



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:15 AM UTC

PDB ID : 4WHY / pdb_00004why
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 types of validation reports are described at

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

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

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

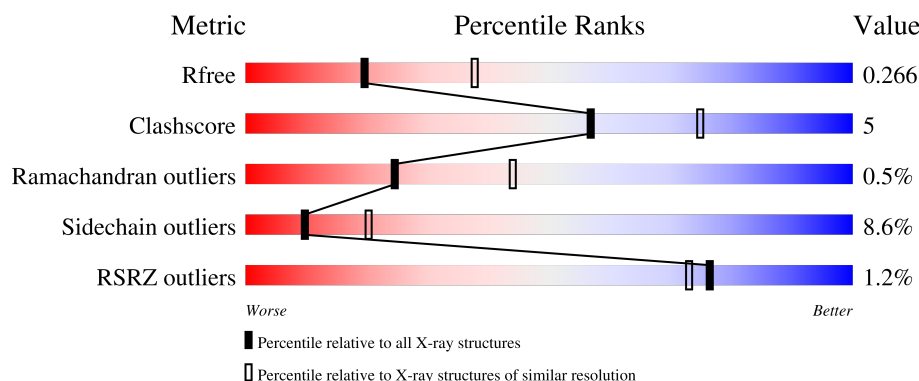
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (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 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	12	
1	B	12	
1	C	12	
1	D	12	
2	G	252	

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Mol	Chain	Length	Quality of chain
2	I	252	67%12%19%
2	K	252	2% 63%15%21%
2	M	252	65%12%21%
3	H	220	77%20%..
3	J	220	81%15%..
3	L	220	% 72%24%..
3	N	220	% 79%16%..

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			

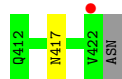
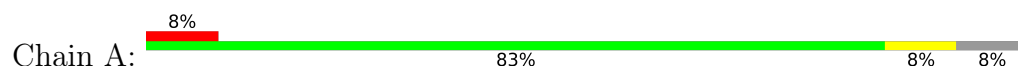
- Molecule 4 is water.

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		

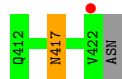
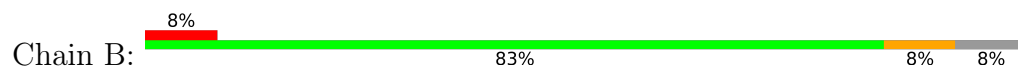
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: epitope peptide



- Molecule 1: epitope peptide



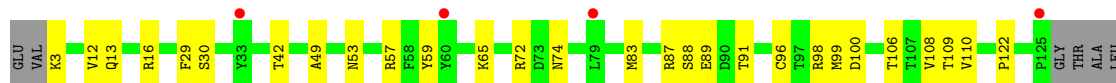
- Molecule 1: epitope peptide

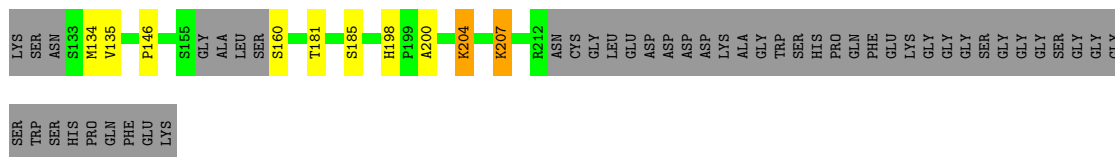


- Molecule 1: epitope peptide

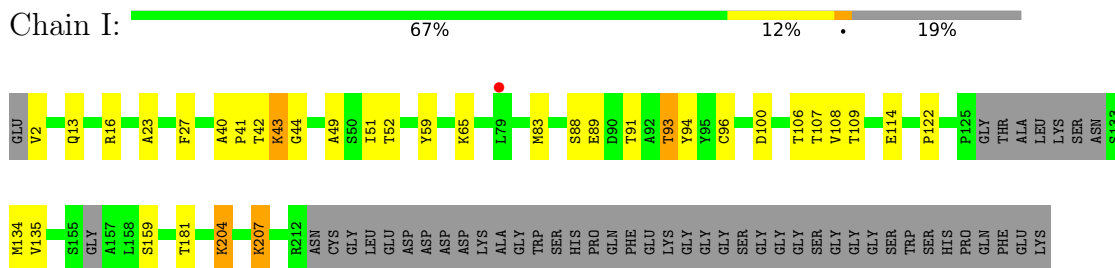


- Molecule 2: Heavy chain of Fab fragment derived from neutralizing antibody 3/11

