



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:56 AM UTC

PDB ID : 4WHT / pdb_00004wht
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 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

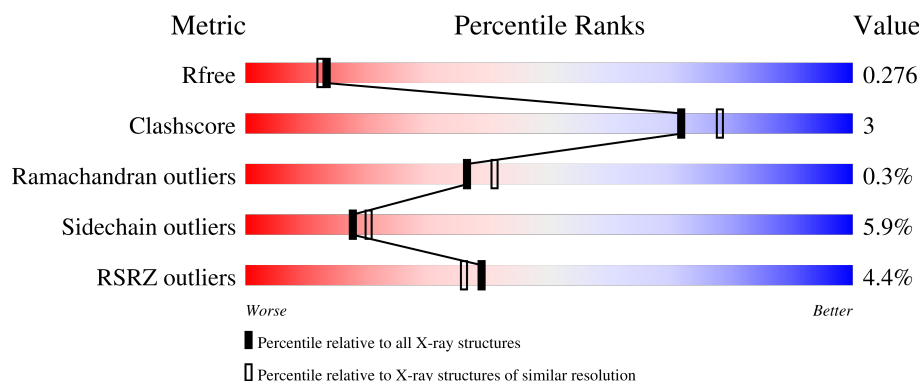
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (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 ≥ 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	 72% 10% 18%
1	C	252	 2% 67% 13% 19%
1	E	252	 2% 72% 10% 17%
1	G	252	 % 71% 11% 18%
1	I	252	 % 68% 13% 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	8% 75% 17% 8%
3	o	12	8% 92% 8%
3	q	12	8% 67% 17% 17%
3	s	12	83% 8% 8%
3	u	12	8% 83% 17%
3	x	12	100%

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

- 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
2	J	215	Total	C	N	O	S	0	0	0
			1634	1014	273	340	7			

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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
3	q	10	Total	C	N	O	0	0	0
			80	51	15	14			
3	s	11	Total	C	N	O	0	0	0
			89	56	17	16			
3	u	10	Total	C	N	O	0	0	0
			80	51	15	14			
3	x	12	Total	C	N	O	0	0	0
			97	60	19	18			

- Molecule 4 is water.

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

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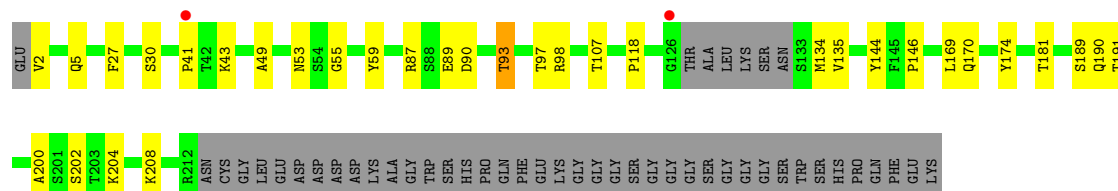
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	48	Total 48	O 48	0	0
4	H	51	Total 51	O 51	0	0
4	L	46	Total 46	O 46	0	0
4	N	24	Total 24	O 24	0	0
4	P	57	Total 57	O 57	0	0
4	R	29	Total 29	O 29	0	0
4	T	32	Total 32	O 32	0	0
4	V	21	Total 21	O 21	0	0
4	Y	40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

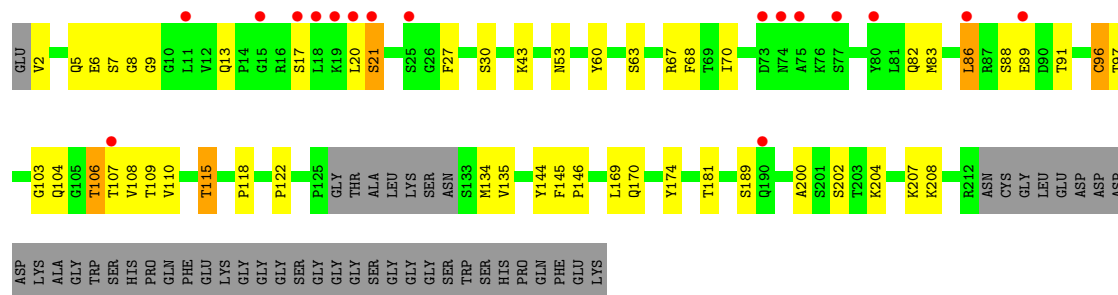
- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11



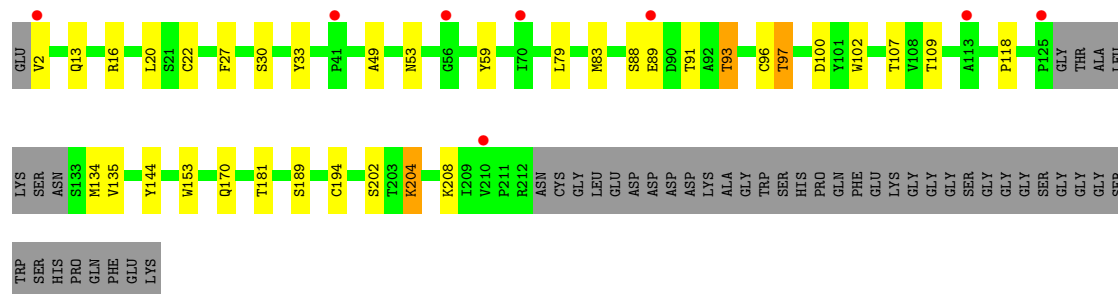
- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11



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

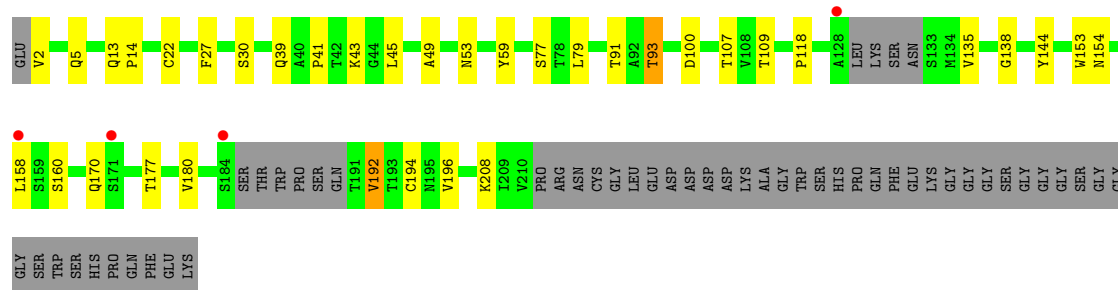


- Molecule 1: Heavy chain of the Fab fragment derived from neutralizing antibody 3/11



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





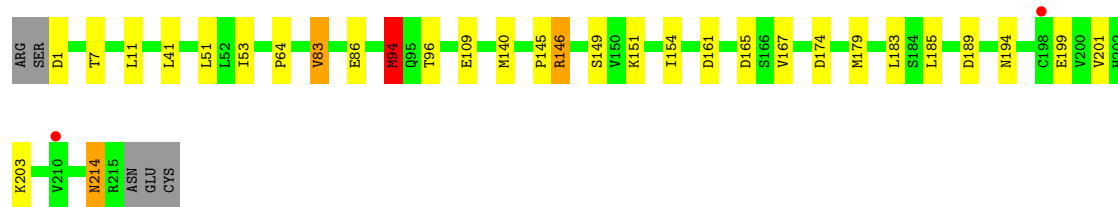
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11

Chain J: 85% 11% ..



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

Chain B: 84% 12% ..



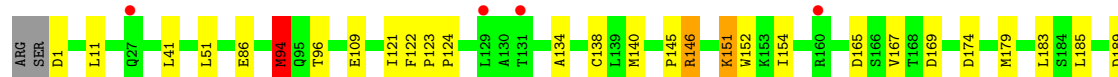
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11

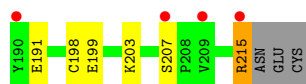
Chain D: 82% 14% ..



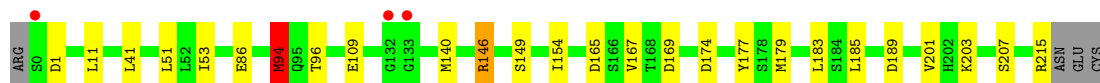
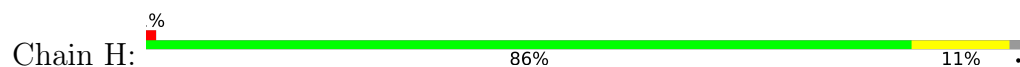
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11

Chain F: 82% 14% ..

