Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2014 – 04:56 AM GMT

PDB ID : 3WI6

Title : Crystal structure of MAPKAP Kinase-2 (MK2) in complex with non-selective inhibitor

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Deposited on : 2013-09-06

Resolution : 2.99 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683
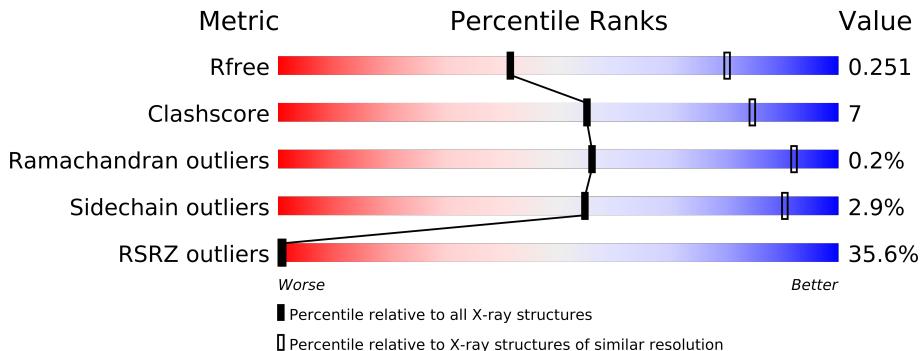
1 Overall quality at a glance ⓘ
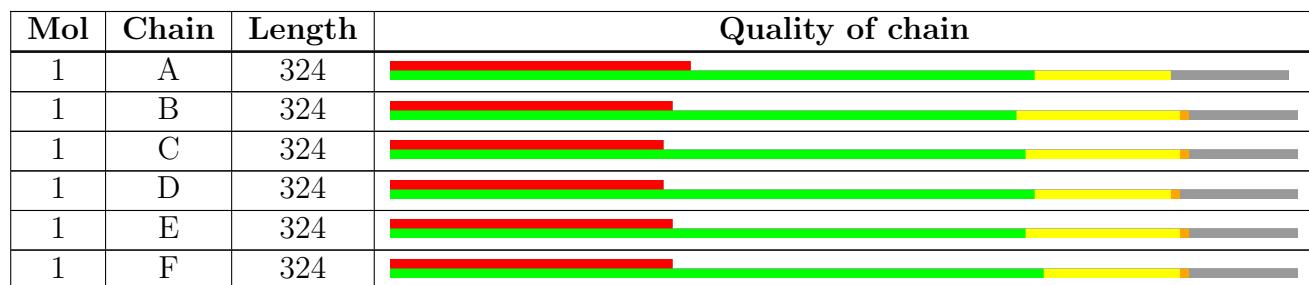
The reported resolution of this entry is 2.99 Å.

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	Percentile Ranks	Value
Rfree		0.251
Clashscore		7
Ramachandran outliers		0.2%
Sidechain outliers		2.9%
RSRZ outliers		35.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	324	
1	B	324	
1	C	324	
1	D	324	
1	E	324	
1	F	324	

2 Entry composition ⓘ
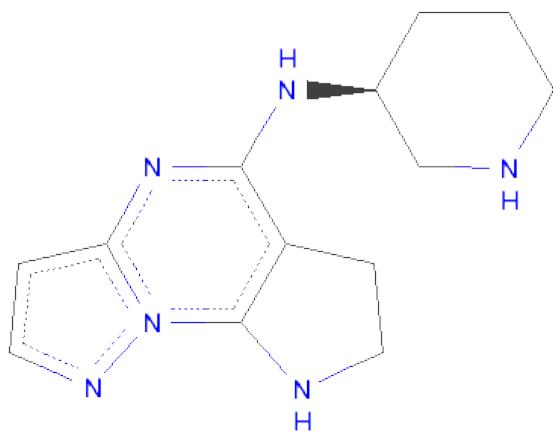
There are 2 unique types of molecules in this entry. The entry contains 13553 atoms, of which 0 are hydrogen and 0 are deuterium.

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 MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2233	1429	380	407	17			
1	B	283	Total	C	N	O	S	0	0	0
			2241	1433	381	410	17			
1	C	283	Total	C	N	O	S	0	0	0
			2237	1431	381	408	17			
1	D	282	Total	C	N	O	S	0	0	0
			2237	1431	380	409	17			
1	E	283	Total	C	N	O	S	0	0	0
			2249	1439	382	411	17			
1	F	283	Total	C	N	O	S	0	0	0
			2242	1434	382	409	17			

- Molecule 2 is N-[(3S)-PIPERIDIN-3-YL]-7,8-DIHYDRO-6H-PYRAZOLO[1,5-A]PYRROLO[3,2-E]PYRIMIDIN-5-AMINE (three-letter code: YRZ) (formula: $C_{13}H_{18}N_6$).
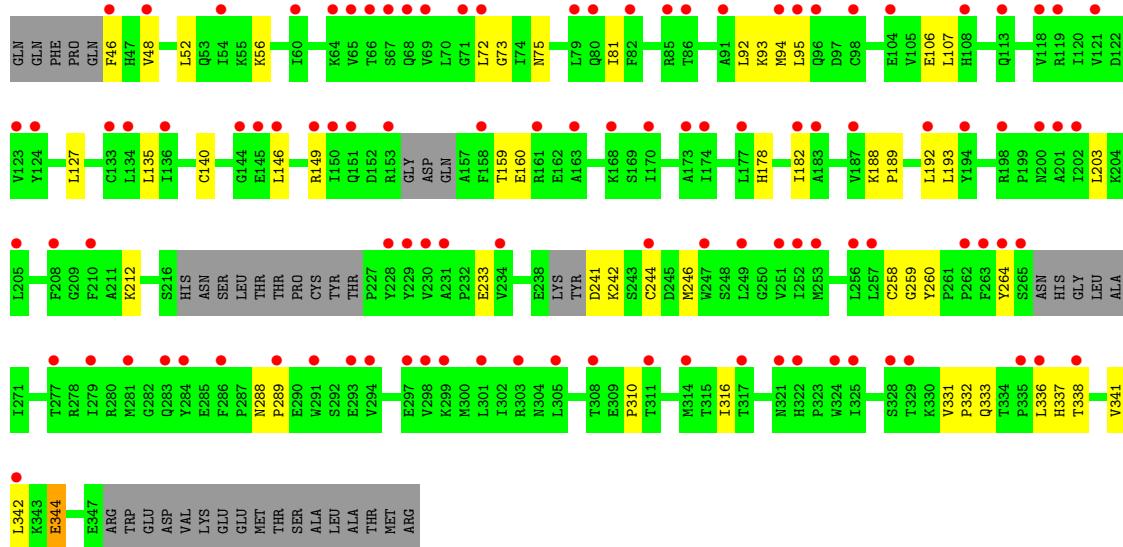
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 19	C 13	N 6	0	0
2	B	1	Total 19	C 13	N 6	0	0
2	C	1	Total 19	C 13	N 6	0	0
2	D	1	Total 19	C 13	N 6	0	0
2	E	1	Total 19	C 13	N 6	0	0
2	F	1	Total 19	C 13	N 6	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
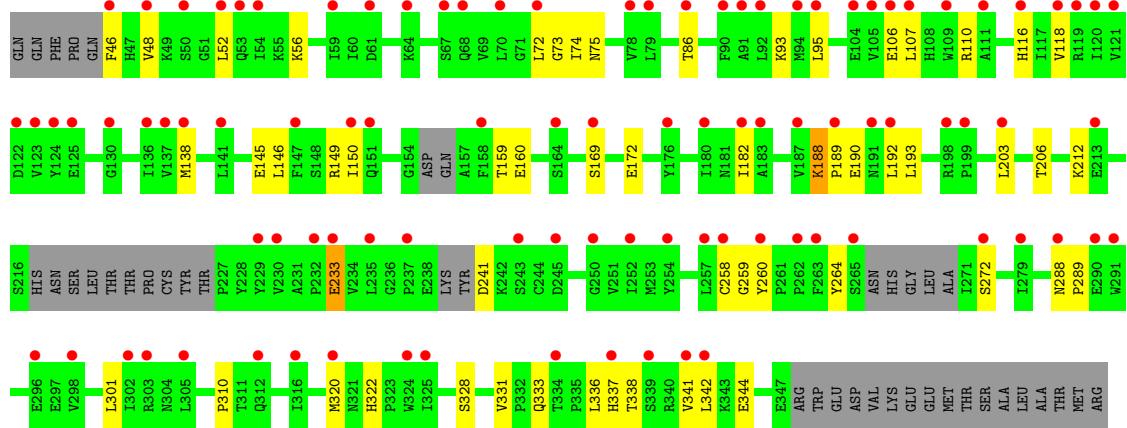
- Molecule 1: MAP kinase-activated protein kinase 2

