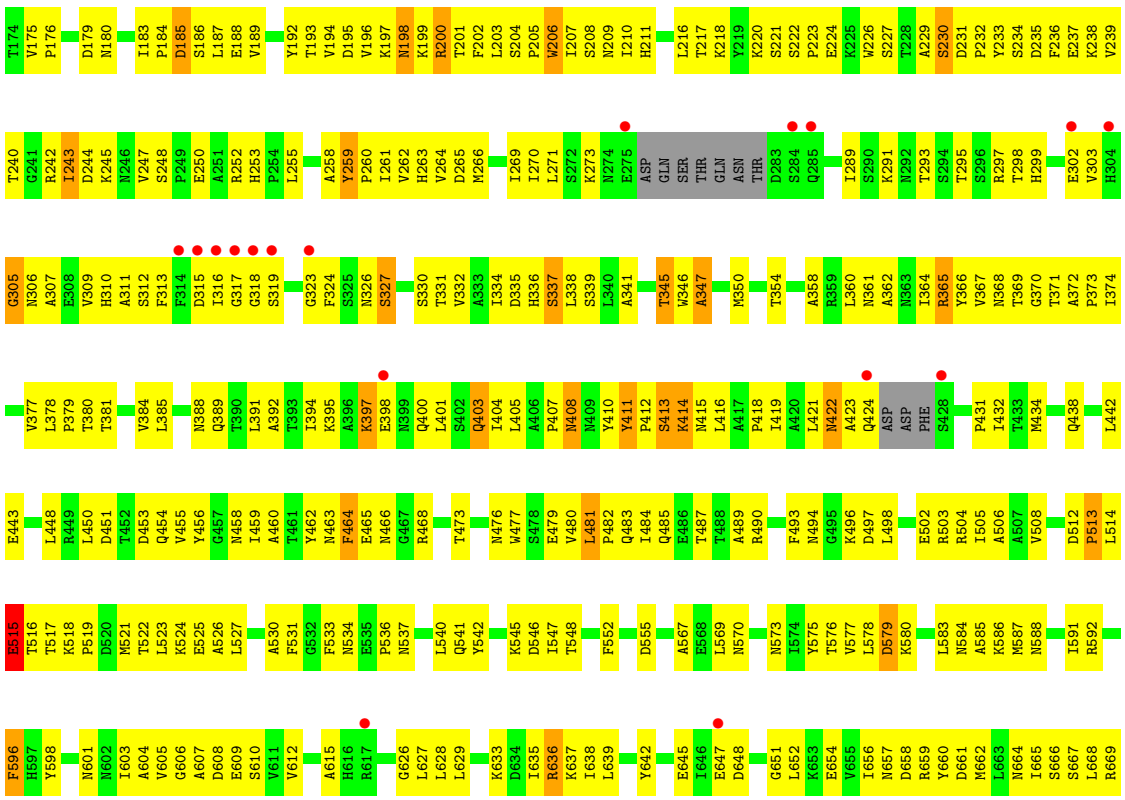


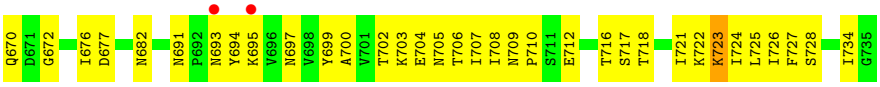
• Molecule 1: Protective antigen



• Molecule 1: Protective antigen

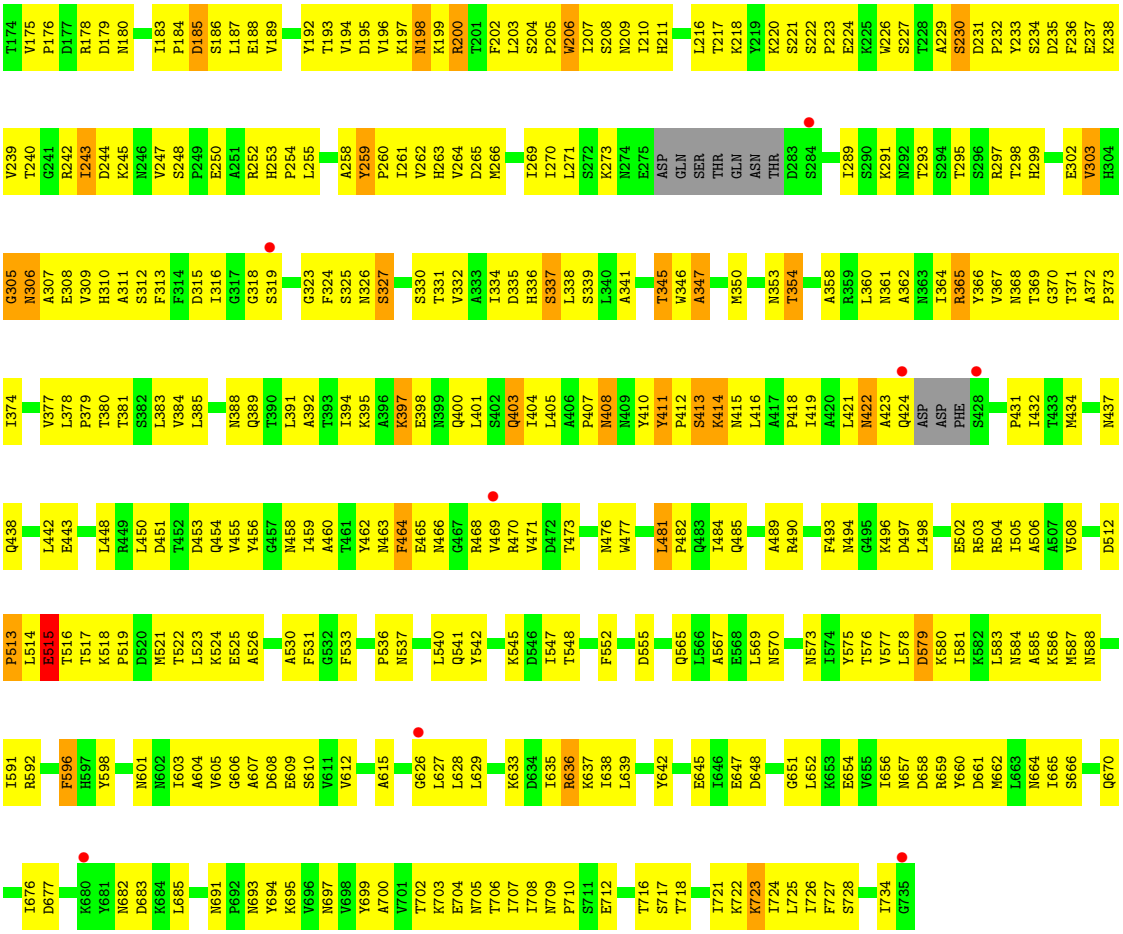
Chain H:





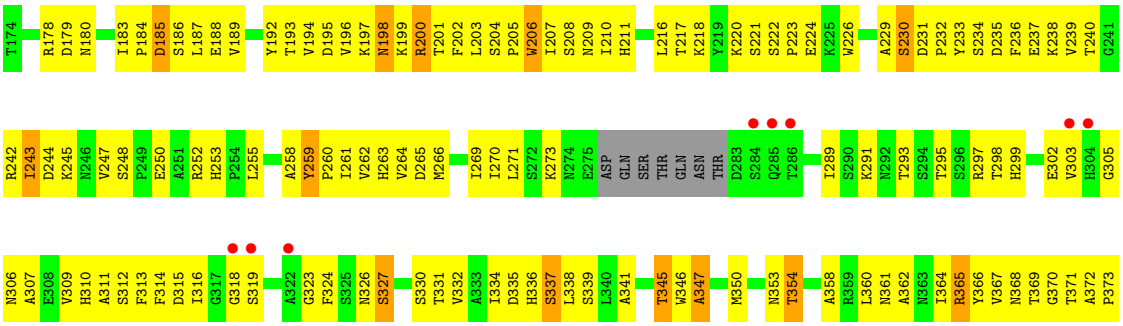
• Molecule 1: Protective antigen

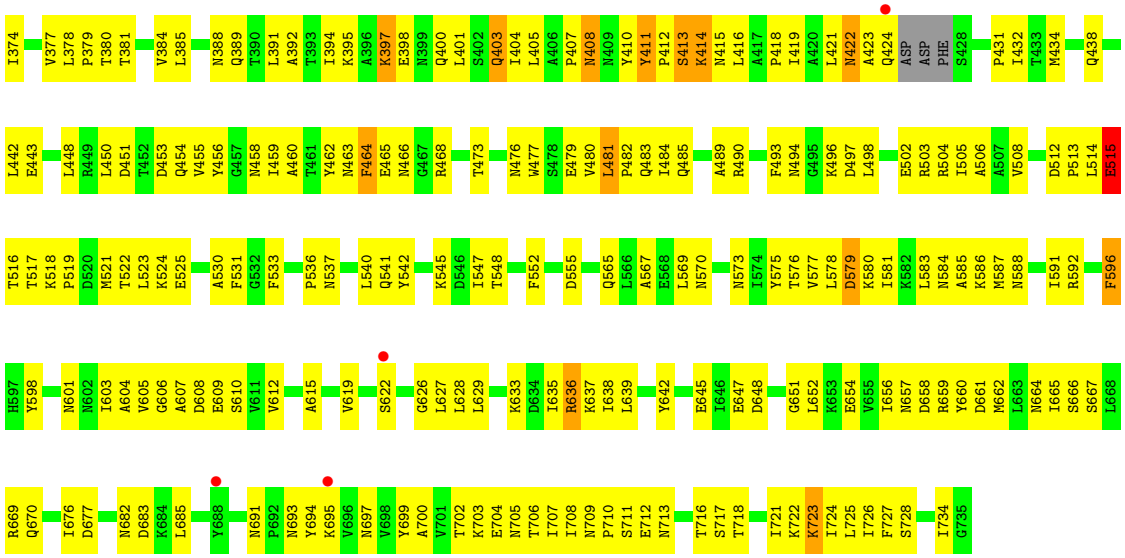
Chain I:



• Molecule 1: Protective antigen

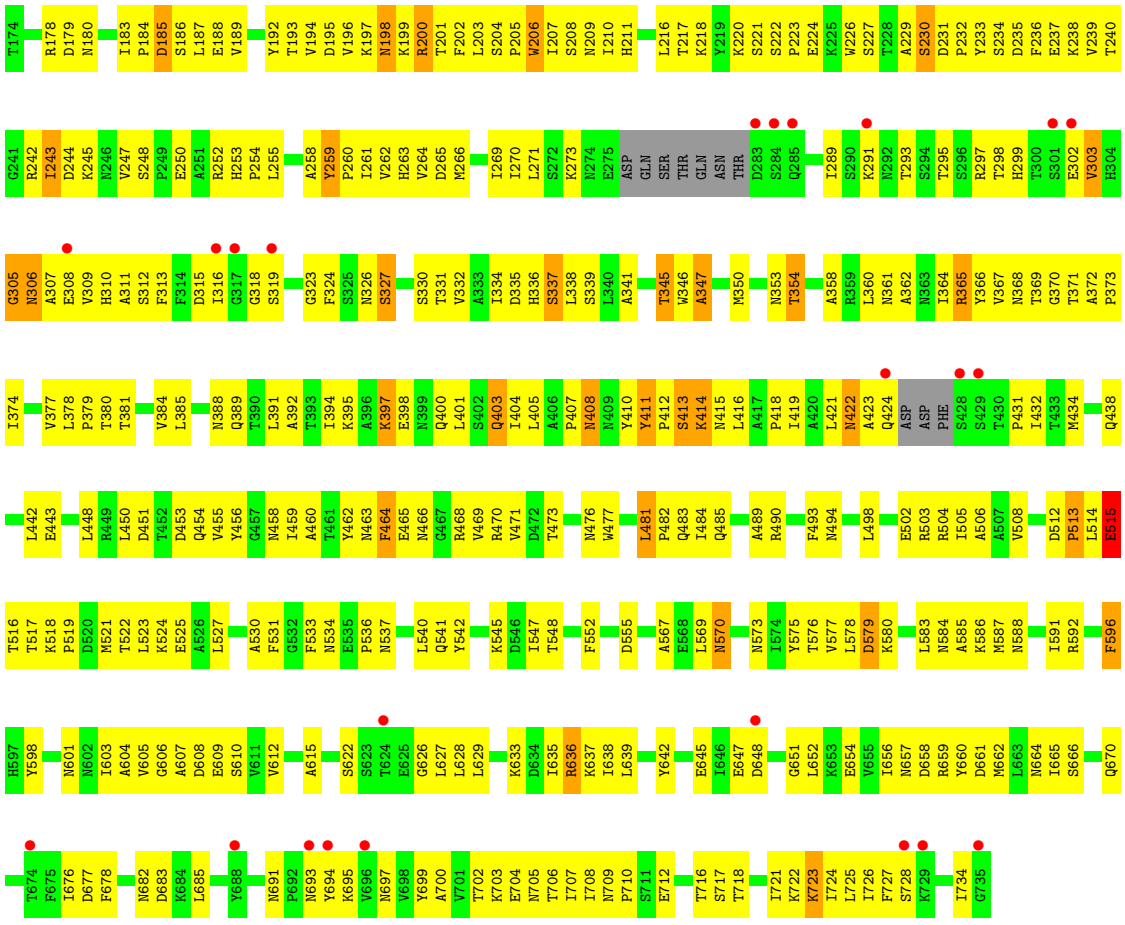
Chain J:





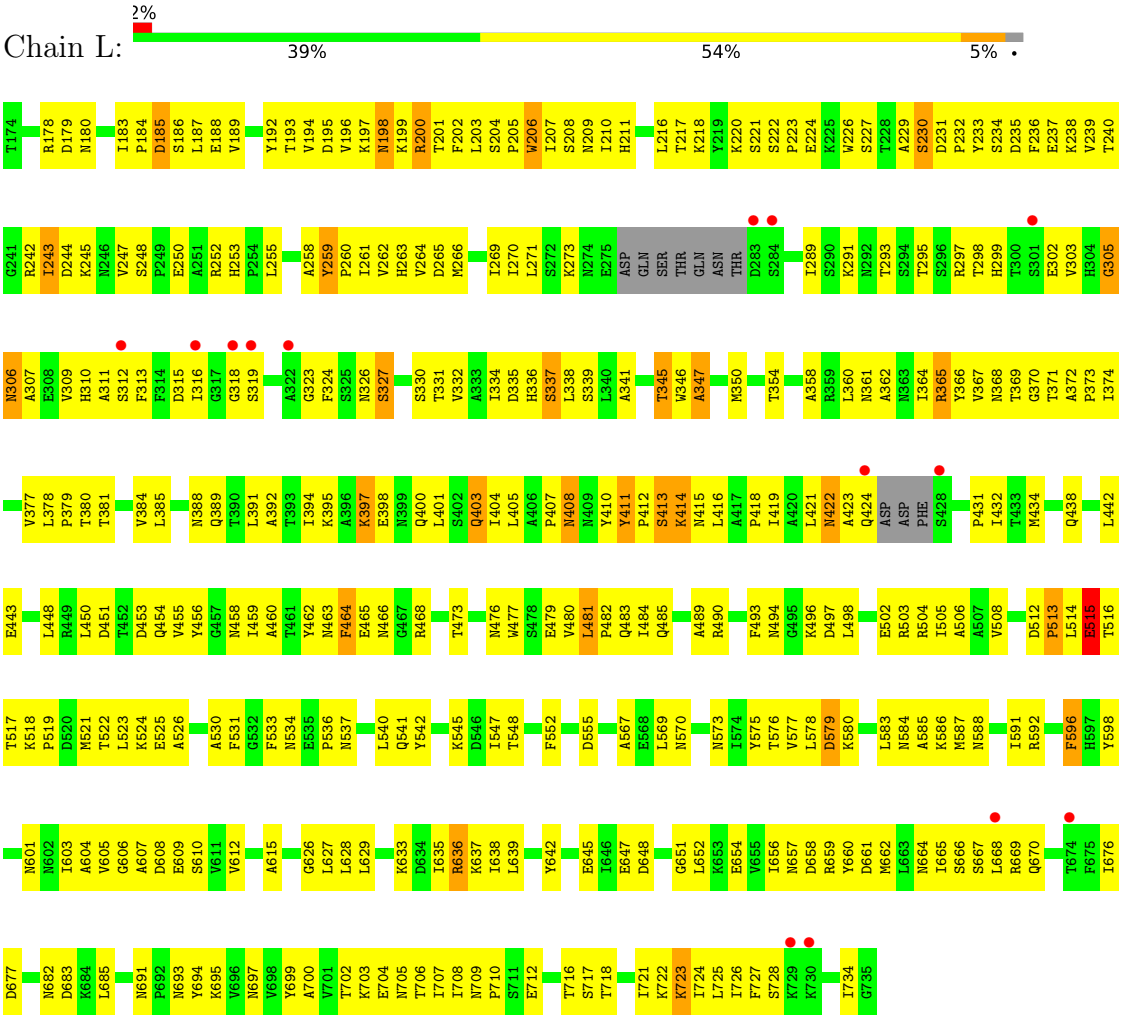
• Molecule 1: Protective antigen

Chain K:



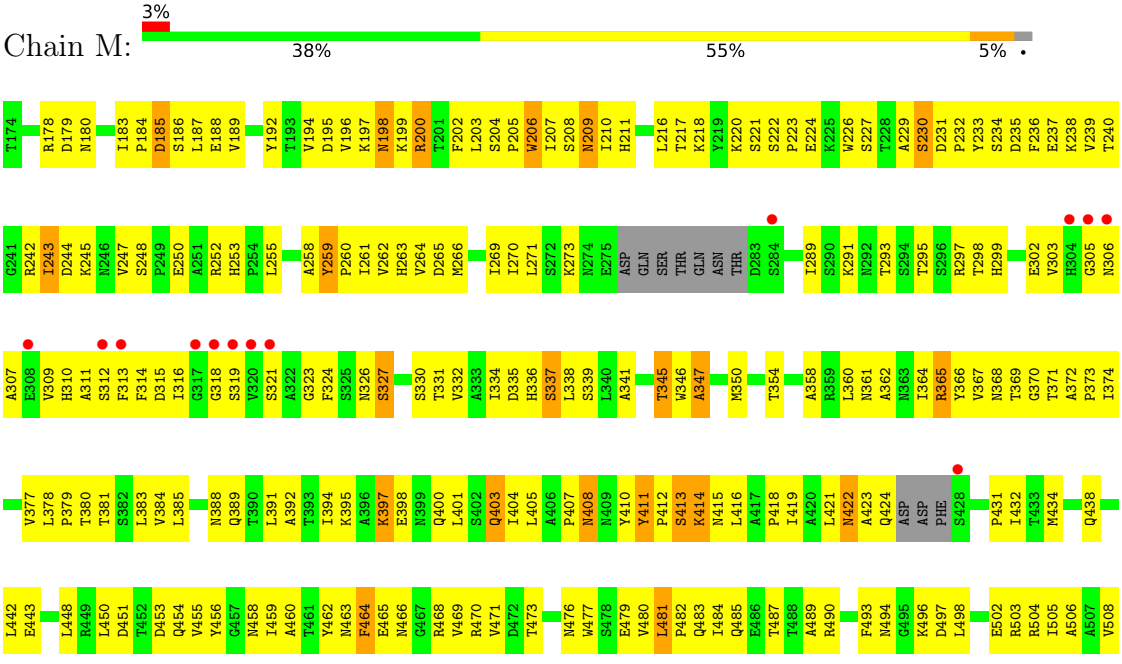
• Molecule 1: Protective antigen

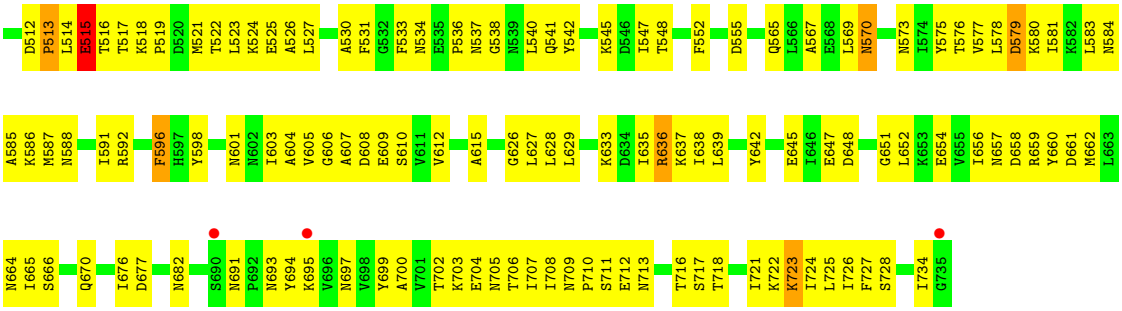
Chain L:



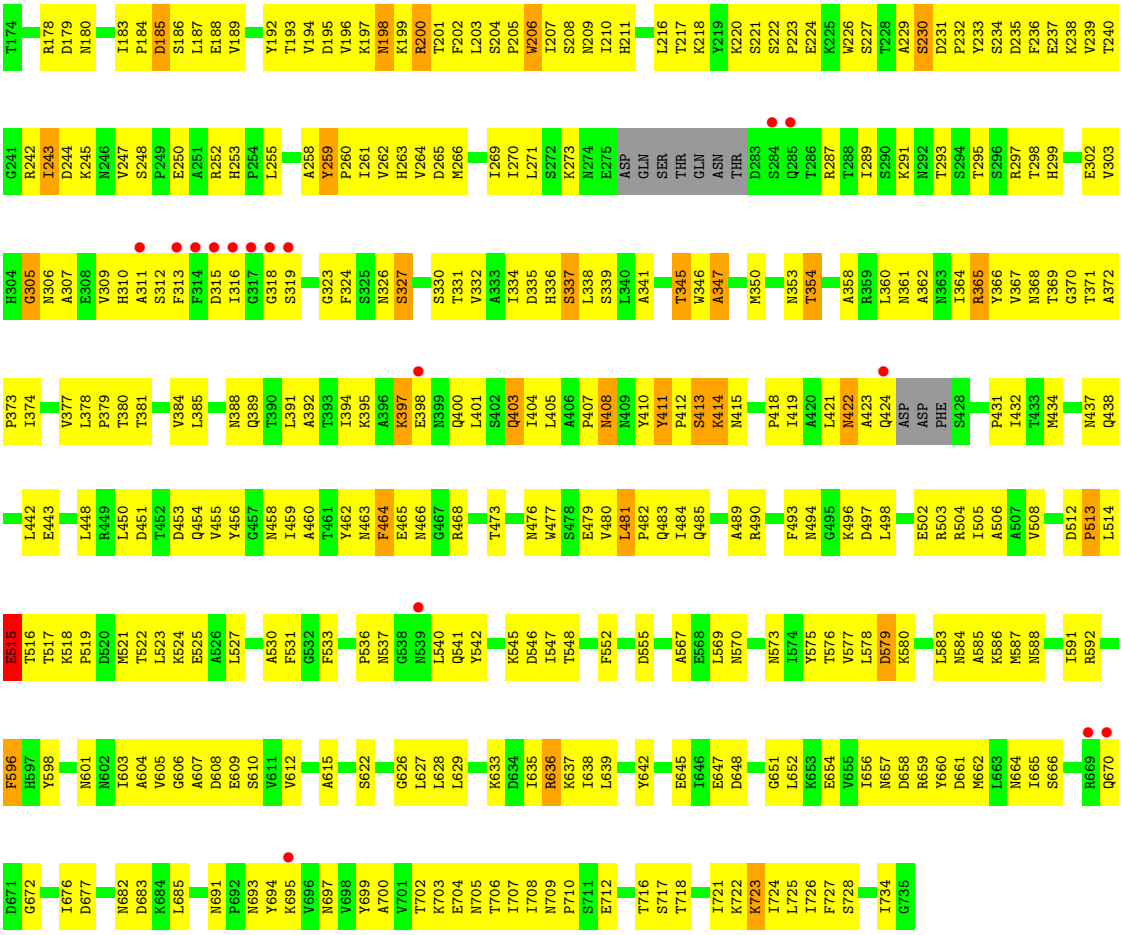
• Molecule 1: Protective antigen

Chain M:

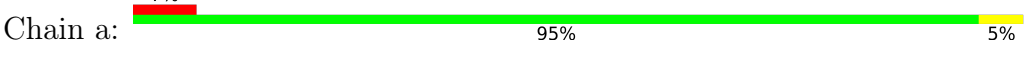




• Molecule 1: Protective antigen

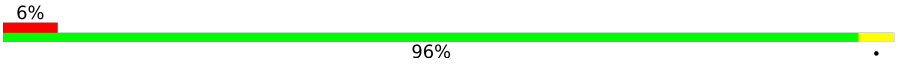


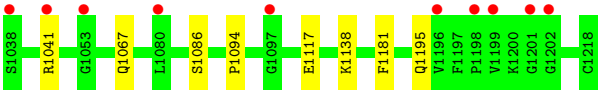
• Molecule 2: Anthrax toxin receptor 2



• Molecule 2: Anthrax toxin receptor 2

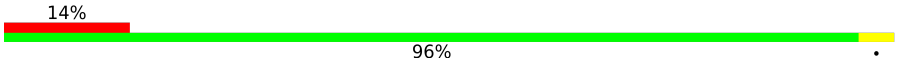
Chain b:

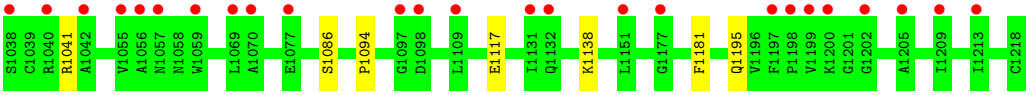




• Molecule 2: Anthrax toxin receptor 2

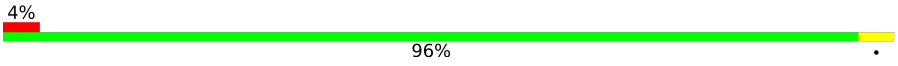
Chain c:

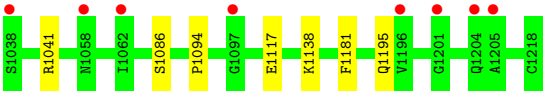




• Molecule 2: Anthrax toxin receptor 2

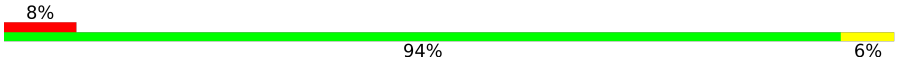
Chain d:

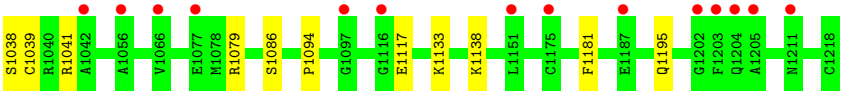




• Molecule 2: Anthrax toxin receptor 2

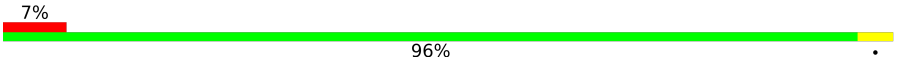
Chain e:

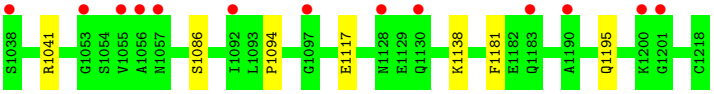




• Molecule 2: Anthrax toxin receptor 2

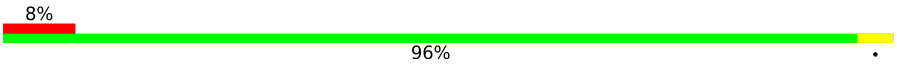
Chain f:

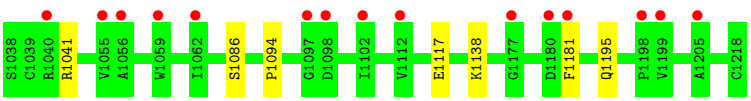




• Molecule 2: Anthrax toxin receptor 2

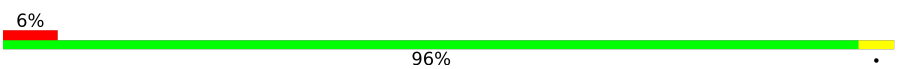
Chain g:

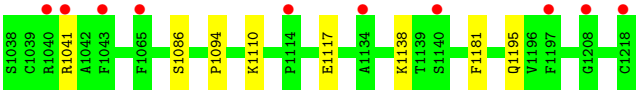




• Molecule 2: Anthrax toxin receptor 2

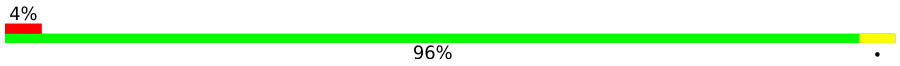
Chain h:

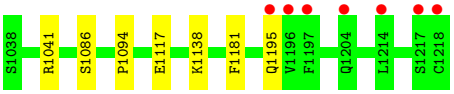




• Molecule 2: Anthrax toxin receptor 2

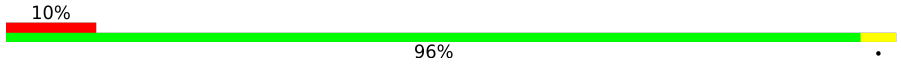
Chain i:

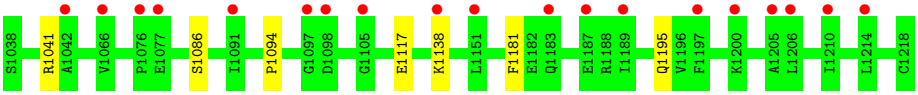




• Molecule 2: Anthrax toxin receptor 2

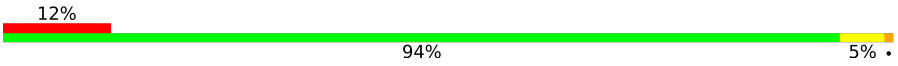
Chain j:

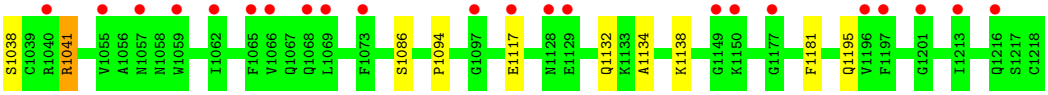




• Molecule 2: Anthrax toxin receptor 2

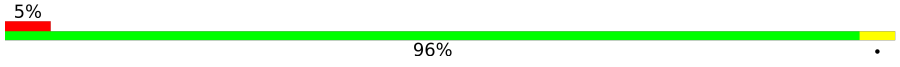
Chain k:

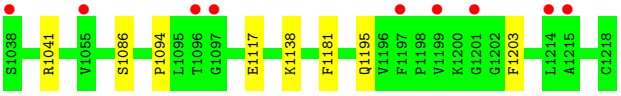




• Molecule 2: Anthrax toxin receptor 2

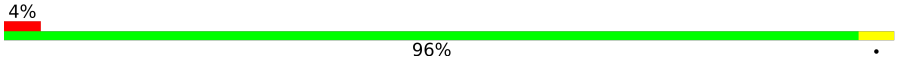
Chain l:

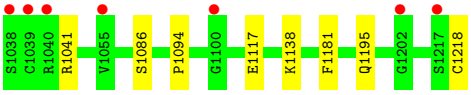




• Molecule 2: Anthrax toxin receptor 2

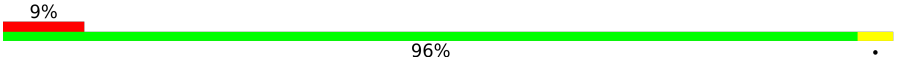
Chain m:

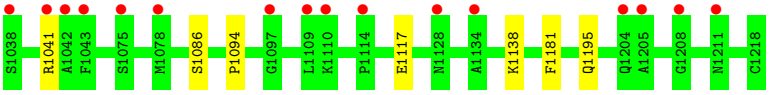




• Molecule 2: Anthrax toxin receptor 2

Chain o:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	158.80Å 158.85Å 214.08Å 69.58° 69.07° 65.58°	Depositor
Resolution (Å)	20.00 – 4.30 19.66 – 4.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-4.30) 94.0 (19.66-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 4.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.322 , 0.330 0.305 , 0.310	Depositor DCC
R_{free} test set	5704 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	81.4	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 8.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.125 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	80570	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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: MG, CA

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	0.27	0/4430	0.51	0/6007
1	B	0.27	0/4430	0.51	0/6007
1	C	0.27	0/4430	0.51	0/6007
1	D	0.27	0/4430	0.51	0/6007
1	E	0.27	0/4430	0.51	0/6007
1	F	0.27	0/4430	0.51	0/6007
1	G	0.27	0/4430	0.51	0/6007
1	H	0.27	0/4430	0.51	0/6007
1	I	0.27	0/4430	0.51	0/6007
1	J	0.27	0/4430	0.51	0/6007
1	K	0.27	0/4430	0.51	0/6007
1	L	0.27	0/4430	0.51	0/6007
1	M	0.27	0/4430	0.51	0/6007
1	O	0.27	0/4430	0.51	0/6007
2	a	0.26	0/1417	0.44	0/1907
2	b	0.26	0/1417	0.44	0/1907
2	c	0.26	0/1417	0.44	0/1907
2	d	0.26	0/1417	0.44	0/1907
2	e	0.26	0/1417	0.44	0/1907
2	f	0.26	0/1417	0.44	0/1907
2	g	0.26	0/1417	0.44	0/1907
2	h	0.26	0/1417	0.44	0/1907
2	i	0.26	0/1417	0.44	0/1907
2	j	0.26	0/1417	0.44	0/1907
2	k	0.26	0/1417	0.44	0/1907
2	l	0.26	0/1417	0.44	0/1907
2	m	0.26	0/1417	0.44	0/1907
2	o	0.26	0/1417	0.44	0/1907
All	All	0.27	0/81858	0.49	0/110796

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4356	0	4314	416	5
1	B	4356	0	4314	406	0
1	C	4356	0	4314	396	2
1	D	4356	0	4314	396	2
1	E	4356	0	4314	390	2
1	F	4356	0	4314	390	9
1	G	4356	0	4314	447	6
1	H	4356	0	4314	452	5
1	I	4356	0	4314	447	0
1	J	4356	0	4314	411	1
1	K	4356	0	4314	419	2
1	L	4356	0	4314	430	0
1	M	4356	0	4314	442	8
1	O	4356	0	4314	409	2
2	a	1396	0	1426	0	2
2	b	1396	0	1426	0	2
2	c	1396	0	1426	0	0
2	d	1396	0	1426	0	0
2	e	1396	0	1426	0	5
2	f	1396	0	1426	0	0
2	g	1396	0	1426	0	0
2	h	1396	0	1426	0	1
2	i	1396	0	1426	0	0
2	j	1396	0	1426	0	0
2	k	1396	0	1426	0	5
2	l	1396	0	1426	0	4
2	m	1396	0	1426	0	1
2	o	1396	0	1426	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	M	2	0	0	0	0
3	O	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
All	All	80570	0	80360	5343	32

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 43.

