



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2026 – 12:45 PM EDT

PDB ID : 9YXW / pdb\_00009yxw  
Title : Crystal structure of HCoV-HKU1 RBD bound by H501-008 Fab  
Authors : Wrapp, D.; McLellan, J.S.  
Deposited on : 2025-10-27  
Resolution : 2.60 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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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

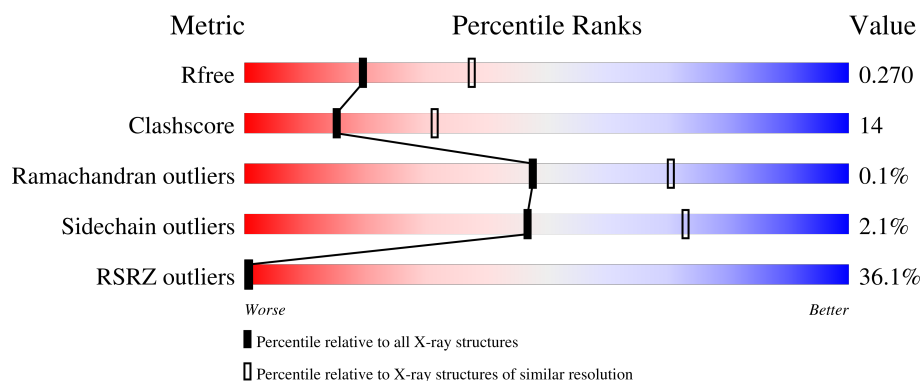
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	305	<div> <div>53%</div> <div>73% 17% 9%</div> </div>
2	H	243	<div> <div>36%</div> <div>71% 22% 5%</div> </div>
3	L	216	<div> <div>4%</div> <div>80% 18% ..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PCA	H	1	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5659 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2152	1339	372	419	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	607	GLY	-	expression tag	UNP Q0ZME7
A	608	SER	-	expression tag	UNP Q0ZME7
A	609	LEU	-	expression tag	UNP Q0ZME7
A	610	GLU	-	expression tag	UNP Q0ZME7
A	611	VAL	-	expression tag	UNP Q0ZME7
A	612	LEU	-	expression tag	UNP Q0ZME7
A	613	PHE	-	expression tag	UNP Q0ZME7
A	614	GLN	-	expression tag	UNP Q0ZME7

- Molecule 2 is a protein called H501-008 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	232	Total	C	N	O	S	0	0	0
			1768	1114	305	341	8			

- Molecule 3 is a protein called H501-008 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1560	974	262	320	4			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		

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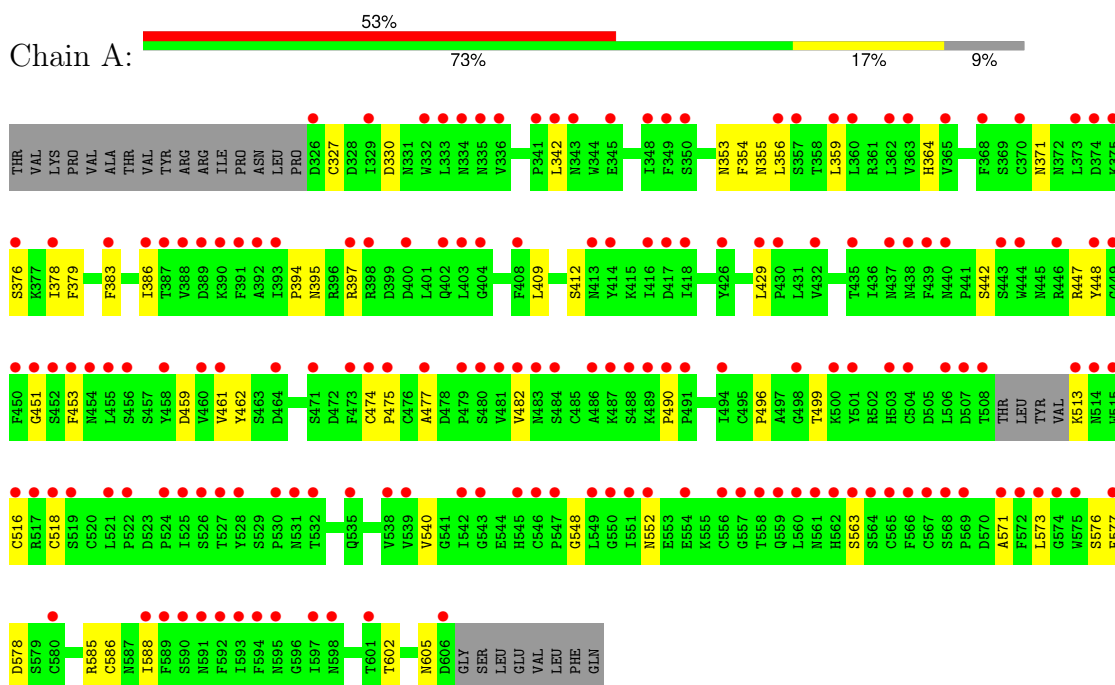
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	77	Total 77	O 77	0	0
4	L	98	Total 98	O 98	0	0

