



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:33 PM GMT

PDB ID : 4LVH
Title : Insight into highly conserved H1 subtype-specific epitopes in influenza virus hemagglutinin
Authors : Kim, K.H.; Cho, K.J.; Kim, S.; Seok, J.H.; Lee, J.-H.
Deposited on : 2013-07-26
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

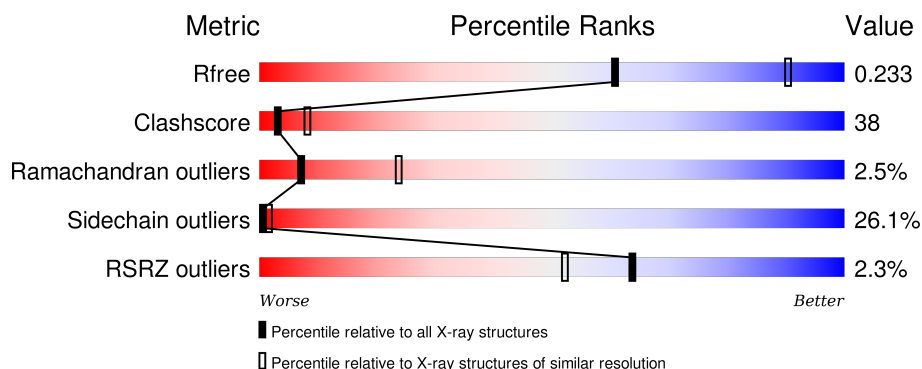
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	518	<div> <div>3%</div> <div>18% 20% 7% 54%</div> </div>
1	D	518	<div> <div>%</div> <div>16% 22% 5% 57%</div> </div>
1	G	518	<div> <div>%</div> <div>17% 22% • 57%</div> </div>
1	J	518	<div> <div>%</div> <div>16% 19% 8% 57%</div> </div>
2	B	222	<div> <div>%</div> <div>34% 44% 19% ••</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	222	
2	H	222	
2	K	222	
3	C	211	
3	F	211	
3	I	211	
3	L	211	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CA	A	601	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20106 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	236	Total	C	N	O	S	0	1	0
			1831	1162	311	352	6			
1	D	222	Total	C	N	O	S	0	1	0
			1762	1121	297	338	6			
1	G	222	Total	C	N	O	S	0	1	0
			1762	1121	297	338	6			
1	J	222	Total	C	N	O	S	0	1	0
			1762	1121	297	338	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	504	ARG	-	EXPRESSION TAG	UNP C5MQE6
D	505	SER	-	EXPRESSION TAG	UNP C5MQE6
D	506	LEU	-	EXPRESSION TAG	UNP C5MQE6
D	507	VAL	-	EXPRESSION TAG	UNP C5MQE6
D	508	PRO	-	EXPRESSION TAG	UNP C5MQE6
D	509	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	504	ARG	-	EXPRESSION TAG	UNP C5MQE6
G	505	SER	-	EXPRESSION TAG	UNP C5MQE6
G	506	LEU	-	EXPRESSION TAG	UNP C5MQE6
G	507	VAL	-	EXPRESSION TAG	UNP C5MQE6
G	508	PRO	-	EXPRESSION TAG	UNP C5MQE6
G	509	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	504	ARG	-	EXPRESSION TAG	UNP C5MQE6
J	505	SER	-	EXPRESSION TAG	UNP C5MQE6
J	506	LEU	-	EXPRESSION TAG	UNP C5MQE6
J	507	VAL	-	EXPRESSION TAG	UNP C5MQE6
J	508	PRO	-	EXPRESSION TAG	UNP C5MQE6
J	509	ARG	-	EXPRESSION TAG	UNP C5MQE6

- Molecule 2 is a protein called MONOCLONAL ANTIBODY H-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1635	1028	280	319	8			
2	E	218	Total	C	N	O	S	0	0	0
			1635	1028	280	319	8			
2	H	218	Total	C	N	O	S	0	0	0
			1635	1028	280	319	8			
2	K	218	Total	C	N	O	S	0	0	0
			1635	1028	280	319	8			

- Molecule 3 is a protein called MONOCLONAL ANTIBODY L-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	210	Total	C	N	O	S	0	0	0
			1610	1007	271	326	6			
3	F	210	Total	C	N	O	S	0	0	0
			1610	1007	271	326	6			
3	I	210	Total	C	N	O	S	0	0	0
			1610	1007	271	326	6			
3	L	209	Total	C	N	O	S	0	0	0
			1604	1004	270	324	6			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Ca	0	0
			1	1		
4	J	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