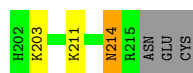
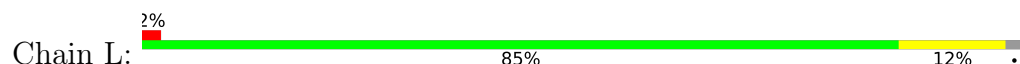




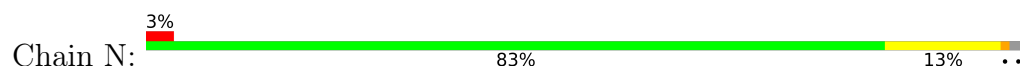
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11



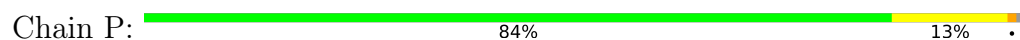
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11



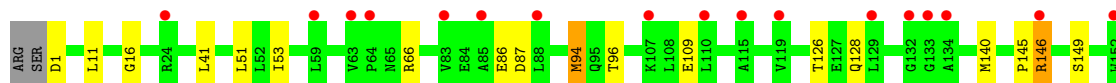
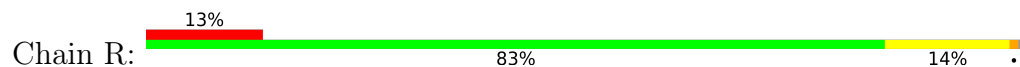
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11

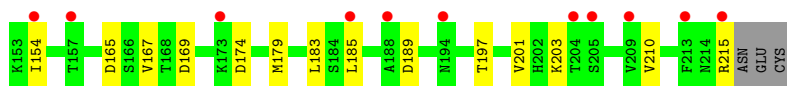


- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11

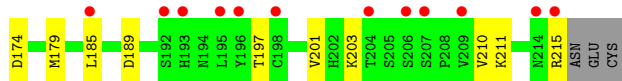
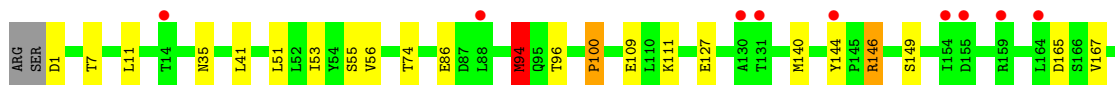
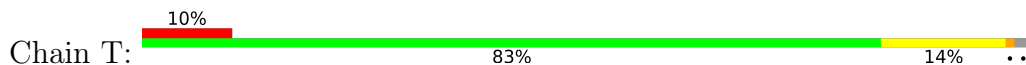


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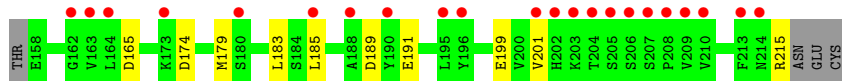
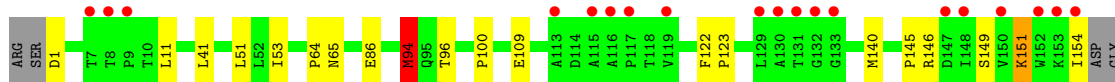
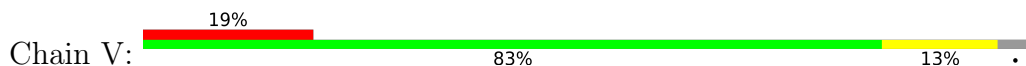




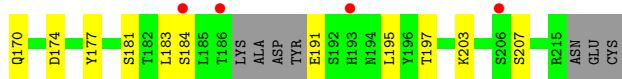
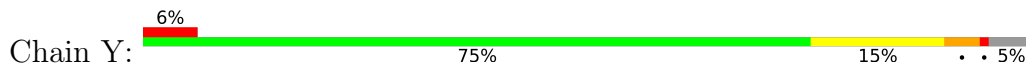
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11



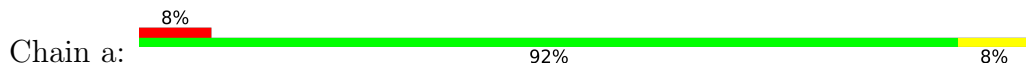
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11



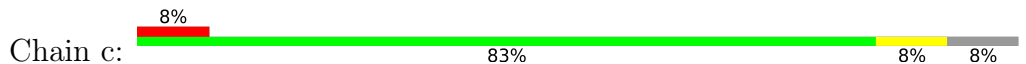
- Molecule 2: Light chain of the Fab fragment derived from neutralizing antibody 3/11

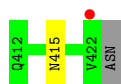


- Molecule 3: Epitope peptide

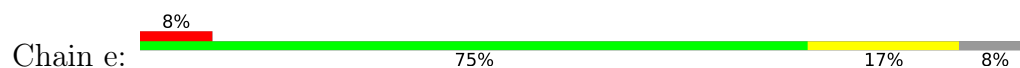


- Molecule 3: Epitope peptide





- Molecule 3: Epitope peptide

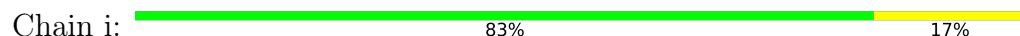


- Molecule 3: Epitope peptide

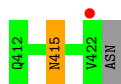
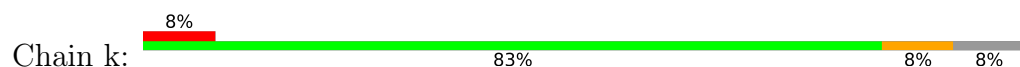


There are no outlier residues recorded for this chain.

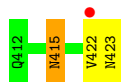
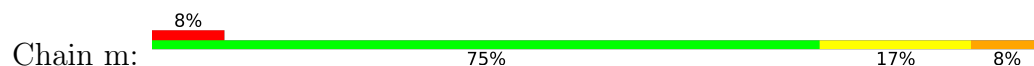
- Molecule 3: Epitope peptide



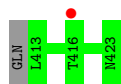
- Molecule 3: Epitope peptide



- Molecule 3: Epitope peptide

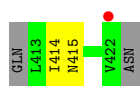


- Molecule 3: Epitope peptide



- Molecule 3: Epitope peptide





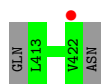
- Molecule 3: Epitope peptide

Chain s:  83% 8% 8%



- Molecule 3: Epitope peptide

Chain u:  8% 83% 17%



- Molecule 3: Epitope peptide

Chain x:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.79Å 128.22Å 163.63Å 88.79° 94.36° 96.15°	Depositor
Resolution (Å)	32.50 – 2.22 32.50 – 2.22	Depositor EDS
% Data completeness (in resolution range)	95.4 (32.50-2.22) 95.4 (32.50-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.22Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.209 , 0.243 0.234 , 0.276	Depositor DCC
R_{free} test set	12380 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	40099	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage'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.*

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	0.83	0/1603	1.20	6/2188 (0.3%)
1	C	0.83	1/1592 (0.1%)	1.20	6/2173 (0.3%)
1	E	0.83	0/1608	1.19	9/2195 (0.4%)
1	G	0.82	1/1605 (0.1%)	1.20	6/2190 (0.3%)
1	I	0.80	0/1588	1.22	7/2167 (0.3%)
1	K	0.83	0/1584	1.22	7/2162 (0.3%)
1	M	0.77	0/1584	1.17	6/2162 (0.3%)
1	O	0.79	0/1588	1.19	6/2167 (0.3%)
1	Q	0.78	0/1595	1.17	5/2177 (0.2%)
1	S	0.85	0/1584	1.20	8/2162 (0.4%)
1	U	0.79	0/1592	1.21	4/2173 (0.2%)
1	X	0.90	0/1528	1.27	5/2082 (0.2%)
2	B	0.89	1/1664 (0.1%)	1.21	9/2264 (0.4%)
2	D	0.87	0/1672	1.25	14/2275 (0.6%)
2	F	0.83	1/1664 (0.1%)	1.20	5/2264 (0.2%)
2	H	0.86	1/1670 (0.1%)	1.19	3/2272 (0.1%)
2	J	0.82	0/1664	1.17	3/2264 (0.1%)
2	L	0.84	1/1664 (0.1%)	1.17	5/2264 (0.2%)
2	N	0.74	0/1664	1.17	7/2264 (0.3%)
2	P	0.79	1/1664 (0.1%)	1.19	6/2264 (0.3%)
2	R	0.77	0/1664	1.17	7/2264 (0.3%)
2	T	0.83	1/1664 (0.1%)	1.22	4/2264 (0.2%)
2	V	0.80	1/1644 (0.1%)	1.17	8/2235 (0.4%)
2	Y	0.99	2/1618 (0.1%)	1.41	17/2199 (0.8%)
3	a	0.75	0/99	1.16	0/135
3	c	0.75	0/91	1.38	2/124 (1.6%)
3	e	0.95	0/91	1.35	1/124 (0.8%)
3	g	0.92	0/99	1.33	0/135
3	i	0.80	0/99	1.40	1/135 (0.7%)
3	k	0.85	0/91	1.45	2/124 (1.6%)
3	m	0.76	0/99	1.46	2/135 (1.5%)
3	o	0.69	0/90	1.16	0/123
3	q	0.78	0/82	1.34	0/112
3	s	0.84	0/91	1.31	0/124

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	u	0.74	0/82	1.25	0/112
3	x	1.11	0/99	1.52	0/135
All	All	0.83	11/40080 (0.0%)	1.21	171/54609 (0.3%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	94	MET	SD-CE	-7.78	1.60	1.79
2	B	94	MET	SD-CE	-7.60	1.60	1.79
2	H	94	MET	SD-CE	-7.33	1.61	1.79
2	L	94	MET	SD-CE	-7.10	1.61	1.79
2	V	94	MET	SD-CE	-6.96	1.62	1.79
2	T	94	MET	SD-CE	-6.71	1.62	1.79
1	G	40	ALA	CA-C	6.21	1.59	1.53
1	C	83	MET	SD-CE	-5.44	1.66	1.79
2	F	94	MET	SD-CE	-5.24	1.66	1.79
2	Y	9	PRO	C-N	5.23	1.40	1.33
2	P	94	MET	CA-C	5.15	1.58	1.52

