



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:39 AM UTC

PDB ID : 4GNX / pdb_00004gnx
Title : Structure of U. maydis Replication protein A bound to ssDNA
Authors : Pavletich, N.P.; Fan, J.
Deposited on : 2012-08-17
Resolution : 2.80 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

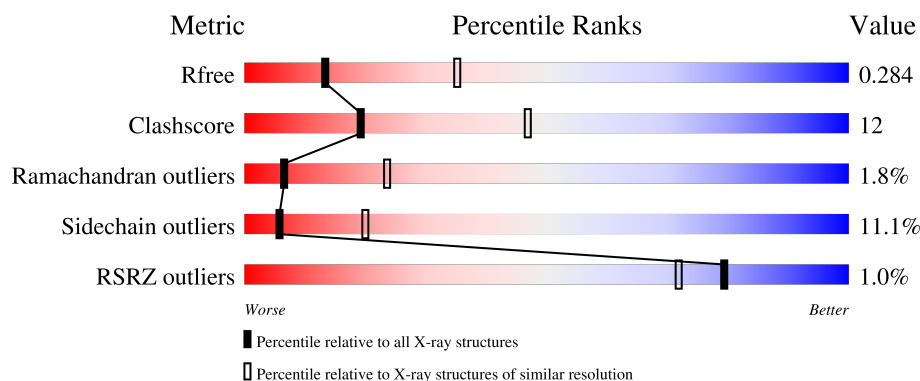
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	114	% 61% 26% 6% • 5%
1	X	114	4% 59% 26% 8% • 5%
2	B	136	% 65% 19% 5% • 10%
2	Y	136	% 64% 21% • • 10%
3	C	444	72% 23% • •

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Mol	Chain	Length	Quality of chain
3	Z	444	
4	K	62	
4	L	62	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11350 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			809	505	132	168	4			
1	X	108	Total	C	N	O	S	0	0	0
			809	505	132	168	4			

- Molecule 2 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	S	0	0	0
			978	609	186	181	2			
2	Y	122	Total	C	N	O	S	0	0	0
			978	609	186	181	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	173	VAL	ALA	conflict	UNP Q4PBD4
Y	173	VAL	ALA	conflict	UNP Q4PBD4

- Molecule 3 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	433	Total	C	N	O	S	0	0	0
			3437	2144	600	675	18			
3	Z	433	Total	C	N	O	S	0	0	0
			3437	2144	600	675	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	314	GLN	THR	conflict	UNP Q4P407
Z	314	GLN	THR	conflict	UNP Q4P407

- Molecule 4 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	25	Total 500	C 250	N 50	O 175	P 25	0	0	0
4	L	20	Total 400	C 200	N 40	O 140	P 20	0	0	0

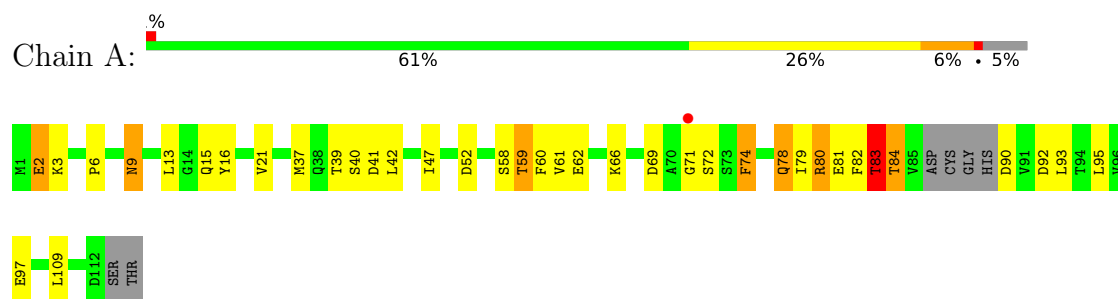
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total 1	Zn 1	0	0
5	Z	1	Total 1	Zn 1	0	0

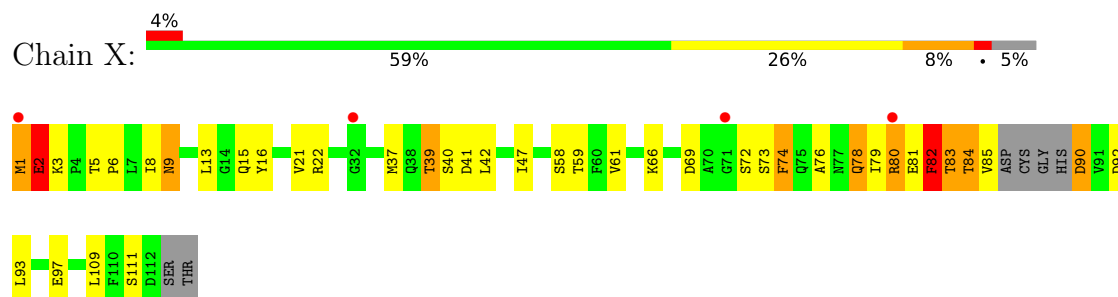
3 Residue-property plots [i](#)

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.

