Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:04 am BST

PDB ID	:	5YEF
Title	:	Crystal structure of CTCF ZFs2-8-Hs5-1aE
Authors	:	Yin, M.; Wang, J.; Wang, M.; Li, X.; Wang, Y.
Deposited on	:	2017-09-17
Resolution	:	2.81 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 following versions of software and data (see references ①) were used in the production of this report:

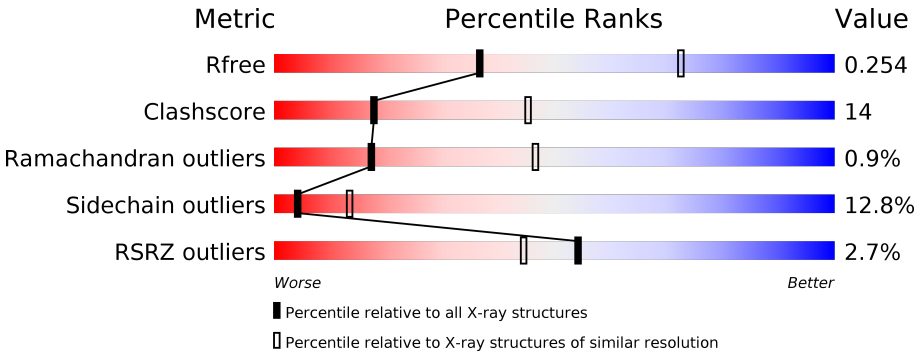
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	199	56% 23% 6% 15%
1	B	199	2% 59% 21% 16%
1	G	199	3% 52% 29% 15%
1	J	199	4% 51% 25% 8% 16%
2	C	27	52% 44%
2	E	27	11% 56% 41%

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Mol	Chain	Length	Quality of chain
2	H	27	63% 37%
2	K	27	52% 37% 11%
3	D	28	71% 21%
3	F	28	7% 79% 18%
3	I	28	61% 29% 7%
3	L	28	7% 64% 29%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9727 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 Transcriptional repressor CTCF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1334	827	263	229	15			
1	B	167	Total	C	N	O	S	0	0	0
			1321	820	261	225	15			
1	G	169	Total	C	N	O	S	0	0	0
			1331	826	263	227	15			
1	J	167	Total	C	N	O	S	0	0	0
			1321	820	261	225	15			

- Molecule 2 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	27	Total	C	N	O	P	0	0	0
			548	262	98	162	26			
2	E	27	Total	C	N	O	P	0	0	0
			548	262	98	162	26			
2	H	27	Total	C	N	O	P	0	0	0
			548	262	98	162	26			
2	K	27	Total	C	N	O	P	0	0	0
			548	262	98	162	26			

- Molecule 3 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	27	Total	C	N	O	P	0	0	0
			551	263	106	156	26			
3	F	27	Total	C	N	O	P	0	0	0
			551	263	106	156	26			
3	I	27	Total	C	N	O	P	0	0	0
			551	263	106	156	26			
3	L	27	Total	C	N	O	P	0	0	0
			551	263	106	156	26			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

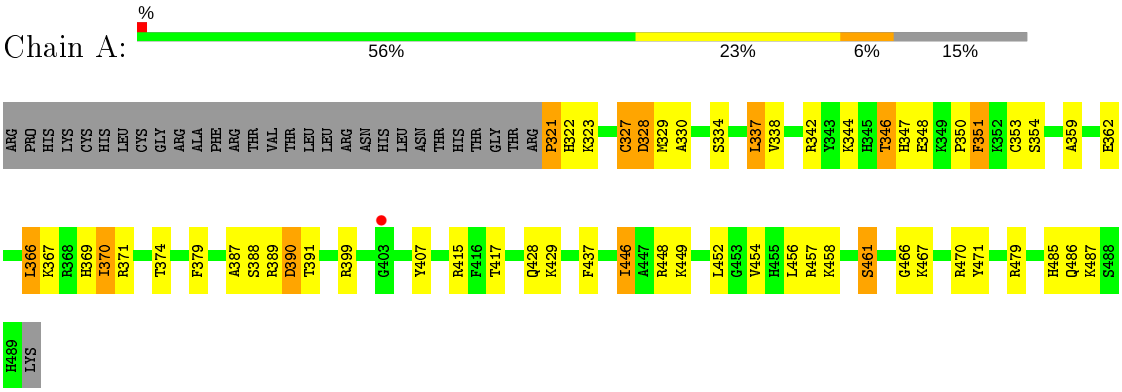
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	6	Total Zn 6 6	0	0
4	B	6	Total Zn 6 6	0	0
4	A	6	Total Zn 6 6	0	0
4	J	6	Total Zn 6 6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

