



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2017 – 01:46 PM EST

PDB ID : 5GZO  
Title : Structure of neutralizing antibody bound to Zika envelope protein  
Authors : Wang, Q.; Yang, H.; Liu, X.; Dai, L.; Ma, T.; Qi, J.; Wong, G.; Peng, R.; Liu, S.; Li, J.; Li, S.; Song, J.; Liu, J.; He, J.; Yuan, H.; Xiong, Y.; Liao, Y.; Li, J.; Yang, J.; Tong, Z.; Griffin, B.; Bi, Y.; Liang, M.; Xu, X.; Cheng, G.; Wang, P.; Qiu, X.; Kobinger, G.; Shi, Y.; Yan, J.; Gao, G.F.  
Deposited on : 2016-09-29  
Resolution : 2.75 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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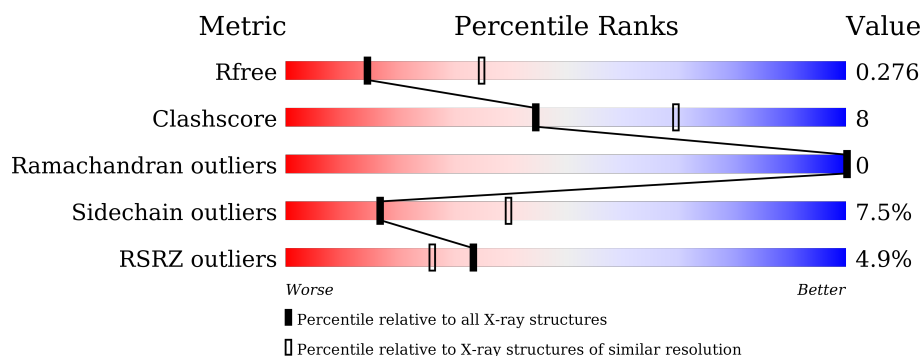
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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## X-RAY DIFFRACTION

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))
$R_{free}$	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	409	<div> <div>4%</div> <div>81%</div> <div>12%</div> <div>5%</div> </div>
1	B	409	<div> <div>12%</div> <div>77%</div> <div>17%</div> <div>5%</div> </div>
2	C	220	<div> <div>2%</div> <div>79%</div> <div>17%</div> <div>2%</div> </div>
2	H	220	<div> <div>79%</div> <div>17%</div> <div>4%</div> </div>
3	D	215	<div> <div>4%</div> <div>80%</div> <div>17%</div> <div>1%</div> </div>
3	L	215	<div> <div>78%</div> <div>18%</div> <div>4%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12422 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			2976	1861	519	571	25			
1	B	390	Total	C	N	O	S	0	0	0
			2976	1861	519	571	25			

- Molecule 2 is a protein called Antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	0	0
			1599	1009	268	318	4			
2	C	214	Total	C	N	O	S	0	0	0
			1599	1009	268	318	4			

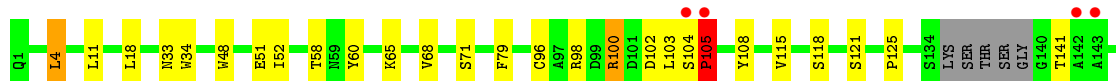
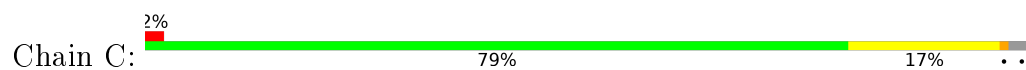
- Molecule 3 is a protein called Antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1636	1019	282	330	5			
3	D	213	Total	C	N	O	S	0	0	0
			1636	1019	282	330	5			

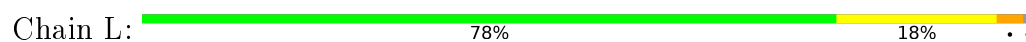




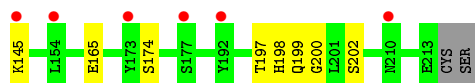
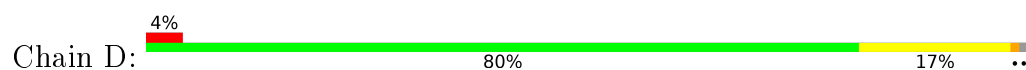
• Molecule 2: Antibody heavy chain



