



# wwPDB X-ray Structure Validation Summary Report

Jun 23, 2024 – 03:00 AM EDT

PDB ID : 4WHT  
Title : Structure of the Hepatitis C virus envelope glycoprotein E2 antigenic region 412-423 bound to the broadly neutralizing antibody 3/11, P1 crystal form  
Authors : Krey, T.; Rey, F.A.  
Deposited on : 2014-09-23  
Resolution : 2.22 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](mailto: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>.

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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 : 2.37.1  
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

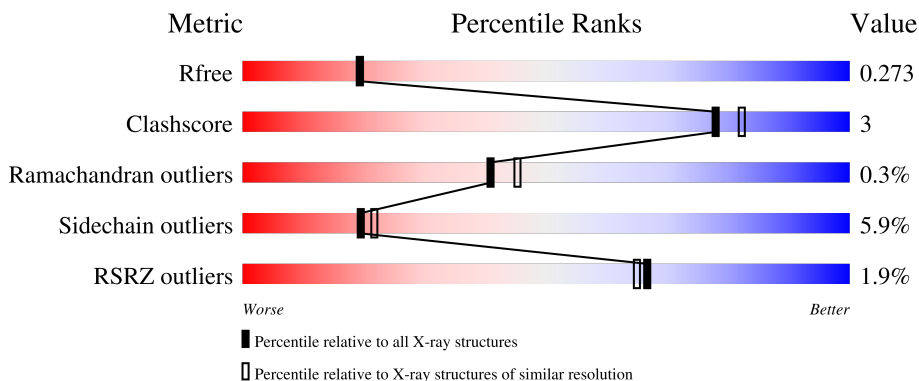
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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  $\geq 3$ , 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	252	73% 9% 18%
1	C	252	69% 12% 19%
1	E	252	73% 9% 17%
1	G	252	73% 9% 18%
1	I	252	71% 11% 19%

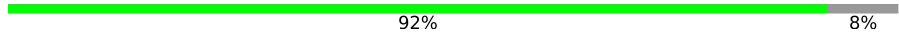

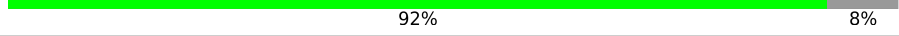
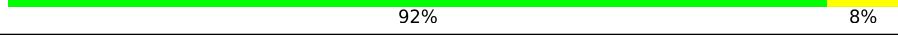
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Mol	Chain	Length	Quality of chain
1	K	252	
1	M	252	
1	O	252	
1	Q	252	
1	S	252	
1	U	252	
1	X	252	
2	B	220	
2	D	220	
2	F	220	
2	H	220	
2	J	220	
2	L	220	
2	N	220	
2	P	220	
2	R	220	
2	T	220	
2	V	220	
2	Y	220	
3	a	12	
3	c	12	
3	e	12	
3	g	12	
3	i	12	
3	k	12	

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Mol	Chain	Length	Quality of chain
3	m	12	 83% 17%
3	o	12	 92% 8%
3	q	12	 83% 17%
3	s	12	 92% 8%
3	u	12	 83% 17%
3	x	12	 92% 8%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 40099 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 Heavy chain of the Fab fragment derived from neutralizing antibody 3/11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	207	1565	988	264	306	7	0	0	0
1	C	205	1554	982	262	303	7	0	0	0
1	E	208	1570	991	265	307	7	0	0	0
1	G	207	1567	989	264	307	7	0	0	0
1	I	205	1550	980	261	302	7	0	0	0
1	K	204	1546	978	260	301	7	0	0	0
1	M	204	1546	978	260	301	7	0	0	0
1	O	205	1550	980	261	302	7	0	0	0
1	Q	206	1557	984	262	304	7	0	0	0
1	S	204	1546	978	260	301	7	0	0	0
1	U	205	1554	982	262	303	7	0	0	0
1	X	199	1495	945	250	293	7	0	0	0

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			
2	D	216	Total	C	N	O	S	0	0	0
			1642	1018	275	342	7			
2	F	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			
2	H	216	Total	C	N	O	S	0	0	0
			1640	1017	274	342	7			
2	L	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			
2	N	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			
2	P	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			
2	R	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			
2	T	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			
2	V	212	Total	C	N	O	S	0	0	0
			1615	1004	270	334	7			
2	Y	210	Total	C	N	O	S	0	0	0
			1591	987	266	331	7			

