Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:48 am BST

PDB ID	:	4WHY
Title	:	Structure of the Hepatitis C virus envelope glycoprotein E2 antigenic region 412-423 bound to the broadly neutralizing antibody 3/11, P21 crystal form
Authors	:	Krey, T.; Rey, F.A.
Deposited on	:	2014-09-24
Resolution	:	2.62 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see references ⓘ) were used in the production of this report:

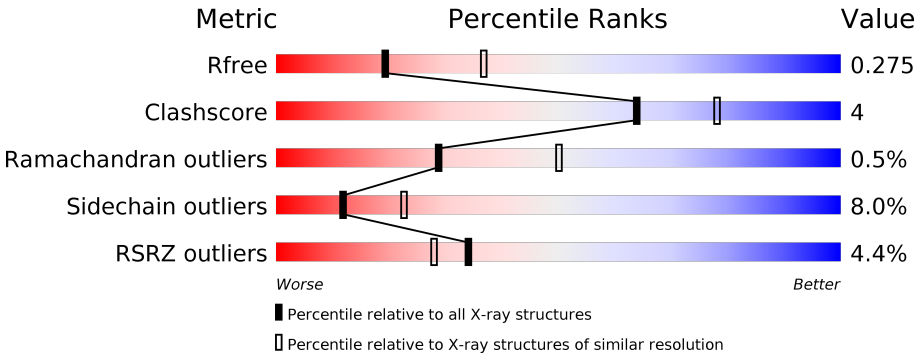
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 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	12	8% 75% 17% 8%
1	B	12	75% 8% 8% 8%
1	C	12	58% 33% 8%
1	D	12	50% 42% 8%
2	G	252	6% 67% 12% 21%
2	I	252	3% 70% 9% • 19%

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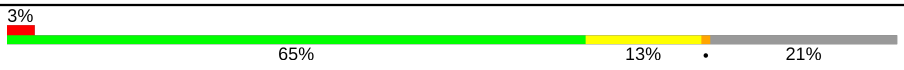
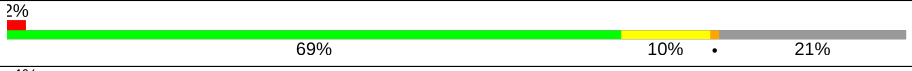
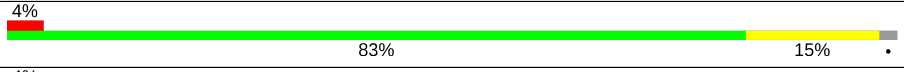
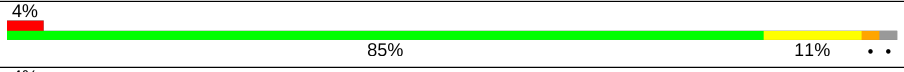
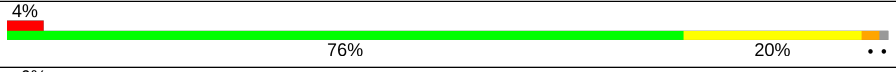
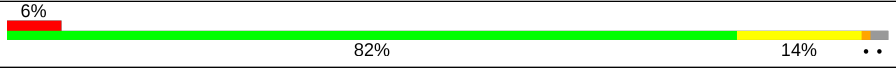
Mol	Chain	Length	Quality of chain
2	K	252	
2	M	252	
3	H	220	
3	J	220	
3	L	220	
3	N	220	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13178 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 epitope peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	11	Total	C	N	O	0	0	0
			89	56	17	16			
1	B	11	Total	C	N	O	0	0	0
			89	56	17	16			
1	C	11	Total	C	N	O	0	0	0
			89	56	17	16			
1	D	11	Total	C	N	O	0	0	0
			89	56	17	16			

- Molecule 2 is a protein called Heavy chain of Fab fragment derived from neutralizing antibody 3/11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	199	Total	C	N	O	S	0	0	0
			1516	959	255	295	7			
2	I	203	Total	C	N	O	S	0	0	0
			1542	976	259	300	7			
2	K	200	Total	C	N	O	S	0	0	0
			1525	967	256	295	7			
2	M	200	Total	C	N	O	S	0	0	0
			1523	964	256	296	7			

- Molecule 3 is a protein called Light chain of Fab fragment derived from neutralizing antibody 3/11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			
3	J	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			
3	L	218	Total	C	N	O	S	0	0	0
			1658	1026	277	347	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			

- Molecule 4 is water.