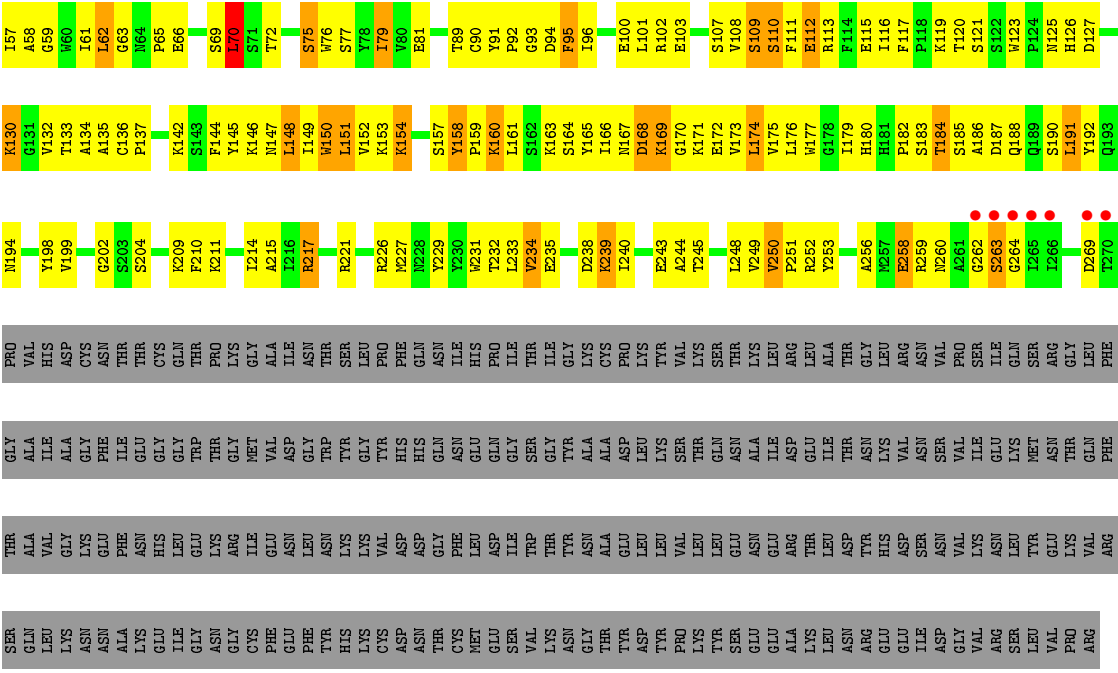
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	1	Total	O	0	0
			1	1		
5	F	1	Total	O	0	0
			1	1		

