



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2022 – 03:06 PM JST

PDB ID : 7YW8  
Title : Crystal structure of zika E protein  
Authors : Wang, X.X.; Yang, Y.X.  
Deposited on : 2022-08-21  
Resolution : 2.50 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

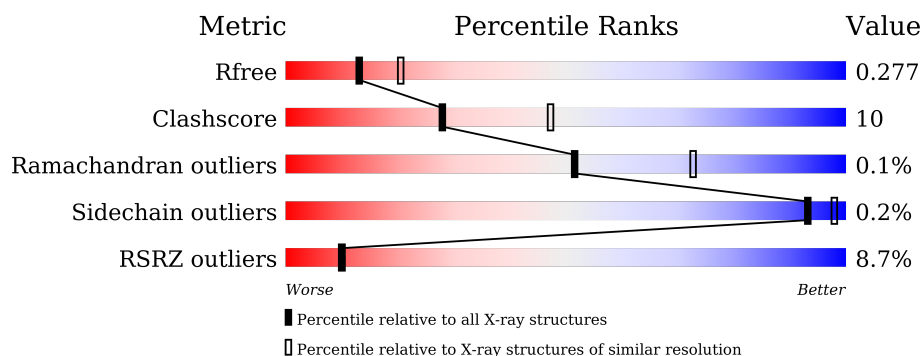
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	410	<div> <div>5%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	B	410	<div> <div>8%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	C	410	<div> <div>10%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
1	D	410	<div> <div>11%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12367 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 Core protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3076	1921	539	589	27			
1	B	404	Total	C	N	O	S	0	0	0
			3058	1911	534	586	27			
1	D	404	Total	C	N	O	S	0	0	0
			3069	1917	538	587	27			
1	C	404	Total	C	N	O	S	0	0	0
			3041	1901	530	583	27			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A0A2Z2DVT8
B	0	MET	-	initiating methionine	UNP A0A2Z2DVT8
D	0	MET	-	initiating methionine	UNP A0A2Z2DVT8
C	0	MET	-	initiating methionine	UNP A0A2Z2DVT8

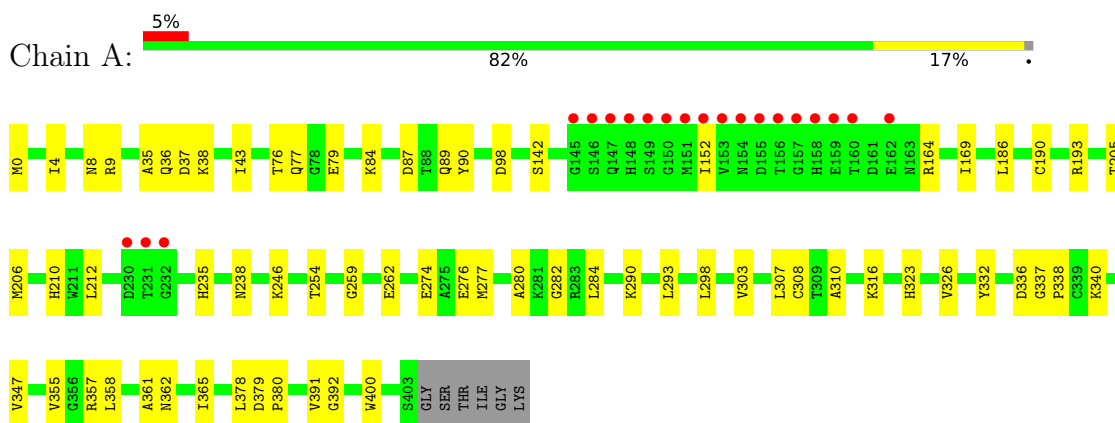
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	46	Total	O	0	0
			46	46		
2	B	33	Total	O	0	0
			33	33		
2	D	22	Total	O	0	0
			22	22		
2	C	22	Total	O	0	0
			22	22		

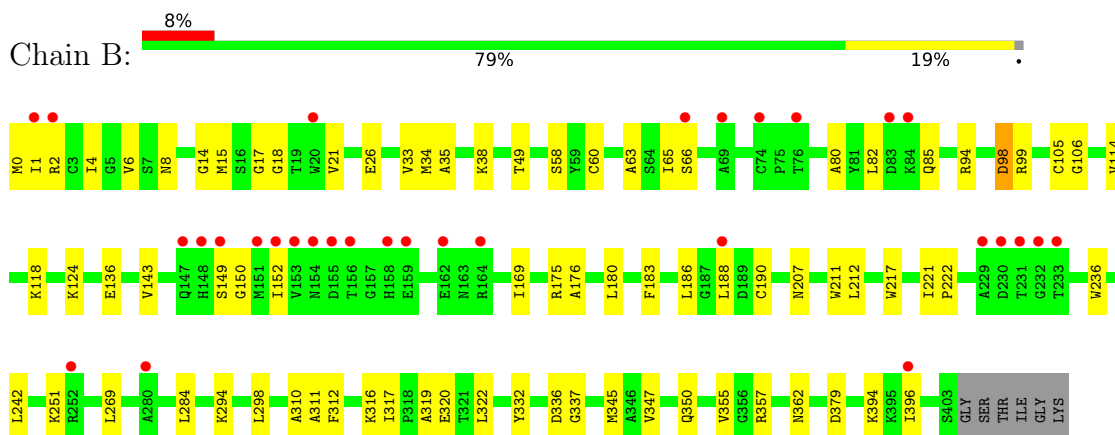
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