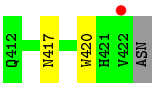
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	C	2	Total	O	0	0
			2	2		
4	G	15	Total	O	0	0
			15	15		
4	H	14	Total	O	0	0
			14	14		
4	I	26	Total	O	0	0
			26	26		
4	J	23	Total	O	0	0
			23	23		
4	K	14	Total	O	0	0
			14	14		
4	L	13	Total	O	0	0
			13	13		
4	M	23	Total	O	0	0
			23	23		
4	N	25	Total	O	0	0
			25	25		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

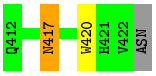
- Molecule 1: epitope peptide

Chain A:



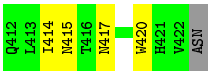
- Molecule 1: epitope peptide

Chain B:



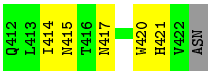
- Molecule 1: epitope peptide

Chain C:



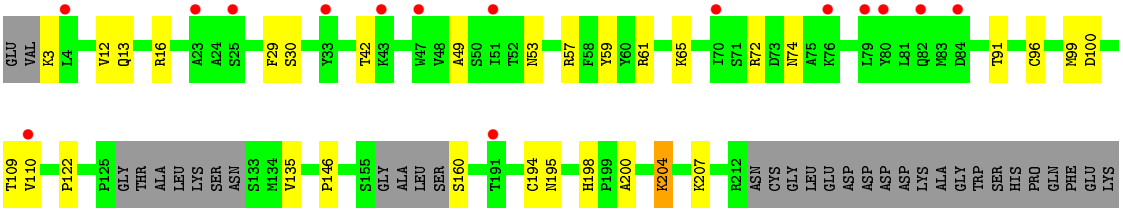
- Molecule 1: epitope peptide

Chain D:

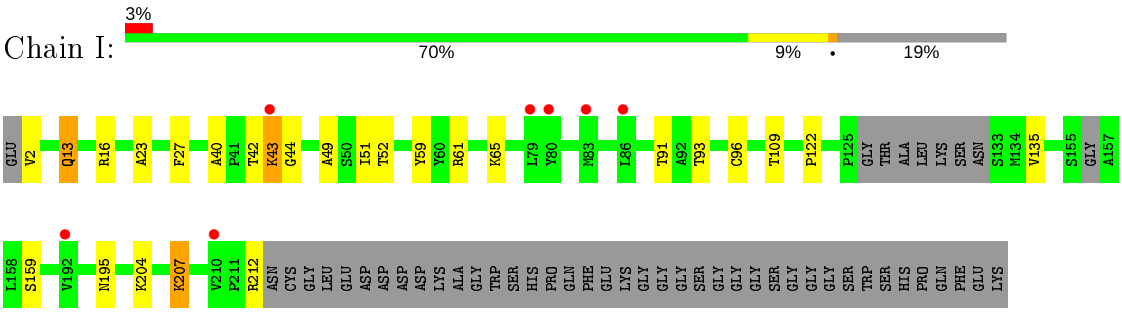


- Molecule 2: Heavy chain of Fab fragment derived from neutralizing antibody 3/11

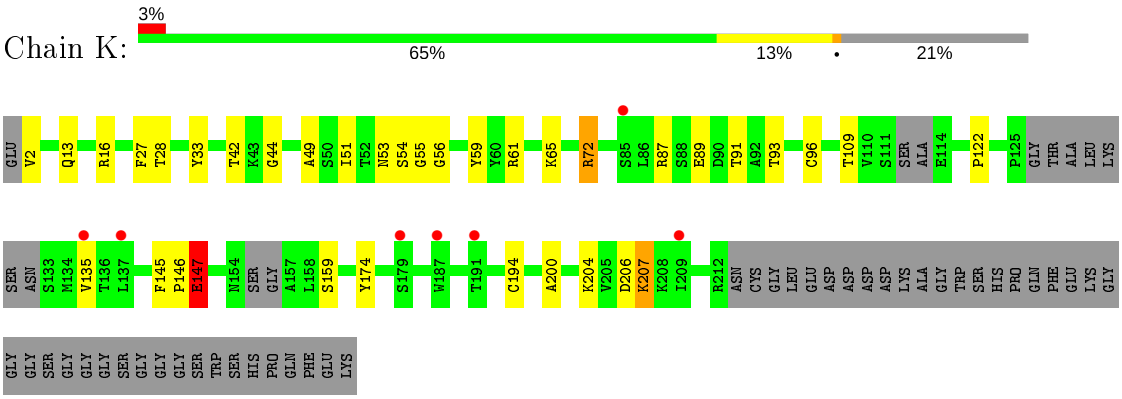
Chain G:



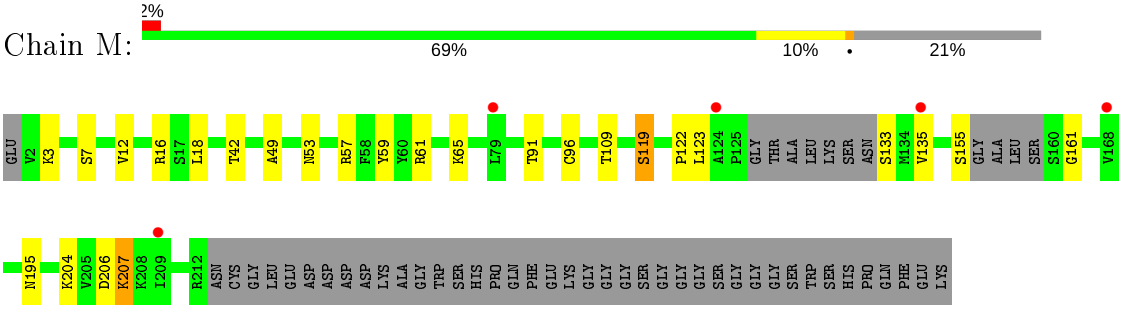
• Molecule 2: Heavy chain of Fab fragment derived from neutralizing antibody 3/11



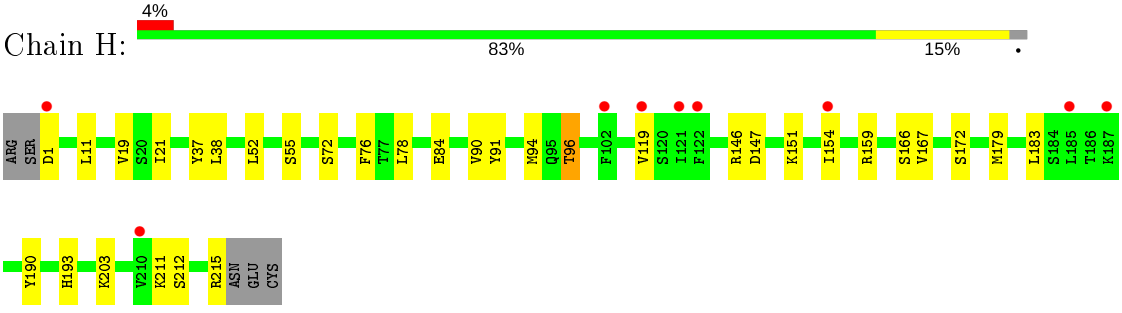
• Molecule 2: Heavy chain of Fab fragment derived from neutralizing antibody 3/11



• Molecule 2: Heavy chain of Fab fragment derived from neutralizing antibody 3/11

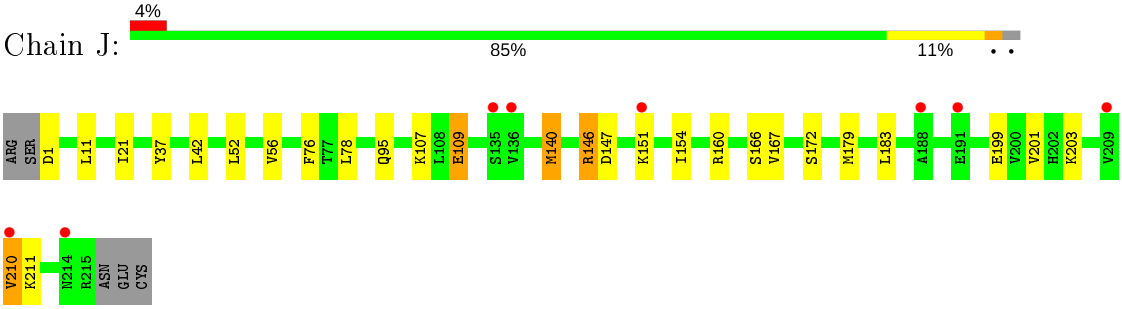


• Molecule 3: Light chain of Fab fragment derived from neutralizing antibody 3/11