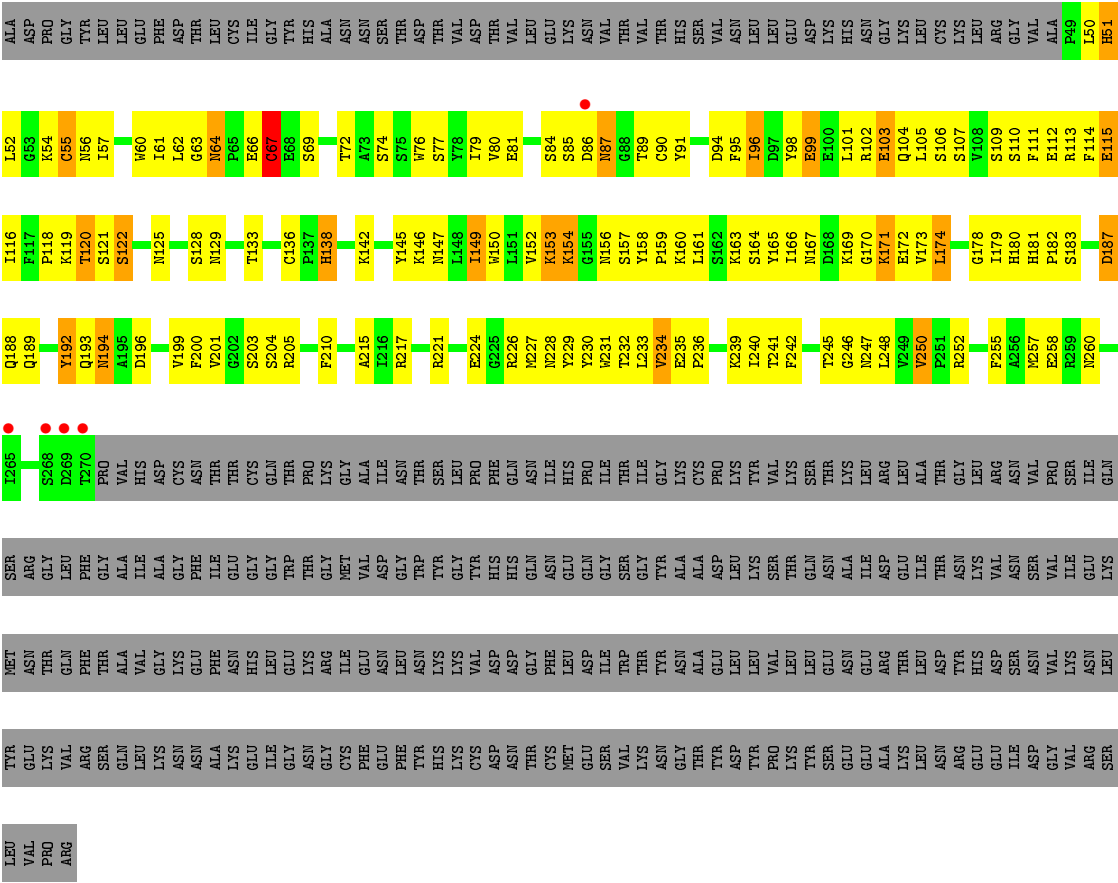
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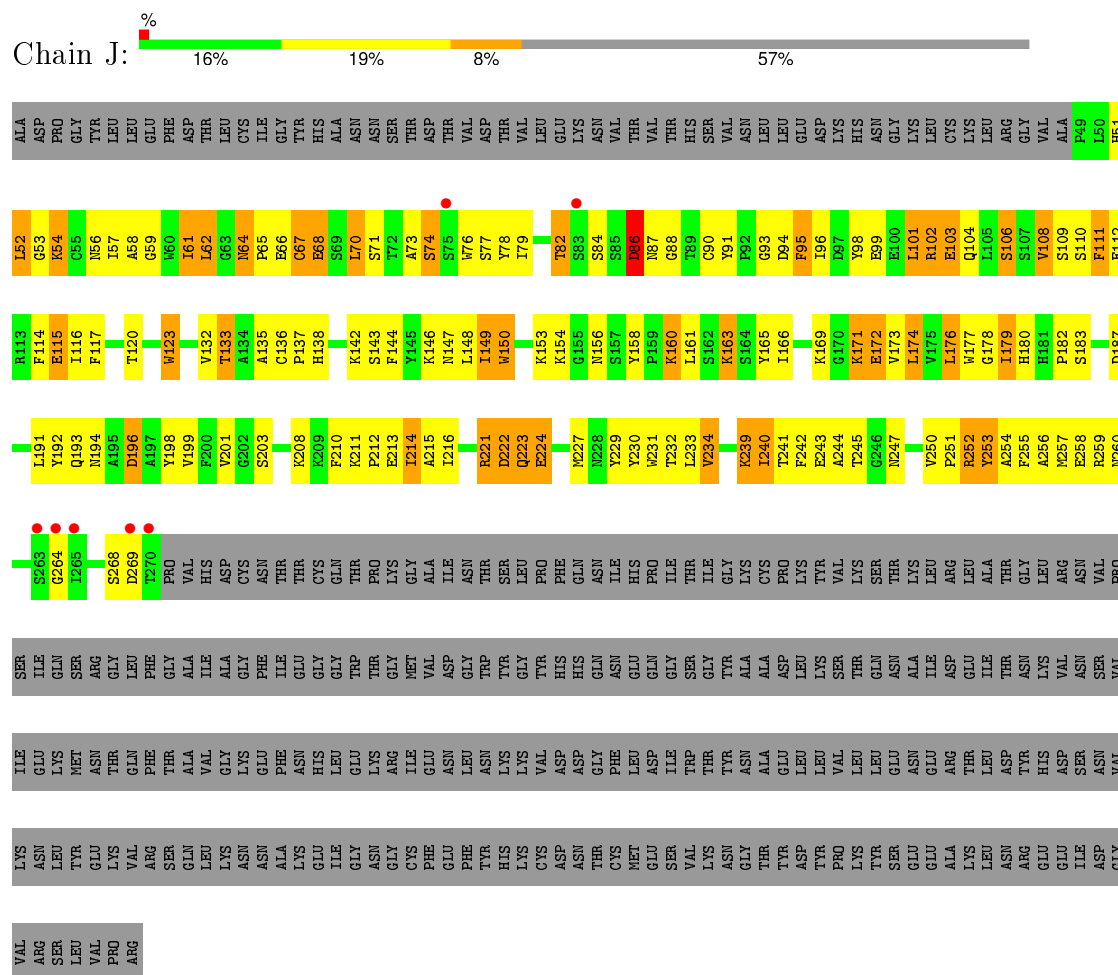
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total 1	O 1	0	0
5	H	3	Total 3	O 3	0	0
5	I	2	Total 2	O 2	0	0
5	K	1	Total 1	O 1	0	0
5	L	1	Total 1	O 1	0	0