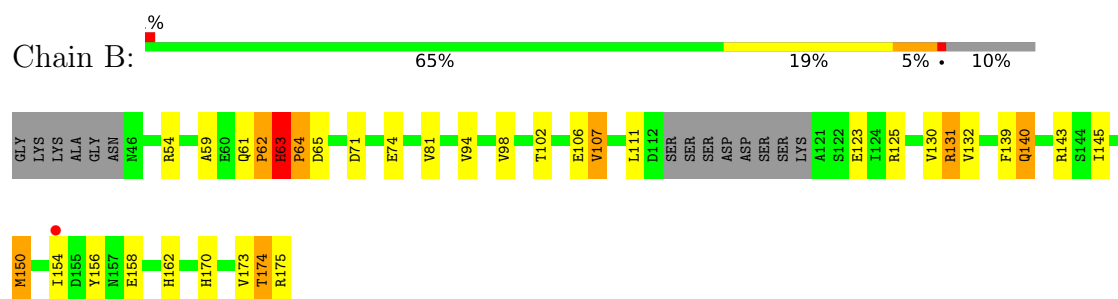
- Molecule 1: Putative uncharacterized protein



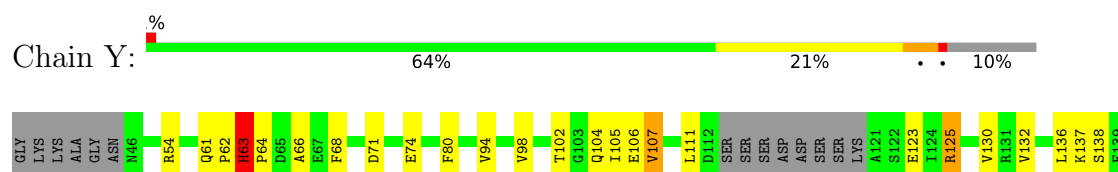
- Molecule 1: Putative uncharacterized protein



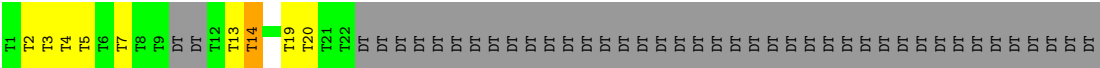
- Molecule 2: Putative uncharacterized protein



- Molecule 2: Putative uncharacterized protein







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.10Å 91.40Å 114.60Å 90.00° 97.80° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.3 (20.00-2.80) 88.2 (20.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.219 , 0.278 0.223 , 0.284	Depositor DCC
R_{free} test set	1498 reflections (3.77%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11350	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7967e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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

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	0.78	0/818	1.03	1/1111 (0.1%)
1	X	0.78	0/818	1.01	1/1111 (0.1%)
2	B	0.85	0/994	0.97	1/1348 (0.1%)
2	Y	0.79	0/994	0.99	3/1348 (0.2%)
3	C	0.67	0/3502	0.89	2/4732 (0.0%)
3	Z	0.66	0/3502	0.91	2/4732 (0.0%)
4	K	0.34	0/549	1.11	4/846 (0.5%)
4	L	0.33	0/438	1.02	1/672 (0.1%)
All	All	0.69	0/11615	0.95	15/15900 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	442	GLY	N-CA-C	9.76	136.31	113.18
2	Y	63	HIS	CA-C-N	9.44	130.42	119.47
2	Y	63	HIS	C-N-CA	9.44	130.42	119.47
3	C	442	GLY	N-CA-C	8.34	132.95	113.18
4	K	11	DT	P-O3'-C3'	6.76	130.34	120.20
4	L	14	DT	P-O3'-C3'	6.26	129.59	120.20
2	B	162	HIS	N-CA-C	5.70	117.49	111.28
1	A	83	THR	N-CA-C	5.67	122.87	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	18	DT	P-O3'-C3'	5.32	128.17	120.20
2	Y	162	HIS	N-CA-C	5.22	116.97	111.28
4	K	4	DT	P-O3'-C3'	5.22	128.03	120.20
4	K	10	DT	P-O3'-C3'	5.18	127.97	120.20
3	Z	430	THR	N-CA-C	5.13	117.91	110.42
3	C	619	ILE	N-CA-C	5.03	115.25	110.42
1	X	111	SER	N-CA-C	5.02	115.16	108.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	441	GLY	Peptide

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	809	0	807	40	0
1	X	809	0	807	35	0
2	B	978	0	970	21	0
2	Y	978	0	970	20	0
3	C	3437	0	3315	71	0
3	Z	3437	0	3315	69	0
4	K	500	0	301	16	0
4	L	400	0	242	12	0
5	C	1	0	0	0	0
5	Z	1	0	0	0	0
All	All	11350	0	10727	259	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 12.

