



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 03:21 PM UTC

PDB ID : 5WKO / pdb_00005wko
Title : Crystal structure of antibody 27F3 recognizing the HA from
A/California/04/2009 (H1N1) influenza virus
Authors : Wilson, I.A.; Lang, S.; Zhu, X.
Deposited on : 2017-07-25
Resolution : 3.49 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

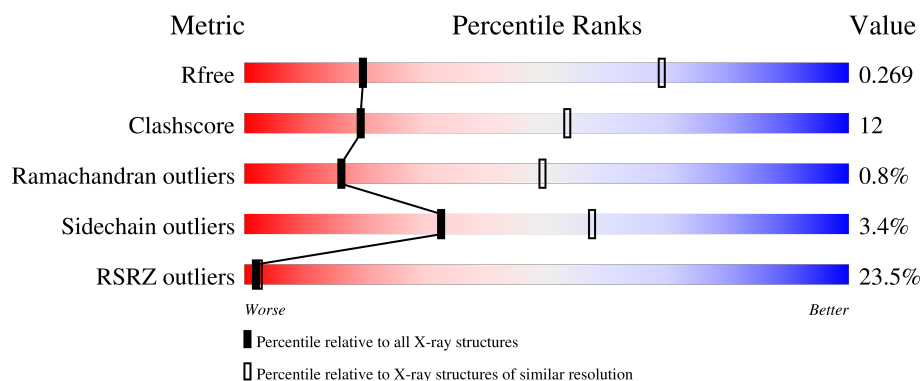
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	225	6% 75% 20% ..
1	C	225	6% 71% 26% ..
1	E	225	6% 76% 23% .
1	G	225	7% 71% 24% .
1	I	225	12% 71% 26% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	225	
2	B	213	
2	D	213	
2	F	213	
2	H	213	
2	J	213	
2	L	213	
3	M	331	
3	N	331	
3	O	331	
3	S	331	
3	T	331	
3	U	331	
4	P	177	
4	Q	177	
4	R	177	
4	V	177	
4	W	177	
4	X	177	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 43322 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 Antibody 27F3 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			
1	C	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			
1	E	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			
1	G	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			
1	I	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			
1	K	225	Total	C	N	O	S	0	0	0
			1675	1061	277	330	7			

- Molecule 2 is a protein called Antibody 27F3 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			
2	D	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			
2	F	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			
2	H	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			
2	J	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			
2	L	213	Total	C	N	O	S	0	0	0
			1628	1020	275	329	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	76	THR	SER	conflict	UNP Q9UL78

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	83	PHE	CYS	conflict	UNP Q9UL78
B	92	VAL	GLY	conflict	UNP Q9UL78
B	94	THR	SER	conflict	UNP Q9UL78
D	76	THR	SER	conflict	UNP Q9UL78
D	83	PHE	CYS	conflict	UNP Q9UL78
D	92	VAL	GLY	conflict	UNP Q9UL78
D	94	THR	SER	conflict	UNP Q9UL78
F	76	THR	SER	conflict	UNP Q9UL78
F	83	PHE	CYS	conflict	UNP Q9UL78
F	92	VAL	GLY	conflict	UNP Q9UL78
F	94	THR	SER	conflict	UNP Q9UL78
H	76	THR	SER	conflict	UNP Q9UL78
H	83	PHE	CYS	conflict	UNP Q9UL78
H	92	VAL	GLY	conflict	UNP Q9UL78
H	94	THR	SER	conflict	UNP Q9UL78
J	76	THR	SER	conflict	UNP Q9UL78
J	83	PHE	CYS	conflict	UNP Q9UL78
J	92	VAL	GLY	conflict	UNP Q9UL78
J	94	THR	SER	conflict	UNP Q9UL78
L	76	THR	SER	conflict	UNP Q9UL78
L	83	PHE	CYS	conflict	UNP Q9UL78
L	92	VAL	GLY	conflict	UNP Q9UL78
L	94	THR	SER	conflict	UNP Q9UL78

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	324	Total	C	N	O	S	0	0	0
			2529	1599	436	483	11			
3	N	323	Total	C	N	O	S	0	0	0
			2523	1596	435	481	11			
3	O	326	Total	C	N	O	S	0	0	0
			2544	1608	438	487	11			
3	S	324	Total	C	N	O	S	0	0	0
			2529	1599	436	483	11			
3	T	323	Total	C	N	O	S	0	0	0
			2523	1596	435	481	11			
3	U	326	Total	C	N	O	S	0	0	0
			2544	1608	438	487	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	7	ALA	-	expression tag	UNP C3W5S1
M	8	ASP	-	expression tag	UNP C3W5S1
M	9	PRO	-	expression tag	UNP C3W5S1
M	10	GLY	-	expression tag	UNP C3W5S1
N	7	ALA	-	expression tag	UNP C3W5S1
N	8	ASP	-	expression tag	UNP C3W5S1
N	9	PRO	-	expression tag	UNP C3W5S1
N	10	GLY	-	expression tag	UNP C3W5S1
O	7	ALA	-	expression tag	UNP C3W5S1
O	8	ASP	-	expression tag	UNP C3W5S1
O	9	PRO	-	expression tag	UNP C3W5S1
O	10	GLY	-	expression tag	UNP C3W5S1
S	7	ALA	-	expression tag	UNP C3W5S1
S	8	ASP	-	expression tag	UNP C3W5S1
S	9	PRO	-	expression tag	UNP C3W5S1
S	10	GLY	-	expression tag	UNP C3W5S1
T	7	ALA	-	expression tag	UNP C3W5S1
T	8	ASP	-	expression tag	UNP C3W5S1
T	9	PRO	-	expression tag	UNP C3W5S1
T	10	GLY	-	expression tag	UNP C3W5S1
U	7	ALA	-	expression tag	UNP C3W5S1
U	8	ASP	-	expression tag	UNP C3W5S1
U	9	PRO	-	expression tag	UNP C3W5S1
U	10	GLY	-	expression tag	UNP C3W5S1