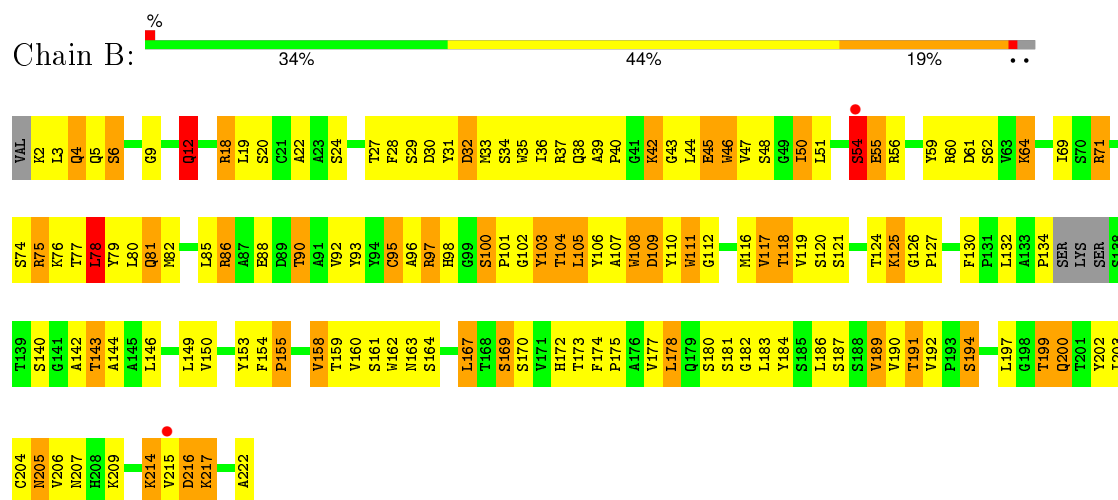
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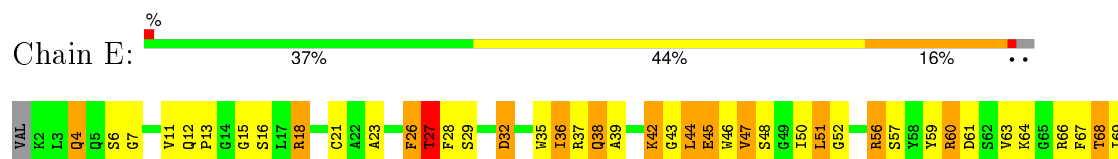
• Molecule 1: Hemagglutinin

