



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 25, 2023 – 05:23 AM EDT

PDB ID : 5WKO
Title : Crystal structure of antibody 27F3 recognizing the HA from
A/California/04/2009 (H1N1) influenza virus
Authors : Wilson, 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

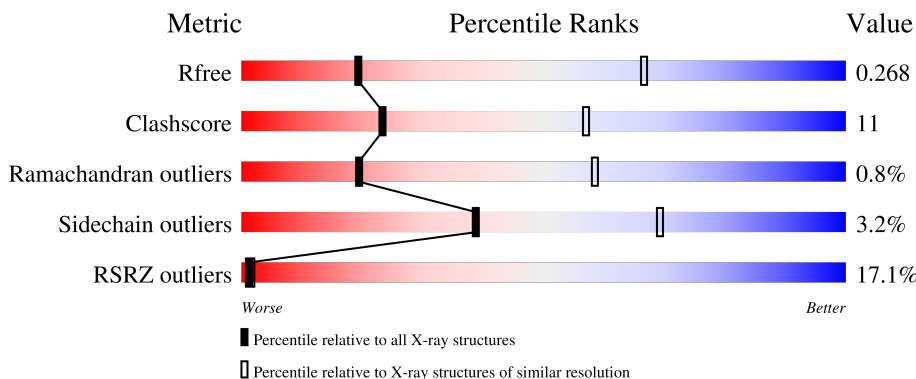
1 Overall quality at a glance

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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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% 74% 21% 5%
1	C	225	 5% 70% 26% 5%
1	E	225	 4% 74% 23% 5%
1	G	225	 5% 70% 25% 5%
1	I	225	 15% 72% 25% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	225	 6% 74% 23% .
2	B	213	 72% 23% ..
2	D	213	 68% 29% .
2	F	213	 78% 21% .
2	H	213	 75% 23% .
2	J	213	 2% 72% 25% ..
2	L	213	 76% 21% .
3	M	331	 44% 77% 20% ..
3	N	331	 41% 81% 16% ..
3	O	331	 50% 76% 21% ..
3	S	331	 34% 79% 18% ..
3	T	331	 34% 83% 13% ..
3	U	331	 35% 79% 18% ..
4	P	177	 6% 79% 20% .
4	Q	177	 6% 80% 17% .
4	R	177	 5% 76% 19% ..
4	V	177	 6% 80% 19% .
4	W	177	 7% 81% 15% ..
4	X	177	 6% 80% 16% ..

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
			Total	C	N	O	S			
1	A	225	1675	1061	277	330	7	0	0	0
1	C	225	1675	1061	277	330	7	0	0	0
1	E	225	1675	1061	277	330	7	0	0	0
1	G	225	1675	1061	277	330	7	0	0	0
1	I	225	1675	1061	277	330	7	0	0	0
1	K	225	1675	1061	277	330	7	0	0	0

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

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

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
			Total	C	N	O	S			
3	M	324	2529	1599	436	483	11	0	0	0
3	N	323	2523	1596	435	481	11	0	0	0
3	O	326	2544	1608	438	487	11	0	0	0
3	S	324	2529	1599	436	483	11	0	0	0
3	T	323	2523	1596	435	481	11	0	0	0
3	U	326	2544	1608	438	487	11	0	0	0

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:

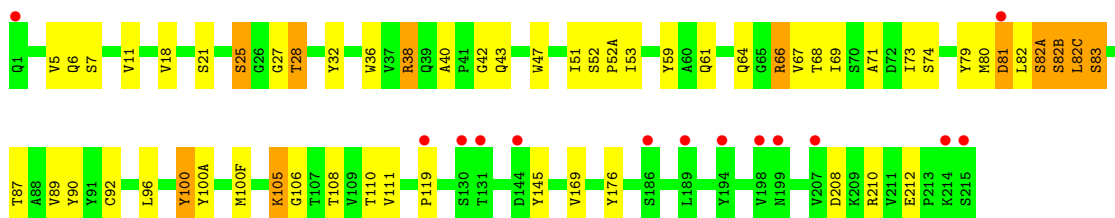
Chain	Residue	Modelled	Actual	Comment	Reference
P	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
P	175	SER	-	expression tag	UNP A0A023ZYH9
P	176	GLY	-	expression tag	UNP A0A023ZYH9
P	177	ARG	-	expression tag	UNP A0A023ZYH9
Q	47	GLY	GLU	engineered mutation	UNP A0A023ZYH9
Q	175	SER	-	expression tag	UNP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

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.