• Molecule 3: Antibody light chain



• Molecule 3: Antibody light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.67Å 97.50Å 165.75Å 90.00° 91.52° 90.00°	Depositor
Resolution (Å)	44.68 – 2.75 44.68 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.68-2.75) 99.8 (44.68-2.76)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.231 , 0.277 0.233 , 0.276	Depositor DCC
$R_{free}$ test set	2591 reflections (4.89%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.3	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12422	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.27% 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	0.29	0/3038	0.52	1/4114 (0.0%)
1	B	0.25	0/3038	0.51	2/4114 (0.0%)
2	C	0.34	1/1640 (0.1%)	0.53	0/2242
2	H	0.36	0/1640	0.57	1/2242 (0.0%)
3	D	0.31	0/1670	0.53	2/2264 (0.1%)
3	L	0.38	0/1670	0.69	5/2264 (0.2%)
All	All	0.31	1/12696 (0.0%)	0.55	11/17240 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	105	PRO	N-CD	5.16	1.55	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	49	TYR	N-CA-C	14.50	150.14	111.00
3	L	51	ALA	CB-CA-C	-10.02	95.07	110.10
2	H	65	LYS	N-CA-CB	-9.15	94.14	110.60
3	L	49	TYR	CB-CA-C	-8.64	93.13	110.40
1	B	143	VAL	CB-CA-C	6.81	124.35	111.40
3	D	49	TYR	N-CA-C	6.49	128.52	111.00
3	L	110	VAL	N-CA-CB	-6.32	97.59	111.50
3	D	110	VAL	N-CA-CB	-6.04	98.22	111.50
1	A	228	GLY	N-CA-C	5.47	126.78	113.10
3	L	11	LEU	CA-CB-CG	5.23	127.32	115.30
1	B	143	VAL	N-CA-C	-5.05	97.36	111.00

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	2976	0	2919	31	1
1	B	2976	0	2919	75	0
2	C	1599	0	1566	27	0
2	H	1599	0	1566	25	0
3	D	1636	0	1597	21	0
3	L	1636	0	1597	31	1
All	All	12422	0	12164	194	1

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.