Chain A:

- Molecule 1: MAP kinase-activated protein kinase 2
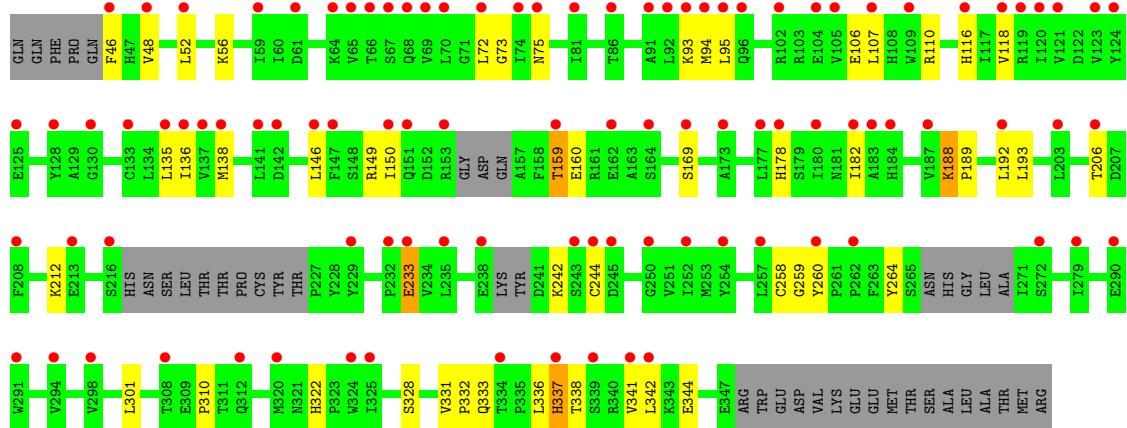
Chain B:

● Molecule 1: MAP kinase-activated protein kinase 2
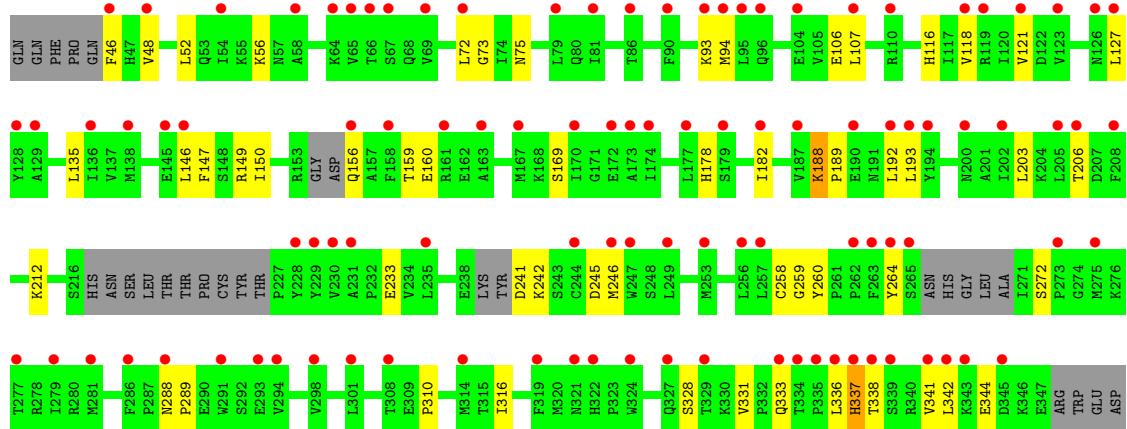
Chain C:

● Molecule 1: MAP kinase-activated protein kinase 2

Chain D:

● Molecule 1: MAP kinase-activated protein kinase 2
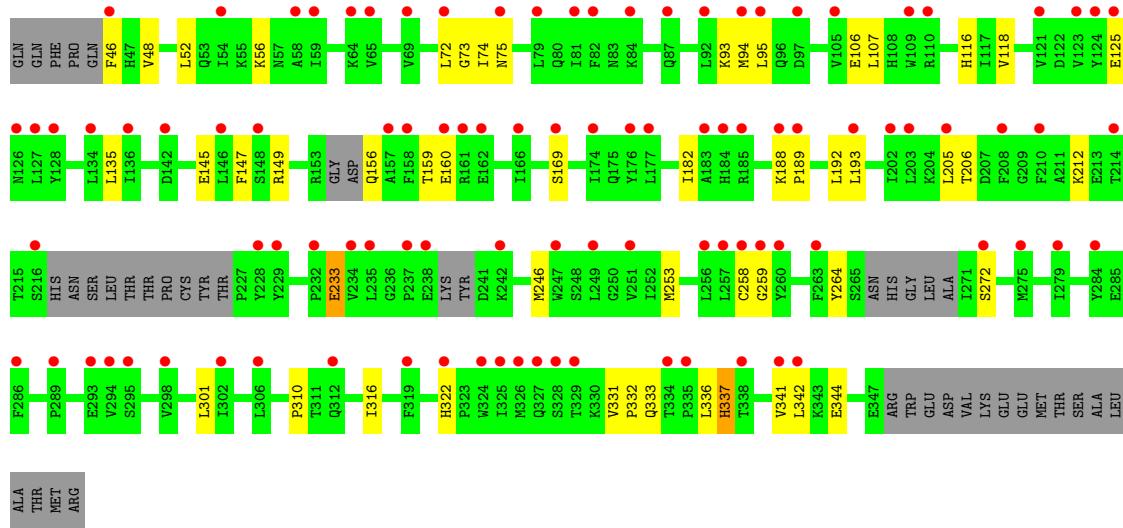
Chain E:

VAL LYS GLU GLU MET THR SER ALA LEU ALA THR MET ARG

• Molecule 1: MAP kinase-activated protein kinase 2

Chain F:

ALA THR MET ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	180.06Å 179.68Å 254.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.99 45.02 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.99) 99.0 (45.02-2.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.28 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.240 , 0.283 0.233 , 0.251	Depositor DCC
R_{free} test set	4136 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	82.4	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.3	EDS
Estimated twinning fraction	0.466 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.467 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.469 for k,h,-l 0.459 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.467 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k	Xtriage
L-test for twinning	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Outliers	0 of 82788 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13553	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5　Model quality ⓘ

5.1　Standard geometry ⓘ

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

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	0.92	2/2280 (0.1%)	0.75	0/3083
1	B	0.91	0/2288	0.77	1/3093 (0.0%)
1	C	0.90	0/2284	0.76	0/3088
1	D	0.91	1/2284 (0.0%)	0.76	0/3088
1	E	0.89	0/2296	0.76	2/3104 (0.1%)
1	F	0.90	1/2289 (0.0%)	0.77	1/3095 (0.0%)
All	All	0.91	4/13721 (0.0%)	0.76	4/18551 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	CYS	CB-SG	-5.23	1.73	1.81
1	A	140	CYS	CB-SG	-5.14	1.73	1.81
1	D	244	CYS	CB-SG	-5.03	1.73	1.81
1	F	125	GLU	CD-OE1	5.03	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	245	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	B	245	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	E	121	VAL	CB-CA-C	-5.18	101.56	111.40
1	F	205	LEU	CB-CG-CD2	-5.12	102.30	111.00

There are no chirality outliers.

There are no planarity outliers.