- Molecule 3 is a protein called Epitope peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	a	12	Total	C	N	O	0	0	0
			97	60	19	18			
3	c	11	Total	C	N	O	0	0	0
			89	56	17	16			
3	e	11	Total	C	N	O	0	0	0
			89	56	17	16			
3	g	12	Total	C	N	O	0	0	0
			97	60	19	18			
3	i	12	Total	C	N	O	0	0	0
			97	60	19	18			
3	k	11	Total	C	N	O	0	0	0
			89	56	17	16			
3	m	12	Total	C	N	O	0	0	0
			97	60	19	18			
3	o	11	Total	C	N	O	0	0	0
			88	55	17	16			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	q	10	Total 80	C 51	N 15	O 14	0	0	0
3	s	11	Total 89	C 56	N 17	O 16	0	0	0
3	u	10	Total 80	C 51	N 15	O 14	0	0	0
3	x	12	Total 97	C 60	N 19	O 18	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total 38	O 38	0	0
4	C	44	Total 44	O 44	0	0
4	E	34	Total 34	O 34	0	0
4	G	29	Total 29	O 29	0	0
4	I	31	Total 31	O 31	0	0
4	J	55	Total 55	O 55	0	0
4	K	13	Total 13	O 13	0	0
4	M	18	Total 18	O 18	0	0
4	O	26	Total 26	O 26	0	0
4	Q	20	Total 20	O 20	0	0
4	S	27	Total 27	O 27	0	0
4	U	14	Total 14	O 14	0	0
4	X	42	Total 42	O 42	0	0
4	B	47	Total 47	O 47	0	0
4	D	62	Total 62	O 62	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	F	48	Total O 48 48	0	0
4	H	51	Total O 51 51	0	0
4	L	46	Total O 46 46	0	0
4	N	24	Total O 24 24	0	0
4	P	57	Total O 57 57	0	0
4	R	29	Total O 29 29	0	0
4	T	32	Total O 32 32	0	0
4	V	21	Total O 21 21	0	0
4	Y	40	Total O 40 40	0	0
4	a	1	Total O 1 1	0	0
4	s	1	Total O 1 1	0	0

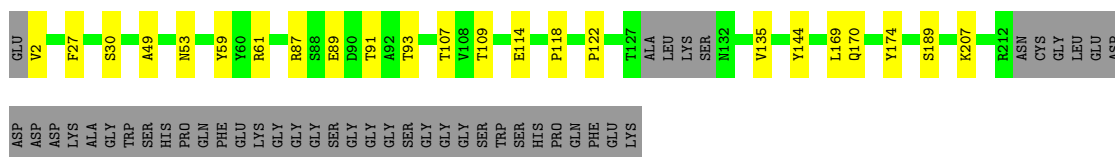


### 3 Residue-property plots [i](#)

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.

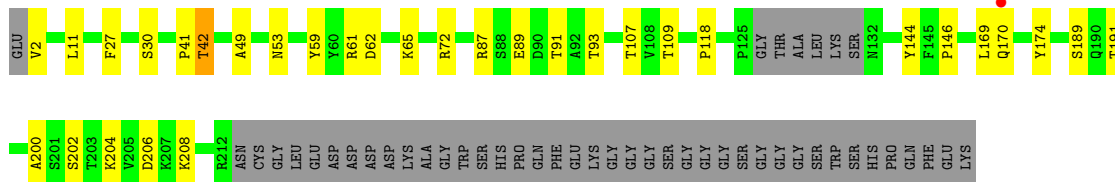
- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11

Chain A:  73% 9% 18%



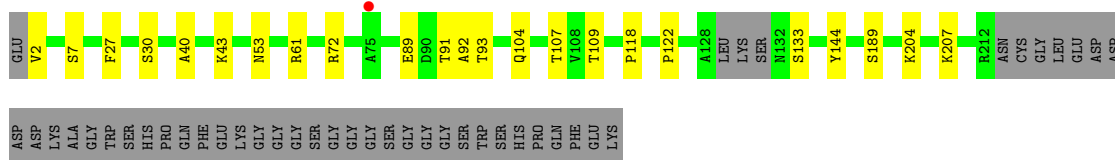
- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11