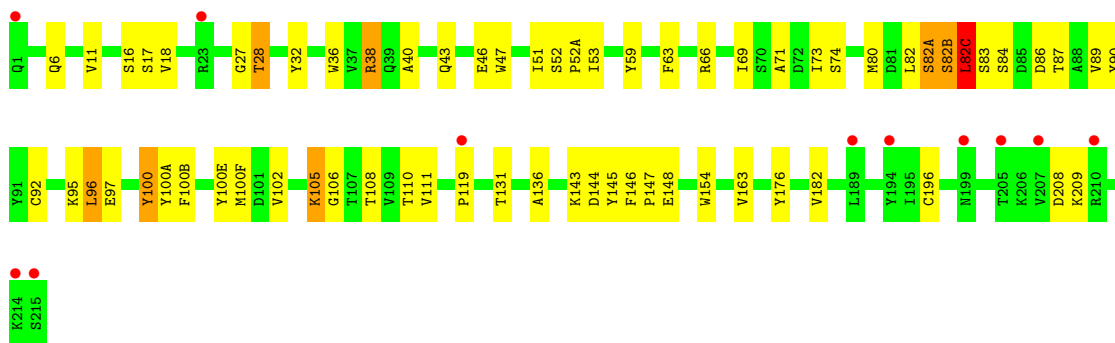
- Molecule 1: Antibody 27F3 heavy chain

Chain A: 




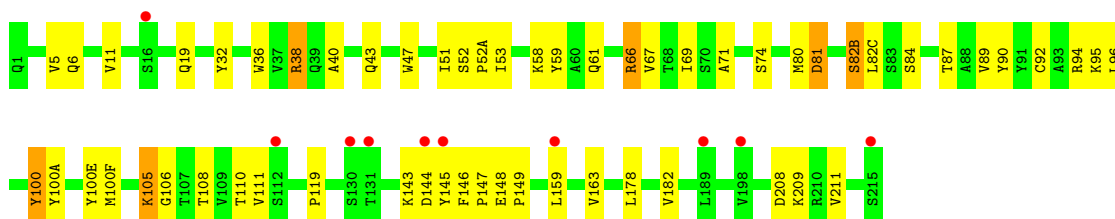
- Molecule 1: Antibody 27F3 heavy chain

Chain C: 

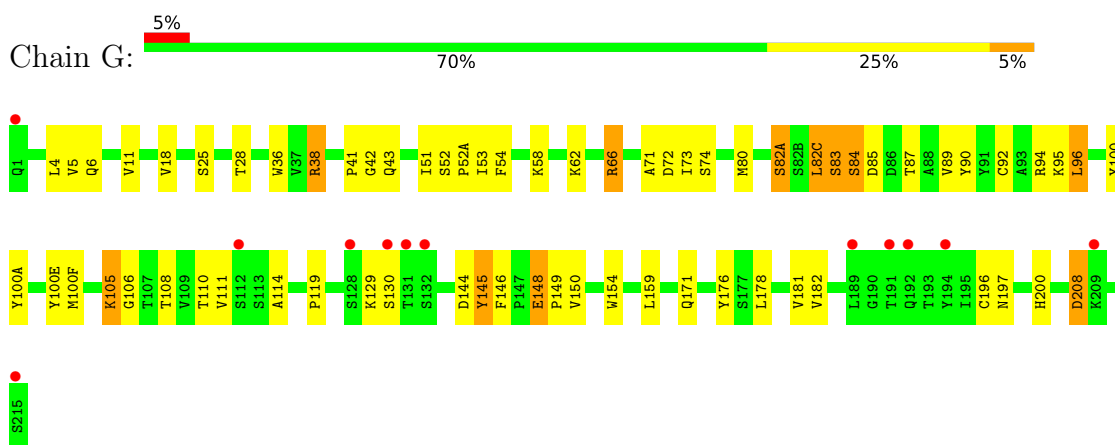


- Molecule 1: Antibody 27F3 heavy chain

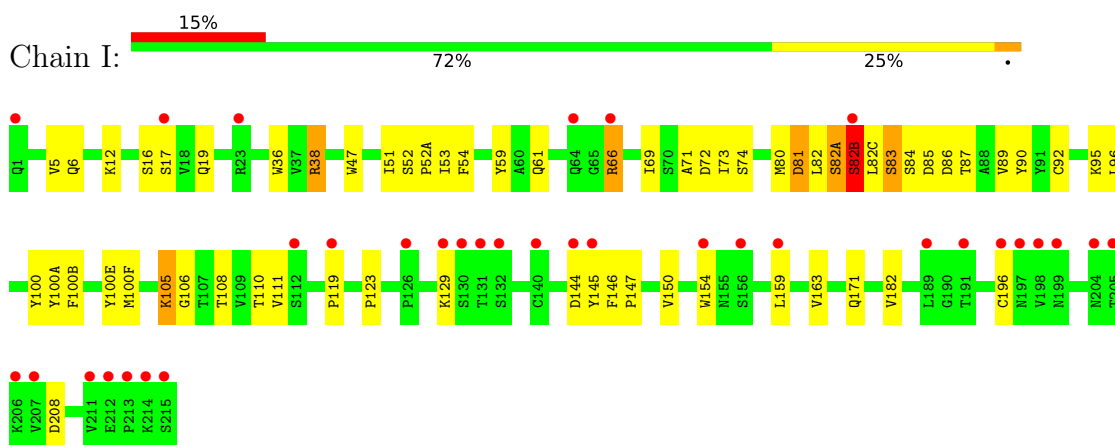
Chain E: 