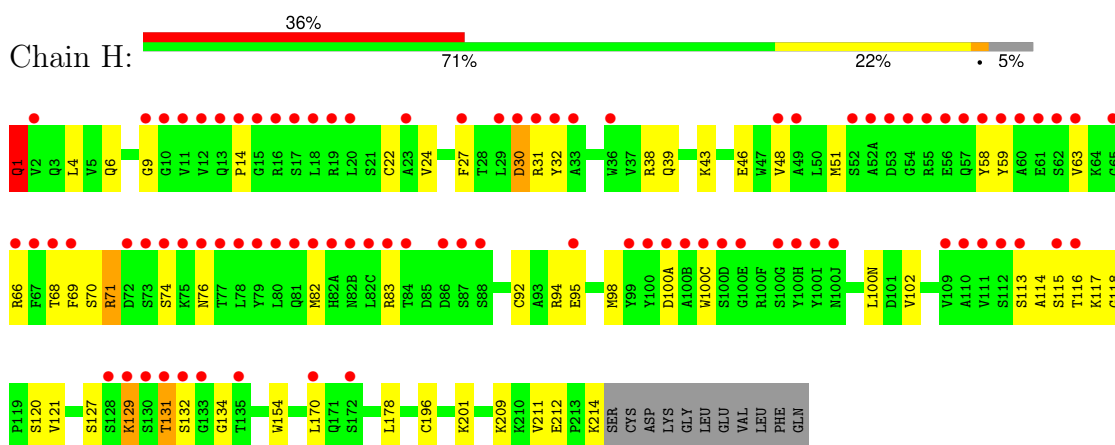
### 3 Residue-property plots

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.

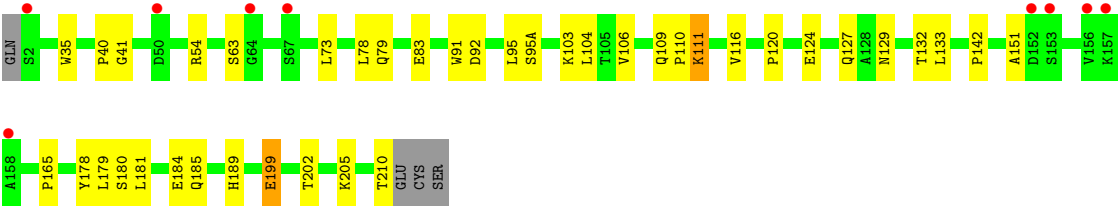
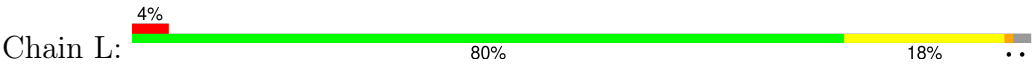
#### • Molecule 1: Spike protein S1



#### • Molecule 2: H501-008 Fab heavy chain



#### • Molecule 3: H501-008 Fab light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.46Å 71.76Å 174.48Å 90.00° 94.58° 90.00°	Depositor
Resolution (Å)	57.97 – 2.60 57.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (57.97-2.60) 99.7 (57.97-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.252 , 0.267 0.257 , 0.270	Depositor DCC
$R_{free}$ test set	1935 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.8	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 75.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5659	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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

