wwPDB X-ray Structure Validation Summary Report (i)

Jun 18, 2024 – 06:19 PM EDT

PDB ID	:	4F15
Title	:	Molecular basis of infectivity of 2009 pandemic H1N1 influenza A viruses
Authors	:	Kim, K.H.; Cho, K.J.; Lee, J.H.; Park, Y.H.; Khan, T.G.; Lee, J.Y.; Kang, S.H.; Alam, I.
Deposited on	:	2012-05-06
Resolution	:	2.81 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:

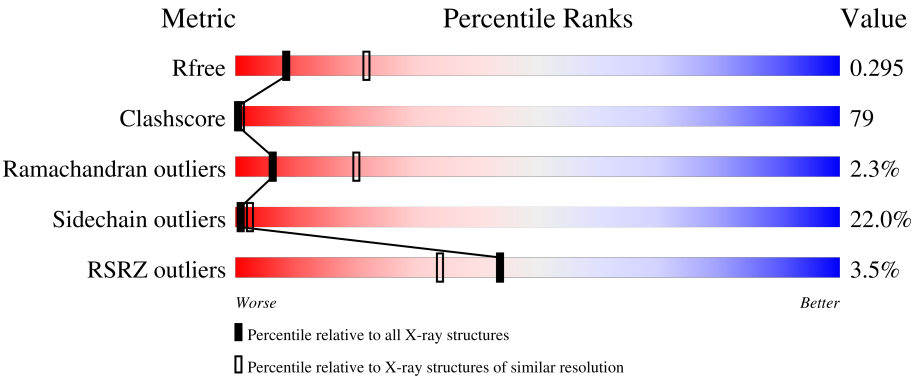
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.81 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	518	3% 16% 24% 5% 55%
1	D	518	5% 15% 26% 6% 53%
1	G	518	% 12% 25% 6% 56%
1	J	518	6% 17% 26% 6% 51%
2	B	219	24% 52% 18% • 5%

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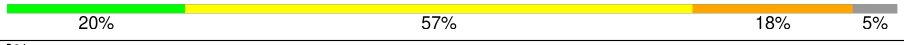
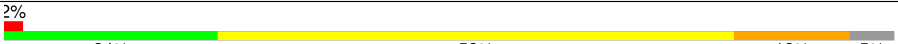
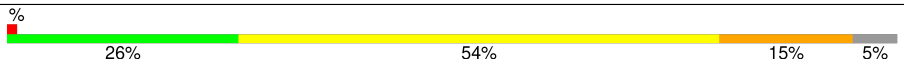
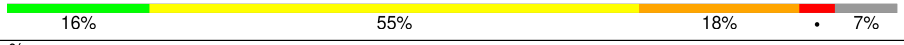
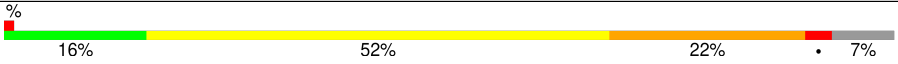
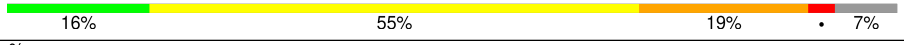
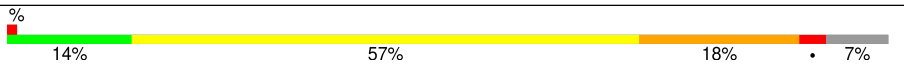
Mol	Chain	Length	Quality of chain
2	E	219	
2	H	219	
2	K	219	
3	C	218	
3	F	218	
3	I	218	
3	L	218	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19900 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1813	1152	311	344	6			
1	D	246	Total	C	N	O	S	0	0	0
			1872	1187	323	356	6			
1	G	227	Total	C	N	O	S	0	0	0
			1778	1131	304	337	6			
1	J	255	Total	C	N	O	S	0	0	0
			1918	1215	332	365	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ALA	-	EXPRESSION TAG	UNP C5MQE6
A	-7	ASP	-	EXPRESSION TAG	UNP C5MQE6
A	-6	PRO	-	EXPRESSION TAG	UNP C5MQE6
A	-5	GLY	-	EXPRESSION TAG	UNP C5MQE6
A	-4	TYR	-	EXPRESSION TAG	UNP C5MQE6
A	-3	LEU	-	EXPRESSION TAG	UNP C5MQE6
A	-2	LEU	-	EXPRESSION TAG	UNP C5MQE6
A	-1	GLU	-	EXPRESSION TAG	UNP C5MQE6
A	0	PHE	-	EXPRESSION TAG	UNP C5MQE6
A	507	ARG	-	EXPRESSION TAG	UNP C5MQE6
A	508	SER	-	EXPRESSION TAG	UNP C5MQE6
A	509	LEU	-	EXPRESSION TAG	UNP C5MQE6
A	510	VAL	-	EXPRESSION TAG	UNP C5MQE6
A	511	PRO	-	EXPRESSION TAG	UNP C5MQE6
A	512	ARG	-	EXPRESSION TAG	UNP C5MQE6
D	-8	ALA	-	EXPRESSION TAG	UNP C5MQE6
D	-7	ASP	-	EXPRESSION TAG	UNP C5MQE6
D	-6	PRO	-	EXPRESSION TAG	UNP C5MQE6
D	-5	GLY	-	EXPRESSION TAG	UNP C5MQE6
D	-4	TYR	-	EXPRESSION TAG	UNP C5MQE6
D	-3	LEU	-	EXPRESSION TAG	UNP C5MQE6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	LEU	-	EXPRESSION TAG	UNP C5MQE6
D	-1	GLU	-	EXPRESSION TAG	UNP C5MQE6
D	0	PHE	-	EXPRESSION TAG	UNP C5MQE6
D	507	ARG	-	EXPRESSION TAG	UNP C5MQE6
D	508	SER	-	EXPRESSION TAG	UNP C5MQE6
D	509	LEU	-	EXPRESSION TAG	UNP C5MQE6
D	510	VAL	-	EXPRESSION TAG	UNP C5MQE6
D	511	PRO	-	EXPRESSION TAG	UNP C5MQE6
D	512	ARG	-	EXPRESSION TAG	UNP C5MQE6
G	-8	ALA	-	EXPRESSION TAG	UNP C5MQE6
G	-7	ASP	-	EXPRESSION TAG	UNP C5MQE6
G	-6	PRO	-	EXPRESSION TAG	UNP C5MQE6
G	-5	GLY	-	EXPRESSION TAG	UNP C5MQE6
G	-4	TYR	-	EXPRESSION TAG	UNP C5MQE6
G	-3	LEU	-	EXPRESSION TAG	UNP C5MQE6
G	-2	LEU	-	EXPRESSION TAG	UNP C5MQE6
G	-1	GLU	-	EXPRESSION TAG	UNP C5MQE6
G	0	PHE	-	EXPRESSION TAG	UNP C5MQE6
G	507	ARG	-	EXPRESSION TAG	UNP C5MQE6
G	508	SER	-	EXPRESSION TAG	UNP C5MQE6
G	509	LEU	-	EXPRESSION TAG	UNP C5MQE6
G	510	VAL	-	EXPRESSION TAG	UNP C5MQE6
G	511	PRO	-	EXPRESSION TAG	UNP C5MQE6
G	512	ARG	-	EXPRESSION TAG	UNP C5MQE6
J	-8	ALA	-	EXPRESSION TAG	UNP C5MQE6
J	-7	ASP	-	EXPRESSION TAG	UNP C5MQE6
J	-6	PRO	-	EXPRESSION TAG	UNP C5MQE6
J	-5	GLY	-	EXPRESSION TAG	UNP C5MQE6
J	-4	TYR	-	EXPRESSION TAG	UNP C5MQE6
J	-3	LEU	-	EXPRESSION TAG	UNP C5MQE6
J	-2	LEU	-	EXPRESSION TAG	UNP C5MQE6
J	-1	GLU	-	EXPRESSION TAG	UNP C5MQE6
J	0	PHE	-	EXPRESSION TAG	UNP C5MQE6
J	507	ARG	-	EXPRESSION TAG	UNP C5MQE6
J	508	SER	-	EXPRESSION TAG	UNP C5MQE6
J	509	LEU	-	EXPRESSION TAG	UNP C5MQE6
J	510	VAL	-	EXPRESSION TAG	UNP C5MQE6
J	511	PRO	-	EXPRESSION TAG	UNP C5MQE6
J	512	ARG	-	EXPRESSION TAG	UNP C5MQE6