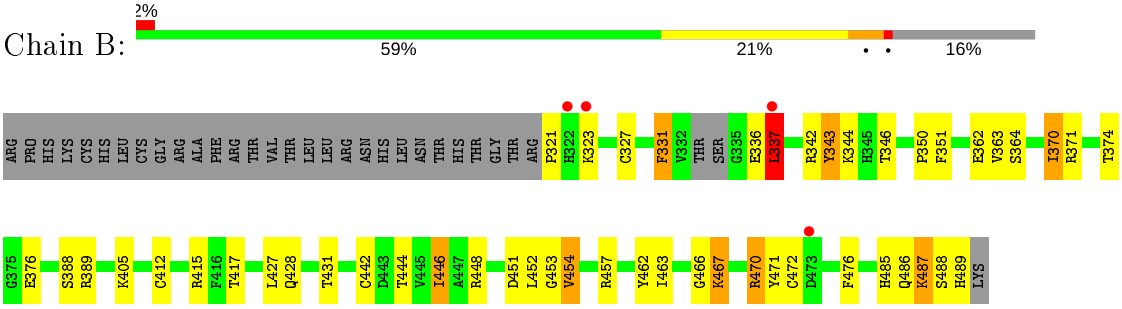
- Molecule 1: Transcriptional repressor CTCF

Chain A:



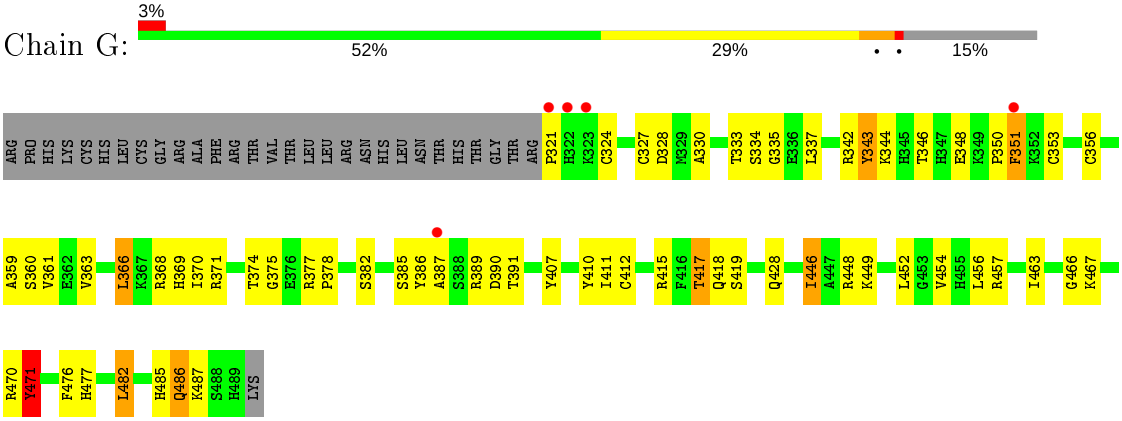
- Molecule 1: Transcriptional repressor CTCF

Chain B:



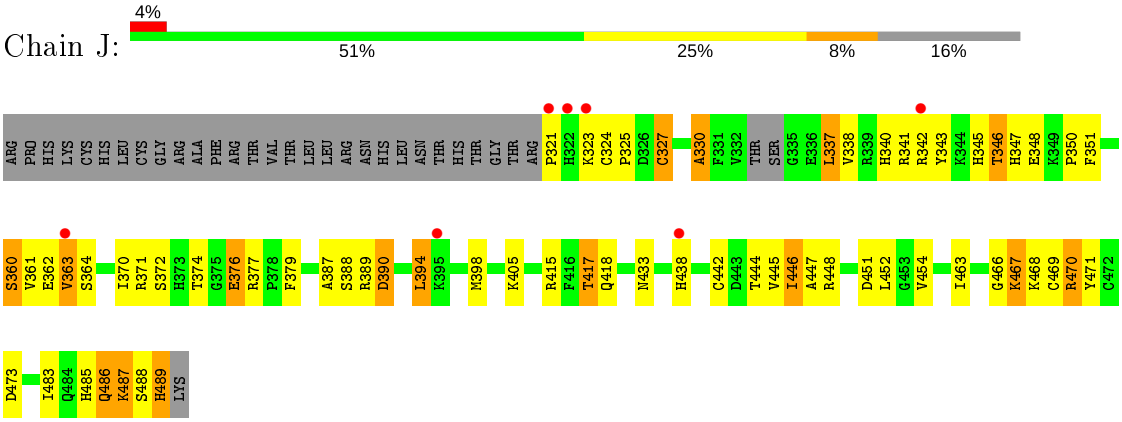
- Molecule 1: Transcriptional repressor CTCF

Chain G:



• Molecule 1: Transcriptional repressor CTCF

Chain J:



• Molecule 2: DNA (27-MER)

Chain C:

• Molecule 2: DNA (27-MER)

Chain E:

• Molecule 2: DNA (27-MER)

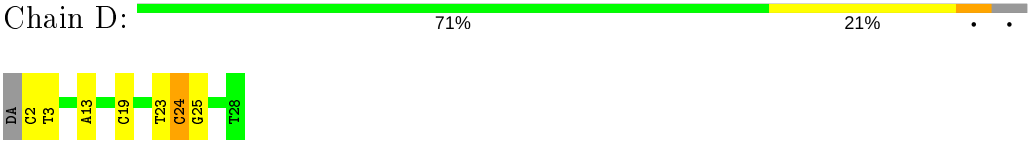
Chain H:

• Molecule 2: DNA (27-MER)

Chain K:

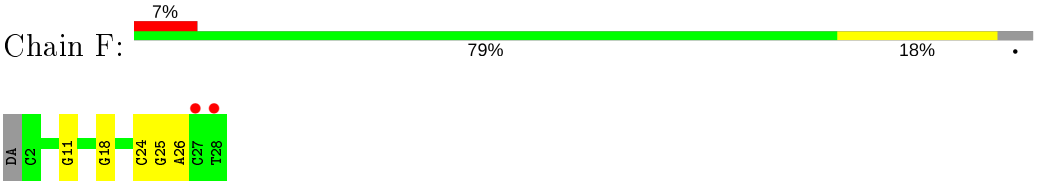
• Molecule 3: DNA (27-MER)

Chain D:



• Molecule 3: DNA (27-MER)

Chain F:

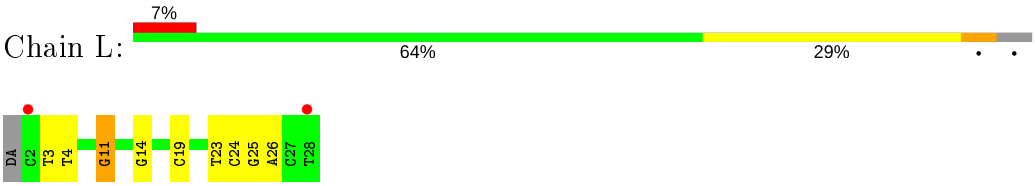


• Molecule 3: DNA (27-MER)

Chain I:

• Molecule 3: DNA (27-MER)

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.11Å 143.06Å 90.23Å 90.00° 119.69° 90.00°	Depositor
Resolution (Å)	45.06 – 2.81 45.06 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.06-2.81) 97.1 (45.06-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.224 , 0.254 0.224 , 0.254	Depositor DCC
R_{free} test set	2455 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	79.1	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 34.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -h-l,k,h 0.027 for l,k,-h-l 0.440 for h,-k,-h-l 0.027 for -h-l,-k,l 0.041 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9727	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.52	1/1369 (0.1%)	0.74	1/1841 (0.1%)
1	B	0.56	1/1355 (0.1%)	0.76	2/1820 (0.1%)
1	G	0.51	1/1366 (0.1%)	0.73	3/1837 (0.2%)
1	J	0.50	0/1355	0.72	1/1820 (0.1%)
2	C	1.02	1/613 (0.2%)	1.17	3/944 (0.3%)
2	E	1.05	1/613 (0.2%)	1.13	2/944 (0.2%)
2	H	0.96	0/613	1.11	1/944 (0.1%)
2	K	1.10	2/613 (0.3%)	1.20	5/944 (0.5%)
3	D	1.03	0/619	1.09	2/951 (0.2%)
3	F	1.07	0/619	1.09	0/951
3	I	1.01	1/619 (0.2%)	1.10	3/951 (0.3%)
3	L	1.11	1/619 (0.2%)	1.09	1/951 (0.1%)
All	All	0.81	9/10373 (0.1%)	0.95	24/14898 (0.2%)

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
1	B	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	412	CYS	CB-SG	-7.57	1.69	1.82
1	G	412	CYS	CB-SG	-6.95	1.70	1.82
2	K	20	DT	C3'-O3'	-6.63	1.35	1.44
3	I	10	DA	C3'-O3'	-5.90	1.36	1.44
3	L	14	DG	C3'-O3'	-5.25	1.37	1.44
1	A	327	CYS	CB-SG	-5.25	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	20	DT	C3'-O3'	-5.07	1.37	1.44
2	C	26	DA	C3'-O3'	-5.05	1.37	1.44
2	K	15	DT	C3'-O3'	-5.01	1.37	1.44

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	18	DG	O5'-P-OP2	6.67	118.71	110.70
3	I	24	DC	O5'-P-OP1	6.62	118.64	110.70
2	C	16	DC	O5'-P-OP1	-6.55	99.81	105.70
2	K	5	DC	O4'-C4'-C3'	-6.49	101.90	104.50
1	J	321	PRO	N-CA-CB	6.23	110.78	103.30
1	G	321	PRO	N-CA-CB	5.94	110.42	103.30
1	A	321	PRO	N-CA-CB	5.89	110.37	103.30
3	D	13	DA	O4'-C1'-N9	5.88	112.12	108.00
1	B	337	LEU	CA-CB-CG	5.69	128.39	115.30
1	B	321	PRO	N-CA-CB	5.58	109.99	103.30
2	E	15	DT	OP1-P-OP2	5.53	127.89	119.60
2	K	27	DA	OP2-P-O3'	5.46	117.22	105.20
3	D	24	DC	O5'-P-OP1	5.35	117.12	110.70
1	G	366	LEU	CB-CG-CD2	5.24	119.91	111.00
2	C	27	DA	O5'-P-OP2	-5.22	101.01	105.70
2	K	20	DT	N3-C4-O4	5.16	123.00	119.90
2	K	15	DT	N3-C4-O4	5.15	122.99	119.90
3	I	7	DA	OP2-P-O3'	5.12	116.46	105.20
2	H	27	DA	O5'-P-OP2	-5.11	101.10	105.70
2	E	15	DT	N3-C4-O4	5.11	122.96	119.90
3	L	11	DG	O5'-P-OP2	-5.09	101.11	105.70
1	G	471	TYR	CA-CB-CG	5.08	123.04	113.40
3	I	23	DT	N3-C4-O4	5.05	122.93	119.90
2	K	5	DC	OP1-P-O3'	5.04	116.28	105.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	331	PHE	Peptide