All (259) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:63:HIS:HB3	2:Y:64:PRO:HD2	1.28	1.12
2:B:62:PRO:O	2:B:64:PRO:HD2	1.51	1.10
3:Z:451:ARG:HG3	3:Z:451:ARG:HH11	1.19	1.06
3:C:451:ARG:HG3	3:C:451:ARG:HH11	1.23	0.99
1:A:62:GLU:HB2	1:A:82:PHE:HZ	1.29	0.96
1:A:60:PHE:HD1	1:A:83:THR:HG1	1.05	0.94
3:C:472:ASN:HB3	3:C:580:MET:HE1	1.50	0.94
1:A:83:THR:HG23	1:A:90:ASP:N	1.82	0.93
1:A:80:ARG:HE	1:A:80:ARG:HA	1.35	0.92
3:Z:472:ASN:HB3	3:Z:580:MET:HE1	1.57	0.86
1:X:9:ASN:HB2	1:X:41:ASP:HB2	1.59	0.85
3:Z:498:LYS:HB2	4:L:14:DT:H5''	1.59	0.84
3:Z:267:PHE:HA	4:L:5:DT:H71	1.59	0.83
3:C:597:ARG:HD3	4:K:17:DT:O4	1.78	0.82
1:A:9:ASN:HB2	1:A:41:ASP:HB2	1.62	0.81
3:Z:602:ARG:HH21	3:Z:604:ALA:HB2	1.46	0.80
3:C:602:ARG:HH21	3:C:604:ALA:HB2	1.45	0.79
1:A:81:GLU:O	1:A:82:PHE:CD2	2.35	0.79
3:C:375:LYS:HG2	3:C:417:TYR:CE2	2.18	0.78
1:X:78:GLN:HE21	1:X:78:GLN:HA	1.49	0.77
3:Z:375:LYS:HG2	3:Z:417:TYR:CE2	2.19	0.77
1:A:83:THR:CG2	1:A:90:ASP:N	2.47	0.77
1:A:78:GLN:HE21	1:A:78:GLN:HA	1.48	0.76
1:A:13:LEU:CD1	1:A:72:SER:HB2	2.15	0.76
1:X:58:SER:HB2	1:X:81:GLU:OE2	1.87	0.75
2:B:61:GLN:O	2:B:63:HIS:N	2.15	0.74
3:Z:514:ARG:NH1	3:Z:515:SER:O	2.20	0.74
3:C:551:MET:HG2	3:C:555:GLU:HB2	1.69	0.73
4:K:12:DT:H2''	4:K:13:DT:OP2	1.89	0.72
3:C:514:ARG:HG2	3:C:515:SER:H	1.54	0.71
3:C:397:SER:HB3	4:K:5:DT:H3	1.55	0.71
2:Y:63:HIS:HB3	2:Y:64:PRO:CD	2.14	0.70
3:Z:451:ARG:HH11	3:Z:451:ARG:CG	2.02	0.69
3:C:448:MET:O	3:C:449:ALA:CB	2.41	0.69
4:L:2:DT:H2''	4:L:3:DT:OP1	1.91	0.69
1:A:2:GLU:OE1	1:A:2:GLU:HA	1.90	0.69
1:X:80:ARG:HE	1:X:80:ARG:HA	1.58	0.68
3:C:595:ARG:HH11	4:K:17:DT:H73	1.58	0.67
3:C:352:ARG:HH21	3:C:429:TYR:HA	1.59	0.67
3:C:451:ARG:HH11	3:C:451:ARG:CG	2.04	0.67
3:Z:352:ARG:HH21	3:Z:429:TYR:HA	1.60	0.66
3:C:442:GLY:O	4:K:8:DT:H5'	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ARG:HA	1:A:80:ARG:NE	2.11	0.64
1:A:15:GLN:HE22	1:X:15:GLN:HE22	1.43	0.64
3:Z:357:THR:OG1	3:Z:444:ALA:HB3	1.97	0.64
4:K:8:DT:H2'	4:K:9:DT:C6	2.33	0.64
2:Y:63:HIS:CB	2:Y:64:PRO:HD2	2.13	0.63
1:X:13:LEU:CD1	1:X:72:SER:HB2	2.29	0.63
1:A:13:LEU:HD13	1:A:72:SER:HB2	1.81	0.62
1:A:62:GLU:HB2	1:A:82:PHE:CZ	2.21	0.62
2:B:71:ASP:OD2	2:B:170:HIS:HD2	1.81	0.62
1:X:13:LEU:HD13	1:X:72:SER:HB2	1.81	0.62
3:C:200:ARG:HB3	3:C:252:VAL:HG22	1.82	0.62
2:B:170:HIS:O	2:B:174:THR:HB	2.00	0.60
3:C:214:ARG:HH12	4:K:2:DT:H4'	1.66	0.60
3:Z:358:LEU:HD22	3:Z:395:MET:HE2	1.82	0.60
3:Z:513:ASP:O	3:Z:514:ARG:HB2	2.00	0.60
3:Z:375:LYS:HE2	3:Z:417:TYR:OH	2.02	0.59
3:Z:447:ASN:HB2	3:Z:450:GLU:OE2	2.02	0.59
1:A:58:SER:HB2	1:A:81:GLU:OE2	2.02	0.59
1:X:2:GLU:HG2	2:Y:104:GLN:HB2	1.84	0.59
3:Z:460:GLU:HB2	3:Z:462:LEU:HD13	1.85	0.59
1:X:2:GLU:OE1	1:X:2:GLU:HA	2.03	0.59
2:Y:107:VAL:HB	2:Y:145:ILE:HB	1.85	0.59