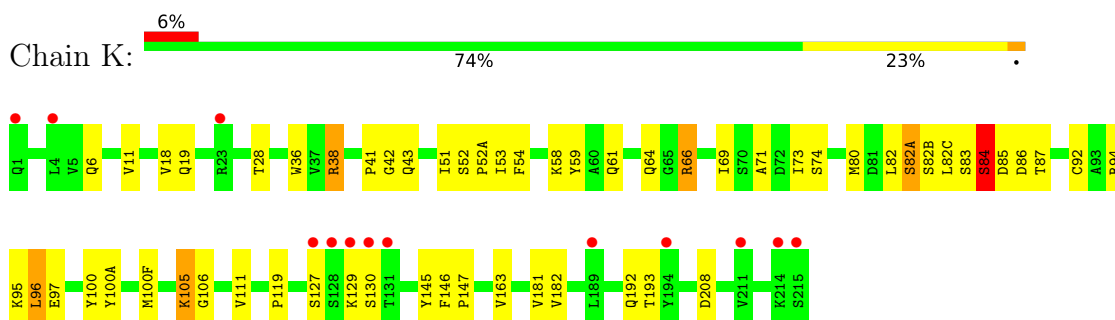
- Molecule 1: Antibody 27F3 heavy chain



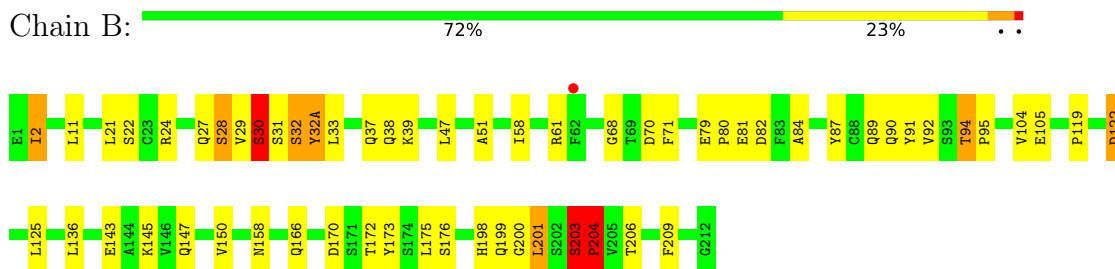
- Molecule 1: Antibody 27F3 heavy chain



- Molecule 1: Antibody 27F3 heavy chain

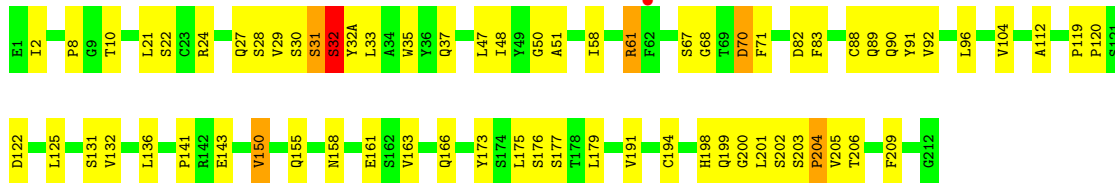


- Molecule 2: Antibody 27F3 light chain




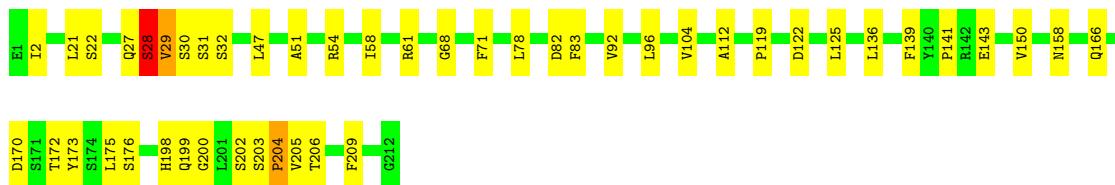
- Molecule 2: Antibody 27F3 light chain