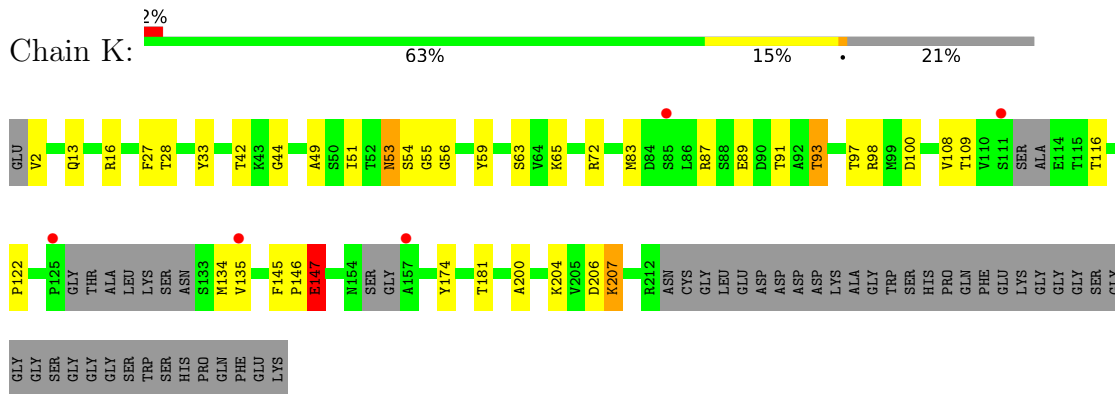




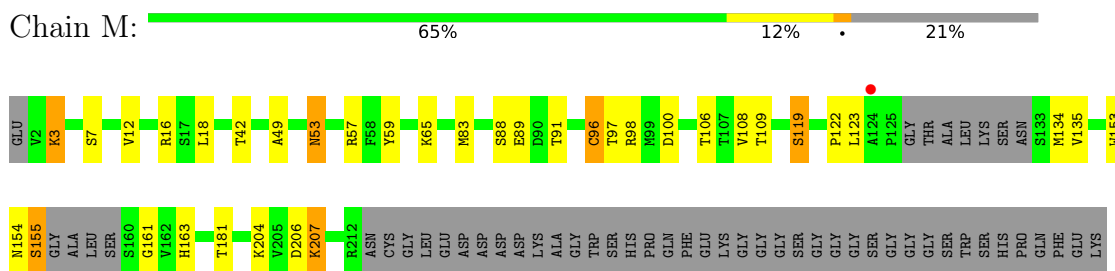
- Molecule 2: Heavy chain of Fab fragment derived from neutralizing antibody 3/11



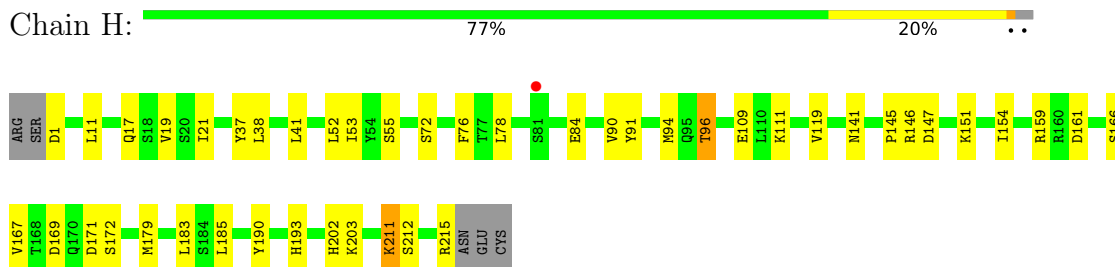
- Molecule 2: Heavy chain of Fab fragment derived from neutralizing antibody 3/11