3:C:267:PHE:HA	4:K:5:DT:H71	1.83	0.59
2:B:131:ARG:HG2	2:B:131:ARG:HH11	1.68	0.59
3:C:448:MET:O	3:C:449:ALA:HB3	2.02	0.59
3:C:397:SER:CB	4:K:5:DT:H3	2.16	0.58
1:X:9:ASN:C	1:X:9:ASN:HD22	2.11	0.58
3:Z:448:MET:O	3:Z:449:ALA:CB	2.50	0.58
3:Z:263:ALA:HA	3:Z:275:GLU:HG2	1.84	0.58
3:C:365:THR:O	3:C:368:THR:HB	2.04	0.58
1:X:9:ASN:HA	1:X:39:THR:HG21	1.86	0.58
3:C:551:MET:HG2	3:C:555:GLU:CB	2.34	0.58
3:Z:551:MET:HG2	3:Z:555:GLU:HB2	1.84	0.58
1:A:6:PRO:HG3	1:A:16:TYR:CE2	2.39	0.57
3:Z:365:THR:O	3:Z:368:THR:HB	2.04	0.57
2:B:130:VAL:HG21	2:B:150:MET:HE2	1.86	0.56
3:C:358:LEU:HD22	3:C:395:MET:HE2	1.87	0.56
2:Y:170:HIS:O	2:Y:174:THR:HB	2.05	0.56
3:Z:200:ARG:HB3	3:Z:252:VAL:HG22	1.88	0.56
1:A:21:VAL:CG2	1:A:74:PHE:HZ	2.18	0.56
3:C:292:ASP:OD1	3:C:292:ASP:N	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:VAL:HB	2:B:145:ILE:HB	1.88	0.56
3:C:460:GLU:HB2	3:C:462:LEU:HD13	1.88	0.56
1:A:37:MET:HE2	1:A:61:VAL:CG1	2.36	0.56
3:C:472:ASN:HB3	3:C:580:MET:CE	2.30	0.56
3:Z:302:ARG:HB2	3:Z:305:GLU:HG3	1.88	0.55
3:C:587:MET:SD	3:C:596:VAL:HG22	2.45	0.55
3:Z:498:LYS:CB	4:L:14:DT:H5''	2.34	0.55
1:X:5:THR:HG22	1:X:5:THR:O	2.07	0.55
1:X:21:VAL:CG2	1:X:74:PHE:HZ	2.18	0.55
2:Y:71:ASP:OD2	2:Y:170:HIS:HD2	1.90	0.55
1:A:13:LEU:HD13	1:A:72:SER:CB	2.37	0.55
3:Z:451:ARG:HG3	3:Z:451:ARG:NH1	1.98	0.54
3:C:261:ASN:ND2	3:C:277:THR:OG1	2.41	0.54
1:A:9:ASN:C	1:A:9:ASN:HD22	2.15	0.54
3:C:498:LYS:HB2	4:K:14:DT:H5''	1.90	0.54
1:X:1:MET:O	1:X:2:GLU:O	2.25	0.54
3:Z:448:MET:O	3:Z:449:ALA:HB3	2.08	0.54
1:A:59:THR:HB	1:A:83:THR:OG1	2.08	0.53
4:K:18:DT:H4'	4:K:19:DT:OP2	2.08	0.53
2:B:61:GLN:C	2:B:63:HIS:H	2.14	0.53
1:X:41:ASP:O	1:X:42:LEU:HB2	2.09	0.53
2:Y:54:ARG:NH1	2:Y:102:THR:O	2.41	0.53
3:Z:498:LYS:HB2	4:L:14:DT:C5'	2.33	0.53
1:A:9:ASN:HA	1:A:39:THR:HG21	1.91	0.53
2:Y:62:PRO:O	2:Y:63:HIS:HB2	2.09	0.53
3:Z:394:SER:HB2	3:Z:445:GLY:HA3	1.89	0.53
3:C:263:ALA:HA	3:C:275:GLU:HG2	1.90	0.52
1:X:58:SER:HB2	1:X:81:GLU:CD	2.34	0.52
3:Z:200:ARG:NH1	3:Z:294:PRO:O	2.42	0.52
1:A:13:LEU:CD1	1:A:72:SER:CB	2.87	0.52
3:C:302:ARG:HB2	3:C:305:GLU:HG3	1.90	0.52
3:Z:261:ASN:ND2	3:Z:277:THR:OG1	2.42	0.52
2:Y:61:GLN:HE21	2:Y:66:ALA:H	1.58	0.52
3:C:595:ARG:NH1	4:K:17:DT:H73	2.26	0.51
1:X:1:MET:O	1:X:2:GLU:C	2.54	0.51
2:Y:105:ILE:HD13	2:Y:145:ILE:HD13	1.92	0.51
3:Z:472:ASN:HB3	3:Z:580:MET:CE	2.36	0.51
1:A:81:GLU:O	1:A:82:PHE:HD2	1.93	0.51
3:C:375:LYS:HE2	3:C:417:TYR:OH	2.11	0.51
3:Z:551:MET:HG2	3:Z:555:GLU:CB	2.41	0.51
2:B:131:ARG:NH1	2:B:158:GLU:OE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:78:GLN:HE21	1:X:78:GLN:CA	2.22	0.51
3:Z:186:GLU:HB2	3:Z:228:SER:HB2	1.93	0.50
1:X:6:PRO:HG3	1:X:16:TYR:CE2	2.47	0.50
3:C:200:ARG:NH1	3:C:294:PRO:O	2.44	0.50
1:X:78:GLN:O	1:X:79:ILE:HG13	2.11	0.50
