



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:46 PM UTC

PDB ID : 7YW8 / pdb_00007yw8
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
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

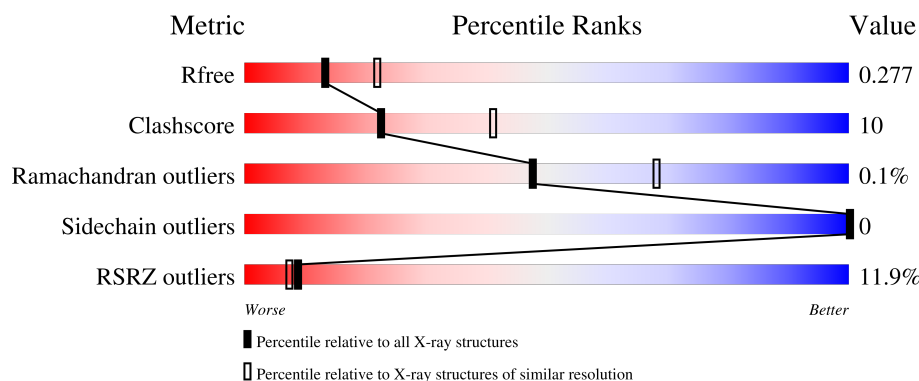
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 ≥ 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	8% 81% 17% .
1	B	410	11% 78% 21% .
1	C	410	15% 80% 19% .
1	D	410	13% 78% 21% .

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

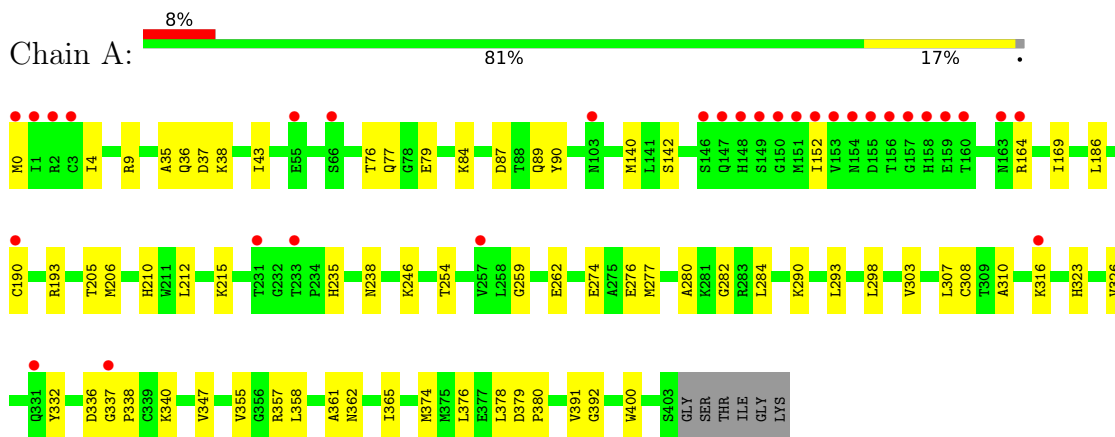
- Molecule 2 is water.