Chain C:  69% 12% 19%



- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11

Chain E:  73% 9% 17%

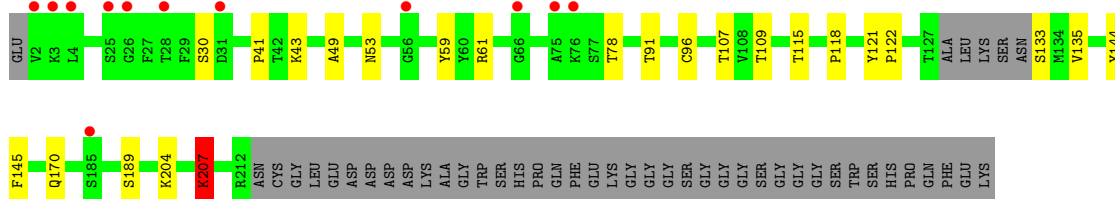
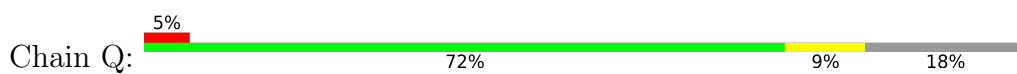


- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11

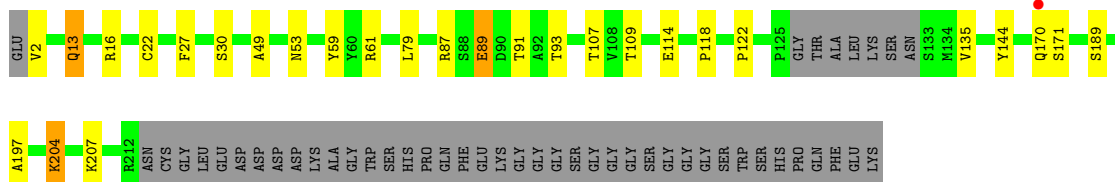
Chain G:  73% 9% 18%



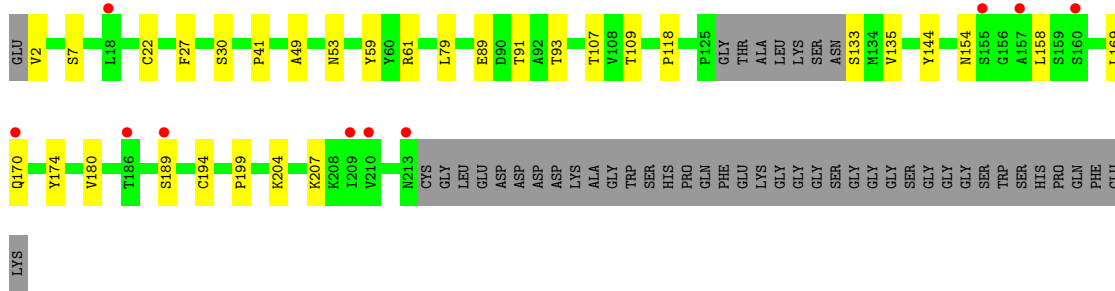




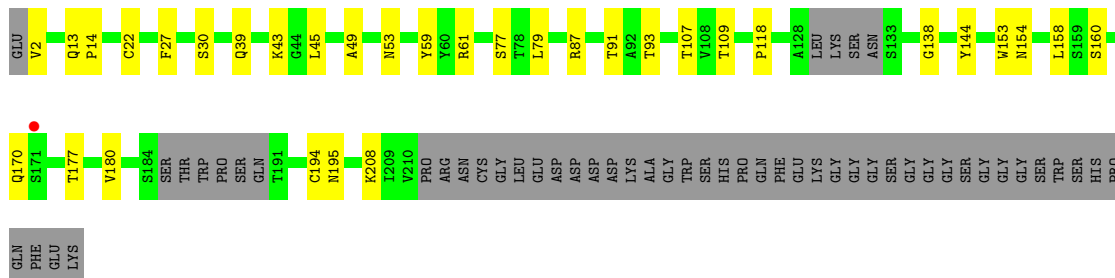
- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11



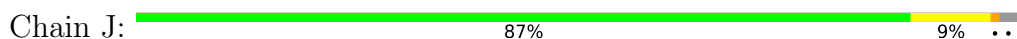
- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11