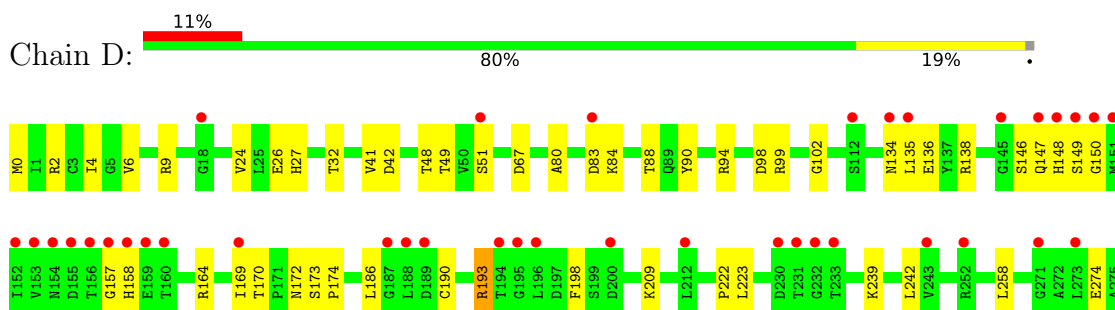
#### • Molecule 1: Core protein

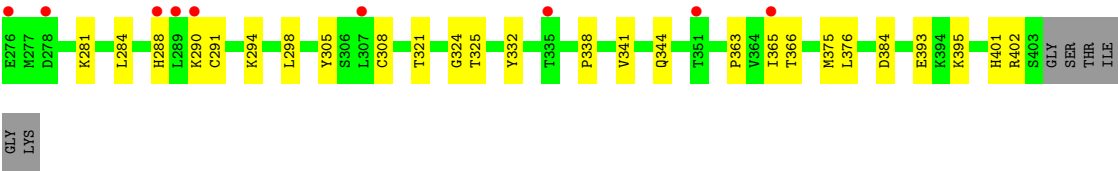


#### • Molecule 1: Core protein

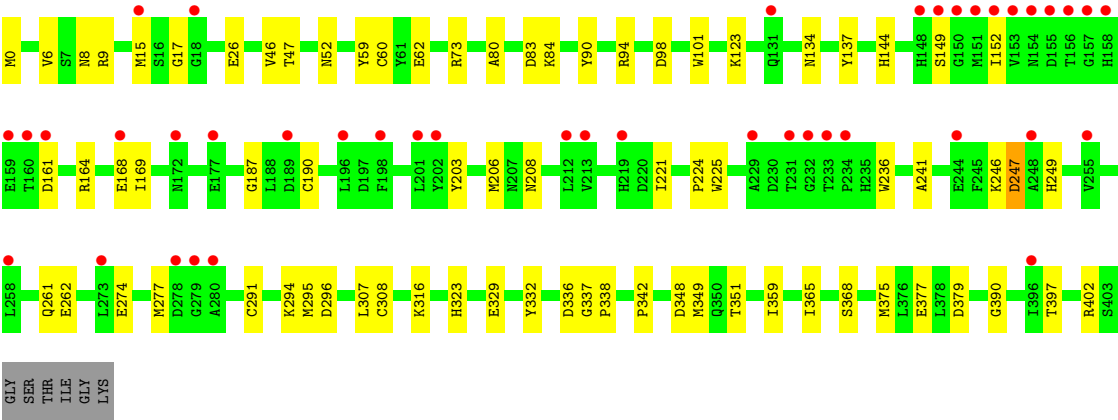
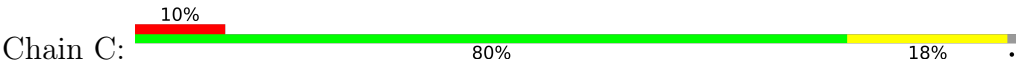


