



# Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2026 – 08:15 PM EDT

PDB ID : 9ZM7 / pdb\_00009zm7  
Title : Crystal structure of Fab 7160 in complex with junctional region from circumsporozoite protein  
Authors : Jain, M.; Wilson, I.A.  
Deposited on : 2025-12-09  
Resolution : 2.30 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](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>.

---

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

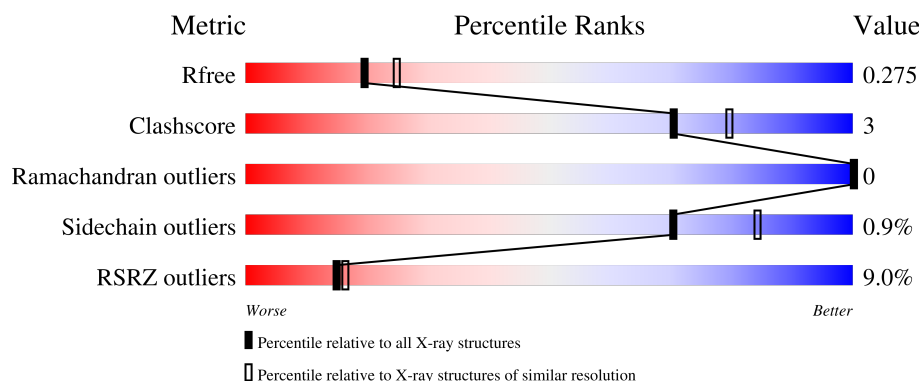
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	230	<div> <div>4%</div> <div>91%</div> <div>5%</div> <div>.</div> </div>
1	D	230	<div> <div>%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	G	230	<div> <div>7%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>
1	I	230	<div> <div>3%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	M	230	<div> <div>12%</div> <div>86%</div> <div>8%</div> <div>6%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	P	230	
1	S	230	
1	V	230	
2	B	219	
2	E	219	
2	H	219	
2	J	219	
2	N	219	
2	Q	219	
2	T	219	
2	W	219	
3	C	16	
3	F	16	
3	K	16	
3	L	16	
3	O	16	
3	R	16	
3	U	16	
3	X	16	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27733 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 Fab 7160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	221	Total	C	N	O	S	0	0	0
			1648	1043	277	322	6			
1	A	221	Total	C	N	O	S	0	0	0
			1648	1043	277	322	6			
1	D	222	Total	C	N	O	S	0	0	0
			1655	1047	278	324	6			
1	G	221	Total	C	N	O	S	0	0	0
			1648	1043	277	322	6			
1	M	217	Total	C	N	O	S	0	0	0
			1623	1029	272	316	6			
1	P	218	Total	C	N	O	S	0	0	0
			1627	1031	273	317	6			
1	S	215	Total	C	N	O	S	0	0	0
			1611	1021	270	314	6			
1	V	221	Total	C	N	O	S	0	0	0
			1649	1044	277	322	6			

- Molecule 2 is a protein called Light Chain of Fab 7160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	219	Total	C	N	O	S	0	0	0
			1703	1070	285	341	7			
2	B	218	Total	C	N	O	S	0	0	0
			1697	1067	284	340	6			
2	E	219	Total	C	N	O	S	0	0	0
			1703	1070	285	341	7			
2	H	219	Total	C	N	O	S	0	0	0
			1703	1070	285	341	7			
2	N	219	Total	C	N	O	S	0	0	0
			1703	1070	285	341	7			
2	Q	218	Total	C	N	O	S	0	0	0
			1697	1067	284	340	6			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	214	Total	C	N	O	S	0	0	0
			1661	1042	276	336	7			
2	W	219	Total	C	N	O	S	0	0	0
			1703	1070	285	341	7			

- Molecule 3 is a protein called Circumsporozoite protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	13	Total	C	N	O	0	0	0
			96	56	18	22			
3	C	11	Total	C	N	O	0	0	0
			81	47	15	19			
3	F	12	Total	C	N	O	0	0	0
			88	52	16	20			
3	L	12	Total	C	N	O	0	0	0
			88	52	16	20			
3	O	12	Total	C	N	O	0	0	0
			88	52	16	20			
3	R	12	Total	C	N	O	0	0	0
			88	52	16	20			
3	U	12	Total	C	N	O	0	0	0
			88	52	16	20			
3	X	14	Total	C	N	O	0	0	0
			101	59	19	23			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	30	Total	O	0	0
			30	30		
4	J	20	Total	O	0	0
			20	20		
4	K	1	Total	O	0	0
			1	1		
4	A	27	Total	O	0	0
			27	27		
4	B	26	Total	O	0	0
			26	26		
4	C	1	Total	O	0	0
			1	1		
4	D	26	Total	O	0	0
			26	26		

*Continued on next page...*

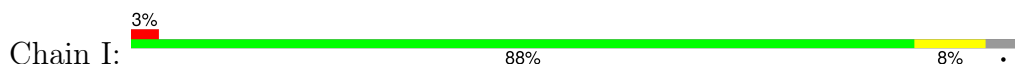
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	32	Total 32	O 32	0	0
4	F	2	Total 2	O 2	0	0
4	G	22	Total 22	O 22	0	0
4	H	12	Total 12	O 12	0	0
4	L	2	Total 2	O 2	0	0
4	M	9	Total 9	O 9	0	0
4	N	4	Total 4	O 4	0	0
4	O	1	Total 1	O 1	0	0
4	P	13	Total 13	O 13	0	0
4	Q	23	Total 23	O 23	0	0
4	R	1	Total 1	O 1	0	0
4	S	33	Total 33	O 33	0	0
4	T	16	Total 16	O 16	0	0
4	U	3	Total 3	O 3	0	0
4	V	23	Total 23	O 23	0	0
4	W	8	Total 8	O 8	0	0
4	X	1	Total 1	O 1	0	0

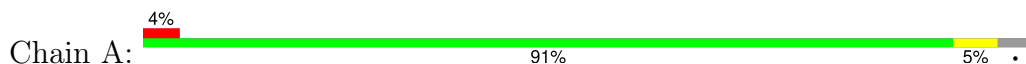
### 3 Residue-property plots [i](#)

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.