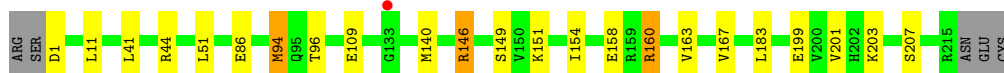


- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11

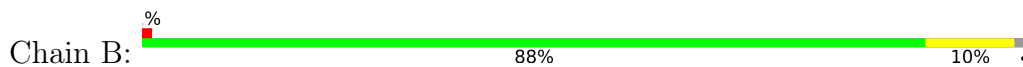


- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11

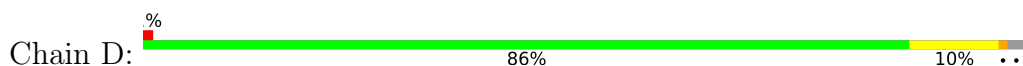




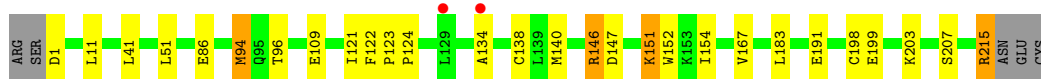
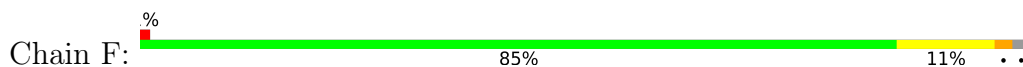
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11



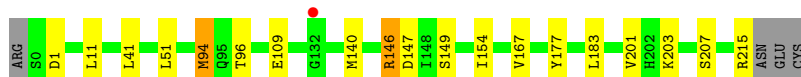
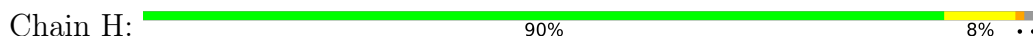
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11



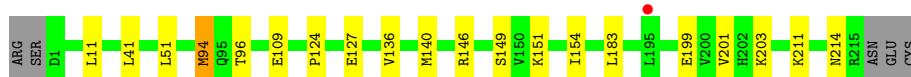
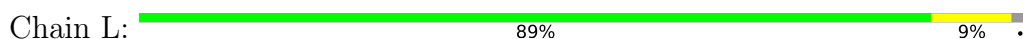
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11



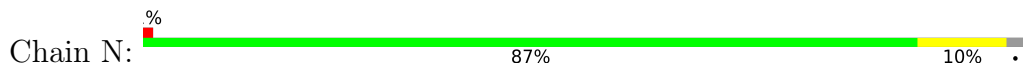
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11




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



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




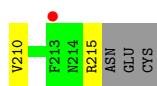
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11

Chain P:  87% 9% ..




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

Chain R:  5% 87% 10% .




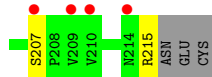
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11

Chain T:  5% 85% 12% .




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

Chain V:  10% 87% 8% ..