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	160	SER	N-CA-C	8.69	120.37	111.07
1	I	55	GLY	N-CA-C	8.55	126.67	115.47
1	X	93	THR	CB-CA-C	7.92	122.79	109.80
2	Y	130	ALA	CA-C-N	7.76	136.37	121.54
2	Y	130	ALA	C-N-CA	7.76	136.37	121.54
1	X	41	PRO	CA-C-N	7.68	130.90	120.38
1	X	41	PRO	C-N-CA	7.68	130.90	120.38
1	I	93	THR	CB-CA-C	7.56	122.22	109.75
2	V	65	ASN	CA-CB-CG	7.43	120.03	112.60
2	Y	161	ASP	CA-CB-CG	7.33	119.94	112.60
1	C	93	THR	CB-CA-C	6.98	121.24	109.80
1	O	93	THR	CB-CA-C	6.96	121.24	109.75
1	U	93	THR	CB-CA-C	6.79	120.93	109.80
1	A	93	THR	CB-CA-C	6.77	120.92	109.75
2	Y	83	VAL	N-CA-CB	6.69	119.09	110.13
2	Y	158	GLU	CA-C-N	6.68	134.30	121.54
2	Y	158	GLU	C-N-CA	6.68	134.30	121.54
2	D	85	ALA	CA-C-N	6.67	131.27	120.60
2	D	85	ALA	C-N-CA	6.67	131.27	120.60
2	Y	100	PRO	N-CA-C	6.64	121.26	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	93	THR	CB-CA-C	6.60	120.63	109.80
1	G	55	GLY	N-CA-C	6.58	124.78	115.30
2	D	132	GLY	CA-C-N	6.58	126.68	121.61
2	D	132	GLY	C-N-CA	6.58	126.68	121.61
1	M	93	THR	CB-CA-C	6.56	120.58	109.75
1	Q	207	LYS	CG-CD-CE	-6.54	96.25	111.30
2	Y	64	PRO	CA-C-N	6.54	129.93	120.38
2	Y	64	PRO	C-N-CA	6.54	129.93	120.38
1	A	88	SER	CA-C-N	6.53	129.68	120.28
1	A	88	SER	C-N-CA	6.53	129.68	120.28
2	D	174	ASP	CA-CB-CG	6.53	119.13	112.60
1	O	88	SER	CA-C-N	6.41	129.50	120.28
1	O	88	SER	C-N-CA	6.41	129.50	120.28
2	Y	158	GLU	N-CA-C	6.40	116.51	108.45
1	M	88	SER	CA-C-N	6.34	129.41	120.28
1	M	88	SER	C-N-CA	6.34	129.41	120.28
2	F	174	ASP	CA-CB-CG	6.28	118.88	112.60
1	E	88	SER	CA-C-N	6.23	129.25	120.28
1	E	88	SER	C-N-CA	6.23	129.25	120.28
2	T	7	THR	N-CA-C	6.23	118.07	111.28
1	S	88	SER	CA-C-N	6.18	129.41	120.38
1	S	88	SER	C-N-CA	6.18	129.41	120.38
1	U	88	SER	CA-C-N	6.15	129.13	120.28
1	U	88	SER	C-N-CA	6.15	129.13	120.28
1	S	93	THR	CB-CA-C	6.15	119.89	109.75
1	K	97	THR	N-CA-C	6.13	118.73	109.23
1	C	115	THR	CB-CA-C	6.10	118.53	110.06
2	R	174	ASP	CA-CB-CG	6.09	118.69	112.60
1	M	97	THR	N-CA-C	6.08	118.65	109.23
1	G	93	THR	CB-CA-C	6.06	119.75	109.75
2	P	94	MET	N-CA-CB	-6.04	100.66	110.81
2	L	174	ASP	CA-CB-CG	6.04	118.64	112.60
1	C	88	SER	CA-C-N	5.97	128.88	120.28
1	C	88	SER	C-N-CA	5.97	128.88	120.28
2	V	64	PRO	CA-C-N	5.97	129.09	120.38
2	V	64	PRO	C-N-CA	5.97	129.09	120.38
2	N	189	ASP	CA-CB-CG	5.96	118.56	112.60
2	Y	174	ASP	CA-CB-CG	5.96	118.56	112.60
2	D	145	PRO	CA-C-N	5.95	128.25	120.28
2	D	145	PRO	C-N-CA	5.95	128.25	120.28
2	F	145	PRO	CA-C-N	5.95	128.25	120.28
2	F	145	PRO	C-N-CA	5.95	128.25	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	100	ASP	CA-CB-CG	5.92	118.52	112.60
2	P	145	PRO	CA-C-N	5.89	128.45	120.38
2	P	145	PRO	C-N-CA	5.89	128.45	120.38
3	m	415	ASN	CA-C-N	5.88	130.00	120.60
3	m	415	ASN	C-N-CA	5.88	130.00	120.60
2	B	174	ASP	CA-CB-CG	5.87	118.47	112.60
2	N	174	ASP	CA-CB-CG	5.87	118.47	112.60
1	K	68	PHE	CA-CB-CG	5.83	119.63	113.80
2	P	174	ASP	CA-CB-CG	5.81	118.41	112.60
2	D	189	ASP	CA-CB-CG	5.78	118.38	112.60
2	D	6	GLN	CA-C-N	5.77	132.57	121.54
2	D	6	GLN	C-N-CA	5.77	132.57	121.54
2	N	145	PRO	CA-C-N	5.77	128.28	120.38
2	N	145	PRO	C-N-CA	5.77	128.28	120.38
1	X	192	VAL	CB-CA-C	5.75	118.18	110.42
1	G	41	PRO	N-CA-C	5.75	124.31	112.47
2	H	174	ASP	CA-CB-CG	5.75	118.35	112.60
2	T	189	ASP	CA-CB-CG	5.73	118.33	112.60
2	V	189	ASP	CA-CB-CG	5.71	118.31	112.60
1	E	127	THR	CA-C-N	5.70	131.96	121.70
1	E	127	THR	C-N-CA	5.70	131.96	121.70
2	F	169	ASP	CA-CB-CG	5.70	118.30	112.60
3	c	415	ASN	CA-C-N	5.69	128.47	120.28
3	c	415	ASN	C-N-CA	5.69	128.47	120.28
2	B	189	ASP	CA-CB-CG	5.68	118.28	112.60
1	M	100	ASP	CA-CB-CG	5.68	118.28	112.60
2	Y	126	THR	N-CA-C	-5.67	105.00	111.07
1	A	96	CYS	N-CA-C	-5.64	100.05	109.24
2	T	174	ASP	CA-CB-CG	5.64	118.24	112.60
2	T	100	PRO	N-CA-C	5.60	119.66	111.03
2	P	189	ASP	CA-CB-CG	5.56	118.16	112.60
1	Q	100	ASP	CA-CB-CG	5.55	118.15	112.60
1	K	43	LYS	N-CA-C	5.54	118.54	110.17
1	I	43	LYS	N-CA-C	5.53	118.61	109.94
1	I	190	GLN	CA-C-N	5.51	128.53	120.71
1	I	190	GLN	C-N-CA	5.51	128.53	120.71
1	C	100	ASP	CA-CB-CG	5.49	118.09	112.60
2	R	189	ASP	CA-CB-CG	5.47	118.07	112.60
2	J	174	ASP	CA-CB-CG	5.46	118.06	112.60
2	N	100	PRO	N-CA-C	5.46	119.44	111.03
2	J	189	ASP	CA-CB-CG	5.46	118.06	112.60
1	O	100	ASP	CA-CB-CG	5.41	118.01	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	145	PRO	CA-C-N	5.41	127.53	120.28
2	B	145	PRO	C-N-CA	5.41	127.53	120.28
2	H	189	ASP	CA-CB-CG	5.40	118.00	112.60
1	G	33	TYR	N-CA-C	-5.40	101.67	110.20
2	R	126	THR	CA-C-N	5.39	127.50	120.28
2	R	126	THR	C-N-CA	5.39	127.50	120.28
2	R	169	ASP	CA-CB-CG	5.36	117.96	112.60
2	F	189	ASP	CA-CB-CG	5.34	117.94	112.60
2	V	145	PRO	CA-C-N	5.34	127.69	120.38
2	V	145	PRO	C-N-CA	5.34	127.69	120.38
1	U	68	PHE	CA-CB-CG	5.33	119.13	113.80
2	L	214	ASN	CA-C-N	5.32	131.27	121.70
2	L	214	ASN	C-N-CA	5.32	131.27	121.70
1	A	97	THR	N-CA-C	5.31	117.32	108.99
3	k	415	ASN	CA-C-N	5.30	127.92	120.28
3	k	415	ASN	C-N-CA	5.30	127.92	120.28
2	Y	119	VAL	N-CA-C	5.29	115.72	107.99
2	V	100	PRO	N-CA-C	5.28	119.87	111.26
2	V	174	ASP	CA-CB-CG	5.27	117.87	112.60
1	Q	33	TYR	N-CA-C	-5.27	101.87	110.20
2	R	145	PRO	CA-C-N	5.27	127.35	120.28
2	R	145	PRO	C-N-CA	5.27	127.35	120.28
2	B	214	ASN	CA-C-N	5.26	131.17	121.70
2	B	214	ASN	C-N-CA	5.26	131.17	121.70
1	G	43	LYS	N-CA-C	5.24	117.99	109.86
2	D	216	ASN	CA-CB-CG	5.24	117.84	112.60
2	L	189	ASP	CA-CB-CG	5.24	117.84	112.60
1	S	100	ASP	CA-CB-CG	5.23	117.83	112.60
1	S	114	GLU	N-CA-C	5.23	118.25	110.14
2	H	169	ASP	CA-CB-CG	5.23	117.83	112.60
2	J	33	ASP	CA-CB-CG	5.23	117.83	112.60
1	K	88	SER	CA-C-N	5.20	127.77	120.28
1	K	88	SER	C-N-CA	5.20	127.77	120.28
1	E	97	THR	N-CA-C	5.20	117.15	108.99
2	D	72	SER	N-CA-C	-5.20	104.52	108.78
3	i	415	ASN	CA-CB-CG	5.20	117.80	112.60
2	L	100	PRO	N-CA-C	5.19	119.03	111.03
1	S	190	GLN	CA-C-N	5.18	128.07	120.71
1	S	190	GLN	C-N-CA	5.18	128.07	120.71
2	N	214	ASN	CA-C-N	5.18	131.03	121.70
2	N	214	ASN	C-N-CA	5.18	131.03	121.70
3	e	415	ASN	CA-CB-CG	5.16	117.76	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	33	TYR	N-CA-C	-5.16	102.05	110.20
1	I	97	THR	N-CA-C	5.15	117.22	109.23
1	G	100	ASP	CA-CB-CG	5.15	117.75	112.60
2	B	64	PRO	CA-C-N	5.13	127.67	120.28
2	B	64	PRO	C-N-CA	5.13	127.67	120.28
2	P	212	SER	N-CA-C	5.13	116.98	109.24
2	B	83	VAL	N-CA-CB	5.12	118.73	110.13
1	C	98	ARG	N-CA-C	-5.11	106.45	113.30
1	S	76	LYS	CG-CD-CE	5.11	123.06	111.30
2	Y	33	ASP	CA-CB-CG	5.10	117.70	112.60
1	I	98	ARG	N-CA-C	-5.09	106.48	113.30
1	O	97	THR	N-CA-C	5.09	116.98	108.99
1	E	43	LYS	N-CA-C	5.08	117.92	109.94
1	K	21	SER	N-CA-C	5.08	115.71	107.23
2	Y	83	VAL	N-CA-C	5.08	116.23	109.37
1	K	115	THR	CB-CA-C	5.07	117.10	110.06
1	E	100	ASP	CA-CB-CG	5.06	117.66	112.60
2	Y	126	THR	CA-C-N	5.06	130.81	121.70
2	Y	126	THR	C-N-CA	5.06	130.81	121.70
1	Q	87	ARG	CA-C-N	5.03	127.53	120.28
1	Q	87	ARG	C-N-CA	5.03	127.53	120.28
1	E	68	PHE	CA-CB-CG	5.02	118.82	113.80
2	D	215	ARG	CA-C-N	5.01	130.73	121.70
2	D	215	ARG	C-N-CA	5.01	130.73	121.70
1	A	157	ALA	N-CA-C	5.01	117.47	111.71

