



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:37 AM UTC

PDB ID : 9IY2 / pdb_00009iy2
Title : Immune complex of HEV-E2s, nAb 8C11 and nAb 8H3
Authors : Minghua, Z.; Lizhi, Z.; Ying, G.; Shaowei, L.
Deposited on : 2024-07-29
Resolution : 3.48 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

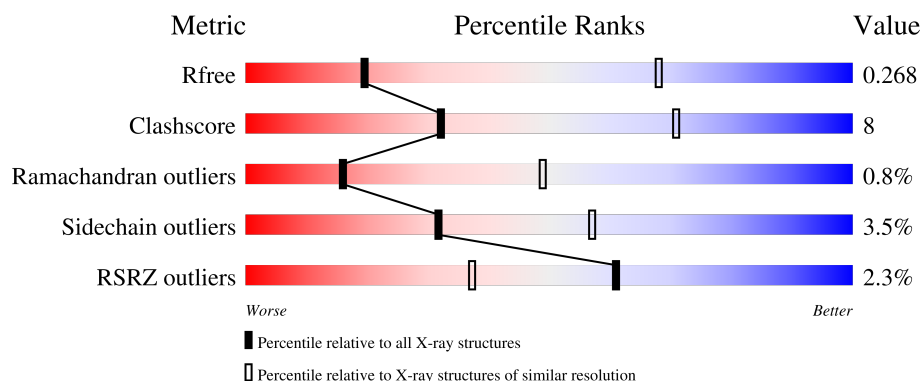
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	214	53%15%32%
1	B	214	57%11%32%
2	D	230	70%23%5%
2	H	230	71%21%5%
3	C	214	60%34%6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	L	214	2% 65% 29% 6%
4	E	221	2% 76% 20% ...
4	G	221	9% 84% 13% ...
5	F	219	83% 15% ..
5	I	219	3% 89% 9% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15430 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 Secreted protein ORF2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	0	0	0
			1096	697	185	214			
1	B	145	Total	C	N	O	0	0	0
			1090	694	184	212			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	393	MET	-	initiating methionine	UNP P33426
A	532	HIS	TYR	conflict	UNP P33426
A	604	PRO	-	expression tag	UNP P33426
A	605	PRO	-	expression tag	UNP P33426
A	606	ARG	-	expression tag	UNP P33426
B	393	MET	-	initiating methionine	UNP P33426
B	532	HIS	TYR	conflict	UNP P33426
B	604	PRO	-	expression tag	UNP P33426
B	605	PRO	-	expression tag	UNP P33426
B	606	ARG	-	expression tag	UNP P33426

- Molecule 2 is a protein called Heavy Chain of mAb 8C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1637	1044	267	320	6			
2	D	218	Total	C	N	O	S	0	0	0
			1637	1044	267	320	6			

- Molecule 3 is a protein called Light Chain of mAb 8C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1656	1034	278	338	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1656	1034	278	338	6			

- Molecule 4 is a protein called Heavy Chain of mAb 8H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	219	Total	C	N	O	S	0	0	0
			1644	1040	271	325	8			
4	G	219	Total	C	N	O	S	0	0	0
			1644	1040	271	325	8			

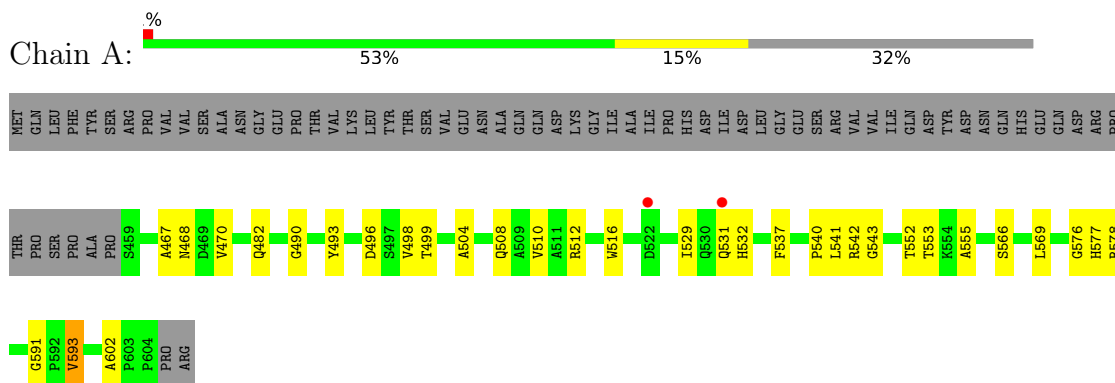
- Molecule 5 is a protein called Light Chain of mAb 8H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	217	Total	C	N	O	S	0	0	0
			1685	1051	282	344	8			
5	I	217	Total	C	N	O	S	0	0	0
			1685	1051	282	344	8			