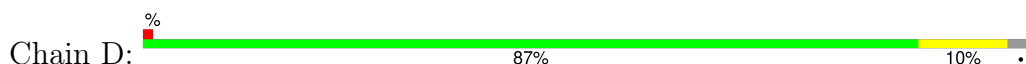
- Molecule 1: Heavy Chain of Fab 7160



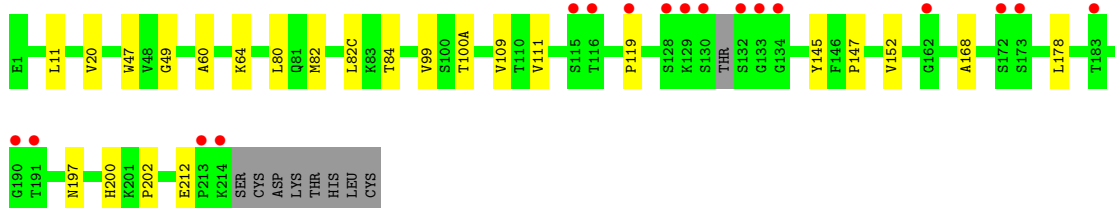
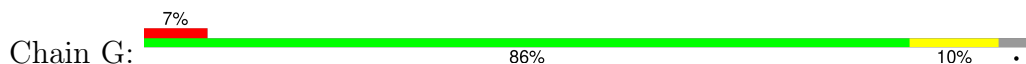
- Molecule 1: Heavy Chain of Fab 7160



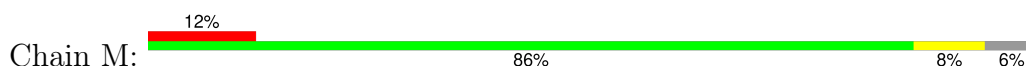
- Molecule 1: Heavy Chain of Fab 7160

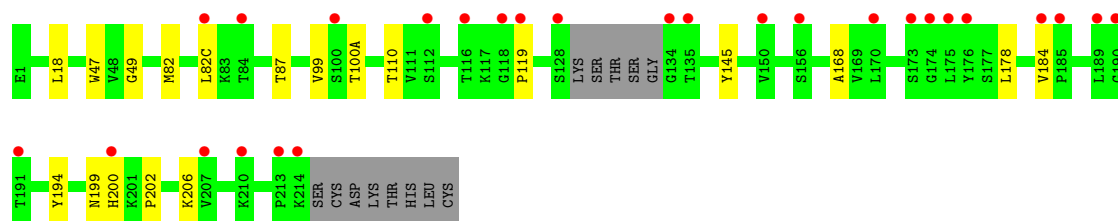


- Molecule 1: Heavy Chain of Fab 7160

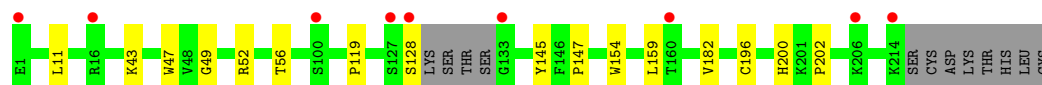
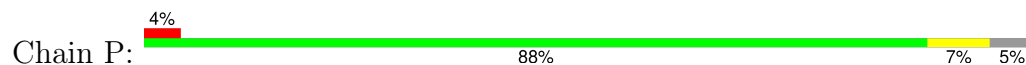


- Molecule 1: Heavy Chain of Fab 7160

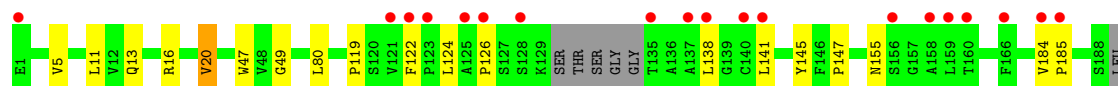
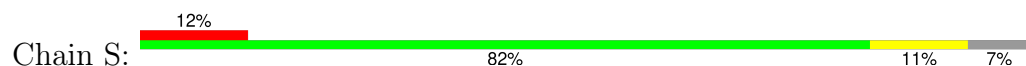




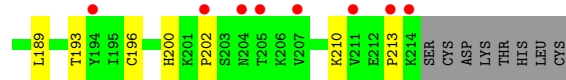
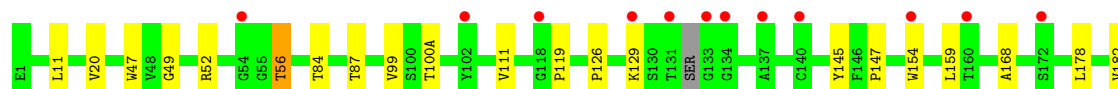
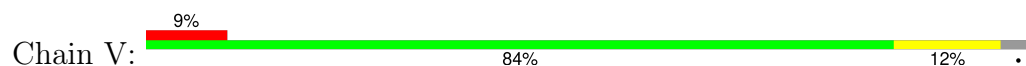
• Molecule 1: Heavy Chain of Fab 7160



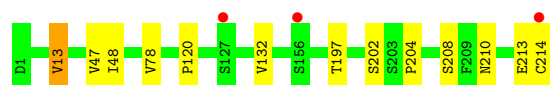
• Molecule 1: Heavy Chain of Fab 7160



• Molecule 1: Heavy Chain of Fab 7160



• Molecule 2: Light Chain of Fab 7160



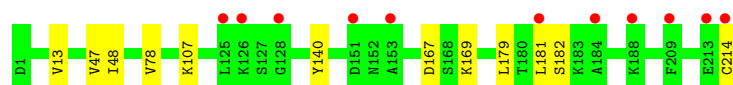
• Molecule 2: Light Chain of Fab 7160



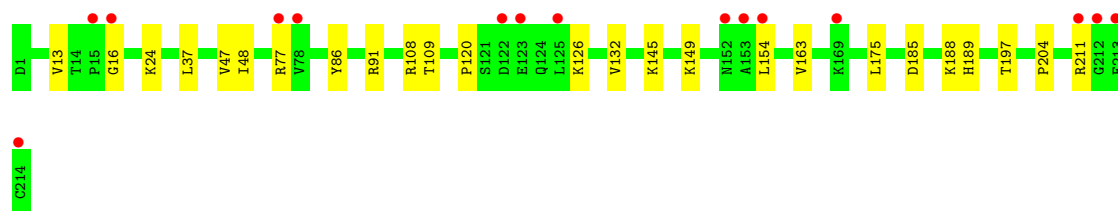
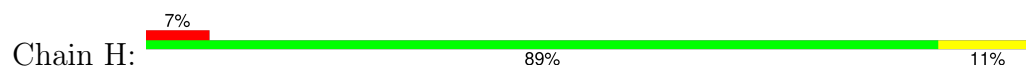




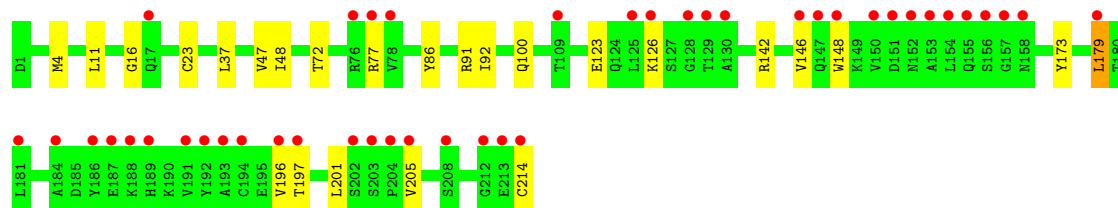
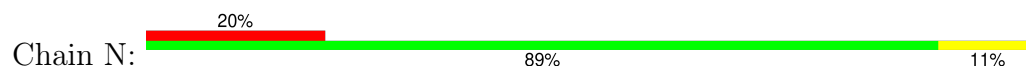
- Molecule 2: Light Chain of Fab 7160



