



## wwPDB EM Validation Summary Report ⓘ

Oct 7, 2024 – 02:50 PM JST

PDB ID : 8YWW  
EMDB ID : EMD-39645  
Title : The structure of HKU1-B S protein with bsAb1  
Authors : Xia, L.Y.; Zhang, Y.Y.; Zhou, Q.  
Deposited on : 2024-04-01  
Resolution : 2.70 Å (reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

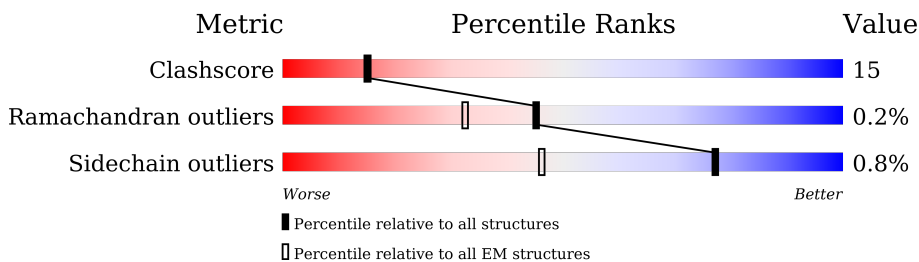
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1210	
1	B	1210	
1	C	1210	
2	E	218	
2	G	218	
3	D	212	
3	F	212	
4	H	245	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 31649 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1024	7754	4980	1288	1451	35	0	0
1	B	1024	7754	4980	1288	1451	35	0	0
1	C	1024	7754	4980	1288	1451	35	0	0

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	variant	UNP P0DTC2
A	78	HIS	ARG	conflict	UNP P0DTC2
A	79	VAL	PHE	conflict	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	658	SER	ASN	conflict	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	GLY	TYR	conflict	UNP P0DTC2
A	1210	SER	ILE	conflict	UNP P0DTC2
B	19	ILE	THR	variant	UNP P0DTC2
B	78	HIS	ARG	conflict	UNP P0DTC2
B	79	VAL	PHE	conflict	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	658	SER	ASN	conflict	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1209	GLY	TYR	conflict	UNP P0DTC2
B	1210	SER	ILE	conflict	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2
C	78	HIS	ARG	conflict	UNP P0DTC2
C	79	VAL	PHE	conflict	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	VAL	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	658	SER	ASN	conflict	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1209	GLY	TYR	conflict	UNP P0DTC2
C	1210	SER	ILE	conflict	UNP P0DTC2

- Molecule 2 is a protein called H4B6 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	218	Total	C	N	O	S	0	0
			1619	1015	278	320	6		
2	G	218	Total	C	N	O	S	0	0
			1619	1015	278	320	6		

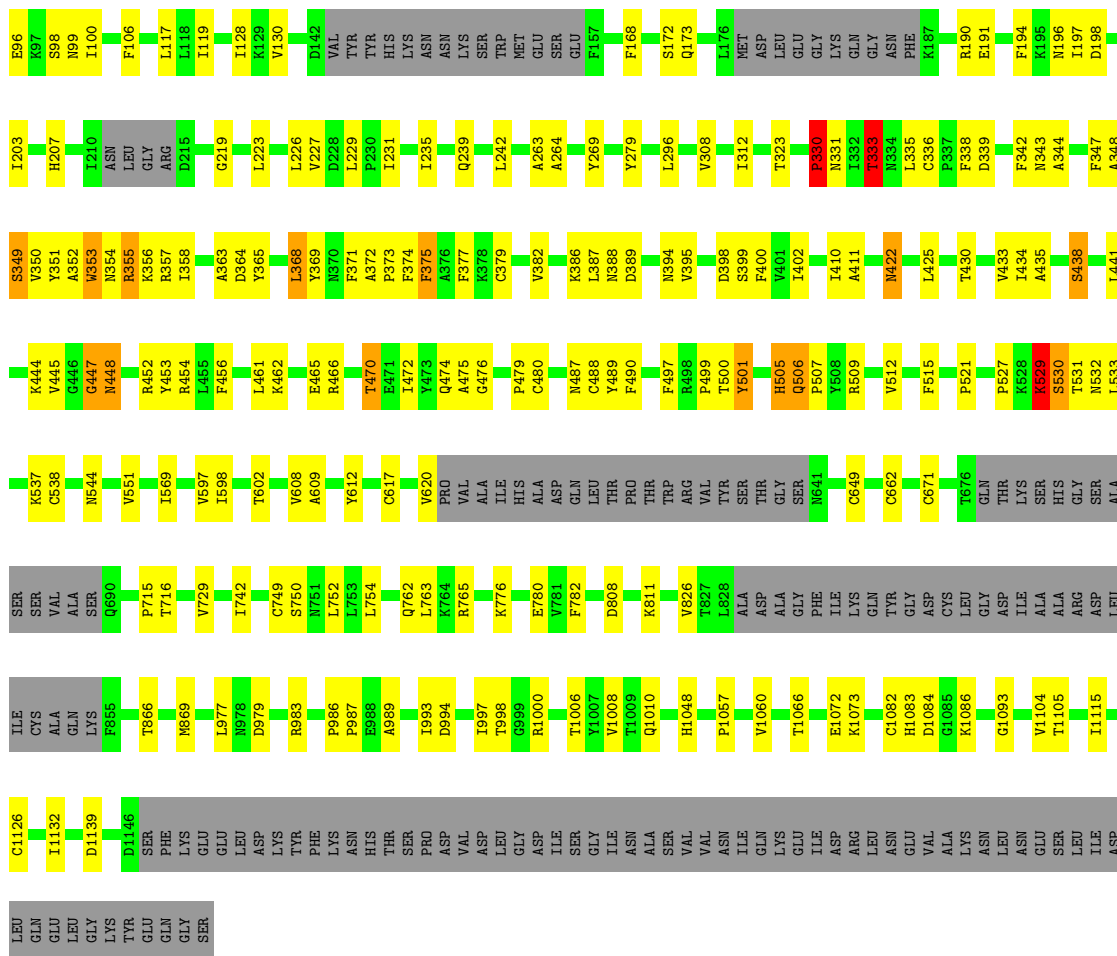
- Molecule 3 is a protein called H4B6 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	212	Total	C	N	O	S	0	0
			1646	1028	278	335	5		
3	F	212	Total	C	N	O	S	0	0
			1646	1028	278	335	5		