3:Z:455:VAL:HB	3:Z:533:THR:HB	1.93	0.50
2:B:54:ARG:NH1	2:B:102:THR:O	2.44	0.50
3:C:186:GLU:HB2	3:C:228:SER:HB2	1.93	0.50
3:C:335:SER:O	3:C:336:GLN:HB2	2.11	0.50
3:C:528:ASN:HD21	3:C:535:GLN:HG2	1.76	0.50
3:C:227:ASP:OD1	3:C:227:ASP:N	2.29	0.49
3:C:394:SER:HB2	3:C:445:GLY:HA3	1.94	0.49
3:Z:428:PRO:O	3:Z:429:TYR:HB2	2.12	0.49
3:Z:447:ASN:HB2	3:Z:450:GLU:CD	2.38	0.49
3:Z:335:SER:HB3	3:Z:337:ARG:HG3	1.94	0.49
3:Z:227:ASP:OD1	3:Z:227:ASP:N	2.36	0.48
3:C:428:PRO:O	3:C:429:TYR:HB2	2.12	0.48
3:Z:460:GLU:CB	3:Z:462:LEU:HD13	2.43	0.48
4:L:19:DT:H2''	4:L:20:DT:O5'	2.12	0.48
2:B:59:ALA:O	2:B:143:ARG:NH2	2.41	0.48
1:X:37:MET:HE2	1:X:61:VAL:CG1	2.43	0.48
1:X:76:ALA:HB1	1:X:79:ILE:HD11	1.96	0.48
3:Z:587:MET:HE1	3:Z:594:ALA:HB1	1.95	0.48
3:C:595:ARG:HH11	4:K:17:DT:C7	2.24	0.48
1:X:81:GLU:CD	1:X:82:PHE:N	2.72	0.48
2:Y:68:PHE:HZ	2:Y:138:SER:HB2	1.78	0.47
3:Z:451:ARG:CG	3:Z:451:ARG:NH1	2.70	0.47
1:A:78:GLN:HE21	1:A:78:GLN:CA	2.23	0.47
1:A:78:GLN:HA	1:A:78:GLN:NE2	2.24	0.47
1:A:81:GLU:CD	1:A:82:PHE:N	2.72	0.47
3:C:470:TYR:CE2	3:C:584:ARG:HB3	2.49	0.47
3:Z:507:TRP:O	3:Z:515:SER:HA	2.14	0.47
3:C:299:GLU:O	3:C:316:ASP:HB2	2.14	0.47
1:X:40:SER:HB2	1:X:97:GLU:HB2	1.95	0.47
1:A:81:GLU:C	1:A:82:PHE:CD2	2.92	0.47
3:Z:292:ASP:OD1	3:Z:292:ASP:N	2.33	0.47
3:Z:327:LEU:HD11	3:Z:364:GLU:HG2	1.97	0.47
3:C:460:GLU:CB	3:C:462:LEU:HD13	2.45	0.47
3:Z:470:TYR:CE2	3:Z:584:ARG:HB3	2.50	0.47
3:Z:528:ASN:HD21	3:Z:535:GLN:HG2	1.79	0.47
3:Z:263:ALA:HA	3:Z:275:GLU:CD	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:263:ALA:HA	3:C:275:GLU:CD	2.40	0.47
3:C:388:PHE:HD1	3:C:448:MET:CG	2.28	0.47
1:A:15:GLN:NE2	1:X:15:GLN:HE22	2.12	0.46
2:B:61:GLN:C	2:B:63:HIS:N	2.72	0.46
3:C:417:TYR:HA	3:C:421:GLY:HA3	1.97	0.46
3:Z:380:PHE:CZ	3:Z:401:MET:HE2	2.51	0.46
3:Z:453:THR:OG1	3:Z:455:VAL:HG12	2.15	0.46
3:C:327:LEU:HD11	3:C:364:GLU:HG2	1.96	0.46
3:Z:303:ILE:HG12	3:Z:348:ASP:OD2	2.16	0.46
3:Z:417:TYR:HA	3:Z:421:GLY:HA3	1.98	0.46
1:A:80:ARG:HE	1:A:80:ARG:CA	2.19	0.46
3:Z:498:LYS:HD2	4:L:14:DT:H4'	1.98	0.46
1:A:40:SER:HB2	1:A:97:GLU:HB2	1.98	0.46
3:C:451:ARG:HG3	3:C:451:ARG:NH1	2.03	0.46
3:C:242:ARG:NH1	3:C:280:ASN:HA	2.31	0.45
3:Z:320:ILE:HD13	3:Z:377:VAL:HG22	1.97	0.45
3:Z:333:LYS:HB2	4:L:7:DT:OP1	2.17	0.45
3:C:320:ILE:HD13	3:C:377:VAL:HG22	1.97	0.45
3:C:455:VAL:HB	3:C:533:THR:HB	1.97	0.45
3:C:488:THR:HG22	3:C:521:TYR:CE2	2.51	0.45
3:Z:299:GLU:O	3:Z:316:ASP:HB2	2.16	0.45
3:Z:491:ALA:HB3	3:Z:516:TYR:CD2	2.52	0.45
3:C:388:PHE:HD1	3:C:448:MET:HG2	1.81	0.45
4:L:3:DT:H2''	4:L:4:DT:O5'	2.16	0.45
2:Y:132:VAL:HG22	2:Y:150:MET:HG3	1.99	0.45
3:Z:607:ASP:C	3:Z:607:ASP:OD1	2.59	0.45
1:A:78:GLN:O	1:A:79:ILE:HG13	2.17	0.45
1:A:83:THR:HB	1:A:84:THR:H	1.33	0.45
3:Z:244:TYR:HB3	3:Z:245:PRO:HD3	1.99	0.45
