



# Full wwPDB X-ray Structure Validation Report i

Oct 31, 2023 – 07:57 PM JST

PDB ID : 5GZN  
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 : 3.00 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 i 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](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

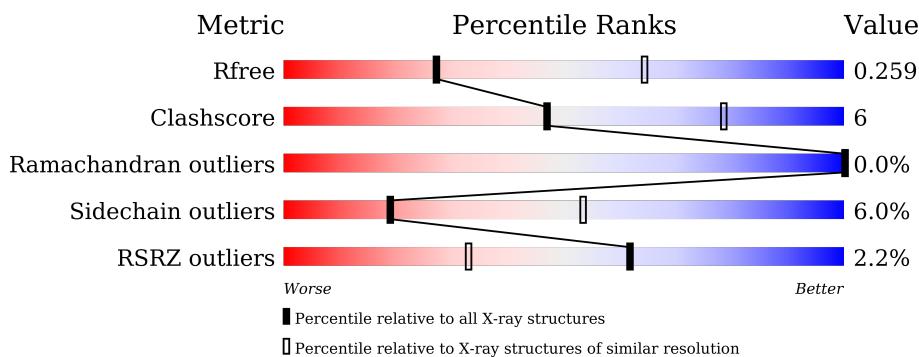
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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.



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Mol	Chain	Length	Quality of chain		
3	D	216	%	81%	17% ..
3	L	216		87%	11% ..

## 2 Entry composition [\(i\)](#)

There are 3 unique types of molecules in this entry. The entry contains 15537 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	402	Total	C	N	O	S	0	0	0
			3071	1915	537	594	25			
1	B	401	Total	C	N	O	S	0	0	0
			3061	1909	534	593	25			
1	E	184	Total	C	N	O	S	0	0	0
			1431	895	250	274	12			
1	G	183	Total	C	N	O	S	0	0	0
			1429	896	249	272	12			

- Molecule 2 is a protein called Antibody Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total	C	N	O	S	0	0	0
			1692	1070	286	330	6			
2	C	223	Total	C	N	O	S	0	0	0
			1686	1067	285	328	6			

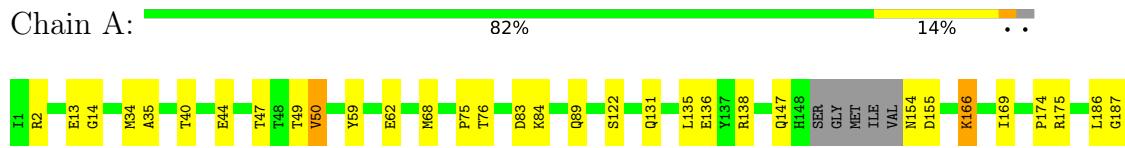
- Molecule 3 is a protein called Antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1579	991	262	322	4			
3	D	214	Total	C	N	O	S	0	0	0
			1588	996	263	325	4			

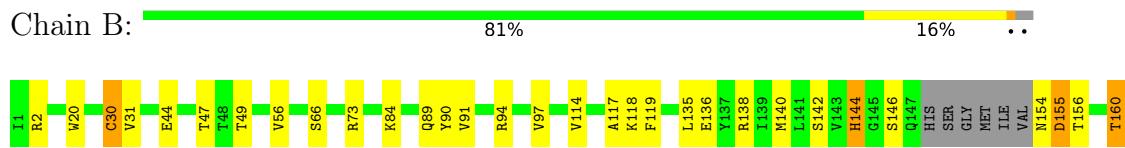
### 3 Residue-property plots

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.