- Molecule 4 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	175	Total	C	N	O	S	0	0	0
			1406	881	238	281	6			
4	Q	171	Total	C	N	O	S	0	0	0
			1375	863	234	272	6			
4	R	171	Total	C	N	O	S	0	0	0
			1375	863	234	272	6			
4	V	175	Total	C	N	O	S	0	0	0
			1406	881	238	281	6			
4	W	171	Total	C	N	O	S	0	0	0
			1375	863	234	272	6			
4	X	171	Total	C	N	O	S	0	0	0
			1375	863	234	272	6			

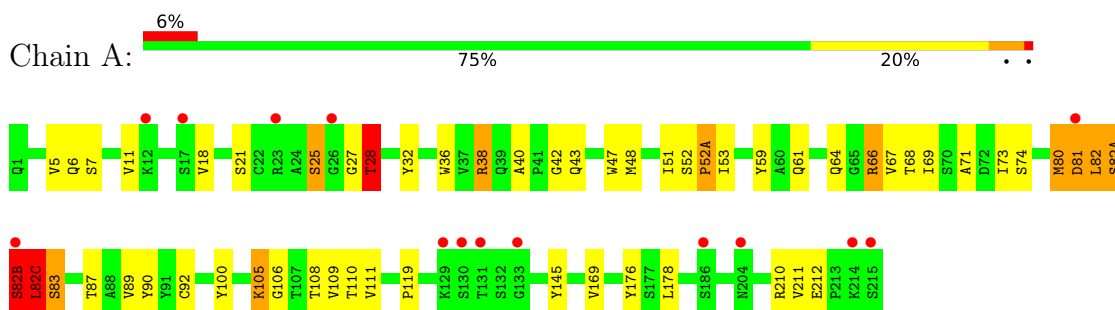
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
P	175	SER	-	expression tag	UNP A0A023ZYH9
P	176	GLY	-	expression tag	UNP A0A023ZYH9
P	177	ARG	-	expression tag	UNP A0A023ZYH9
Q	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
Q	175	SER	-	expression tag	UNP A0A023ZYH9
Q	176	GLY	-	expression tag	UNP A0A023ZYH9
Q	177	ARG	-	expression tag	UNP A0A023ZYH9
R	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
R	175	SER	-	expression tag	UNP A0A023ZYH9
R	176	GLY	-	expression tag	UNP A0A023ZYH9
R	177	ARG	-	expression tag	UNP A0A023ZYH9
V	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
V	175	SER	-	expression tag	UNP A0A023ZYH9
V	176	GLY	-	expression tag	UNP A0A023ZYH9
V	177	ARG	-	expression tag	UNP A0A023ZYH9
W	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
W	175	SER	-	expression tag	UNP A0A023ZYH9
W	176	GLY	-	expression tag	UNP A0A023ZYH9
W	177	ARG	-	expression tag	UNP A0A023ZYH9
X	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
X	175	SER	-	expression tag	UNP A0A023ZYH9
X	176	GLY	-	expression tag	UNP A0A023ZYH9
X	177	ARG	-	expression tag	UNP A0A023ZYH9

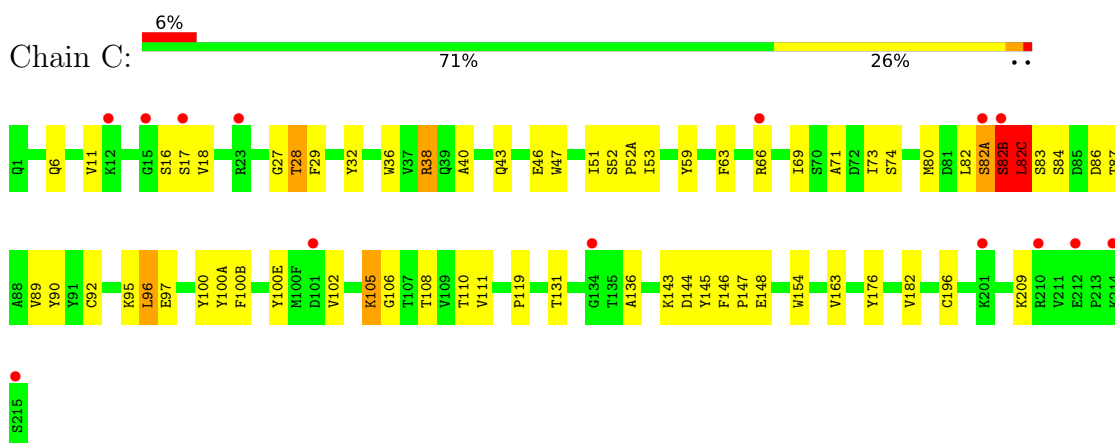
3 Residue-property plots [i](#)

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.