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

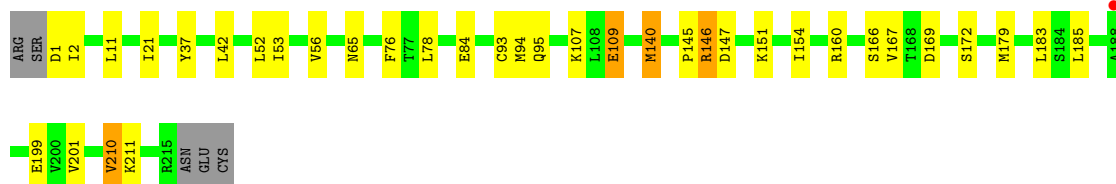


- Molecule 3: Light chain of Fab fragment derived from neutralizing antibody 3/11



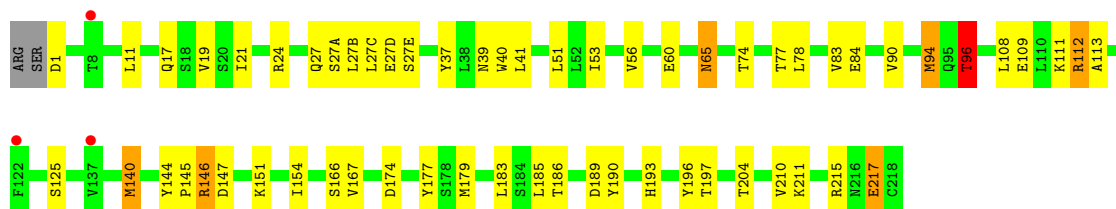
- Molecule 3: Light chain of Fab fragment derived from neutralizing antibody 3/11

Chain J:  81% 15% ..



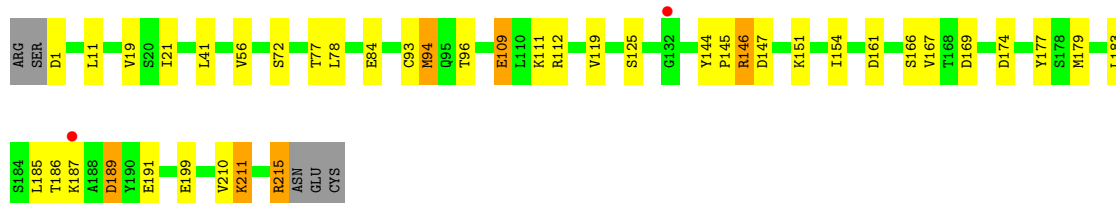
- Molecule 3: Light chain of Fab fragment derived from neutralizing antibody 3/11

Chain L:  72% 24% ..



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

Chain N:  79% 16% ..



4 Data and refinement statistics

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) 96.9 (47.97-2.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.204 , 0.258 (Not available) , 0.266	Depositor DCC
R_{free} test set	2541 reflections (4.83%)	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)	0.34 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.78	0/91	1.32	0/124
1	B	0.81	0/91	1.31	0/124
1	C	0.84	0/91	1.27	0/124
1	D	0.76	0/91	1.32	0/124
2	G	0.78	0/1553	1.21	6/2118 (0.3%)
2	I	0.83	0/1579	1.25	9/2154 (0.4%)
2	K	0.79	0/1561	1.24	6/2128 (0.3%)
2	M	0.84	0/1560	1.29	15/2128 (0.7%)
3	H	0.83	0/1664	1.29	9/2264 (0.4%)
3	J	0.92	1/1664 (0.1%)	1.26	4/2264 (0.2%)
3	L	0.83	0/1688	1.29	10/2295 (0.4%)
3	N	0.91	1/1664 (0.1%)	1.26	7/2264 (0.3%)
All	All	0.84	2/13297 (0.0%)	1.26	66/18111 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	94	MET	SD-CE	-6.75	1.62	1.79
3	N	94	MET	SD-CE	-5.98	1.64	1.79