Chain D:  68% 29%




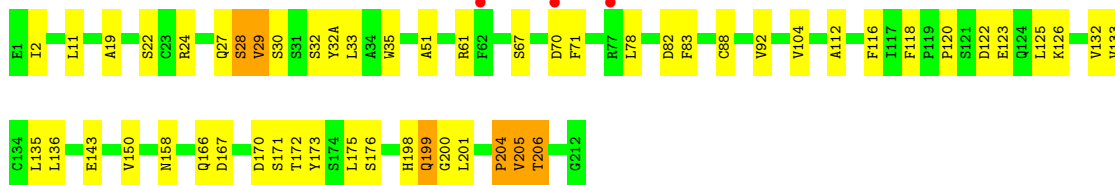
• Molecule 2: Antibody 27F3 light chain

Chain F:  78% 21%



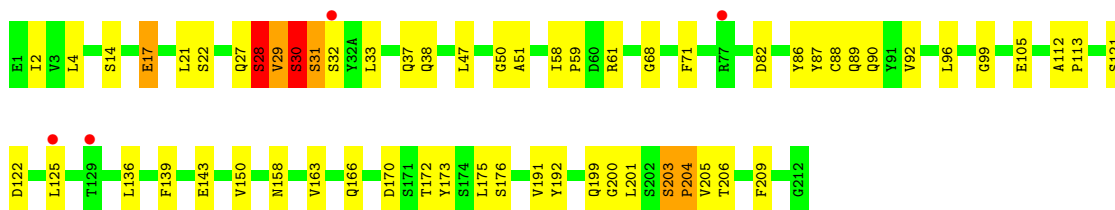
• Molecule 2: Antibody 27F3 light chain

Chain H:  75% 23%



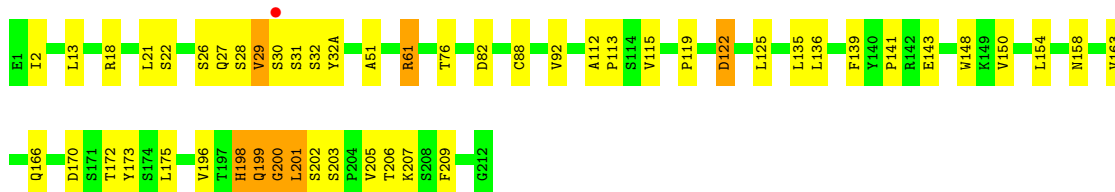
• Molecule 2: Antibody 27F3 light chain

Chain J:  72% 25%