All (194) 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:B:301:LYS:NZ	1:B:366:THR:CG2	2.12	1.12
1:B:301:LYS:NZ	1:B:366:THR:HG21	1.67	1.08
1:B:301:LYS:HZ1	1:B:366:THR:HG21	1.06	1.07
1:B:301:LYS:HZ2	1:B:366:THR:HG22	1.24	1.02
2:C:60:TYR:CD1	2:C:65:LYS:HD3	1.98	0.98
1:B:301:LYS:HE3	1:B:364:VAL:CG1	1.97	0.95
1:B:144:HIS:HD2	1:B:360:THR:HA	1.33	0.94
1:B:144:HIS:HD2	1:B:360:THR:CA	1.84	0.91
3:L:6:GLN:HB2	3:L:100:GLN:OE1	1.74	0.87
1:B:301:LYS:HZ2	1:B:366:THR:CG2	1.79	0.86
1:B:144:HIS:CD2	1:B:360:THR:HA	2.12	0.85
1:B:302:GLY:O	1:B:303:VAL:HG23	1.79	0.83
1:B:301:LYS:NZ	1:B:366:THR:HG22	1.89	0.81
1:A:145:GLY:O	1:A:146:SER:OG	1.98	0.81
1:B:58:SER:HB2	1:B:226:HIS:CE1	2.17	0.79
1:A:118:LYS:NZ	2:H:51:GLU:OE2	2.16	0.77
1:B:301:LYS:HZ1	1:B:366:THR:CG2	1.80	0.77
1:B:308:CYS:SG	1:B:340:LYS:O	2.42	0.77
1:B:144:HIS:CD2	1:B:360:THR:CA	2.69	0.74
1:B:144:HIS:CD2	1:B:360:THR:CG2	2.70	0.74
1:B:46:VAL:HG12	1:B:47:THR:HG23	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:ILE:CD1	1:B:144:HIS:O	2.37	0.71
2:H:105:PRO:CB	3:L:36:TYR:OH	2.39	0.70
1:B:301:LYS:HE3	1:B:364:VAL:HB	1.72	0.70
1:B:301:LYS:CD	1:B:364:VAL:HG11	2.21	0.70
2:H:105:PRO:HB2	3:L:36:TYR:OH	1.92	0.69
1:B:144:HIS:NE2	1:B:359:ILE:HG22	2.08	0.69
1:B:301:LYS:HE3	1:B:364:VAL:CB	2.21	0.69
1:B:144:HIS:CD2	1:B:360:THR:HG23	2.29	0.67
3:L:108:ARG:NH2	3:L:170:ASP:O	2.26	0.67
1:A:145:GLY:O	1:A:146:SER:CB	2.42	0.66
1:B:144:HIS:HD2	1:B:360:THR:N	1.93	0.66
2:C:100:ARG:HB3	2:C:104:SER:OG	1.96	0.65
3:L:6:GLN:CB	3:L:100:GLN:OE1	2.44	0.65
1:B:302:GLY:O	1:B:303:VAL:CG2	2.44	0.65
3:D:40:PRO:HG2	3:D:165:GLU:HG2	1.78	0.64
3:D:19:VAL:HB	3:D:75:ILE:HG23	1.79	0.63
1:A:37:ASP:C	1:A:300:LEU:HD21	2.18	0.63
2:H:206:HIS:ND1	2:H:209:SER:HB3	2.13	0.63
2:C:48:TRP:HZ2	2:C:51:GLU:HB2	1.62	0.63
3:D:37:GLN:HB2	3:D:47:LEU:HD11	1.82	0.62
3:D:50:ALA:O	3:D:51:ALA:HB3	1.98	0.62
2:H:201:ILE:HG12	2:H:216:ARG:HG3	1.81	0.62
1:B:301:LYS:HE3	1:B:364:VAL:HG11	1.80	0.62
3:L:40:PRO:HG2	3:L:165:GLU:HG2	1.82	0.61
3:L:19:VAL:HB	3:L:75:ILE:HG23	1.82	0.61
3:D:145:LYS:HB2	3:D:197:THR:HB	1.82	0.61
3:L:6:GLN:N	3:L:100:GLN:OE1	2.32	0.61
2:C:125:PRO:HB3	2:C:151:TYR:HB3	1.82	0.61
1:B:301:LYS:CE	1:B:364:VAL:HB	2.30	0.60
1:B:144:HIS:CD2	1:B:360:THR:N	2.70	0.60
2:C:18:LEU:HD12	2:C:115:VAL:HG11	1.84	0.60
1:A:300:LEU:H	1:A:300:LEU:CD2	2.16	0.59
3:L:6:GLN:CA	3:L:100:GLN:OE1	2.51	0.59
1:A:57:ARG:NH1	1:A:59:TYR:OH	2.35	0.59
1:B:85:GLN:OE1	1:B:94:ARG:NH2	2.32	0.59
3:L:83:PHE:HZ	3:L:165:GLU:HG3	1.67	0.59
1:A:194:THR:HG21	1:A:290:LYS:HE2	1.85	0.59
1:A:186:LEU:HD21	1:A:298:LEU:HD22	1.84	0.59
3:D:49:TYR:HB2	3:D:55:GLN:NE2	2.18	0.58
2:H:105:PRO:HB3	3:L:36:TYR:OH	2.04	0.58
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LYS:HD3	1:B:305:TYR:CE2	2.39	0.58