Bond lengths and bond angles in the following residue types are not validated in this section: PCA

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	0/2207	0.78	0/3000
2	H	0.45	0/1806	0.92	5/2459 (0.2%)
3	L	0.47	0/1598	0.83	0/2188
All	All	0.42	0/5611	0.84	5/7647 (0.1%)

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
2	H	0	2
3	L	0	1
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	LYS	CB-CG-CD	-5.42	98.84	111.30
2	H	131	THR	CA-C-N	5.21	128.49	121.05
2	H	131	THR	C-N-CA	5.21	128.49	121.05
2	H	100(N)	LEU	CA-C-N	5.18	127.22	120.28
2	H	100(N)	LEU	C-N-CA	5.18	127.22	120.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	1	PCA	Mainchain
2	H	31	ARG	Sidechain
3	L	54	ARG	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	2152	0	2001	33	1
2	H	1768	0	1717	73	0
3	L	1560	0	1511	41	1
4	A	4	0	0	1	0
4	H	77	0	0	43	2
4	L	98	0	0	33	3
All	All	5659	0	5229	146	4

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 14.

All (146) 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)
2:H:71:ARG:HB2	4:H:305:HOH:O	1.28	1.26
3:L:180:SER:OG	4:L:301:HOH:O	1.71	1.09
3:L:178:TYR:OH	4:L:302:HOH:O	1.74	1.05
3:L:124:GLU:HG3	4:L:349:HOH:O	1.58	1.03
3:L:180:SER:CB	4:L:301:HOH:O	2.10	1.00
2:H:38:ARG:CZ	4:H:306:HOH:O	2.09	0.98
2:H:117:LYS:HE2	4:H:303:HOH:O	1.61	0.97
3:L:109:GLN:NE2	4:L:303:HOH:O	1.97	0.97
2:H:118:GLY:O	4:H:303:HOH:O	1.81	0.96
2:H:83:ARG:HB3	4:H:325:HOH:O	1.63	0.96
2:H:71:ARG:N	4:H:305:HOH:O	2.00	0.94
3:L:210:THR:HB	4:L:320:HOH:O	1.70	0.90
2:H:38:ARG:NH1	4:H:306:HOH:O	2.03	0.89
2:H:46:GLU:HB3	4:H:306:HOH:O	1.72	0.89
3:L:91:TRP:CE2	4:L:316:HOH:O	2.25	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:129:LYS:HG3	4:H:313:HOH:O	1.74	0.88
2:H:1:PCA:CD	4:H:309:HOH:O	2.21	0.87
2:H:63:VAL:HG12	2:H:66:ARG:HH12	1.38	0.87
2:H:1:PCA:N	4:H:309:HOH:O	2.07	0.84
3:L:41:GLY:N	4:L:305:HOH:O	2.01	0.84
2:H:39:GLN:OE1	4:H:304:HOH:O	1.96	0.83
3:L:127:GLN:OE1	4:L:304:HOH:O	1.98	0.80
2:H:71:ARG:CB	4:H:305:HOH:O	2.03	0.80
2:H:98:MET:SD	4:H:348:HOH:O	2.40	0.79
3:L:199:GLU:O	4:L:306:HOH:O	2.03	0.76
2:H:1:PCA:CB	4:H:309:HOH:O	2.35	0.74
3:L:199:GLU:OE2	4:L:307:HOH:O	2.06	0.74
2:H:1:PCA:CA	4:H:309:HOH:O	2.34	0.74
3:L:91:TRP:NE1	4:L:316:HOH:O	2.22	0.72
1:A:353:ASN:HD21	1:A:605:ASN:HB3	1.55	0.72
1:A:330:ASP:HB3	1:A:359:LEU:HD11	1.72	0.71
1:A:376:SER:HA	1:A:379:PHE:CE2	2.26	0.70
2:H:114:ALA:HB2	4:H:322:HOH:O	1.92	0.70
3:L:210:THR:C	4:L:320:HOH:O	2.34	0.70
2:H:46:GLU:CG	4:H:306:HOH:O	2.41	0.69