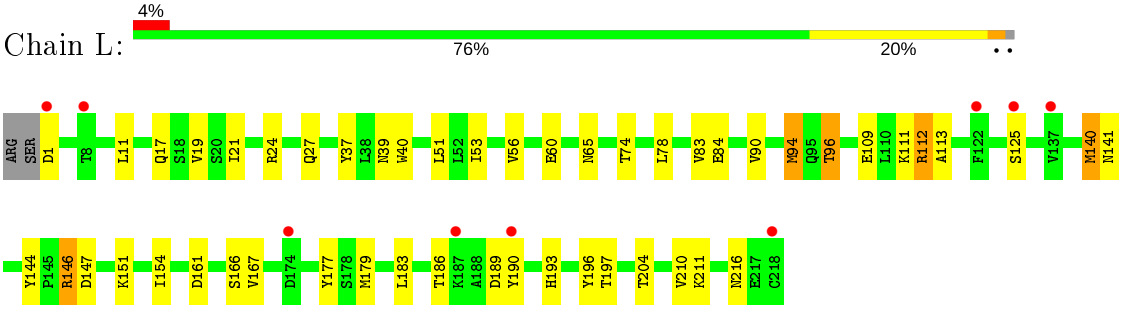
• Molecule 3: Light chain of Fab fragment derived from neutralizing antibody 3/11

Chain J:



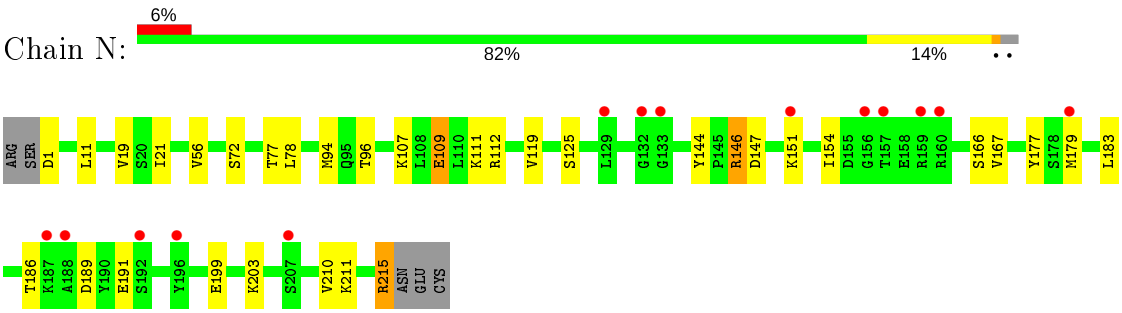
• Molecule 3: Light chain of Fab fragment derived from neutralizing antibody 3/11

Chain L:



• Molecule 3: Light chain of Fab fragment derived from neutralizing antibody 3/11

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.76Å 205.51Å 69.02Å 90.00° 103.18° 90.00°	Depositor
Resolution (Å)	47.97 – 2.62 47.97 – 2.62	Depositor EDS
% Data completeness (in resolution range)	96.6 (47.97-2.62) 97.0 (47.97-2.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.204 , 0.258 0.219 , 0.275	Depositor DCC
R_{free} test set	2541 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	53.3	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 67.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13178	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.47	0/91	0.68	0/124
1	B	0.50	0/91	0.70	0/124
1	C	0.52	0/91	0.68	0/124
1	D	0.44	0/91	0.67	0/124
2	G	0.46	0/1553	0.71	0/2118
2	I	0.51	0/1579	0.74	0/2154
2	K	0.47	0/1561	0.76	0/2128
2	M	0.51	0/1560	0.77	1/2128 (0.0%)
3	H	0.48	0/1664	0.76	0/2264
3	J	0.55	0/1664	0.77	0/2264
3	L	0.50	0/1688	0.78	0/2295
3	N	0.55	0/1664	0.78	0/2264
All	All	0.51	0/13297	0.76	1/18111 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	119	SER	N-CA-C	-5.42	96.38	111.00

There are no chirality outliers.

There are no planarity outliers.

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	89	0	82	0	0
1	B	89	0	82	1	0
1	C	89	0	82	3	0
1	D	89	0	82	4	0
2	G	1516	0	1486	12	0
2	I	1542	0	1516	12	0
2	K	1525	0	1500	21	0
2	M	1523	0	1495	10	0
3	H	1634	0	1593	14	0
3	J	1634	0	1593	11	0
3	L	1658	0	1610	25	0
3	N	1634	0	1593	12	0
4	A	1	0	0	1	0
4	C	2	0	0	0	0
4	G	15	0	0	0	0
4	H	14	0	0	0	0
4	I	26	0	0	1	0
4	J	23	0	0	1	0
4	K	14	0	0	0	0
4	L	13	0	0	1	0
4	M	23	0	0	0	0
4	N	25	0	0	1	0
All	All	13178	0	12714	108	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 4.