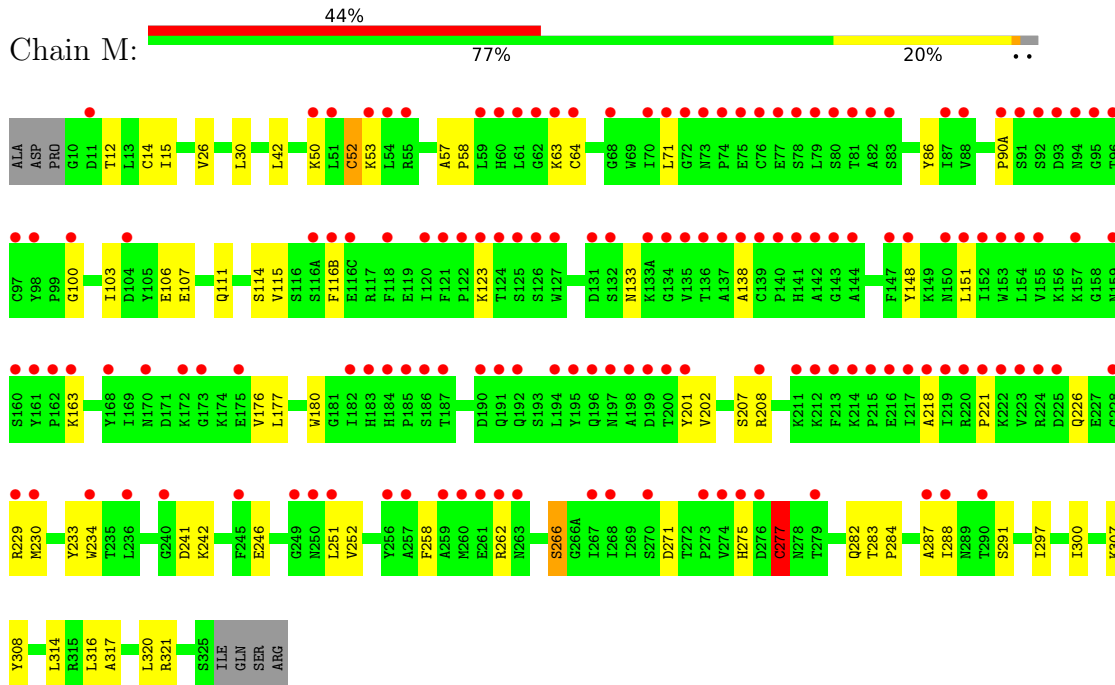


• Molecule 2: Antibody 27F3 light chain

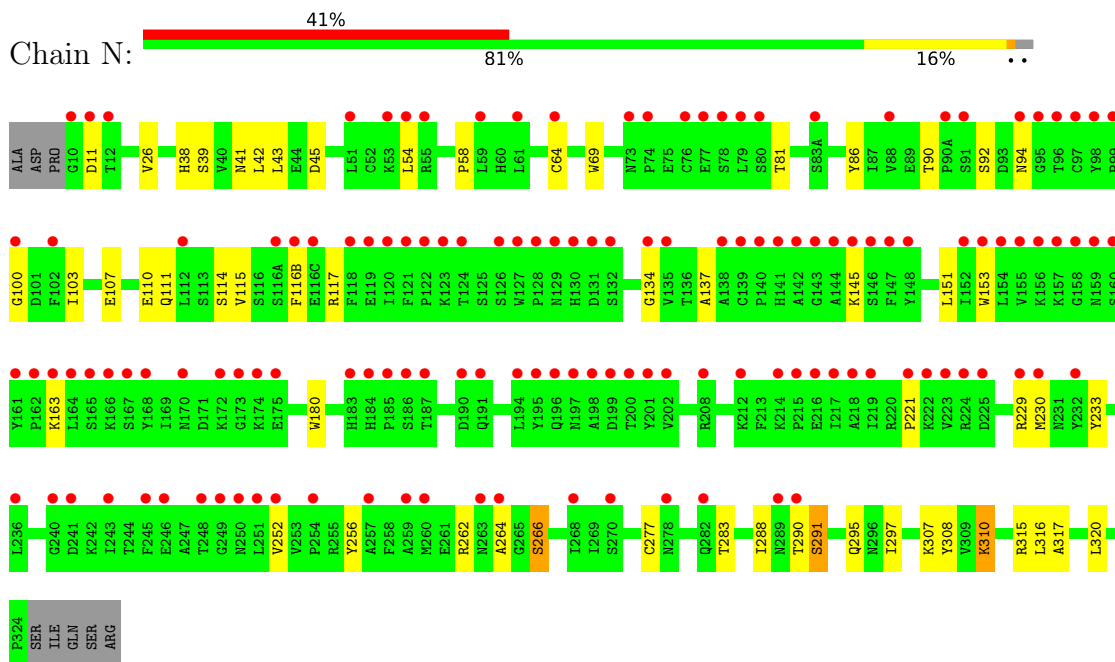
Chain L:  76% 21%



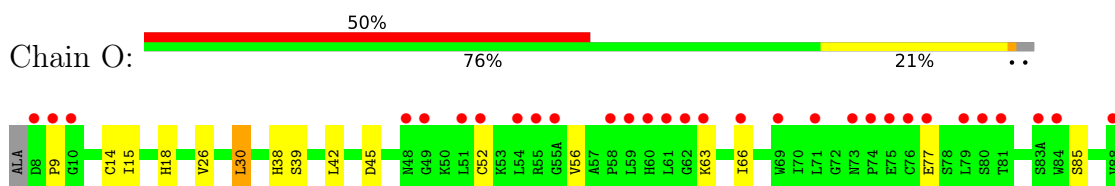
- Molecule 3: Hemagglutinin

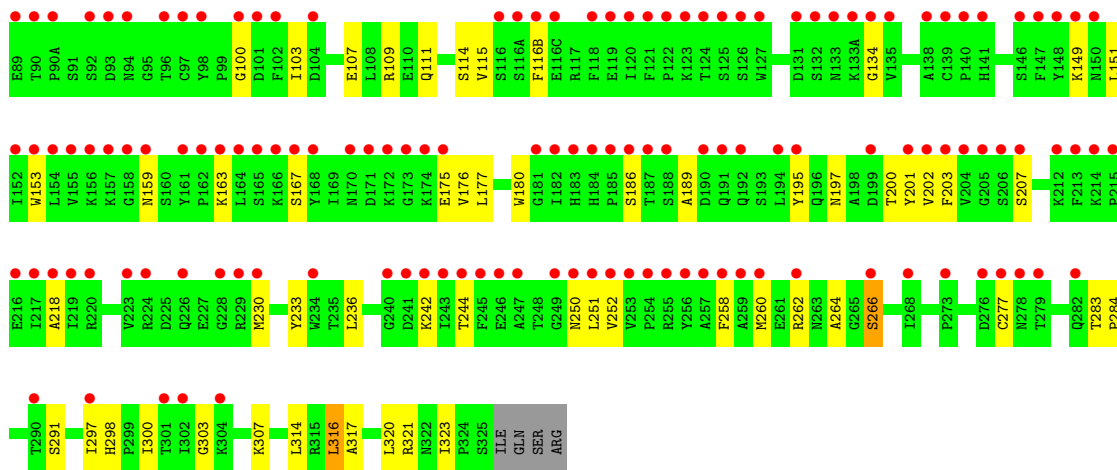


- Molecule 3: Hemagglutinin

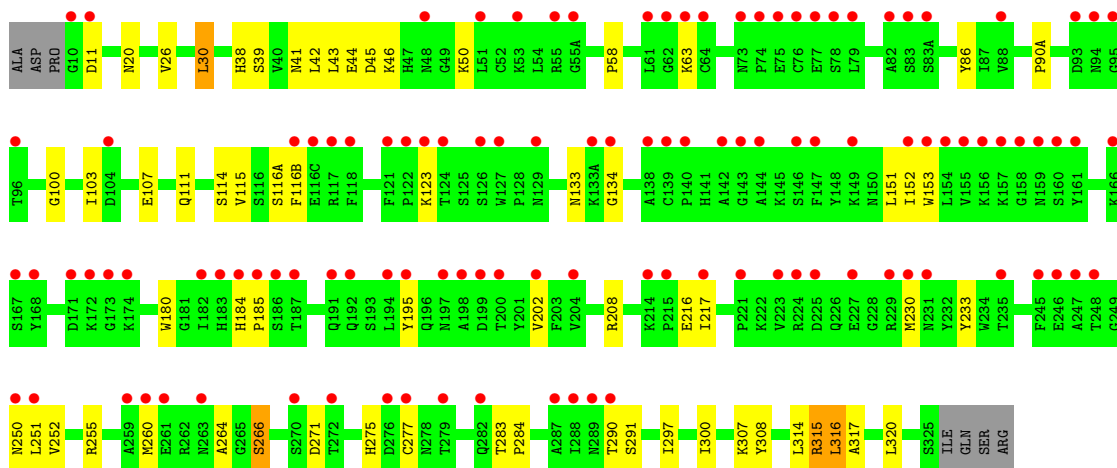
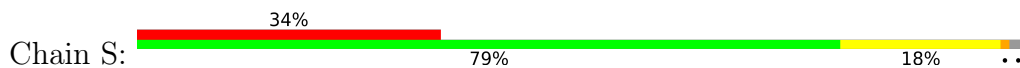