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	119	SER	N-CA-C	-7.68	96.38	108.90
3	L	65	ASN	CA-CB-CG	7.10	119.70	112.60
2	M	3	LYS	N-CA-C	6.91	120.75	110.52
2	K	93	THR	CB-CA-C	6.87	121.32	110.19
3	H	141	ASN	N-CA-C	6.71	120.39	109.59
3	N	169	ASP	CA-CB-CG	6.19	118.79	112.60
2	I	41	PRO	CA-C-N	6.15	129.66	120.31
2	I	41	PRO	C-N-CA	6.15	129.66	120.31
3	H	145	PRO	CA-C-N	6.13	128.78	120.38
3	H	145	PRO	C-N-CA	6.13	128.78	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	202	HIS	CA-C-N	6.10	128.78	120.54
3	H	202	HIS	C-N-CA	6.10	128.78	120.54
2	I	93	THR	CB-CA-C	6.08	119.78	109.75
2	M	88	SER	CA-C-N	6.05	129.00	120.28
2	M	88	SER	C-N-CA	6.05	129.00	120.28
3	L	108	LEU	CA-C-N	5.88	132.64	122.64
3	L	108	LEU	C-N-CA	5.88	132.64	122.64
2	I	94	TYR	N-CA-C	5.87	118.29	108.73
2	M	53	ASN	CA-CB-CG	5.87	118.47	112.60
3	J	169	ASP	CA-CB-CG	5.86	118.46	112.60
3	J	93	CYS	N-CA-C	-5.76	102.00	110.52
3	H	169	ASP	CA-CB-CG	5.75	118.35	112.60
2	M	106	THR	CB-CA-C	5.70	119.63	110.16
2	K	98	ARG	N-CA-C	-5.66	105.06	112.41
2	K	97	THR	CA-C-N	5.64	131.35	122.49
2	K	97	THR	C-N-CA	5.64	131.35	122.49
3	L	145	PRO	CA-C-N	5.62	128.09	120.38
3	L	145	PRO	C-N-CA	5.62	128.09	120.38
2	K	53	ASN	CA-CB-CG	5.61	118.21	112.60
3	L	215	ARG	N-CA-C	5.60	119.86	113.19
2	M	97	THR	CA-C-N	5.59	130.96	122.08
2	M	97	THR	C-N-CA	5.59	130.96	122.08
3	N	174	ASP	N-CA-C	5.58	120.20	113.17
2	M	154	ASN	CA-C-N	5.50	131.60	121.70
2	M	154	ASN	C-N-CA	5.50	131.60	121.70
3	N	189	ASP	CA-CB-CG	5.46	118.06	112.60
2	I	107	THR	CB-CA-C	5.44	118.72	109.80
2	I	106	THR	CB-CA-C	5.38	118.10	110.24
2	M	98	ARG	N-CA-C	-5.38	105.01	113.02
3	N	93	CYS	N-CA-C	-5.38	102.56	110.52
2	I	88	SER	CA-C-N	5.38	128.23	120.38
2	I	88	SER	C-N-CA	5.38	128.23	120.38
3	H	161	ASP	CA-CB-CG	5.37	117.97	112.60
2	G	88	SER	CA-C-N	5.32	128.14	120.38
2	G	88	SER	C-N-CA	5.32	128.14	120.38
2	G	98	ARG	N-CA-C	-5.29	105.48	112.94
3	L	174	ASP	CA-CB-CG	5.27	117.87	112.60
3	L	217	GLU	N-CA-C	5.25	118.28	110.14
2	M	3	LYS	CA-C-N	5.24	130.14	121.86
2	M	3	LYS	C-N-CA	5.24	130.14	121.86
2	K	100	ASP	CA-CB-CG	5.22	117.82	112.60
2	M	96	CYS	N-CA-C	-5.19	100.27	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	96	THR	CB-CA-C	5.17	118.12	109.80
2	G	185	SER	CA-C-N	5.14	127.94	120.79
2	G	185	SER	C-N-CA	5.14	127.94	120.79
2	I	100	ASP	CA-CB-CG	5.09	117.69	112.60
3	H	171	ASP	CA-C-N	5.06	127.47	120.29
3	H	171	ASP	C-N-CA	5.06	127.47	120.29
3	J	145	PRO	CA-C-N	5.06	127.31	120.38
3	J	145	PRO	C-N-CA	5.06	127.31	120.38
3	N	145	PRO	CA-C-N	5.03	127.27	120.38
3	N	145	PRO	C-N-CA	5.03	127.27	120.38
3	N	161	ASP	N-CA-C	5.02	117.91	110.48
2	G	106	THR	CB-CA-C	5.02	117.87	110.14
3	L	77	THR	N-CA-C	5.01	116.58	108.26
2	M	100	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

There are no planarity outliers.