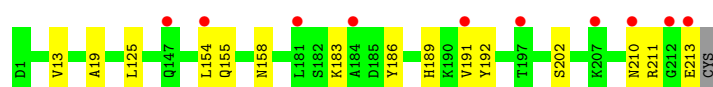
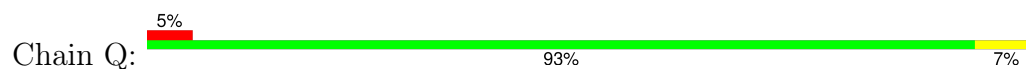
- Molecule 2: Light Chain of Fab 7160



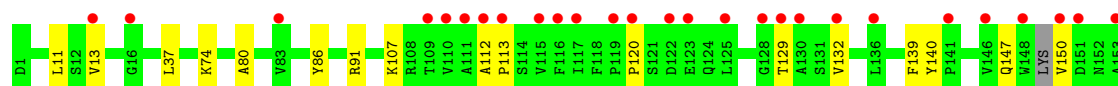
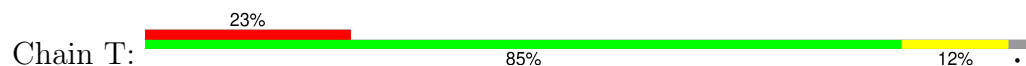
- Molecule 2: Light Chain of Fab 7160

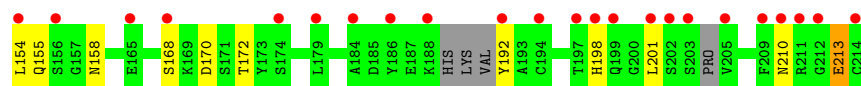


- Molecule 2: Light Chain of Fab 7160

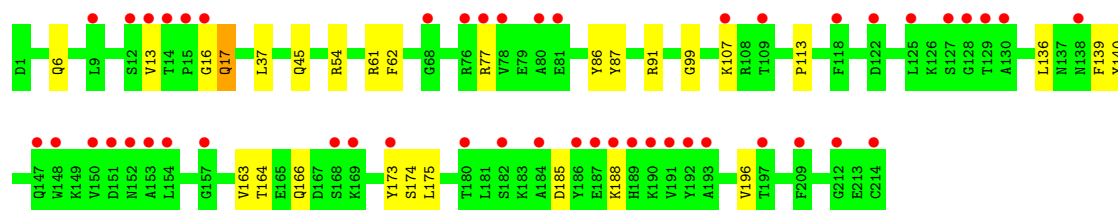
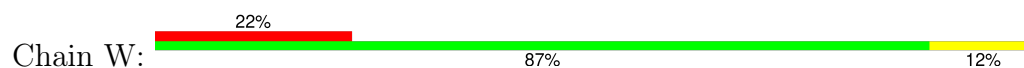


- Molecule 2: Light Chain of Fab 7160

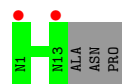
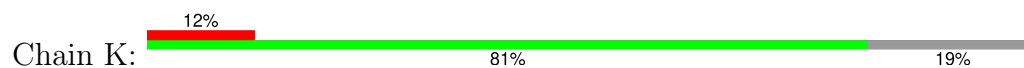




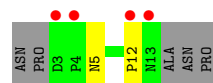
- Molecule 2: Light Chain of Fab 7160



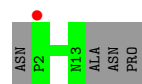
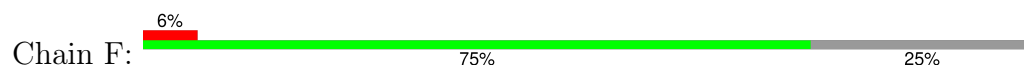
- Molecule 3: Circumsporozoite protein



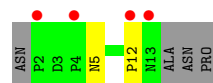
- Molecule 3: Circumsporozoite protein



- Molecule 3: Circumsporozoite protein

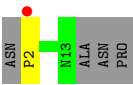


- Molecule 3: Circumsporozoite protein

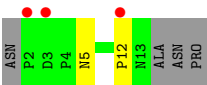


- Molecule 3: Circumsporozoite protein

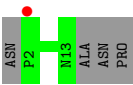




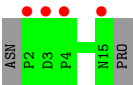
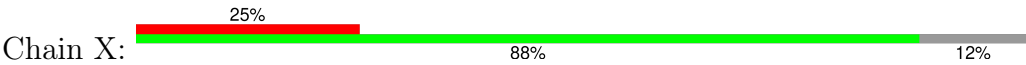
● Molecule 3: Circumsporozoite protein



● Molecule 3: Circumsporozoite protein



● Molecule 3: Circumsporozoite protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.19Å 105.13Å 405.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.30 29.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.88-2.30) 95.9 (29.88-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, $R_{free}$	0.229 , 0.275 0.229 , 0.275	Depositor DCC
$R_{free}$ test set	2000 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 26.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	27733	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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

### 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	0.11	0/1687	0.28	0/2294
1	D	0.11	0/1695	0.28	0/2307
1	G	0.11	0/1687	0.28	0/2294
1	I	0.11	0/1687	0.29	0/2294
1	M	0.10	0/1662	0.27	0/2262
1	P	0.10	0/1666	0.28	0/2267
1	S	0.13	0/1649	0.30	0/2243
1	V	0.12	0/1688	0.29	0/2296
2	B	0.10	0/1734	0.28	0/2354
2	E	0.10	0/1740	0.30	0/2362
2	H	0.09	0/1740	0.29	0/2362
2	J	0.10	0/1740	0.30	0/2362
2	N	0.12	0/1740	0.30	0/2362
2	Q	0.11	0/1734	0.30	0/2354
2	T	0.13	0/1693	0.30	0/2294
2	W	0.11	0/1740	0.30	0/2362
3	C	0.12	0/83	0.30	0/116
3	F	0.10	0/91	0.28	0/127
3	K	0.11	0/99	0.28	0/139
3	L	0.11	0/91	0.31	0/127
3	O	0.15	0/91	0.37	0/127
3	R	0.12	0/91	0.27	0/127
3	U	0.11	0/91	0.29	0/127
3	X	0.10	0/104	0.31	0/145
All	All	0.11	0/28023	0.29	0/38104

There are no bond length outliers.

There are no bond angle outliers.