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		

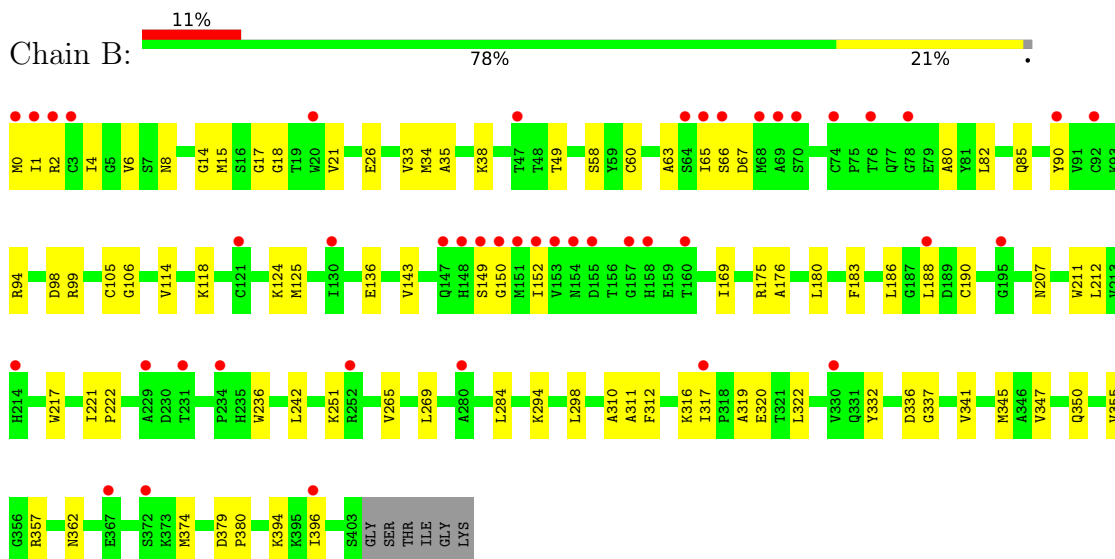
3 Residue-property plots

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.

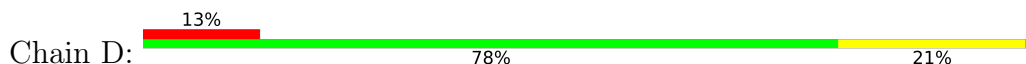
• Molecule 1: Core protein

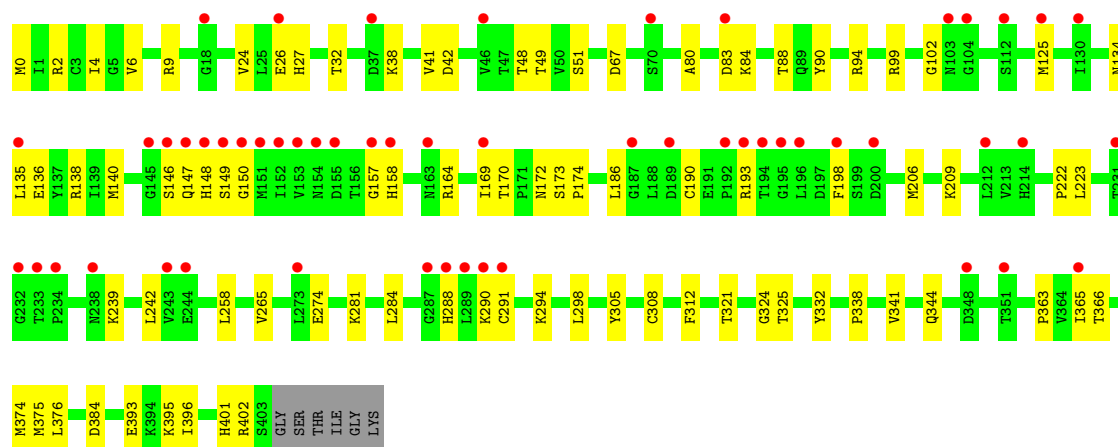


• Molecule 1: Core protein

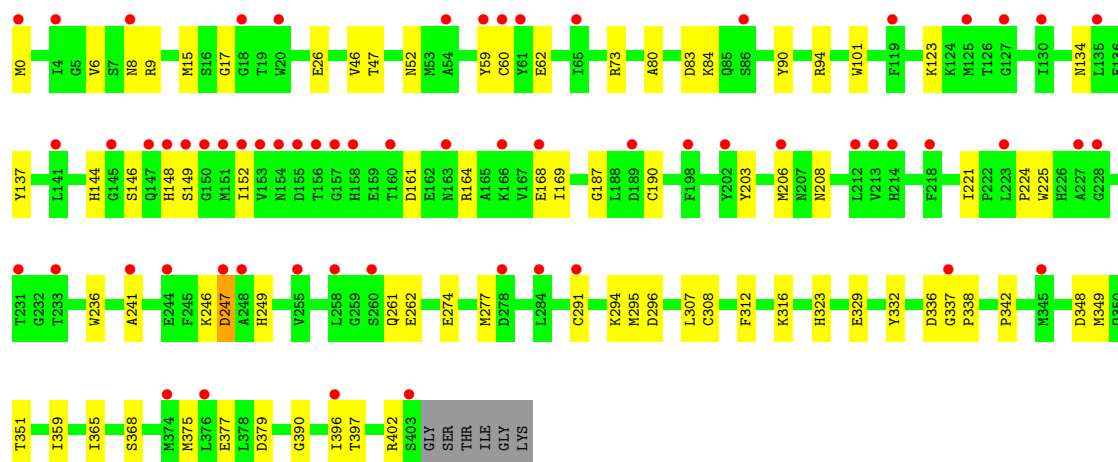
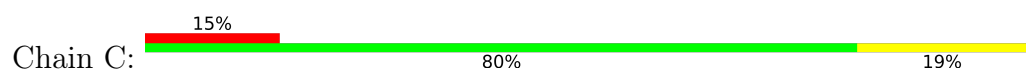