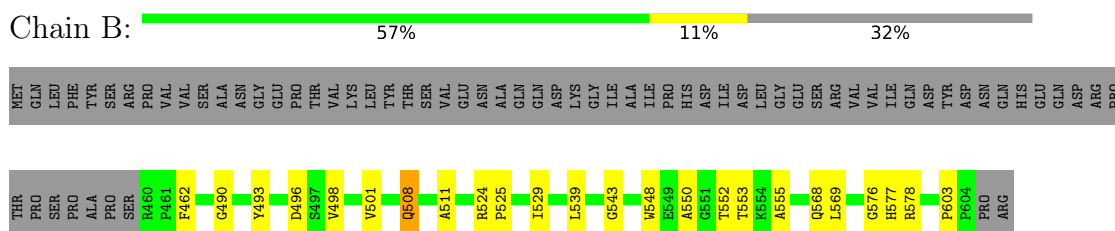
3 Residue-property plots [i](#)

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: Secreted protein ORF2



- Molecule 1: Secreted protein ORF2

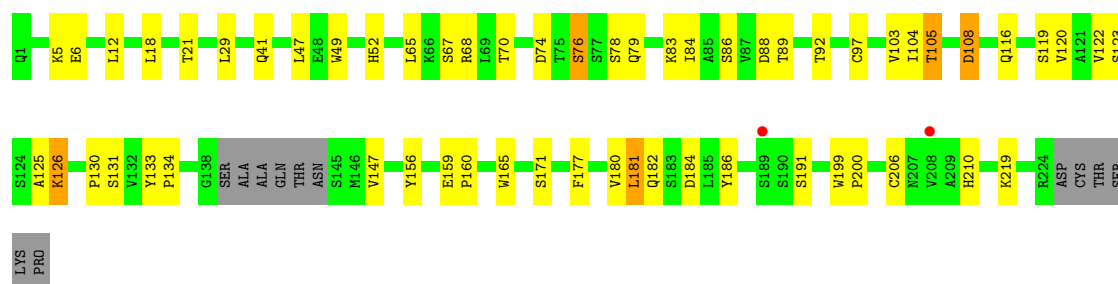


- Molecule 2: Heavy Chain of mAb 8C11

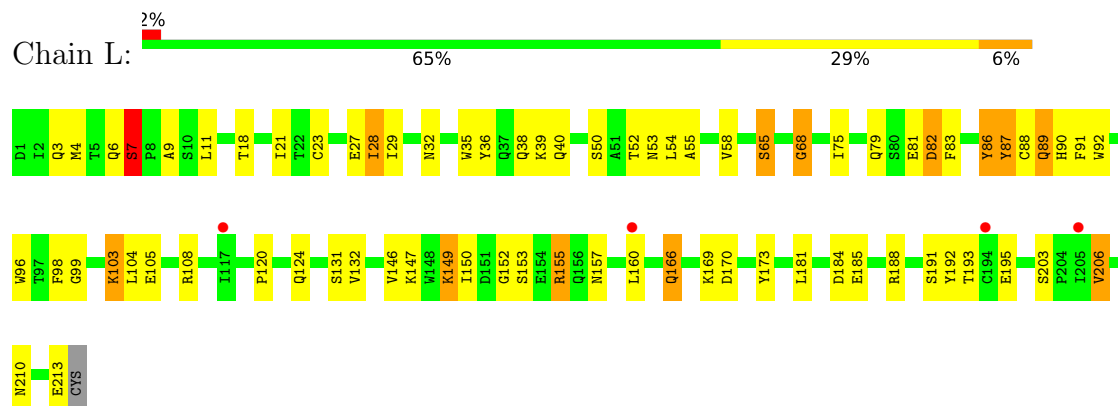


- Molecule 2: Heavy Chain of mAb 8C11

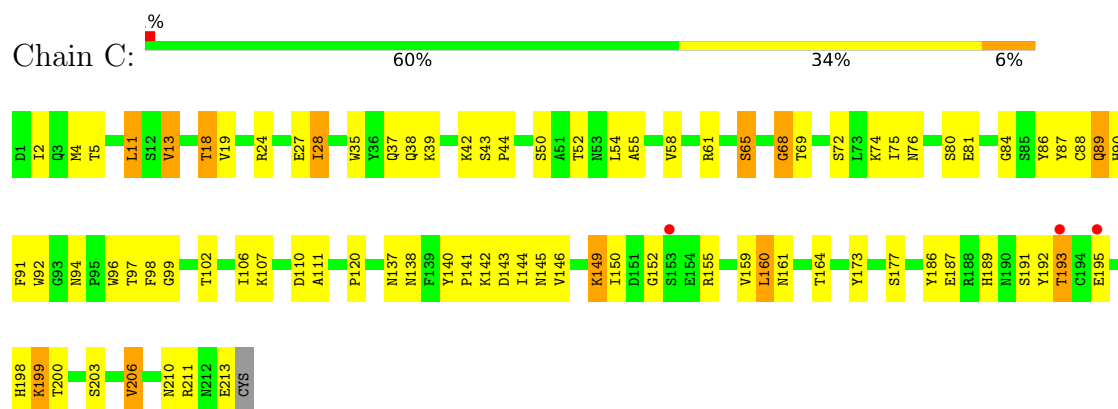




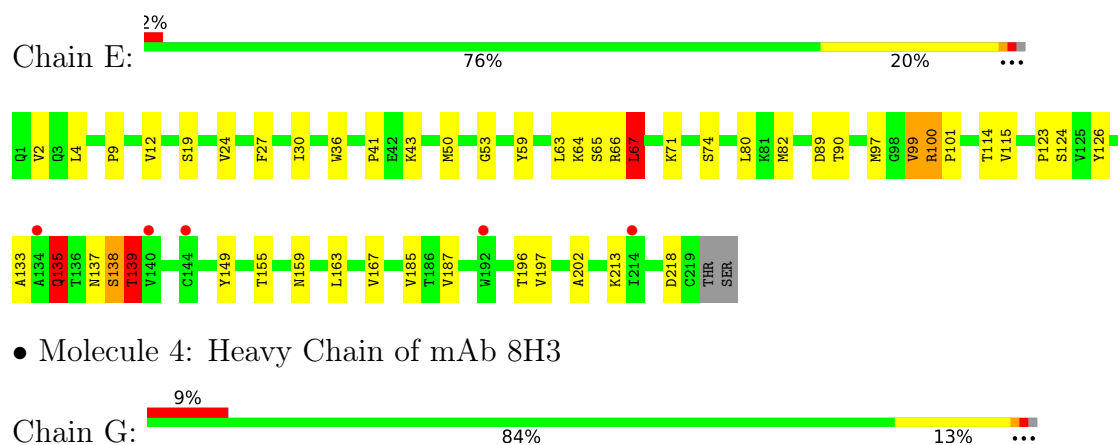
• Molecule 3: Light Chain of mAb 8C11



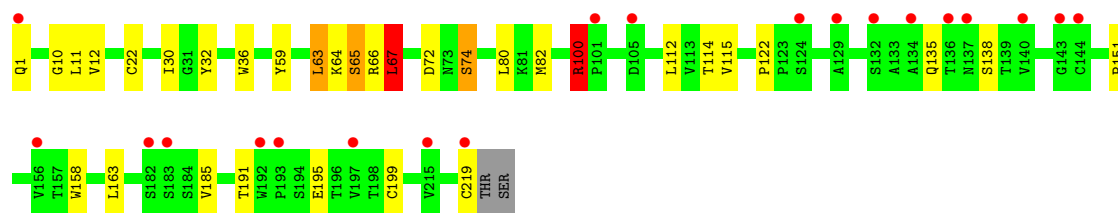
• Molecule 3: Light Chain of mAb 8C11



• Molecule 4: Heavy Chain of mAb 8H3



• Molecule 4: Heavy Chain of mAb 8H3



• Molecule 5: Light Chain of mAb 8H3

Chain F: 83% 15% ..



• Molecule 5: Light Chain of mAb 8H3

Chain I: 3% 89% 9% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.47Å 248.94Å 76.84Å 90.00° 94.07° 90.00°	Depositor
Resolution (Å)	36.65 – 3.48 36.65 – 3.48	Depositor EDS
% Data completeness (in resolution range)	93.4 (36.65-3.48) 93.3 (36.65-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.223 , 0.269 0.229 , 0.268	Depositor DCC
R_{free} test set	1542 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	72.4	Xtriage
Anisotropy	0.692	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.2	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	0.90	EDS
Total number of atoms	15430	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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	0.62	0/1122	1.14	7/1540 (0.5%)
1	B	0.68	0/1116	1.16	6/1532 (0.4%)
2	D	0.52	0/1680	0.91	3/2299 (0.1%)
2	H	0.53	0/1680	0.93	0/2299
3	C	0.64	0/1695	1.44	31/2302 (1.3%)
3	L	0.57	0/1695	1.29	24/2302 (1.0%)
4	E	0.69	1/1687 (0.1%)	1.22	8/2311 (0.3%)
4	G	0.59	0/1687	1.06	9/2311 (0.4%)
5	F	0.57	0/1723	1.01	3/2338 (0.1%)
5	I	0.54	0/1723	0.97	3/2338 (0.1%)
All	All	0.59	1/15808 (0.0%)	1.12	94/21572 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	137	ASN	N-CA	5.17	1.54	1.46