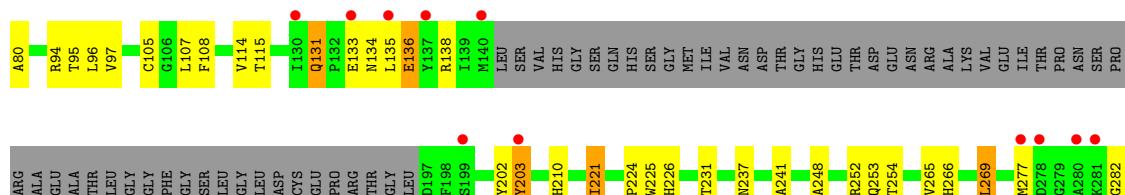
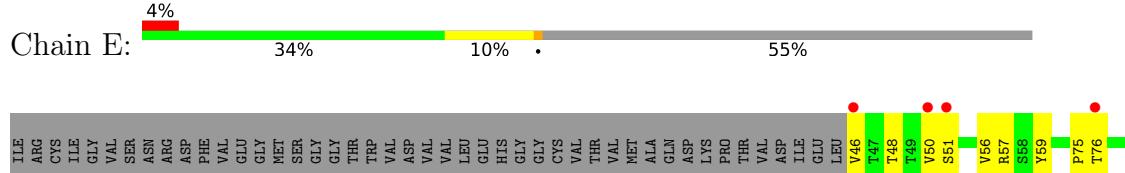
- Molecule 1: Genome polyprotein



- Molecule 1: Genome polyprotein



- Molecule 1: Genome polyprotein







- Molecule 3: Antibody light chain

Chain L: 87% 11% ..



- Molecule 3: Antibody light chain

Chain D: 81% 17% .. %



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.71Å    129.38Å    428.71Å 90.00°    90.00°    90.00°	Depositor
Resolution (Å)	42.08 – 3.00 42.87 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.3 (42.08-3.00) 98.2 (42.87-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.28 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
$R$ , $R_{free}$	0.223 , 0.258 0.228 , 0.259	Depositor DCC
$R_{free}$ test set	3491 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	88.7	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.052 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15537	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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 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	0.24	0/3135	0.46	0/4247
1	B	0.26	0/3124	0.58	2/4232 (0.0%)
1	E	0.24	0/1463	0.45	0/1977
1	G	0.23	0/1460	0.45	0/1971
2	C	0.24	0/1730	0.49	1/2359 (0.0%)
2	H	0.26	0/1736	0.45	0/2367
3	D	0.24	0/1628	0.45	0/2226
3	L	0.25	0/1619	0.47	0/2214
All	All	0.25	0/15895	0.49	3/21593 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	146	SER	N-CA-CB	-21.96	77.56	110.50
2	C	160	PHE	C-N-CD	-7.01	105.17	120.60
1	B	144	HIS	CB-CA-C	-5.35	99.69	110.40

There are no chirality outliers.

There are no planarity outliers.

### 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	3071	0	2996	32	0
1	B	3061	0	2989	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1431	0	1370	24	0
1	G	1429	0	1372	20	0
2	C	1686	0	1632	30	0
2	H	1692	0	1637	20	0
3	D	1588	0	1546	19	0
3	L	1579	0	1540	18	0
All	All	15537	0	15082	190	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 6.