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	1565	0	1536	7	0
1	C	1554	0	1526	15	0
1	E	1570	0	1541	8	0
1	G	1567	0	1538	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1550	0	1523	11	0
1	K	1546	0	1520	21	0
1	M	1546	0	1520	14	0
1	O	1550	0	1523	10	0
1	Q	1557	0	1530	10	0
1	S	1546	0	1520	13	0
1	U	1554	0	1526	11	0
1	X	1495	0	1472	13	0
2	B	1634	0	1593	8	0
2	D	1642	0	1599	15	0
2	F	1634	0	1593	12	0
2	H	1640	0	1598	7	0
2	J	1634	0	1593	10	0
2	L	1634	0	1593	8	0
2	N	1634	0	1593	11	0
2	P	1634	0	1593	12	0
2	R	1634	0	1593	11	0
2	T	1634	0	1593	12	0
2	V	1615	0	1578	8	0
2	Y	1591	0	1552	10	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	1	0
3	m	97	0	88	1	0
3	o	88	0	80	0	0
3	q	80	0	74	2	0
3	s	89	0	82	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	254	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.

All (254) 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
2:D:94:MET:HE3	2:D:96:THR:HG23	1.59	0.81
1:C:202:SER:HB3	1:I:208:LYS:HB3	1.65	0.76
2:Y:94:MET:HE3	2:Y:96:THR:HG23	1.70	0.73
2:J:44:ARG:NH1	2:J:86:GLU:O	2.23	0.71
2:L:94:MET:HE3	2:L:96:THR:HG23	1.73	0.71
2:V:94:MET:HE3	2:V:96:THR:HG23	1.74	0.70
2:F:94:MET:HE3	2:F:96:THR:HG23	1.75	0.69
2:P:94:MET:HE1	2:P:96:THR:HG23	1.75	0.68
2:J:94:MET:HE3	2:J:96:THR:HG23	1.76	0.68
2:N:94:MET:HE3	2:N:96:THR:HG23	1.76	0.67
2:H:94:MET:HE3	2:H:96:THR:HG23	1.77	0.66
1:K:208:LYS:HB3	1:M:202:SER:HB3	1.75	0.66
2:L:154:ILE:HD11	2:L:183:LEU:HD21	1.78	0.66
2:J:160:ARG:HH21	2:J:163:VAL:HG11	1.62	0.65
2:F:191:GLU:HA	2:F:215:ARG:HH22	1.62	0.65
2:V:191:GLU:HA	2:V:215:ARG:HH22	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:214:ASN:O	2:D:215:ARG:HB2	1.95	0.64
2:Y:127:GLU:O	2:Y:129:LEU:N	2.31	0.63
2:R:94:MET:HE3	2:R:96:THR:HG23	1.80	0.63
2:B:94:MET:HE3	2:B:96:THR:HG23	1.81	0.62
1:G:30:SER:O	1:G:53:ASN:HB2	2.00	0.62
1:U:118:PRO:HB3	1:U:144:TYR:HB3	1.83	0.61
1:M:97:THR:HG21	1:M:102:TRP:CD2	2.37	0.60
2:T:165:ASP:HB3	2:T:179:MET:HE3	1.84	0.59
1:G:118:PRO:HB3	1:G:144:TYR:HB3	1.84	0.59
1:I:118:PRO:HB3	1:I:144:TYR:HB3	1.84	0.59
1:S:118:PRO:HB3	1:S:144:TYR:HB3	1.83	0.59
2:P:94:MET:HE1	2:P:96:THR:CG2	2.33	0.59
1:S:171:SER:HB3	2:Y:159:ARG:HG3	1.84	0.58
1:Q:30:SER:O	1:Q:53:ASN:HB2	2.04	0.57
1:M:30:SER:O	1:M:53:ASN:HB2	2.04	0.57
1:O:30:SER:O	1:O:53:ASN:HB2	2.03	0.57
1:Q:118:PRO:HB3	1:Q:144:TYR:HB3	1.87	0.57
1:X:118:PRO:HB3	1:X:144:TYR:HB3	1.86	0.56
2:T:197:THR:HG23	2:T:210:VAL:HG13	1.88	0.56
2:D:165:ASP:HB3	2:D:179:MET:HE3	1.88	0.56
2:L:165:ASP:HB3	2:L:179:MET:HE3	1.88	0.56
1:U:30:SER:O	1:U:53:ASN:HB2	2.06	0.56
2:N:154:ILE:HD11	2:N:183:LEU:HD21	1.88	0.56
1:A:118:PRO:HB3	1:A:144:TYR:HB3	1.88	0.55
1:O:118:PRO:HB3	1:O:144:TYR:HB3	1.88	0.55
2:F:165:ASP:HB3	2:F:179:MET:HE3	1.89	0.55
1:S:30:SER:O	1:S:53:ASN:HB2	2.06	0.55
1:K:118:PRO:HB3	1:K:144:TYR:HB3	1.89	0.55
1:C:208:LYS:HB3	1:I:202:SER:HB3	1.88	0.55
1:I:30:SER:O	1:I:53:ASN:HB2	2.06	0.55
1:E:118:PRO:HB3	1:E:144:TYR:HB3	1.87	0.55
2:J:165:ASP:HB3	2:J:179:MET:HE3	1.89	0.55
1:X:30:SER:O	1:X:53:ASN:HB2	2.06	0.55
1:X:22:CYS:HB3	1:X:79:LEU:HB3	1.89	0.54
2:B:146:ARG:HD3	2:B:167:VAL:HG11	1.90	0.54
2:N:146:ARG:HD3	2:N:167:VAL:HG11	1.89	0.54
1:C:206:ASP:HB2	1:I:204:LYS:HB2	1.88	0.54
1:O:202:SER:HB3	1:X:208:LYS:HB3	1.89	0.54
1:C:118:PRO:HB3	1:C:144:TYR:HB3	1.89	0.54
2:D:154:ILE:HD11	2:D:183:LEU:HD21	1.89	0.54
2:P:165:ASP:HB3	2:P:179:MET:HE3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:55:SER:O	2:T:56:VAL:HG12	2.07	0.54
1:A:30:SER:O	1:A:53:ASN:HB2	2.07	0.53
2:N:165:ASP:HB3	2:N:179:MET:HE3	1.91	0.53
2:D:190:TYR:CE2	2:D:216:ASN:CB	2.91	0.53
2:R:197:THR:HG23	2:R:210:VAL:HG13	1.91	0.53
1:K:146:PRO:HD2	1:K:200:ALA:CB	2.39	0.53
2:D:190:TYR:CE2	2:D:216:ASN:HB3	2.44	0.53
1:M:118:PRO:HB3	1:M:144:TYR:HB3	1.89	0.53
2:B:165:ASP:HB3	2:B:179:MET:HE3	1.92	0.52
2:R:146:ARG:HD3	2:R:167:VAL:HG11	1.90	0.52
1:U:22:CYS:HB3	1:U:79:LEU:HB3	1.92	0.52
2:H:146:ARG:HG2	2:H:177:TYR:CE1	2.45	0.52
2:J:146:ARG:HD3	2:J:167:VAL:HG11	1.92	0.52
2:F:121:ILE:HD12	2:F:198:CYS:HB2	1.90	0.52
2:T:111:LYS:HA	2:T:144:TYR:OH	2.10	0.52
2:Y:124:PRO:HD3	2:Y:136:VAL:HG22	1.92	0.52
1:Q:122:PRO:HD3	1:Q:207:LYS:HE3	1.92	0.51
2:D:146:ARG:HD3	2:D:167:VAL:HG11	1.91	0.51
2:P:154:ILE:HD11	2:P:183:LEU:HD21	1.92	0.51
1:S:13:GLN:HG2	1:S:16:ARG:HD3	1.92	0.51
1:K:6:GLU:OE1	1:K:103:GLY:HA3	2.10	0.51
1:X:177:THR:HG21	2:Y:139:LEU:HD21	1.93	0.51
2:D:39:ASN:OD1	2:D:54:TYR:HA	2.09	0.51
2:H:154:ILE:HD11	2:H:183:LEU:HD21	1.92	0.51
1:U:158:LEU:HD23	1:U:180:VAL:HG21	1.93	0.51
1:S:87:ARG:HG3	1:S:89:GLU:HB3	1.93	0.51
2:B:154:ILE:HD11	2:B:183:LEU:HD21	1.93	0.51
2:V:151:LYS:HB3	2:V:199:GLU:HB3	1.93	0.51
1:A:91:THR:HG23	1:A:109:THR:HA	1.91	0.51
1:X:154:ASN:HB2	1:X:158:LEU:HD13	1.92	0.50
2:H:165:ASP:HB3	2:H:179:MET:HE3	1.94	0.50
2:F:151:LYS:HB3	2:F:199:GLU:HB3	1.91	0.50
2:R:154:ILE:HD11	2:R:183:LEU:HD21	1.93	0.50
2:L:124:PRO:HD3	2:L:136:VAL:HG22	1.94	0.50
2:N:42:LEU:HB2	2:N:52:LEU:HD11	1.94	0.50
2:R:165:ASP:HB3	2:R:179:MET:HE3	1.94	0.50
1:C:30:SER:O	1:C:53:ASN:HB2	2.11	0.50
1:K:2:VAL:HG13	1:K:27:PHE:CD1	2.48	0.49
2:R:16:GLY:HA2	4:R:320:HOH:O	2.12	0.49
1:X:39:GLN:HB2	1:X:45:LEU:HD23	1.95	0.49
2:V:165:ASP:HB3	2:V:179:MET:HE3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:13:GLN:HG3	1:O:16:ARG:HD3	1.95	0.49
1:E:134:MET:HE3	1:E:181:THR:HG22	1.94	0.49
2:F:154:ILE:HD11	2:F:183:LEU:HD21	1.95	0.49
1:O:41:PRO:O	1:O:42:THR:HB	2.13	0.48
1:G:134:MET:HE3	1:G:181:THR:HG22	1.94	0.48
2:D:190:TYR:CE2	2:D:216:ASN:HB2	2.49	0.48
2:V:154:ILE:HD11	2:V:183:LEU:HD21	1.95	0.48
2:J:154:ILE:HD11	2:J:183:LEU:HD21	1.95	0.48
1:K:63:SER:O	1:K:67:ARG:NH2	2.46	0.48
1:S:22:CYS:HB3	1:S:79:LEU:HB3	1.95	0.48
1:U:2:VAL:HG13	1:U:27:PHE:CD1	2.49	0.48
2:T:35:ASN:HB3	4:T:327:HOH:O	2.14	0.48
1:S:134:MET:HE3	1:S:181:THR:HG22	1.96	0.48
1:K:134:MET:HE3	1:K:181:THR:HG22	1.96	0.47
1:E:2:VAL:HG13	1:E:27:PHE:CD1	2.49	0.47
1:E:91:THR:HG23	1:E:109:THR:HA	1.97	0.47
1:K:30:SER:O	1:K:53:ASN:HB2	2.14	0.47
1:S:2:VAL:HG13	1:S:27:PHE:CD1	2.49	0.47
2:D:151:LYS:HB3	2:D:199:GLU:HB3	1.96	0.47
1:K:115:THR:HA	1:K:145:PHE:O	2.14	0.47
1:E:30:SER:O	1:E:53:ASN:HB2	2.13	0.47
1:I:2:VAL:HG13	1:I:27:PHE:CD1	2.49	0.47
2:J:151:LYS:HB3	2:J:199:GLU:HB3	1.96	0.47