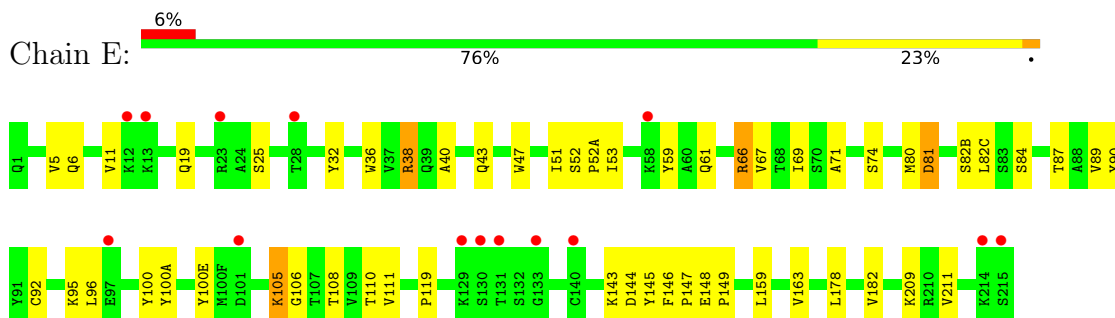
- Molecule 1: Antibody 27F3 heavy chain



- Molecule 1: Antibody 27F3 heavy chain



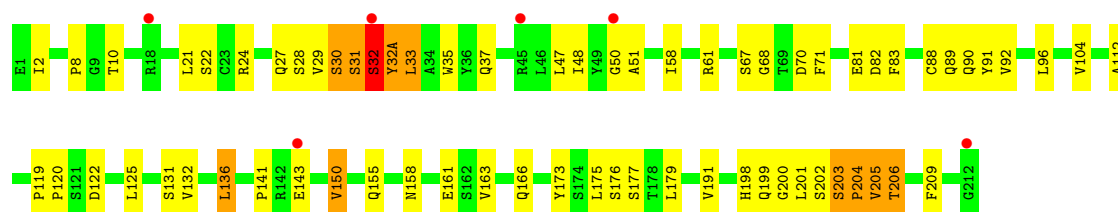
- Molecule 1: Antibody 27F3 heavy chain



- Molecule 1: Antibody 27F3 heavy chain

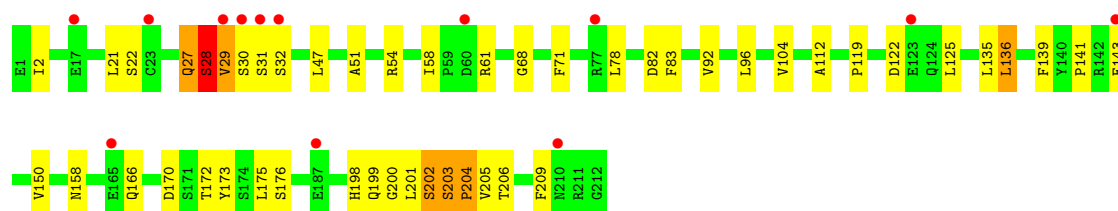
- Molecule 2: Antibody 27F3 light chain

Chain D: 



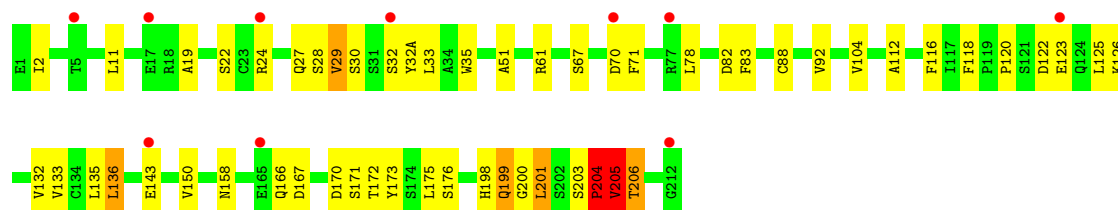
- Molecule 2: Antibody 27F3 light chain

Chain F: 



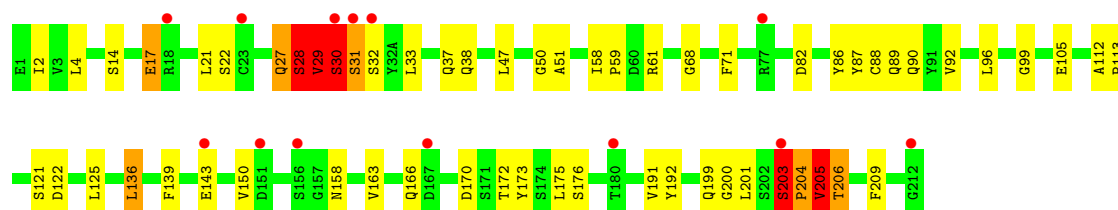
- Molecule 2: Antibody 27F3 light chain

Chain H: 



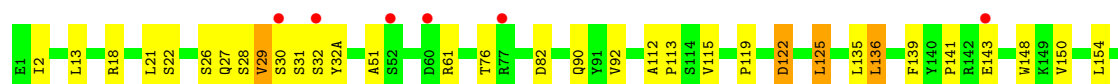
- Molecule 2: Antibody 27F3 light chain

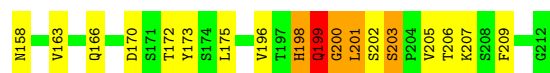
Chain J: 



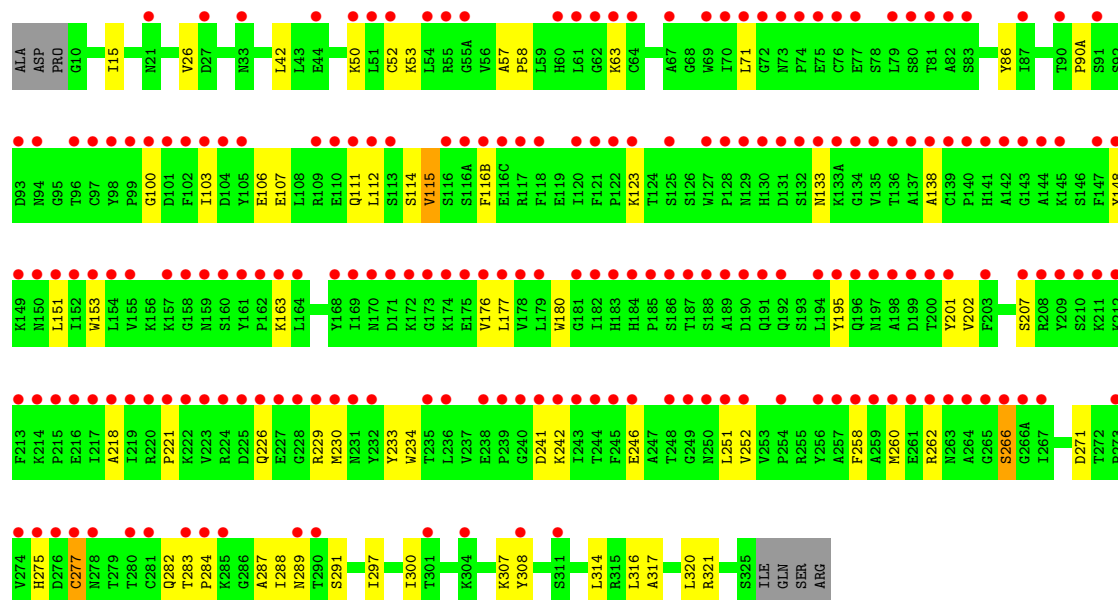
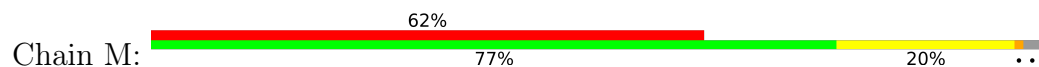
- Molecule 2: Antibody 27F3 light chain