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

Chain Y:  2% 78% 14% 5%



- Molecule 3: Epitope peptide

Chain a:  92% 8%




- Molecule 3: Epitope peptide

Chain c:  92% 8%



- Molecule 3: Epitope peptide

Chain e:  83% 8% 8%



- Molecule 3: Epitope peptide

Chain g:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Epitope peptide

Chain i:  92% 8%




- Molecule 3: Epitope peptide

Chain k:  92% 8%



- Molecule 3: Epitope peptide

Chain m:  83% 17%

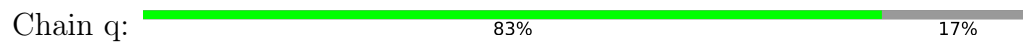


- Molecule 3: Epitope peptide

Chain o:  92% 8%



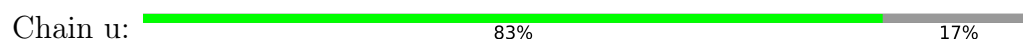
- Molecule 3: Epitope peptide



- Molecule 3: Epitope peptide



- Molecule 3: Epitope peptide



- Molecule 3: Epitope peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.79Å 128.22Å 163.63Å 88.79° 94.36° 96.15°	Depositor
Resolution (Å)	32.50 – 2.22 48.74 – 2.22	Depositor EDS
% Data completeness (in resolution range)	95.4 (32.50-2.22) 95.4 (48.74-2.22)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.22Å)	Xtrriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.209 , 0.243 0.233 , 0.273	Depositor DCC
$R_{free}$ test set	12380 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtrriage
Anisotropy	0.254	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	40099	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.51	0/1603	0.76	0/2188
1	C	0.52	0/1592	0.75	0/2173
1	E	0.51	0/1608	0.74	0/2195
1	G	0.50	0/1605	0.75	0/2190
1	I	0.50	0/1588	0.75	1/2167 (0.0%)
1	K	0.51	0/1584	0.74	0/2162
1	M	0.47	0/1584	0.73	0/2162
1	O	0.49	0/1588	0.74	0/2167
1	Q	0.48	0/1595	0.73	1/2177 (0.0%)
1	S	0.53	0/1584	0.75	0/2162
1	U	0.49	0/1592	0.75	0/2173
1	X	0.56	0/1528	0.82	0/2082
2	B	0.53	0/1664	0.74	0/2264
2	D	0.52	0/1672	0.74	0/2275
2	F	0.51	0/1664	0.72	0/2264
2	H	0.51	0/1670	0.73	0/2272
2	J	0.51	0/1664	0.73	0/2264
2	L	0.51	0/1664	0.72	0/2264
2	N	0.44	0/1664	0.71	0/2264
2	P	0.48	0/1664	0.73	1/2264 (0.0%)
2	R	0.45	0/1664	0.71	0/2264
2	T	0.50	0/1664	0.73	0/2264
2	V	0.47	0/1644	0.69	0/2235
2	Y	0.61	0/1618	0.88	2/2199 (0.1%)
3	a	0.51	0/99	0.67	0/135
3	c	0.48	0/91	0.71	0/124
3	e	0.57	0/91	0.71	0/124
3	g	0.56	0/99	0.70	0/135
3	i	0.50	0/99	0.75	0/135
3	k	0.55	0/91	0.78	0/124
3	m	0.45	0/99	0.75	0/135
3	o	0.45	0/90	0.64	0/123
3	q	0.46	0/82	0.73	0/112
3	s	0.52	0/91	0.74	0/124

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	u	0.49	0/82	0.73	0/112
3	x	0.67	0/99	0.82	0/135
All	All	0.51	0/40080	0.74	5/54609 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	130	ALA	C-N-CA	5.87	136.37	121.70
2	P	94	MET	N-CA-CB	-5.52	100.66	110.60
1	I	55	GLY	N-CA-C	5.43	126.67	113.10
1	Q	207	LYS	CG-CD-CE	-5.22	96.25	111.90
2	Y	158	GLU	C-N-CA	5.04	134.30	121.70

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	1565	0	1536	7	0
1	C	1554	0	1526	14	0
1	E	1570	0	1541	7	0
1	G	1567	0	1538	6	0
1	I	1550	0	1523	10	0
1	K	1546	0	1520	18	0
1	M	1546	0	1520	12	0
1	O	1550	0	1523	9	0
1	Q	1557	0	1530	7	0
1	S	1546	0	1520	12	0
1	U	1554	0	1526	10	0
1	X	1495	0	1472	13	0
2	B	1634	0	1593	6	0
2	D	1642	0	1599	15	0
2	F	1634	0	1593	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1640	0	1598	6	0
2	J	1634	0	1593	10	0
2	L	1634	0	1593	7	0
2	N	1634	0	1593	8	0
2	P	1634	0	1593	10	0
2	R	1634	0	1593	8	0
2	T	1634	0	1593	9	0
2	V	1615	0	1578	8	0
2	Y	1591	0	1552	11	0
3	a	97	0	88	0	0
3	c	89	0	82	0	0
3	e	89	0	82	0	0
3	g	97	0	88	0	0
3	i	97	0	88	0	0
3	k	89	0	82	0	0
3	m	97	0	88	0	0
3	o	88	0	80	0	0
3	q	80	0	74	0	0
3	s	89	0	82	0	0
3	u	80	0	74	0	0
3	x	97	0	88	0	0
4	A	38	0	0	0	0
4	B	47	0	0	0	0
4	C	44	0	0	2	0
4	D	62	0	0	1	0
4	E	34	0	0	0	0
4	F	48	0	0	0	0
4	G	29	0	0	0	0
4	H	51	0	0	0	0
4	I	31	0	0	0	0
4	J	55	0	0	0	0
4	K	13	0	0	0	0
4	L	46	0	0	0	0
4	M	18	0	0	1	0
4	N	24	0	0	0	0
4	O	26	0	0	0	0
4	P	57	0	0	0	0
4	Q	20	0	0	0	0
4	R	29	0	0	1	0
4	S	27	0	0	1	0
4	T	32	0	0	1	0
4	U	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	V	21	0	0	0	0
4	X	42	0	0	0	0
4	Y	40	0	0	0	0
4	a	1	0	0	0	0
4	s	1	0	0	0	0
All	All	40099	0	38342	223	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 3.