1:X:91:THR:HG23	1:X:109:THR:HA	1.97	0.47
2:F:146:ARG:HD3	2:F:167:VAL:HG11	1.95	0.47
1:A:2:VAL:HG13	1:A:27:PHE:CD1	2.50	0.47
1:X:2:VAL:HG13	1:X:27:PHE:CD1	2.50	0.46
1:A:49:ALA:HA	1:A:59:TYR:O	2.15	0.46
1:O:2:VAL:HG13	1:O:27:PHE:CD1	2.51	0.46
1:Q:134:MET:HE3	1:Q:181:THR:HG22	1.96	0.46
1:E:122:PRO:HD3	1:E:207:LYS:HE3	1.98	0.46
2:L:149:SER:HB3	2:L:201:VAL:HB	1.97	0.46
2:L:151:LYS:HB3	2:L:199:GLU:HB3	1.97	0.46
1:C:49:ALA:HA	1:C:59:TYR:O	2.16	0.46
1:G:49:ALA:HA	1:G:59:TYR:O	2.15	0.46
1:K:83:MET:HE1	1:K:108:VAL:HG21	1.96	0.46
1:M:2:VAL:HG13	1:M:27:PHE:CD1	2.50	0.46
1:U:199:PRO:HD2	4:U:306:HOH:O	2.16	0.46
2:D:94:MET:CE	2:D:96:THR:HG23	2.38	0.46
2:P:147:ASP:O	2:P:202:HIS:CD2	2.68	0.46
1:Q:20:LEU:HG	1:Q:83:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:91:THR:HG23	1:U:109:THR:HA	1.97	0.45
1:C:91:THR:HG23	1:C:109:THR:HA	1.98	0.45
1:S:91:THR:HG23	1:S:109:THR:HA	1.98	0.45
1:X:49:ALA:HA	1:X:59:TYR:O	2.17	0.45
2:R:41:LEU:HD23	2:R:51:LEU:HA	1.98	0.45
2:Y:170:GLN:HB2	2:Y:177:TYR:CZ	2.52	0.45
1:K:91:THR:HG23	1:K:109:THR:HA	1.98	0.45
1:Q:49:ALA:HA	1:Q:59:TYR:O	2.17	0.45
2:H:146:ARG:HD3	2:H:167:VAL:HG11	1.97	0.45
1:M:204:LYS:HG2	4:M:303:HOH:O	2.16	0.45
1:O:91:THR:HG23	1:O:109:THR:HA	1.99	0.45
1:G:91:THR:HG23	1:G:109:THR:HA	1.98	0.45
1:Q:91:THR:HG23	1:Q:109:THR:HA	1.98	0.45
2:P:214:ASN:O	2:P:215:ARG:HB2	2.17	0.45
1:K:9:GLY:HA3	1:K:106:THR:HG23	1.98	0.45
2:P:147:ASP:O	2:P:202:HIS:HD2	2.00	0.45
1:K:122:PRO:HD3	1:K:207:LYS:HE3	1.99	0.45
1:C:11:LEU:HD11	4:C:325:HOH:O	2.17	0.45
1:I:49:ALA:HA	1:I:59:TYR:O	2.17	0.45
2:P:149:SER:HB3	2:P:201:VAL:HB	1.99	0.45
2:T:96:THR:HG23	2:T:100:PRO:HG3	1.99	0.45
2:T:96:THR:HG21	3:s:414:ILE:HG23	1.99	0.45
1:X:138:GLY:HA2	1:X:153:TRP:CH2	2.53	0.44
2:N:151:LYS:HB3	2:N:199:GLU:HB3	1.99	0.44
1:M:91:THR:HG23	1:M:109:THR:HA	2.00	0.44
2:B:194:ASN:O	2:B:214:ASN:HA	2.17	0.44
1:C:2:VAL:HG13	1:C:27:PHE:CD1	2.53	0.44
2:P:151:LYS:HB3	2:P:199:GLU:HB3	2.00	0.44
1:C:134:MET:HE3	1:C:181:THR:HG22	1.99	0.44
2:B:149:SER:HB3	2:B:201:VAL:HB	1.99	0.44
1:O:134:MET:HE3	1:O:181:THR:HG22	1.99	0.44
2:N:151:LYS:HG2	2:N:158:GLU:HG3	2.00	0.44
1:M:49:ALA:HA	1:M:59:TYR:O	2.18	0.44
1:X:13:GLN:HG3	1:X:14:PRO:HD2	2.00	0.44
1:I:134:MET:HE3	1:I:181:THR:HG22	1.98	0.43
2:Y:122:PHE:HA	2:Y:123:PRO:HD3	1.92	0.43
1:C:41:PRO:O	1:C:42:THR:HG22	2.18	0.43
1:K:86:LEU:HG	1:K:110:VAL:HG21	2.00	0.43
2:R:96:THR:O	3:q:415:ASN:HB3	2.18	0.43
2:V:149:SER:HB3	2:V:201:VAL:HB	2.01	0.43
2:N:37:TYR:CG	3:m:415:ASN:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:87:ARG:O	1:I:90:ASP:HB2	2.19	0.43
1:K:60:TYR:CE1	1:K:70:ILE:HG22	2.54	0.43
2:B:151:LYS:HB3	2:B:199:GLU:HB3	2.00	0.43
2:T:94:MET:HE3	2:T:96:THR:OG1	2.18	0.43
2:H:149:SER:HB3	2:H:201:VAL:HB	2.00	0.43
1:O:49:ALA:HA	1:O:59:TYR:O	2.19	0.43
1:Q:121:TYR:CD2	2:R:128:GLN:HG3	2.54	0.43
2:F:124:PRO:HG3	2:F:134:ALA:HB1	2.01	0.43
1:C:146:PRO:HD2	1:C:200:ALA:CB	2.49	0.43
1:E:40:ALA:HB3	1:E:43:LYS:HB2	2.00	0.43
1:S:197:ALA:HB2	1:S:204:LYS:HE2	2.01	0.43
1:U:49:ALA:HA	1:U:59:TYR:O	2.19	0.43
2:N:41:LEU:HD23	2:N:51:LEU:HA	2.00	0.43
1:X:153:TRP:CZ3	1:X:194:CYS:HB3	2.53	0.42
2:B:41:LEU:HD23	2:B:51:LEU:HA	2.00	0.42
2:D:149:SER:HB3	2:D:201:VAL:HB	2.00	0.42
2:J:151:LYS:HG2	2:J:158:GLU:HG3	2.01	0.42
1:K:20:LEU:HG	1:K:83:MET:HE2	2.01	0.42
2:D:146:ARG:HB2	4:D:340:HOH:O	2.19	0.42
2:T:41:LEU:HD23	2:T:51:LEU:HA	2.02	0.42
2:T:146:ARG:HD3	2:T:167:VAL:HG11	2.02	0.42
1:K:202:SER:HB3	1:M:208:LYS:HB3	2.00	0.42
1:A:122:PRO:HD3	1:A:207:LYS:HE3	2.02	0.42
1:K:7:SER:OG	1:K:8:GLY:N	2.53	0.42
1:G:12:VAL:CG2	1:G:18:LEU:HD13	2.48	0.42
2:J:41:LEU:HD23	2:J:51:LEU:HA	2.00	0.42
1:S:49:ALA:HA	1:S:59:TYR:O	2.20	0.42
2:V:41:LEU:HD23	2:V:51:LEU:HA	2.02	0.42
2:P:41:LEU:HD23	2:P:51:LEU:HA	2.01	0.42
2:P:107:LYS:HE3	2:P:109:GLU:HB3	2.02	0.42
1:M:20:LEU:HG	1:M:83:MET:HE2	2.02	0.42
1:U:134:MET:HE3	1:U:181:THR:HG22	2.02	0.42
1:U:154:ASN:HB2	1:U:158:LEU:HD13	2.02	0.42
2:R:66:ARG:NE	2:R:87:ASP:OD2	2.46	0.42
2:T:149:SER:HB3	2:T:201:VAL:HB	2.02	0.42
1:A:169:LEU:HG	1:A:174:TYR:CE1	2.54	0.41
1:C:62:ASP:HA	1:C:65:LYS:HD2	2.00	0.41
1:K:169:LEU:HG	1:K:174:TYR:CE1	2.55	0.41
4:S:304:HOH:O	2:T:127:GLU:HG3	2.19	0.41
1:C:169:LEU:HG	1:C:174:TYR:CE1	2.55	0.41
1:O:115:THR:HA	1:O:145:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:149:SER:HB3	2:N:201:VAL:HB	2.01	0.41
2:L:41:LEU:HD23	2:L:51:LEU:HA	2.02	0.41
1:G:169:LEU:HG	1:G:174:TYR:CE1	2.55	0.41
2:Y:154:ILE:HD11	2:Y:183:LEU:HD21	2.01	0.41
1:E:91:THR:O	1:E:92:ALA:HB2	2.21	0.41
1:K:6:GLU:HG3	1:K:96:CYS:HB3	2.03	0.41
2:P:151:LYS:HG2	2:P:158:GLU:HG3	2.02	0.41
2:Y:129:LEU:O	2:Y:131:THR:N	2.53	0.41
2:R:149:SER:HB3	2:R:201:VAL:HB	2.03	0.41
2:J:149:SER:HB3	2:J:201:VAL:HB	2.02	0.41
2:D:190:TYR:HE2	2:D:216:ASN:HB3	1.86	0.41
2:F:94:MET:CE	2:F:96:THR:HG23	2.48	0.41
2:F:122:PHE:HA	2:F:123:PRO:HD3	1.97	0.41
1:M:134:MET:HE3	1:M:181:THR:HG22	2.02	0.41
1:S:122:PRO:HD3	1:S:207:LYS:HE3	2.03	0.41
2:H:41:LEU:HD23	2:H:51:LEU:HA	2.02	0.41
1:U:169:LEU:HG	1:U:174:TYR:CE1	2.56	0.40
2:L:96:THR:O	3:k:415:ASN:HB3	2.21	0.40
1:C:191:THR:HA	4:C:327:HOH:O	2.21	0.40
1:I:146:PRO:HD2	1:I:200:ALA:CB	2.51	0.40
1:M:22:CYS:HB3	1:M:79:LEU:HB3	2.03	0.40
1:M:153:TRP:CH2	1:M:194:CYS:HB3	2.56	0.40
1:Q:99:MET:HB2	3:q:414:ILE:HD11	2.02	0.40
2:D:128:GLN:HG2	2:D:133:GLY:O	2.21	0.40
2:F:138:CYS:HB2	2:F:152:TRP:CH2	2.56	0.40
2:V:122:PHE:HA	2:V:123:PRO:HD3	1.98	0.40
2:N:122:PHE:HA	2:N:123:PRO:HD3	2.00	0.40
2:F:41:LEU:HD23	2:F:51:LEU:HA	2.03	0.40
1:I:169:LEU:HG	1:I:174:TYR:CE1	2.56	0.40
1:K:17:SER:HB3	1:K:82:GLN:HE22	1.87	0.40
1:Q:115:THR:HA	1:Q:145:PHE:O	2.22	0.40
1:S:171:SER:CB	2:Y:159:ARG:HG3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	12	11
1	I	201/252 (80%)	197 (98%)	3 (2%)	1 (0%)	24	26
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%)	24	26
1	S	200/252 (79%)	196 (98%)	4 (2%)	0	100	100
1	U	201/252 (80%)	197 (98%)	3 (2%)	1 (0%)	24	26
1	X	193/252 (77%)	189 (98%)	2 (1%)	2 (1%)	12	11
2	B	213/220 (97%)	208 (98%)	5 (2%)	0	100	100
2	D	214/220 (97%)	208 (97%)	4 (2%)	2 (1%)	14	13
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%)	3	1
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
All	All	5064/5808 (87%)	4926 (97%)	123 (2%)	15 (0%)	36	41