All (108) 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:L:51:LEU:HD23	3:L:60:GLU:HG3	1.59	0.83
3:L:40:TRP:HB2	3:L:53:ILE:HG13	1.60	0.81
2:K:146:PRO:O	2:K:147:GLU:HB2	1.82	0.77
2:I:13:GLN:HG3	2:I:16:ARG:HD3	1.74	0.69
3:J:140:MET:HG3	3:J:179:MET:HB3	1.77	0.66
3:L:140:MET:HG3	3:L:179:MET:HB3	1.78	0.65
3:H:154:ILE:HD12	3:H:159:ARG:HD3	1.79	0.65
3:L:154:ILE:HD11	3:L:183:LEU:HD21	1.80	0.64
2:K:51:ILE:HD13	2:K:72:ARG:HG2	1.81	0.61
3:L:112:ARG:HD3	3:L:113:ALA:O	1.99	0.61
2:K:54:SER:O	2:K:56:GLY:N	2.34	0.61
2:G:198:HIS:CE1	2:G:200:ALA:HB3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:154:ILE:HD11	3:H:183:LEU:HD21	1.85	0.59
3:H:193:HIS:O	3:H:215:ARG:NH2	2.37	0.58
3:J:154:ILE:HD11	3:J:183:LEU:HD21	1.86	0.57
2:M:122:PRO:HD3	2:M:207:LYS:HE2	1.86	0.57
3:L:40:TRP:HB2	3:L:53:ILE:CG1	2.33	0.57
2:K:2:VAL:HG22	2:K:27:PHE:HB3	1.87	0.56
3:L:109:GLU:HG3	3:L:177:TYR:OH	2.06	0.56
3:J:56:VAL:HG13	3:J:76:PHE:HD1	1.71	0.55
2:M:123:LEU:HA	4:N:319:HOH:O	2.07	0.54
2:K:122:PRO:HD3	2:K:207:LYS:HE2	1.90	0.53
3:N:154:ILE:HD11	3:N:183:LEU:HD21	1.89	0.53
1:D:415:ASN:H	3:H:96:THR:HG23	1.73	0.53
3:L:190:TYR:O	3:L:196:TYR:OH	2.26	0.53
2:G:122:PRO:HD3	2:G:207:LYS:HE2	1.90	0.53
2:K:51:ILE:HG23	2:K:72:ARG:HH21	1.74	0.53
2:I:122:PRO:HD3	2:I:207:LYS:HE2	1.92	0.52
3:L:37:TYR:HB3	3:L:96:THR:HG22	1.91	0.52
2:K:146:PRO:HD2	2:K:200:ALA:CB	2.40	0.52
1:D:415:ASN:H	3:H:96:THR:CG2	2.23	0.52
2:K:146:PRO:O	2:K:174:TYR:CE2	2.63	0.52
3:L:40:TRP:CD1	3:L:53:ILE:HD11	2.44	0.52
2:I:44:GLY:HA2	4:I:307:HOH:O	2.09	0.51
3:L:186:THR:HG23	3:L:189:ASP:H	1.76	0.51
3:J:199:GLU:HB3	3:J:210:VAL:HG12	1.91	0.51
3:N:199:GLU:HB3	3:N:210:VAL:HG12	1.93	0.51
2:I:91:THR:HG23	2:I:109:THR:HA	1.92	0.50
3:L:197:THR:HG23	3:L:210:VAL:HG13	1.93	0.50
2:G:13:GLN:HB2	2:G:16:ARG:HD3	1.93	0.49
3:N:186:THR:HG23	3:N:189:ASP:H	1.77	0.49
3:N:191:GLU:HA	3:N:215:ARG:HE	1.78	0.48
1:D:414:ILE:HA	3:H:96:THR:HG21	1.95	0.48
2:K:159:SER:HG	2:M:133:SER:N	2.12	0.48
2:K:44:GLY:HA2	4:L:303:HOH:O	2.14	0.48
2:M:12:VAL:HG21	2:M:18:LEU:HD13	1.96	0.48
3:H:37:TYR:HB3	3:H:96:THR:HG22	1.96	0.48
2:G:204:LYS:HB2	2:K:206:ASP:HB2	1.96	0.47
2:K:13:GLN:HB2	2:K:16:ARG:HD3	1.96	0.47
3:N:167:VAL:HG22	3:N:179:MET:HG3	1.97	0.47
2:I:40:ALA:HB3	2:I:43:LYS:HB2	1.97	0.47
2:G:12:VAL:HG23	2:G:110:VAL:HG22	1.97	0.46