• Molecule 1: Core protein





● Molecule 1: Core protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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	2906 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.16	0/3141	0.35	0/4256
1	B	0.15	0/3123	0.38	0/4235
1	C	0.16	0/3106	0.37	0/4216
1	D	0.16	0/3134	0.38	0/4248
All	All	0.16	0/12504	0.37	0/16955

There are no bond length outliers.

There are no bond angle outliers.

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	55	9
1	B	3058	0	2977	70	0
1	C	3041	0	2942	60	9
1	D	3069	0	2994	68	0
2	A	46	0	0	28	1
2	B	33	0	0	33	0
2	C	22	0	0	24	1
2	D	22	0	0	21	0
All	All	12367	0	11920	253	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 (253) 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	1.16
1:B:221:ILE:C	2:B:503:HOH:O	1.93	1.11
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: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:B:65:ILE:C	2:B:501:HOH:O	2.09	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: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: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:A:87:ASP:CG	2:A:503:HOH:O	2.15	0.88
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
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: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:A:323:HIS:ND1	2:A:508:HOH:O	1.99	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:B:337:GLY:N	2:B:502:HOH:O	2.01	0.82
1:C:351:THR:OG1	2:C:504:HOH:O	1.96	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLU:OE1	2:A:507:HOH:O	1.99	0.81
1:B:175:ARG:C	2:B:505:HOH:O	2.21	0.80
1:A:336:ASP:C	2:A:504:HOH:O	2.20	0.79
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:391:VAL:HA	2:A:502:HOH:O	1.84	0.77
1:C:294:LYS:C	2:C:502:HOH:O	2.27	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:D:305:TYR:OH	2:D:506:HOH:O	2.03	0.75
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:B:222:PRO:N	2:B:503:HOH:O	2.16	0.72
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:D:88:THR:O	1:D:239:LYS:NZ	2.23	0.71
1:B:17:GLY:C	2:B:508:HOH:O	2.32	0.70
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:B:98:ASP:CG	2:B:506:HOH:O	2.35	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: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
1:D:170:THR:HG23	1:D:173:SER:H	1.59	0.66
1:A:362:ASN:N	2:A:509:HOH:O	2.01	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:125:MET:HE1	1:D:265:VAL:HG11	1.83	0.61
1:D:27:HIS:NE2	1:D:48:THR:OG1	2.27	0.61
1:B:18:GLY:C	2:B:508:HOH:O	2.44	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: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:A:215:LYS:NZ	2:A:512:HOH:O	2.30	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:C:0:MET:HE1	1:C:375:MET:HE2	1.84	0.57
1:D:190:CYS:CB	1:D:291:CYS:HA	2.33	0.57
1:A:206:MET:HE2	1:A:262:GLU:HG3	1.87	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: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:A:140:MET:HE3	1:A:164:ARG:HD3	1.89	0.54
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:B:312:PHE:C	1:B:396:ILE:HD11	2.32	0.54
1:B:341:VAL:HG21	1:B:374:MET:HE1	1.89	0.54
1:D:0:MET:N	1:D:149:SER:O	2.40	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ILE:HG21	1:B:190:CYS:HB2	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:C:349:MET:HE2	1:C:397:THR:HG22	1.92	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: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:N	1:B:336:ASP:OD1	2.46	0.49
1:C:0:MET:HG3	2:C:510:HOH:O	1.93	0.49
1:D:38:LYS:NZ	1:D:298:LEU:O	2.41	0.48
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:D:341:VAL:HG21	1:D:374:MET:HE2	1.96	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	1:C:83:ASP:N	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:D:146:SER:C	1:D:148:HIS:H	2.23	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:295:MET:C	2:C:502:HOH:O	2.56	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:125:MET:HE1	1:B:265:VAL:HG21	1.97	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:B:345:MET:HE2	1:B:380:PRO:HB3	1.98	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:312:PHE:C	1:C:396:ILE:HD11	2.41	0.45
1:C:329:GLU:HG3	1:C:375:MET:HG2	1.99	0.45
1:D:67:ASP:OD2	1:D:90:TYR:OH	2.32	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: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:B:67:ASP:OD2	1:B:90:TYR:OH	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:80:ALA:O	1:C:94:ARG:NH1	2.51	0.43
1:A:374:MET:HE1	1:A:376:LEU:HD21	2.00	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:140:MET:HE3	1:D:164:ARG:HB2	2.02	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:C:146:SER:C	1:C:148:HIS:H	2.27	0.42
1:A:84:LYS:HG3	1:A:90:TYR:CZ	2.55	0.42
1:D:125:MET:HE2	1:D:206:MET:SD	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:LEU:HD23	1:B:322:LEU:HA	1.94	0.40
1:D:312:PHE:C	1:D:396:ILE:HD11	2.46	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
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%)	43	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	402/410 (98%)	393 (98%)	9 (2%)	0	100	100
All	All	1608/1640 (98%)	1566 (97%)	41 (2%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	247	ASP