All (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
2	Y	156	GLY
1	X	43	LYS
2	Y	130	ALA
2	Y	131	THR
2	Y	184	SER
2	Y	9	PRO
1	I	41	PRO
1	U	41	PRO
1	G	41	PRO
1	Q	41	PRO

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	176/208 (85%)	168 (96%)	8 (4%)	24	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	175/208 (84%)	167 (95%)	8 (5%)	24	30
1	E	176/208 (85%)	169 (96%)	7 (4%)	28	36
1	G	176/208 (85%)	168 (96%)	8 (4%)	24	31
1	I	174/208 (84%)	166 (95%)	8 (5%)	24	30
1	K	174/208 (84%)	161 (92%)	13 (8%)	12	13
1	M	174/208 (84%)	164 (94%)	10 (6%)	18	21
1	O	174/208 (84%)	163 (94%)	11 (6%)	16	18
1	Q	175/208 (84%)	165 (94%)	10 (6%)	18	21
1	S	174/208 (84%)	163 (94%)	11 (6%)	16	18
1	U	175/208 (84%)	164 (94%)	11 (6%)	16	18
1	X	167/208 (80%)	158 (95%)	9 (5%)	20	23
2	B	191/196 (97%)	178 (93%)	13 (7%)	14	16
2	D	192/196 (98%)	183 (95%)	9 (5%)	23	29
2	F	191/196 (97%)	179 (94%)	12 (6%)	16	18
2	H	192/196 (98%)	180 (94%)	12 (6%)	16	18
2	J	191/196 (97%)	180 (94%)	11 (6%)	18	21
2	L	191/196 (97%)	179 (94%)	12 (6%)	16	18
2	N	191/196 (97%)	181 (95%)	10 (5%)	21	25
2	P	191/196 (97%)	180 (94%)	11 (6%)	18	21
2	R	191/196 (97%)	180 (94%)	11 (6%)	18	21
2	T	191/196 (97%)	178 (93%)	13 (7%)	14	16
2	V	189/196 (96%)	179 (95%)	10 (5%)	20	24
2	Y	187/196 (95%)	163 (87%)	24 (13%)	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	7
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%)	2	1
3	o	10/11 (91%)	10 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	11 (100%)	0	100	100
All	All	4501/4980 (90%)	4234 (94%)	267 (6%)	18	20