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5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2233	0	2209	28	0
1	B	2241	0	2216	35	0
1	C	2237	0	2212	35	0
1	D	2237	0	2213	31	0
1	E	2249	0	2230	29	0
1	F	2242	0	2217	29	0
2	A	19	0	0	0	0
2	B	19	0	0	0	0
2	C	19	0	0	0	0
2	D	19	0	0	0	0
2	E	19	0	0	0	0
2	F	19	0	0	0	0
All	All	13553	0	13297	179	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (179) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:337:HIS:O	1:C:341:VAL:HG23	1.81	0.81
1:E:337:HIS:O	1:E:341:VAL:HG23	1.83	0.79
1:A:337:HIS:O	1:A:341:VAL:HG23	1.83	0.78
1:D:337:HIS:O	1:D:341:VAL:HG23	1.85	0.77
1:D:159:THR:HG22	1:D:333:GLN:O	1.86	0.74
1:A:159:THR:HG22	1:A:333:GLN:O	1.87	0.73
1:E:159:THR:HG22	1:E:333:GLN:O	1.90	0.70
1:B:337:HIS:O	1:B:341:VAL:HG23	1.95	0.67
1:D:52:LEU:HD23	1:D:106:GLU:OE2	1.98	0.64
1:E:344:GLU:N	1:E:344:GLU:OE2	2.31	0.64
1:D:344:GLU:OE2	1:D:344:GLU:N	2.31	0.63
1:B:72:LEU:HD23	1:B:73:GLY:N	2.13	0.63
1:A:344:GLU:OE2	1:A:344:GLU:N	2.33	0.61
1:B:160:GLU:HA	1:B:336:LEU:HD21	1.84	0.60
1:B:301:LEU:HD13	1:B:322:HIS:CD2	2.37	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:192:LEU:C	1:B:193:LEU:HD23	2.23	0.59
1:C:110:ARG:HG2	1:E:127:LEU:HD11	1.84	0.59
1:F:301:LEU:HD13	1:F:322:HIS:CD2	2.37	0.59
1:D:72:LEU:HD23	1:D:73:GLY:N	2.18	0.59
1:A:127:LEU:HD11	1:D:110:ARG:HG2	1.83	0.59
1:C:344:GLU:N	1:C:344:GLU:OE2	2.35	0.59
1:C:192:LEU:C	1:C:193:LEU:HD23	2.23	0.59
1:B:344:GLU:OE2	1:B:344:GLU:N	2.36	0.58
1:E:146:LEU:HD13	1:E:203:LEU:HD21	1.85	0.58
1:F:192:LEU:C	1:F:193:LEU:HD23	2.24	0.58
1:C:160:GLU:HA	1:C:336:LEU:HD21	1.85	0.58
1:D:160:GLU:HA	1:D:336:LEU:HD21	1.86	0.58
1:C:146:LEU:O	1:C:150:ILE:HD13	2.04	0.58
1:F:337:HIS:O	1:F:341:VAL:HG23	2.04	0.57
1:D:107:LEU:HD22	1:D:182:ILE:HG12	1.86	0.57
1:A:258:CYS:SG	1:A:259:GLY:N	2.78	0.57
1:A:94:MET:HG2	1:A:135:LEU:HD22	1.85	0.57
1:C:301:LEU:HD13	1:C:322:HIS:CD2	2.38	0.57
1:F:344:GLU:OE2	1:F:344:GLU:N	2.37	0.56
1:F:258:CYS:SG	1:F:259:GLY:N	2.78	0.56
1:C:52:LEU:HD23	1:C:106:GLU:OE2	2.06	0.56
1:D:75:ASN:HB3	1:D:95:LEU:HD22	1.88	0.55
1:E:94:MET:HG2	1:E:135:LEU:HD22	1.88	0.55
1:B:178:HIS:CE1	1:B:242:LYS:HB2	2.42	0.54
1:D:146:LEU:O	1:D:150:ILE:HD13	2.08	0.54
1:C:146:LEU:HD13	1:C:203:LEU:HD21	1.90	0.54
1:C:107:LEU:HD22	1:C:182:ILE:HG12	1.89	0.54
1:A:160:GLU:HA	1:A:336:LEU:HD21	1.90	0.54
1:B:159:THR:HG22	1:B:333:GLN:O	2.07	0.54
1:C:338:THR:O	1:C:342:LEU:HB2	2.08	0.54
1:F:107:LEU:HD22	1:F:182:ILE:HG12	1.89	0.54
1:F:159:THR:HG22	1:F:333:GLN:O	2.07	0.53
1:D:72:LEU:HD23	1:D:73:GLY:H	1.72	0.53
1:A:310:PRO:HG3	1:C:233:GLU:HG2	1.89	0.53
1:F:72:LEU:HD23	1:F:73:GLY:N	2.24	0.53
1:F:75:ASN:HB3	1:F:95:LEU:HD22	1.91	0.53
1:B:94:MET:HG2	1:B:135:LEU:HD22	1.89	0.53
1:B:107:LEU:HD22	1:B:182:ILE:HG12	1.90	0.53
1:F:193:LEU:N	1:F:193:LEU:HD23	2.24	0.53
1:B:193:LEU:HD23	1:B:193:LEU:N	2.23	0.52
1:C:72:LEU:HD23	1:C:73:GLY:H	1.74	0.52
1:C:258:CYS:SG	1:C:260:TYR:CE2	3.02	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:75:ASN:HB3	1:C:95:LEU:HD22	1.92	0.52
1:B:258:CYS:SG	1:B:259:GLY:N	2.84	0.51
1:D:328:SER:O	1:D:331:VAL:HG12	2.11	0.51
1:A:72:LEU:HD23	1:A:73:GLY:H	1.76	0.51
1:C:46:PHE:CE1	1:C:48:VAL:HG21	2.46	0.50
1:F:147:PHE:HB3	1:F:342:LEU:HD21	1.92	0.50
1:F:94:MET:HG2	1:F:135:LEU:HD22	1.94	0.50
1:A:188:LYS:HB2	1:A:189:PRO:CD	2.42	0.50
1:F:246:MET:HE1	1:F:316:ILE:HA	1.94	0.50
1:E:258:CYS:SG	1:E:259:GLY:N	2.85	0.49
1:A:75:ASN:HD22	1:A:93:LYS:CE	2.25	0.49
1:E:233:GLU:HG2	1:F:310:PRO:HG3	1.93	0.49
1:D:94:MET:HG2	1:D:135:LEU:HD22	1.93	0.49
1:F:72:LEU:HD23	1:F:73:GLY:H	1.77	0.49
1:E:75:ASN:HD22	1:E:93:LYS:HE3	1.78	0.49
1:B:52:LEU:HD23	1:B:106:GLU:OE2	2.13	0.49
1:E:46:PHE:CE1	1:E:48:VAL:HG21	2.47	0.49
1:F:160:GLU:HA	1:F:336:LEU:HD21	1.94	0.49
1:B:46:PHE:CE1	1:B:48:VAL:HG21	2.48	0.49
1:D:178:HIS:CE1	1:D:242:LYS:HB2	2.47	0.49
1:D:310:PRO:HG3	1:F:233:GLU:HG2	1.96	0.48
1:C:159:THR:HG22	1:C:333:GLN:O	2.12	0.48
1:D:301:LEU:HD13	1:D:322:HIS:CD2	2.49	0.48
1:F:253:MET:HE1	1:F:301:LEU:CD2	2.44	0.48
1:E:52:LEU:HD23	1:E:106:GLU:OE2	2.14	0.48
1:D:258:CYS:SG	1:D:259:GLY:N	2.87	0.47
1:D:233:GLU:HG2	1:E:310:PRO:HG3	1.95	0.47
1:C:72:LEU:HD23	1:C:73:GLY:N	2.30	0.47
1:B:93:LYS:HD3	1:B:138:MET:HE1	1.96	0.47
1:A:178:HIS:CE1	1:A:242:LYS:HB2	2.50	0.47
1:C:258:CYS:SG	1:C:259:GLY:N	2.87	0.47
1:B:75:ASN:HD22	1:B:93:LYS:HE3	1.79	0.47
1:B:233:GLU:HG2	1:C:310:PRO:HG3	1.96	0.47
1:E:107:LEU:HD22	1:E:182:ILE:HG12	1.95	0.47
1:C:75:ASN:HD22	1:C:93:LYS:HE3	1.80	0.47
1:C:188:LYS:HB2	1:C:189:PRO:CD	2.45	0.47
1:A:46:PHE:CE1	1:A:48:VAL:HG21	2.50	0.47
1:B:188:LYS:HB2	1:B:189:PRO:CD	2.46	0.46
1:D:116:HIS:CE1	1:D:169:SER:HB2	2.50	0.46
1:B:338:THR:O	1:B:342:LEU:HB2	2.15	0.46
1:B:146:LEU:HD13	1:B:203:LEU:HD21	1.98	0.46
1:A:192:LEU:C	1:A:193:LEU:HD23	2.36	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:338:THR:O	1:D:342:LEU:HB2	2.16	0.46
1:B:149:ARG:NH2	1:B:198:ARG:O	2.49	0.46
1:E:160:GLU:HA	1:E:336:LEU:HD21	1.97	0.46
1:A:233:GLU:HG2	1:B:310:PRO:HG3	1.98	0.46
1:C:328:SER:O	1:C:331:VAL:HG12	2.16	0.46
1:B:174:ILE:HD11	1:B:187:VAL:HG21	1.97	0.45
1:C:93:LYS:HD3	1:C:138:MET:HE1	1.97	0.45
1:D:192:LEU:C	1:D:193:LEU:HD23	2.37	0.45
1:E:178:HIS:CE1	1:E:242:LYS:HB2	2.52	0.45
1:E:338:THR:O	1:E:342:LEU:HB2	2.17	0.45
1:F:46:PHE:CE1	1:F:48:VAL:HG21	2.52	0.45
1:A:246:MET:HE1	1:A:316:ILE:HA	1.98	0.45
1:B:328:SER:O	1:B:331:VAL:HG12	2.17	0.45
1:F:253:MET:HE1	1:F:301:LEU:HD21	1.99	0.44
1:A:146:LEU:HD13	1:A:203:LEU:HD21	1.99	0.44
1:E:192:LEU:C	1:E:193:LEU:HD23	2.38	0.44
1:E:258:CYS:SG	1:E:260:TYR:CE2	3.07	0.44
1:A:75:ASN:HD22	1:A:93:LYS:HE3	1.82	0.44
1:F:52:LEU:HD23	1:F:106:GLU:OE2	2.17	0.44
1:A:75:ASN:HB3	1:A:95:LEU:HD22	2.00	0.44
1:C:172:GLU:HG3	1:C:320:MET:HE1	2.00	0.44
1:B:116:HIS:CE1	1:B:169:SER:HB2	2.53	0.44
1:C:160:GLU:CA	1:C:336:LEU:HD21	2.47	0.43
1:F:74:ILE:H	1:F:74:ILE:HD12	1.83	0.43
1:E:188:LYS:HB2	1:E:189:PRO:CD	2.47	0.43
1:D:258:CYS:SG	1:D:260:TYR:CE2	3.06	0.43
1:E:147:PHE:HB3	1:E:342:LEU:HD21	2.00	0.43
1:C:288:ASN:HB3	1:C:289:PRO:HA	2.01	0.43
1:C:116:HIS:CE1	1:C:169:SER:HB2	2.53	0.43
1:C:74:ILE:H	1:C:74:ILE:HD12	1.83	0.43
1:F:75:ASN:HD22	1:F:93:LYS:HE3	1.84	0.43
1:B:46:PHE:CE1	1:B:48:VAL:CG2	3.02	0.43
1:D:188:LYS:HB2	1:D:189:PRO:CD	2.48	0.43
1:B:258:CYS:SG	1:B:260:TYR:CE2	3.12	0.43
1:C:190:GLU:OE1	1:C:190:GLU:N	2.49	0.43
1:A:81:ILE:HD13	1:A:92:LEU:HB2	2.00	0.43
1:A:288:ASN:HB3	1:A:289:PRO:HA	1.99	0.43
1:D:331:VAL:HG23	1:D:332:PRO:HD2	2.01	0.42
1:C:46:PHE:CE1	1:C:48:VAL:CG2	3.02	0.42
1:E:246:MET:HE1	1:E:316:ILE:HA	2.00	0.42
1:F:145:GLU:HA	1:F:193:LEU:HD22	2.00	0.42
1:A:107:LEU:HD22	1:A:182:ILE:HG12	2.00	0.42