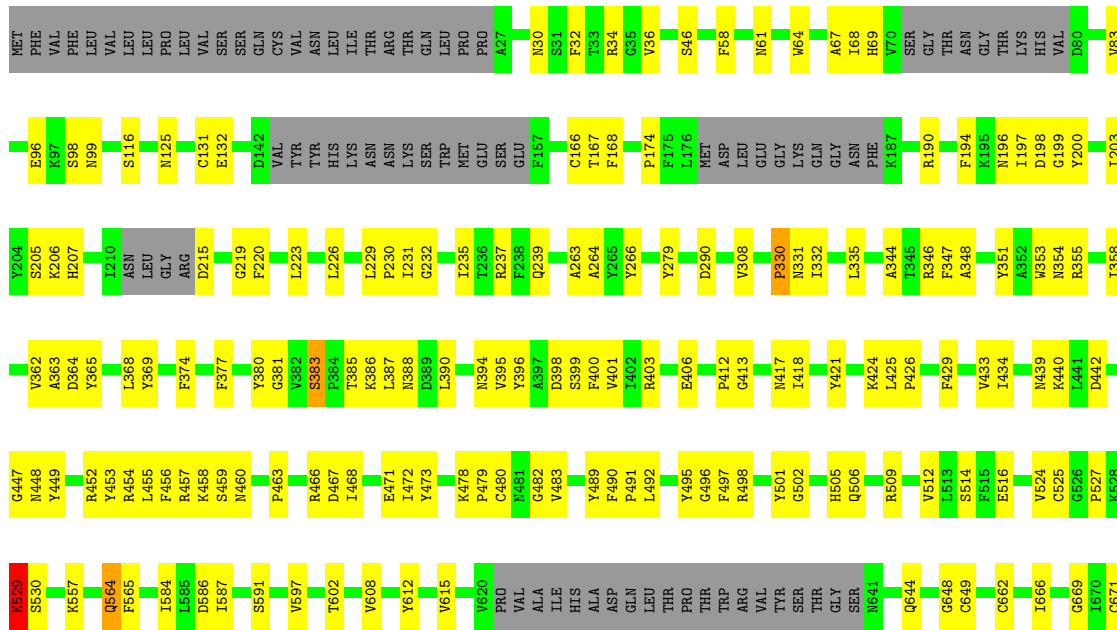
- Molecule 4 is a protein called the scfv of H4D12.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	245	Total	C	N	O	S	0	0
			1857	1160	324	364	9		