2:H:48:TRP:HZ2	2:H:51:GLU:HB2	1.67	0.58
2:C:60:TYR:HD1	2:C:65:LYS:HD3	1.65	0.58
1:B:301:LYS:HD2	1:B:364:VAL:HG21	1.86	0.57
1:B:65:ILE:HA	2:C:103:LEU:HD12	1.87	0.57
1:B:186:LEU:HD21	1:B:298:LEU:HD22	1.87	0.56
3:L:80:PRO:HA	3:L:106:ILE:HD13	1.88	0.55
1:B:301:LYS:CE	1:B:364:VAL:HG11	2.35	0.55
3:L:83:PHE:CZ	3:L:165:GLU:HG3	2.41	0.55
1:B:50:VAL:HG11	1:B:130:ILE:HG23	1.88	0.55
2:C:166:THR:HG23	2:C:167:SER:N	2.20	0.55
3:D:46:ARG:NH2	3:D:56:SER:O	2.39	0.55
1:A:85:GLN:OE1	1:A:94:ARG:NH2	2.41	0.54
1:B:118:LYS:NZ	2:C:51:GLU:OE2	2.37	0.54
1:B:144:HIS:CG	1:B:360:THR:HG22	2.43	0.54
1:A:300:LEU:HD23	1:A:300:LEU:H	1.72	0.54
1:A:308:CYS:HB3	1:A:332:TYR:CZ	2.42	0.54
1:B:301:LYS:HE3	1:B:364:VAL:HG12	1.85	0.53
1:A:145:GLY:C	1:A:146:SER:OG	2.47	0.53
1:B:144:HIS:CD2	1:B:360:THR:HG22	2.44	0.53
1:B:40:THR:HB	1:B:144:HIS:HB2	1.90	0.53
1:B:1:ILE:HD12	1:B:144:HIS:O	2.07	0.52
3:L:61:ARG:NH2	3:L:82:ASP:OD1	2.33	0.52
2:C:4:LEU:HD11	2:C:108:TYR:HB3	1.92	0.52
1:B:30:CYS:SG	1:B:31:VAL:N	2.83	0.51
2:H:8:GLY:HA3	2:H:20:LEU:HD23	1.92	0.51
1:B:227:ALA:O	1:B:228:GLY:C	2.49	0.51
1:A:27:HIS:HB2	1:A:287:GLY:H	1.75	0.51
1:A:300:LEU:CD2	1:A:300:LEU:N	2.73	0.51
1:B:301:LYS:CE	1:B:364:VAL:CG1	2.79	0.50
2:C:11:LEU:HD11	2:C:118:SER:HB3	1.91	0.50
3:L:40:PRO:CG	3:L:165:GLU:HG2	2.40	0.50
1:B:118:LYS:HB3	2:C:103:LEU:HD13	1.94	0.50
3:L:6:GLN:O	3:L:100:GLN:OE1	2.29	0.50
2:C:52:ILE:HD12	2:C:58:THR:HG22	1.94	0.50
3:L:32:ASP:HB2	3:L:92:ASN:HB2	1.93	0.50
2:C:206:HIS:CD2	2:C:208:PRO:HD2	2.45	0.50
2:C:165:LEU:HD12	2:C:165:LEU:C	2.32	0.49
3:D:59:PRO:HB2	3:D:61:ARG:HG2	1.94	0.49
3:D:40:PRO:CG	3:D:165:GLU:HG2	2.43	0.49
1:A:67:ASP:OD2	3:L:96:ARG:NH2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LYS:NZ	2:H:58:THR:O	2.45	0.49
1:A:228:GLY:O	1:A:229:ALA:HB3	2.13	0.49
3:D:50:ALA:O	3:D:51:ALA:CB	2.61	0.49
2:C:79:PHE:CZ	2:C:96:CYS:HB2	2.48	0.48
3:L:145:LYS:HB2	3:L:197:THR:HB	1.93	0.48
2:C:33:ASN:HD22	2:C:98:ARG:HD2	1.79	0.48
1:B:1:ILE:HD11	1:B:144:HIS:O	2.13	0.48
1:B:73:ARG:HD3	1:B:80:ALA:HA	1.94	0.48
2:H:39:ARG:HB3	2:H:49:ILE:HD11	1.96	0.48
1:B:308:CYS:HB3	1:B:332:TYR:CZ	2.48	0.48
3:L:11:LEU:HD11	3:L:19:VAL:HG13	1.96	0.47
1:B:336:ASP:N	1:B:336:ASP:OD1	2.43	0.47
1:A:82:LEU:O	1:A:85:GLN:HB2	2.14	0.47
2:H:100:ARG:HB3	2:H:104:SER:OG	2.14	0.47
1:A:67:ASP:OD2	1:A:118:LYS:NZ	2.40	0.47
1:B:65:ILE:CA	2:C:103:LEU:HD12	2.44	0.47
1:A:312:PHE:C	1:A:396:ILE:HD11	2.35	0.47
1:B:305:TYR:HB2	1:B:340:LYS:HG3	1.98	0.46
1:B:144:HIS:NE2	1:B:359:ILE:CG2	2.78	0.46
1:B:312:PHE:C	1:B:396:ILE:HD11	2.35	0.46
1:B:79:GLU:HB3	1:B:94:ARG:NH1	2.31	0.46
1:B:301:LYS:CE	1:B:366:THR:CG2	2.90	0.46
1:B:85:GLN:HA	1:B:92:CYS:SG	2.56	0.46
3:D:83:PHE:CZ	3:D:165:GLU:HG3	2.51	0.46
1:B:118:LYS:HE3	2:C:34:TRP:CD1	2.51	0.45
3:D:198:HIS:CD2	3:D:200:GLY:H	2.34	0.45