#### • Molecule 1: Core protein





● Molecule 1: Core protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.57Å 134.48Å 214.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.51 – 2.50 41.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.9 (41.51-2.50) 93.9 (41.51-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, $R_{free}$	0.257 , 0.280 0.256 , 0.277	Depositor DCC
$R_{free}$ test set	2903 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.7	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12367	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.47% 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	0.27	0/3141	0.50	1/4256 (0.0%)
1	B	0.26	0/3123	0.49	1/4235 (0.0%)
1	C	0.26	0/3106	0.50	1/4216 (0.0%)
1	D	0.26	0/3134	0.51	1/4248 (0.0%)
All	All	0.26	0/12504	0.50	4/16955 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	98	ASP	CB-CG-OD2	5.18	122.97	118.30
1	B	98	ASP	CB-CG-OD2	5.18	122.97	118.30
1	D	98	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	98	ASP	CB-CG-OD2	5.13	122.91	118.30

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	3076	0	3007	52	9
1	B	3058	0	2977	67	0
1	C	3041	0	2942	57	9
1	D	3069	0	2994	62	0
2	A	46	0	0	27	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	33	0	0	34	0
2	C	22	0	0	24	1
2	D	22	0	0	21	0
All	All	12367	0	11920	238	10

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 10.

All (238) 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:221:ILE:HB	2:C:505:HOH:O	1.23	1.34
1:A:277:MET:HA	2:A:506:HOH:O	1.17	1.30
1:B:336:ASP:C	2:B:502:HOH:O	1.86	1.12
1:D:190:CYS:SG	2:D:522:HOH:O	2.09	1.11
1:C:59:TYR:CZ	2:C:505:HOH:O	2.04	1.11
1:B:66:SER:N	2:B:501:HOH:O	1.84	1.10
1:B:221:ILE:C	2:B:503:HOH:O	1.93	1.06
1:C:0:MET:SD	2:C:510:HOH:O	2.12	1.06
1:B:176:ALA:N	2:B:505:HOH:O	1.91	1.03
1:C:348:ASP:CB	2:C:504:HOH:O	2.03	1.03
1:A:337:GLY:N	2:A:504:HOH:O	1.94	0.99
1:D:305:TYR:CZ	2:D:501:HOH:O	2.16	0.96
1:A:76:THR:OG1	2:A:501:HOH:O	1.81	0.96
1:C:390:GLY:O	2:C:501:HOH:O	1.83	0.96
1:D:305:TYR:OH	2:D:501:HOH:O	1.83	0.95
1:C:0:MET:CG	2:C:510:HOH:O	2.13	0.95
1:B:65:ILE:HA	2:B:501:HOH:O	1.68	0.94
1:B:337:GLY:O	2:B:502:HOH:O	1.84	0.94
1:A:323:HIS:ND1	2:A:508:HOH:O	1.99	0.93
1:D:172:ASN:O	2:D:502:HOH:O	1.87	0.92
1:B:18:GLY:N	2:B:508:HOH:O	2.02	0.91
1:B:337:GLY:N	2:B:502:HOH:O	2.01	0.90
1:B:65:ILE:C	2:B:501:HOH:O	2.09	0.90
1:C:294:LYS:O	2:C:502:HOH:O	1.89	0.89
1:B:65:ILE:CA	2:B:501:HOH:O	2.19	0.89
1:B:350:GLN:O	2:B:504:HOH:O	1.91	0.89
1:B:221:ILE:O	2:B:503:HOH:O	1.85	0.88
1:D:102:GLY:O	2:D:503:HOH:O	1.93	0.86
1:A:152:ILE:HG21	1:A:164:ARG:HH12	1.39	0.86
1:A:276:GLU:O	2:A:506:HOH:O	1.95	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:LYS:O	2:D:504:HOH:O	1.94	0.84
1:C:208:ASN:OD1	2:C:503:HOH:O	1.95	0.84
1:A:87:ASP:CG	2:A:503:HOH:O	2.15	0.84
1:D:172:ASN:HB2	2:D:508:HOH:O	1.77	0.83
1:B:118:LYS:O	2:B:501:HOH:O	1.96	0.83
1:A:77:GLN:NE2	2:A:501:HOH:O	2.04	0.83
1:B:175:ARG:HB3	2:B:505:HOH:O	1.78	0.83
1:A:282:GLY:HA2	2:A:506:HOH:O	1.78	0.82
1:B:98:ASP:OD2	2:B:506:HOH:O	1.96	0.82
1:C:351:THR:OG1	2:C:504:HOH:O	1.96	0.82
1:A:79:GLU:OE1	2:A:507:HOH:O	1.99	0.81
1:D:172:ASN:CB	2:D:508:HOH:O	2.30	0.79
1:A:361:ALA:HA	2:A:509:HOH:O	1.82	0.78
1:A:392:GLY:N	2:A:502:HOH:O	1.90	0.78
1:A:336:ASP:C	2:A:504:HOH:O	2.20	0.77
1:A:391:VAL:HA	2:A:502:HOH:O	1.84	0.77
1:D:190:CYS:HB3	1:D:291:CYS:HA	1.67	0.76
1:C:295:MET:CA	2:C:502:HOH:O	2.34	0.76
1:B:175:ARG:C	2:B:505:HOH:O	2.21	0.76
1:D:305:TYR:OH	2:D:506:HOH:O	2.03	0.75
1:B:222:PRO:N	2:B:503:HOH:O	2.16	0.74
1:A:280:ALA:O	2:A:510:HOH:O	2.04	0.73
1:C:168:GLU:O	2:C:506:HOH:O	2.06	0.73
1:C:59:TYR:OH	2:C:505:HOH:O	2.01	0.73
1:D:324:GLY:O	2:D:507:HOH:O	2.06	0.73
1:D:305:TYR:CE2	2:D:501:HOH:O	2.40	0.72
1:B:186:LEU:HD21	1:B:298:LEU:HD22	1.72	0.72
1:A:36:GLN:NE2	1:A:37:ASP:OD2	2.22	0.71