- Molecule 3: Hemagglutinin

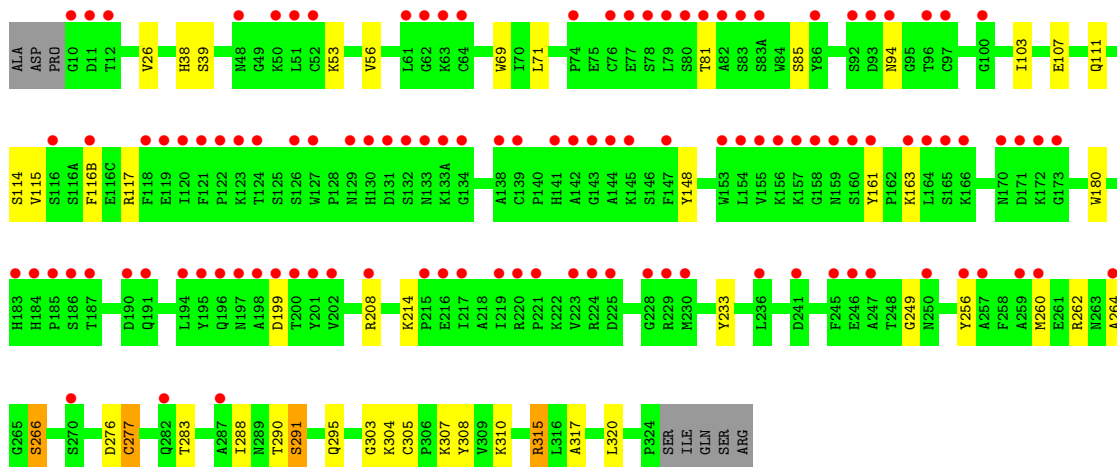
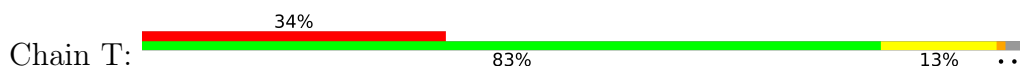




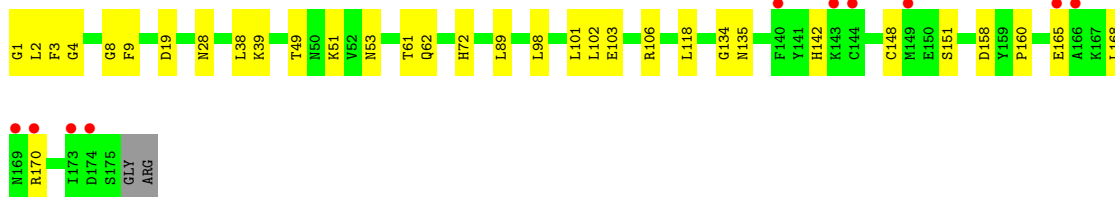
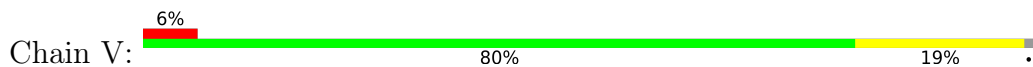
• Molecule 3: Hemagglutinin



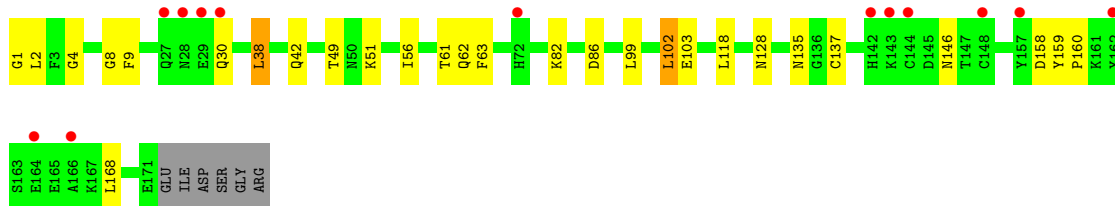
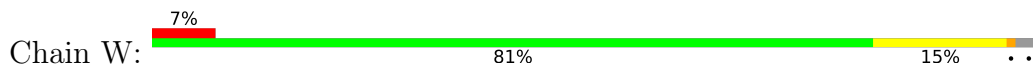
• Molecule 3: Hemagglutinin



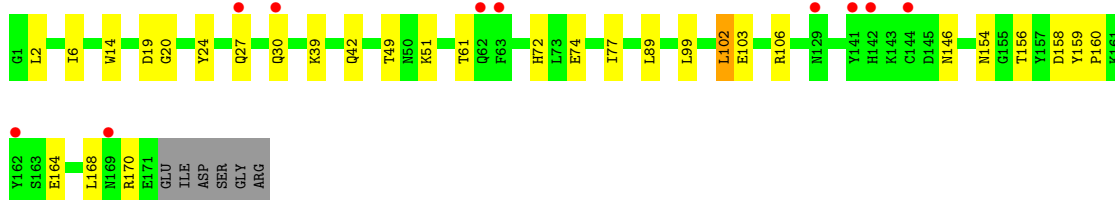
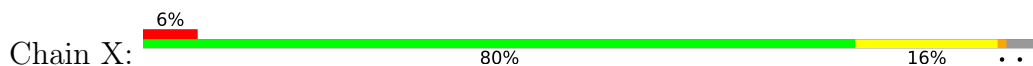
• Molecule 4: Hemagglutinin