- Molecule 2 is a protein called Fab fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	0	0
			1544	962	268	307	7			
2	E	208	Total	C	N	O	S	0	0	0
			1544	962	268	307	7			
2	H	208	Total	C	N	O	S	0	0	0
			1544	962	268	307	7			
2	K	208	Total	C	N	O	S	0	0	0
			1544	962	268	307	7			

- Molecule 3 is a protein called Fab fragment, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	203	Total	C	N	O	S	0	0	0
			1557	975	263	313	6			
3	F	203	Total	C	N	O	S	0	0	0
			1557	975	263	313	6			
3	I	203	Total	C	N	O	S	0	0	0
			1557	975	263	313	6			
3	L	203	Total	C	N	O	S	0	0	0
			1557	975	263	313	6			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	8	Total	O	0	0
			8	8		
4	C	11	Total	O	0	0
			11	11		
4	D	7	Total	O	0	0
			7	7		
4	E	11	Total	O	0	0
			11	11		
4	F	9	Total	O	0	0
			9	9		
4	G	8	Total	O	0	0
			8	8		
4	H	10	Total	O	0	0
			10	10		
4	I	12	Total	O	0	0
			12	12		
4	J	7	Total	O	0	0
			7	7		

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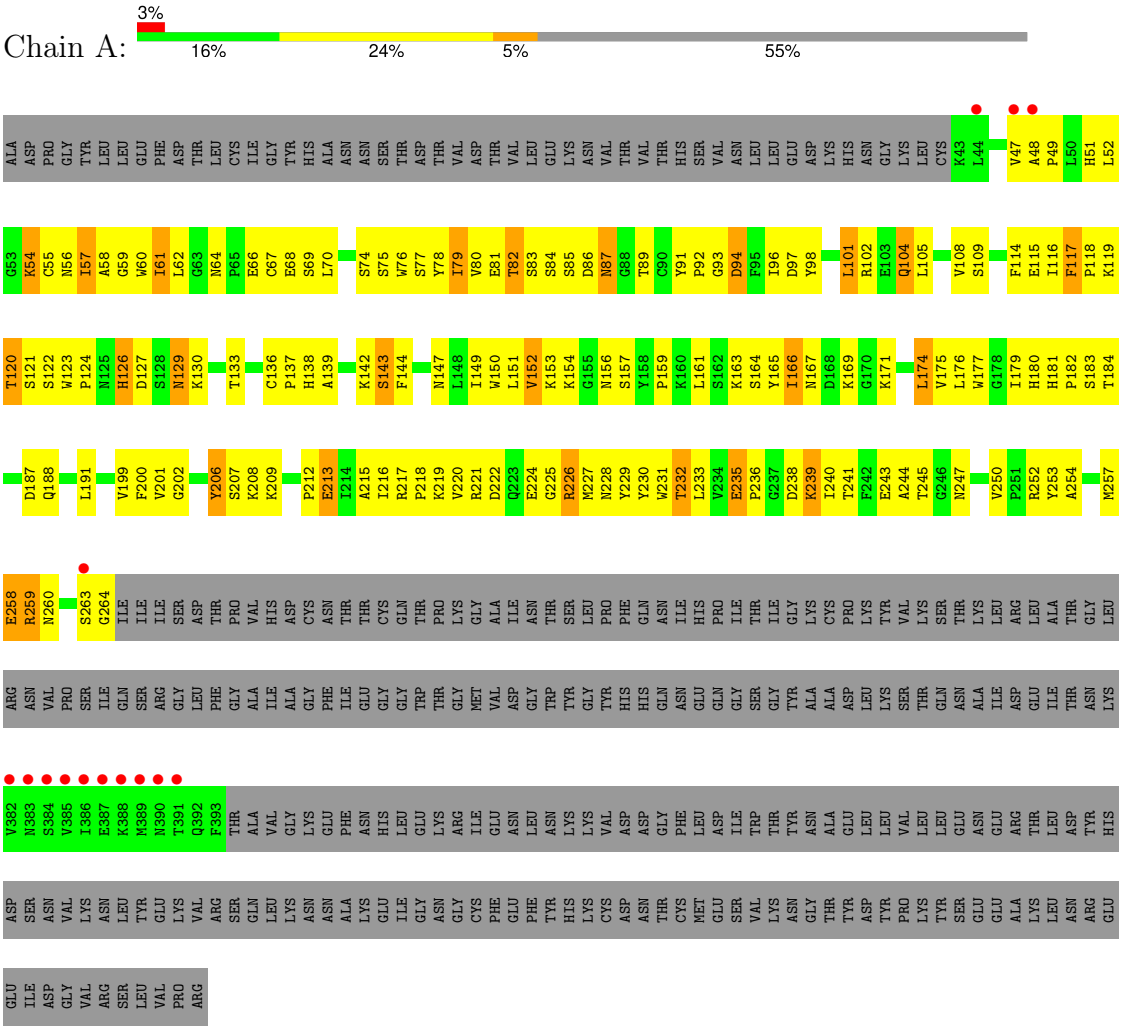
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	6	Total O 6 6	0	0
4	L	15	Total O 15 15	0	0

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.

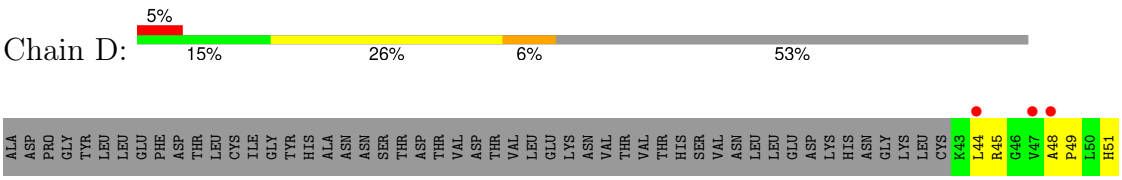
• Molecule 1: Hemagglutinin

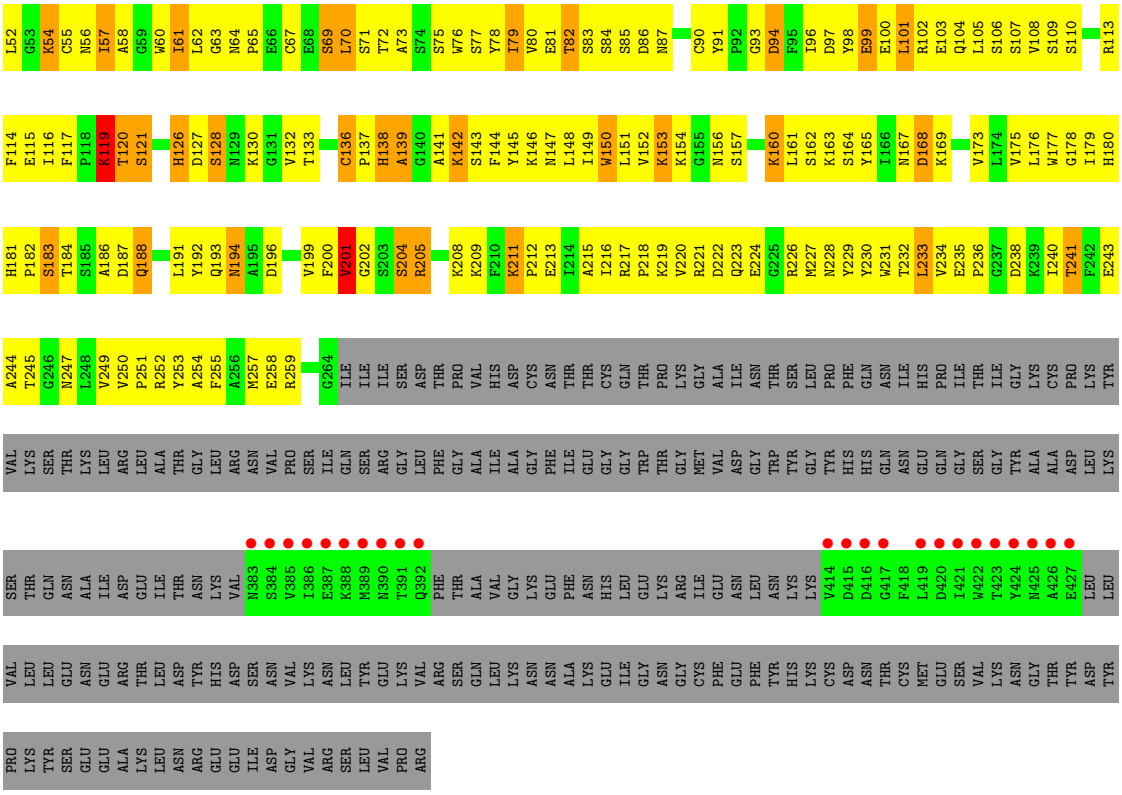
Chain A:



• Molecule 1: Hemagglutinin

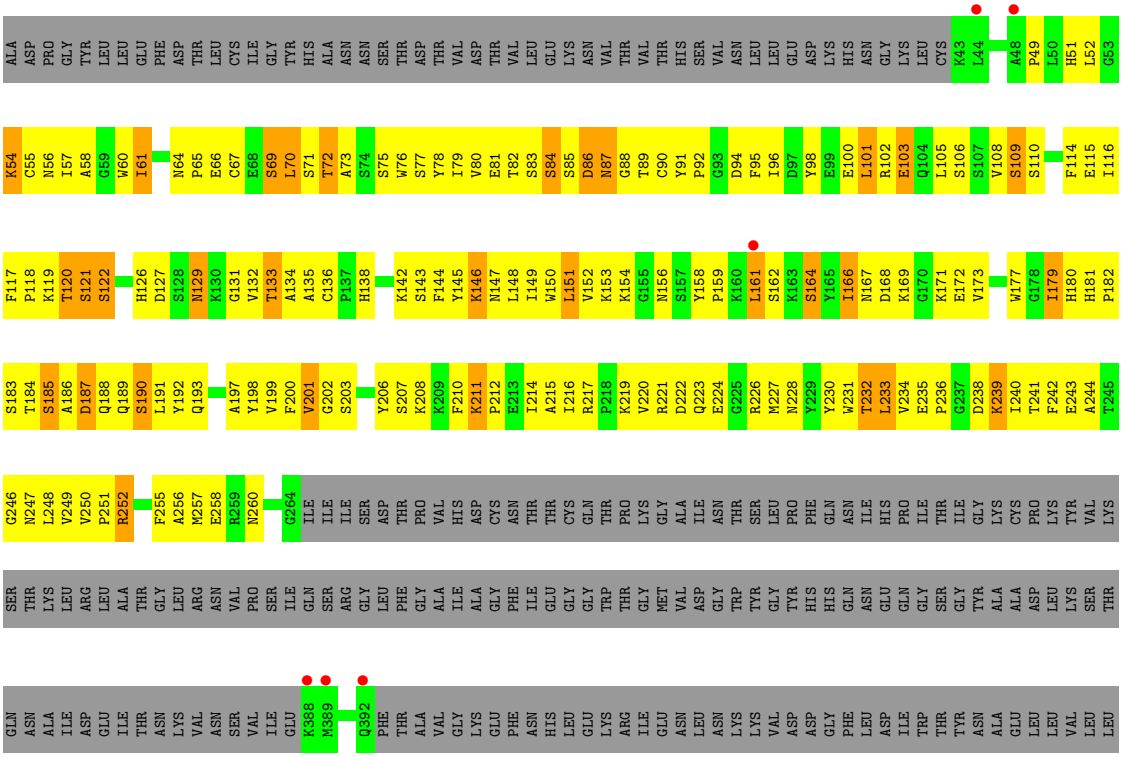
Chain D:

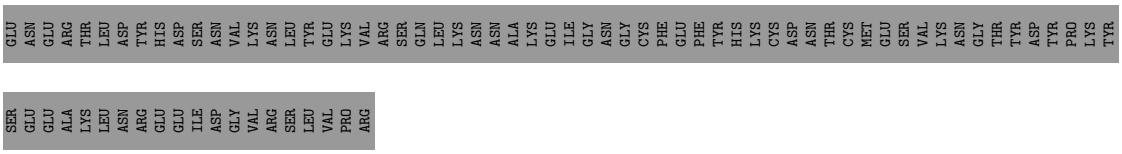




• Molecule 1: Hemagglutinin

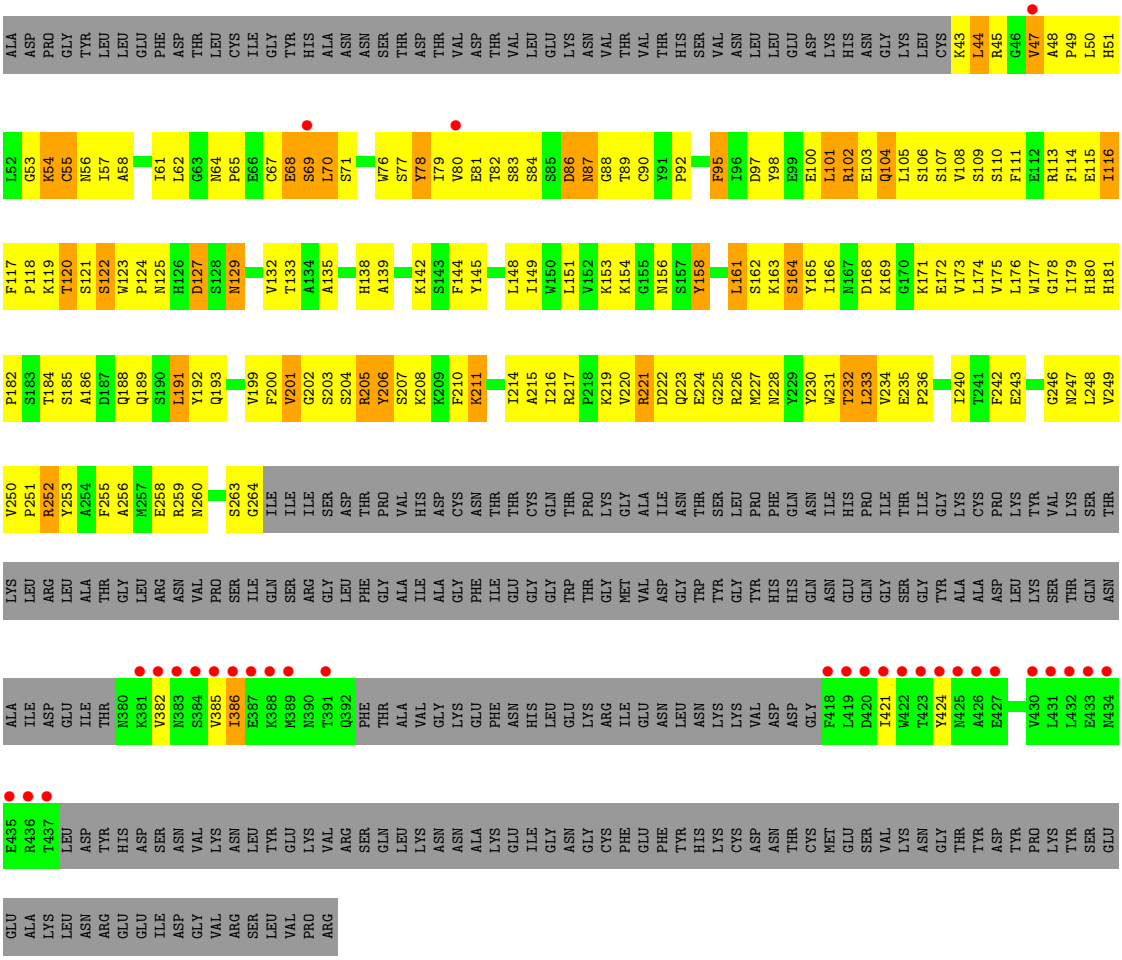
Chain G:





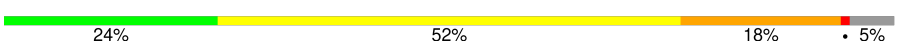
• Molecule 1: Hemagglutinin

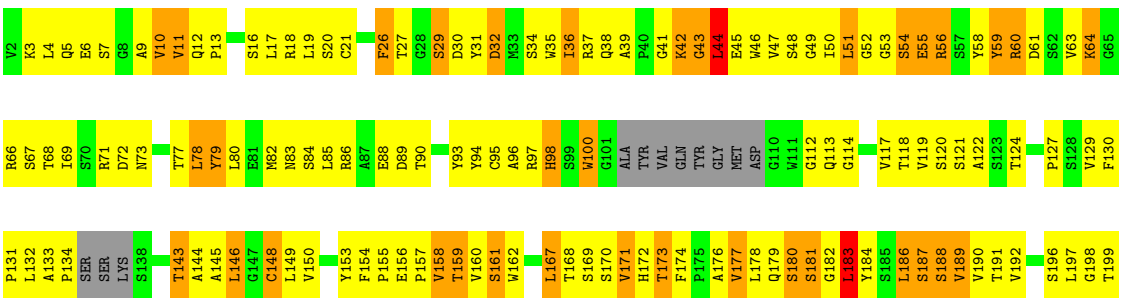
Chain J:

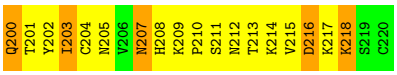


• Molecule 2: Fab fragment, heavy chain

Chain B:

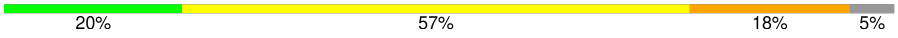


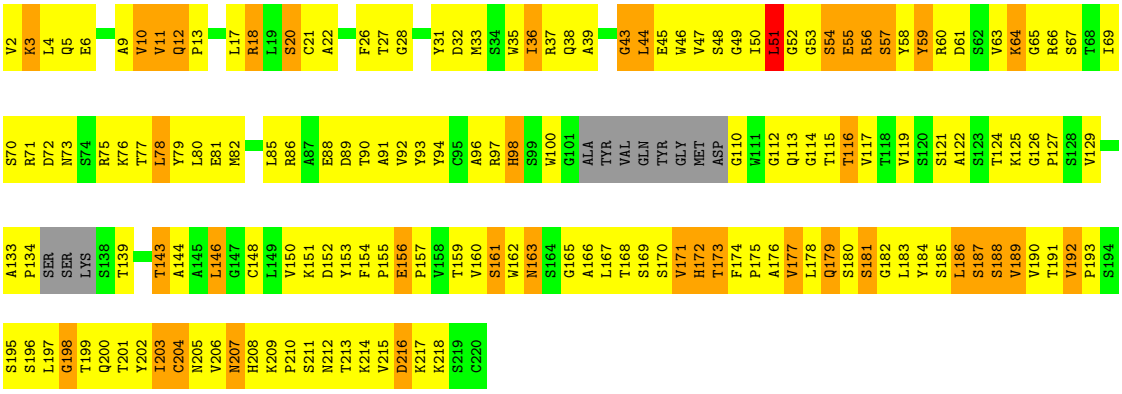




• Molecule 2: Fab fragment, heavy chain

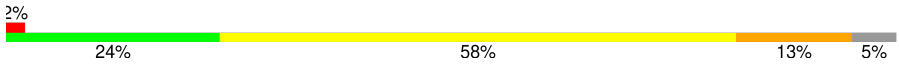
Chain E:

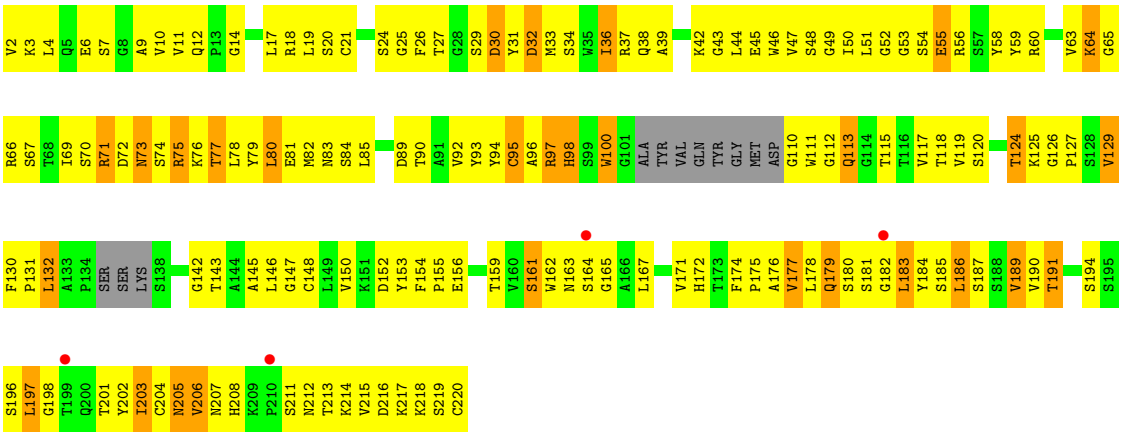




• Molecule 2: Fab fragment, heavy chain

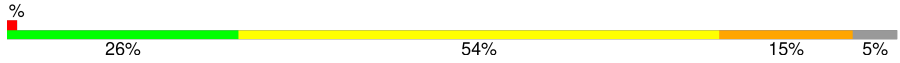
Chain H:

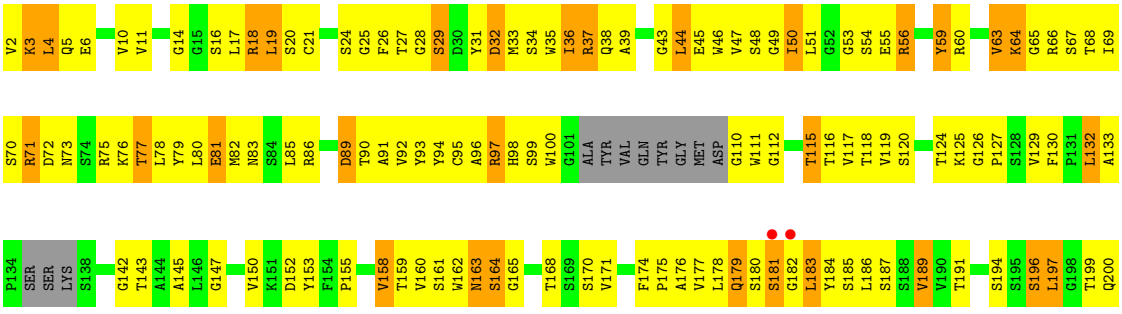


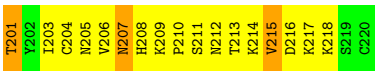


• Molecule 2: Fab fragment, heavy chain

Chain K:

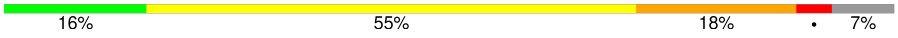


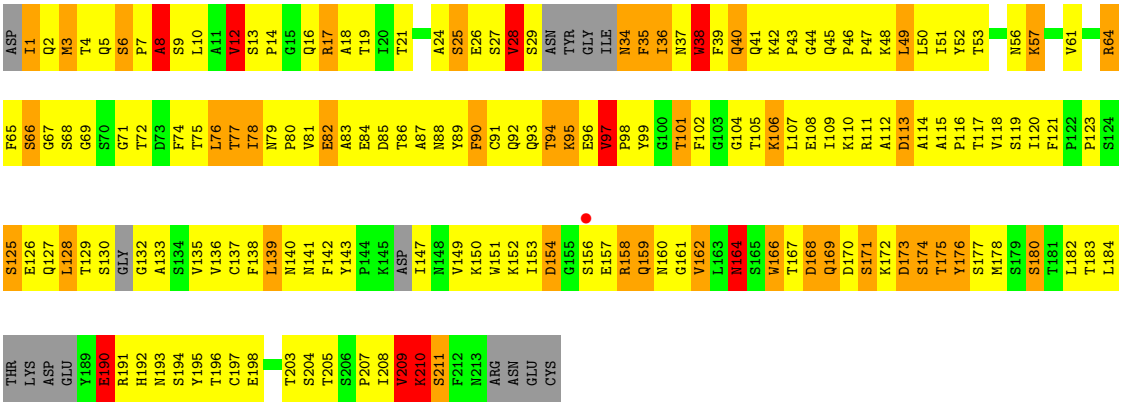




• Molecule 3: Fab fragment, light chain

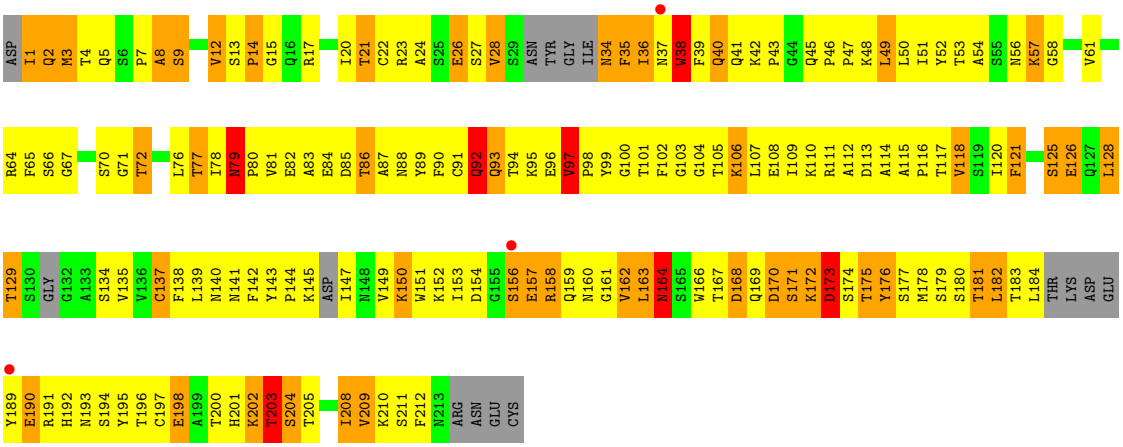
Chain C:





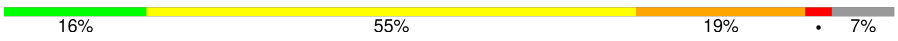
• Molecule 3: Fab fragment, light chain

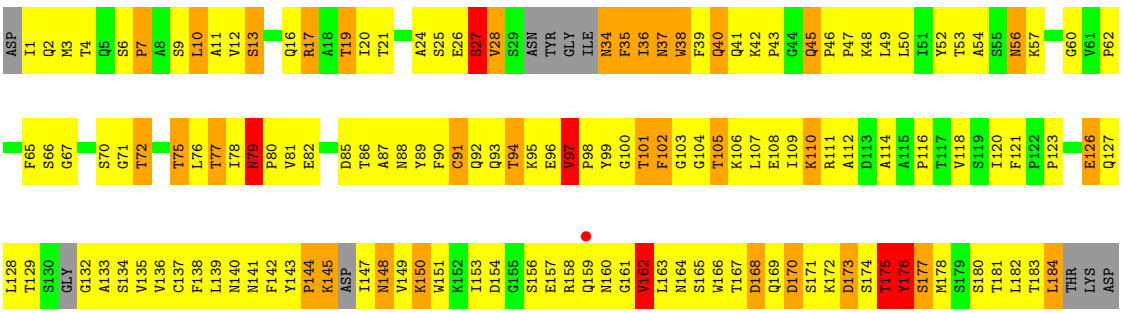
Chain F:



• Molecule 3: Fab fragment, light chain

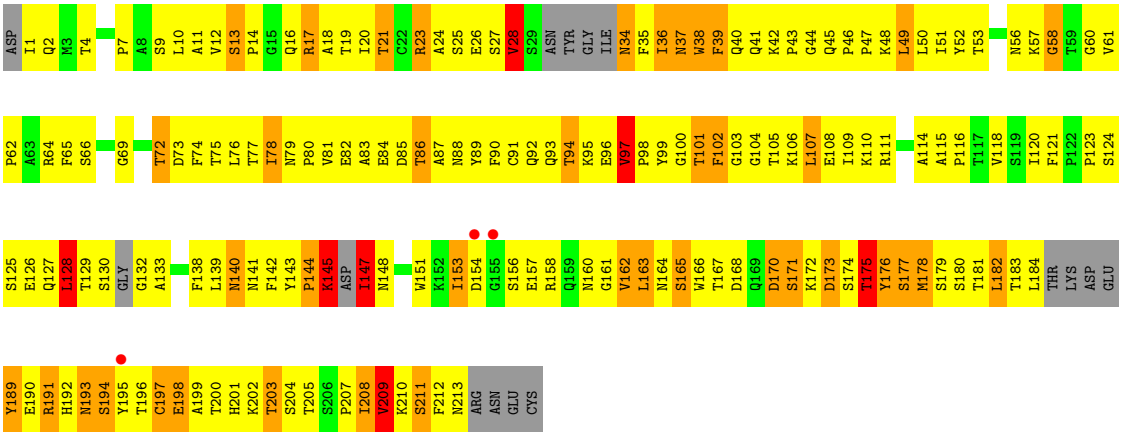
Chain I:





• Molecule 3: Fab fragment, light chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.70Å 90.13Å 238.18Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	49.68 – 2.81 49.68 – 2.81	Depositor EDS
% Data completeness (in resolution range)	87.5 (49.68-2.81) 84.4 (49.68-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.233 , 0.289 0.236 , 0.295	Depositor DCC
R_{free} test set	3381 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 21.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.457 for h,-k,-l	Xtriage
Reported twinning fraction	0.492 for h,-k,-l	Depositor
Outliers	2 of 66880 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	19900	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1107e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (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	0.39	0/1861	0.63	0/2523
1	D	0.41	0/1919	0.67	0/2602
1	G	0.42	0/1826	0.69	0/2474
1	J	0.41	0/1965	0.67	1/2667 (0.0%)
2	B	0.45	0/1577	0.76	3/2141 (0.1%)
2	E	0.42	0/1577	0.74	3/2141 (0.1%)
2	H	0.43	0/1577	0.73	0/2141
2	K	0.43	0/1577	0.72	0/2141
3	C	0.50	0/1590	0.86	4/2157 (0.2%)
3	F	0.51	0/1590	0.79	1/2157 (0.0%)
3	I	0.78	1/1591 (0.1%)	0.85	5/2160 (0.2%)
3	L	0.84	1/1591 (0.1%)	0.90	7/2160 (0.3%)
All	All	0.52	2/20241 (0.0%)	0.75	24/27464 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	3
1	G	0	3
1	J	0	2
2	B	0	1
2	E	0	1
2	H	0	1
2	K	0	1
3	C	0	8
3	F	0	13
3	I	0	6
3	L	0	2
All	All	0	43

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	145	LYS	C-N	27.80	1.98	1.34
3	I	145	LYS	C-N	24.11	1.89	1.34

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	145	LYS	O-C-N	-12.89	102.07	122.70
3	L	145	LYS	C-N-CA	9.08	144.39	121.70
2	E	43	GLY	N-CA-C	-6.80	96.09	113.10
2	B	43	GLY	N-CA-C	-6.76	96.19	113.10
3	C	94	THR	N-CA-C	-6.63	93.11	111.00