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:118:VAL:HB	1:D:206:THR:HG22	2.00	0.42
1:D:93:LYS:HD3	1:D:138:MET:HE1	2.01	0.42
1:E:46:PHE:CE1	1:E:48:VAL:CG2	3.03	0.42
1:B:75:ASN:HB3	1:B:95:LEU:HD22	2.00	0.42
1:D:136:ILE:HG21	1:D:138:MET:HE2	2.01	0.42
1:D:46:PHE:CE1	1:D:48:VAL:HG21	2.54	0.42
1:D:160:GLU:CA	1:D:336:LEU:HD21	2.47	0.42
1:E:116:HIS:CE1	1:E:169:SER:HB2	2.55	0.42
1:D:159:THR:HG21	1:D:333:GLN:HB3	2.02	0.42
1:F:118:VAL:HB	1:F:206:THR:HG22	2.02	0.42
1:B:74:ILE:H	1:B:74:ILE:HD12	1.85	0.41
1:C:145:GLU:HA	1:C:193:LEU:HD22	2.01	0.41
1:E:146:LEU:HD13	1:E:203:LEU:CD2	2.49	0.41
1:E:72:LEU:HD23	1:E:73:GLY:H	1.85	0.41
1:A:258:CYS:SG	1:A:260:TYR:CE2	3.10	0.41
1:E:328:SER:O	1:E:331:VAL:HG12	2.20	0.41
1:E:118:VAL:HB	1:E:206:THR:HG22	2.02	0.41
1:D:188:LYS:HB2	1:D:189:PRO:HD2	2.01	0.41
1:A:338:THR:O	1:A:342:LEU:HB2	2.20	0.41
1:F:46:PHE:CE1	1:F:48:VAL:CG2	3.04	0.41
1:A:52:LEU:HD23	1:A:106:GLU:OE2	2.21	0.41
1:F:331:VAL:HG23	1:F:332:PRO:HD2	2.03	0.41
1:F:188:LYS:HB2	1:F:189:PRO:CD	2.51	0.41
1:B:72:LEU:HD23	1:B:73:GLY:H	1.84	0.41
1:C:193:LEU:HD23	1:C:193:LEU:N	2.35	0.41
1:B:192:LEU:HD21	1:B:205:LEU:HD13	2.02	0.41
1:A:331:VAL:HG23	1:A:332:PRO:HD2	2.03	0.41
1:E:288:ASN:HB3	1:E:289:PRO:HA	2.02	0.41
1:B:147:PHE:HB3	1:B:342:LEU:HD21	2.03	0.41
1:B:146:LEU:O	1:B:150:ILE:HD13	2.21	0.41
1:F:116:HIS:CE1	1:F:169:SER:HB2	2.56	0.41
1:E:146:LEU:O	1:E:150:ILE:HD13	2.21	0.41
1:A:75:ASN:HB3	1:A:95:LEU:CD2	2.51	0.40
1:B:90:PHE:CE2	1:B:121:VAL:HG21	2.56	0.40
1:B:145:GLU:HA	1:B:193:LEU:HD22	2.03	0.40
1:C:258:CYS:SG	1:C:260:TYR:CD2	3.14	0.40
1:C:118:VAL:HB	1:C:206:THR:HG22	2.03	0.40
1:A:72:LEU:HD23	1:A:73:GLY:N	2.36	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	272/324 (84%)	258 (95%)	14 (5%)	0	100	100
1	B	273/324 (84%)	258 (94%)	14 (5%)	1 (0%)	43	87
1	C	273/324 (84%)	257 (94%)	15 (6%)	1 (0%)	43	87
1	D	272/324 (84%)	257 (94%)	15 (6%)	0	100	100
1	E	273/324 (84%)	260 (95%)	12 (4%)	1 (0%)	43	87
1	F	273/324 (84%)	261 (96%)	11 (4%)	1 (0%)	43	87
All	All	1636/1944 (84%)	1551 (95%)	81 (5%)	4 (0%)	56	92