3:J:42:LEU:HB2	3:J:52:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:109:GLU:HG3	3:N:177:TYR:OH	2.15	0.46
2:M:91:THR:HG23	2:M:109:THR:HA	1.98	0.46
3:N:119:VAL:O	3:N:211:LYS:HD2	2.16	0.45
2:G:91:THR:HG23	2:G:109:THR:HA	1.98	0.45
3:J:146:ARG:HD3	3:J:167:VAL:HG11	1.98	0.45
3:H:21:ILE:HD13	3:H:78:LEU:HD23	1.98	0.45
1:D:421:HIS:HB3	2:G:57:ARG:HB3	1.97	0.45
3:H:119:VAL:O	3:H:211:LYS:HD2	2.17	0.45
1:C:415:ASN:H	3:L:96:THR:CG2	2.30	0.45
1:B:417:ASN:HA	2:M:57:ARG:HH12	1.82	0.44
3:J:107:LYS:HE2	3:J:109:GLU:HB3	1.98	0.44
2:I:159:SER:HB3	2:K:28:THR:HG23	1.98	0.44
3:J:21:ILE:HD13	3:J:78:LEU:HD23	1.98	0.44
2:K:2:VAL:HG13	2:K:27:PHE:CD1	2.52	0.44
2:K:49:ALA:HA	2:K:59:TYR:O	2.17	0.44
2:K:91:THR:HG23	2:K:109:THR:HA	1.99	0.44
3:L:111:LYS:HA	3:L:144:TYR:OH	2.17	0.44
3:H:52:LEU:HD11	3:H:91:TYR:HE1	1.82	0.44
3:H:190:TYR:O	3:H:215:ARG:NH2	2.48	0.43
2:I:13:GLN:HG3	2:I:16:ARG:CD	2.45	0.43
3:J:201:VAL:HG13	4:J:322:HOH:O	2.18	0.43
2:K:122:PRO:HD2	3:L:125:SER:HB3	2.00	0.43
3:L:39:ASN:HB2	3:L:94:MET:HG3	2.00	0.43
2:K:145:PHE:CG	2:K:146:PRO:HA	2.54	0.43
3:L:146:ARG:HD3	3:L:167:VAL:HG11	2.00	0.43
2:M:122:PRO:HD2	3:N:125:SER:CB	2.49	0.43
4:A:501:HOH:O	3:J:37:TYR:HA	2.18	0.43
3:N:94:MET:CE	3:N:96:THR:HG23	2.49	0.43
3:N:146:ARG:HD3	3:N:167:VAL:HG11	1.99	0.43
2:I:49:ALA:HA	2:I:59:TYR:O	2.19	0.43
3:H:167:VAL:HG22	3:H:179:MET:HG3	2.00	0.42
2:G:29:PHE:CD2	2:G:74:ASN:HA	2.54	0.42
2:G:99:MET:SD	3:H:94:MET:HE1	2.58	0.42
2:M:12:VAL:HG13	2:M:16:ARG:HB2	2.01	0.42
3:L:167:VAL:HG22	3:L:179:MET:HG3	2.01	0.42
3:H:38:LEU:HG	3:H:76:PHE:CG	2.54	0.42
2:I:23:ALA:HB3	3:L:65:ASN:HB2	2.00	0.42
2:I:2:VAL:HG13	2:I:27:PHE:CD1	2.55	0.42
3:J:167:VAL:HG22	3:J:179:MET:HG3	2.01	0.42
2:K:122:PRO:HD2	3:L:125:SER:CB	2.50	0.42
3:L:17:GLN:O	3:L:83:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:ILE:HG21	2:K:33:TYR:CE1	2.55	0.42
3:N:111:LYS:HA	3:N:144:TYR:OH	2.20	0.42
2:M:49:ALA:HA	2:M:59:TYR:O	2.19	0.41
2:G:146:PRO:HD2	2:G:200:ALA:CB	2.50	0.41
2:I:51:ILE:HG12	2:I:52:THR:H	1.84	0.41
1:C:415:ASN:CB	3:L:96:THR:HG23	2.50	0.41
3:N:21:ILE:HD13	3:N:78:LEU:HD23	2.02	0.41
2:I:204:LYS:HB3	2:M:206:ASP:HB2	2.02	0.41
2:G:49:ALA:HA	2:G:59:TYR:O	2.21	0.41
3:L:21:ILE:HD13	3:L:78:LEU:HD23	2.02	0.41
2:G:30:SER:HB3	2:G:74:ASN:HB3	2.03	0.40
3:L:140:MET:CG	3:L:179:MET:HB3	2.48	0.40
3:L:189:ASP:O	3:L:193:HIS:CD2	2.74	0.40
2:K:146:PRO:O	2:K:147:GLU:CB	2.60	0.40