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	1334	0	1239	35	0
1	B	1321	0	1231	36	0
1	G	1331	0	1237	42	0
1	J	1321	0	1231	49	0
2	C	548	0	306	10	0
2	E	548	0	306	11	0
2	H	548	0	306	10	0
2	K	548	0	306	20	0
3	D	551	0	304	6	0
3	F	551	0	304	8	0
3	I	551	0	304	9	0
3	L	551	0	304	11	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	G	6	0	0	0	0
4	J	6	0	0	0	0
All	All	9727	0	7378	232	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 14.

All (232) 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:K:2:DA:H2'	2:K:3:DG:C8	2.01	0.95
2:K:26:DA:H2"	2:K:27:DA:N7	1.84	0.93
2:E:2:DA:H2'	2:E:3:DG:C8	2.08	0.89
1:A:329:MET:HA	1:A:330:ALA:HB3	1.56	0.86
3:I:24:DC:H2"	3:I:25:DG:C8	2.11	0.85
1:J:371:ARG:NH1	1:J:389:ARG:O	2.12	0.82
2:H:2:DA:H2'	2:H:3:DG:C8	2.16	0.80
1:G:470:ARG:HE	1:G:471:TYR:HE2	1.30	0.80
3:D:24:DC:H2"	3:D:25:DG:C8	2.16	0.80
3:L:3:DT:H2"	3:L:4:DT:C5	2.17	0.79
1:J:379:PHE:HB3	1:J:394:LEU:HD12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2:DA:H2'	2:C:3:DG:C8	2.18	0.78
3:L:24:DC:H2"	3:L:25:DG:C8	2.19	0.77
1:J:483:ILE:O	1:J:486:GLN:NE2	2.16	0.77
2:K:26:DA:H2"	2:K:27:DA:C8	2.19	0.76
1:B:371:ARG:NH1	1:B:389:ARG:O	2.18	0.76
1:J:342:ARG:HA	1:J:346:THR:HG23	1.69	0.75
1:G:485:HIS:O	1:G:487:LYS:N	2.20	0.75
1:A:470:ARG:NH2	1:A:471:TYR:OH	2.21	0.74
1:G:327:CYS:SG	1:G:328:ASP:N	2.55	0.73
1:J:405:LYS:NZ	3:L:11:DG:OP1	2.21	0.73
1:A:346:THR:O	1:A:346:THR:OG1	2.05	0.72
1:G:356:CYS:SG	1:G:369:HIS:NE2	2.63	0.72
1:B:487:LYS:N	1:B:487:LYS:HD3	2.07	0.70
1:J:338:VAL:O	1:J:342:ARG:HG2	1.91	0.70
1:B:342:ARG:HA	1:B:346:THR:HG22	1.74	0.70
2:K:2:DA:H2'	2:K:3:DG:H8	1.57	0.69
1:A:327:CYS:SG	1:A:328:ASP:N	2.65	0.69
1:B:417:THR:HG21	3:F:11:DG:H2'	1.76	0.68
1:A:323:LYS:O	1:A:337:LEU:HD11	1.93	0.67
3:F:24:DC:H2"	3:F:25:DG:C8	2.29	0.67
2:K:27:DA:H2"	2:K:28:DG:OP2	1.94	0.67
1:B:446:ILE:HD11	1:B:452:LEU:N	2.10	0.67
1:J:340:HIS:ND1	3:L:19:DC:OP1	2.24	0.66
1:J:346:THR:O	1:J:348:GLU:N	2.29	0.65
1:J:471:TYR:HD2	1:J:489:HIS:CD2	2.15	0.65
1:B:470:ARG:HD2	1:B:471:TYR:CE2	2.31	0.64
2:K:5:DC:H2'	2:K:6:DG:C8	2.32	0.64
1:B:342:ARG:HA	1:B:346:THR:CG2	2.28	0.64
1:A:446:ILE:HD11	1:A:452:LEU:HB2	1.77	0.64
1:A:485:HIS:O	1:A:487:LYS:N	2.27	0.63
1:J:324:CYS:HB3	1:J:327:CYS:O	1.98	0.62
1:J:470:ARG:HG2	1:J:471:TYR:CE1	2.35	0.62
1:J:341:ARG:HA	1:J:345:HIS:CD2	2.34	0.62
1:J:405:LYS:O	1:J:415:ARG:NH1	2.33	0.62
1:B:405:LYS:O	1:B:415:ARG:NH1	2.33	0.61
2:E:20:DT:H2"	2:E:21:DG:C8	2.36	0.61
1:B:470:ARG:HD2	1:B:471:TYR:CZ	2.36	0.61
2:C:7:DA:H1'	2:C:8:DC:H5'	1.81	0.61
1:J:323:LYS:O	1:J:337:LEU:HD21	2.01	0.61
1:A:350:PRO:HG2	1:A:351:PHE:CE2	2.36	0.60
3:D:2:DC:H2'	3:D:3:DT:H72	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:323:LYS:O	1:J:337:LEU:HD11	2.01	0.60
3:L:25:DG:H2"	3:L:26:DA:C8	2.36	0.60
2:C:5:DC:H2'	2:C:6:DG:C8	2.37	0.60
1:J:341:ARG:HA	1:J:345:HIS:HD2	1.65	0.60
1:G:350:PRO:HG2	1:G:351:PHE:CE2	2.36	0.60
1:A:329:MET:HA	1:A:330:ALA:CB	2.29	0.60
2:K:20:DT:H2"	2:K:21:DG:C8	2.37	0.60
1:B:405:LYS:NZ	3:F:11:DG:OP1	2.33	0.60
2:H:7:DA:H1'	2:H:8:DC:H5'	1.82	0.59
3:I:24:DC:H2"	3:I:25:DG:N7	2.17	0.59
3:D:24:DC:H2"	3:D:25:DG:N7	2.17	0.59
2:H:6:DG:H2"	2:H:7:DA:OP2	2.01	0.59
2:E:26:DA:H2"	2:E:27:DA:C8	2.37	0.59
2:E:5:DC:H2'	2:E:6:DG:C8	2.37	0.59
1:J:346:THR:O	1:J:346:THR:OG1	2.20	0.59
2:C:2:DA:H2'	2:C:3:DG:H8	1.68	0.59
2:H:5:DC:H2'	2:H:6:DG:C8	2.38	0.59
1:A:388:SER:OG	1:A:390:ASP:O	2.21	0.58
1:A:371:ARG:NH1	1:A:389:ARG:O	2.36	0.58
1:G:333:THR:O	1:G:335:GLY:N	2.36	0.58
1:B:470:ARG:NH1	1:B:471:TYR:OH	2.37	0.57
2:E:7:DA:H1'	2:E:8:DC:H5'	1.87	0.57
1:A:370:ILE:O	1:A:374:THR:HG23	2.05	0.57