3:C:597:ARG:CD	4:K:17:DT:O4	2.58	0.45
3:C:607:ASP:OD1	3:C:607:ASP:C	2.60	0.44
3:Z:578:MET:HE3	3:Z:578:MET:HB2	1.87	0.44
3:C:327:LEU:CD1	3:C:364:GLU:HA	2.47	0.44
3:Z:468:PRO:HB3	3:Z:586:LYS:HG2	2.00	0.44
1:A:82:PHE:CE2	2:B:156:TYR:CD1	3.06	0.44
3:C:602:ARG:HH21	3:C:604:ALA:CB	2.23	0.44
2:Y:62:PRO:O	2:Y:63:HIS:CB	2.64	0.44
3:Z:394:SER:CB	3:Z:445:GLY:HA3	2.47	0.44
1:X:78:GLN:HA	1:X:78:GLN:NE2	2.25	0.44
3:Z:263:ALA:HA	3:Z:275:GLU:CG	2.47	0.44
1:X:2:GLU:OE1	1:X:2:GLU:CA	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:HIS:O	2:B:64:PRO:C	2.61	0.44
3:C:375:LYS:HG2	3:C:417:TYR:HE2	1.78	0.43
1:X:21:VAL:CG2	1:X:74:PHE:CZ	3.01	0.43
2:Y:125:ARG:HH11	2:Y:125:ARG:HB2	1.83	0.43
1:A:81:GLU:CD	1:A:82:PHE:H	2.26	0.43
3:C:208:ARG:HH21	4:K:4:DT:P	2.41	0.43
3:C:219:LEU:C	3:C:219:LEU:HD12	2.44	0.43
3:C:280:ASN:HA	3:C:280:ASN:HD22	1.62	0.43
2:Y:71:ASP:OD2	2:Y:170:HIS:CD2	2.70	0.43
1:A:92:ASP:C	1:A:92:ASP:OD1	2.60	0.43
1:X:83:THR:HG22	1:X:84:THR:H	1.84	0.42
2:Y:130:VAL:HG21	2:Y:150:MET:HE2	2.00	0.42
3:C:379:ALA:O	3:C:401:MET:HA	2.19	0.42
3:C:595:ARG:HD2	4:K:17:DT:H72	2.01	0.42
1:X:5:THR:HG22	1:X:22:ARG:HB2	2.00	0.42
3:Z:327:LEU:CD1	3:Z:364:GLU:HA	2.49	0.42
2:B:131:ARG:HG2	2:B:131:ARG:NH1	2.31	0.42
3:C:514:ARG:HG2	3:C:515:SER:N	2.27	0.42
2:Y:80:PHE:HA	2:Y:162:HIS:CE1	2.53	0.42
3:Z:525:LEU:O	3:Z:539:SER:HA	2.19	0.42
4:L:3:DT:O2	4:L:4:DT:H71	2.20	0.42
2:B:139:PHE:C	2:B:140:GLN:HG3	2.43	0.42
1:X:82:PHE:HB2	1:X:83:THR:H	1.54	0.42
3:C:327:LEU:HD12	3:C:364:GLU:HA	2.02	0.42
3:Z:267:PHE:HA	4:L:5:DT:C7	2.39	0.42
2:B:94:VAL:HG23	2:B:111:LEU:HD21	2.01	0.42
1:A:37:MET:HE2	1:A:61:VAL:HG13	2.02	0.42
3:C:457:VAL:HA	3:C:462:LEU:HD22	2.02	0.42
3:Z:352:ARG:NH2	3:Z:429:TYR:HA	2.32	0.42
3:C:244:TYR:HB3	3:C:245:PRO:HD3	2.02	0.42
3:Z:389:GLY:HA2	3:Z:431:ASN:H	1.85	0.42
2:Y:94:VAL:HG23	2:Y:111:LEU:HD21	2.01	0.42
3:Z:233:ALA:HA	3:Z:276:ILE:O	2.19	0.41
3:C:357:THR:OG1	3:C:444:ALA:HB3	2.19	0.41
3:Z:384:LYS:HE3	3:Z:445:GLY:O	2.20	0.41
1:A:41:ASP:O	1:A:42:LEU:HB2	2.20	0.41
2:B:81:VAL:HA	2:B:130:VAL:O	2.20	0.41
1:X:84:THR:HG22	1:X:85:VAL:H	1.85	0.41
1:X:92:ASP:OD1	1:X:92:ASP:C	2.63	0.41
3:Z:587:MET:CE	3:Z:594:ALA:HB1	2.51	0.41
1:X:6:PRO:HB2	1:X:8:ILE:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:366:PHE:HB3	3:Z:367:PRO:HD3	2.03	0.41
1:A:21:VAL:CG2	1:A:74:PHE:CZ	3.01	0.41
1:A:95:LEU:O	1:A:95:LEU:HD12	2.20	0.41
3:C:263:ALA:HA	3:C:275:GLU:CG	2.51	0.41
2:B:131:ARG:HH11	2:B:131:ARG:CG	2.32	0.40
3:C:322:ASP:HA	3:C:375:LYS:HE3	2.03	0.40
1:X:83:THR:HG23	1:X:90:ASP:HA	2.03	0.40
4:L:13:DT:H2'	4:L:14:DT:H72	2.04	0.40
2:B:154:ILE:HD12	3:C:608:PHE:HE1	1.86	0.40
2:B:132:VAL:HG22	2:B:150:MET:HE3	2.04	0.40
3:C:380:PHE:HB3	3:C:383:VAL:HG21	2.04	0.40
2:Y:136:LEU:O	2:Y:137:LYS:HG2	2.21	0.40