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	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	14	0
2	I	1542	0	1516	15	0
2	K	1525	0	1500	22	0
2	M	1523	0	1495	12	0
3	H	1634	0	1593	15	0
3	J	1634	0	1593	11	0
3	L	1658	0	1610	25	0
3	N	1634	0	1593	14	0
4	A	1	0	0	1	0
4	C	2	0	0	0	0
4	G	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	119	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 5.

All (119) 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:G:99:MET:SD	3:H:94:MET:HE1	2.28	0.73
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
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
2:M:134:MET:HE3	2:M:181:THR:HG22	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:G:134:MET:HE3	2:G:181:THR:HG22	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:K:134:MET:HE3	2:K:181:THR:HG22	1.90	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
2:I:134:MET:HE3	2:I:181:THR:HG22	1.93	0.49
3:N:186:THR:HG23	3:N:189:ASP:H	1.77	0.49
2:I:83:MET:HE1	2:I:108:VAL:HG21	1.95	0.48
2:I:114:GLU:OE1	3:N:187:LYS:NZ	2.40	0.48
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: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:83:MET:HE1	2:G:108:VAL:HG21	1.95	0.47
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
2:M:83:MET:HE1	2:M:108:VAL:HG21	1.97	0.47
2:K:83:MET:HE1	2:K:108:VAL:HG21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:159:SER:HB3	2:K:28:THR:HG23	1.98	0.44
3:J:107:LYS:HE2	3:J:109:GLU:HB3	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: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:2:VAL:HG13	2:I:27:PHE:CD1	2.55	0.42
2:I:23:ALA:HB3	3:L:65:ASN:HB2	2.00	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
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
2:M:153:TRP:C	2:M:155:SER:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:H:94:MET:HE3	3:H:94:MET:HB3	1.85	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
3:N:94:MET:HE2	3:N:96:THR:HG23	2.03	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%)	24	44
2	I	197/252 (78%)	190 (96%)	7 (4%)	0	100	100
2	K	192/252 (76%)	185 (96%)	4 (2%)	3 (2%)	7	15
2	M	194/252 (77%)	186 (96%)	6 (3%)	2 (1%)	12	26
3	H	213/220 (97%)	202 (95%)	10 (5%)	1 (0%)	24	44
3	J	213/220 (97%)	205 (96%)	8 (4%)	0	100	100
3	L	216/220 (98%)	207 (96%)	8 (4%)	1 (0%)	24	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	N	213/220 (97%)	204 (96%)	8 (4%)	1 (0%)	24	44
All	All	1667/1936 (86%)	1600 (96%)	58 (4%)	9 (0%)	24	44

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 ⓘ

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%)	9 (90%)	1 (10%)	7	15
1	B	10/11 (91%)	9 (90%)	1 (10%)	7	15
1	C	10/11 (91%)	9 (90%)	1 (10%)	7	15
1	D	10/11 (91%)	9 (90%)	1 (10%)	7	15
2	G	171/208 (82%)	159 (93%)	12 (7%)	14	29
2	I	174/208 (84%)	165 (95%)	9 (5%)	21	42
2	K	172/208 (83%)	161 (94%)	11 (6%)	16	33
2	M	172/208 (83%)	160 (93%)	12 (7%)	14	29
3	H	191/196 (97%)	170 (89%)	21 (11%)	6	12
3	J	191/196 (97%)	173 (91%)	18 (9%)	8	17
3	L	194/196 (99%)	168 (87%)	26 (13%)	4	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	191/196 (97%)	175 (92%)	16 (8%)	10	21
All	All	1496/1660 (90%)	1367 (91%)	129 (9%)	10	20

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	417	ASN
1	B	417	ASN
1	C	417	ASN
1	D	417	ASN
2	G	3	LYS
2	G	42	THR
2	G	65	LYS
2	G	72	ARG
2	G	87	ARG
2	G	89	GLU
2	G	96	CYS
2	G	100	ASP
2	G	135	VAL
2	G	160	SER
2	G	204	LYS
2	G	207	LYS
3	H	1	ASP
3	H	11	LEU
3	H	17	GLN
3	H	19	VAL
3	H	41	LEU
3	H	53	ILE
3	H	55	SER
3	H	84	GLU
3	H	90	VAL
3	H	96	THR
3	H	109	GLU
3	H	111	LYS
3	H	146	ARG
3	H	147	ASP
3	H	151	LYS
3	H	166	SER
3	H	172	SER
3	H	185	LEU
3	H	203	LYS
3	H	211	LYS