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	9/12 (75%)	9 (100%)	0	0	100	100
1	B	9/12 (75%)	9 (100%)	0	0	100	100
1	C	9/12 (75%)	9 (100%)	0	0	100	100
1	D	9/12 (75%)	9 (100%)	0	0	100	100
2	G	193/252 (77%)	185 (96%)	7 (4%)	1 (0%)	29	50
2	I	197/252 (78%)	190 (96%)	7 (4%)	0	100	100
2	K	192/252 (76%)	185 (96%)	4 (2%)	3 (2%)	9	18
2	M	194/252 (77%)	186 (96%)	6 (3%)	2 (1%)	15	30
3	H	213/220 (97%)	202 (95%)	10 (5%)	1 (0%)	29	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	213/220 (97%)	205 (96%)	8 (4%)	0	100	100
3	L	216/220 (98%)	207 (96%)	8 (4%)	1 (0%)	29	50
3	N	213/220 (97%)	204 (96%)	8 (4%)	1 (0%)	29	50
All	All	1667/1936 (86%)	1600 (96%)	58 (4%)	9 (0%)	29	50

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	55	GLY
2	M	53	ASN
2	G	53	ASN
2	K	147	GLU
3	L	204	THR
2	M	161	GLY
3	N	72	SER
3	H	72	SER
2	K	53	ASN

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	10/11 (91%)	8 (80%)	2 (20%)	1	2
1	B	10/11 (91%)	8 (80%)	2 (20%)	1	2
1	C	10/11 (91%)	8 (80%)	2 (20%)	1	2
1	D	10/11 (91%)	8 (80%)	2 (20%)	1	2
2	G	171/208 (82%)	159 (93%)	12 (7%)	15	29
2	I	174/208 (84%)	163 (94%)	11 (6%)	18	35
2	K	172/208 (83%)	159 (92%)	13 (8%)	13	25
2	M	172/208 (83%)	160 (93%)	12 (7%)	15	29
3	H	191/196 (97%)	177 (93%)	14 (7%)	14	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	J	191/196 (97%)	177 (93%)	14 (7%)	14 27
3	L	194/196 (99%)	173 (89%)	21 (11%)	6 11
3	N	191/196 (97%)	177 (93%)	14 (7%)	14 27
All	All	1496/1660 (90%)	1377 (92%)	119 (8%)	12 23

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	417	ASN
1	A	420	TRP
1	B	417	ASN
1	B	420	TRP
1	C	417	ASN
1	C	420	TRP
1	D	417	ASN
1	D	420	TRP
2	G	3	LYS
2	G	42	THR
2	G	61	ARG
2	G	65	LYS
2	G	72	ARG
2	G	96	CYS
2	G	100	ASP
2	G	135	VAL
2	G	160	SER
2	G	194	CYS
2	G	195	ASN
2	G	204	LYS
3	H	1	ASP
3	H	11	LEU
3	H	19	VAL
3	H	55	SER
3	H	84	GLU
3	H	90	VAL
3	H	96	THR
3	H	146	ARG
3	H	147	ASP
3	H	151	LYS
3	H	166	SER
3	H	172	SER
3	H	203	LYS

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Mol	Chain	Res	Type
3	H	212	SER
2	I	13	GLN
2	I	42	THR
2	I	43	LYS
2	I	61	ARG
2	I	65	LYS
2	I	93	THR
2	I	96	CYS
2	I	135	VAL
2	I	195	ASN
2	I	207	LYS
2	I	212	ARG
3	J	1	ASP
3	J	11	LEU
3	J	95	GLN
3	J	109	GLU
3	J	140	MET
3	J	146	ARG
3	J	147	ASP
3	J	151	LYS
3	J	160	ARG
3	J	166	SER
3	J	172	SER
3	J	203	LYS
3	J	210	VAL
3	J	211	LYS
2	K	42	THR
2	K	61	ARG
2	K	65	LYS
2	K	72	ARG
2	K	87	ARG
2	K	89	GLU
2	K	93	THR
2	K	96	CYS
2	K	135	VAL
2	K	147	GLU
2	K	194	CYS
2	K	204	LYS
2	K	207	LYS
3	L	1	ASP
3	L	11	LEU
3	L	19	VAL