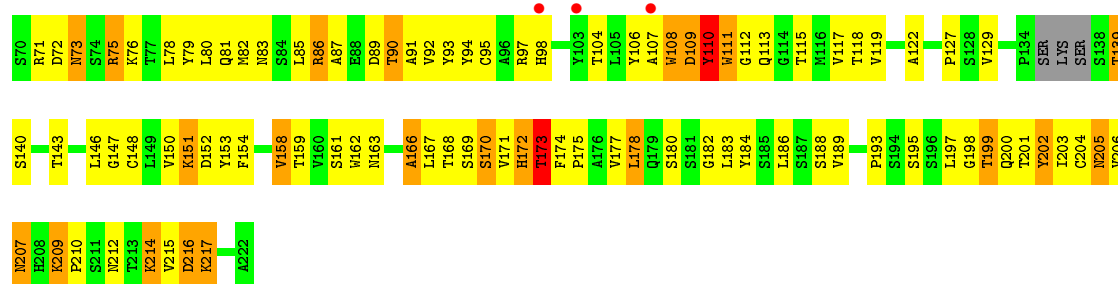


• Molecule 2: MONOCLONAL ANTIBODY H-CHAIN

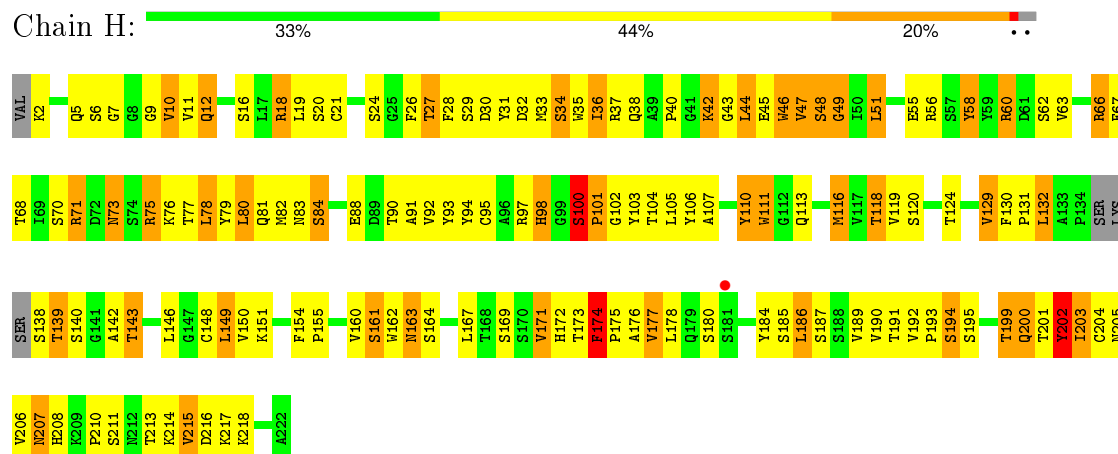


- Molecule 2: MONOCLONAL ANTIBODY H-CHAIN

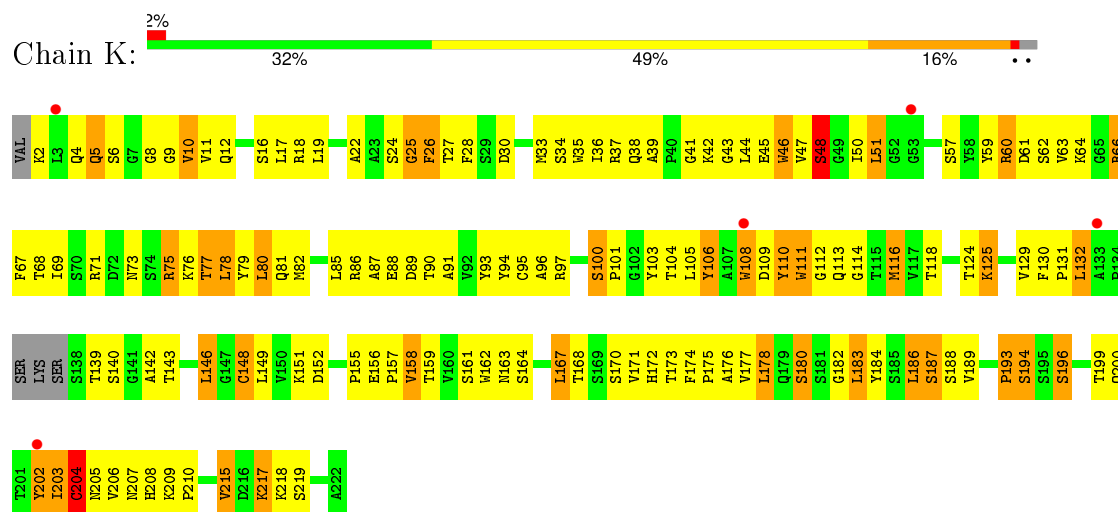




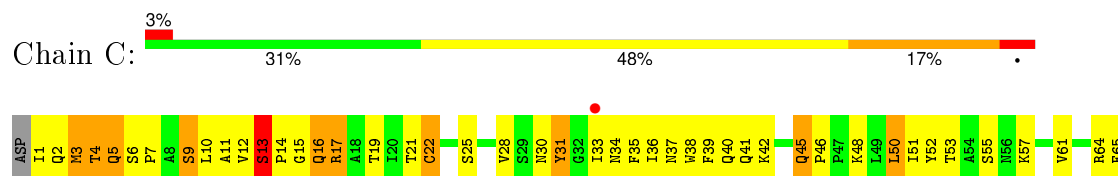
• Molecule 2: MONOCLONAL ANTIBODY H-CHAIN