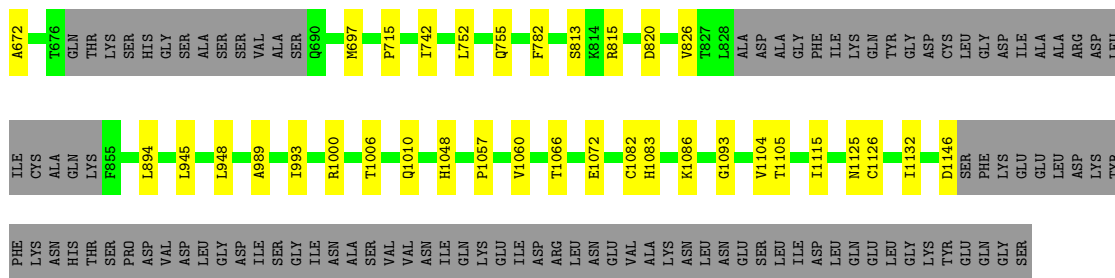




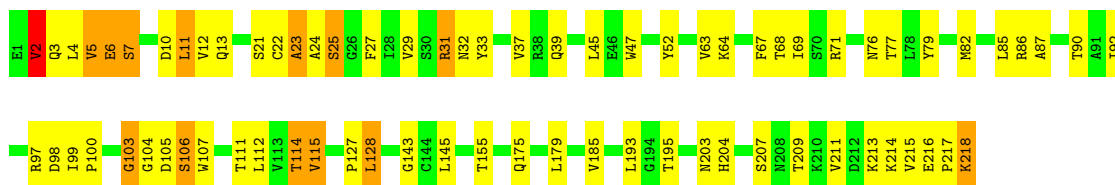
• Molecule 1: Spike glycoprotein



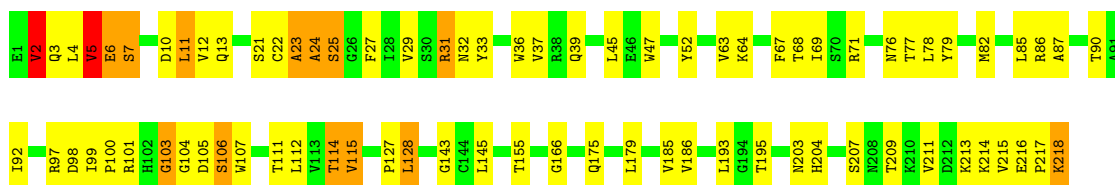




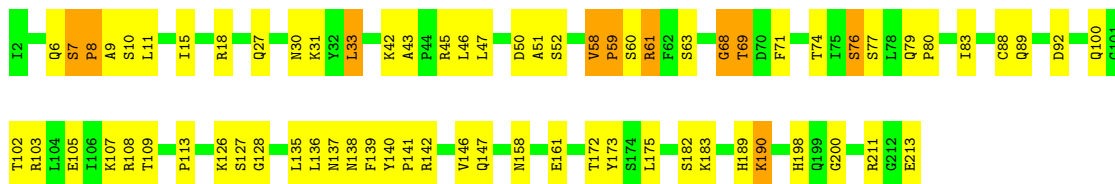
• Molecule 2: H4B6 heavy chain



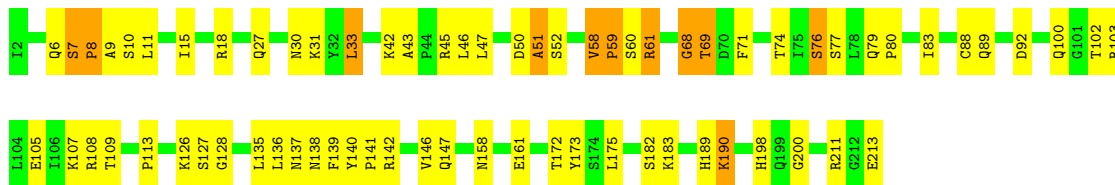
• Molecule 2: H4B6 heavy chain



• Molecule 3: H4B6 light chain

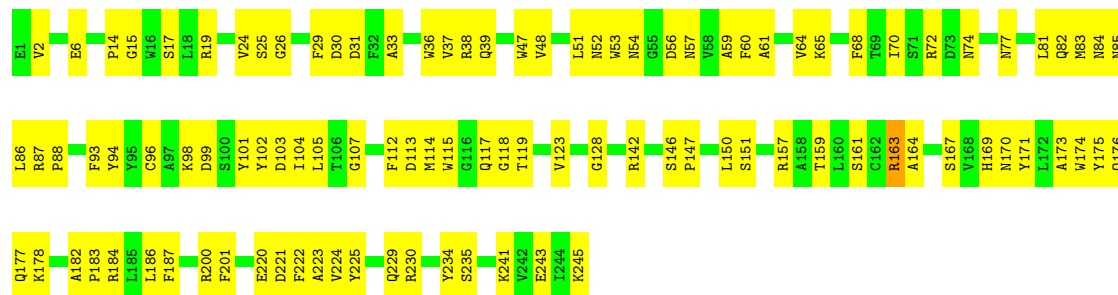


• Molecule 3: H4B6 light chain



- Molecule 4: the scfv of H4D12

Chain H:  58% 42%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	368678	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