Chain L: 

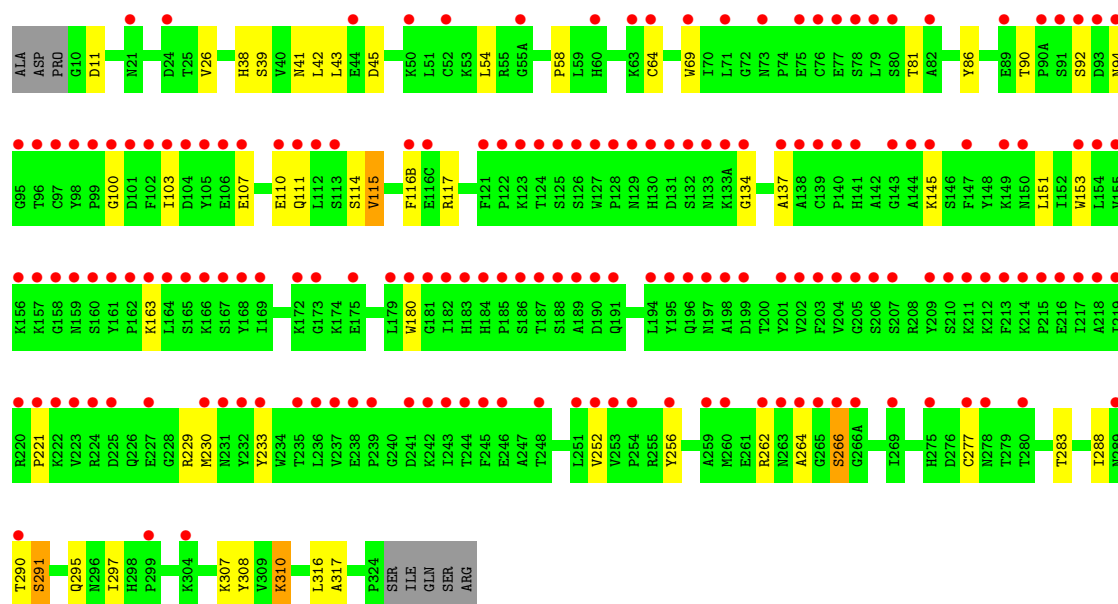
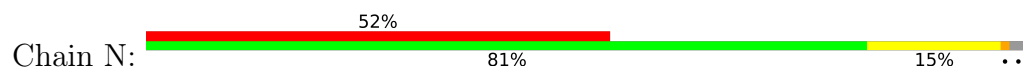