2:H:46:GLU:CB	4:H:306:HOH:O	2.37	0.67
3:L:124:GLU:OE1	4:L:308:HOH:O	2.10	0.67
2:H:120:SER:HA	4:H:328:HOH:O	1.94	0.67
3:L:92:ASP:OD2	3:L:95:LEU:HD12	1.95	0.67
3:L:40:PRO:CA	4:L:305:HOH:O	2.43	0.66
3:L:40:PRO:HA	4:L:305:HOH:O	1.96	0.65
2:H:27:PHE:HE2	2:H:32:TYR:HB2	1.62	0.65
2:H:116:THR:N	4:H:308:HOH:O	2.05	0.65
2:H:127:SER:OG	4:H:301:HOH:O	1.64	0.64
3:L:165:PRO:HD3	4:L:358:HOH:O	1.97	0.64
1:A:330:ASP:HB3	1:A:359:LEU:CD1	2.28	0.63
1:A:429:LEU:HD23	1:A:588:ILE:HD12	1.79	0.63
2:H:117:LYS:HG2	4:H:303:HOH:O	1.98	0.63
3:L:180:SER:HB3	4:L:301:HOH:O	1.84	0.63
2:H:211:VAL:O	4:H:311:HOH:O	2.15	0.63
2:H:63:VAL:HG12	2:H:66:ARG:NH1	2.13	0.61
2:H:1:PCA:OE	4:H:312:HOH:O	2.16	0.61
2:H:38:ARG:HG3	4:H:306:HOH:O	2.00	0.60
3:L:83:GLU:CD	4:L:324:HOH:O	2.44	0.59
2:H:43:LYS:HE2	4:H:318:HOH:O	2.00	0.59
2:H:27:PHE:CE2	2:H:32:TYR:HB2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:210:THR:CA	4:L:320:HOH:O	2.50	0.59
2:H:43:LYS:NZ	4:H:318:HOH:O	2.36	0.58
3:L:110:PRO:O	4:L:309:HOH:O	2.16	0.58
3:L:63:SER:OG	4:L:310:HOH:O	2.17	0.58
1:A:356:LEU:HD21	1:A:378:ILE:HG22	1.85	0.58
2:H:63:VAL:CG1	2:H:66:ARG:HH12	2.13	0.57
2:H:113:SER:C	4:H:322:HOH:O	2.47	0.57
3:L:132:THR:O	4:L:312:HOH:O	2.18	0.57
3:L:129:ASN:OD1	4:L:311:HOH:O	2.18	0.57
3:L:91:TRP:CD1	4:L:316:HOH:O	2.58	0.56
1:A:354:PHE:CE2	1:A:359:LEU:HD13	2.41	0.55
2:H:131:THR:N	4:H:313:HOH:O	2.26	0.55
3:L:103:LYS:NZ	4:L:323:HOH:O	2.38	0.55
1:A:342:LEU:HD23	1:A:461:VAL:HG12	1.89	0.54
1:A:394:PRO:HG2	1:A:397:ARG:HB2	1.89	0.53
2:H:6:GLN:HE22	2:H:92:CYS:H	1.57	0.53
1:A:563:SER:HA	4:A:701:HOH:O	2.08	0.53
2:H:43:LYS:CE	4:H:318:HOH:O	2.57	0.53
1:A:364:HIS:CE1	1:A:585:ARG:HH22	2.27	0.52
2:H:1:PCA:HB2	4:H:309:HOH:O	2.03	0.52
2:H:38:ARG:HG2	2:H:48:VAL:CG2	2.39	0.52
3:L:120:PRO:O	4:L:313:HOH:O	2.18	0.52
1:A:412:SER:HA	1:A:540:VAL:HG23	1.92	0.51
2:H:6:GLN:NE2	2:H:92:CYS:H	2.08	0.51
2:H:121:VAL:O	2:H:209:LYS:HE3	2.10	0.51
3:L:106:VAL:O	4:L:314:HOH:O	2.19	0.51
2:H:129:LYS:HB2	2:H:132:SER:HB2	1.92	0.51
2:H:94:ARG:HB3	2:H:102:VAL:HG22	1.92	0.50
2:H:127:SER:CB	4:H:301:HOH:O	2.39	0.50
1:A:354:PHE:CD2	1:A:355:ASN:N	2.78	0.50
2:H:38:ARG:NH2	2:H:46:GLU:OE2	2.45	0.49
3:L:78:LEU:HD11	3:L:104:LEU:HD21	1.94	0.49
3:L:79:GLN:NE2	4:L:322:HOH:O	2.36	0.49
1:A:395:ASN:HB2	1:A:578:ASP:OD2	2.14	0.48
2:H:70:SER:C	4:H:305:HOH:O	2.50	0.48
3:L:133:LEU:HB2	3:L:179:LEU:HB3	1.96	0.48
2:H:129:LYS:HE3	2:H:132:SER:O	2.14	0.48
3:L:202:THR:HG21	4:L:332:HOH:O	2.13	0.48