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	272	SER
1	F	272	SER
1	B	272	SER
1	C	272	SER

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	243/293 (83%)	237 (98%)	6 (2%)	60	92
1	B	244/293 (83%)	238 (98%)	6 (2%)	60	92
1	C	243/293 (83%)	235 (97%)	8 (3%)	50	88
1	D	244/293 (83%)	236 (97%)	8 (3%)	50	88
1	E	246/293 (84%)	238 (97%)	8 (3%)	50	88
1	F	244/293 (83%)	237 (97%)	7 (3%)	55	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1464/1758 (83%)	1421 (97%)	43 (3%)	55	90

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
1	A	149	ARG
1	A	212	LYS
1	A	241	ASP
1	A	264	TYR
1	A	344	GLU
1	B	56	LYS
1	B	149	ARG
1	B	212	LYS
1	B	241	ASP
1	B	264	TYR
1	B	336	LEU
1	C	56	LYS
1	C	86	THR
1	C	149	ARG
1	C	188	LYS
1	C	212	LYS
1	C	233	GLU
1	C	241	ASP
1	C	264	TYR
1	D	56	LYS
1	D	149	ARG
1	D	159	THR
1	D	188	LYS
1	D	212	LYS
1	D	233	GLU
1	D	264	TYR
1	D	337	HIS
1	E	56	LYS
1	E	149	ARG
1	E	156	GLN
1	E	188	LYS
1	E	212	LYS
1	E	241	ASP
1	E	264	TYR
1	E	337	HIS
1	F	56	LYS

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Mol	Chain	Res	Type
1	F	149	ARG
1	F	156	GLN
1	F	212	LYS
1	F	233	GLU
1	F	264	TYR
1	F	337	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	68	GLN
1	A	75	ASN
1	A	80	GLN
1	A	87	GLN
1	A	184	HIS
1	A	304	ASN
1	B	53	GLN
1	B	75	ASN
1	B	80	GLN
1	B	87	GLN
1	B	184	HIS
1	B	304	ASN
1	C	53	GLN
1	C	75	ASN
1	C	80	GLN
1	C	87	GLN
1	C	126	ASN
1	C	184	HIS
1	C	304	ASN
1	D	53	GLN
1	D	68	GLN
1	D	75	ASN
1	D	80	GLN
1	D	87	GLN
1	D	184	HIS
1	D	304	ASN
1	E	53	GLN
1	E	68	GLN
1	E	75	ASN
1	E	80	GLN
1	E	87	GLN

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Mol	Chain	Res	Type
1	E	184	HIS
1	E	304	ASN
1	F	53	GLN
1	F	68	GLN
1	F	75	ASN
1	F	80	GLN
1	F	87	GLN
1	F	184	HIS
1	F	304	ASN

5.3.3　RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6　Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	YRZ	A	901	-	22,22,22	5.54	6 (27%)	25,31,31	2.14	10 (40%)
2	YRZ	B	901	-	22,22,22	4.97	5 (22%)	25,31,31	2.28	9 (36%)
2	YRZ	C	901	-	22,22,22	4.43	6 (27%)	25,31,31	2.15	7 (28%)
2	YRZ	D	901	-	22,22,22	4.85	6 (27%)	25,31,31	2.21	9 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	YRZ	E	901	-	22,22,22	5.62	5 (22%)	25,31,31	2.24	10 (40%)
2	YRZ	F	901	-	22,22,22	6.14	5 (22%)	25,31,31	2.34	9 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	YRZ	A	901	-	-	0/4/18/18	0/1/4/4
2	YRZ	B	901	-	-	0/4/18/18	0/1/4/4
2	YRZ	C	901	-	-	0/4/18/18	0/1/4/4
2	YRZ	D	901	-	-	0/4/18/18	0/1/4/4
2	YRZ	E	901	-	-	0/4/18/18	0/1/4/4
2	YRZ	F	901	-	-	0/4/18/18	0/1/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	901	YRZ	C14-C13	27.82	1.42	1.39
2	E	901	YRZ	C14-C13	25.17	1.42	1.39
2	A	901	YRZ	C14-C13	24.77	1.42	1.39
2	B	901	YRZ	C14-C13	21.97	1.42	1.39
2	D	901	YRZ	C14-C13	21.33	1.42	1.39
2	C	901	YRZ	C14-C13	19.51	1.41	1.39
2	E	901	YRZ	N16-N12	4.56	1.43	1.36
2	F	901	YRZ	C13-N12	-4.24	1.31	1.38
2	D	901	YRZ	C13-N12	-4.21	1.31	1.38
2	C	901	YRZ	C13-N12	-4.15	1.31	1.38
2	A	901	YRZ	N16-N12	4.05	1.42	1.36
2	B	901	YRZ	C13-N12	-3.96	1.32	1.38
2	A	901	YRZ	C13-N12	-3.88	1.32	1.38
2	B	901	YRZ	N16-N12	3.80	1.42	1.36
2	E	901	YRZ	C13-N12	-3.79	1.32	1.38
2	D	901	YRZ	N16-N12	3.70	1.41	1.36
2	F	901	YRZ	N16-N12	3.69	1.41	1.36
2	B	901	YRZ	C17-N18	3.55	1.36	1.31
2	D	901	YRZ	C17-N18	3.48	1.36	1.31
2	A	901	YRZ	C17-N18	3.29	1.35	1.31
2	E	901	YRZ	C17-N18	3.14	1.35	1.31
2	C	901	YRZ	C17-N18	2.98	1.35	1.31
2	C	901	YRZ	N16-N12	2.76	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	901	YRZ	C2-N12	-2.45	1.33	1.38
2	C	901	YRZ	C2-N12	-2.21	1.33	1.38
2	F	901	YRZ	C17-N18	2.19	1.34	1.31
2	B	901	YRZ	C1-C17	2.16	1.47	1.42
2	C	901	YRZ	C1-C17	2.15	1.47	1.42
2	D	901	YRZ	C1-C17	2.06	1.47	1.42
2	D	901	YRZ	C2-N12	-2.06	1.34	1.38
2	A	901	YRZ	C1-C17	2.03	1.47	1.42
2	E	901	YRZ	C1-C17	2.01	1.47	1.42
2	A	901	YRZ	C2-N12	-2.01	1.34	1.38