All (190) 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:L:155:ASP:OD2	3:L:192:HIS:HB3	1.67	0.93
3:L:155:ASP:OD2	3:L:192:HIS:CB	2.27	0.82
2:C:160:PHE:HD2	2:C:161:PRO:HD3	1.47	0.80
2:C:160:PHE:CD2	2:C:161:PRO:HD3	2.18	0.78
3:L:155:ASP:CG	3:L:192:HIS:HB3	2.04	0.76
2:H:91:THR:HG23	2:H:124:THR:HA	1.68	0.73
1:A:405:SER:OG	1:A:406:THR:N	2.21	0.73
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.21	0.73
2:C:91:THR:HG23	2:C:124:THR:HA	1.71	0.72
3:L:155:ASP:OD2	3:L:192:HIS:CD2	2.43	0.72
1:E:51:SER:HB2	1:E:134:ASN:HB3	1.74	0.70
1:A:406:THR:O	1:A:406:THR:OG1	2.13	0.67
1:E:80:ALA:O	1:E:94:ARG:NH1	2.29	0.66
1:B:311:ALA:HB2	1:B:394:LYS:HD3	1.78	0.65
3:D:26:SER:HA	3:D:30:GLY:HA3	1.79	0.64
2:C:160:PHE:CE2	2:C:161:PRO:HB3	2.31	0.64
1:G:75:PRO:O	1:G:76:THR:HG22	1.96	0.64
1:A:2:ARG:NE	1:A:44:GLU:OE2	2.22	0.64
3:L:155:ASP:OD1	3:L:193:ARG:N	2.31	0.63
1:A:138:ARG:HD3	1:A:166:LYS:HE2	1.79	0.63
3:L:1:GLN:O	3:L:1:GLN:HG2	1.98	0.63
1:B:161:ASP:OD2	1:B:162:GLU:N	2.32	0.62
2:C:29:PHE:O	2:C:72:ARG:NH2	2.33	0.62
1:B:144:HIS:ND1	1:B:360:THR:HG22	2.14	0.62
2:C:160:PHE:CD2	2:C:161:PRO:CD	2.83	0.62
2:C:160:PHE:CD2	2:C:161:PRO:HB3	2.34	0.62
3:L:155:ASP:OD1	3:L:192:HIS:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:GLU:OE2	1:E:138:ARG:NH2	2.32	0.62
3:L:155:ASP:OD2	3:L:192:HIS:CG	2.53	0.61
1:B:283:ARG:NH1	2:C:111:GLU:OE1	2.33	0.61
1:G:115:THR:OG1	1:G:253:GLN:NE2	2.33	0.61
1:E:75:PRO:O	1:E:76:THR:HG22	2.00	0.61
1:G:95:THR:OG1	1:G:96:LEU:N	2.36	0.59
1:B:56:VAL:HG21	1:B:202:TYR:HE1	1.70	0.56
2:H:103:TRP:HA	2:H:108:SER:HB2	1.88	0.56
1:G:52:ASN:N	1:G:52:ASN:OD1	2.40	0.55
1:A:14:GLY:HA3	1:A:35:ALA:HA	1.88	0.55
1:E:115:THR:HG21	1:E:253:GLN:HB3	1.89	0.55
2:C:35:HIS:NE2	2:C:99:ASP:OD1	2.38	0.54
2:C:133:PRO:HB3	2:C:159:TYR:HB3	1.90	0.54
1:A:135:LEU:HD21	1:A:198:PHE:HD2	1.72	0.54
1:A:169:ILE:HG23	1:A:174:PRO:HA	1.89	0.53
2:H:133:PRO:HB3	2:H:159:TYR:HB3	1.89	0.53
1:E:135:LEU:HD22	1:E:136:GLU:H	1.74	0.53
1:B:155:ASP:OD2	1:B:155:ASP:N	2.41	0.53
1:G:46:VAL:HB	1:G:138:ARG:HG2	1.91	0.52
1:B:210:HIS:CD2	1:B:277:MET:HB2	2.44	0.52
3:D:79:LEU:HD11	3:D:107:LEU:HD21	1.90	0.52
1:G:224:PRO:HD3	1:G:241:ALA:HB3	1.91	0.52
1:E:59:TYR:CG	1:E:221:ILE:HD11	2.45	0.52
1:A:62:GLU:HG2	1:A:122:SER:HB2	1.91	0.52
1:A:210:HIS:CD2	1:A:277:MET:HB2	2.45	0.52
1:B:278:ASP:OD2	2:C:108:SER:HB3	2.10	0.52
2:H:24:ALA:HB1	2:H:27:PHE:CZ	2.46	0.51
1:B:30:CYS:SG	1:B:31:VAL:N	2.83	0.51
3:D:46:LYS:HE2	3:D:59:ILE:HD11	1.92	0.51
1:B:2:ARG:NE	1:B:44:GLU:OE2	2.27	0.51
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.93	0.51
1:B:186:LEU:HD22	1:B:293:LEU:HD12	1.93	0.50
1:B:138:ARG:HD3	1:B:166:LYS:HE2	1.92	0.50
1:B:169:ILE:HG23	1:B:174:PRO:HA	1.92	0.50
1:B:194:THR:HG21	1:B:290:LYS:HE2	1.94	0.50