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	1648	0	1629	6	0
1	D	1655	0	1637	11	0
1	G	1648	0	1629	13	0
1	I	1648	0	1629	10	0
1	M	1623	0	1603	11	0
1	P	1627	0	1606	8	0
1	S	1611	0	1588	23	0
1	V	1649	0	1631	18	0
2	B	1697	0	1659	7	0
2	E	1703	0	1664	5	0
2	H	1703	0	1664	14	0
2	J	1703	0	1664	6	0
2	N	1703	0	1664	14	0
2	Q	1697	0	1659	8	0
2	T	1661	0	1612	15	0
2	W	1703	0	1664	16	0
3	C	81	0	66	2	0
3	F	88	0	74	0	0
3	K	96	0	82	0	0
3	L	88	0	74	1	0
3	O	88	0	74	1	0
3	R	88	0	74	1	0
3	U	88	0	74	0	0
3	X	101	0	85	0	0
4	A	27	0	0	0	0
4	B	26	0	0	0	0
4	C	1	0	0	0	0
4	D	26	0	0	0	0
4	E	32	0	0	0	0
4	F	2	0	0	0	0
4	G	22	0	0	0	0
4	H	12	0	0	0	0
4	I	30	0	0	0	0
4	J	20	0	0	0	0
4	K	1	0	0	0	0
4	L	2	0	0	0	0
4	M	9	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	4	0	0	0	0
4	O	1	0	0	0	0
4	P	13	0	0	0	0
4	Q	23	0	0	0	0
4	R	1	0	0	0	0
4	S	33	0	0	0	0
4	T	16	0	0	0	0
4	U	3	0	0	0	0
4	V	23	0	0	0	0
4	W	8	0	0	0	0
4	X	1	0	0	0	0
All	All	27733	0	26805	186	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 (186) 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:S:126:PRO:HB3	1:S:138:LEU:CD2	2.06	0.86
1:I:16:ARG:HD3	1:I:17:SER:H	1.43	0.82
1:V:87:THR:HG22	1:V:111:VAL:H	1.42	0.82
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.77	0.66
2:T:210:ASN:HB2	2:T:213:GLU:HB2	1.76	0.66
2:Q:155:GLN:HB3	2:Q:158:ASN:HD21	1.61	0.65
1:S:119:PRO:HB3	1:S:145:TYR:HB3	1.77	0.65
1:V:193:THR:HG23	1:V:210:LYS:HD2	1.78	0.64
1:S:124:LEU:HD21	1:S:141:LEU:HB2	1.79	0.64
1:V:159:LEU:HD21	1:V:182:VAL:HG21	1.78	0.64
2:J:13:VAL:HG11	2:J:78:VAL:HG21	1.82	0.62
1:A:193:THR:HG23	1:A:210:LYS:HE3	1.82	0.62
1:P:119:PRO:HB3	1:P:145:TYR:HB3	1.80	0.62
1:G:168:ALA:HB2	1:G:178:LEU:HD23	1.82	0.62
3:C:5:ASN:HD21	3:C:12:PRO:HB3	1.66	0.60
1:P:11:LEU:HB2	1:P:147:PRO:HG3	1.83	0.60
2:W:6:GLN:HE22	2:W:87:TYR:HA	1.64	0.60
2:J:197:THR:HG22	2:J:204:PRO:HB3	1.84	0.60
2:T:80:ALA:HB1	2:T:168:SER:O	2.01	0.60
1:I:119:PRO:HB3	1:I:145:TYR:HB3	1.83	0.59
1:S:126:PRO:CG	1:S:138:LEU:HD22	2.32	0.59
1:V:119:PRO:HB3	1:V:145:TYR:HB3	1.83	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:MET:HB3	1:G:82(C):LEU:HD21	1.85	0.59
2:J:47:VAL:HG12	2:J:48:ILE:HG13	1.85	0.58
2:H:47:VAL:HG12	2:H:48:ILE:HG13	1.85	0.58
1:G:119:PRO:HB3	1:G:145:TYR:HB3	1.85	0.58
1:V:129:LYS:H	1:V:129:LYS:HD2	1.67	0.58
2:H:16:GLY:HA2	2:H:77:ARG:HD2	1.84	0.58
2:E:47:VAL:HG12	2:E:48:ILE:HG13	1.85	0.58
2:H:197:THR:HG22	2:H:204:PRO:HB3	1.84	0.58
2:T:120:PRO:HD3	2:T:132:VAL:HG22	1.87	0.57
1:M:119:PRO:HB3	1:M:145:TYR:HB3	1.86	0.57
2:B:197:THR:HG22	2:B:204:PRO:HB3	1.86	0.57
2:W:16:GLY:HA2	2:W:77:ARG:HD2	1.86	0.57
1:S:20:VAL:HG13	1:S:80:LEU:HB3	1.87	0.56
2:B:6:GLN:H	2:B:100:GLN:NE2	2.03	0.56
2:Q:125:LEU:HB3	2:Q:183:LYS:HE3	1.87	0.56
2:W:185:ASP:HA	2:W:188:LYS:HE2	1.87	0.56
1:S:126:PRO:CB	1:S:138:LEU:CD2	2.81	0.56
1:V:126:PRO:HG2	1:V:213:PRO:HA	1.88	0.56
1:G:200:HIS:CE1	1:G:202:PRO:HG2	2.41	0.55
2:W:113:PRO:HB3	2:W:139:PHE:HB3	1.90	0.54
1:G:168:ALA:HA	1:G:178:LEU:HB3	1.88	0.54
1:S:193:THR:HG23	1:S:210:LYS:HE2	1.89	0.54
2:N:16:GLY:HA2	2:N:77:ARG:HG3	1.90	0.53
1:G:84:THR:HA	1:G:111:VAL:HB	1.91	0.53
2:J:120:PRO:HD3	2:J:132:VAL:HG22	1.90	0.53
1:V:11:LEU:HB2	1:V:147:PRO:HG3	1.90	0.52
1:S:126:PRO:HB3	1:S:138:LEU:HD21	1.86	0.52
2:J:210:ASN:HB2	2:J:213:GLU:HG3	1.91	0.52
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.92	0.52
1:S:11:LEU:HB2	1:S:147:PRO:HG3	1.92	0.52
1:D:200:HIS:CE1	1:D:202:PRO:HG2	2.45	0.52
1:I:40:ALA:HB3	1:I:43:LYS:HG3	1.92	0.52
2:T:147:GLN:HB3	2:T:154:LEU:HD11	1.92	0.52
1:I:82:MET:HB3	1:I:82(C):LEU:HD21	1.92	0.52
1:D:119:PRO:HB3	1:D:145:TYR:HB3	1.91	0.52
1:M:200:HIS:CE1	1:M:202:PRO:HG2	2.44	0.52
2:B:5:THR:HA	2:B:100:GLN:HE22	1.74	0.51
1:M:168:ALA:HA	1:M:178:LEU:HB3	1.91	0.51
1:P:200:HIS:CE1	1:P:202:PRO:HG2	2.44	0.51
2:T:91:ARG:O	2:T:91:ARG:HD2	2.11	0.51
1:G:99:VAL:HG12	1:G:100(A):THR:HG22	1.93	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:126:PRO:CD	1:S:138:LEU:HD22	2.41	0.51
2:N:123:GLU:HA	2:N:126:LYS:HE2	1.93	0.51
2:T:150:VAL:HG22	2:T:192:TYR:HB2	1.93	0.51
2:W:6:GLN:HE21	2:W:99:GLY:HA3	1.76	0.51
2:H:108:ARG:HH21	2:H:109:THR:HG22	1.76	0.50
1:S:122:PHE:HD2	1:S:141:LEU:HD23	1.77	0.50
1:D:82:MET:HB3	1:D:82(C):LEU:HD21	1.93	0.50
2:N:201:LEU:HD13	2:N:205:VAL:HG12	1.93	0.50
1:I:47:TRP:CZ2	1:I:49:GLY:HA2	2.46	0.50
1:P:47:TRP:CZ2	1:P:49:GLY:HA2	2.46	0.50
2:H:91:ARG:O	2:H:91:ARG:HD2	2.12	0.50
2:W:136:LEU:HD22	2:W:175:LEU:HD22	1.92	0.50
2:Q:210:ASN:HB2	2:Q:213:GLU:HG3	1.92	0.50
1:S:126:PRO:HD3	1:S:138:LEU:HD22	1.93	0.50
1:P:52:ARG:HH11	1:P:56:THR:HG23	1.77	0.49
2:W:163:VAL:HG22	2:W:175:LEU:HD12	1.94	0.49
1:I:12:VAL:HG11	1:I:18:LEU:HB2	1.94	0.49
1:D:12:VAL:HG11	1:D:18:LEU:HB2	1.95	0.49
2:W:164:THR:HG22	2:W:174:SER:H	1.76	0.49
2:H:24:LYS:NZ	2:N:197:THR:HG21	2.27	0.49
1:M:82:MET:HB3	1:M:82(C):LEU:HD21	1.94	0.49
1:D:193:THR:HG23	1:D:210:LYS:HE3	1.95	0.49
3:R:5:ASN:ND2	3:R:12:PRO:HB3	2.28	0.49
1:G:20:VAL:HG23	1:G:80:LEU:HB3	1.94	0.48
1:S:47:TRP:CZ2	1:S:49:GLY:HA2	2.48	0.48
2:E:13:VAL:HG21	2:E:78:VAL:HG21	1.95	0.48
1:V:52:ARG:HH11	1:V:56:THR:HG23	1.77	0.48
1:I:16:ARG:HD3	1:I:17:SER:N	2.21	0.48
1:S:210:LYS:NZ	1:S:212:GLU:HG2	2.28	0.48
1:I:200:HIS:CE1	1:I:202:PRO:HG2	2.48	0.48
1:S:126:PRO:HG2	1:S:213:PRO:HA	1.96	0.48
2:T:170:ASP:HB2	2:T:172:THR:HG22	1.96	0.48
1:D:47:TRP:CZ2	1:D:49:GLY:HA2	2.48	0.48
1:V:154:TRP:CH2	1:V:196:CYS:HB3	2.49	0.48
2:H:120:PRO:HD3	2:H:132:VAL:HG22	1.96	0.47
2:B:163:VAL:HG22	2:B:175:LEU:HD12	1.95	0.47
1:D:168:ALA:HA	1:D:178:LEU:HB3	1.95	0.47
1:V:47:TRP:CZ2	1:V:49:GLY:HA2	2.49	0.47
2:B:145:LYS:HB3	2:B:145:LYS:HE3	1.69	0.47
1:V:168:ALA:HB2	1:V:178:LEU:HD23	1.95	0.47
1:A:20:VAL:HG13	1:A:80:LEU:HB3	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:87:THR:HG23	1:M:110:THR:HA	1.97	0.47