1:J:350:PRO:HG2	1:J:351:PHE:CE2	2.40	0.57
1:B:442:CYS:SG	1:B:444:THR:HG23	2.45	0.56
2:C:6:DG:H2"	2:C:7:DA:OP2	2.05	0.56
3:I:23:DT:H2"	3:I:24:DC:O4'	2.05	0.56
2:K:6:DG:H2"	2:K:7:DA:OP2	2.04	0.56
1:J:471:TYR:HD2	1:J:489:HIS:HD2	1.51	0.56
1:J:470:ARG:HG2	1:J:471:TYR:CD1	2.40	0.56
2:K:26:DA:H8	2:K:26:DA:OP2	1.89	0.56
1:J:466:GLY:O	1:J:467:LYS:HD3	2.06	0.55
2:E:6:DG:H2"	2:E:7:DA:OP2	2.05	0.55
1:G:371:ARG:HH12	1:G:378:PRO:HG3	1.72	0.55
1:G:466:GLY:O	1:G:467:LYS:HD3	2.07	0.54
2:H:7:DA:H1'	2:H:8:DC:C5'	2.36	0.54
1:B:466:GLY:O	1:B:467:LYS:HD2	2.07	0.54
1:B:486:GLN:O	1:B:489:HIS:HB2	2.08	0.54
2:E:5:DC:H4'	2:E:6:DG:OP1	2.07	0.54
2:H:2:DA:H2'	2:H:3:DG:H8	1.73	0.54
1:G:446:ILE:HD11	1:G:452:LEU:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:488:SER:N	1:J:489:HIS:HA	2.22	0.54
1:J:324:CYS:SG	1:J:325:PRO:HD2	2.48	0.53
1:J:468:LYS:HG2	1:J:469:CYS:O	2.08	0.53
2:C:7:DA:H1'	2:C:8:DC:C5'	2.38	0.53
1:J:330:ALA:HB1	1:J:337:LEU:HD22	1.91	0.53
2:K:7:DA:H1'	2:K:8:DC:H5'	1.91	0.53
1:B:451:ASP:HA	1:B:454:VAL:HG13	1.91	0.53
1:J:360:SER:OG	1:J:361:VAL:N	2.40	0.53
1:A:446:ILE:HD11	1:A:452:LEU:CB	2.39	0.53
1:B:371:ARG:HG2	1:B:376:GLU:HB2	1.90	0.53
1:G:486:GLN:O	1:G:487:LYS:HD2	2.08	0.53
2:K:5:DC:H4'	2:K:6:DG:OP1	2.08	0.53
3:I:2:DC:H2'	3:I:3:DT:H72	1.90	0.52
1:J:370:ILE:O	1:J:374:THR:HG23	2.08	0.52
1:J:471:TYR:CD2	1:J:489:HIS:HD2	2.27	0.52
1:J:486:GLN:OE1	1:J:487:LYS:N	2.43	0.52
2:C:5:DC:H4'	2:C:6:DG:OP1	2.09	0.52
1:J:374:THR:OG1	1:J:376:GLU:HG2	2.10	0.52
2:H:5:DC:H4'	2:H:6:DG:OP1	2.09	0.51
1:G:446:ILE:HD11	1:G:452:LEU:CA	2.41	0.51
1:A:457:ARG:O	1:A:461:SER:HB3	2.11	0.51
1:B:370:ILE:O	1:B:374:THR:HG23	2.10	0.51
1:G:485:HIS:C	1:G:487:LYS:H	2.09	0.51
1:B:417:THR:HG22	3:F:11:DG:OP2	2.11	0.51
3:D:23:DT:H2"	3:D:24:DC:O4'	2.11	0.51
1:A:353:CYS:SG	1:A:354:SER:N	2.82	0.51
1:J:340:HIS:HD1	3:L:19:DC:P	2.33	0.51
2:K:5:DC:H2"	2:K:6:DG:H5'	1.93	0.51
2:K:5:DC:H3'	2:K:6:DG:C8	2.46	0.50
1:A:366:LEU:HD22	1:A:370:ILE:HD12	1.91	0.50
3:F:25:DG:H2"	3:F:26:DA:C8	2.46	0.50
1:B:331:PHE:HA	1:B:336:GLU:CB	2.41	0.50
1:G:342:ARG:HD2	1:G:348:GLU:CB	2.42	0.50
1:B:463:ILE:HG21	1:B:467:LYS:HD3	1.94	0.50
1:B:371:ARG:CG	1:B:376:GLU:HB2	2.42	0.49
1:G:368:ARG:O	1:G:371:ARG:HD2	2.12	0.49
1:G:350:PRO:HG2	1:G:351:PHE:CD2	2.47	0.49
1:G:344:LYS:HE3	3:I:18:DG:O3'	2.13	0.49
1:G:476:PHE:CE1	1:G:485:HIS:CD2	3.01	0.49
1:J:417:THR:HG22	1:J:418:GLN:HG3	1.93	0.49
1:G:482:LEU:O	1:G:486:GLN:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:TYR:CD2	1:J:346:THR:HB	2.47	0.49
2:K:5:DC:C3'	2:K:6:DG:C8	2.95	0.49
1:G:377:ARG:HD3	1:G:387:ALA:O	2.13	0.49
1:J:446:ILE:HG12	1:J:447:ALA:N	2.28	0.48
1:A:328:ASP:N	1:A:328:ASP:OD2	2.46	0.48
2:K:6:DG:C4	2:K:7:DA:N7	2.82	0.48
1:B:351:PHE:CE1	1:B:363:VAL:HB	2.48	0.48
1:J:446:ILE:HD11	1:J:448:ARG:O	2.13	0.48
1:G:343:TYR:CD1	3:I:18:DG:H2'	2.47	0.48
1:B:344:LYS:HE3	3:F:18:DG:O3'	2.13	0.48
3:F:24:DC:OP1	3:F:24:DC:H4'	2.12	0.48
1:B:487:LYS:HA	1:B:488:SER:C	2.34	0.48
1:A:344:LYS:NZ	3:D:19:DC:OP1	2.44	0.47
1:G:353:CYS:SG	1:G:369:HIS:CD2	3.07	0.47
3:I:24:DC:H4'	3:I:24:DC:OP1	2.13	0.47
1:J:470:ARG:H	1:J:470:ARG:HD2	1.79	0.47
1:J:351:PHE:CE1	1:J:363:VAL:HG22	2.50	0.47
3:L:24:DC:H2"	3:L:25:DG:N7	2.29	0.47
1:G:417:THR:HG22	1:G:418:GLN:HG3	1.97	0.47
3:L:24:DC:OP1	3:L:24:DC:H4'	2.14	0.46
1:G:428:GLN:HG3	1:G:448:ARG:CZ	2.46	0.46
3:L:25:DG:H2"	3:L:26:DA:H8	1.79	0.46
1:B:471:TYR:O	1:B:472:CYS:HB3	2.15	0.46
1:A:466:GLY:O	1:A:467:LYS:HD3	2.16	0.46
2:E:5:DC:H2"	2:E:6:DG:H5'	1.97	0.46
1:J:470:ARG:HG2	1:J:471:TYR:CZ	2.51	0.46
2:K:4:DT:H2"	2:K:5:DC:H6	1.81	0.46
1:A:367:LYS:O	1:A:371:ARG:HD2	2.16	0.46