2:C:214:HIS:CD2	2:C:216:PRO:HD2	2.47	0.50
1:B:136:GLU:OE2	3:D:33:TYR:OH	2.30	0.49
1:A:147:GLN:OE1	1:E:252:ARG:NH2	2.45	0.49
3:L:155:ASP:OD2	3:L:192:HIS:HD2	1.96	0.49
2:C:36:TRP:HE1	2:C:79:LEU:HD22	1.78	0.48
3:D:4:LEU:HD11	3:D:91:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:108:THR:HG21	3:D:145:PRO:HB3	1.96	0.48
2:H:141:SER:OG	2:H:142:SER:N	2.45	0.48
3:D:21:SER:HB3	3:D:73:THR:HG22	1.95	0.48
1:E:224:PRO:HD3	1:E:241:ALA:HB3	1.96	0.48
1:A:155:ASP:OD1	1:A:155:ASP:N	2.40	0.48
2:C:160:PHE:CD2	2:C:161:PRO:CB	2.97	0.47
1:A:136:GLU:OE2	3:L:33:TYR:OH	2.29	0.47
3:L:119:VAL:O	3:L:208:LYS:NZ	2.46	0.47
1:G:59:TYR:CG	1:G:221:ILE:HD11	2.50	0.47
1:A:135:LEU:HD11	1:A:198:PHE:HE2	1.79	0.47
2:H:133:PRO:HD2	2:H:219:THR:HG21	1.97	0.47
2:C:67:ARG:NH2	2:C:90:ASP:OD2	2.48	0.47
3:D:153:LYS:HB2	3:D:196:SER:HB2	1.96	0.47
1:G:49:THR:HG21	1:G:281:LYS:HD3	1.97	0.47
1:G:97:VAL:HG12	1:G:248:ALA:HB1	1.97	0.47
2:H:165:THR:HG23	2:H:213:ASN:HB3	1.97	0.47
1:A:59:TYR:CD1	1:A:225:TRP:HB3	2.51	0.46
2:C:89:GLU:OE1	2:C:89:GLU:N	2.46	0.46
1:A:187:GLY:HA3	1:A:294:LYS:HB3	1.97	0.46
1:A:227:ALA:O	1:A:228:GLY:C	2.51	0.46
1:A:50:VAL:HG13	1:A:135:LEU:HD13	1.98	0.46
1:E:59:TYR:CD1	1:E:225:TRP:HB3	2.50	0.46
2:H:103:TRP:HA	2:H:108:SER:CB	2.46	0.46
1:B:224:PRO:HD3	1:B:241:ALA:HB3	1.98	0.46
3:D:6:GLN:HG2	3:D:22:CYS:HB3	1.98	0.46
2:H:105:SER:OG	2:H:106:ILE:N	2.48	0.46
1:E:57:ARG:HD3	1:E:59:TYR:CZ	2.51	0.46
1:G:75:PRO:O	1:G:76:THR:CG2	2.63	0.46
1:A:283:ARG:NH1	2:H:111:GLU:OE1	2.49	0.45
1:B:308:CYS:HB3	1:B:332:TYR:CE1	2.52	0.45
2:C:52:SER:O	2:C:72:ARG:NH1	2.49	0.45
1:G:62:GLU:HB3	1:G:123:LYS:HB2	1.97	0.45
2:H:29:PHE:O	2:H:72:ARG:NH2	2.49	0.45
2:C:160:PHE:HA	2:C:161:PRO:HA	1.56	0.45
1:E:48:THR:HB	1:E:284:LEU:HB2	1.99	0.45
1:B:305:TYR:HB2	1:B:340:LYS:HG3	1.98	0.45
1:E:277:MET:HA	1:E:282:GLY:HA2	1.99	0.45
1:E:46:VAL:N	1:E:138:ARG:O	2.50	0.44
1:G:47:THR:HB	1:G:138:ARG:HD2	1.98	0.44
3:L:84:GLU:HG2	3:L:108:THR:HA	1.98	0.44
3:L:96:LEU:HD23	1:E:108:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:42:GLY:O	3:D:167:THR:HG21	2.17	0.44
1:A:331:GLN:HA	1:A:372:SER:O	2.17	0.44
1:G:58:SER:HB2	1:G:226:HIS:NE2	2.33	0.44
2:H:198:VAL:HG11	2:H:208:TYR:CE1	2.53	0.44
1:G:49:THR:HG23	1:G:281:LYS:HB3	2.00	0.44
1:B:161:ASP:OD2	1:B:163:ASN:N	2.51	0.44
1:B:89:GLN:O	1:B:119:PHE:N	2.35	0.43
3:D:84:GLU:CG	3:D:109:VAL:H	2.31	0.43
3:D:48:LEU:HD23	3:D:48:LEU:HA	1.88	0.43
1:B:90:TYR:HA	1:B:117:ALA:O	2.18	0.43
1:A:186:LEU:HG	1:A:298:LEU:HD13	2.01	0.43
2:C:6:GLU:OE2	2:C:6:GLU:N	2.51	0.43
3:D:29:ILE:HG23	3:D:34:VAL:HG21	1.99	0.43
1:E:203:TYR:HE1	1:E:210:HIS:HB3	1.83	0.43
1:B:138:ARG:NH1	1:B:168:GLU:OE2	2.52	0.43
1:B:308:CYS:HB3	1:B:332:TYR:CZ	2.53	0.43
1:G:59:TYR:CD1	1:G:225:TRP:HB3	2.52	0.43