The worst 5 of 223 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:M:97:THR:HG21	1:M:102:TRP:CE3	2.13	0.83
1:C:202:SER:HB3	1:I:208:LYS:HB3	1.65	0.76
2:J:44:ARG:NH1	2:J:86:GLU:O	2.23	0.71
1:K:208:LYS:HB3	1:M:202:SER:HB3	1.75	0.66
2:D:214:ASN:O	2:D:215:ARG:HB2	1.95	0.66

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	203/252 (81%)	195 (96%)	8 (4%)	0	100	100
1	C	201/252 (80%)	195 (97%)	6 (3%)	0	100	100
1	E	204/252 (81%)	197 (97%)	7 (3%)	0	100	100
1	G	203/252 (81%)	197 (97%)	4 (2%)	2 (1%)	15	13
1	I	201/252 (80%)	197 (98%)	3 (2%)	1 (0%)	29	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	200/252 (79%)	194 (97%)	6 (3%)	0	100	100
1	M	200/252 (79%)	196 (98%)	4 (2%)	0	100	100
1	O	201/252 (80%)	196 (98%)	5 (2%)	0	100	100
1	Q	202/252 (80%)	199 (98%)	2 (1%)	1 (0%)	29	30
1	S	200/252 (79%)	196 (98%)	4 (2%)	0	100	100
1	U	201/252 (80%)	197 (98%)	3 (2%)	1 (0%)	29	30
1	X	193/252 (77%)	189 (98%)	2 (1%)	2 (1%)	15	13
2	B	213/220 (97%)	208 (98%)	5 (2%)	0	100	100
2	D	214/220 (97%)	208 (97%)	4 (2%)	2 (1%)	17	15
2	F	213/220 (97%)	208 (98%)	5 (2%)	0	100	100
2	H	214/220 (97%)	212 (99%)	2 (1%)	0	100	100
2	J	213/220 (97%)	208 (98%)	5 (2%)	0	100	100
2	L	213/220 (97%)	210 (99%)	3 (1%)	0	100	100
2	N	213/220 (97%)	208 (98%)	5 (2%)	0	100	100
2	P	213/220 (97%)	206 (97%)	7 (3%)	0	100	100
2	R	213/220 (97%)	206 (97%)	7 (3%)	0	100	100
2	T	213/220 (97%)	207 (97%)	6 (3%)	0	100	100
2	V	208/220 (94%)	203 (98%)	5 (2%)	0	100	100
2	Y	204/220 (93%)	186 (91%)	12 (6%)	6 (3%)	4	2
3	a	10/12 (83%)	10 (100%)	0	0	100	100
3	c	9/12 (75%)	9 (100%)	0	0	100	100
3	e	9/12 (75%)	9 (100%)	0	0	100	100
3	g	10/12 (83%)	10 (100%)	0	0	100	100
3	i	10/12 (83%)	10 (100%)	0	0	100	100
3	k	9/12 (75%)	8 (89%)	1 (11%)	0	100	100
3	m	10/12 (83%)	10 (100%)	0	0	100	100
3	o	9/12 (75%)	8 (89%)	1 (11%)	0	100	100
3	q	8/12 (67%)	7 (88%)	1 (12%)	0	100	100
3	s	9/12 (75%)	9 (100%)	0	0	100	100
3	u	8/12 (67%)	8 (100%)	0	0	100	100
3	x	10/12 (83%)	10 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5064/5808 (87%)	4926 (97%)	123 (2%)	15 (0%)	41	45

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	7	THR
2	D	215	ARG
2	Y	159	ARG
1	G	125	PRO
1	X	160	SER