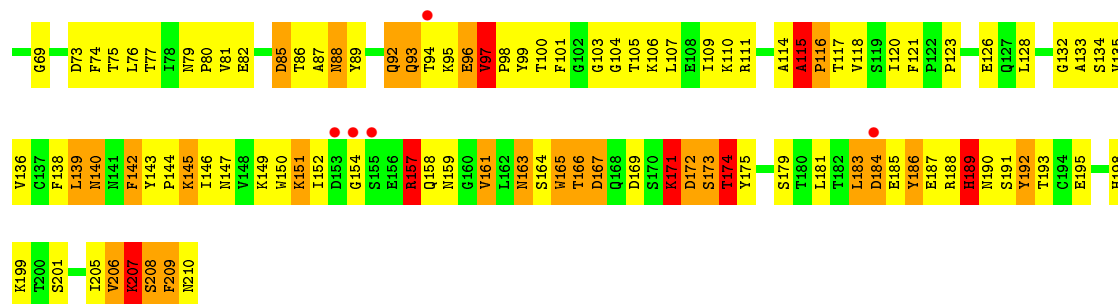


• Molecule 2: MONOCLONAL ANTIBODY H-CHAIN

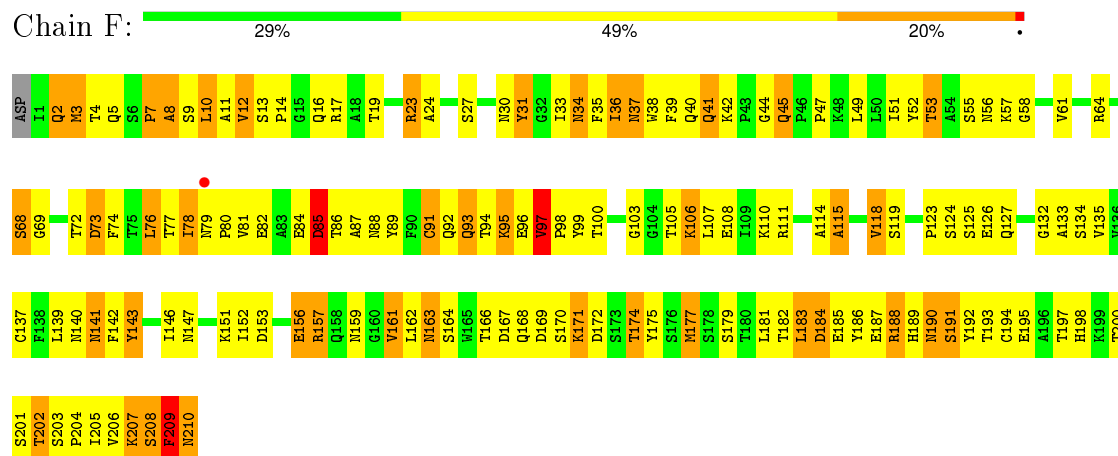


• Molecule 3: MONOCLONAL ANTIBODY L-CHAIN

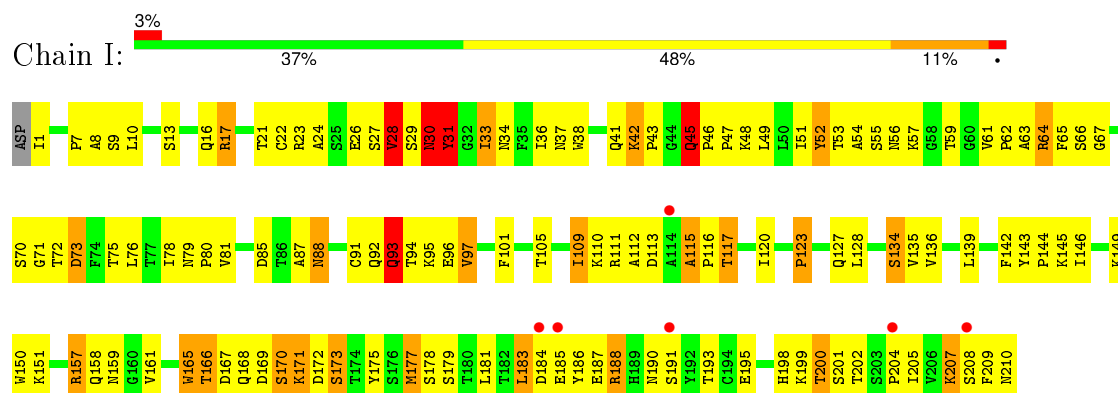




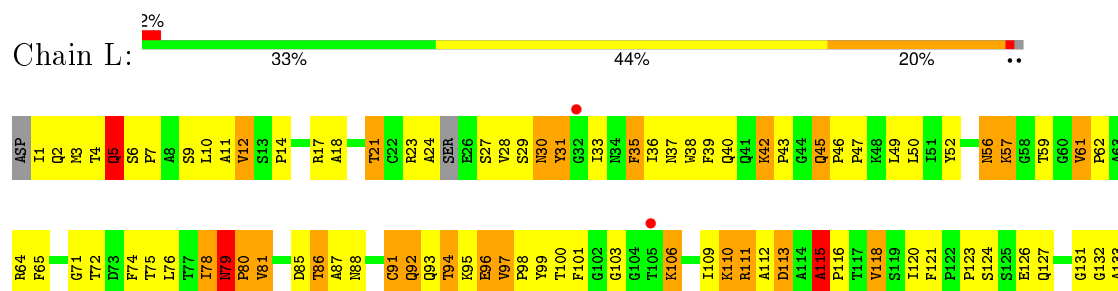
• Molecule 3: MONOCLONAL ANTIBODY L-CHAIN