1:B:1:ILE:HD12	1:B:4:ILE:HD11	1.74	0.70
1:B:222:PRO:CA	2:B:503:HOH:O	2.40	0.70
1:C:295:MET:HA	2:C:502:HOH:O	1.93	0.69
1:D:157:GLY:O	1:D:164:ARG:NH2	2.25	0.68
1:B:106:GLY:O	2:B:509:HOH:O	2.10	0.68
1:A:358:LEU:HD23	2:A:509:HOH:O	1.93	0.68
1:A:89:GLN:N	2:A:503:HOH:O	1.93	0.68
1:B:251:LYS:HE2	2:B:515:HOH:O	1.93	0.67
1:C:144:HIS:CE1	2:C:510:HOH:O	2.47	0.67
1:A:391:VAL:CA	2:A:502:HOH:O	2.39	0.67
1:C:294:LYS:C	2:C:502:HOH:O	2.27	0.67
1:B:362:ASN:N	2:B:510:HOH:O	2.15	0.66
1:C:161:ASP:OD2	1:C:164:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:THR:HG23	1:D:173:SER:H	1.59	0.66
1:B:17:GLY:C	2:B:508:HOH:O	2.32	0.66
1:A:362:ASN:N	2:A:509:HOH:O	2.01	0.66
1:B:98:ASP:CG	2:B:506:HOH:O	2.35	0.65
1:A:87:ASP:OD1	2:A:503:HOH:O	2.15	0.64
1:A:89:GLN:CB	2:A:503:HOH:O	2.45	0.64
1:B:320:GLU:N	2:B:507:HOH:O	1.97	0.64
1:C:359:ILE:HD11	1:C:379:ASP:HB2	1.80	0.64
1:D:173:SER:HA	2:D:502:HOH:O	1.98	0.64
1:D:88:THR:O	1:D:239:LYS:NZ	2.23	0.64
1:B:242:LEU:HD13	2:B:513:HOH:O	1.98	0.63
1:D:242:LEU:HA	1:D:258:LEU:HD12	1.81	0.63
1:D:26:GLU:OE2	1:D:288:HIS:ND1	2.32	0.63
1:A:89:GLN:HB2	2:A:503:HOH:O	1.99	0.62
1:A:186:LEU:HD21	1:A:298:LEU:HD22	1.81	0.62
1:B:222:PRO:HA	2:B:503:HOH:O	1.98	0.61
1:C:84:LYS:HD3	1:C:90:TYR:CZ	2.35	0.60
1:C:149:SER:HA	1:C:152:ILE:HB	1.83	0.60
1:A:206:MET:HE1	1:A:262:GLU:HA	1.83	0.60
1:A:323:HIS:CE1	2:A:508:HOH:O	2.46	0.60
1:A:307:LEU:HD23	1:A:340:LYS:HB3	1.84	0.60
1:D:27:HIS:NE2	1:D:48:THR:OG1	2.27	0.60
1:B:49:THR:HB	1:B:136:GLU:HG2	1.84	0.60
1:B:207:ASN:N	2:B:511:HOH:O	2.36	0.58
1:B:319:ALA:HA	2:B:507:HOH:O	2.04	0.58
1:D:190:CYS:CB	1:D:291:CYS:HA	2.33	0.57
1:B:80:ALA:O	1:B:94:ARG:NH2	2.31	0.56
1:B:212:LEU:HD11	1:B:284:LEU:HD22	1.87	0.56
1:B:18:GLY:C	2:B:508:HOH:O	2.44	0.56
1:B:357:ARG:HB2	1:B:379:ASP:HB3	1.86	0.56
1:C:73:ARG:NH2	2:C:509:HOH:O	2.37	0.56
1:A:169:ILE:HG21	1:A:190:CYS:HB2	1.87	0.56
1:A:35:ALA:HB3	1:A:38:LYS:HB2	1.88	0.55
1:C:187:GLY:HA3	1:C:294:LYS:HE3	1.89	0.55
1:C:137:TYR:HB2	1:C:169:ILE:HB	1.87	0.55
1:D:173:SER:CA	2:D:502:HOH:O	2.53	0.55
1:C:8:ASN:ND2	1:C:26:GLU:OE1	2.20	0.55
1:D:321:THR:OG1	1:D:325:THR:OG1	2.18	0.55
1:D:341:VAL:HB	1:D:363:PRO:HB2	1.89	0.54
1:D:186:LEU:HG	1:D:298:LEU:HD13	1.89	0.54
1:D:0:MET:N	1:D:149:SER:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:VAL:HG12	1:C:47:THR:HG23	1.89	0.54
1:A:246:LYS:HB2	1:A:254:THR:OG1	2.08	0.54
1:D:344:GLN:HG2	2:D:505:HOH:O	2.08	0.53
1:B:149:SER:HA	1:B:152:ILE:HD12	1.89	0.53
1:B:169:ILE:HG21	1:B:190:CYS:HB2	1.90	0.53
1:C:349:MET:HE2	1:C:397:THR:HG22	1.90	0.53
1:C:52:ASN:HB2	1:C:134:ASN:ND2	2.24	0.53
1:B:347:VAL:HG23	1:B:355:VAL:HG21	1.90	0.52
1:C:247:ASP:HB3	1:C:249:HIS:CE1	2.44	0.52
1:A:336:ASP:N	2:A:504:HOH:O	2.41	0.52
1:B:14:GLY:N	1:B:34:MET:O	2.42	0.52
1:D:172:ASN:N	2:D:508:HOH:O	2.13	0.52
1:D:49:THR:HG21	1:D:281:LYS:HE2	1.92	0.52
1:A:43:ILE:HD11	1:A:293:LEU:HD21	1.91	0.52
1:D:363:PRO:HB3	1:D:376:LEU:HD21	1.92	0.51
1:D:174:PRO:HB2	1:D:190:CYS:O	2.11	0.51
1:D:402:ARG:HD2	2:D:507:HOH:O	2.10	0.51
1:A:308:CYS:HB3	1:A:332:TYR:CZ	2.46	0.51
1:B:85:GLN:OE1	1:B:94:ARG:NH2	2.36	0.51
1:B:2:ARG:O	1:B:6:VAL:HG23	2.11	0.51
1:C:144:HIS:NE2	1:C:377:GLU:OE1	2.44	0.51
1:A:0:MET:O	1:A:4:ILE:HG12	2.11	0.51
1:D:51:SER:O	1:D:134:ASN:ND2	2.45	0.50
1:D:308:CYS:HB3	1:D:332:TYR:CZ	2.46	0.50
1:C:307:LEU:HD22	1:C:342:PRO:HG3	1.93	0.50
1:C:390:GLY:N	2:C:501:HOH:O	2.44	0.50
1:B:312:PHE:C	1:B:396:ILE:HD11	2.32	0.50
1:D:170:THR:HG23	2:D:508:HOH:O	2.11	0.50
1:C:332:TYR:OH	1:C:336:ASP:OD2	2.29	0.50
1:A:212:LEU:HD11	1:A:284:LEU:HD22	1.92	0.50
1:B:98:ASP:OD1	2:B:506:HOH:O	2.18	0.50
1:B:294:LYS:HE2	2:B:519:HOH:O	2.10	0.50
1:C:59:TYR:CD1	1:C:225:TRP:HB3	2.47	0.50
1:B:217:TRP:CH2	1:B:269:LEU:HD11	2.46	0.49
1:D:4:ILE:HA	1:D:9:ARG:HH11	1.77	0.49
1:D:209:LYS:NZ	1:D:274:GLU:OE2	2.45	0.49