The worst 5 of 5343 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:414:LYS:HG3	1:M:319:SER:N	1.35	1.39
1:G:305:GLY:HA2	1:H:670:GLN:NE2	1.42	1.34
1:G:414:LYS:CG	1:M:319:SER:H	1.41	1.32
1:H:483:GLN:NE2	1:I:469:VAL:HG21	1.47	1.28
1:L:305:GLY:HA2	1:M:670:GLN:CG	1.64	1.25

The worst 5 of 32 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:546:ASP:OD2	2:l:1203:PHE:CE1[1_455]	0.85	1.35
1:F:570:ASN:CG	1:G:197:LYS:NZ[1_544]	1.33	0.87
2:b:1067:GLN:OE1	1:E:537:ASN:OD1[1_455]	1.36	0.84
1:A:197:LYS:NZ	1:M:570:ASN:ND2[1_544]	1.37	0.83
1:A:197:LYS:NZ	1:M:570:ASN:CG[1_544]	1.45	0.75

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	546/562 (97%)	374 (68%)	132 (24%)	40 (7%)	1	16
1	B	546/562 (97%)	374 (68%)	132 (24%)	40 (7%)	1	16
1	C	546/562 (97%)	373 (68%)	133 (24%)	40 (7%)	1	16
1	D	546/562 (97%)	374 (68%)	132 (24%)	40 (7%)	1	16
1	E	546/562 (97%)	374 (68%)	132 (24%)	40 (7%)	1	16
1	F	546/562 (97%)	373 (68%)	133 (24%)	40 (7%)	1	16
1	G	546/562 (97%)	374 (68%)	132 (24%)	40 (7%)	1	16
1	H	546/562 (97%)	374 (68%)	132 (24%)	40 (7%)	1	16
1	I	546/562 (97%)	374 (68%)	132 (24%)	40 (7%)	1	16
1	J	546/562 (97%)	374 (68%)	132 (24%)	40 (7%)	1	16
1	K	546/562 (97%)	374 (68%)	132 (24%)	40 (7%)	1	16
1	L	546/562 (97%)	374 (68%)	132 (24%)	40 (7%)	1	16
1	M	546/562 (97%)	373 (68%)	133 (24%)	40 (7%)	1	16
1	O	546/562 (97%)	374 (68%)	132 (24%)	40 (7%)	1	16
2	a	179/181 (99%)	144 (80%)	29 (16%)	6 (3%)	3	29
2	b	179/181 (99%)	144 (80%)	29 (16%)	6 (3%)	3	29
2	c	179/181 (99%)	143 (80%)	30 (17%)	6 (3%)	3	29
2	d	179/181 (99%)	144 (80%)	29 (16%)	6 (3%)	3	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	e	179/181 (99%)	144 (80%)	29 (16%)	6 (3%)	3	29
2	f	179/181 (99%)	144 (80%)	29 (16%)	6 (3%)	3	29
2	g	179/181 (99%)	144 (80%)	29 (16%)	6 (3%)	3	29
2	h	179/181 (99%)	144 (80%)	29 (16%)	6 (3%)	3	29
2	i	179/181 (99%)	144 (80%)	29 (16%)	6 (3%)	3	29
2	j	179/181 (99%)	144 (80%)	29 (16%)	6 (3%)	3	29
2	k	179/181 (99%)	144 (80%)	29 (16%)	6 (3%)	3	29
2	l	179/181 (99%)	144 (80%)	29 (16%)	6 (3%)	3	29
2	m	179/181 (99%)	144 (80%)	29 (16%)	6 (3%)	3	29
2	o	179/181 (99%)	144 (80%)	29 (16%)	6 (3%)	3	29
All	All	10150/10402 (98%)	7248 (71%)	2258 (22%)	644 (6%)	1	19

5 of 644 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	LYS
1	A	209	ASN
1	A	422	ASN
1	A	656	ILE
2	a	1086	SER

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	491/501 (98%)	476 (97%)	15 (3%)	40	63
1	B	491/501 (98%)	476 (97%)	15 (3%)	40	63
1	C	491/501 (98%)	476 (97%)	15 (3%)	40	63
1	D	491/501 (98%)	476 (97%)	15 (3%)	40	63
1	E	491/501 (98%)	476 (97%)	15 (3%)	40	63
1	F	491/501 (98%)	476 (97%)	15 (3%)	40	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	491/501 (98%)	476 (97%)	15 (3%)	40	63
1	H	491/501 (98%)	476 (97%)	15 (3%)	40	63
1	I	491/501 (98%)	476 (97%)	15 (3%)	40	63
1	J	491/501 (98%)	476 (97%)	15 (3%)	40	63
1	K	491/501 (98%)	476 (97%)	15 (3%)	40	63
1	L	491/501 (98%)	476 (97%)	15 (3%)	40	63
1	M	491/501 (98%)	476 (97%)	15 (3%)	40	63
1	O	491/501 (98%)	476 (97%)	15 (3%)	40	63
2	a	152/152 (100%)	151 (99%)	1 (1%)	84	90
2	b	152/152 (100%)	151 (99%)	1 (1%)	84	90
2	c	152/152 (100%)	151 (99%)	1 (1%)	84	90
2	d	152/152 (100%)	151 (99%)	1 (1%)	84	90
2	e	152/152 (100%)	151 (99%)	1 (1%)	84	90
2	f	152/152 (100%)	151 (99%)	1 (1%)	84	90
2	g	152/152 (100%)	151 (99%)	1 (1%)	84	90
2	h	152/152 (100%)	151 (99%)	1 (1%)	84	90
2	i	152/152 (100%)	151 (99%)	1 (1%)	84	90
2	j	152/152 (100%)	151 (99%)	1 (1%)	84	90
2	k	152/152 (100%)	151 (99%)	1 (1%)	84	90
2	l	152/152 (100%)	151 (99%)	1 (1%)	84	90
2	m	152/152 (100%)	151 (99%)	1 (1%)	84	90
2	o	152/152 (100%)	151 (99%)	1 (1%)	84	90
All	All	9002/9142 (98%)	8778 (98%)	224 (2%)	47	68