1:S:13:GLN:HB3	1:S:16:ARG:HG3	1.97	0.47
3:C:5:ASN:ND2	3:C:12:PRO:HB3	2.30	0.47
1:D:59:TYR:HB2	1:D:64:LYS:HG3	1.96	0.47
2:H:37:LEU:HD13	2:H:86:TYR:CZ	2.49	0.47
1:S:126:PRO:HB3	1:S:138:LEU:HD23	1.94	0.47
2:T:112:ALA:HB1	2:T:201:LEU:HD23	1.96	0.47
2:W:91:ARG:HD2	2:W:91:ARG:O	2.15	0.47
1:I:20:VAL:HG13	1:I:80:LEU:HB3	1.96	0.47
2:N:91:ARG:O	2:N:91:ARG:HD2	2.15	0.46
2:Q:191:VAL:HG22	2:Q:210:ASN:HD21	1.80	0.46
2:N:148:TRP:CE3	2:N:179:LEU:HD12	2.51	0.46
1:S:126:PRO:HG3	1:S:138:LEU:HD22	1.98	0.46
1:A:200:HIS:CE1	1:A:202:PRO:HG2	2.51	0.46
2:H:189:HIS:O	2:H:211:ARG:HD3	2.16	0.46
2:E:107:LYS:HA	2:E:140:TYR:OH	2.16	0.45
2:N:142:ARG:HD3	2:N:173:TYR:CD2	2.51	0.45
1:I:201:LYS:HD2	1:I:201:LYS:HA	1.80	0.45
1:S:200:HIS:CE1	1:S:202:PRO:HG2	2.52	0.45
2:B:145:LYS:HD3	2:B:147:GLN:HG3	1.98	0.45
1:G:47:TRP:CZ2	1:G:49:GLY:HA2	2.52	0.45
2:N:47:VAL:HG12	2:N:48:ILE:HG13	1.99	0.45
3:L:5:ASN:ND2	3:L:12:PRO:HB3	2.32	0.45
2:T:37:LEU:HD13	2:T:86:TYR:CZ	2.52	0.45
2:W:166:GLN:HG3	2:W:173:TYR:CZ	2.52	0.45
2:T:107:LYS:HA	2:T:140:TYR:OH	2.17	0.44
2:W:107:LYS:HA	2:W:140:TYR:OH	2.17	0.44
1:M:47:TRP:CZ2	1:M:49:GLY:HA2	2.53	0.44
2:H:154:LEU:HD12	2:H:154:LEU:HA	1.87	0.44
2:N:146:VAL:HG22	2:N:196:VAL:HG22	1.99	0.44
1:S:184:VAL:HG21	1:S:194:TYR:CZ	2.52	0.44
1:G:11:LEU:HB2	1:G:147:PRO:HG3	2.00	0.44
1:V:189:LEU:HD23	1:V:189:LEU:HA	1.81	0.44
2:H:185:ASP:O	2:H:188:LYS:HG2	2.18	0.43
1:V:200:HIS:CE1	1:V:202:PRO:HG2	2.53	0.43
1:A:47:TRP:CZ2	1:A:49:GLY:HA2	2.53	0.43
1:V:84:THR:O	1:V:87:THR:HG23	2.17	0.43
2:Q:13:VAL:HG21	2:Q:19:ALA:HB2	2.00	0.43
2:Q:186:TYR:HA	2:Q:192:TYR:OH	2.19	0.43
2:H:126:LYS:HB2	2:H:126:LYS:HE3	1.77	0.43
1:V:154:TRP:HB3	1:V:159:LEU:HD23	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:37:LEU:O	2:W:45:GLN:HG2	2.18	0.43
2:W:61:ARG:HD2	2:W:77:ARG:O	2.18	0.43
1:M:199:ASN:OD1	1:M:206:LYS:HE3	2.19	0.43
2:H:163:VAL:HG22	2:H:175:LEU:HD12	2.00	0.43
2:T:155:GLN:HB3	2:T:158:ASN:HD21	1.83	0.43
2:Q:189:HIS:O	2:Q:211:ARG:HD3	2.19	0.43
2:N:92:ILE:HG12	3:O:2:PRO:HB3	2.01	0.42
1:V:168:ALA:HA	1:V:178:LEU:HB3	2.01	0.42
1:G:60:ALA:O	1:G:64:LYS:HG3	2.19	0.42
1:M:119:PRO:HB3	1:M:145:TYR:HD2	1.83	0.42
1:D:11:LEU:HB2	1:D:147:PRO:HG3	2.00	0.42
1:G:82:MET:HE1	1:G:109:VAL:HG21	2.01	0.42
1:P:154:TRP:CH2	1:P:196:CYS:HB3	2.54	0.42
2:T:74:LYS:HB3	2:T:74:LYS:HE2	1.67	0.42
2:W:17:GLN:NE2	2:W:17:GLN:HA	2.34	0.42
2:T:113:PRO:HB3	2:T:139:PHE:HB3	2.00	0.42
1:V:129:LYS:H	1:V:129:LYS:CD	2.31	0.42
1:M:184:VAL:HG11	1:M:194:TYR:CE1	2.55	0.42
1:S:184:VAL:HG22	1:S:185:PRO:HD2	2.02	0.42
2:J:202:SER:HB3	1:S:5:VAL:HG22	2.02	0.41
2:T:11:LEU:HD23	2:T:11:LEU:HA	1.88	0.41
1:P:159:LEU:HD21	1:P:182:VAL:HG21	2.01	0.41
1:P:43:LYS:HE2	1:P:43:LYS:HB3	1.83	0.41
1:A:43:LYS:HE3	1:A:44:GLY:H	1.86	0.41
1:D:201:LYS:N	1:D:202:PRO:HD2	2.35	0.41
2:E:167:ASP:OD2	2:E:169:LYS:HG2	2.20	0.41
1:V:99:VAL:HG12	1:V:100(A):THR:HG22	2.01	0.41
2:H:145:LYS:HZ1	2:N:72:THR:HG21	1.86	0.41
2:W:37:LEU:HD13	2:W:86:TYR:CZ	2.56	0.41
2:W:54:ARG:HD3	2:W:62:PHE:O	2.21	0.41
1:M:168:ALA:HB2	1:M:178:LEU:HD23	2.03	0.41
2:T:140:TYR:O	2:T:198:HIS:HE1	2.04	0.41
2:N:4:MET:HE3	2:N:23:CYS:SG	2.61	0.40
2:N:37:LEU:HD13	2:N:86:TYR:CZ	2.55	0.40
2:E:179:LEU:HG	2:E:181:LEU:HD13	2.02	0.40
2:Q:191:VAL:HG22	2:Q:210:ASN:ND2	2.36	0.40
1:D:129:LYS:HE3	1:D:129:LYS:HB3	1.91	0.40
1:G:152:VAL:HA	1:G:197:ASN:O	2.22	0.40
1:S:155:ASN:HD21	1:S:194:TYR:HD1	1.69	0.40
1:M:99:VAL:HG12	1:M:100(A):THR:HG22	2.02	0.40
2:N:11:LEU:HD23	2:N:11:LEU:HA	1.92	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	217/230 (94%)	212 (98%)	5 (2%)	0	100	100
1	D	220/230 (96%)	218 (99%)	2 (1%)	0	100	100
1	G	217/230 (94%)	212 (98%)	5 (2%)	0	100	100
1	I	217/230 (94%)	212 (98%)	5 (2%)	0	100	100
1	M	213/230 (93%)	209 (98%)	4 (2%)	0	100	100
1	P	214/230 (93%)	209 (98%)	5 (2%)	0	100	100
1	S	209/230 (91%)	206 (99%)	3 (1%)	0	100	100
1	V	217/230 (94%)	214 (99%)	3 (1%)	0	100	100
2	B	216/219 (99%)	213 (99%)	3 (1%)	0	100	100
2	E	217/219 (99%)	211 (97%)	6 (3%)	0	100	100
2	H	217/219 (99%)	215 (99%)	2 (1%)	0	100	100
2	J	217/219 (99%)	213 (98%)	4 (2%)	0	100	100
2	N	217/219 (99%)	214 (99%)	3 (1%)	0	100	100
2	Q	216/219 (99%)	212 (98%)	4 (2%)	0	100	100
2	T	206/219 (94%)	199 (97%)	7 (3%)	0	100	100
2	W	217/219 (99%)	212 (98%)	5 (2%)	0	100	100
3	C	9/16 (56%)	9 (100%)	0	0	100	100
3	F	10/16 (62%)	10 (100%)	0	0	100	100
3	K	11/16 (69%)	11 (100%)	0	0	100	100
3	L	10/16 (62%)	10 (100%)	0	0	100	100
3	O	10/16 (62%)	10 (100%)	0	0	100	100
3	R	10/16 (62%)	10 (100%)	0	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	U	10/16 (62%)	10 (100%)	0	0	100	100
3	X	12/16 (75%)	12 (100%)	0	0	100	100
All	All	3529/3720 (95%)	3463 (98%)	66 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	184/193 (95%)	184 (100%)	0	100	100
1	D	185/193 (96%)	183 (99%)	2 (1%)	65	81
1	G	184/193 (95%)	183 (100%)	1 (0%)	81	90
1	I	184/193 (95%)	183 (100%)	1 (0%)	81	90
1	M	181/193 (94%)	180 (99%)	1 (1%)	78	89
1	P	181/193 (94%)	180 (99%)	1 (1%)	78	89
1	S	180/193 (93%)	178 (99%)	2 (1%)	65	81
1	V	184/193 (95%)	182 (99%)	2 (1%)	65	81
2	B	195/196 (100%)	194 (100%)	1 (0%)	81	90
2	E	196/196 (100%)	194 (99%)	2 (1%)	68	82
2	H	196/196 (100%)	194 (99%)	2 (1%)	68	82
2	J	196/196 (100%)	193 (98%)	3 (2%)	57	75
2	N	196/196 (100%)	193 (98%)	3 (2%)	57	75
2	Q	195/196 (100%)	193 (99%)	2 (1%)	68	82
2	T	191/196 (97%)	188 (98%)	3 (2%)	55	73
2	W	196/196 (100%)	193 (98%)	3 (2%)	57	75
3	C	10/14 (71%)	10 (100%)	0	100	100
3	F	11/14 (79%)	11 (100%)	0	100	100
3	K	12/14 (86%)	12 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	11/14 (79%)	11 (100%)	0	100	100
3	O	11/14 (79%)	11 (100%)	0	100	100
3	R	11/14 (79%)	11 (100%)	0	100	100
3	U	11/14 (79%)	11 (100%)	0	100	100
3	X	12/14 (86%)	12 (100%)	0	100	100
All	All	3113/3224 (97%)	3084 (99%)	29 (1%)	70	84