1:B:336:ASP:OD1	1:B:336:ASP:N	2.46	0.49
1:C:0:MET:HG3	2:C:510:HOH:O	1.93	0.49
1:D:24:VAL:HG22	1:D:290:LYS:HG3	1.94	0.48
1:D:48:THR:HB	1:D:284:LEU:HB2	1.95	0.48
1:B:175:ARG:CB	2:B:505:HOH:O	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:GLU:N	2:D:509:HOH:O	2.47	0.47
1:A:338:PRO:HA	1:A:365:ILE:O	2.15	0.47
1:B:143:VAL:HG23	1:B:180:LEU:HD23	1.96	0.47
1:D:136:GLU:OE1	1:D:138:ARG:NH1	2.44	0.47
1:D:338:PRO:HA	1:D:365:ILE:O	2.15	0.47
1:C:203:TYR:OH	1:C:277:MET:HG2	2.14	0.47
1:B:143:VAL:HG21	1:B:183:PHE:CD2	2.49	0.47
1:C:83:ASP:N	1:C:83:ASP:OD1	2.47	0.46
1:B:319:ALA:CA	2:B:507:HOH:O	2.61	0.46
1:D:9:ARG:NH2	1:D:32:THR:HG21	2.30	0.46
1:C:338:PRO:HA	1:C:365:ILE:O	2.15	0.46
1:D:41:VAL:HG11	1:D:186:LEU:HD11	1.97	0.46
1:D:80:ALA:O	1:D:94:ARG:NH1	2.48	0.46
1:C:296:ASP:OD2	2:C:507:HOH:O	2.21	0.45
1:D:193:ARG:HH22	1:D:198:PHE:N	2.14	0.45
1:C:221:ILE:CB	2:C:505:HOH:O	2.11	0.45
1:B:211:TRP:CD2	1:B:269:LEU:HD23	2.52	0.45
1:A:303:VAL:O	1:A:340:LYS:NZ	2.33	0.45
1:C:261:GLN:OE1	2:C:508:HOH:O	2.21	0.45
1:A:205:THR:HG23	1:A:210:HIS:CE1	2.52	0.45
1:C:6:VAL:HG23	1:C:9:ARG:HB2	1.99	0.45
1:D:67:ASP:OD2	1:D:84:LYS:NZ	2.28	0.45
1:C:15:MET:SD	1:C:17:GLY:N	2.70	0.45
1:D:222:PRO:O	1:D:223:LEU:HD23	2.17	0.45
1:C:329:GLU:HG3	1:C:375:MET:HG2	1.99	0.45
1:C:59:TYR:CE2	2:C:505:HOH:O	2.52	0.45
1:C:224:PRO:HD3	1:C:241:ALA:HB3	1.98	0.44
1:C:295:MET:N	2:C:502:HOH:O	2.45	0.44
1:D:67:ASP:OD2	1:D:90:TYR:OH	2.32	0.44
1:C:316:LYS:HB2	1:C:329:GLU:HB3	2.00	0.44
1:B:0:MET:HG2	1:B:150:GLY:HA2	1.99	0.44
1:B:8:ASN:ND2	1:B:26:GLU:OE2	2.37	0.44
1:B:311:ALA:HB2	1:B:394:LYS:HD2	1.98	0.44
1:C:59:TYR:CE1	1:C:225:TRP:HB3	2.52	0.44
1:B:99:ARG:HB3	1:B:105:CYS:SG	2.58	0.44
1:A:238:ASN:OD1	2:A:511:HOH:O	2.20	0.43
1:B:316:LYS:HD2	1:B:317:ILE:H	1.84	0.43
1:D:294:LYS:O	2:D:510:HOH:O	2.21	0.43
1:D:83:ASP:N	1:D:83:ASP:OD1	2.50	0.43
1:B:175:ARG:HA	1:B:188:LEU:O	2.19	0.43
1:A:259:GLY:N	2:A:505:HOH:O	1.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ALA:O	1:C:94:ARG:NH1	2.51	0.43
1:C:295:MET:C	2:C:502:HOH:O	2.56	0.43
1:D:384:ASP:OD1	1:D:401:HIS:ND1	2.49	0.43
1:C:206:MET:CE	1:C:262:GLU:HG3	2.49	0.43
1:A:193:ARG:HA	1:A:290:LYS:HE2	2.01	0.43
1:C:337:GLY:HA2	1:C:368:SER:HA	2.01	0.43
1:A:310:ALA:HB3	1:A:332:TYR:CE1	2.53	0.42
1:A:326:VAL:HG22	1:A:400:TRP:CZ2	2.54	0.42
1:D:150:GLY:HA3	1:D:375:MET:SD	2.59	0.42
1:D:147:GLN:OE1	1:D:366:THR:N	2.49	0.42
1:B:35:ALA:HB3	1:B:38:LYS:HB2	2.01	0.42
1:D:2:ARG:O	1:D:6:VAL:HG23	2.20	0.42
1:B:82:LEU:HD12	1:B:114:VAL:HG13	2.01	0.42
1:D:99:ARG:HA	1:D:99:ARG:HD2	1.88	0.42
1:C:379:ASP:OD1	1:C:402:ARG:NH1	2.49	0.42
1:D:158:HIS:CD2	1:D:158:HIS:H	2.36	0.42
1:A:9:ARG:HB3	1:A:323:HIS:CE1	2.55	0.42
1:A:357:ARG:HB2	1:A:379:ASP:HB3	2.01	0.42
1:D:135:LEU:HD11	1:D:198:PHE:HD2	1.84	0.42
1:C:308:CYS:HB3	1:C:332:TYR:CZ	2.54	0.42
1:D:146:SER:C	1:D:148:HIS:H	2.23	0.42
1:A:84:LYS:HG3	1:A:90:TYR:CZ	2.55	0.42
1:A:336:ASP:N	1:A:336:ASP:OD1	2.44	0.41
1:A:378:LEU:O	1:A:380:PRO:HD3	2.20	0.41
1:B:310:ALA:HB3	1:B:332:TYR:CE1	2.55	0.41
1:B:58:SER:HB3	1:B:124:LYS:HE3	2.02	0.41
1:B:21:VAL:HG21	1:B:33:VAL:HG11	2.03	0.41
1:B:63:ALA:N	2:B:513:HOH:O	2.40	0.41
1:D:172:ASN:CA	2:D:508:HOH:O	2.54	0.41
1:C:62:GLU:HB3	1:C:123:LYS:HB2	2.02	0.41
1:A:142:SER:OG	1:A:164:ARG:NE	2.54	0.41
1:A:347:VAL:HG23	1:A:355:VAL:HG21	2.02	0.41
1:B:345:MET:HB2	1:B:355:VAL:O	2.21	0.41
1:D:4:ILE:HA	1:D:9:ARG:NH1	2.36	0.41
1:C:60:CYS:HB2	1:C:236:TRP:CZ3	2.56	0.41
1:D:169:ILE:HG13	2:D:522:HOH:O	2.20	0.41
1:C:190:CYS:HA	1:C:291:CYS:HA	2.03	0.41
1:B:322:LEU:HD23	1:B:322:LEU:HA	1.94	0.40
1:A:235:HIS:HA	2:A:518:HOH:O	2.21	0.40
1:D:32:THR:HG22	1:D:42:ASP:OD1	2.21	0.40
1:C:9:ARG:HB3	1:C:323:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:GLY:O	2:A:504:HOH:O	2.22	0.40
1:B:14:GLY:O	1:B:15:MET:HB3	2.22	0.40
1:B:60:CYS:HB2	1:B:236:TRP:CZ3	2.57	0.40

