



wwPDB X-ray Structure Validation Summary Report ⓘ

May 20, 2026 – 08:14 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 wwPDB X-ray Structure Validation Summary 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

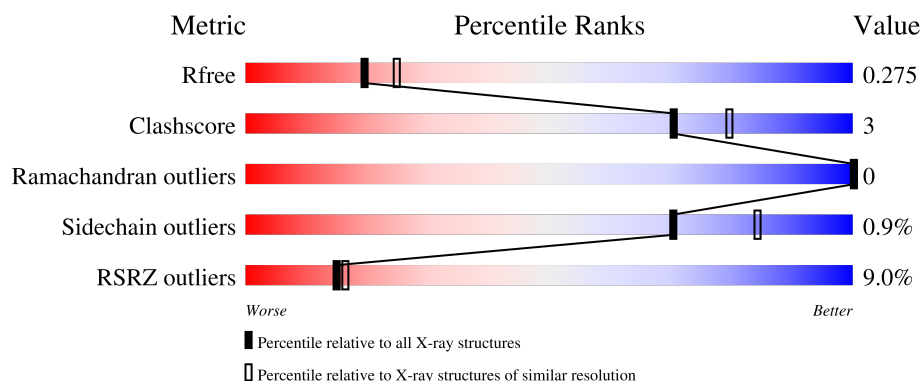
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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 ≥ 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>

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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			

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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		

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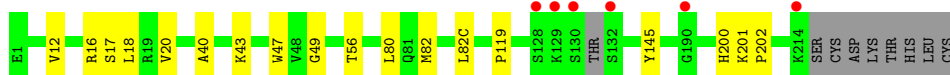
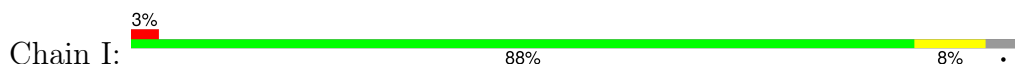
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	32	Total 32	O 32	0	0
4	F	2	Total 2	O 2	0	0
4	G	22	Total 22	O 22	0	0
4	H	12	Total 12	O 12	0	0
4	L	2	Total 2	O 2	0	0
4	M	9	Total 9	O 9	0	0
4	N	4	Total 4	O 4	0	0
4	O	1	Total 1	O 1	0	0
4	P	13	Total 13	O 13	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

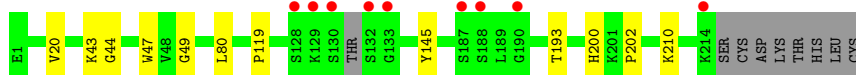
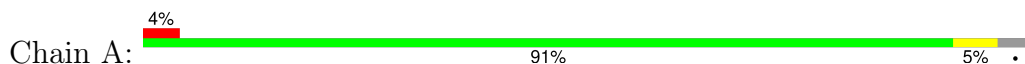
3 Residue-property plots [i](#)

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.

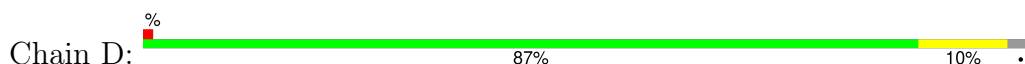
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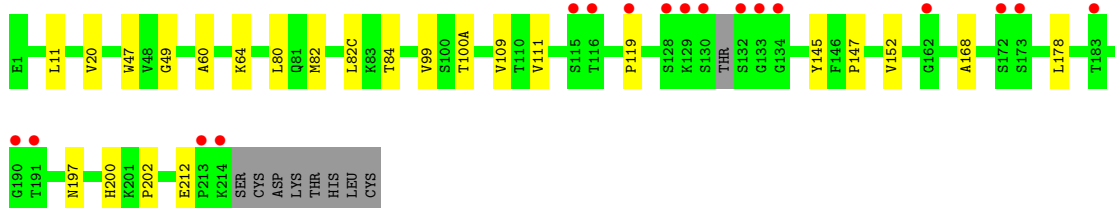
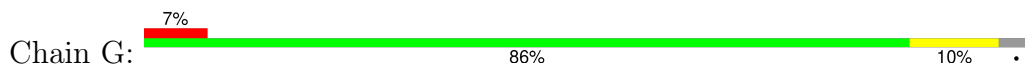
- Molecule 1: Heavy Chain of Fab 7160



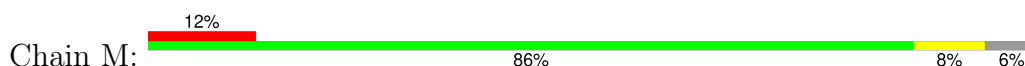
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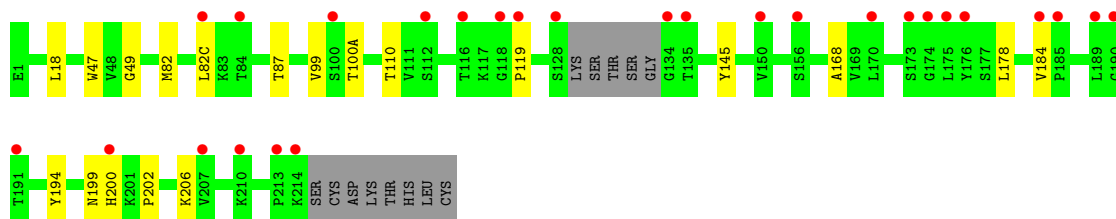