2:H:129:LYS:CG	4:H:313:HOH:O	2.46	0.47
1:A:496:PRO:O	1:A:499:THR:HG22	2.14	0.47
1:A:364:HIS:CD2	1:A:585:ARG:HH12	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:184:GLU:HA	4:L:365:HOH:O	2.14	0.47
2:H:100(A):ASP:CG	2:H:100(C):TRP:HE3	2.23	0.46
2:H:30:ASP:OD1	2:H:30:ASP:C	2.59	0.46
1:A:383:PHE:CZ	1:A:386:ILE:HD11	2.50	0.46
2:H:1:PCA:CG	4:H:309:HOH:O	2.58	0.46
1:A:356:LEU:HD21	1:A:378:ILE:CG2	2.46	0.46
2:H:95:GLU:HG3	4:H:348:HOH:O	2.16	0.46
2:H:24:VAL:HG12	2:H:76:ASN:HB3	1.99	0.45
3:L:91:TRP:CD2	4:L:316:HOH:O	2.63	0.45
3:L:210:THR:CB	4:L:320:HOH:O	2.41	0.45
2:H:9:GLY:N	4:H:307:HOH:O	2.04	0.44
1:A:447:ARG:HG3	2:H:100(C):TRP:CD2	2.52	0.44
2:H:27:PHE:HB2	4:H:343:HOH:O	2.17	0.44
1:A:474:CYS:HB2	1:A:499:THR:OG1	2.18	0.44
2:H:51:MET:SD	2:H:69:PHE:CD2	3.11	0.44
2:H:129:LYS:O	4:H:313:HOH:O	2.21	0.44
3:L:116:VAL:O	3:L:205:LYS:HE3	2.18	0.44
2:H:51:MET:HE1	2:H:68:THR:HA	2.00	0.43
3:L:111:LYS:HG2	3:L:142:PRO:HD3	2.01	0.43
1:A:448:TYR:CE2	1:A:475:PRO:HD2	2.53	0.43
2:H:27:PHE:CD2	2:H:32:TYR:CD1	3.07	0.43
2:H:63:VAL:HG12	2:H:63:VAL:O	2.19	0.43
3:L:35:TRP:CD2	3:L:73:LEU:HB2	2.53	0.43
1:A:327:CYS:HB2	1:A:354:PHE:CD1	2.54	0.43
1:A:462:TYR:CZ	1:A:576:SER:HB3	2.54	0.43
2:H:14:PRO:HD2	2:H:113:SER:HA	2.00	0.43
1:A:459:ASP:OD1	1:A:577:PHE:HE2	2.02	0.43
1:A:383:PHE:HE1	1:A:602:THR:HG22	1.84	0.42
2:H:70:SER:OG	2:H:74:SER:HB3	2.20	0.42
2:H:132:SER:C	2:H:134:GLY:H	2.27	0.42
1:A:459:ASP:OD1	1:A:577:PHE:CE2	2.72	0.42
2:H:115:SER:N	4:H:308:HOH:O	2.52	0.42
1:A:552:ASN:HB2	1:A:573:LEU:HD21	2.01	0.42
1:A:477:ALA:HB1	1:A:482:VAL:HG11	2.00	0.42
1:A:571:ALA:O	1:A:573:LEU:HD22	2.20	0.42
2:H:46:GLU:HG2	4:H:306:HOH:O	2.14	0.42
2:H:4:LEU:HD12	2:H:22:CYS:SG	2.60	0.41
2:H:214:LYS:HE3	2:H:214:LYS:HB3	1.87	0.41
1:A:490:PRO:HG3	1:A:518:CYS:SG	2.60	0.41
3:L:151:ALA:HB1	3:L:189:HIS:CD2	2.56	0.41
2:H:46:GLU:CD	4:H:306:HOH:O	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:91:TRP:CZ2	3:L:95(A):SER:C	2.99	0.41
2:H:58:TYR:C	2:H:59:TYR:CD1	2.99	0.41
2:H:83:ARG:HD3	2:H:83:ARG:HA	1.79	0.41
1:A:442:SER:HB2	1:A:548:GLY:HA2	2.03	0.40
2:H:82:MET:HE2	2:H:82:MET:HB3	1.86	0.40
1:A:359:LEU:HA	1:A:359:LEU:HD12	1.41	0.40
1:A:397:ARG:HB3	1:A:409:LEU:HD11	2.04	0.40
2:H:154:TRP:CH2	2:H:196:CYS:HB3	2.57	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:385:HOH:O	4:L:398:HOH:O[4_345]	1.73	0.47
4:H:365:HOH:O	4:L:384:HOH:O[4_345]	1.81	0.39
4:H:351:HOH:O	4:L:370:HOH:O[4_345]	2.06	0.14
1:A:513:LYS:NZ	3:L:185:GLN:OE1[3_555]	2.12	0.08