5 of 224 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	259	TYR
1	O	596	PHE
2	i	1041	ARG
1	O	464	PHE
1	M	397	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 376 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	584	ASN
1	K	697	ASN
2	i	1183	GLN
1	J	697	ASN
1	L	415	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 42 ligands modelled in this entry, 42 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	552/562 (98%)	-0.06	8 (1%) 75 66	1, 36, 166, 200	0
1	B	552/562 (98%)	-0.05	19 (3%) 45 36	1, 36, 166, 200	0
1	C	552/562 (98%)	0.09	23 (4%) 36 29	1, 36, 166, 200	0
1	D	552/562 (98%)	-0.09	7 (1%) 77 68	1, 36, 166, 200	0
1	E	552/562 (98%)	-0.07	10 (1%) 68 60	1, 36, 166, 200	0
1	F	552/562 (98%)	0.04	13 (2%) 59 49	1, 36, 166, 200	0
1	G	552/562 (98%)	0.03	21 (3%) 40 32	1, 36, 166, 200	0
1	H	552/562 (98%)	-0.01	19 (3%) 45 36	1, 36, 166, 200	0
1	I	552/562 (98%)	-0.09	8 (1%) 75 66	1, 36, 166, 200	0
1	J	552/562 (98%)	-0.07	12 (2%) 62 52	1, 36, 166, 200	0
1	K	552/562 (98%)	0.02	23 (4%) 36 29	1, 36, 166, 200	0
1	L	552/562 (98%)	-0.01	14 (2%) 57 48	1, 36, 166, 200	0
1	M	552/562 (98%)	0.02	16 (2%) 51 41	1, 36, 166, 200	0
1	O	552/562 (98%)	-0.02	16 (2%) 51 41	1, 36, 166, 200	0
2	a	181/181 (100%)	0.21	13 (7%) 15 12	6, 92, 179, 200	0
2	b	181/181 (100%)	0.30	10 (5%) 25 22	6, 92, 179, 200	0
2	c	181/181 (100%)	0.79	25 (13%) 2 3	6, 92, 179, 200	0
2	d	181/181 (100%)	0.21	8 (4%) 34 28	6, 92, 179, 200	0
2	e	181/181 (100%)	0.35	14 (7%) 13 11	6, 92, 179, 200	0
2	f	181/181 (100%)	0.50	13 (7%) 15 12	6, 92, 179, 200	0
2	g	181/181 (100%)	0.51	15 (8%) 11 10	6, 92, 179, 200	0
2	h	181/181 (100%)	0.22	10 (5%) 25 22	6, 92, 179, 200	0
2	i	181/181 (100%)	0.12	7 (3%) 39 31	6, 92, 179, 200	0
2	j	181/181 (100%)	0.57	19 (10%) 6 6	6, 92, 179, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	k	181/181 (100%)	0.60	22 (12%) 4 5	6, 92, 179, 200	0
2	l	181/181 (100%)	0.33	9 (4%) 28 25	6, 92, 179, 200	0
2	m	181/181 (100%)	0.19	7 (3%) 39 31	6, 92, 179, 200	0
2	o	181/181 (100%)	0.36	16 (8%) 10 9	6, 92, 179, 200	0
All	All	10262/10402 (98%)	0.08	397 (3%) 39 31	1, 54, 174, 200	0

The worst 5 of 397 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	319	SER	12.1
1	F	285	GLN	10.8
1	J	319	SER	9.2
1	C	695	LYS	8.9
1	I	319	SER	7.8

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, 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(Å^2)	Q<0.9
4	MG	G	738	1/1	0.69	0.24	0,0,0,0	0
4	MG	J	738	1/1	0.71	0.11	0,0,0,0	0
4	MG	I	738	1/1	0.76	0.22	0,0,0,0	0
4	MG	K	738	1/1	0.78	0.14	0,0,0,0	0
4	MG	B	738	1/1	0.81	0.17	0,0,0,0	0
4	MG	C	738	1/1	0.83	0.18	0,0,0,0	0
4	MG	M	738	1/1	0.83	0.07	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	E	738	1/1	0.84	0.11	0,0,0,0	0
4	MG	O	738	1/1	0.84	0.11	0,0,0,0	0
4	MG	F	738	1/1	0.86	0.17	0,0,0,0	0
3	CA	H	737	1/1	0.90	0.10	0,0,0,0	0
4	MG	A	738	1/1	0.90	0.13	0,0,0,0	0
3	CA	A	737	1/1	0.90	0.11	0,0,0,0	0
3	CA	B	736	1/1	0.90	0.07	0,0,0,0	0
3	CA	F	737	1/1	0.90	0.10	0,0,0,0	0
3	CA	G	737	1/1	0.90	0.12	0,0,0,0	0
3	CA	E	737	1/1	0.91	0.14	0,0,0,0	0
3	CA	F	736	1/1	0.91	0.07	0,0,0,0	0
3	CA	B	737	1/1	0.92	0.11	0,0,0,0	0
4	MG	D	738	1/1	0.93	0.05	0,0,0,0	0
4	MG	L	738	1/1	0.93	0.26	0,0,0,0	0
3	CA	I	736	1/1	0.93	0.12	0,0,0,0	0
3	CA	G	736	1/1	0.93	0.09	0,0,0,0	0
3	CA	L	737	1/1	0.94	0.13	0,0,0,0	0
3	CA	J	736	1/1	0.94	0.06	0,0,0,0	0
3	CA	J	737	1/1	0.95	0.10	0,0,0,0	0
4	MG	H	738	1/1	0.95	0.07	0,0,0,0	0
3	CA	I	737	1/1	0.95	0.07	0,0,0,0	0
3	CA	M	737	1/1	0.95	0.09	0,0,0,0	0
3	CA	C	737	1/1	0.96	0.12	0,0,0,0	0
3	CA	D	737	1/1	0.96	0.07	0,0,0,0	0
3	CA	O	737	1/1	0.97	0.04	0,0,0,0	0
3	CA	K	737	1/1	0.97	0.07	0,0,0,0	0
3	CA	D	736	1/1	0.97	0.05	0,0,0,0	0
3	CA	K	736	1/1	0.97	0.06	0,0,0,0	0
3	CA	O	736	1/1	0.97	0.03	0,0,0,0	0
3	CA	H	736	1/1	0.98	0.10	0,0,0,0	0
3	CA	E	736	1/1	0.98	0.08	0,0,0,0	0
3	CA	L	736	1/1	0.98	0.09	0,0,0,0	0
3	CA	M	736	1/1	0.99	0.07	0,0,0,0	0
3	CA	C	736	1/1	0.99	0.12	0,0,0,0	0
3	CA	A	736	1/1	0.99	0.10	0,0,0,0	0

6.5 Other polymers (i)

There are no such residues in this entry.