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	138	SER	N-CA-C	-14.15	89.51	110.46
3	L	75	ILE	N-CA-C	9.15	121.27	106.72
3	C	203	SER	CA-C-N	-9.06	110.44	119.78
3	C	203	SER	C-N-CA	-9.06	110.44	119.78
3	C	206	VAL	N-CA-C	8.80	120.57	107.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	482	GLN	Sidechain

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	1096	0	1085	21	0
1	B	1090	0	1080	15	0
2	D	1637	0	1630	35	0
2	H	1637	0	1630	36	0
3	C	1656	0	1576	43	0
3	L	1656	0	1576	42	0
4	E	1644	0	1618	33	0
4	G	1644	0	1618	24	0
5	F	1685	0	1617	18	0
5	I	1685	0	1617	9	0
All	All	15430	0	15047	243	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 8.

The worst 5 of 243 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:GLN:HE22	2:D:41:GLN:HE22	1.13	0.88
1:A:529:ILE:HD12	4:G:30:ILE:HD12	1.55	0.88
3:C:195:GLU:HG2	3:C:206:VAL:HG22	1.54	0.87
1:A:552:THR:HB	4:E:100:ARG:HB2	1.57	0.84
3:L:195:GLU:HG2	3:L:206:VAL:HG22	1.64	0.80

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	144/214 (67%)	138 (96%)	5 (4%)	1 (1%)	18	51
1	B	143/214 (67%)	137 (96%)	5 (4%)	1 (1%)	18	51
2	D	214/230 (93%)	195 (91%)	16 (8%)	3 (1%)	9	38
2	H	214/230 (93%)	192 (90%)	19 (9%)	3 (1%)	9	38
3	C	211/214 (99%)	205 (97%)	5 (2%)	1 (0%)	24	58
3	L	211/214 (99%)	203 (96%)	7 (3%)	1 (0%)	24	58
4	E	217/221 (98%)	213 (98%)	2 (1%)	2 (1%)	14	47
4	G	217/221 (98%)	213 (98%)	2 (1%)	2 (1%)	14	47
5	F	215/219 (98%)	206 (96%)	8 (4%)	1 (0%)	24	58
5	I	215/219 (98%)	206 (96%)	8 (4%)	1 (0%)	24	58
All	All	2001/2196 (91%)	1908 (95%)	77 (4%)	16 (1%)	16	49

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	75	THR
2	H	182	GLN
4	E	64	LYS
4	E	100	ARG
4	G	64	LYS

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	119/180 (66%)	116 (98%)	3 (2%)	42	63
1	B	118/180 (66%)	117 (99%)	1 (1%)	73	76
2	D	189/199 (95%)	181 (96%)	8 (4%)	26	52
2	H	189/199 (95%)	180 (95%)	9 (5%)	23	49
3	C	188/189 (100%)	175 (93%)	13 (7%)	14	40
3	L	188/189 (100%)	179 (95%)	9 (5%)	23	49
4	E	190/192 (99%)	186 (98%)	4 (2%)	47	66
4	G	190/192 (99%)	187 (98%)	3 (2%)	55	70
5	F	193/195 (99%)	188 (97%)	5 (3%)	40	63
5	I	193/195 (99%)	187 (97%)	6 (3%)	35	60
All	All	1757/1910 (92%)	1696 (96%)	61 (4%)	32	57

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	107	LYS
5	I	19	VAL
2	D	29	LEU
4	G	219	CYS
5	I	208	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	161	ASN
4	E	39	GLN
3	C	189	HIS
2	D	13	GLN
5	F	37	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, 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	146/214 (68%)	0.09	2 (1%) 73 49	47, 59, 74, 87	0
1	B	145/214 (67%)	-0.07	0 100 100	45, 57, 68, 77	0
2	D	218/230 (94%)	0.15	2 (0%) 81 58	50, 67, 116, 130	0
2	H	218/230 (94%)	0.21	4 (1%) 67 43	51, 66, 122, 134	0
3	C	213/214 (99%)	0.26	3 (1%) 73 49	53, 83, 114, 122	0
3	L	213/214 (99%)	0.26	4 (1%) 66 42	57, 97, 151, 162	0
4	E	219/221 (99%)	0.40	5 (2%) 61 37	53, 78, 136, 162	0
4	G	219/221 (99%)	0.61	20 (9%) 15 10	57, 79, 179, 208	0
5	F	217/219 (99%)	0.30	0 100 100	54, 82, 162, 173	0
5	I	217/219 (99%)	0.44	6 (2%) 55 32	51, 92, 212, 251	0
All	All	2025/2196 (92%)	0.28	46 (2%) 61 37	45, 74, 163, 251	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	137	VAL	4.3
3	L	194	CYS	3.6
4	G	129	ALA	3.4
4	G	182	SER	3.4
4	G	136	THR	3.2

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.