## 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	273/305 (90%)	269 (98%)	3 (1%)	1 (0%)	30	51
2	H	230/243 (95%)	214 (93%)	16 (7%)	0	100	100
3	L	210/216 (97%)	205 (98%)	5 (2%)	0	100	100
All	All	713/764 (93%)	688 (96%)	24 (3%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	GLY

### 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	257/283 (91%)	253 (98%)	4 (2%)	55	79
2	H	194/204 (95%)	188 (97%)	6 (3%)	35	63
3	L	175/179 (98%)	172 (98%)	3 (2%)	53	78
All	All	626/666 (94%)	613 (98%)	13 (2%)	47	73

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	371	ASN
1	A	453	PHE
1	A	516	CYS
1	A	586	CYS
2	H	30	ASP
2	H	71	ARG
2	H	129	LYS
2	H	170	LEU
2	H	178	LEU
2	H	212	GLU
3	L	111	LYS
3	L	181	LEU
3	L	199	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	ASN
1	A	371	ASN
1	A	395	ASN
1	A	410	GLN
1	A	424	GLN
1	A	433	ASN
1	A	437	ASN
1	A	591	ASN

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Mol	Chain	Res	Type
2	H	6	GLN
2	H	13	GLN
2	H	81	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PCA	H	1	2	7,8,9	0.73	0	9,10,12	1.70	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	PCA	O-C-CA	-4.20	113.96	124.77

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	PCA	7	0

## 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	277/305 (90%)	2.34	163 (58%) <b>0</b> <b>0</b>	99, 188, 256, 270	0
2	H	231/243 (95%)	1.73	88 (38%) <b>1</b> <b>0</b>	28, 77, 145, 169	0
3	L	212/216 (98%)	0.55	9 (4%) 40 35	28, 46, 91, 112	0
All	All	720/764 (94%)	1.61	260 (36%) <b>1</b> <b>0</b>	28, 98, 234, 270	0