2:H:60:TYR:HB2	2:H:65:LYS:HD2	1.99	0.45
1:B:359:ILE:HD11	1:B:379:ASP:HB2	1.99	0.45
1:A:73:ARG:HD3	1:A:80:ALA:HA	1.99	0.45
1:B:302:GLY:C	1:B:303:VAL:HG23	2.35	0.45
3:L:108:ARG:HG3	3:L:109:THR:O	2.17	0.44
1:A:169:ILE:HG23	1:A:174:PRO:HA	1.99	0.44
3:L:50:ALA:O	3:L:51:ALA:CB	2.65	0.44
1:B:195:GLY:O	1:B:288:HIS:HB3	2.18	0.44
1:B:353:THR:HA	1:B:354:PRO:HD3	1.84	0.44
1:B:84:LYS:HA	1:B:87:ASP:HB2	1.99	0.43
3:D:49:TYR:HB2	3:D:55:GLN:HE21	1.83	0.43
2:H:157:THR:OG1	2:H:205:ASN:HB3	2.19	0.43
1:B:224:PRO:HD3	1:B:241:ALA:HB3	2.00	0.43
1:B:211:TRP:CD2	1:B:269:LEU:HD13	2.53	0.43
1:B:186:LEU:HG	1:B:298:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:PRO:HA	1:B:237:ASN:O	2.18	0.43
2:C:166:THR:CG2	2:C:167:SER:N	2.81	0.43
3:D:140:TYR:CG	3:D:141:PRO:HA	2.54	0.43
3:D:23:CYS:HB2	3:D:35:TRP:CH2	2.54	0.43
1:B:359:ILE:HB	1:B:377:GLU:HB3	2.01	0.43
1:A:39:PRO:HD3	1:A:300:LEU:HD22	2.00	0.42
2:H:102:ASP:OD2	2:H:102:ASP:N	2.49	0.42
2:H:64:LEU:O	2:H:68:VAL:HG22	2.18	0.42
1:A:38:LYS:NZ	1:A:298:LEU:O	2.41	0.42
2:C:79:PHE:HZ	2:C:96:CYS:HB2	1.84	0.42
1:B:301:LYS:HD3	1:B:364:VAL:HG11	1.98	0.42
1:B:33:VAL:HB	1:B:41:VAL:HG23	2.01	0.42
2:C:102:ASP:OD2	2:C:102:ASP:N	2.38	0.42
3:L:11:LEU:HD22	3:L:104:VAL:HG22	2.01	0.42
3:D:32:ASP:HB2	3:D:92:ASN:HB2	2.02	0.42
1:A:329:GLU:HG3	1:A:375:MET:HG2	2.01	0.42
3:D:54:LEU:HD11	3:D:58:VAL:O	2.20	0.42
1:A:118:LYS:HB3	2:H:103:LEU:HD13	2.02	0.42
1:A:217:TRP:CH2	1:A:269:LEU:HD21	2.55	0.41
1:A:217:TRP:CZ3	1:A:221:ILE:HD11	2.55	0.41
3:L:61:ARG:HH21	3:L:82:ASP:CG	2.17	0.41
2:C:105:PRO:O	2:C:105:PRO:HG2	2.20	0.41
3:D:113:PRO:HD3	3:D:198:HIS:CD2	2.55	0.41
3:L:50:ALA:O	3:L:51:ALA:HB3	2.20	0.41
3:L:46:ARG:NH2	3:L:56:SER:O	2.53	0.41
3:D:61:ARG:CZ	3:D:79:GLN:HG3	2.50	0.41
2:H:100:ARG:NH2	3:L:55:GLN:OE1	2.53	0.41
1:B:3:CYS:SG	1:B:42:ASP:HB3	2.61	0.41
1:B:75:PRO:O	1:B:76:THR:OG1	2.30	0.41
2:C:65:LYS:HA	2:C:68:VAL:HG22	2.02	0.41
3:L:100:GLN:H	3:L:100:GLN:HG3	1.50	0.41
1:B:64:SER:HA	1:B:257:VAL:HG11	2.02	0.41
1:B:94:ARG:HB3	1:B:94:ARG:HE	1.63	0.41
1:B:65:ILE:HA	2:C:103:LEU:CD1	2.49	0.41
3:L:78:LEU:HD23	3:L:78:LEU:HA	1.76	0.41
1:A:66:SER:HB2	3:L:91:HIS:HD2	1.86	0.41
2:H:102:ASP:C	2:H:104:SER:H	2.23	0.41
3:D:78:LEU:HA	3:D:78:LEU:HD23	1.85	0.41
1:A:233:THR:HG21	2:H:53:TYR:HE2	1.86	0.41
1:B:42:ASP:HB2	1:B:142:SER:OG	2.20	0.41
2:C:100:ARG:HD2	2:C:102:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:152:PHE:HA	2:C:153:PRO:HA	1.90	0.40
2:H:158:VAL:HG11	2:H:186:SER:HB2	2.02	0.40
2:H:195:LEU:HD12	2:H:195:LEU:HA	1.89	0.40
2:H:48:TRP:CZ2	2:H:51:GLU:HB2	2.51	0.40
1:A:14:GLY:HA2	1:A:21:VAL:HG11	2.03	0.40
2:H:125:PRO:HB3	2:H:151:TYR:HB3	2.03	0.40
2:H:22:CYS:O	2:H:78:GLN:HB2	2.22	0.40
3:D:83:PHE:HZ	3:D:165:GLU:HG3	1.85	0.40
2:H:122:THR:HG22	2:H:153:PRO:HD3	2.03	0.40