• 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) 98.1 (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)	Xtrriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.246 , 0.268 0.246 , 0.268	Depositor DCC
R_{free} test set	8910 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	90.1	Xtrriage
Anisotropy	0.148	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.008 for k,h,-l	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	1.09	3/1719 (0.2%)	0.83	2/2344 (0.1%)
1	C	0.92	0/1719	0.82	1/2344 (0.0%)
1	E	0.96	1/1719 (0.1%)	0.81	2/2344 (0.1%)
1	G	0.92	1/1719 (0.1%)	0.81	2/2344 (0.1%)
1	I	0.83	0/1719	0.75	1/2344 (0.0%)
1	K	1.05	1/1719 (0.1%)	0.82	1/2344 (0.0%)
2	B	1.19	0/1663	0.93	4/2260 (0.2%)
2	D	0.98	1/1663 (0.1%)	0.85	2/2260 (0.1%)
2	F	0.99	0/1663	0.83	0/2260
2	H	1.00	0/1663	0.84	0/2260
2	J	0.99	1/1663 (0.1%)	0.87	1/2260 (0.0%)
2	L	1.14	1/1663 (0.1%)	0.88	2/2260 (0.1%)
3	M	0.62	3/2593 (0.1%)	0.72	3/3524 (0.1%)
3	N	0.62	0/2587	0.79	3/3516 (0.1%)
3	O	0.57	1/2609 (0.0%)	0.74	2/3547 (0.1%)
3	S	0.62	0/2593	0.73	4/3524 (0.1%)
3	T	0.64	1/2587 (0.0%)	0.83	6/3516 (0.2%)
3	U	0.60	0/2609	0.75	1/3547 (0.0%)
4	P	1.01	1/1434 (0.1%)	0.87	0/1932
4	Q	1.04	1/1403 (0.1%)	0.86	2/1890 (0.1%)
4	R	0.94	2/1403 (0.1%)	0.86	1/1890 (0.1%)
4	V	0.99	0/1434	0.90	3/1932 (0.2%)
4	W	0.96	1/1403 (0.1%)	0.84	3/1890 (0.2%)
4	X	0.90	1/1403 (0.1%)	0.89	3/1890 (0.2%)
All	All	0.88	20/44350 (0.0%)	0.82	49/60222 (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 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	TYR	CE1-CZ	-8.04	1.28	1.38
1	E	211	VAL	C-N	7.65	1.51	1.34
2	J	17	GLU	CB-CG	-7.09	1.38	1.52
3	M	14	CYS	CB-SG	-6.31	1.71	1.82
4	Q	21	TRP	CB-CG	-6.09	1.39	1.50

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	277	CYS	CA-CB-SG	-15.68	85.77	114.00
3	S	277	CYS	CA-CB-SG	-8.97	97.85	114.00
3	T	320	LEU	CB-CG-CD2	-8.45	96.64	111.00
1	I	82(B)	SER	N-CA-C	-8.29	88.63	111.00
3	S	30	LEU	CB-CG-CD2	-7.80	97.73	111.00

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 [\(i\)](#)

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	1675	0	1642	62	0
1	C	1675	0	1642	67	0
1	E	1675	0	1643	43	0
1	G	1675	0	1643	77	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	69	0
1	K	1675	0	1642	45	0
2	B	1628	0	1592	63	0
2	D	1628	0	1591	65	0
2	F	1628	0	1592	30	0
2	H	1628	0	1592	35	0
2	J	1628	0	1590	63	0
2	L	1628	0	1592	36	0
3	M	2529	0	2479	46	0
3	N	2523	0	2474	37	0
3	O	2544	0	2490	54	0
3	S	2529	0	2479	43	0
3	T	2523	0	2474	30	0
3	U	2544	0	2490	47	0
4	P	1406	0	1326	32	0
4	Q	1375	0	1300	28	0
4	R	1375	0	1300	32	0
4	V	1406	0	1326	33	0
4	W	1375	0	1300	23	0
4	X	1375	0	1300	26	0
All	All	43322	0	42142	966	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 11.

The worst 5 of 966 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 [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	223/225 (99%)	204 (92%)	16 (7%)	3 (1%)	12	48
1	C	223/225 (99%)	200 (90%)	20 (9%)	3 (1%)	12	48
1	E	223/225 (99%)	207 (93%)	15 (7%)	1 (0%)	34	72
1	G	223/225 (99%)	203 (91%)	18 (8%)	2 (1%)	17	56
1	I	223/225 (99%)	205 (92%)	17 (8%)	1 (0%)	34	72
1	K	223/225 (99%)	203 (91%)	17 (8%)	3 (1%)	12	48
2	B	211/213 (99%)	189 (90%)	16 (8%)	6 (3%)	5	32
2	D	211/213 (99%)	191 (90%)	17 (8%)	3 (1%)	11	46
2	F	211/213 (99%)	192 (91%)	16 (8%)	3 (1%)	11	46
2	H	211/213 (99%)	192 (91%)	17 (8%)	2 (1%)	17	56
2	J	211/213 (99%)	190 (90%)	15 (7%)	6 (3%)	5	32
2	L	211/213 (99%)	193 (92%)	15 (7%)	3 (1%)	11	46
3	M	322/331 (97%)	312 (97%)	10 (3%)	0	100	100
3	N	321/331 (97%)	312 (97%)	8 (2%)	1 (0%)	41	75
3	O	324/331 (98%)	312 (96%)	10 (3%)	2 (1%)	25	64
3	S	322/331 (97%)	312 (97%)	9 (3%)	1 (0%)	41	75
3	T	321/331 (97%)	312 (97%)	8 (2%)	1 (0%)	41	75
3	U	324/331 (98%)	312 (96%)	10 (3%)	2 (1%)	25	64
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%)	19	58