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	335/342 (98%)	335 (100%)	0	100	100
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%)	333 (100%)	0	100	100
All	All	1326/1368 (97%)	1326 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	288	HIS
1	A	344	GLN
1	A	398	HIS
1	B	238	ASN
1	D	219	HIS
1	D	344	GLN
1	D	398	HIS
1	C	134	ASN
1	C	210	HIS

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Mol	Chain	Res	Type
1	C	323	HIS
1	C	344	GLN
1	C	398	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 95th 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 ²)	Q<0.9
1	A	404/410 (98%)	0.78	31 (7%) 19 17	35, 54, 85, 132	0
1	B	404/410 (98%)	0.92	44 (10%) 10 9	37, 62, 92, 123	0
1	C	404/410 (98%)	1.14	63 (15%) 5 4	40, 68, 96, 130	0
1	D	404/410 (98%)	1.12	54 (13%) 7 5	42, 68, 103, 131	0
All	All	1616/1640 (98%)	0.99	192 (11%) 9 7	35, 62, 98, 132	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	150	GLY	9.1
1	A	153	VAL	7.0
1	C	153	VAL	6.9
1	C	150	GLY	6.7
1	C	149	SER	6.3
1	A	154	ASN	6.1
1	D	153	VAL	5.9
1	C	152	ILE	5.8
1	C	151	MET	5.7
1	B	2	ARG	5.6
1	B	153	VAL	5.4
1	C	154	ASN	5.2
1	D	149	SER	5.2
1	D	192	PRO	4.9
1	A	149	SER	4.7
1	B	1	ILE	4.6
1	B	147	GLN	4.5
1	D	233	THR	4.3
1	A	152	ILE	4.3
1	B	149	SER	4.3
1	D	196	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	147	GLN	4.1
1	A	159	GLU	4.1
1	D	351	THR	4.0
1	A	160	THR	3.9
1	A	0	MET	3.8
1	D	152	ILE	3.8
1	A	157	GLY	3.8
1	C	248	ALA	3.8
1	D	194	THR	3.7
1	C	18	GLY	3.6
1	D	125	MET	3.6
1	C	54	ALA	3.6
1	C	148	HIS	3.5
1	C	198	PHE	3.5
1	C	213	VAL	3.5
1	A	1	ILE	3.5
1	B	160	THR	3.4
1	A	146	SER	3.4
1	A	231	THR	3.4
1	C	396	ILE	3.3
1	D	232	GLY	3.3
1	D	348	ASP	3.3
1	C	160	THR	3.3
1	D	146	SER	3.2
1	A	158	HIS	3.2
1	B	0	MET	3.2
1	D	187	GLY	3.2
1	D	83	ASP	3.2
1	C	145	GLY	3.2
1	B	152	ILE	3.2
1	D	231	THR	3.1
1	D	155	ASP	3.1
1	C	155	ASP	3.1
1	A	150	GLY	3.1
1	C	156	THR	3.0
1	C	244	GLU	3.0
1	D	148	HIS	3.0
1	D	135	LEU	3.0
1	D	289	LEU	3.0
1	B	330	VAL	3.0
1	D	151	MET	3.0
1	A	337	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	20	TRP	3.0
1	C	374	MET	3.0
1	D	169	ILE	3.0
1	C	189	ASP	2.9
1	D	112	SER	2.9
1	B	154	ASN	2.9
1	C	214	HIS	2.9
1	C	125	MET	2.9