All (10) 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:316:LYS:NZ	1:C:101:TRP:NE1[4_545]	1.47	0.73
1:A:316:LYS:NZ	1:C:101:TRP:CE2[4_545]	1.60	0.60
1:A:316:LYS:NZ	1:C:101:TRP:CD1[4_545]	1.77	0.43
2:A:519:HOH:O	2:C:513:HOH:O[4_545]	1.84	0.36
1:A:274:GLU:OE2	1:C:246:LYS:NZ[4_545]	1.85	0.35
1:A:316:LYS:NZ	1:C:101:TRP:CD2[4_545]	1.95	0.25
1:A:316:LYS:NZ	1:C:101:TRP:CG[4_545]	2.05	0.15
1:A:316:LYS:CE	1:C:101:TRP:CE2[4_545]	2.11	0.09
1:A:246:LYS:NZ	1:C:274:GLU:OE2[4_545]	2.13	0.07
1:A:316:LYS:CE	1:C:101:TRP:NE1[4_545]	2.15	0.05

## 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	402/410 (98%)	394 (98%)	8 (2%)	0	100	100
1	B	402/410 (98%)	389 (97%)	13 (3%)	0	100	100
1	C	402/410 (98%)	390 (97%)	11 (3%)	1 (0%)	47	68
1	D	402/410 (98%)	393 (98%)	9 (2%)	0	100	100
All	All	1608/1640 (98%)	1566 (97%)	41 (2%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	247	ASP