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ASN	Peptide
1	A	74	SER	Peptide
2	B	44	LEU	Peptide
3	C	28	VAL	Peptide
3	C	8	ALA	Peptide

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	1813	0	1716	191	0
1	D	1872	0	1743	214	0
1	G	1778	0	1702	239	0
1	J	1918	0	1760	219	0
2	B	1544	0	1505	262	0
2	E	1544	0	1505	254	0
2	H	1544	0	1505	274	0
2	K	1544	0	1505	247	0
3	C	1557	0	1503	343	0
3	F	1557	0	1503	355	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	1557	0	1503	317	0
3	L	1557	0	1503	332	0
4	A	11	0	0	2	0
4	B	8	0	0	3	0
4	C	11	0	0	3	0
4	D	7	0	0	1	0
4	E	11	0	0	3	0
4	F	9	0	0	5	0
4	G	8	0	0	2	0
4	H	10	0	0	3	0
4	I	12	0	0	2	0
4	J	7	0	0	3	0
4	K	6	0	0	4	0
4	L	15	0	0	8	0
All	All	19900	0	18953	3059	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 79.

The worst 5 of 3059 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)
3:I:145:LYS:C	3:I:147:ILE:N	1.89	1.25
3:C:38:TRP:CD2	3:C:39:PHE:HA	1.74	1.21
2:B:171:VAL:HG21	3:C:176:TYR:CE1	1.76	1.19
3:L:145:LYS:C	3:L:147:ILE:N	1.98	1.16
2:E:32:ASP:HB3	2:E:51:LEU:HA	1.27	1.15

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	230/518 (44%)	198 (86%)	29 (13%)	3 (1%)	12 34
1	D	240/518 (46%)	199 (83%)	35 (15%)	6 (2%)	5 18
1	G	223/518 (43%)	193 (86%)	27 (12%)	3 (1%)	12 34
1	J	249/518 (48%)	211 (85%)	35 (14%)	3 (1%)	13 37
2	B	202/219 (92%)	175 (87%)	25 (12%)	2 (1%)	15 42
2	E	202/219 (92%)	172 (85%)	29 (14%)	1 (0%)	29 59
2	H	202/219 (92%)	174 (86%)	26 (13%)	2 (1%)	15 42
2	K	202/219 (92%)	177 (88%)	21 (10%)	4 (2%)	7 23
3	C	193/218 (88%)	150 (78%)	37 (19%)	6 (3%)	4 13
3	F	193/218 (88%)	142 (74%)	38 (20%)	13 (7%)	1 3
3	I	195/218 (89%)	141 (72%)	45 (23%)	9 (5%)	2 7
3	L	195/218 (89%)	145 (74%)	44 (23%)	6 (3%)	4 13
All	All	2526/3820 (66%)	2077 (82%)	391 (16%)	58 (2%)	6 20

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	8	ALA
3	F	173	ASP
3	L	144	PRO
3	L	147	ILE
1	A	120	THR

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	190/451 (42%)	161 (85%)	29 (15%)	2 8
1	D	190/451 (42%)	154 (81%)	36 (19%)	1 4
1	G	190/451 (42%)	157 (83%)	33 (17%)	2 5
1	J	190/451 (42%)	156 (82%)	34 (18%)	2 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	173/182 (95%)	130 (75%)	43 (25%)	0 1
2	E	173/182 (95%)	129 (75%)	44 (25%)	0 1
2	H	173/182 (95%)	140 (81%)	33 (19%)	1 4
2	K	173/182 (95%)	139 (80%)	34 (20%)	1 4
3	C	177/190 (93%)	128 (72%)	49 (28%)	0 1
3	F	177/190 (93%)	135 (76%)	42 (24%)	1 2
3	I	177/190 (93%)	130 (73%)	47 (27%)	0 1
3	L	177/190 (93%)	125 (71%)	52 (29%)	0 1
All	All	2160/3292 (66%)	1684 (78%)	476 (22%)	1 2

5 of 476 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	158	ARG
3	L	97	VAL
2	H	80	LEU
3	L	72	THR
3	L	209	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	223	GLN
3	I	141	ASN
3	I	37	ASN
3	I	201	HIS
3	C	193	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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

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	234/518 (45%)	0.03	14 (5%) 21 14	19, 35, 59, 76	8 (3%)
1	D	246/518 (47%)	0.25	26 (10%) 6 3	18, 32, 58, 95	21 (8%)
1	G	227/518 (43%)	-0.28	6 (2%) 56 46	18, 32, 57, 70	2 (0%)
1	J	255/518 (49%)	0.30	31 (12%) 4 2	21, 33, 57, 71	30 (11%)
2	B	208/219 (94%)	-0.37	0 100 100	13, 29, 44, 58	0
2	E	208/219 (94%)	-0.44	0 100 100	19, 30, 42, 62	0
2	H	208/219 (94%)	-0.40	4 (1%) 66 59	20, 29, 43, 53	0
2	K	208/219 (94%)	-0.35	2 (0%) 82 77	21, 29, 41, 48	0
3	C	203/218 (93%)	-0.29	1 (0%) 91 88	13, 28, 50, 68	0
3	F	203/218 (93%)	-0.25	3 (1%) 73 67	20, 29, 49, 58	0
3	I	203/218 (93%)	-0.23	1 (0%) 91 88	20, 30, 53, 71	0
3	L	203/218 (93%)	-0.22	3 (1%) 73 67	18, 30, 57, 75	0
All	All	2606/3820 (68%)	-0.17	91 (3%) 44 34	13, 31, 54, 95	61 (2%)

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	388	LYS	13.4
1	J	387	GLU	12.3
1	A	389	MET	12.2
1	D	419	LEU	11.1
1	D	389	MET	10.9

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

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.