## 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	0.36	2/7937 (0.0%)	0.80	30/10832 (0.3%)
1	B	0.37	4/7939 (0.1%)	0.84	34/10839 (0.3%)
1	C	0.52	2/7939 (0.0%)	0.77	3/10839 (0.0%)
2	E	0.48	2/1656 (0.1%)	1.43	33/2251 (1.5%)
2	G	0.48	2/1656 (0.1%)	1.43	33/2251 (1.5%)
3	D	0.32	0/1680	0.98	24/2280 (1.1%)
3	F	0.32	0/1680	0.98	24/2280 (1.1%)
4	H	0.27	0/1901	0.55	0/2573
All	All	0.41	12/32388 (0.0%)	0.89	181/44145 (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	2
1	B	0	4
1	C	0	1
2	E	0	3
2	G	0	3
All	All	0	13

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	330	PRO	C-N	27.88	1.98	1.34
1	C	529	LYS	C-N	-27.09	0.71	1.34
2	E	103	GLY	C-N	-11.18	1.12	1.33
2	G	103	GLY	C-N	-11.16	1.12	1.33
1	B	529	LYS	C-N	6.42	1.48	1.34

The worst 5 of 181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	529	LYS	CA-C-N	-47.33	13.09	117.20
1	C	529	LYS	C-N-CA	-38.82	24.66	121.70
1	B	529	LYS	O-C-N	-36.60	64.14	122.70
1	A	529	LYS	O-C-N	-32.55	70.62	122.70
2	G	24	ALA	CB-CA-C	-21.67	77.59	110.10

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	529	LYS	Peptide,Mainchain
1	B	330	PRO	Mainchain
1	B	333	THR	Peptide,Mainchain
1	B	529	LYS	Mainchain
1	C	529	LYS	Mainchain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7754	0	7362	223	0
1	B	7754	0	7366	215	0
1	C	7754	0	7361	243	0
2	E	1619	0	1592	70	0
2	G	1619	0	1592	77	0
3	D	1646	0	1596	49	0
3	F	1646	0	1596	50	0
4	H	1857	0	1759	130	0
All	All	31649	0	30224	907	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 15.

The worst 5 of 907 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:C:495:TYR:CE1	4:H:105:LEU:HD11	1.46	1.50

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:TYR:CZ	4:H:105:LEU:HD11	1.46	1.50
1:B:382:VAL:HG11	1:B:387:LEU:CD2	1.41	1.45
1:B:364:ASP:CG	1:B:527:PRO:HG3	1.09	1.45
1:A:382:VAL:HG11	1:A:387:LEU:CD2	1.41	1.45

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1000/1210 (83%)	962 (96%)	36 (4%)	2 (0%)	44	68
1	B	1004/1210 (83%)	973 (97%)	28 (3%)	3 (0%)	37	61
1	C	1004/1210 (83%)	934 (93%)	67 (7%)	3 (0%)	37	61
2	E	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
2	G	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
3	D	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
3	F	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
4	H	243/245 (99%)	221 (91%)	22 (9%)	0	100	100
All	All	4103/4735 (87%)	3910 (95%)	185 (4%)	8 (0%)	45	68

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	529	LYS
1	C	529	LYS
1	A	529	LYS
1	A	530	SER
1	B	530	SER

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	820/1055 (78%)	811 (99%)	9 (1%)	70	87
1	B	820/1055 (78%)	811 (99%)	9 (1%)	70	87
1	C	820/1055 (78%)	820 (100%)	0	100	100
2	E	182/182 (100%)	181 (100%)	1 (0%)	86	95
2	G	182/182 (100%)	181 (100%)	1 (0%)	86	95
3	D	187/187 (100%)	185 (99%)	2 (1%)	70	87
3	F	187/187 (100%)	185 (99%)	2 (1%)	70	87
4	H	193/193 (100%)	191 (99%)	2 (1%)	73	89
All	All	3391/4096 (83%)	3365 (99%)	26 (1%)	77	91

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	433	VAL
1	B	488	CYS
4	H	142	ARG
1	B	472	ILE
2	E	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	76	ASN
2	G	32	ASN
1	C	460	ASN
3	F	27	GLN
1	C	439	ASN

### 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4
1	C	4
1	B	2
2	E	2
2	G	2

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	321:GLN	C	322:PRO	N	3.93
1	C	333:THR	C	334:ASN	N	3.40
1	A	526:GLY	C	527:PRO	N	3.36
1	B	322:PRO	C	323:THR	N	3.26
1	A	333:THR	C	334:ASN	N	2.99