### 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	335/342 (98%)	334 (100%)	1 (0%)	92	97
1	B	331/342 (97%)	331 (100%)	0	100	100
1	C	327/342 (96%)	327 (100%)	0	100	100
1	D	333/342 (97%)	332 (100%)	1 (0%)	92	97
All	All	1326/1368 (97%)	1324 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	D	193	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	404/410 (98%)	0.59	20 (4%)	28 30	35, 54, 85, 132	0
1	B	404/410 (98%)	0.60	31 (7%)	13 13	37, 62, 92, 123	0
1	C	404/410 (98%)	0.86	42 (10%)	6 6	40, 68, 96, 130	0
1	D	404/410 (98%)	0.85	47 (11%)	4 4	42, 68, 103, 131	0
All	All	1616/1640 (98%)	0.73	140 (8%)	10 10	35, 62, 98, 132	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	ASN	26.9
1	A	153	VAL	16.6
1	C	154	ASN	14.1
1	C	153	VAL	13.8
1	B	154	ASN	13.1
1	D	153	VAL	12.8
1	A	156	THR	12.8
1	D	233	THR	12.6
1	C	151	MET	12.3
1	C	160	THR	11.5
1	B	153	VAL	10.7
1	C	150	GLY	10.5
1	D	150	GLY	9.5
1	A	151	MET	9.1
1	A	159	GLU	8.8
1	D	157	GLY	8.5
1	C	156	THR	8.3
1	C	149	SER	8.2
1	D	156	THR	8.0
1	C	155	ASP	7.4
1	D	155	ASP	7.3