1:A:147:GLN:HE21	1:A:147:GLN:HB2	1.66	0.43
2:C:198:VAL:HG11	2:C:208:TYR:CE1	2.54	0.43
3:D:148:VAL:HG12	3:D:201:HIS:HB2	2.00	0.43
1:A:191:GLU:HB3	1:A:194:THR:HG22	2.01	0.43
1:B:91:VAL:HB	1:B:239:LYS:HD2	2.00	0.43
1:B:155:ASP:HB2	1:B:156:THR:H	1.52	0.43
2:H:160:PHE:HA	2:H:161:PRO:HA	1.83	0.43
1:B:294:LYS:HE2	1:B:296:ASP:OD1	2.18	0.43
2:C:99:ASP:C	2:C:101:LEU:H	2.23	0.43
1:E:75:PRO:O	1:E:76:THR:CG2	2.66	0.43
1:A:195:GLY:HA2	1:A:288:HIS:O	2.19	0.42
3:L:117:PRO:HA	3:L:143:PHE:HB3	2.00	0.42
1:B:94:ARG:HD2	1:B:114:VAL:HG23	2.01	0.42
1:B:142:SER:HA	1:B:163:ASN:O	2.18	0.42
1:B:202:TYR:CD2	1:B:215:LYS:HA	2.54	0.42
2:C:105:SER:OG	2:C:106:ILE:N	2.52	0.42
2:C:109:ALA:HB3	2:C:110:PRO:HD3	2.00	0.42
1:A:211:TRP:CD2	1:A:269:LEU:HD13	2.55	0.42
2:H:14:PRO:HG3	2:H:127:SER:HB3	2.01	0.42
1:G:80:ALA:O	1:G:94:ARG:NH1	2.49	0.42
1:A:34:MET:HG2	1:A:40:THR:HG23	2.02	0.42
1:B:20:TRP:CZ3	1:B:294:LYS:HB2	2.54	0.42
1:B:144:HIS:HB3	1:B:360:THR:HG22	2.00	0.42
1:E:107:LEU:H	1:E:107:LEU:HD23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:ARG:HD3	1:G:59:TYR:CZ	2.55	0.42
3:D:59:ILE:HA	3:D:60:PRO:HD3	1.93	0.42
1:A:308:CYS:HB3	1:A:332:TYR:CE1	2.54	0.42
2:H:22:CYS:HB3	2:H:79:LEU:HB3	2.02	0.42
1:B:66:SER:O	1:B:118:LYS:HB2	2.20	0.42
2:C:165:THR:HG23	2:C:213:ASN:HB3	2.01	0.42
1:E:131:GLN:C	1:E:133:GLU:H	2.23	0.42
1:G:135:LEU:HD22	1:G:136:GLU:H	1.84	0.42
2:H:16:ARG:HB3	2:H:17:SER:H	1.66	0.42
1:B:97:VAL:HG21	1:B:249:HIS:O	2.19	0.42
1:A:345:MET:O	1:A:355:VAL:HG22	2.20	0.41
1:A:378:LEU:O	1:A:380:PRO:HD3	2.19	0.41
1:B:191:GLU:HB3	1:B:194:THR:HG22	2.01	0.41
1:E:56:VAL:HG21	1:E:202:TYR:CE1	2.54	0.41
3:L:108:THR:HG21	3:L:145:PRO:HB3	2.02	0.41
3:L:142:ASP:HA	3:L:175:LYS:HB3	2.03	0.41
1:B:202:TYR:HD2	1:B:215:LYS:HA	1.85	0.41
1:A:75:PRO:O	1:A:76:THR:OG1	2.36	0.41
1:A:308:CYS:HB3	1:A:332:TYR:CZ	2.55	0.41
1:A:246:LYS:HB3	1:A:247:ASP:H	1.65	0.41
2:C:179:THR:HG23	2:C:194:SER:HB2	2.02	0.41
1:E:80:ALA:HB3	1:E:114:VAL:HG12	2.01	0.41
1:E:95:THR:OG1	1:E:96:LEU:N	2.53	0.41
2:H:183:VAL:HB	3:L:166:THR:HG22	2.03	0.41
3:D:139:LEU:HD23	3:D:179:SER:HB3	2.02	0.41
1:A:191:GLU:HA	1:A:192:PRO:HD3	1.86	0.41
3:L:17:LYS:HG3	3:L:18:VAL:N	2.36	0.41
1:B:160:THR:HG22	1:B:161:ASP:H	1.86	0.41
1:B:351:THR:HG23	1:B:353:THR:H	1.85	0.41
2:C:32:TYR:CG	2:C:98:ARG:HD3	2.56	0.41
2:C:47:TRP:CZ3	3:D:98:VAL:HG13	2.56	0.41
2:C:140:PRO:HG3	2:C:152:LEU:HB3	2.02	0.41
1:G:204:LEU:HD23	1:G:269:LEU:HD21	2.04	0.40
1:E:265:VAL:O	1:E:269:LEU:HD12	2.21	0.40
3:D:167:THR:HA	3:D:168:PRO:HD2	1.81	0.40
1:E:97:VAL:HG12	1:E:248:ALA:HB1	2.02	0.40
2:H:52:SER:O	2:H:72:ARG:NH1	2.54	0.40
2:H:214:HIS:CD2	2:H:216:PRO:HD2	2.57	0.40
3:D:66:SER:OG	3:D:73:THR:OG1	2.40	0.40
1:G:67:ASP:OD2	1:G:90:TYR:OH	2.29	0.40