All (267) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	93	THR
1	A	104	GLN
1	A	107	THR
1	A	114	GLU
1	A	135	VAL
1	A	170	GLN
1	A	189	SER
1	C	42	THR
1	C	89	GLU
1	C	93	THR
1	C	107	THR
1	C	170	GLN
1	C	189	SER
1	C	191	THR
1	C	204	LYS
1	E	89	GLU
1	E	93	THR
1	E	104	GLN
1	E	107	THR
1	E	133	SER
1	E	189	SER
1	E	204	LYS
1	G	88	SER
1	G	93	THR
1	G	107	THR
1	G	135	VAL
1	G	170	GLN
1	G	189	SER
1	G	191	THR
1	G	204	LYS
1	I	5	GLN

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Mol	Chain	Res	Type
1	I	89	GLU
1	I	93	THR
1	I	107	THR
1	I	135	VAL
1	I	170	GLN
1	I	189	SER
1	I	191	THR
2	J	1	ASP
2	J	11	LEU
2	J	53	ILE
2	J	86	GLU
2	J	94	MET
2	J	109	GLU
2	J	140	MET
2	J	146	ARG
2	J	160	ARG
2	J	185	LEU
2	J	203	LYS
1	K	5	GLN
1	K	13	GLN
1	K	21	SER
1	K	86	LEU
1	K	89	GLU
1	K	96	CYS
1	K	104	GLN
1	K	106	THR
1	K	107	THR
1	K	135	VAL
1	K	170	GLN
1	K	189	SER
1	K	204	LYS
1	M	13	GLN
1	M	16	ARG
1	M	89	GLU
1	M	93	THR
1	M	96	CYS
1	M	107	THR
1	M	135	VAL
1	M	170	GLN
1	M	189	SER
1	M	204	LYS
1	O	5	GLN

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Mol	Chain	Res	Type
1	O	13	GLN
1	O	89	GLU
1	O	93	THR
1	O	107	THR
1	O	135	VAL
1	O	170	GLN
1	O	171	SER
1	O	189	SER
1	O	195	ASN
1	O	204	LYS
1	Q	43	LYS
1	Q	78	THR
1	Q	96	CYS
1	Q	107	THR
1	Q	133	SER
1	Q	135	VAL
1	Q	170	GLN
1	Q	189	SER
1	Q	191	THR
1	Q	207	LYS
1	S	13	GLN
1	S	61	ARG
1	S	89	GLU
1	S	93	THR
1	S	104	GLN
1	S	107	THR
1	S	114	GLU
1	S	135	VAL
1	S	189	SER
1	S	191	THR
1	S	204	LYS
1	U	7	SER
1	U	89	GLU
1	U	93	THR
1	U	107	THR
1	U	133	SER
1	U	135	VAL
1	U	170	GLN
1	U	189	SER
1	U	191	THR
1	U	204	LYS
1	U	207	LYS

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Mol	Chain	Res	Type
1	X	5	GLN
1	X	77	SER
1	X	93	THR
1	X	107	THR
1	X	135	VAL
1	X	170	GLN
1	X	180	VAL
1	X	192	VAL
1	X	196	VAL
2	B	1	ASP
2	B	7	THR
2	B	11	LEU
2	B	53	ILE
2	B	83	VAL
2	B	86	GLU
2	B	94	MET
2	B	109	GLU
2	B	140	MET
2	B	146	ARG
2	B	161	ASP
2	B	185	LEU
2	B	203	LYS
2	D	1	ASP
2	D	11	LEU
2	D	53	ILE
2	D	94	MET
2	D	109	GLU
2	D	140	MET
2	D	146	ARG
2	D	203	LYS
2	D	207	SER
2	F	1	ASP
2	F	11	LEU
2	F	86	GLU
2	F	94	MET
2	F	109	GLU
2	F	140	MET
2	F	146	ARG
2	F	151	LYS
2	F	185	LEU
2	F	203	LYS
2	F	207	SER

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Mol	Chain	Res	Type
2	F	215	ARG
2	H	1	ASP
2	H	11	LEU
2	H	53	ILE
2	H	86	GLU
2	H	94	MET
2	H	109	GLU
2	H	140	MET
2	H	146	ARG
2	H	185	LEU
2	H	203	LYS
2	H	207	SER
2	H	215	ARG
2	L	11	LEU
2	L	53	ILE
2	L	94	MET
2	L	109	GLU
2	L	127	GLU
2	L	131	THR
2	L	140	MET
2	L	146	ARG
2	L	185	LEU
2	L	203	LYS
2	L	211	LYS
2	L	214	ASN
2	N	1	ASP
2	N	11	LEU
2	N	53	ILE
2	N	86	GLU
2	N	94	MET
2	N	109	GLU
2	N	140	MET
2	N	146	ARG
2	N	211	LYS
2	N	214	ASN
2	P	1	ASP
2	P	11	LEU
2	P	53	ILE
2	P	86	GLU
2	P	94	MET
2	P	109	GLU
2	P	140	MET

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Mol	Chain	Res	Type
2	P	146	ARG
2	P	161	ASP
2	P	185	LEU
2	P	212	SER
2	R	1	ASP
2	R	11	LEU
2	R	53	ILE
2	R	86	GLU
2	R	94	MET
2	R	109	GLU
2	R	140	MET
2	R	146	ARG
2	R	185	LEU
2	R	203	LYS
2	R	215	ARG
2	T	1	ASP
2	T	11	LEU
2	T	53	ILE
2	T	74	THR
2	T	86	GLU
2	T	94	MET
2	T	109	GLU
2	T	140	MET
2	T	146	ARG
2	T	185	LEU
2	T	203	LYS
2	T	211	LYS
2	T	215	ARG
2	V	1	ASP
2	V	11	LEU
2	V	53	ILE
2	V	86	GLU
2	V	94	MET
2	V	109	GLU
2	V	140	MET
2	V	146	ARG
2	V	151	LYS
2	V	185	LEU
2	Y	1	ASP
2	Y	8	THR
2	Y	11	LEU
2	Y	21	ILE

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Mol	Chain	Res	Type
2	Y	25	SER
2	Y	35	ASN
2	Y	41	LEU
2	Y	53	ILE
2	Y	83	VAL
2	Y	94	MET
2	Y	109	GLU
2	Y	126	THR
2	Y	127	GLU
2	Y	129	LEU
2	Y	157	THR
2	Y	158	GLU
2	Y	159	ARG
2	Y	161	ASP
2	Y	181	SER
2	Y	191	GLU
2	Y	195	LEU
2	Y	197	THR
2	Y	203	LYS
2	Y	207	SER
3	a	422	VAL
3	e	422	VAL
3	i	423	ASN
3	m	422	VAL
3	m	423	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	163	HIS
1	C	170	GLN
1	G	170	GLN
1	I	170	GLN
1	K	5	GLN
1	K	13	GLN
1	K	39	GLN
1	K	82	GLN
1	K	170	GLN
1	M	170	GLN
1	O	13	GLN
1	S	170	GLN
1	U	13	GLN

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Mol	Chain	Res	Type
1	U	170	GLN
2	B	194	ASN
2	D	98	HIS
2	D	142	ASN
2	F	27	GLN
2	H	27	GLN
2	L	27	GLN
2	L	43	GLN
2	L	47	GLN
2	P	214	ASN
2	R	27	GLN
2	R	43	GLN
2	R	65	ASN
2	T	47	GLN
2	V	27	GLN
2	V	35	ASN
2	Y	50	GLN
2	Y	98	HIS
2	Y	193	HIS

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	207/252 (82%)	0.20	1 (0%) 87 86	21, 35, 49, 66	0
1	C	205/252 (81%)	0.13	5 (2%) 59 57	20, 32, 51, 80	0
1	E	208/252 (82%)	0.39	6 (2%) 53 51	21, 37, 57, 79	0
1	G	207/252 (82%)	0.44	2 (0%) 79 78	22, 41, 62, 84	0
1	I	205/252 (81%)	0.23	2 (0%) 79 78	23, 36, 52, 69	0
1	K	204/252 (80%)	0.88	17 (8%) 17 15	28, 48, 71, 93	0
1	M	204/252 (80%)	0.77	8 (3%) 43 40	29, 46, 63, 78	0
1	O	205/252 (81%)	0.51	7 (3%) 48 45	23, 40, 61, 75	0
1	Q	206/252 (81%)	0.85	17 (8%) 17 15	25, 46, 73, 84	0
1	S	204/252 (80%)	0.18	3 (1%) 72 70	18, 34, 55, 78	0
1	U	205/252 (81%)	0.89	14 (6%) 23 20	24, 49, 73, 103	0
1	X	199/252 (78%)	0.13	4 (2%) 65 63	18, 34, 54, 87	0
2	B	215/220 (97%)	0.22	2 (0%) 81 79	18, 35, 59, 74	0
2	D	216/220 (98%)	0.12	3 (1%) 73 72	18, 31, 55, 87	0
2	F	215/220 (97%)	0.26	8 (3%) 45 42	20, 34, 62, 90	0
2	H	216/220 (98%)	0.13	3 (1%) 73 72	18, 35, 56, 69	0
2	J	215/220 (97%)	0.14	1 (0%) 87 86	18, 33, 56, 75	0
2	L	215/220 (97%)	0.31	4 (1%) 66 64	22, 39, 57, 68	0
2	N	215/220 (97%)	0.77	7 (3%) 49 46	30, 49, 68, 80	0
2	P	215/220 (97%)	0.23	1 (0%) 87 86	23, 37, 61, 75	0
2	R	215/220 (97%)	1.09	28 (13%) 7 5	30, 54, 78, 88	0
2	T	215/220 (97%)	0.77	21 (9%) 13 10	21, 44, 76, 90	0
2	V	212/220 (96%)	1.10	41 (19%) 3 2	27, 52, 88, 106	0
2	Y	210/220 (95%)	0.26	14 (6%) 24 21	15, 33, 72, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	a	12/12 (100%)	0.11	1 (8%) 17 15	23, 31, 50, 79	0
3	c	11/12 (91%)	0.28	1 (9%) 15 12	25, 28, 51, 52	0
3	e	11/12 (91%)	0.38	1 (9%) 15 12	23, 30, 56, 56	0
3	g	12/12 (100%)	0.05	0 100 100	26, 30, 46, 48	0
3	i	12/12 (100%)	0.16	0 100 100	30, 34, 50, 65	0
3	k	11/12 (91%)	0.70	1 (9%) 15 12	24, 36, 58, 59	0
3	m	12/12 (100%)	1.01	1 (8%) 17 15	39, 47, 69, 78	0
3	o	11/12 (91%)	0.75	1 (9%) 15 12	34, 43, 59, 61	0
3	q	10/12 (83%)	1.10	1 (10%) 12 10	42, 50, 56, 68	0
3	s	11/12 (91%)	0.21	0 100 100	27, 32, 45, 48	0
3	u	10/12 (83%)	0.63	1 (10%) 12 10	32, 37, 40, 54	0
3	x	12/12 (100%)	0.11	0 100 100	23, 29, 57, 59	0
All	All	5168/5808 (88%)	0.46	227 (4%) 39 36	15, 40, 67, 106	0