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	56	THR
2	J	13	VAL
2	J	208	SER
2	J	214	CYS
2	B	13	VAL
1	D	56	THR
1	D	130	SER
2	E	182	SER
2	E	214	CYS
1	G	212	GLU
2	H	13	VAL
2	H	149	LYS
1	M	18	LEU
2	N	100	GLN
2	N	179	LEU
2	N	214	CYS
1	P	128	SER
2	Q	154	LEU
2	Q	202	SER
1	S	20	VAL
1	S	195	ILE
2	T	13	VAL
2	T	129	THR
2	T	213	GLU
1	V	20	VAL
1	V	56	THR
2	W	13	VAL
2	W	17	GLN
2	W	196	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	39	GLN
1	I	192	GLN
2	J	38	GLN
2	J	147	GLN
1	A	39	GLN
1	A	192	GLN
2	B	38	GLN
2	B	42	GLN
2	B	100	GLN
3	C	5	ASN
3	L	5	ASN
1	M	164	HIS
1	M	171	GLN
1	M	192	GLN
2	N	137	ASN
1	P	39	GLN
2	Q	38	GLN
2	Q	45	GLN
2	Q	210	ASN
3	R	5	ASN
2	T	45	GLN
2	T	160	GLN
1	V	3	GLN
1	V	164	HIS
2	W	6	GLN
2	W	17	GLN
2	W	42	GLN
2	W	137	ASN
2	W	199	GLN
2	W	210	ASN
3	X	13	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 [i](#)