### 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	176/208 (85%)	167 (95%)	9 (5%)	24	27
1	C	175/208 (84%)	165 (94%)	10 (6%)	20	23
1	E	176/208 (85%)	166 (94%)	10 (6%)	20	23
1	G	176/208 (85%)	167 (95%)	9 (5%)	24	27
1	I	174/208 (84%)	166 (95%)	8 (5%)	27	32
1	K	174/208 (84%)	161 (92%)	13 (8%)	13	13
1	M	174/208 (84%)	161 (92%)	13 (8%)	13	13
1	O	174/208 (84%)	162 (93%)	12 (7%)	15	15
1	Q	175/208 (84%)	164 (94%)	11 (6%)	18	19
1	S	174/208 (84%)	164 (94%)	10 (6%)	20	23
1	U	175/208 (84%)	163 (93%)	12 (7%)	15	15
1	X	167/208 (80%)	159 (95%)	8 (5%)	25	30
2	B	191/196 (97%)	180 (94%)	11 (6%)	20	22
2	D	192/196 (98%)	182 (95%)	10 (5%)	23	27
2	F	191/196 (97%)	179 (94%)	12 (6%)	18	19
2	H	192/196 (98%)	182 (95%)	10 (5%)	23	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	191/196 (97%)	182 (95%)	9 (5%)	26	31
2	L	191/196 (97%)	182 (95%)	9 (5%)	26	31
2	N	191/196 (97%)	182 (95%)	9 (5%)	26	31
2	P	191/196 (97%)	181 (95%)	10 (5%)	23	27
2	R	191/196 (97%)	181 (95%)	10 (5%)	23	27
2	T	191/196 (97%)	178 (93%)	13 (7%)	16	16
2	V	189/196 (96%)	181 (96%)	8 (4%)	30	36
2	Y	187/196 (95%)	164 (88%)	23 (12%)	4	3
3	a	11/11 (100%)	10 (91%)	1 (9%)	9	8
3	c	10/11 (91%)	10 (100%)	0	100	100
3	e	10/11 (91%)	9 (90%)	1 (10%)	7	6
3	g	11/11 (100%)	11 (100%)	0	100	100
3	i	11/11 (100%)	10 (91%)	1 (9%)	9	8
3	k	10/11 (91%)	10 (100%)	0	100	100
3	m	11/11 (100%)	9 (82%)	2 (18%)	1	1
3	o	10/11 (91%)	10 (100%)	0	100	100
3	q	9/11 (82%)	9 (100%)	0	100	100
3	s	10/11 (91%)	10 (100%)	0	100	100
3	u	9/11 (82%)	9 (100%)	0	100	100
3	x	11/11 (100%)	10 (91%)	1 (9%)	9	8
All	All	4501/4980 (90%)	4236 (94%)	265 (6%)	19	22

5 of 265 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	V	109	GLU
2	Y	11	LEU
3	e	422	VAL
1	Q	107	THR
1	Q	61	ARG