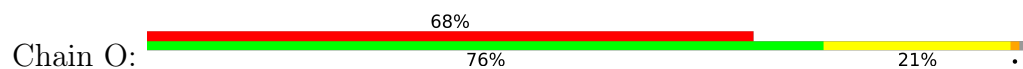
• Molecule 3: Hemagglutinin

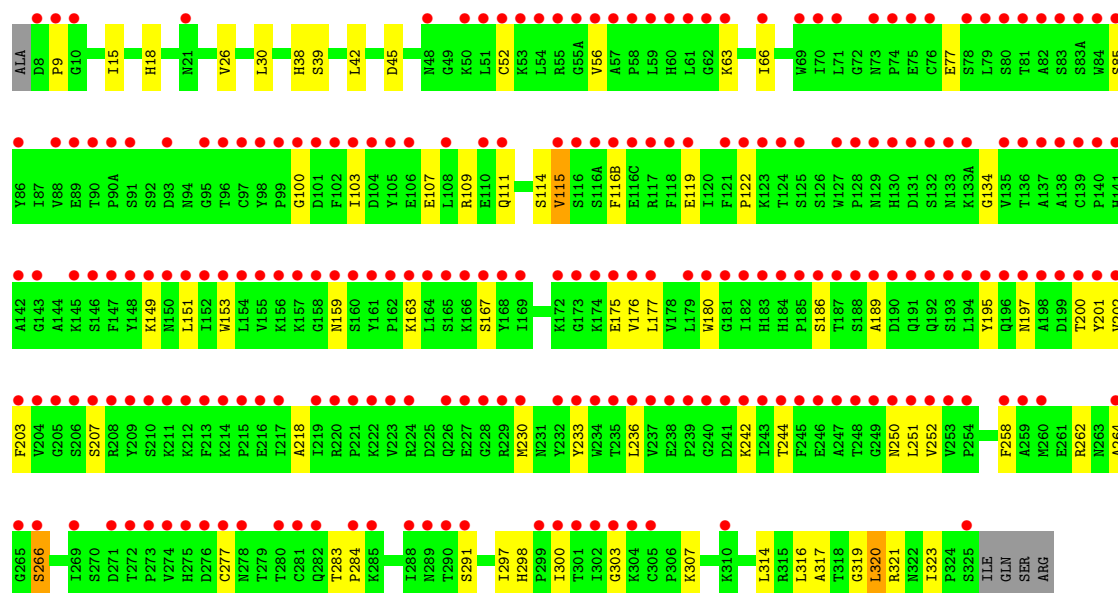


• Molecule 3: Hemagglutinin



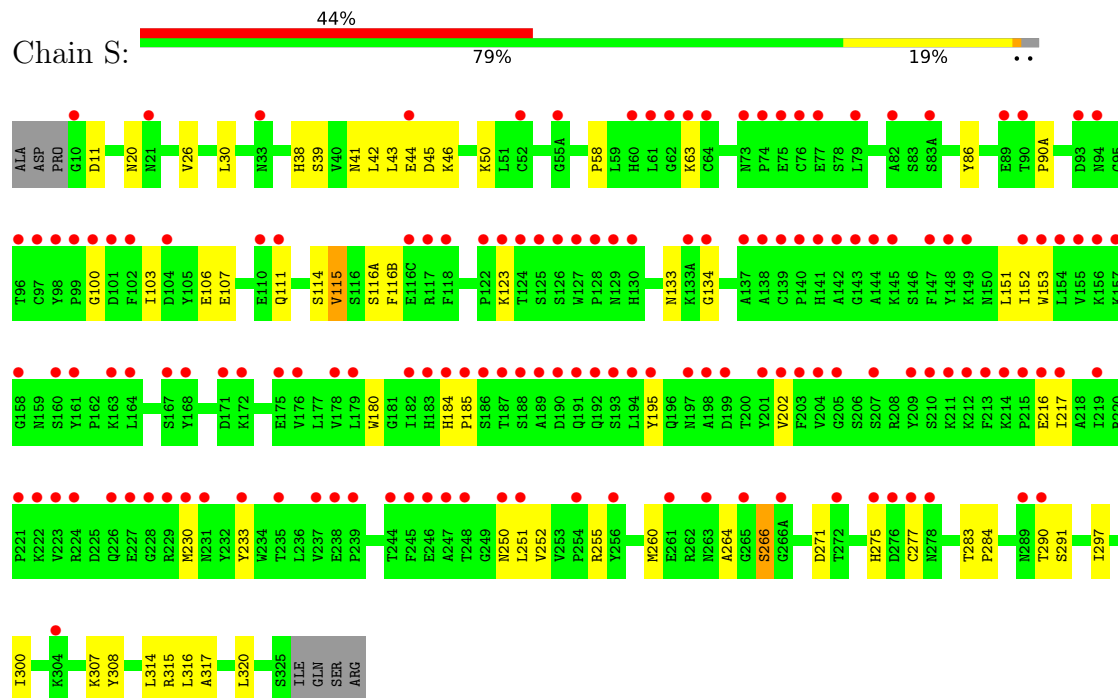
• Molecule 3: Hemagglutinin





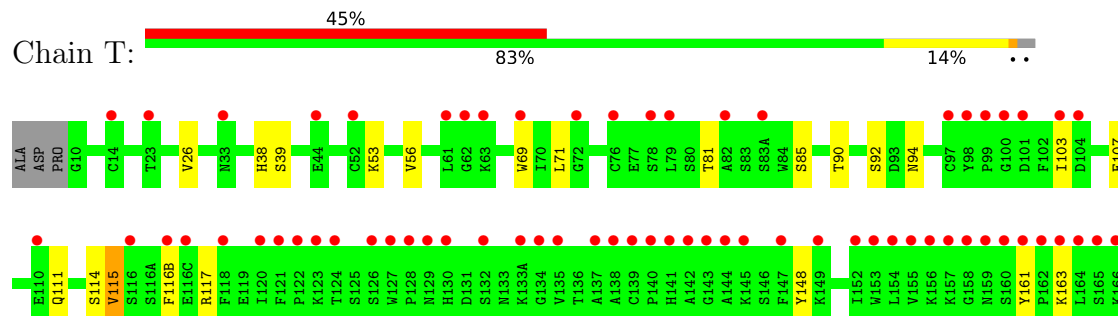
• Molecule 3: Hemagglutinin

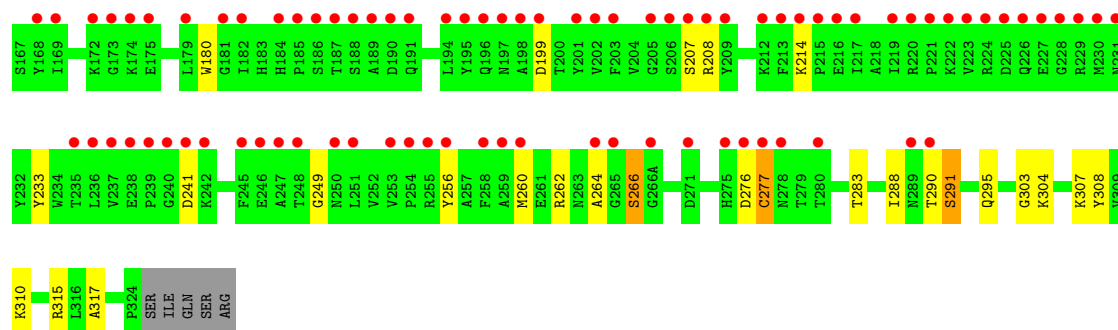
Chain S:



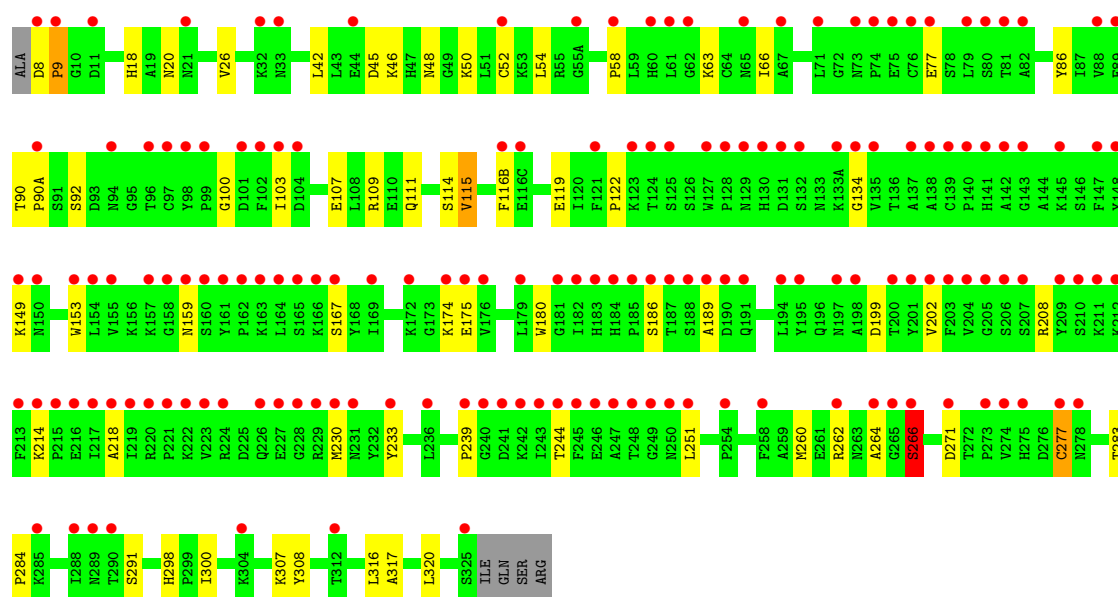
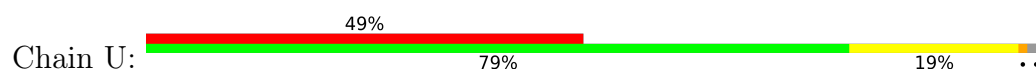
• Molecule 3: Hemagglutinin