1:G:324:CYS:SG	1:G:327:CYS:HB3	2.55	0.46
1:G:410:TYR:CE1	1:G:411:ILE:HG13	2.51	0.46
1:J:446:ILE:HD11	1:J:452:LEU:N	2.30	0.46
1:G:330:ALA:CB	1:G:337:LEU:HD12	2.45	0.45
2:H:25:DA:H2"	2:H:26:DA:OP2	2.15	0.45
1:A:346:THR:O	1:A:348:GLU:N	2.50	0.45
3:D:24:DC:H4'	3:D:24:DC:OP1	2.15	0.45
2:E:26:DA:H2"	2:E:27:DA:H8	1.79	0.45
2:E:25:DA:H2"	2:E:26:DA:OP2	2.16	0.45
3:L:3:DT:H2"	3:L:4:DT:C6	2.51	0.45
2:E:7:DA:H1'	2:E:8:DC:C5'	2.45	0.45
2:K:2:DA:C6	2:K:3:DG:C6	3.04	0.45
1:A:371:ARG:HD2	1:A:371:ARG:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:470:ARG:H	1:J:470:ARG:CD	2.30	0.45
1:J:350:PRO:HG2	1:J:351:PHE:CD2	2.51	0.45
1:B:476:PHE:CZ	1:B:485:HIS:CG	3.05	0.45
1:G:351:PHE:O	1:G:359:ALA:HA	2.17	0.44
1:G:386:TYR:OH	3:I:14:DG:OP2	2.29	0.44
1:J:323:LYS:H	1:J:337:LEU:HD21	1.83	0.44
1:A:428:GLN:HG3	1:A:448:ARG:CZ	2.48	0.43
2:K:5:DC:C2'	2:K:6:DG:C8	3.00	0.43
3:L:23:DT:H2"	3:L:24:DC:O4'	2.17	0.43
1:B:323:LYS:O	1:B:337:LEU:HD21	2.18	0.43
1:G:374:THR:OG1	1:G:375:GLY:N	2.50	0.43
1:A:485:HIS:C	1:A:487:LYS:H	2.18	0.43
1:J:377:ARG:HD3	1:J:387:ALA:O	2.19	0.43
1:A:321:PRO:N	1:A:322:HIS:HA	2.33	0.43
1:A:446:ILE:HD11	1:A:452:LEU:CA	2.48	0.43
1:G:353:CYS:SG	1:G:369:HIS:HD2	2.42	0.43
1:A:351:PHE:O	1:A:359:ALA:HA	2.19	0.43
1:A:374:THR:HB	1:B:376:GLU:CG	2.49	0.43
1:G:476:PHE:CE1	1:G:485:HIS:HD2	2.37	0.43
1:G:370:ILE:O	1:G:374:THR:HG23	2.18	0.42
1:B:337:LEU:HD12	1:B:337:LEU:O	2.19	0.42
1:B:350:PRO:HG2	1:B:351:PHE:CE2	2.55	0.42
1:J:451:ASP:HA	1:J:454:VAL:HG22	2.01	0.42
2:K:26:DA:H2"	2:K:27:DA:C5	2.54	0.42
1:A:351:PHE:HB2	1:A:366:LEU:HD12	2.02	0.42
1:A:379:PHE:O	1:A:387:ALA:HA	2.19	0.42
1:G:389:ARG:NH1	3:I:15:DA:P	2.93	0.42
2:C:25:DA:H2"	2:C:26:DA:OP2	2.19	0.42
1:G:368:ARG:HA	1:G:371:ARG:HD2	2.00	0.42
1:G:446:ILE:HD11	1:G:452:LEU:HB2	2.02	0.42
1:A:334:SER:O	1:A:338:VAL:HG23	2.19	0.42
1:A:353:CYS:SG	1:A:369:HIS:CD2	3.12	0.42
1:B:453:GLY:O	1:B:457:ARG:HG3	2.20	0.42
2:C:20:DT:H2"	2:C:21:DG:C8	2.55	0.42
1:A:437:PHE:HB3	1:A:452:LEU:HD22	2.02	0.42
1:B:350:PRO:HG2	1:B:351:PHE:CD2	2.54	0.42
1:J:372:SER:HA	1:J:389:ARG:NH1	2.35	0.42
1:G:371:ARG:HH12	1:G:378:PRO:CG	2.33	0.41
2:K:8:DC:H2'	2:K:8:DC:H6	1.70	0.41
1:J:388:SER:OG	1:J:390:ASP:O	2.37	0.41
1:B:428:GLN:HG3	1:B:448:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:463:ILE:HG13	1:G:477:HIS:O	2.19	0.41
1:G:407:TYR:O	1:G:415:ARG:HD3	2.21	0.41
1:G:446:ILE:HD11	1:G:452:LEU:CB	2.51	0.41
2:H:4:DT:H2"	2:H:5:DC:H6	1.85	0.41
1:A:407:TYR:O	1:A:415:ARG:HD3	2.21	0.41
1:A:458:LYS:O	1:A:479:ARG:HD3	2.21	0.41
2:C:2:DA:C6	2:C:3:DG:C6	3.09	0.41
1:J:442:CYS:SG	1:J:444:THR:HG23	2.61	0.41
1:B:427:LEU:O	1:B:431:THR:HB	2.21	0.41
1:J:376:GLU:O	1:J:389:ARG:HD3	2.20	0.41
1:J:438:HIS:CG	1:J:445:VAL:HG12	2.56	0.41
2:H:2:DA:H8	2:H:2:DA:HO5'	1.66	0.40
1:G:454:VAL:HG12	1:G:457:ARG:NH2	2.36	0.40
1:B:343:TYR:CD1	3:F:18:DG:H2'	2.55	0.40
1:G:330:ALA:HB3	1:G:337:LEU:HD12	2.03	0.40
1:G:343:TYR:CE2	1:G:361:VAL:HB	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	167/199 (84%)	152 (91%)	13 (8%)	2 (1%)	13 39
1	B	163/199 (82%)	154 (94%)	9 (6%)	0	100 100
1	G	167/199 (84%)	158 (95%)	7 (4%)	2 (1%)	13 39
1	J	163/199 (82%)	152 (93%)	9 (6%)	2 (1%)	13 39
All	All	660/796 (83%)	616 (93%)	38 (6%)	6 (1%)	17 46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	347	HIS
1	G	486	GLN
1	A	347	HIS
1	A	486	GLN
1	G	334	SER
1	J	330	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	137/182 (75%)	119 (87%)	18 (13%)	4 12
1	B	136/182 (75%)	124 (91%)	12 (9%)	10 29
1	G	136/182 (75%)	119 (88%)	17 (12%)	4 14
1	J	136/182 (75%)	113 (83%)	23 (17%)	2 6
All	All	545/728 (75%)	475 (87%)	70 (13%)	4 13