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	901	YRZ	N18-C13-N12	5.88	127.60	122.20
2	B	901	YRZ	N18-C13-N12	5.73	127.47	122.20
2	C	901	YRZ	N18-C13-N12	5.48	127.24	122.20
2	A	901	YRZ	N18-C13-N12	5.41	127.17	122.20
2	D	901	YRZ	N18-C13-N12	5.28	127.06	122.20
2	E	901	YRZ	N18-C13-N12	5.12	126.91	122.20
2	F	901	YRZ	C1-C17-N18	-4.04	115.74	122.63
2	F	901	YRZ	C13-N12-N16	3.93	115.50	111.08
2	E	901	YRZ	C1-C17-N18	-3.79	116.17	122.63
2	C	901	YRZ	C13-N12-N16	3.79	115.33	111.08
2	D	901	YRZ	C1-C17-N18	-3.71	116.31	122.63
2	D	901	YRZ	C13-N12-N16	3.66	115.19	111.08
2	C	901	YRZ	C1-C17-N18	-3.59	116.50	122.63
2	B	901	YRZ	C1-C17-N18	-3.56	116.56	122.63
2	B	901	YRZ	C13-N12-N16	3.51	115.02	111.08
2	A	901	YRZ	C1-C17-N18	-3.49	116.67	122.63
2	E	901	YRZ	C13-N12-N16	3.43	114.93	111.08
2	B	901	YRZ	C5-C4-N3	3.40	108.47	103.57
2	F	901	YRZ	C7-N8-C9	3.37	117.22	111.59
2	A	901	YRZ	C13-N12-N16	3.35	114.84	111.08
2	F	901	YRZ	C5-C4-N3	3.32	108.36	103.57
2	B	901	YRZ	C7-N8-C9	3.29	117.08	111.59
2	C	901	YRZ	C7-N8-C9	3.28	117.07	111.59
2	D	901	YRZ	C5-C4-N3	3.25	108.27	103.57
2	C	901	YRZ	C5-C4-N3	3.20	108.18	103.57
2	F	901	YRZ	C14-C13-N12	-3.15	102.42	108.08
2	E	901	YRZ	C5-C4-N3	3.12	108.06	103.57
2	A	901	YRZ	C14-C13-N12	-3.08	102.53	108.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	901	YRZ	C14-C13-N12	-3.02	102.64	108.08
2	E	901	YRZ	C7-N8-C9	3.00	116.61	111.59
2	C	901	YRZ	C14-C13-N12	-3.00	102.68	108.08
2	B	901	YRZ	C14-C13-N12	-2.98	102.71	108.08
2	E	901	YRZ	C4-C5-C1	-2.88	100.21	103.67
2	B	901	YRZ	C4-C5-C1	-2.88	100.21	103.67
2	E	901	YRZ	C14-C13-N12	-2.87	102.92	108.08
2	A	901	YRZ	C7-N8-C9	2.67	116.05	111.59
2	F	901	YRZ	C4-C5-C1	-2.67	100.46	103.67
2	A	901	YRZ	C5-C4-N3	2.65	107.39	103.57
2	D	901	YRZ	C7-N8-C9	2.60	115.93	111.59
2	D	901	YRZ	C4-C5-C1	-2.59	100.55	103.67
2	C	901	YRZ	C4-C5-C1	-2.49	100.68	103.67
2	E	901	YRZ	C17-N18-C13	2.40	120.37	117.24
2	A	901	YRZ	C4-C5-C1	-2.30	100.90	103.67
2	B	901	YRZ	C17-N19-C6	-2.29	120.99	123.84
2	A	901	YRZ	C4-N3-C2	2.21	112.01	108.06
2	B	901	YRZ	N19-C17-N18	2.19	124.01	118.39
2	E	901	YRZ	C6-C7-N8	-2.15	108.02	111.46
2	D	901	YRZ	N19-C17-N18	2.14	123.87	118.39
2	F	901	YRZ	N19-C17-N18	2.13	123.85	118.39
2	F	901	YRZ	C17-N18-C13	2.09	119.96	117.24
2	A	901	YRZ	C6-C7-N8	-2.08	108.12	111.46
2	D	901	YRZ	C11-C6-C7	-2.08	106.64	109.59
2	A	901	YRZ	N19-C17-N18	2.05	123.64	118.39
2	E	901	YRZ	C17-N19-C6	-2.03	121.32	123.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	282/324 (87%)	1.80	107 (37%)	1	0	49, 75, 116, 133	0
1	B	283/324 (87%)	1.75	101 (35%)	1	0	49, 76, 116, 131	0
1	C	283/324 (87%)	1.70	96 (33%)	1	0	49, 76, 115, 130	0
1	D	282/324 (87%)	1.70	98 (34%)	1	0	48, 75, 113, 130	0
1	E	283/324 (87%)	1.79	102 (36%)	1	0	49, 76, 118, 132	0
1	F	283/324 (87%)	1.67	99 (34%)	1	0	49, 76, 119, 131	0
All	All	1696/1944 (87%)	1.74	603 (35%)	1	0	48, 76, 117, 133	0