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	15	GLY	7.1
1	A	563	SER	7.1
1	A	562	HIS	6.6
1	A	560	LEU	6.6
2	H	132	SER	6.4
2	H	100(G)	SER	5.7
1	A	571	ALA	5.6
1	A	439	PHE	5.6
1	A	486	ALA	5.5
2	H	100	TYR	5.4
2	H	14	PRO	5.2
2	H	63	VAL	5.1
2	H	74	SER	5.1
2	H	111	VAL	5.0
1	A	573	LEU	4.9
2	H	82(C)	LEU	4.9
1	A	564	SER	4.8
2	H	115	SER	4.8
2	H	12	VAL	4.8
1	A	597	ILE	4.7
1	A	513	LYS	4.7
1	A	333	LEU	4.7
1	A	551	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
3	L	158	ALA	4.5
2	H	62	SER	4.5
2	H	172	SER	4.5
1	A	446	ARG	4.5
2	H	133	GLY	4.5
1	A	391	PHE	4.4
1	A	378	ILE	4.4
1	A	508	THR	4.4
2	H	82(B)	ASN	4.3
2	H	100(D)	SER	4.3
2	H	17	SER	4.3
2	H	11	VAL	4.3
1	A	373	LEU	4.2
2	H	65	GLY	4.2
1	A	390	LYS	4.2
1	A	360	LEU	4.2
2	H	82	MET	4.2
2	H	130	SER	4.2
2	H	75	LYS	4.2
1	A	574	GLY	4.1
1	A	542	ILE	4.1
3	L	2	SER	4.1
2	H	30	ASP	4.1
1	A	575	TRP	4.1
2	H	9	GLY	4.1
1	A	430	PRO	4.0
1	A	569	PRO	4.0
2	H	18	LEU	4.0
1	A	454	ASN	4.0
1	A	416	ILE	4.0
2	H	72	ASP	4.0
1	A	460	VAL	3.9
1	A	501	TYR	3.9
1	A	566	PHE	3.8
2	H	55	ARG	3.8
1	A	506	LEU	3.8
2	H	100(H)	TYR	3.7
1	A	487	LYS	3.7
1	A	559	GLN	3.7
1	A	567	CYS	3.6
1	A	488	SER	3.6
2	H	16	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	449	GLY	3.6
1	A	535	GLN	3.6
2	H	68	THR	3.6
2	H	100(J)	ASN	3.6
1	A	528	TYR	3.6
2	H	73	SER	3.6
1	A	550	GLY	3.5
1	A	341	PRO	3.5
1	A	450	PHE	3.5
1	A	334	ASN	3.5
2	H	100(A)	ASP	3.5
1	A	547	PRO	3.5
1	A	561	ASN	3.5
1	A	477	ALA	3.5
1	A	572	PHE	3.5
1	A	375	LYS	3.4
1	A	557	GLY	3.4
2	H	79	TYR	3.4
2	H	113	SER	3.4
2	H	128	SER	3.4
1	A	558	THR	3.4
1	A	403	LEU	3.4
2	H	29	LEU	3.4
2	H	67	PHE	3.4
1	A	458	TYR	3.3
1	A	389	ASP	3.3
1	A	594	PHE	3.3
1	A	538	VAL	3.3
1	A	481	VAL	3.2
2	H	27	PHE	3.2
1	A	437	ASN	3.2
2	H	129	LYS	3.2
2	H	58	TYR	3.2
2	H	76	ASN	3.1
1	A	489	LYS	3.1
1	A	480	SER	3.1
1	A	479	PRO	3.1
1	A	539	VAL	3.1
1	A	522	PRO	3.1
1	A	515	TRP	3.1
1	A	590	SER	3.1
1	A	490	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	414	TYR	3.0
1	A	455	LEU	3.0
1	A	443	SER	3.0
2	H	61	GLU	3.0
1	A	417	ASP	2.9
2	H	52(A)	ALA	2.9
1	A	491	PRO	2.9
1	A	498	GLY	2.9
2	H	110	ALA	2.9
1	A	365	VAL	2.9
1	A	453	PHE	2.9
2	H	78	LEU	2.9
3	L	157	LYS	2.9
2	H	112	SER	2.9
1	A	549	LEU	2.9
2	H	19	ARG	2.9
1	A	376	SER	2.9
1	A	342	LEU	2.9
1	A	448	TYR	2.8
2	H	100(B)	ALA	2.8
2	H	66	ARG	2.8
2	H	23	ALA	2.8
1	A	521	LEU	2.8
1	A	601	THR	2.8
1	A	363	VAL	2.8