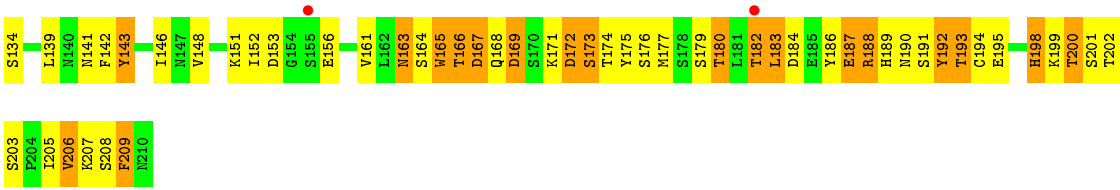


• Molecule 3: MONOCLONAL ANTIBODY L-CHAIN



• Molecule 3: MONOCLONAL ANTIBODY L-CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.75Å 237.81Å 94.23Å 90.00° 110.31° 90.00°	Depositor
Resolution (Å)	43.49 – 2.80 43.49 – 2.69	Depositor EDS
% Data completeness (in resolution range)	76.8 (43.49-2.80) 84.5 (43.49-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.232 , 0.274 0.228 , 0.233	Depositor DCC
R_{free} test set	3466 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 41.3	EDS
Estimated twinning fraction	0.844 for H, K, L 0.156 for -H, -K, H+L 0.004 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.844 for H, K, L 0.156 for -H, -K, H+L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 69841 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	20106	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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 22.72 % 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 5.3778e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.57	0/1879	0.91	1/2549 (0.0%)
1	D	0.53	0/1811	0.84	2/2456 (0.1%)
1	G	0.57	0/1811	0.85	1/2456 (0.0%)
1	J	0.54	0/1811	0.82	1/2456 (0.0%)
2	B	0.59	0/1675	0.95	3/2277 (0.1%)
2	E	0.60	0/1675	0.92	0/2277
2	H	0.59	0/1675	0.90	3/2277 (0.1%)
2	K	0.59	0/1675	0.93	2/2277 (0.1%)
3	C	0.62	0/1648	1.00	8/2242 (0.4%)
3	F	0.60	0/1648	0.99	3/2242 (0.1%)
3	I	0.58	0/1648	0.95	2/2242 (0.1%)
3	L	0.60	0/1641	0.99	4/2231 (0.2%)
All	All	0.58	0/20597	0.92	30/27982 (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	6
1	D	0	1
1	G	0	1
1	J	0	3
2	B	0	7
2	E	0	2
2	H	0	5
2	K	0	6
3	C	0	7
3	F	0	6
3	I	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	7
All	All	0	55

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	9	GLY	N-CA-C	8.66	134.76	113.10
1	D	70	LEU	CA-CB-CG	8.16	134.06	115.30
3	L	97	VAL	C-N-CD	7.60	144.37	128.40
3	F	115	ALA	C-N-CD	-7.54	104.01	120.60
2	H	7	GLY	N-CA-C	7.47	131.78	113.10

There are no chirality outliers.

5 of 55 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	ASN	Peptide
1	A	203	SER	Peptide
1	A	221	ARG	Sidechain
1	A	65	PRO	Peptide
1	A	74	SER	Peptide

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	1831	0	1725	135	0
1	D	1762	0	1694	107	0
1	G	1762	0	1694	115	0
1	J	1762	0	1694	109	0
2	B	1635	0	1587	132	0
2	E	1635	0	1587	150	0
2	H	1635	0	1587	149	0
2	K	1635	0	1587	141	0
3	C	1610	0	1549	166	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1610	0	1549	158	0
3	I	1610	0	1549	135	0
3	L	1604	0	1543	122	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	3	0	0	0	0
5	I	2	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
All	All	20106	0	19345	1503	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 38.