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	ASP
1	A	337	LEU
1	A	342	ARG
1	A	346	THR
1	A	351	PHE
1	A	362	GLU
1	A	366	LEU
1	A	370	ILE
1	A	390	ASP
1	A	391	THR
1	A	399	ARG
1	A	417	THR
1	A	429	LYS
1	A	446	ILE
1	A	449	LYS
1	A	454	VAL

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Mol	Chain	Res	Type
1	A	456	LEU
1	A	461	SER
1	B	327	CYS
1	B	337	LEU
1	B	343	TYR
1	B	362	GLU
1	B	364	SER
1	B	370	ILE
1	B	388	SER
1	B	446	ILE
1	B	454	VAL
1	B	467	LYS
1	B	470	ARG
1	B	487	LYS
1	G	343	TYR
1	G	346	THR
1	G	351	PHE
1	G	360	SER
1	G	363	VAL
1	G	366	LEU
1	G	382	SER
1	G	385	SER
1	G	390	ASP
1	G	391	THR
1	G	417	THR
1	G	419	SER
1	G	446	ILE
1	G	449	LYS
1	G	456	LEU
1	G	471	TYR
1	G	482	LEU
1	J	327	CYS
1	J	337	LEU
1	J	343	TYR
1	J	346	THR
1	J	360	SER
1	J	362	GLU
1	J	363	VAL
1	J	364	SER
1	J	376	GLU
1	J	390	ASP
1	J	394	LEU