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Mol	Chain	Res	Type
3	L	24	ARG
3	L	27	GLN
3	L	56	VAL
3	L	74	THR
3	L	84	GLU
3	L	90	VAL
3	L	94	MET
3	L	96	THR
3	L	112	ARG
3	L	140	MET
3	L	141	ASN
3	L	146	ARG
3	L	147	ASP
3	L	151	LYS
3	L	161	ASP
3	L	166	SER
3	L	211	LYS
3	L	216	ASN
2	M	3	LYS
2	M	7	SER
2	M	42	THR
2	M	61	ARG
2	M	65	LYS
2	M	96	CYS
2	M	119	SER
2	M	135	VAL
2	M	155	SER
2	M	195	ASN
2	M	204	LYS
2	M	207	LYS
3	N	1	ASP
3	N	11	LEU
3	N	19	VAL
3	N	56	VAL
3	N	77	THR
3	N	107	LYS
3	N	109	GLU
3	N	112	ARG
3	N	146	ARG
3	N	147	ASP
3	N	151	LYS
3	N	166	SER

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Mol	Chain	Res	Type
3	N	203	LYS
3	N	215	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	412	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	11/12 (91%)	0.43	1 (9%) 9 6	40, 52, 69, 71	0
1	B	11/12 (91%)	0.59	0 100 100	34, 49, 70, 73	0
1	C	11/12 (91%)	-0.10	0 100 100	49, 58, 67, 67	0
1	D	11/12 (91%)	0.47	0 100 100	56, 61, 69, 75	0
2	G	199/252 (78%)	0.45	15 (7%) 14 10	41, 67, 85, 106	0
2	I	203/252 (80%)	0.23	7 (3%) 45 38	32, 56, 76, 90	0
2	K	200/252 (79%)	0.22	7 (3%) 44 37	38, 58, 76, 88	0
2	M	200/252 (79%)	0.06	5 (2%) 57 51	32, 50, 72, 94	0
3	H	215/220 (97%)	0.32	9 (4%) 36 30	40, 66, 87, 106	0
3	J	215/220 (97%)	0.20	8 (3%) 41 35	27, 55, 83, 97	0
3	L	218/220 (99%)	0.30	9 (4%) 37 31	41, 61, 82, 105	0
3	N	215/220 (97%)	0.30	14 (6%) 18 14	31, 51, 78, 102	0
All	All	1709/1936 (88%)	0.26	75 (4%) 34 28	27, 58, 82, 106	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	218	CYS	6.8
3	N	156	GLY	5.2
3	L	8	THR	4.8
3	L	1	ASP	4.7
3	J	188	ALA	4.2
3	H	1	ASP	4.1
3	N	132	GLY	3.9
3	H	119	VAL	3.6
2	I	79	LEU	3.5
2	I	43	LYS	3.4
2	K	191	THR	3.4

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Mol	Chain	Res	Type	RSRZ
2	K	187	TRP	3.3
3	L	190	TYR	3.3
2	K	137	LEU	3.3
3	L	137	VAL	3.1
2	G	79	LEU	3.1
3	N	187	LYS	3.0
3	N	207	SER	3.0
3	H	185	LEU	3.0
2	G	23	ALA	2.9
2	G	51	ILE	2.9
2	G	47	TRP	2.9
3	J	214	ASN	2.9
2	G	70	ILE	2.8
2	G	84	ASP	2.8
2	K	135	VAL	2.7
2	K	209	ILE	2.7
2	G	191	THR	2.7
3	N	179	MET	2.7
2	K	85	SER	2.7
3	H	121	ILE	2.7
2	G	4	LEU	2.6
3	N	160	ARG	2.6
3	N	133	GLY	2.6
3	N	157	THR	2.6
3	L	122	PHE	2.6
3	J	135	SER	2.6
3	N	192	SER	2.6
2	M	209	ILE	2.6
2	I	80	TYR	2.6
2	M	124	ALA	2.6
3	N	129	LEU	2.6
2	G	33	TYR	2.5
2	M	135	VAL	2.5
3	J	191	GLU	2.4
3	N	196	TYR	2.4
3	L	125	SER	2.4
3	H	122	PHE	2.4
3	J	210	VAL	2.3
3	H	154	ILE	2.3
2	I	210	VAL	2.3
3	N	159	ARG	2.3
3	H	210	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	N	188	ALA	2.3
3	L	187	LYS	2.2
2	I	192	VAL	2.2
2	K	179	SER	2.2
3	J	136	VAL	2.2
3	L	174	ASP	2.2
2	G	76	LYS	2.1
2	M	168	VAL	2.1
3	J	209	VAL	2.1
2	M	79	LEU	2.1
2	G	80	TYR	2.1
2	G	110	VAL	2.1
2	G	25	SER	2.1
2	G	82	GLN	2.1
2	I	86	LEU	2.1
3	J	151	LYS	2.1
1	A	422	VAL	2.0
3	H	187	LYS	2.0
3	N	151	LYS	2.0
3	H	102	PHE	2.0
2	I	83	MET	2.0
2	G	43	LYS	2.0

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 carbohydrates 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.