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Mol	Chain	Res	Type
3	H	212	SER
2	I	42	THR
2	I	43	LYS
2	I	65	LYS
2	I	89	GLU
2	I	93	THR
2	I	96	CYS
2	I	135	VAL
2	I	204	LYS
2	I	207	LYS
3	J	1	ASP
3	J	2	ILE
3	J	11	LEU
3	J	53	ILE
3	J	65	ASN
3	J	84	GLU
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	185	LEU
3	J	210	VAL
3	J	211	LYS
2	K	42	THR
2	K	63	SER
2	K	65	LYS
2	K	87	ARG
2	K	89	GLU
2	K	93	THR
2	K	116	THR
2	K	135	VAL
2	K	147	GLU
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	27(A)	SER
3	L	27(B)	LEU
3	L	27(C)	LEU
3	L	27(D)	GLU
3	L	27(E)	SER
3	L	41	LEU
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	146	ARG
3	L	147	ASP
3	L	151	LYS
3	L	166	SER
3	L	185	LEU
3	L	211	LYS
3	L	217	GLU
2	M	3	LYS
2	M	7	SER
2	M	42	THR
2	M	65	LYS
2	M	89	GLU
2	M	96	CYS
2	M	119	SER
2	M	135	VAL
2	M	155	SER
2	M	163	HIS
2	M	204	LYS
2	M	207	LYS
3	N	1	ASP
3	N	11	LEU
3	N	19	VAL
3	N	41	LEU
3	N	56	VAL
3	N	77	THR
3	N	84	GLU

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Mol	Chain	Res	Type
3	N	109	GLU
3	N	112	ARG
3	N	146	ARG
3	N	147	ASP
3	N	151	LYS
3	N	166	SER
3	N	185	LEU
3	N	211	LYS
3	N	215	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	412	GLN
2	G	13	GLN
2	G	53	ASN
2	G	170	GLN
3	H	47	GLN
2	I	5	GLN
3	J	47	GLN
3	J	50	GLN
2	K	13	GLN
2	K	82	GLN
3	L	194	ASN
3	N	47	GLN
3	N	214	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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, 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	11/12 (91%)	0.19	1 (9%) 15 11	40, 52, 69, 71	0
1	B	11/12 (91%)	0.26	1 (9%) 15 11	34, 49, 70, 73	0
1	C	11/12 (91%)	-0.09	0 100 100	49, 58, 67, 67	0
1	D	11/12 (91%)	0.69	1 (9%) 15 11	56, 61, 69, 75	0
2	G	199/252 (78%)	0.38	4 (2%) 65 60	41, 67, 85, 106	0
2	I	203/252 (80%)	0.20	1 (0%) 87 85	32, 56, 76, 90	0
2	K	200/252 (79%)	0.15	5 (2%) 58 53	38, 58, 76, 88	0
2	M	200/252 (79%)	0.07	1 (0%) 87 85	32, 50, 72, 94	0
3	H	215/220 (97%)	0.31	1 (0%) 87 85	40, 66, 87, 106	0
3	J	215/220 (97%)	0.17	1 (0%) 87 85	27, 55, 83, 97	0
3	L	218/220 (99%)	0.24	3 (1%) 73 70	41, 61, 82, 105	0
3	N	215/220 (97%)	0.09	2 (0%) 81 78	31, 51, 78, 102	0
All	All	1709/1936 (88%)	0.20	21 (1%) 76 73	27, 58, 82, 106	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	188	ALA	3.1
2	K	85	SER	3.1
1	A	422	VAL	3.1
3	L	8	THR	3.1
3	N	132	GLY	2.9
1	D	422	VAL	2.9
2	K	125	PRO	2.8
3	L	137	VAL	2.7
2	K	111	SER	2.5
1	B	422	VAL	2.5
2	M	124	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	G	79	LEU	2.4
2	K	135	VAL	2.2
2	I	79	LEU	2.2
2	G	33	TYR	2.2
3	L	122	PHE	2.2
2	G	125	PRO	2.1
3	H	81	SER	2.1
2	G	60	TYR	2.1
2	K	157	ALA	2.0
3	N	187	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.