There are no oligosaccharides 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	221/230 (96%)	0.23	9 (4%) 41 43	21, 34, 51, 89	0
1	D	222/230 (96%)	0.34	3 (1%) 73 75	26, 37, 51, 74	0
1	G	221/230 (96%)	0.78	17 (7%) 19 21	25, 45, 67, 91	0
1	I	221/230 (96%)	0.24	6 (2%) 56 58	25, 34, 47, 72	0
1	M	217/230 (94%)	1.10	27 (12%) 8 9	30, 52, 69, 82	0
1	P	218/230 (94%)	0.66	9 (4%) 41 43	29, 43, 57, 75	0
1	S	215/230 (93%)	0.72	28 (13%) 7 8	25, 38, 68, 77	0
1	V	221/230 (96%)	0.75	20 (9%) 15 16	24, 39, 65, 74	0
2	B	218/219 (99%)	0.20	4 (1%) 67 69	23, 33, 47, 61	0
2	E	219/219 (100%)	0.32	11 (5%) 34 35	24, 33, 58, 73	0
2	H	219/219 (100%)	0.82	15 (6%) 23 25	29, 46, 63, 79	0
2	J	219/219 (100%)	0.24	3 (1%) 73 75	23, 34, 52, 70	0
2	N	219/219 (100%)	1.37	43 (19%) 3 3	35, 55, 76, 83	0
2	Q	218/219 (99%)	0.47	10 (4%) 37 39	23, 35, 65, 83	0
2	T	214/219 (97%)	1.24	50 (23%) 2 2	30, 59, 77, 83	0
2	W	219/219 (100%)	1.21	48 (21%) 2 2	31, 51, 74, 83	0
3	C	11/16 (68%)	1.11	4 (36%) 1 1	30, 34, 56, 63	0
3	F	12/16 (75%)	1.00	1 (8%) 17 19	33, 46, 61, 64	0
3	K	13/16 (81%)	0.62	2 (15%) 5 6	30, 43, 58, 71	0
3	L	12/16 (75%)	1.23	4 (33%) 1 1	32, 50, 58, 66	0
3	O	12/16 (75%)	0.95	1 (8%) 17 19	36, 51, 63, 71	0
3	R	12/16 (75%)	1.16	3 (25%) 2 2	34, 46, 59, 60	0
3	U	12/16 (75%)	0.65	1 (8%) 17 19	33, 37, 43, 47	0
3	X	14/16 (87%)	1.09	4 (28%) 1 1	32, 47, 56, 59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3599/3720 (96%)	0.67	323 (8%) 15 16	21, 40, 68, 91	0