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 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	398/409 (97%)	366 (92%)	32 (8%)	0	100 100
1	B	397/409 (97%)	363 (91%)	34 (9%)	0	100 100
1	E	180/409 (44%)	168 (93%)	12 (7%)	0	100 100
1	G	177/409 (43%)	166 (94%)	11 (6%)	0	100 100
2	C	219/228 (96%)	192 (88%)	26 (12%)	1 (0%)	29 68
2	H	220/228 (96%)	194 (88%)	26 (12%)	0	100 100
3	D	212/216 (98%)	200 (94%)	12 (6%)	0	100 100
3	L	211/216 (98%)	200 (95%)	11 (5%)	0	100 100
All	All	2014/2524 (80%)	1849 (92%)	164 (8%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	161	PRO

### 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 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	336/341 (98%)	314 (94%)	22 (6%)	17 50
1	B	335/341 (98%)	317 (95%)	18 (5%)	22 57
1	E	152/341 (45%)	140 (92%)	12 (8%)	12 41
1	G	152/341 (45%)	141 (93%)	11 (7%)	14 45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	187/192 (97%)	179 (96%)	8 (4%)	29	66
2	H	188/192 (98%)	177 (94%)	11 (6%)	19	54
3	D	180/182 (99%)	169 (94%)	11 (6%)	18	53
3	L	179/182 (98%)	169 (94%)	10 (6%)	21	56
All	All	1709/2112 (81%)	1606 (94%)	103 (6%)	19	53