Chain T:

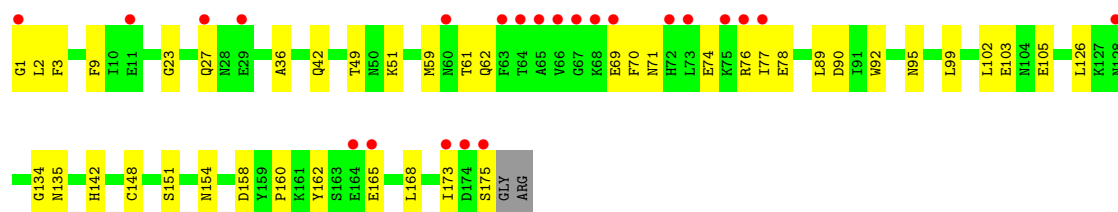
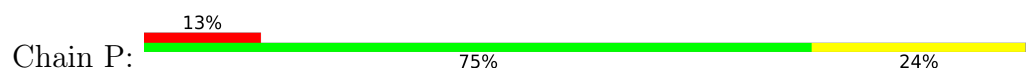




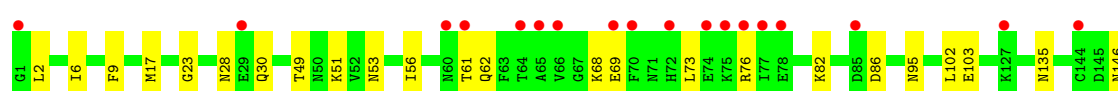
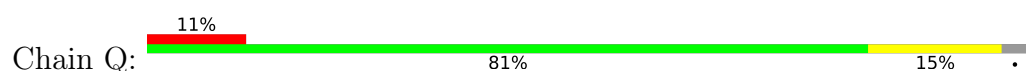
• Molecule 3: Hemagglutinin



• Molecule 4: Hemagglutinin

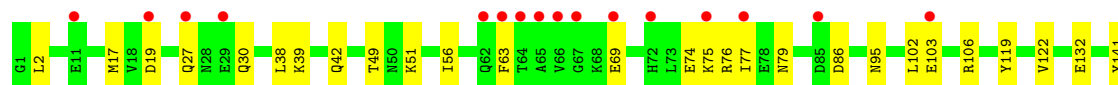
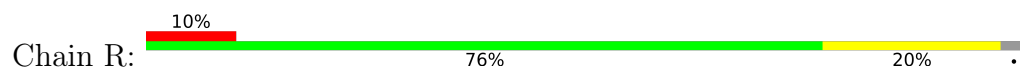


• Molecule 4: Hemagglutinin

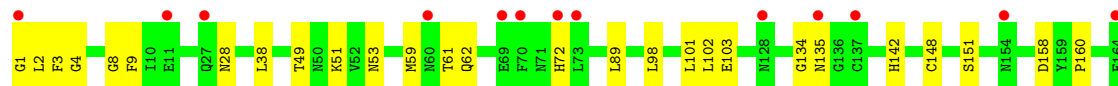
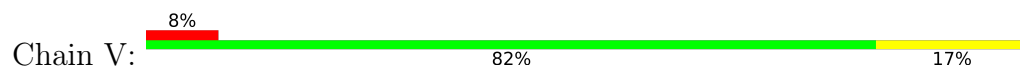




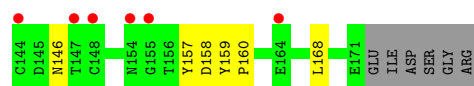
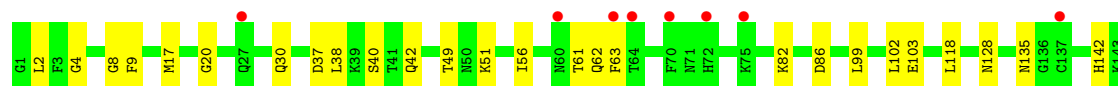
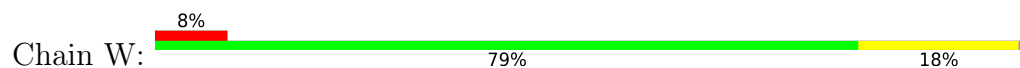
• Molecule 4: Hemagglutinin



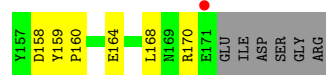
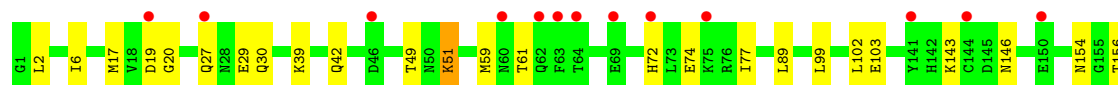
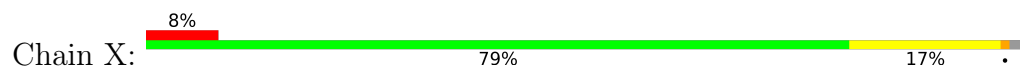
• Molecule 4: Hemagglutinin