- Molecule 1: Heavy Chain of Fab 7160

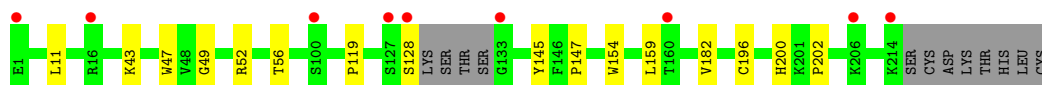
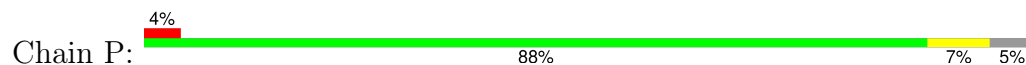


- Molecule 1: Heavy Chain of Fab 7160

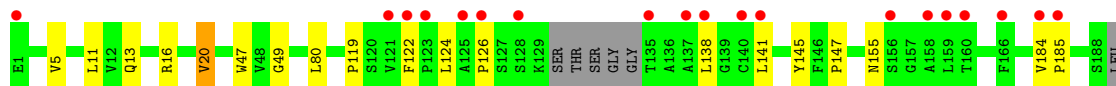
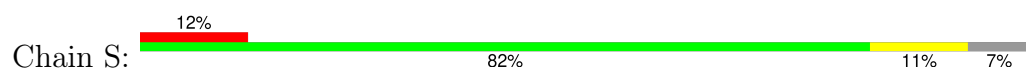




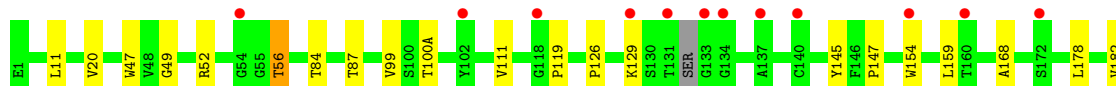
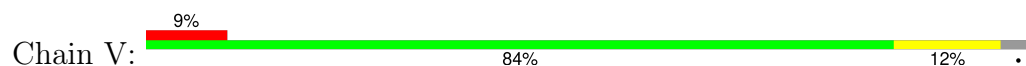
• Molecule 1: Heavy Chain of Fab 7160



• Molecule 1: Heavy Chain of Fab 7160



• Molecule 1: Heavy Chain of Fab 7160



• Molecule 2: Light Chain of Fab 7160

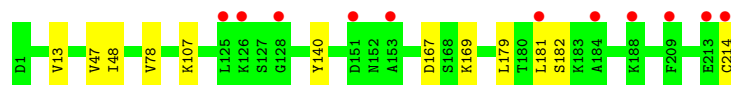


• Molecule 2: Light Chain of Fab 7160

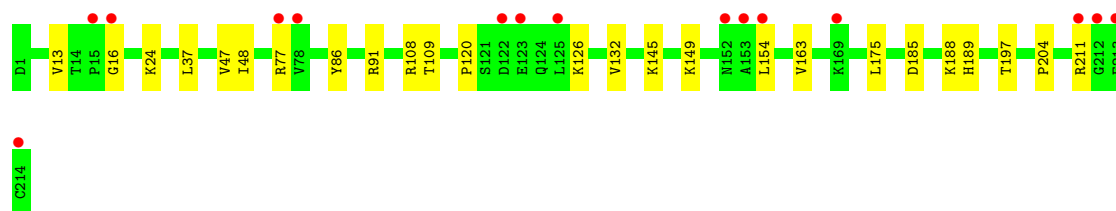
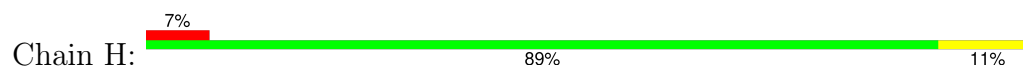




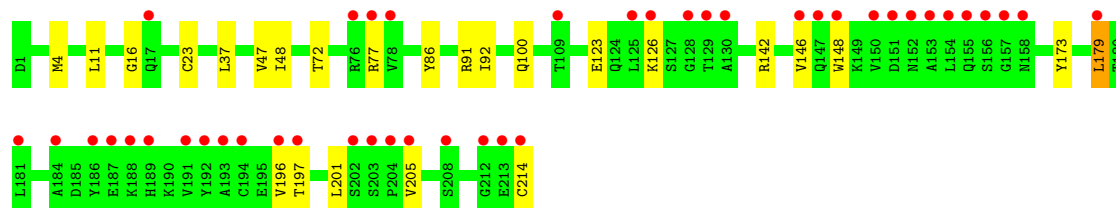
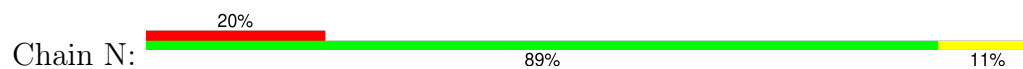
- Molecule 2: Light Chain of Fab 7160