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	47	THR
1	A	49	THR
1	A	50	VAL
1	A	68	MET
1	A	83	ASP
1	A	84	LYS
1	A	89	GLN
1	A	131	GLN
1	A	154	ASN
1	A	166	LYS
1	A	175	ARG
1	A	191	GLU
1	A	238	ASN
1	A	247	ASP
1	A	276	GLU
1	A	283	ARG
1	A	293	LEU
1	A	304	SER
1	A	372	SER
1	A	406	THR
1	A	407	ILE
2	H	18	LEU
2	H	76	LYS
2	H	79	LEU
2	H	84	ASN
2	H	98	ARG
2	H	129	SER
2	H	173	LEU
2	H	186	SER
2	H	195	VAL
2	H	207	THR

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Mol	Chain	Res	Type
2	H	211	ASN
3	L	2	SER
3	L	48	LEU
3	L	77	THR
3	L	84	GLU
3	L	86	ASP
3	L	99	TRP
3	L	100	VAL
3	L	114	LYS
3	L	155	ASP
3	L	171	GLN
1	B	30	CYS
1	B	47	THR
1	B	49	THR
1	B	73	ARG
1	B	84	LYS
1	B	135	LEU
1	B	140	MET
1	B	154	ASN
1	B	155	ASP
1	B	160	THR
1	B	166	LYS
1	B	230	ASP
1	B	233	THR
1	B	246	LYS
1	B	276	GLU
1	B	300	LEU
1	B	304	SER
1	B	406	THR
2	C	18	LEU
2	C	53	TYR
2	C	76	LYS
2	C	79	LEU
2	C	84	ASN
2	C	173	LEU
2	C	210	CYS
2	C	221	VAL
3	D	2	SER
3	D	6	GLN
3	D	64	SER
3	D	77	THR
3	D	81	THR

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Mol	Chain	Res	Type
3	D	84	GLU
3	D	99	TRP
3	D	100	VAL
3	D	114	LYS
3	D	171	GLN
3	D	179	SER
1	E	50	VAL
1	E	105	CYS
1	E	131	GLN
1	E	136	GLU
1	E	203	TYR
1	E	221	ILE
1	E	226	HIS
1	E	231	THR
1	E	237	ASN
1	E	254	THR
1	E	266	HIS
1	E	269	LEU
1	G	52	ASN
1	G	95	THR
1	G	107	LEU
1	G	115	THR
1	G	131	GLN
1	G	203	TYR
1	G	221	ILE
1	G	237	ASN
1	G	266	HIS
1	G	269	LEU
1	G	276	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	158	HIS
1	E	226	HIS
1	E	249	HIS
1	G	253	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 monosaccharides 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 [\(i\)](#)

### 6.1 Protein, DNA and RNA chains [\(i\)](#)

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	402/409 (98%)	-0.17	1 (0%)	95	87	52, 84, 131, 224
1	B	401/409 (98%)	-0.10	2 (0%)	91	75	54, 85, 135, 203
1	E	184/409 (44%)	0.42	15 (8%)	11	3	76, 114, 186, 242
1	G	183/409 (44%)	0.29	18 (9%)	7	2	74, 108, 182, 219
2	C	223/228 (97%)	-0.06	3 (1%)	77	51	56, 97, 147, 179
2	H	224/228 (98%)	-0.11	3 (1%)	77	51	60, 98, 142, 192
3	D	214/216 (99%)	-0.14	3 (1%)	75	49	52, 79, 163, 202
3	L	213/216 (98%)	-0.17	0	100	100	48, 73, 144, 212
All	All	2044/2524 (80%)	-0.04	45 (2%)	62	33	48, 91, 154, 242
							0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	137	TYR	7.2
1	E	135	LEU	5.8
2	C	146	SER	5.5
1	G	137	TYR	5.4
1	G	135	LEU	4.3
1	E	203	TYR	4.1
2	H	126	SER	3.6
1	E	281	LYS	3.6
2	C	147	GLY	3.5
2	C	126	SER	3.3
1	E	133	GLU	3.3
1	A	231	THR	3.3
1	E	277	MET	3.2
1	E	130	ILE	3.2
1	G	50	VAL	3.1
1	G	46	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	277	MET	2.9
1	G	281	LYS	2.9
2	H	146	SER	2.9
1	E	46	VAL	2.8
1	G	54	ALA	2.8
3	D	195	TYR	2.7
1	E	51	SER	2.7
3	D	194	SER	2.7
1	E	140	MET	2.7
1	G	133	GLU	2.6
1	E	278	ASP	2.6
1	G	139	ILE	2.5
1	G	127	GLY	2.5
1	E	50	VAL	2.4
1	G	278	ASP	2.4
1	G	128	LYS	2.4
1	B	232	GLY	2.3
1	G	52	ASN	2.2
1	G	203	TYR	2.2
1	G	132	PRO	2.2
1	G	53	MET	2.1
1	E	280	ALA	2.1
3	D	193	ARG	2.1
1	B	231	THR	2.1
2	H	224	ARG	2.1
1	E	199	SER	2.1
1	G	273	LEU	2.1
1	E	76	THR	2.0
1	G	280	ALA	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 monosaccharides 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.