There are no symmetry-related clashes.

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	104/114 (91%)	92 (88%)	10 (10%)	2 (2%)	6	22
1	X	104/114 (91%)	93 (89%)	9 (9%)	2 (2%)	6	22
2	B	118/136 (87%)	111 (94%)	3 (2%)	4 (3%)	3	11
2	Y	118/136 (87%)	111 (94%)	6 (5%)	1 (1%)	16	44
3	C	429/444 (97%)	399 (93%)	21 (5%)	9 (2%)	5	20
3	Z	429/444 (97%)	398 (93%)	25 (6%)	6 (1%)	9	30
All	All	1302/1388 (94%)	1204 (92%)	74 (6%)	24 (2%)	6	23

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	THR

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Mol	Chain	Res	Type
2	B	63	HIS
2	B	65	ASP
3	C	216	GLU
3	C	336	GLN
3	C	449	ALA
3	Z	449	ALA
3	C	448	MET
1	X	2	GLU
3	C	212	ASN
3	Z	514	ARG
2	B	62	PRO
2	B	64	PRO
3	C	237	ASN
3	C	429	TYR
3	C	591	ASN
1	X	82	PHE
3	Z	420	ASP
3	Z	429	TYR
3	Z	593	THR
3	C	420	ASP
2	Y	63	HIS
3	Z	237	ASN
1	A	71	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	96/101 (95%)	81 (84%)	15 (16%)	2	9
1	X	96/101 (95%)	77 (80%)	19 (20%)	1	5
2	B	107/118 (91%)	94 (88%)	13 (12%)	5	16
2	Y	107/118 (91%)	94 (88%)	13 (12%)	5	16
3	C	370/374 (99%)	336 (91%)	34 (9%)	8	27
3	Z	370/374 (99%)	337 (91%)	33 (9%)	9	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1146/1186 (97%)	1019 (89%)	127 (11%)	6 20

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	3	LYS
1	A	9	ASN
1	A	47	ILE
1	A	52	ASP
1	A	59	THR
1	A	66	LYS
1	A	69	ASP
1	A	74	PHE
1	A	78	GLN
1	A	80	ARG
1	A	83	THR
1	A	84	THR
1	A	93	LEU
1	A	109	LEU
2	B	63	HIS
2	B	74	GLU
2	B	98	VAL
2	B	106	GLU
2	B	107	VAL
2	B	123	GLU
2	B	125	ARG
2	B	131	ARG
2	B	140	GLN
2	B	150	MET
2	B	173	VAL
2	B	174	THR
2	B	175	ARG
3	C	198	LYS
3	C	213	GLN
3	C	222	VAL
3	C	227	ASP
3	C	249	GLU
3	C	257	LYS
3	C	288	THR
3	C	291	THR
3	C	292	ASP