All (1) 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)
1:A:278:ASP:OD1	3:L:69:THR:OG1[2_758]	2.00	0.20

## 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	386/409 (94%)	375 (97%)	11 (3%)	0	100	100
1	B	386/409 (94%)	359 (93%)	27 (7%)	0	100	100
2	C	210/220 (96%)	201 (96%)	9 (4%)	0	100	100
2	H	210/220 (96%)	203 (97%)	7 (3%)	0	100	100
3	D	211/215 (98%)	202 (96%)	9 (4%)	0	100	100
3	L	211/215 (98%)	203 (96%)	8 (4%)	0	100	100
All	All	1614/1688 (96%)	1543 (96%)	71 (4%)	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	325/341 (95%)	298 (92%)	27 (8%)	14	35
1	B	325/341 (95%)	301 (93%)	24 (7%)	17	40
2	C	185/190 (97%)	172 (93%)	13 (7%)	19	44
2	H	185/190 (97%)	173 (94%)	12 (6%)	21	48
3	D	186/188 (99%)	174 (94%)	12 (6%)	21	48
3	L	186/188 (99%)	170 (91%)	16 (9%)	13	33
All	All	1392/1438 (97%)	1288 (92%)	104 (8%)	17	40

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	30	CYS
1	A	37	ASP
1	A	49	THR
1	A	50	VAL
1	A	73	ARG
1	A	85	GLN
1	A	94	ARG
1	A	107	LEU
1	A	122	SER
1	A	131	GLN
1	A	146	SER
1	A	205	THR
1	A	233	THR
1	A	249	HIS
1	A	252	ARG
1	A	255	VAL
1	A	256	VAL
1	A	258	LEU
1	A	283	ARG
1	A	289	LEU
1	A	293	LEU

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Mol	Chain	Res	Type
1	A	300	LEU
1	A	317	ILE
1	A	351	THR
1	A	353	THR
1	A	403	SER
2	H	2	VAL
2	H	64	LEU
2	H	69	THR
2	H	78	GLN
2	H	141	THR
2	H	178	SER
2	H	187	VAL
2	H	199	THR
2	H	209	SER
2	H	210	ASN
2	H	211	THR
2	H	215	LYS
3	L	18	ARG
3	L	30	ARG
3	L	42	LYS
3	L	46	ARG
3	L	52	SER
3	L	67	SER
3	L	69	THR
3	L	70	GLU
3	L	75	ILE
3	L	78	LEU
3	L	85	THR
3	L	100	GLN
3	L	147	GLN
3	L	168	SER
3	L	187	GLU
3	L	199	GLN
1	B	10	ASP
1	B	27	HIS
1	B	30	CYS
1	B	49	THR
1	B	50	VAL
1	B	73	ARG
1	B	94	ARG
1	B	107	LEU
1	B	118	LYS