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	75	ALA	5.1
1	G	126	GLY	5.0
3	e	422	VAL	4.4
2	V	209	VAL	4.4
1	U	157	ALA	4.2
2	T	131	THR	4.1
2	Y	129	LEU	4.0
1	Q	2	VAL	3.9
3	q	422	VAL	3.9
2	V	201	VAL	3.7
2	Y	156	GLY	3.6
3	k	422	VAL	3.6
2	Y	9	PRO	3.6
2	R	85	ALA	3.4
2	V	154	ILE	3.4
2	D	216	ASN	3.4
1	Q	26	GLY	3.4
1	K	20	LEU	3.4
2	V	162	GLY	3.4
2	R	115	ALA	3.3
2	R	119	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	V	115	ALA	3.3
2	V	150	VAL	3.3
2	V	8	THR	3.2
2	V	205	SER	3.2
1	M	41	PRO	3.2
1	E	128	ALA	3.1
2	D	207	SER	3.1
2	L	35	ASN	3.1
2	N	133	GLY	3.1
2	V	113	ALA	3.1
2	T	204	THR	3.1
1	Q	56	GLY	3.1
2	R	133	GLY	3.1
2	T	130	ALA	3.0
2	Y	127	GLU	3.0
3	u	422	VAL	3.0
2	N	1	ASP	3.0
2	R	134	ALA	2.9
2	V	131	THR	2.9
2	T	154	ILE	2.8
2	V	132	GLY	2.8
2	V	208	PRO	2.8
2	T	196	TYR	2.8
2	T	195	LEU	2.8
2	R	152	TRP	2.8
2	H	132	GLY	2.8
1	O	89	GLU	2.8
1	O	212	ARG	2.8
1	S	42	THR	2.7
1	Q	54	SER	2.7
1	Q	172	GLY	2.7
1	K	18	LEU	2.7
2	V	164	LEU	2.7
1	Q	31	ASP	2.7
3	c	422	VAL	2.7
1	K	89	GLU	2.6
1	X	184	SER	2.6
2	V	206	SER	2.6
1	U	173	LEU	2.6
1	U	145	PHE	2.6
2	F	215	ARG	2.6
1	C	55	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	U	204	LYS	2.6
2	V	163	VAL	2.6
2	R	154	ILE	2.6
1	M	89	GLU	2.6
1	M	125	PRO	2.6
2	F	131	THR	2.6
2	R	132	GLY	2.6
2	R	204	THR	2.6
2	V	210	VAL	2.6
1	K	80	TYR	2.6
2	Y	157	THR	2.5
1	Q	185	SER	2.5
2	R	173	LYS	2.5
2	V	203	LYS	2.5
2	V	148	ILE	2.5
2	V	214	ASN	2.5
2	V	195	LEU	2.5
1	X	128	ALA	2.5
2	T	198	CYS	2.5
2	V	202	HIS	2.5
1	Q	127	THR	2.5
2	Y	186	THR	2.5
1	U	160	SER	2.5
2	R	213	PHE	2.5
2	T	192	SER	2.5
2	T	144	TYR	2.5
1	K	86	LEU	2.5
1	Q	24	ALA	2.5
2	V	133	GLY	2.5
1	K	107	THR	2.4
1	U	186	THR	2.4
1	E	7	SER	2.4
1	K	21	SER	2.4
2	N	56	VAL	2.4
1	K	11	LEU	2.4
2	V	190	TYR	2.4
2	L	188	ALA	2.4
2	V	204	THR	2.4
2	T	206	SER	2.4
2	V	207	SER	2.4
1	U	162	VAL	2.4
2	R	83	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	V	153	LYS	2.4
2	Y	193	HIS	2.4
1	U	213	ASN	2.4
2	T	214	ASN	2.4
1	K	15	GLY	2.4
1	O	126	GLY	2.4
2	R	188	ALA	2.4
1	U	18	LEU	2.4
1	K	74	ASN	2.4
1	U	89	GLU	2.4
1	E	42	THR	2.4
2	F	190	TYR	2.3
2	V	196	TYR	2.3
2	R	64	PRO	2.3
2	H	133	GLY	2.3
2	N	8	THR	2.3
2	Y	184	SER	2.3
1	Q	64	VAL	2.3
2	B	198	CYS	2.3
1	S	170	GLN	2.3
2	F	129	LEU	2.3
2	Y	158	GLU	2.3
1	I	41	PRO	2.3
3	o	416	THR	2.3
1	X	171	SER	2.3
2	V	180	SER	2.3
2	B	210	VAL	2.3
1	S	169	LEU	2.3
1	U	169	LEU	2.3
1	G	213	ASN	2.3
2	V	9	PRO	2.3
1	Q	55	GLY	2.3
2	V	152	TRP	2.3
2	V	116	ALA	2.3
1	M	70	ILE	2.3
2	R	63	VAL	2.3
2	V	119	VAL	2.3
1	O	86	LEU	2.3
2	R	185	LEU	2.3
1	Q	75	ALA	2.3
2	F	160	ARG	2.3
2	V	130	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	N	7	THR	2.3
1	K	17	SER	2.3
2	D	206	SER	2.3
1	C	168	VAL	2.3
1	Q	4	LEU	2.2
2	T	185	LEU	2.2
2	T	209	VAL	2.3
1	K	73	ASP	2.2
3	a	423	ASN	2.2
1	M	56	GLY	2.2
1	K	190	GLN	2.2
2	Y	206	SER	2.2
2	T	88	LEU	2.2
3	m	422	VAL	2.2
2	P	215	ARG	2.2
2	T	215	ARG	2.2
1	K	19	LYS	2.2
2	V	129	LEU	2.2
1	O	29	PHE	2.2
1	Q	58	PHE	2.2
2	R	194	ASN	2.2
2	Y	155	ASP	2.2
2	R	205	SER	2.2
2	Y	7	THR	2.2
2	L	65	ASN	2.2
1	E	127	THR	2.2
1	M	113	ALA	2.2
2	R	157	THR	2.2
2	T	14	THR	2.2
1	U	174	TYR	2.1
2	R	215	ARG	2.1
2	T	155	ASP	2.1
1	Q	3	LYS	2.1
1	Q	65	LYS	2.1
2	F	27	GLN	2.1
1	K	77	SER	2.1
2	F	207	SER	2.1
2	N	10	THR	2.1
1	E	212	ARG	2.1
2	L	195	LEU	2.1
2	R	110	LEU	2.1
2	T	164	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	2	VAL	2.1
2	V	213	PHE	2.1
1	C	172	GLY	2.1
1	U	150	THR	2.1
2	R	24	ARG	2.1
2	R	107	LYS	2.1
2	V	147	ASP	2.1
1	A	156	GLY	2.1
1	K	25	SER	2.1
2	H	0	SER	2.1
2	V	188	ALA	2.1
1	X	158	LEU	2.1
2	N	27	GLN	2.1
2	R	59	LEU	2.1
2	R	88	LEU	2.1
1	M	210	VAL	2.1
1	Q	161	GLY	2.1
1	U	56	GLY	2.1
2	R	146	ARG	2.1
2	T	159	ARG	2.1
2	Y	160	ARG	2.1
2	V	173	LYS	2.0
2	J	192	SER	2.0
2	V	7	THR	2.0
1	C	75	ALA	2.0
1	E	24	ALA	2.0
1	O	11	LEU	2.0
2	F	209	VAL	2.0
2	R	209	VAL	2.0
1	I	126	GLY	2.0
1	O	68	PHE	2.0
2	T	207	SER	2.0
2	Y	8	THR	2.0
1	C	170	GLN	2.0
2	T	193	HIS	2.0
2	R	129	LEU	2.0
2	V	185	LEU	2.0
2	V	117	PRO	2.0

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 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.