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Mol	Chain	Res	Type
3	C	315	CYS
3	C	330	ILE
3	C	355	LYS
3	C	362	THR
3	C	372	VAL
3	C	381	LYS
3	C	398	SER
3	C	400	THR
3	C	401	MET
3	C	406	ASP
3	C	407	ILE
3	C	429	TYR
3	C	451	ARG
3	C	462	LEU
3	C	478	VAL
3	C	483	GLU
3	C	485	LEU
3	C	520	GLU
3	C	524	ILE
3	C	535	GLN
3	C	556	LEU
3	C	586	LYS
3	C	589	THR
3	C	593	THR
3	C	610	LYS
1	X	1	MET
1	X	2	GLU
1	X	3	LYS
1	X	9	ASN
1	X	39	THR
1	X	47	ILE
1	X	59	THR
1	X	66	LYS
1	X	69	ASP
1	X	73	SER
1	X	74	PHE
1	X	78	GLN
1	X	80	ARG
1	X	82	PHE
1	X	83	THR
1	X	84	THR
1	X	90	ASP

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Mol	Chain	Res	Type
1	X	93	LEU
1	X	109	LEU
2	Y	74	GLU
2	Y	98	VAL
2	Y	106	GLU
2	Y	107	VAL
2	Y	123	GLU
2	Y	125	ARG
2	Y	140	GLN
2	Y	142	ARG
2	Y	145	ILE
2	Y	146	SER
2	Y	173	VAL
2	Y	174	THR
2	Y	175	ARG
3	Z	198	LYS
3	Z	213	GLN
3	Z	222	VAL
3	Z	227	ASP
3	Z	249	GLU
3	Z	257	LYS
3	Z	288	THR
3	Z	291	THR
3	Z	292	ASP
3	Z	315	CYS
3	Z	328	SER
3	Z	330	ILE
3	Z	339	VAL
3	Z	355	LYS
3	Z	362	THR
3	Z	372	VAL
3	Z	381	LYS
3	Z	398	SER
3	Z	400	THR
3	Z	401	MET
3	Z	406	ASP
3	Z	407	ILE
3	Z	429	TYR
3	Z	451	ARG
3	Z	462	LEU
3	Z	478	VAL
3	Z	483	GLU

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Mol	Chain	Res	Type
3	Z	485	LEU
3	Z	520	GLU
3	Z	535	GLN
3	Z	556	LEU
3	Z	586	LYS
3	Z	610	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	44	ASN
1	A	75	GLN
1	A	78	GLN
2	B	93	ASN
2	B	104	GLN
2	B	109	GLN
2	B	170	HIS
3	C	192	GLN
3	C	223	ASN
3	C	261	ASN
3	C	266	GLN
3	C	280	ASN
3	C	313	GLN
3	C	351	ASN
3	C	528	ASN
3	C	557	HIS
1	X	9	ASN
1	X	15	GLN
1	X	44	ASN
1	X	78	GLN
2	Y	61	GLN
2	Y	104	GLN
2	Y	109	GLN
2	Y	149	HIS
2	Y	170	HIS
3	Z	209	HIS
3	Z	261	ASN
3	Z	266	GLN
3	Z	280	ASN
3	Z	313	GLN
3	Z	351	ASN

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Mol	Chain	Res	Type
3	Z	369	ASN
3	Z	528	ASN
3	Z	557	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	108/114 (94%)	-0.22	1 (0%) 81 74	28, 47, 87, 108	0
1	X	108/114 (94%)	-0.09	4 (3%) 45 36	28, 54, 94, 125	0
2	B	122/136 (89%)	-0.43	1 (0%) 82 75	22, 45, 96, 120	0
2	Y	122/136 (89%)	-0.42	1 (0%) 82 75	24, 46, 87, 120	0
3	C	433/444 (97%)	-0.11	2 (0%) 87 82	28, 68, 121, 150	0
3	Z	433/444 (97%)	-0.05	3 (0%) 84 77	26, 67, 122, 172	0
4	K	25/62 (40%)	0.78	2 (8%) 18 13	65, 119, 165, 194	0
4	L	20/62 (32%)	0.77	0 100 100	79, 128, 166, 180	0
All	All	1371/1512 (90%)	-0.13	14 (1%) 79 72	22, 62, 121, 194	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Z	448	MET	4.5
3	Z	422	ALA	3.6
1	X	71	GLY	2.8
1	X	32	GLY	2.6
3	C	590	PHE	2.4
4	K	21	DT	2.3
3	Z	330	ILE	2.2
2	B	154	ILE	2.2
3	C	430	THR	2.2
4	K	22	DT	2.2
1	X	80	ARG	2.1
1	A	71	GLY	2.1
2	Y	140	GLN	2.0
1	X	1	MET	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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	C	701	1/1	0.99	0.03	72,72,72,72	0
5	ZN	Z	701	1/1	0.99	0.03	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.