2	H	100(I)	TYR	2.8
2	H	20	LEU	2.8
1	A	432	VAL	2.8
1	A	554	GLU	2.8
1	A	546	CYS	2.7
1	A	494	ILE	2.7
1	A	593	ILE	2.7
2	H	95	GLU	2.7
1	A	517	ARG	2.7
1	A	589	PHE	2.7
1	A	451	GLY	2.7
1	A	519	SER	2.7
1	A	552	ASN	2.7
1	A	398	ARG	2.7
1	A	368	PHE	2.7
1	A	482	VAL	2.7
2	H	32	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	504	CYS	2.7
2	H	109	VAL	2.7
1	A	362	LEU	2.7
2	H	131	THR	2.7
2	H	86	ASP	2.7
1	A	356	LEU	2.6
2	H	13	GLN	2.6
1	A	475	PRO	2.6
2	H	100(C)	TRP	2.6
3	L	50	ASP	2.6
2	H	31	ARG	2.6
1	A	516	CYS	2.6
1	A	348	ILE	2.5
1	A	577	PHE	2.5
1	A	326	ASP	2.5
1	A	525	ILE	2.5
1	A	524	PRO	2.5
1	A	461	VAL	2.5
3	L	156	VAL	2.5
2	H	69	PHE	2.5
3	L	67	SER	2.5
1	A	386	ILE	2.5
1	A	500	LYS	2.5
1	A	503	HIS	2.5
2	H	82(A)	HIS	2.5
2	H	59	TYR	2.5
1	A	592	PHE	2.5
2	H	49	ALA	2.5
1	A	343	ASN	2.5
1	A	387	THR	2.5
1	A	359	LEU	2.5
1	A	568	SER	2.5
2	H	88	SER	2.5
1	A	444	TRP	2.5
1	A	388	VAL	2.5
1	A	595	ASN	2.4
2	H	36	TRP	2.4
1	A	408	PHE	2.4
1	A	565	CYS	2.4
1	A	580	CYS	2.4
3	L	64	GLY	2.4
2	H	83	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	84	THR	2.4
1	A	357	SER	2.4
1	A	484	SER	2.4
1	A	438	ASN	2.4
1	A	374	ASP	2.4
1	A	606	ASP	2.4
3	L	152	ASP	2.4
1	A	543	GLY	2.4
1	A	531	ASN	2.3
2	H	81	GLN	2.3
1	A	452	SER	2.3
1	A	464	ASP	2.3
2	H	48	VAL	2.3
1	A	392	ALA	2.3
2	H	60	ALA	2.3
1	A	400	ASP	2.3
2	H	87	SER	2.3
1	A	393	ILE	2.3
1	A	526	SER	2.3
2	H	10	GLY	2.3
2	H	80	LEU	2.3
1	A	556	CYS	2.2
1	A	588	ILE	2.2
1	A	345	GLU	2.2
1	A	507	ASP	2.2
1	A	336	VAL	2.2
1	A	435	THR	2.2
1	A	527	THR	2.2
1	A	532	THR	2.2
1	A	471	SER	2.2
3	L	153	SER	2.2
1	A	429	LEU	2.2
1	A	329	ILE	2.2
2	H	77	THR	2.2
1	A	397	ARG	2.2
1	A	530	PRO	2.2
2	H	100(E)	GLY	2.2
1	A	456	SER	2.2
1	A	545	HIS	2.2
1	A	349	PHE	2.2
1	A	370	CYS	2.1
1	A	474	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	335	ASN	2.1
2	H	54	GLY	2.1
1	A	418	ILE	2.1
2	H	33	ALA	2.1
2	H	116	THR	2.1
1	A	402	GLN	2.1
1	A	518	CYS	2.1
1	A	440	ASN	2.1
1	A	483	ASN	2.1
1	A	404	GLY	2.1
2	H	2	VAL	2.1
2	H	53	ASP	2.1
1	A	383	PHE	2.1
2	H	57	GLN	2.1
1	A	413	ASN	2.1
1	A	591	ASN	2.1
1	A	350	SER	2.1
2	H	52	SER	2.1
1	A	426	TYR	2.1
2	H	99	TYR	2.1
1	A	473	PHE	2.1
2	H	56	GLU	2.0
2	H	135	THR	2.0
2	H	170	LEU	2.0
1	A	598	ASN	2.0
1	A	332	TRP	2.0
1	A	514	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	PCA	H	1	8/9	0.78	0.21	46,49,57,57	0

## 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.