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Mol	Chain	Res	Type
1	B	131	GLN
1	B	144	HIS
1	B	191	GLU
1	B	205	THR
1	B	233	THR
1	B	249	HIS
1	B	258	LEU
1	B	293	LEU
1	B	304	SER
1	B	313	THR
1	B	353	THR
1	B	357	ARG
1	B	370	GLU
1	B	376	LEU
1	B	393	GLU
2	C	4	LEU
2	C	71	SER
2	C	100	ARG
2	C	105	PRO
2	C	121	SER
2	C	141	THR
2	C	165	LEU
2	C	178	SER
2	C	199	THR
2	C	209	SER
2	C	210	ASN
2	C	211	THR
2	C	215	LYS
3	D	9	SER
3	D	14	SER
3	D	33	LEU
3	D	42	LYS
3	D	46	ARG
3	D	49	TYR
3	D	75	ILE
3	D	85	THR
3	D	109	THR
3	D	174	SER
3	D	199	GLN
3	D	202	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:



Mol	Chain	Res	Type
2	H	59	ASN
2	H	78	GLN
2	H	111	GLN
3	L	91	HIS
1	B	144	HIS
1	B	226	HIS
2	C	5	GLN
2	C	33	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 carbohydrates 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	390/409 (95%)	0.18	16 (4%) 41 34	24, 59, 119, 189	0
1	B	390/409 (95%)	0.72	50 (12%) 5 3	49, 82, 159, 199	0
2	C	214/220 (97%)	0.23	4 (1%) 70 64	41, 74, 118, 151	0
2	H	214/220 (97%)	-0.21	1 (0%) 91 90	18, 37, 68, 95	0
3	D	213/215 (99%)	0.27	8 (3%) 44 37	38, 76, 128, 160	0
3	L	213/215 (99%)	-0.19	1 (0%) 91 90	23, 48, 84, 118	0
All	All	1634/1688 (96%)	0.23	80 (4%) 33 26	18, 65, 132, 199	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	TRP	8.8
1	B	178	ALA	5.9
1	A	405	SER	5.7
1	A	302	GLY	5.7
1	B	180	LEU	5.5
1	B	295	MET	5.4
2	H	105	PRO	5.2
1	B	293	LEU	5.1
1	B	18	GLY	4.9
1	B	169	ILE	4.9
1	B	403	SER	4.7
1	B	401	HIS	4.6
2	C	143	ALA	4.6
1	B	248	ALA	4.5
1	B	349	MET	4.3
1	A	229	ALA	4.2
3	D	145	LYS	4.1
1	B	347	VAL	4.1
1	B	399	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	303	VAL	3.9
1	B	301	LYS	3.8
1	B	22	ASP	3.8
1	B	186	LEU	3.6
1	A	404	GLY	3.6
1	B	144	HIS	3.5
1	B	15	MET	3.5
1	B	193	ARG	3.4
1	B	19	THR	3.3
1	B	303	VAL	3.3
1	A	247	ASP	3.3
1	B	21	VAL	3.3
3	D	173	TYR	3.2
1	B	227	ALA	3.2
1	B	196	LEU	3.1
1	A	164	ARG	3.1
1	B	188	LEU	3.0
1	B	24	VAL	2.9
1	B	250	ALA	2.9
1	B	167	VAL	2.9
1	B	384	ASP	2.9
2	C	104	SER	2.8
1	A	180	LEU	2.8
1	B	292	ARG	2.8
1	B	195	GLY	2.7
2	C	142	ALA	2.7
1	A	304	SER	2.6
1	B	232	GLY	2.6
3	D	154	LEU	2.6
1	A	1	ILE	2.6
1	B	302	GLY	2.6
1	B	304	SER	2.6
1	B	381	PRO	2.6
2	C	105	PRO	2.6
1	B	366	THR	2.6
1	B	405	SER	2.6
1	A	20	TRP	2.5
1	B	14	GLY	2.5
1	A	15	MET	2.5
1	A	230	ASP	2.5
3	D	177	SER	2.5
1	B	16	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	383	GLY	2.4
1	B	374	MET	2.4
3	D	192	TYR	2.3
1	B	249	HIS	2.3
1	B	231	THR	2.3
1	A	186	LEU	2.2
1	A	162	GLU	2.2
1	B	385	SER	2.1
1	B	364	VAL	2.1
3	L	49	TYR	2.1
3	D	135	LEU	2.1
1	B	1	ILE	2.1
1	A	248	ALA	2.1
3	D	210	ASN	2.1
1	B	13	GLU	2.1
3	D	106	ILE	2.1
1	B	394	LYS	2.0
1	B	23	VAL	2.0
1	B	299	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.