All (603) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	157	ALA	8.7
1	A	264	TYR	8.2
1	E	229	TYR	7.9
1	E	158	PHE	7.8
1	C	235	LEU	7.8
1	E	264	TYR	7.3
1	F	326	MET	7.3
1	B	328	SER	6.8
1	B	46	PHE	6.8
1	A	230	VAL	6.8
1	B	157	ALA	6.7
1	D	46	PHE	6.6
1	E	336	LEU	6.4
1	F	46	PHE	6.1
1	E	54	ILE	5.9
1	C	46	PHE	5.8
1	A	158	PHE	5.8
1	A	256	LEU	5.7
1	C	339	SER	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	235	LEU	5.7
1	D	150	ILE	5.7
1	D	68	GLN	5.7
1	A	329	THR	5.6
1	F	234	VAL	5.6
1	C	120	ILE	5.6
1	B	146	LEU	5.6
1	E	338	THR	5.5
1	C	147	PHE	5.3
1	E	205	LEU	5.2
1	B	294	VAL	5.2
1	F	75	ASN	5.2
1	A	231	ALA	5.1
1	A	249	LEU	5.1
1	E	256	LEU	5.1
1	F	294	VAL	5.1
1	D	339	SER	5.1
1	A	48	VAL	5.0
1	C	337	HIS	4.9
1	D	70	LEU	4.9
1	A	336	LEU	4.9
1	A	163	ALA	4.9
1	E	228	TYR	4.8
1	C	124	TYR	4.8
1	A	265	SER	4.8
1	C	59	ILE	4.7
1	B	234	VAL	4.7
1	A	257	LEU	4.6
1	E	48	VAL	4.6
1	A	104	GLU	4.6
1	D	147	PHE	4.6
1	C	150	ILE	4.6
1	A	205	LEU	4.5
1	E	230	VAL	4.5
1	B	259	GLY	4.5
1	D	153	ARG	4.5
1	A	228	TYR	4.5
1	D	342	LEU	4.5
1	F	259	GLY	4.5
1	E	257	LEU	4.4
1	E	339	SER	4.4
1	D	203	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	229	TYR	4.4
1	A	200	ASN	4.4
1	B	128	TYR	4.4
1	E	46	PHE	4.3
1	E	298	VAL	4.3
1	A	301	LEU	4.3
1	F	249	LEU	4.3
1	A	46	PHE	4.2
1	B	201	ALA	4.2
1	E	249	LEU	4.1
1	B	261	PRO	4.1
1	C	229	TYR	4.1
1	E	118	VAL	4.1
1	A	96	GLN	4.1
1	B	326	MET	4.1
1	D	243	SER	4.1
1	F	228	TYR	4.0
1	B	237	PRO	4.0
1	C	342	LEU	4.0
1	E	66	THR	4.0
1	D	245	ASP	4.0
1	B	338	THR	4.0
1	C	334	THR	4.0
1	B	94	MET	4.0
1	F	94	MET	4.0
1	A	66	THR	4.0
1	F	289	PRO	4.0
1	D	120	ILE	3.9
1	E	279	ILE	3.9
1	A	294	VAL	3.9
1	D	119	ARG	3.9
1	B	279	ILE	3.9
1	C	61	ASP	3.9
1	E	277	THR	3.9
1	C	109	TRP	3.9
1	E	64	LYS	3.9
1	C	233	GLU	3.8
1	A	121	VAL	3.8
1	E	90	PHE	3.8
1	C	298	VAL	3.8
1	B	72	LEU	3.8
1	F	95	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	334	THR	3.8
1	D	61	ASP	3.7
1	F	237	PRO	3.7
1	E	96	GLN	3.7
1	A	321	ASN	3.7
1	C	182	ILE	3.7
1	E	126	ASN	3.7
1	A	279	ILE	3.7
1	A	151	GLN	3.7
1	B	289	PRO	3.7
1	C	243	SER	3.7
1	E	65	VAL	3.7
1	E	294	VAL	3.7
1	D	279	ILE	3.7
1	D	232	PRO	3.6
1	E	263	PHE	3.6
1	F	328	SER	3.6
1	B	244	CYS	3.6
1	D	182	ILE	3.6
1	E	327	GLN	3.6
1	F	272	SER	3.6
1	F	295	SER	3.6
1	D	95	LEU	3.6
1	F	188	LYS	3.6
1	A	64	LYS	3.5
1	C	48	VAL	3.5
1	D	164	SER	3.5
1	E	301	LEU	3.5
1	F	263	PHE	3.5
1	F	79	LEU	3.5
1	C	151	GLN	3.5
1	A	229	TYR	3.5
1	F	128	TYR	3.5
1	D	121	VAL	3.5
1	F	72	LEU	3.5
1	C	52	LEU	3.5
1	F	312	GLN	3.5
1	E	94	MET	3.5
1	E	127	LEU	3.5
1	A	170	ILE	3.5
1	B	302	ILE	3.5
1	F	174	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	258	CYS	3.4
1	B	174	ILE	3.4
1	B	272	SER	3.4
1	E	182	ILE	3.4
1	B	325	ILE	3.4
1	D	180	ILE	3.4
1	E	329	THR	3.4
1	F	136	ILE	3.4
1	F	235	LEU	3.4
1	B	298	VAL	3.4
1	E	123	VAL	3.4
1	B	158	PHE	3.4
1	B	79	LEU	3.4
1	A	174	ILE	3.4
1	F	146	LEU	3.4
1	E	163	ALA	3.4
1	B	251	VAL	3.4
1	F	329	THR	3.3
1	A	314	MET	3.3
1	E	265	SER	3.3
1	D	133	CYS	3.3
1	D	324	TRP	3.3
1	B	150	ILE	3.3
1	E	293	GLU	3.3
1	F	286	PHE	3.3
1	E	79	LEU	3.3
1	B	183	ALA	3.3
1	D	48	VAL	3.3
1	D	75	ASN	3.3
1	D	169	SER	3.3
1	D	192	LEU	3.3
1	E	129	ALA	3.3
1	F	298	VAL	3.3
1	D	52	LEU	3.3
1	A	113	GLN	3.3
1	E	145	GLU	3.3
1	F	216	SER	3.3
1	E	202	ILE	3.2
1	A	118	VAL	3.2
1	E	253	MET	3.2
1	B	329	THR	3.2
1	B	232	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	94	MET	3.2
1	A	291	TRP	3.2
1	B	229	TYR	3.2
1	B	249	LEU	3.2
1	B	154	GLY	3.2
1	F	338	THR	3.2
1	A	85	ARG	3.2
1	A	67	SER	3.2
1	B	202	ILE	3.2
1	A	253	MET	3.2
1	C	305	LEU	3.2
1	D	229	TYR	3.2
1	F	324	TRP	3.2
1	C	187	VAL	3.2
1	D	116	HIS	3.2
1	B	306	LEU	3.2
1	F	134	LEU	3.2
1	A	123	VAL	3.2
1	C	121	VAL	3.2
1	E	200	ASN	3.2
1	E	194	TYR	3.2
1	C	136	ILE	3.2
1	F	302	ILE	3.2
1	F	123	VAL	3.2
1	A	54	ILE	3.2
1	B	148	SER	3.1
1	E	67	SER	3.1
1	F	258	CYS	3.1
1	C	324	TRP	3.1
1	A	293	GLU	3.1
1	B	228	TYR	3.1
1	D	159	THR	3.1
1	C	180	ILE	3.1
1	E	314	MET	3.1
1	A	283	GLN	3.1
1	A	82	PHE	3.1
1	A	328	SER	3.1
1	D	86	THR	3.1
1	E	275	MET	3.1
1	C	70	LEU	3.1
1	B	193	LEU	3.1
1	B	235	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	95	LEU	3.1
1	F	325	ILE	3.1
1	C	91	ALA	3.1
1	A	145	GLU	3.1
1	C	119	ARG	3.1
1	D	102	ARG	3.1
1	A	194	TYR	3.1
1	C	176	TYR	3.1
1	B	105	VAL	3.1
1	A	149	ARG	3.1
1	A	153	ARG	3.1
1	E	192	LEU	3.1
1	B	64	LYS	3.1
1	B	84	LYS	3.1
1	F	54	ILE	3.1
1	B	263	PHE	3.0
1	D	257	LEU	3.0
1	C	290	GLU	3.0
1	E	174	ILE	3.0
1	F	335	PRO	3.0
1	F	193	LEU	3.0
1	C	68	GLN	3.0
1	D	74	ILE	3.0
1	A	146	LEU	3.0
1	F	84	LYS	3.0
1	B	63	TYR	3.0
1	D	187	VAL	3.0
1	C	72	LEU	3.0
1	C	312	GLN	3.0
1	F	279	ILE	3.0
1	E	119	ARG	3.0
1	C	232	PRO	3.0
1	E	235	LEU	3.0
1	C	320	MET	3.0
1	F	257	LEU	3.0
1	A	60	ILE	3.0
1	B	118	VAL	3.0
1	A	79	LEU	3.0
1	C	141	LEU	3.0
1	A	94	MET	3.0
1	A	136	ILE	3.0
1	E	136	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	308	THR	3.0
1	D	124	TYR	3.0
1	D	59	ILE	2.9
1	D	312	GLN	2.9
1	D	294	VAL	2.9
1	F	92	LEU	2.9
1	D	252	ILE	2.9
1	A	308	THR	2.9
1	B	95	LEU	2.9
1	C	272	SER	2.9
1	A	187	VAL	2.9
1	B	304	ASN	2.9
1	F	322	HIS	2.9
1	B	203	LEU	2.9
1	B	256	LEU	2.9
1	F	169	SER	2.9
1	F	81	ILE	2.9
1	B	286	PHE	2.9
1	C	90	PHE	2.9
1	E	128	TYR	2.9
1	B	162	GLU	2.9
1	B	136	ILE	2.9
1	B	324	TRP	2.9
1	C	257	LEU	2.9
1	B	334	THR	2.8
1	C	199	PRO	2.8
1	D	162	GLU	2.8
1	A	202	ILE	2.8
1	B	134	LEU	2.8
1	A	65	VAL	2.8
1	B	214	THR	2.8
1	A	161	ARG	2.8
1	D	72	LEU	2.8
1	D	92	LEU	2.8
1	F	205	LEU	2.8
1	F	256	LEU	2.8
1	A	338	THR	2.8
1	C	92	LEU	2.8
1	E	146	LEU	2.8
1	A	263	PHE	2.8