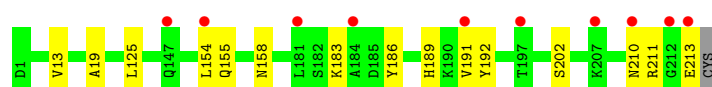
- Molecule 2: Light Chain of Fab 7160



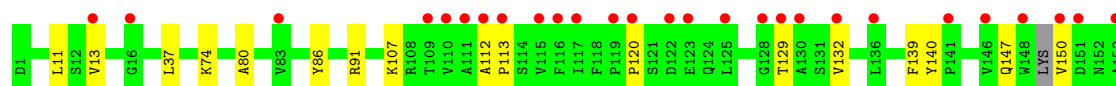
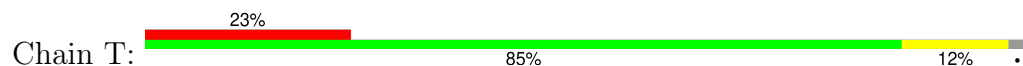
- Molecule 2: Light Chain of Fab 7160

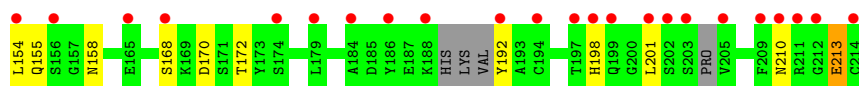


- Molecule 2: Light Chain of Fab 7160

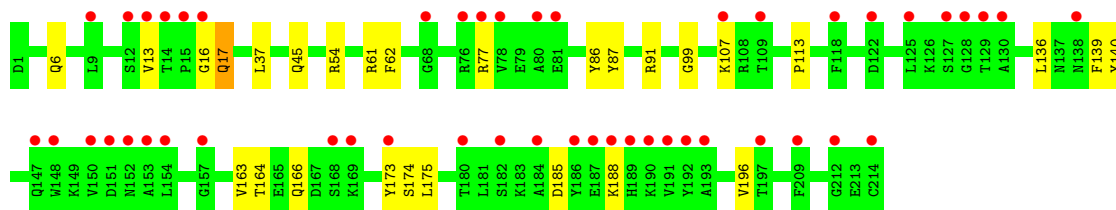
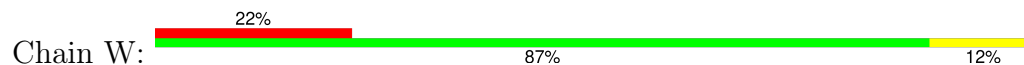


- Molecule 2: Light Chain of Fab 7160

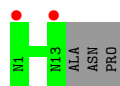
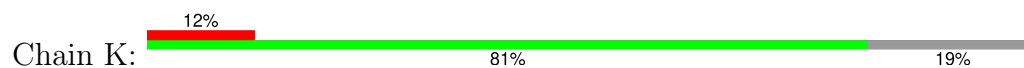




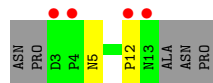
- Molecule 2: Light Chain of Fab 7160



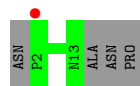
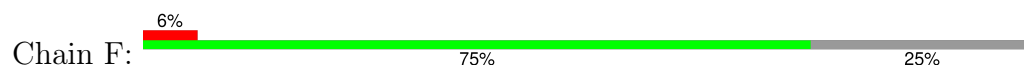
- Molecule 3: Circumsporozoite protein



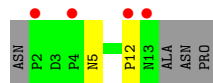
- Molecule 3: Circumsporozoite protein



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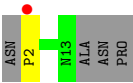


- Molecule 3: Circumsporozoite protein

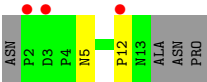


- Molecule 3: Circumsporozoite protein

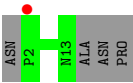




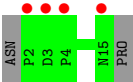
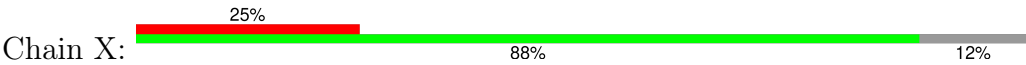
● Molecule 3: Circumsporozoite protein



● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	35.2	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.11	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

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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.

The worst 5 of 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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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
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

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	179	LEU
2	W	17	GLN
2	Q	154	LEU
1	V	20	VAL
1	P	128	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	137	ASN
2	W	137	ASN
2	Q	45	GLN
2	W	210	ASN
2	W	6	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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, 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	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

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

The worst 5 of 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

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.