The worst 5 of 1503 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:115:GLU:HB3	3:I:96:GLU:HB3	1.37	1.07
2:H:216:ASP:O	2:H:217:LYS:HG3	1.56	1.06
2:K:63:VAL:HA	2:K:66:ARG:NH2	1.71	1.02
2:K:63:VAL:HA	2:K:66:ARG:HH21	1.18	1.02
2:E:39:ALA:HB2	2:E:44:LEU:HB2	1.42	1.01

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	233/518 (45%)	191 (82%)	40 (17%)	2 (1%)	21	55
1	D	221/518 (43%)	183 (83%)	38 (17%)	0	100	100
1	G	221/518 (43%)	189 (86%)	30 (14%)	2 (1%)	21	55
1	J	221/518 (43%)	187 (85%)	32 (14%)	2 (1%)	21	55
2	B	214/222 (96%)	180 (84%)	29 (14%)	5 (2%)	8	26
2	E	214/222 (96%)	176 (82%)	35 (16%)	3 (1%)	14	42
2	H	214/222 (96%)	173 (81%)	35 (16%)	6 (3%)	6	21
2	K	214/222 (96%)	164 (77%)	47 (22%)	3 (1%)	14	42
3	C	208/211 (99%)	147 (71%)	50 (24%)	11 (5%)	2	7
3	F	208/211 (99%)	150 (72%)	47 (23%)	11 (5%)	2	7
3	I	208/211 (99%)	157 (76%)	41 (20%)	10 (5%)	3	9
3	L	205/211 (97%)	152 (74%)	44 (22%)	9 (4%)	3	10
All	All	2581/3804 (68%)	2049 (79%)	468 (18%)	64 (2%)	7	24

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	34	ASN
2	K	48	SER
3	L	5	GLN
3	L	45	GLN
3	L	79	ASN

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	193/451 (43%)	140 (72%)	53 (28%)	0	1
1	D	193/451 (43%)	149 (77%)	44 (23%)	1	3
1	G	193/451 (43%)	153 (79%)	40 (21%)	1	4
1	J	193/451 (43%)	141 (73%)	52 (27%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	180/184 (98%)	126 (70%)	54 (30%)	0	1
2	E	180/184 (98%)	131 (73%)	49 (27%)	0	1
2	H	180/184 (98%)	126 (70%)	54 (30%)	0	1
2	K	180/184 (98%)	136 (76%)	44 (24%)	1	2
3	C	182/183 (100%)	137 (75%)	45 (25%)	1	2
3	F	182/183 (100%)	134 (74%)	48 (26%)	0	1
3	I	182/183 (100%)	137 (75%)	45 (25%)	1	2
3	L	181/183 (99%)	131 (72%)	50 (28%)	0	1
All	All	2219/3272 (68%)	1641 (74%)	578 (26%)	0	1

5 of 578 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	95	LYS
1	G	174	LEU
3	L	29	SER
3	F	141	ASN
1	G	51	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	81	GLN
1	G	64	ASN
3	L	93	GLN
2	E	163	ASN
3	F	5	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	236/518 (45%)	-0.09	14 (5%)	26 16	6, 15, 85, 123	0
1	D	222/518 (42%)	-0.26	7 (3%)	51 39	8, 18, 41, 108	0
1	G	222/518 (42%)	-0.29	5 (2%)	64 52	7, 16, 47, 88	0
1	J	222/518 (42%)	-0.21	7 (3%)	51 39	6, 19, 50, 110	0
2	B	218/222 (98%)	-0.41	2 (0%)	85 79	8, 16, 30, 47	0
2	E	218/222 (98%)	-0.32	3 (1%)	78 69	7, 17, 37, 50	0
2	H	218/222 (98%)	-0.30	1 (0%)	91 88	6, 19, 37, 48	0
2	K	218/222 (98%)	-0.18	5 (2%)	64 52	10, 23, 41, 64	0
3	C	210/211 (99%)	-0.22	6 (2%)	55 43	10, 20, 47, 78	0
3	F	210/211 (99%)	-0.23	1 (0%)	91 88	8, 21, 41, 56	0
3	I	210/211 (99%)	-0.16	6 (2%)	55 43	11, 23, 49, 69	0
3	L	209/211 (99%)	-0.19	4 (1%)	70 59	11, 24, 44, 82	0
All	All	2613/3804 (68%)	-0.24	61 (2%)	64 52	6, 19, 44, 123	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	425	ASN	10.6
1	A	427	GLU	10.6
1	J	264	GLY	7.6
1	A	420	ASP	6.7
1	A	417	GLY	6.6

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	A	601	1/1	0.99	0.22	3.21	9,9,9,9	0
4	CA	J	601	1/1	1.00	0.19	1.06	3,3,3,3	0
4	CA	D	601	1/1	0.99	0.19	0.91	7,7,7,7	0
4	CA	G	601	1/1	0.99	0.15	-0.96	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.