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 [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	189/189 (100%)	175 (93%)	14 (7%)	13	44
1	C	189/189 (100%)	177 (94%)	12 (6%)	18	51
1	E	189/189 (100%)	180 (95%)	9 (5%)	25	60
1	G	189/189 (100%)	176 (93%)	13 (7%)	15	47
1	I	189/189 (100%)	179 (95%)	10 (5%)	22	55
1	K	189/189 (100%)	178 (94%)	11 (6%)	20	53
2	B	184/184 (100%)	176 (96%)	8 (4%)	29	62
2	D	184/184 (100%)	175 (95%)	9 (5%)	25	59
2	F	184/184 (100%)	174 (95%)	10 (5%)	22	55
2	H	184/184 (100%)	173 (94%)	11 (6%)	19	52
2	J	184/184 (100%)	175 (95%)	9 (5%)	25	59
2	L	184/184 (100%)	171 (93%)	13 (7%)	14	46
3	M	284/290 (98%)	278 (98%)	6 (2%)	53	79
3	N	283/290 (98%)	279 (99%)	4 (1%)	67	85
3	O	286/290 (99%)	283 (99%)	3 (1%)	76	88
3	S	284/290 (98%)	279 (98%)	5 (2%)	59	81
3	T	283/290 (98%)	280 (99%)	3 (1%)	73	88
3	U	286/290 (99%)	283 (99%)	3 (1%)	76	88
4	P	150/151 (99%)	150 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Q	146/151 (97%)	145 (99%)	1 (1%)	84	93
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%)	84	93
4	X	146/151 (97%)	146 (100%)	0	100	100
All	All	4828/4884 (99%)	4673 (97%)	155 (3%)	39	69

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	208	ASP
3	S	63	LYS
2	L	28	SER
3	M	208	ARG
3	T	291	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
4	P	95	ASN
3	S	133	ASN
4	Q	53	ASN
4	R	25	HIS
3	T	226	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	225/225 (100%)	0.56	14 (6%) 20 18	51, 74, 96, 116	0
1	C	225/225 (100%)	0.53	11 (4%) 29 26	59, 78, 95, 114	0
1	E	225/225 (100%)	0.54	10 (4%) 34 30	55, 79, 99, 111	0
1	G	225/225 (100%)	0.64	12 (5%) 26 24	54, 81, 105, 124	0
1	I	225/225 (100%)	0.92	34 (15%) 2 3	59, 91, 116, 128	0
1	K	225/225 (100%)	0.55	13 (5%) 23 20	51, 72, 98, 114	0
2	B	213/213 (100%)	0.23	1 (0%) 91 88	53, 61, 76, 85	0
2	D	213/213 (100%)	0.38	1 (0%) 91 88	62, 71, 83, 94	0
2	F	213/213 (100%)	0.30	0 100 100	58, 68, 83, 92	0
2	H	213/213 (100%)	0.29	3 (1%) 75 69	54, 68, 86, 98	0
2	J	213/213 (100%)	0.33	4 (1%) 66 61	55, 71, 89, 106	0
2	L	213/213 (100%)	0.17	1 (0%) 91 88	51, 61, 76, 88	0
3	M	324/331 (97%)	2.28	146 (45%) 0 0	55, 175, 212, 218	0
3	N	323/331 (97%)	2.01	137 (42%) 0 0	50, 168, 205, 211	0
3	O	326/331 (98%)	2.48	165 (50%) 0 0	54, 196, 228, 232	0
3	S	324/331 (97%)	1.69	114 (35%) 0 0	55, 153, 182, 186	0
3	T	323/331 (97%)	1.72	114 (35%) 0 0	52, 157, 192, 196	0
3	U	326/331 (98%)	1.73	116 (35%) 0 0	55, 159, 190, 197	0
4	P	175/177 (98%)	0.62	11 (6%) 20 18	51, 73, 141, 170	0
4	Q	171/177 (96%)	0.53	10 (5%) 23 20	50, 72, 133, 157	0
4	R	171/177 (96%)	0.51	8 (4%) 31 28	51, 74, 134, 156	0
4	V	175/177 (98%)	0.57	10 (5%) 23 21	52, 77, 128, 147	0
4	W	171/177 (96%)	0.57	13 (7%) 13 14	51, 72, 113, 141	0
4	X	171/177 (96%)	0.52	10 (5%) 23 20	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%)	1.01	958 (17%) 1 1	50, 80, 199, 232	0

The worst 5 of 958 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	165	SER	13.2
3	O	164	LEU	11.8
3	N	198	ALA	11.7
3	O	250	ASN	10.9
3	M	127	TRP	9.4

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.