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Mol	Chain	Res	Type	RSRZ
1	B	158	HIS	7.1
1	A	157	GLY	7.1
1	D	148	HIS	7.1
1	D	147	GLN	6.8
1	B	149	SER	6.7
1	A	150	GLY	6.5
1	D	231	THR	6.5
1	C	152	ILE	6.4
1	D	154	ASN	6.2
1	A	155	ASP	6.1
1	C	148	HIS	6.0
1	C	213	VAL	5.9
1	D	151	MET	5.8
1	C	202	TYR	5.4
1	A	152	ILE	5.3
1	D	196	LEU	5.1
1	C	198	PHE	5.1
1	D	158	HIS	5.1
1	C	278	ASP	4.9
1	D	194	THR	4.9
1	D	159	GLU	4.7
1	D	230	ASP	4.7
1	B	152	ILE	4.6
1	A	160	THR	4.6
1	B	2	ARG	4.6
1	C	159	GLU	4.6
1	C	233	THR	4.5
1	C	231	THR	4.5
1	D	160	THR	4.4
1	D	232	GLY	4.4
1	A	148	HIS	4.3
1	B	229	ALA	4.3
1	B	232	GLY	4.2
1	D	149	SER	4.1
1	A	149	SER	4.1
1	C	229	ALA	4.1
1	C	248	ALA	4.0
1	B	147	GLN	4.0
1	C	157	GLY	4.0
1	D	195	GLY	3.9
1	B	151	MET	3.8
1	B	233	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	83	ASP	3.8
1	A	231	THR	3.8
1	A	158	HIS	3.8
1	D	273	LEU	3.8
1	C	196	LEU	3.7
1	C	280	ALA	3.7
1	B	156	THR	3.6
1	C	18	GLY	3.6
1	B	252	ARG	3.5
1	D	271	GLY	3.4
1	B	155	ASP	3.4
1	B	1	ILE	3.3
1	C	189	ASP	3.2
1	C	158	HIS	3.2
1	C	244	GLU	3.2
1	A	230	ASP	3.1
1	C	131	GLN	3.0
1	C	212	LEU	3.0
1	D	290	LYS	3.0
1	D	51	SER	3.0
1	D	200	ASP	3.0
1	B	164	ARG	3.0
1	A	147	GLN	3.0
1	B	69	ALA	3.0
1	B	162	GLU	2.9
1	B	148	HIS	2.9
1	B	84	LYS	2.9
1	B	159	GLU	2.9
1	D	18	GLY	2.8
1	C	161	ASP	2.8
1	C	232	GLY	2.6
1	A	232	GLY	2.6
1	D	189	ASP	2.6
1	D	212	LEU	2.6
1	D	112	SER	2.6
1	D	145	GLY	2.5
1	C	279	GLY	2.5
1	D	187	GLY	2.5
1	B	188	LEU	2.4
1	C	172	ASN	2.4
1	D	335	THR	2.4
1	D	276	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	177	GLU	2.4
1	B	231	THR	2.4
1	D	288	HIS	2.4
1	B	280	ALA	2.3
1	B	83	ASP	2.3
1	D	152	ILE	2.3
1	C	396	ILE	2.3
1	C	168	GLU	2.3
1	D	169	ILE	2.3
1	C	258	LEU	2.3
1	D	134	ASN	2.2
1	C	255	VAL	2.2
1	B	20	TRP	2.2
1	C	219	HIS	2.2
1	D	289	LEU	2.2
1	C	201	LEU	2.2
1	D	243	VAL	2.2
1	D	252	ARG	2.2
1	B	66	SER	2.2
1	C	15	MET	2.2
1	B	230	ASP	2.2
1	B	76	THR	2.2
1	D	351	THR	2.2
1	D	135	LEU	2.2
1	A	146	SER	2.2
1	D	278	ASP	2.1
1	D	365	ILE	2.1
1	C	273	LEU	2.1
1	A	145	GLY	2.1
1	D	307	LEU	2.1
1	C	234	PRO	2.1
1	D	188	LEU	2.0
1	B	74	CYS	2.0
1	A	162	GLU	2.0
1	B	396	ILE	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no 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.