• Molecule 4: Hemagglutinin



• Molecule 4: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	190.58Å 191.49Å 391.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.45 – 3.49 49.45 – 3.49	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.45-3.49) 98.0 (49.45-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.246 , 0.268 0.247 , 0.269	Depositor DCC
R_{free} test set	8912 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	90.1	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	43322	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.16% 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	1.01	2/1719 (0.1%)	0.94	3/2344 (0.1%)
1	C	0.88	0/1719	0.90	2/2344 (0.1%)
1	E	0.89	1/1719 (0.1%)	0.91	0/2344
1	G	0.87	1/1719 (0.1%)	0.90	0/2344
1	I	0.79	0/1719	0.88	2/2344 (0.1%)
1	K	0.96	1/1719 (0.1%)	0.95	4/2344 (0.2%)
2	B	1.22	5/1663 (0.3%)	1.21	16/2260 (0.7%)
2	D	0.99	2/1663 (0.1%)	1.01	5/2260 (0.2%)
2	F	0.98	0/1663	0.97	3/2260 (0.1%)
2	H	0.99	1/1663 (0.1%)	0.94	2/2260 (0.1%)
2	J	0.99	1/1663 (0.1%)	1.02	7/2260 (0.3%)
2	L	1.14	1/1663 (0.1%)	1.01	5/2260 (0.2%)
3	M	0.58	0/2593	0.76	0/3524
3	N	0.62	0/2587	0.83	1/3516 (0.0%)
3	O	0.53	0/2609	0.77	2/3547 (0.1%)
3	S	0.57	0/2593	0.73	1/3524 (0.0%)
3	T	0.63	1/2587 (0.0%)	0.87	3/3516 (0.1%)
3	U	0.58	0/2609	0.81	2/3547 (0.1%)
4	P	0.95	0/1434	0.94	1/1932 (0.1%)
4	Q	0.97	0/1403	0.90	0/1890
4	R	0.89	0/1403	0.86	0/1890
4	V	0.94	0/1434	0.93	0/1932
4	W	0.94	0/1403	0.89	0/1890
4	X	0.87	0/1403	0.91	1/1890 (0.1%)
All	All	0.85	16/44350 (0.0%)	0.90	60/60222 (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	G	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
All	All	0	2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	211	VAL	C-N	8.74	1.51	1.33
1	A	80	MET	CA-C	-8.30	1.42	1.52
2	H	205	VAL	C-O	-6.42	1.17	1.24
2	L	199	GLN	CA-C	-6.33	1.45	1.52
2	J	205	VAL	C-O	-6.14	1.17	1.24

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	82(B)	SER	N-CA-C	-14.12	88.63	108.54
2	B	203	SER	CA-C-N	12.73	135.75	119.84
2	B	203	SER	C-N-CA	12.73	135.75	119.84
3	T	277	CYS	CA-CB-SG	-12.45	85.77	114.40
2	B	94	THR	CA-C-N	11.72	134.49	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	148	GLU	Peptide
2	L	198	HIS	Mainchain

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	1675	0	1642	66	0
1	C	1675	0	1642	68	0
1	E	1675	0	1643	45	0
1	G	1675	0	1643	76	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1675	0	1643	73	0
1	K	1675	0	1642	47	0
2	B	1628	0	1592	62	0
2	D	1628	0	1591	66	0
2	F	1628	0	1592	32	0
2	H	1628	0	1592	36	0
2	J	1628	0	1590	64	0
2	L	1628	0	1592	37	0
3	M	2529	0	2479	49	0
3	N	2523	0	2474	37	0
3	O	2544	0	2490	54	0
3	S	2529	0	2479	44	0
3	T	2523	0	2474	33	0
3	U	2544	0	2490	48	0
4	P	1406	0	1326	35	0
4	Q	1375	0	1300	28	0
4	R	1375	0	1300	33	0
4	V	1406	0	1326	34	0
4	W	1375	0	1300	26	0
4	X	1375	0	1300	29	0
All	All	43322	0	42142	1003	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 12.

The worst 5 of 1003 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)
2:J:30:SER:OG	2:J:92:VAL:CG1	1.64	1.44
2:B:94:THR:CB	2:B:95:PRO:HD3	1.33	1.34
1:I:66:ARG:HB3	1:I:82(B):SER:CB	1.59	1.33
2:B:94:THR:CB	2:B:95:PRO:CD	2.07	1.32
1:I:17:SER:CB	1:I:82(A):SER:OG	1.76	1.31

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	223/225 (99%)	204 (92%)	16 (7%)	3 (1%)	9	39
1	C	223/225 (99%)	200 (90%)	20 (9%)	3 (1%)	9	39
1	E	223/225 (99%)	207 (93%)	15 (7%)	1 (0%)	30	62
1	G	223/225 (99%)	203 (91%)	18 (8%)	2 (1%)	14	47
1	I	223/225 (99%)	205 (92%)	17 (8%)	1 (0%)	30	62
1	K	223/225 (99%)	203 (91%)	17 (8%)	3 (1%)	9	39
2	B	211/213 (99%)	189 (90%)	16 (8%)	6 (3%)	4	26
2	D	211/213 (99%)	191 (90%)	17 (8%)	3 (1%)	9	38
2	F	211/213 (99%)	192 (91%)	16 (8%)	3 (1%)	9	38
2	H	211/213 (99%)	192 (91%)	17 (8%)	2 (1%)	14	47
2	J	211/213 (99%)	190 (90%)	15 (7%)	6 (3%)	4	26
2	L	211/213 (99%)	193 (92%)	15 (7%)	3 (1%)	9	38
3	M	322/331 (97%)	312 (97%)	10 (3%)	0	100	100
3	N	321/331 (97%)	312 (97%)	8 (2%)	1 (0%)	36	67
3	O	324/331 (98%)	312 (96%)	10 (3%)	2 (1%)	21	54
3	S	322/331 (97%)	312 (97%)	9 (3%)	1 (0%)	36	67
3	T	321/331 (97%)	312 (97%)	8 (2%)	1 (0%)	36	67
3	U	324/331 (98%)	312 (96%)	10 (3%)	2 (1%)	21	54
4	P	173/177 (98%)	169 (98%)	4 (2%)	0	100	100
4	Q	169/177 (96%)	167 (99%)	2 (1%)	0	100	100
4	R	169/177 (96%)	167 (99%)	2 (1%)	0	100	100
4	V	173/177 (98%)	169 (98%)	4 (2%)	0	100	100
4	W	169/177 (96%)	166 (98%)	3 (2%)	0	100	100
4	X	169/177 (96%)	167 (99%)	2 (1%)	0	100	100
All	All	5560/5676 (98%)	5246 (94%)	271 (5%)	43 (1%)	16	49