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

Mol	Chain	Res	Type
1	E	163	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	207/252 (82%)	-0.14	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	21, 35, 49, 66	0
1	C	205/252 (81%)	-0.10	1 (0%) <span style="border: 1px solid blue; padding: 2px;">91</span> <span style="border: 1px solid blue; padding: 2px;">90</span>	20, 32, 51, 80	0
1	E	208/252 (82%)	0.03	1 (0%) <span style="border: 1px solid blue; padding: 2px;">91</span> <span style="border: 1px solid blue; padding: 2px;">90</span>	21, 37, 57, 79	0
1	G	207/252 (82%)	-0.03	1 (0%) <span style="border: 1px solid blue; padding: 2px;">91</span> <span style="border: 1px solid blue; padding: 2px;">90</span>	22, 41, 62, 84	0
1	I	205/252 (81%)	-0.12	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	23, 36, 52, 69	0
1	K	204/252 (80%)	0.38	6 (2%) <span style="border: 1px solid gray; padding: 2px;">51</span> <span style="border: 1px solid gray; padding: 2px;">49</span>	28, 48, 71, 93	0
1	M	204/252 (80%)	0.26	2 (0%) <span style="border: 1px solid blue; padding: 2px;">82</span> <span style="border: 1px solid blue; padding: 2px;">81</span>	29, 46, 63, 78	0
1	O	205/252 (81%)	0.16	3 (1%) <span style="border: 1px solid blue; padding: 2px;">73</span> <span style="border: 1px solid blue; padding: 2px;">72</span>	23, 40, 61, 75	0
1	Q	206/252 (81%)	0.43	12 (5%) <span style="border: 1px solid red; padding: 2px;">23</span> <span style="border: 1px solid red; padding: 2px;">21</span>	25, 46, 73, 84	0
1	S	204/252 (80%)	-0.05	1 (0%) <span style="border: 1px solid blue; padding: 2px;">91</span> <span style="border: 1px solid blue; padding: 2px;">90</span>	18, 34, 55, 78	0
1	U	205/252 (81%)	0.42	10 (4%) <span style="border: 1px solid red; padding: 2px;">29</span> <span style="border: 1px solid red; padding: 2px;">28</span>	24, 49, 73, 103	0
1	X	199/252 (78%)	-0.06	1 (0%) <span style="border: 1px solid blue; padding: 2px;">91</span> <span style="border: 1px solid blue; padding: 2px;">90</span>	18, 34, 54, 87	0
2	B	215/220 (97%)	0.01	2 (0%) <span style="border: 1px solid blue; padding: 2px;">84</span> <span style="border: 1px solid blue; padding: 2px;">83</span>	18, 35, 59, 74	0
2	D	216/220 (98%)	0.01	2 (0%) <span style="border: 1px solid blue; padding: 2px;">84</span> <span style="border: 1px solid blue; padding: 2px;">83</span>	18, 31, 55, 87	0
2	F	215/220 (97%)	0.01	2 (0%) <span style="border: 1px solid blue; padding: 2px;">84</span> <span style="border: 1px solid blue; padding: 2px;">83</span>	20, 34, 62, 90	0
2	H	216/220 (98%)	-0.11	1 (0%) <span style="border: 1px solid blue; padding: 2px;">91</span> <span style="border: 1px solid blue; padding: 2px;">90</span>	18, 35, 56, 69	0
2	J	215/220 (97%)	-0.06	1 (0%) <span style="border: 1px solid blue; padding: 2px;">91</span> <span style="border: 1px solid blue; padding: 2px;">90</span>	18, 33, 56, 75	0
2	L	215/220 (97%)	0.03	1 (0%) <span style="border: 1px solid blue; padding: 2px;">91</span> <span style="border: 1px solid blue; padding: 2px;">90</span>	22, 39, 57, 68	0
2	N	215/220 (97%)	0.23	3 (1%) <span style="border: 1px solid blue; padding: 2px;">75</span> <span style="border: 1px solid blue; padding: 2px;">73</span>	30, 49, 68, 80	0
2	P	215/220 (97%)	-0.11	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	23, 37, 61, 75	0
2	R	215/220 (97%)	0.41	10 (4%) <span style="border: 1px solid red; padding: 2px;">31</span> <span style="border: 1px solid red; padding: 2px;">29</span>	30, 54, 78, 88	0
2	T	215/220 (97%)	0.38	12 (5%) <span style="border: 1px solid red; padding: 2px;">24</span> <span style="border: 1px solid red; padding: 2px;">23</span>	21, 44, 76, 90	0
2	V	212/220 (96%)	0.64	21 (9%) <span style="border: 1px solid red; padding: 2px;">7</span> <span style="border: 1px solid red; padding: 2px;">6</span>	27, 52, 88, 106	0
2	Y	210/220 (95%)	0.04	5 (2%) <span style="border: 1px solid blue; padding: 2px;">59</span> <span style="border: 1px solid blue; padding: 2px;">57</span>	15, 33, 72, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9	
3	a	12/12 (100%)	-0.03	0	100 100	23, 31, 50, 79	0
3	c	11/12 (91%)	-0.06	0	100 100	25, 28, 51, 52	0
3	e	11/12 (91%)	0.08	0	100 100	23, 30, 56, 56	0
3	g	12/12 (100%)	-0.34	0	100 100	26, 30, 46, 48	0
3	i	12/12 (100%)	-0.05	0	100 100	30, 34, 50, 65	0
3	k	11/12 (91%)	0.36	0	100 100	24, 36, 58, 59	0
3	m	12/12 (100%)	0.24	0	100 100	39, 47, 69, 78	0
3	o	11/12 (91%)	0.22	0	100 100	34, 43, 59, 61	0
3	q	10/12 (83%)	0.34	0	100 100	42, 50, 56, 68	0
3	s	11/12 (91%)	0.04	0	100 100	27, 32, 45, 48	0
3	u	10/12 (83%)	0.14	0	100 100	32, 37, 40, 54	0
3	x	12/12 (100%)	-0.09	0	100 100	23, 29, 57, 59	0
All	All	5168/5808 (88%)	0.11	98 (1%)	66 65	15, 40, 67, 106	0

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	75	ALA	5.6
1	Q	31	ASP	4.9
2	Y	157	THR	4.3
2	H	132	GLY	4.3
2	Y	156	GLY	4.2

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.