1	C	135	LEU	2.8
1	A	156	THR	2.8
1	B	396	ILE	2.8
1	D	365	ILE	2.8
1	B	234	PRO	2.8
1	C	227	ALA	2.8
1	A	164	ARG	2.8
1	D	145	GLY	2.8
1	C	0	MET	2.8
1	C	130	ILE	2.7
1	C	59	TYR	2.7
1	B	20	TRP	2.7
1	D	18	GLY	2.7
1	C	157	GLY	2.7
1	B	317	ILE	2.7
1	B	188	LEU	2.7
1	B	158	HIS	2.7
1	B	229	ALA	2.7
1	C	233	THR	2.7
1	D	189	ASP	2.6
1	D	291	CYS	2.6
1	C	278	ASP	2.6
1	B	65	ILE	2.6
1	B	372	SER	2.6
1	A	155	ASP	2.6
1	C	65	ILE	2.6
1	D	158	HIS	2.6
1	C	202	TYR	2.6
1	B	64	SER	2.6
1	C	212	LEU	2.5
1	C	403	SER	2.5
1	A	316	LYS	2.5
1	B	157	GLY	2.5
1	C	127	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	231	THR	2.5
1	C	345	MET	2.5
1	B	195	GLY	2.5
1	C	337	GLY	2.5
1	D	273	LEU	2.5
1	D	198	PHE	2.5
1	C	119	PHE	2.5
1	B	66	SER	2.5
1	C	231	THR	2.5
1	D	288	HIS	2.4
1	A	103	ASN	2.4
1	D	154	ASN	2.4
1	A	55	GLU	2.4
1	A	3	CYS	2.4
1	D	290	LYS	2.4
1	B	151	MET	2.4
1	B	280	ALA	2.4
1	B	148	HIS	2.4
1	B	68	MET	2.4
1	C	255	VAL	2.4
1	B	150	GLY	2.4
1	C	158	HIS	2.4
1	C	241	ALA	2.4
1	D	193	ARG	2.3
1	C	147	GLN	2.3
1	A	233	THR	2.3
1	B	76	THR	2.3
1	D	130	ILE	2.3
1	C	141	LEU	2.3
1	C	258	LEU	2.3
1	A	190	CYS	2.3
1	D	26	GLU	2.3
1	D	157	GLY	2.3
1	C	260	SER	2.3
1	D	163	ASN	2.3
1	D	212	LEU	2.3
1	A	257	VAL	2.3
1	A	163	ASN	2.2
1	B	69	ALA	2.2
1	A	148	HIS	2.2
1	B	214	HIS	2.2
1	A	66	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	238	ASN	2.2
1	C	8	ASN	2.2
1	C	291	CYS	2.2
1	A	331	GLN	2.2
1	D	287	GLY	2.2
1	C	376	LEU	2.2
1	B	130	ILE	2.2
1	D	37	ASP	2.2
1	D	243	VAL	2.2
1	A	147	GLN	2.2
1	B	3	CYS	2.2
1	D	104	GLY	2.2
1	C	223	LEU	2.2
1	C	284	LEU	2.2
1	C	168	GLU	2.2
1	B	47	THR	2.2
1	B	74	CYS	2.2
1	B	78	GLY	2.2
1	B	155	ASP	2.2
1	C	218	PHE	2.2
1	D	214	HIS	2.1
1	D	195	GLY	2.1
1	C	166	LYS	2.1
1	D	244	GLU	2.1
1	D	70	SER	2.1
1	C	247	ASP	2.1
1	D	234	PRO	2.1
1	C	163	ASN	2.1
1	A	2	ARG	2.1
1	B	90	TYR	2.1
1	D	46	VAL	2.1
1	B	252	ARG	2.1
1	C	4	ILE	2.1
1	B	70	SER	2.1
1	B	92	CYS	2.1
1	B	121	CYS	2.1
1	A	151	MET	2.1
1	D	200	ASP	2.0
1	C	86	SER	2.0
1	C	206	MET	2.0
1	C	60	CYS	2.0
1	B	367	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	103	ASN	2.0
1	C	228	GLY	2.0
1	C	61	TYR	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 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.