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82(B)	SER
2	B	30	SER
2	B	94	THR
1	C	28	THR
1	G	149	PRO

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	189/189 (100%)	176 (93%)	13 (7%)	14	39
1	C	189/189 (100%)	180 (95%)	9 (5%)	23	49
1	E	189/189 (100%)	184 (97%)	5 (3%)	40	62
1	G	189/189 (100%)	176 (93%)	13 (7%)	14	39
1	I	189/189 (100%)	182 (96%)	7 (4%)	30	56
1	K	189/189 (100%)	178 (94%)	11 (6%)	18	44
2	B	184/184 (100%)	172 (94%)	12 (6%)	15	42
2	D	184/184 (100%)	174 (95%)	10 (5%)	20	46
2	F	184/184 (100%)	173 (94%)	11 (6%)	17	44
2	H	184/184 (100%)	171 (93%)	13 (7%)	13	38
2	J	184/184 (100%)	172 (94%)	12 (6%)	15	42
2	L	184/184 (100%)	170 (92%)	14 (8%)	12	37
3	M	284/290 (98%)	278 (98%)	6 (2%)	47	66
3	N	283/290 (98%)	278 (98%)	5 (2%)	51	69
3	O	286/290 (99%)	281 (98%)	5 (2%)	53	70
3	S	284/290 (98%)	279 (98%)	5 (2%)	51	69
3	T	283/290 (98%)	279 (99%)	4 (1%)	59	71
3	U	286/290 (99%)	281 (98%)	5 (2%)	53	70
4	P	150/151 (99%)	149 (99%)	1 (1%)	76	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Q	146/151 (97%)	145 (99%)	1 (1%)	76	78
4	R	146/151 (97%)	146 (100%)	0	100	100
4	V	150/151 (99%)	150 (100%)	0	100	100
4	W	146/151 (97%)	145 (99%)	1 (1%)	76	78
4	X	146/151 (97%)	146 (100%)	0	100	100
All	All	4828/4884 (99%)	4665 (97%)	163 (3%)	32	57

5 of 163 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	105	LYS
3	O	266	SER
2	L	28	SER
3	M	63	LYS
3	S	266	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
3	N	94	ASN
4	V	53	ASN
4	P	95	ASN
4	V	43	ASN
4	W	95	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 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(Å²)	Q<0.9
1	A	225/225 (100%)	0.50	14 (6%)	26	16	51, 74, 96, 116	0
1	C	225/225 (100%)	0.60	14 (6%)	26	16	59, 78, 95, 114	0
1	E	225/225 (100%)	0.49	14 (6%)	26	16	55, 79, 99, 111	0
1	G	225/225 (100%)	0.51	16 (7%)	22	14	54, 81, 105, 124	0
1	I	225/225 (100%)	0.90	26 (11%)	9	6	59, 91, 116, 128	0
1	K	225/225 (100%)	0.42	13 (5%)	29	17	51, 72, 98, 114	0
2	B	213/213 (100%)	0.28	10 (4%)	36	20	53, 61, 76, 85	0
2	D	213/213 (100%)	0.43	6 (2%)	55	32	62, 71, 83, 94	0
2	F	213/213 (100%)	0.36	13 (6%)	27	16	58, 68, 83, 92	0
2	H	213/213 (100%)	0.31	10 (4%)	36	20	54, 68, 86, 98	0
2	J	213/213 (100%)	0.49	13 (6%)	27	16	55, 71, 89, 106	0
2	L	213/213 (100%)	0.16	6 (2%)	55	32	51, 61, 76, 88	0
3	M	324/331 (97%)	2.47	204 (62%)	0	0	55, 175, 212, 218	0
3	N	323/331 (97%)	2.20	172 (53%)	0	0	50, 168, 205, 211	0
3	O	326/331 (98%)	2.88	226 (69%)	0	0	54, 196, 228, 232	0
3	S	324/331 (97%)	1.83	147 (45%)	0	1	55, 153, 182, 186	0
3	T	323/331 (97%)	1.88	149 (46%)	0	1	52, 157, 192, 196	0
3	U	326/331 (98%)	2.07	163 (50%)	0	1	55, 159, 190, 197	0
4	P	175/177 (98%)	0.59	23 (13%)	7	6	51, 73, 141, 170	0
4	Q	171/177 (96%)	0.66	20 (11%)	9	6	50, 72, 133, 157	0
4	R	171/177 (96%)	0.61	18 (10%)	11	8	51, 74, 134, 156	0
4	V	175/177 (98%)	0.57	15 (8%)	16	11	52, 77, 128, 147	0
4	W	171/177 (96%)	0.55	14 (8%)	17	11	51, 72, 113, 141	0
4	X	171/177 (96%)	0.57	14 (8%)	17	11	53, 77, 116, 142	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	5608/5676 (98%)	1.09	1320 (23%) 2 2	50, 80, 199, 232	0

The worst 5 of 1320 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	155	VAL	8.6
3	O	243	ILE	8.4
3	O	179	LEU	8.3
3	M	154	LEU	8.2
3	M	195	TYR	8.1

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 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.