All (323) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	133	GLY	5.6
2	T	192	TYR	4.5
2	N	156	SER	4.5
2	N	181	LEU	4.5
2	N	154	LEU	4.4
2	T	201	LEU	4.4
1	S	138	LEU	4.4
1	G	190	GLY	4.4
2	N	214	CYS	4.2
3	F	2	PRO	4.2
2	N	157	GLY	4.2
1	A	128	SER	4.1
2	E	214	CYS	4.1
1	G	132	SER	4.0
1	S	126	PRO	4.0
2	T	16	GLY	3.9
2	N	150	VAL	3.9
2	H	154	LEU	3.9
2	N	193	ALA	3.9
2	N	148	TRP	3.9
1	G	214	LYS	3.8
2	H	153	ALA	3.8
2	N	151	ASP	3.8
2	W	184	ALA	3.8
1	G	173	SER	3.8
1	M	112	SER	3.8
2	T	214	CYS	3.8
1	V	134	GLY	3.8
2	W	191	VAL	3.8
2	N	153	ALA	3.8
2	W	214	CYS	3.7
1	V	207	VAL	3.7
2	T	209	PHE	3.6
2	H	16	GLY	3.6
2	H	152	ASN	3.6
2	T	132	VAL	3.6
1	M	191	THR	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	N	129	THR	3.6
2	N	158	ASN	3.6
1	M	173	SER	3.6
2	W	154	LEU	3.6
1	A	132	SER	3.6
2	H	212	GLY	3.6
1	A	130	SER	3.5
2	N	191	VAL	3.5
2	H	214	CYS	3.5
2	T	150	VAL	3.5
2	N	186	TYR	3.5
1	A	214	LYS	3.4
2	T	205	VAL	3.4
2	W	157	GLY	3.4
2	W	125	LEU	3.4
2	T	194	CYS	3.4
3	R	12	PRO	3.3
2	W	76	ARG	3.3
1	A	190	GLY	3.3
1	M	134	GLY	3.3
2	T	113	PRO	3.3
2	W	80	ALA	3.3
3	C	12	PRO	3.3
3	X	2	PRO	3.3
2	N	189	HIS	3.3
1	I	132	SER	3.3
2	W	122	ASP	3.3
2	H	77	ARG	3.3
1	A	129	LYS	3.3
2	W	16	GLY	3.2
2	N	125	LEU	3.2
3	O	2	PRO	3.2
2	T	184	ALA	3.2
2	N	188	LYS	3.2
2	N	184	ALA	3.2
1	S	135	THR	3.2
2	T	203	SER	3.1
2	T	110	VAL	3.1
1	S	195	ILE	3.1
2	T	188	LYS	3.1
2	W	182	SER	3.1
2	T	111	ALA	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	S	121	VAL	3.1
1	M	176	TYR	3.1
2	B	88	CYS	3.1
2	T	186	TYR	3.0
1	M	135	THR	3.0
1	P	128	SER	3.0
1	V	118	GLY	3.0
1	S	125	ALA	3.0
2	T	115	VAL	3.0
1	S	210	LYS	3.0
2	T	168	SER	3.0
1	S	122	PHE	3.0
2	W	152	ASN	3.0
2	E	125	LEU	2.9
2	W	129	THR	2.9
1	G	133	GLY	2.9
2	W	148	TRP	2.9
1	P	214	LYS	2.9
1	V	131	THR	2.9
1	S	1	GLU	2.9
2	W	127	SER	2.9
3	C	4	PRO	2.9
1	S	158	ALA	2.9
2	W	153	ALA	2.9
3	R	3	ASP	2.9
2	T	120	PRO	2.9
2	E	184	ALA	2.9
2	T	153	ALA	2.9
2	T	154	LEU	2.9
1	G	130	SER	2.8
3	X	3	ASP	2.9
3	L	2	PRO	2.8
2	Q	154	LEU	2.8
1	M	116	THR	2.8
2	B	127	SER	2.8
1	M	207	VAL	2.8
1	I	214	LYS	2.8
1	A	133	GLY	2.8
1	P	127	SER	2.8
1	S	213	PRO	2.8
2	E	213	GLU	2.8
2	Q	213	GLU	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	S	140	CYS	2.8
2	W	188	LYS	2.8
2	W	130	ALA	2.8
2	T	156	SER	2.7
2	N	194	CYS	2.7
2	N	204	PRO	2.7
2	Q	184	ALA	2.7
2	N	212	GLY	2.7
1	V	202	PRO	2.7
2	W	169	LYS	2.7
2	N	196	VAL	2.7
2	T	151	ASP	2.7
2	T	117	ILE	2.7
1	G	129	LYS	2.7
2	T	112	ALA	2.7
1	M	185	PRO	2.7
1	V	154	TRP	2.7
2	W	186	TYR	2.6
2	N	146	VAL	2.6
2	W	150	VAL	2.6
1	G	128	SER	2.6
1	G	213	PRO	2.6
1	P	100	SER	2.6
2	N	203	SER	2.6
2	W	107	LYS	2.6
3	L	13	ASN	2.6
3	X	15	ASN	2.6
1	V	205	THR	2.6
1	A	188	SER	2.6
1	M	175	LEU	2.6
2	H	125	LEU	2.6
2	E	128	GLY	2.6
2	H	78	VAL	2.6
2	T	13	VAL	2.6
2	J	214	CYS	2.5
1	V	204	ASN	2.5
2	W	209	PHE	2.5
3	U	2	PRO	2.5
2	W	78	VAL	2.5
1	M	189	LEU	2.5
1	P	133	GLY	2.5
2	E	126	LYS	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	T	212	GLY	2.5
2	W	212	GLY	2.5
2	N	202	SER	2.5
1	P	1	GLU	2.5
2	W	173	TYR	2.5
2	N	130	ALA	2.5
1	S	193	THR	2.5
2	N	197	THR	2.5
2	Q	147	GLN	2.5
2	W	14	THR	2.5
1	M	156	SER	2.5
2	T	146	VAL	2.5
2	W	13	VAL	2.5
2	T	136	LEU	2.5
2	W	68	GLY	2.5
3	R	2	PRO	2.5
2	N	77	ARG	2.4
1	M	170	LEU	2.4
1	S	141	LEU	2.4
1	D	214	LYS	2.4
3	K	1	ASN	2.4
1	M	174	GLY	2.4
1	V	54	GLY	2.4
2	N	76	ARG	2.4
2	N	187	GLU	2.4
2	T	119	PRO	2.4
1	A	187	SER	2.4
2	Q	191	VAL	2.4
2	N	126	LYS	2.4
1	S	192	GLN	2.4
2	H	213	GLU	2.4
1	G	134	GLY	2.4
1	G	116	THR	2.4
2	T	129	THR	2.4
1	I	130	SER	2.4
2	T	148	TRP	2.4
1	M	213	PRO	2.4
1	M	214	LYS	2.4
1	V	211	VAL	2.4
1	M	128	SER	2.3
2	W	12	SER	2.3
2	N	205	VAL	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	T	198	HIS	2.3
2	W	189	HIS	2.3
1	I	128	SER	2.3
1	S	211	VAL	2.3
2	N	17	GLN	2.3
2	W	9	LEU	2.3
1	G	119	PRO	2.3
2	T	130	ALA	2.3
1	M	100	SER	2.3
2	J	127	SER	2.3
2	J	156	SER	2.3
2	N	208	SER	2.3
1	S	166	PHE	2.3
2	E	188	LYS	2.3
2	Q	210	ASN	2.3
2	W	128	GLY	2.3
1	P	16	ARG	2.3
1	S	137	ALA	2.3
2	W	193	ALA	2.3
1	M	210	LYS	2.3
1	S	184	VAL	2.3
2	E	151	ASP	2.2
2	T	210	ASN	2.2
2	T	197	THR	2.2
2	W	109	THR	2.2
2	W	192	TYR	2.2
1	M	82(C)	LEU	2.2
1	M	150	VAL	2.2
2	B	201	LEU	2.2
2	N	179	LEU	2.2
1	S	123	PRO	2.2
2	T	141	PRO	2.2
1	M	118	GLY	2.2
2	H	123	GLU	2.2
1	G	191	THR	2.2
1	M	84	THR	2.2
1	V	102	TYR	2.2
1	V	172	SER	2.2
2	T	83	VAL	2.2
2	H	211	ARG	2.2
2	W	138	ASN	2.2
1	V	213	PRO	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	129	LYS	2.2
1	S	206	LYS	2.2
1	D	128	SER	2.2
1	G	115	SER	2.2
2	N	192	TYR	2.2
2	T	179	LEU	2.2
2	W	77	ARG	2.2
2	H	122	ASP	2.2
2	N	152	ASN	2.2
2	W	118	PHE	2.2
3	X	4	PRO	2.2
2	T	165	GLU	2.2
1	G	162	GLY	2.2
2	Q	212	GLY	2.2
2	T	199	GLN	2.2
1	P	160	THR	2.2
2	N	109	THR	2.2
2	Q	181	LEU	2.1
2	N	213	GLU	2.1
2	W	190	LYS	2.1
1	M	119	PRO	2.1
2	H	15	PRO	2.1
3	L	4	PRO	2.1
2	E	153	ALA	2.1
2	T	211	ARG	2.1
1	S	159	LEU	2.1
3	C	3	ASP	2.1
1	S	185	PRO	2.1
2	W	15	PRO	2.1
2	W	147	GLN	2.1
1	M	190	GLY	2.1
1	D	131	THR	2.1
1	G	172	SER	2.1
2	W	197	THR	2.1
1	V	137	ALA	2.1
2	E	181	LEU	2.1
2	T	125	LEU	2.1
2	T	122	ASP	2.1
3	C	13	ASN	2.1
2	N	155	GLN	2.1
2	T	116	PHE	2.1
1	S	128	SER	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	S	160	THR	2.1
2	T	202	SER	2.1
2	H	169	LYS	2.1
1	S	212	GLU	2.1
2	T	123	GLU	2.1
1	M	200	HIS	2.1
2	N	147	GLN	2.1
2	W	151	ASP	2.1
1	V	194	TYR	2.1
2	N	78	VAL	2.1
1	I	190	GLY	2.1
2	N	128	GLY	2.1
1	V	129	LYS	2.0
1	V	214	LYS	2.0
1	G	183	THR	2.0
1	S	156	SER	2.0
2	Q	197	THR	2.0
2	T	174	SER	2.0
2	W	168	SER	2.0
1	V	140	CYS	2.0
2	W	81	GLU	2.0
3	K	13	ASN	2.0
3	L	12	PRO	2.0
1	M	184	VAL	2.0
2	T	128	GLY	2.0
2	E	209	PHE	2.0
2	Q	207	LYS	2.0
1	V	160	THR	2.0
2	B	202	SER	2.0
2	T	109	THR	2.0
2	W	180	THR	2.0
2	W	187	GLU	2.0
1	S	196	CYS	2.0
1	P	206	LYS	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.