1	A	324	TRP	2.8
1	B	248	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	262	PRO	2.8
1	E	110	ARG	2.8
1	B	59	ILE	2.8
1	C	325	ILE	2.8
1	B	287	PRO	2.8
1	C	302	ILE	2.8
1	C	291	TRP	2.8
1	D	66	THR	2.8
1	C	123	VAL	2.8
1	C	252	ILE	2.8
1	E	281	MET	2.8
1	A	299	LYS	2.8
1	E	179	SER	2.8
1	C	138	MET	2.7
1	C	258	CYS	2.7
1	D	123	VAL	2.7
1	D	130	GLY	2.7
1	E	69	VAL	2.7
1	C	262	PRO	2.7
1	A	201	ALA	2.7
1	C	137	VAL	2.7
1	C	260	TYR	2.7
1	E	291	TRP	2.7
1	D	184	HIS	2.7
1	C	118	VAL	2.7
1	B	54	ILE	2.7
1	D	81	ILE	2.7
1	D	128	TYR	2.7
1	B	278	ARG	2.7
1	C	303	ARG	2.7
1	D	216	SER	2.7
1	A	198	ARG	2.7
1	E	273	PRO	2.7
1	C	203	LEU	2.6
1	B	80	GLN	2.6
1	C	316	ILE	2.6
1	F	124	TYR	2.6
1	C	288	ASN	2.6
1	C	53	GLN	2.6
1	D	67	SER	2.6
1	A	289	PRO	2.6
1	D	337	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	69	VAL	2.6
1	C	265	SER	2.6
1	B	177	LEU	2.6
1	E	95	LEU	2.6
1	C	169	SER	2.6
1	D	208	PHE	2.6
1	F	69	VAL	2.6
1	F	166	ILE	2.6
1	D	291	TRP	2.6
1	F	232	PRO	2.6
1	B	215	THR	2.6
1	C	111	ALA	2.6
1	D	173	ALA	2.6
1	E	58	ALA	2.6
1	A	68	GLN	2.6
1	F	275	MET	2.6
1	C	341	VAL	2.6
1	E	170	ILE	2.6
1	F	158	PHE	2.6
1	A	192	LEU	2.6
1	B	92	LEU	2.6
1	C	94	MET	2.6
1	D	138	MET	2.6
1	F	148	SER	2.5
1	E	324	TRP	2.5
1	B	108	HIS	2.5
1	E	337	HIS	2.5
1	B	65	VAL	2.5
1	C	245	ASP	2.5
1	E	187	VAL	2.5
1	A	72	LEU	2.5
1	A	277	THR	2.5
1	B	260	TYR	2.5
1	B	69	VAL	2.5
1	C	116	HIS	2.5
1	A	208	PHE	2.5
1	A	234	VAL	2.5
1	F	306	LEU	2.5
1	F	342	LEU	2.5
1	C	125	GLU	2.5
1	A	252	ILE	2.5
1	E	81	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	321	ASN	2.5
1	A	144	GLY	2.5
1	C	107	LEU	2.5
1	D	107	LEU	2.5
1	B	335	PRO	2.5
1	E	104	GLU	2.5
1	E	208	PHE	2.5
1	E	247	TRP	2.5
1	E	286	PHE	2.5
1	B	68	GLN	2.5
1	E	121	VAL	2.5
1	F	162	GLU	2.5
1	E	231	ALA	2.5
1	E	319	PHE	2.5
1	E	72	LEU	2.5
1	C	67	SER	2.5
1	B	327	GLN	2.5
1	F	105	VAL	2.5
1	B	81	ILE	2.4
1	F	176	TYR	2.4
1	F	293	GLU	2.4
1	A	298	VAL	2.4
1	E	86	THR	2.4
1	F	334	THR	2.4
1	B	166	ILE	2.4
1	E	341	VAL	2.4
1	E	206	THR	2.4
1	D	151	GLN	2.4
1	A	182	ILE	2.4
1	A	183	ALA	2.4
1	F	260	TYR	2.4
1	B	342	LEU	2.4
1	F	125	GLU	2.4
1	D	250	GLY	2.4
1	E	246	MET	2.4
1	A	134	LEU	2.4
1	D	109	TRP	2.4
1	D	125	GLU	2.4
1	D	272	SER	2.4
1	B	142	ASP	2.4
1	F	203	LEU	2.4
1	A	297	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	345	ASP	2.4
1	B	264	TYR	2.4
1	C	78	VAL	2.4
1	B	66	THR	2.4
1	C	50	SER	2.4
1	F	161	ARG	2.4
1	B	75	ASN	2.4
1	C	105	VAL	2.4
1	D	137	VAL	2.4
1	E	288	ASN	2.4
1	F	82	PHE	2.4
1	E	190	GLU	2.4
1	A	91	ALA	2.4
1	E	138	MET	2.4
1	F	109	TRP	2.3
1	F	341	VAL	2.3
1	C	130	GLY	2.3
1	A	177	LEU	2.3
1	C	79	LEU	2.3
1	C	183	ALA	2.3
1	A	284	TYR	2.3
1	D	65	VAL	2.3
1	F	319	PHE	2.3
1	B	185	ARG	2.3
1	B	121	VAL	2.3
1	B	123	VAL	2.3
1	D	298	VAL	2.3
1	E	93	LYS	2.3
1	D	142	ASP	2.3
1	F	247	TRP	2.3
1	C	122	ASP	2.3
1	D	177	LEU	2.3
1	C	296	GLU	2.3
1	F	208	PHE	2.3
1	A	168	LYS	2.3
1	D	141	LEU	2.3
1	F	160	GLU	2.3
1	F	327	GLN	2.3
1	A	71	GLY	2.3
1	A	210	PHE	2.3
1	A	95	LEU	2.3
1	D	136	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	142	ASP	2.3
1	F	183	ALA	2.3
1	D	64	LYS	2.2
1	F	126	ASN	2.2
1	E	322	HIS	2.2
1	E	262	PRO	2.2
1	A	86	THR	2.2
1	A	124	TYR	2.2
1	A	286	PHE	2.2
1	D	341	VAL	2.2
1	A	311	THR	2.2
1	C	192	LEU	2.2
1	D	320	MET	2.2
1	D	213	GLU	2.2
1	E	193	LEU	2.2
1	B	161	ARG	2.2
1	B	82	PHE	2.2
1	C	158	PHE	2.2
1	D	118	VAL	2.2
1	E	177	LEU	2.2
1	D	325	ILE	2.2
1	F	202	ILE	2.2
1	B	125	GLU	2.2
1	C	237	PRO	2.2
1	C	230	VAL	2.2
1	D	69	VAL	2.2
1	B	87	GLN	2.2
1	B	312	GLN	2.2
1	D	93	LYS	2.2
1	B	301	LEU	2.2
1	A	150	ILE	2.2
1	A	247	TRP	2.2
1	B	109	TRP	2.2
1	B	271	ILE	2.2
1	E	161	ARG	2.2
1	C	263	PHE	2.2
1	B	173	ALA	2.2
1	F	87	GLN	2.2
1	E	107	LEU	2.2
1	C	54	ILE	2.2
1	D	206	THR	2.2
1	D	91	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	65	VAL	2.2
1	F	121	VAL	2.2
1	F	251	VAL	2.2
1	D	135	LEU	2.2
1	E	334	THR	2.2
1	F	110	ARG	2.2
1	D	146	LEU	2.2
1	D	290	GLU	2.2
1	A	80	GLN	2.1
1	B	262	PRO	2.1
1	D	233	GLU	2.1
1	F	189	PRO	2.1
1	B	124	TYR	2.1
1	F	284	TYR	2.1
1	B	83	ASN	2.1
1	F	59	ILE	2.1
1	A	119	ARG	2.1
1	A	317	THR	2.1
1	A	322	HIS	2.1
1	F	214	THR	2.1
1	B	164	SER	2.1
1	D	238	GLU	2.1
1	E	333	GLN	2.1
1	A	281	MET	2.1
1	B	341	VAL	2.1
1	D	183	ALA	2.1
1	A	108	HIS	2.1
1	F	64	LYS	2.1
1	C	164	SER	2.1
1	E	167	MET	2.1
1	A	133	CYS	2.1
1	B	284	TYR	2.1
1	C	213	GLU	2.1
1	D	96	GLN	2.1
1	D	178	HIS	2.1
1	A	335	PRO	2.1
1	E	342	LEU	2.1
1	B	56	LYS	2.1
1	C	104	GLU	2.1
1	D	104	GLU	2.1
1	C	189	PRO	2.1
1	E	173	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	58	ALA	2.1
1	A	325	ILE	2.1
1	A	244	CYS	2.1
1	F	127	LEU	2.1
1	C	106	GLU	2.1
1	F	238	GLU	2.1
1	A	262	PRO	2.1
1	C	86	THR	2.1
1	D	308	THR	2.1
1	E	343	LYS	2.1
1	B	257	LEU	2.1
1	C	250	GLY	2.1
1	A	98	CYS	2.1
1	D	105	VAL	2.0
1	E	335	PRO	2.0
1	C	254	TYR	2.0
1	A	305	LEU	2.0
1	A	342	LEU	2.0
1	A	251	VAL	2.0
1	C	64	LYS	2.0
1	D	244	CYS	2.0
1	C	198	ARG	2.0
1	B	145	GLU	2.0
1	C	191	ASN	2.0
1	E	172	GLU	2.0
1	F	177	LEU	2.0
1	F	185	ARG	2.0
1	E	244	CYS	2.0
1	F	210	PHE	2.0
1	F	184	HIS	2.0
1	E	156	GLN	2.0
1	F	97	ASP	2.0
1	A	303	ARG	2.0
1	C	279	ILE	2.0
1	A	173	ALA	2.0
1	D	254	TYR	2.0
1	D	260	TYR	2.0
1	F	242	LYS	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	YRZ	A	901	19/19	0.42	1.73	67,68,71,73	0
2	YRZ	E	901	19/19	0.44	1.27	66,68,74,74	0
2	YRZ	F	901	19/19	0.36	0.95	69,70,76,76	0
2	YRZ	B	901	19/19	0.33	0.17	72,73,76,77	0
2	YRZ	C	901	19/19	0.32	-0.03	71,72,79,80	0
2	YRZ	D	901	19/19	0.29	-0.40	68,70,72,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.