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Mol	Chain	Res	Type
1	J	398	MET
1	J	417	THR
1	J	433	ASN
1	J	446	ILE
1	J	463	ILE
1	J	467	LYS
1	J	470	ARG
1	J	473	ASP
1	J	485	HIS
1	J	486	GLN
1	J	487	LYS
1	J	489	HIS

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 24 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, 95^{th} 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	169/199 (84%)	-0.22	1 (0%) 89 86	46, 86, 141, 180	0
1	B	167/199 (83%)	-0.32	4 (2%) 59 49	40, 74, 141, 191	0
1	G	169/199 (84%)	-0.05	5 (2%) 50 40	43, 89, 144, 187	0
1	J	167/199 (83%)	-0.16	7 (4%) 36 26	40, 78, 156, 208	0
2	C	27/27 (100%)	-0.60	0 100 100	61, 116, 209, 224	0
2	E	27/27 (100%)	-0.04	3 (11%) 5 3	61, 108, 296, 309	0
2	H	27/27 (100%)	-0.62	0 100 100	61, 121, 231, 249	0
2	K	27/27 (100%)	-0.22	0 100 100	50, 115, 295, 310	0
3	D	27/28 (96%)	-0.72	0 100 100	57, 87, 174, 191	0
3	F	27/28 (96%)	-0.14	2 (7%) 14 8	50, 84, 277, 326	0
3	I	27/28 (96%)	-0.66	0 100 100	59, 91, 182, 201	0
3	L	27/28 (96%)	0.13	2 (7%) 14 8	50, 88, 261, 302	0
All	All	888/1016 (87%)	-0.23	24 (2%) 54 44	40, 85, 182, 326	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	28	DT	8.5
1	G	321	PRO	7.6
3	F	28	DT	7.1
1	J	322	HIS	6.1
3	L	2	DC	5.5
2	E	2	DA	5.1
2	E	3	DG	5.1
1	J	363	VAL	3.6
2	E	4	DT	3.0
1	B	337	LEU	3.0
3	F	27	DC	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	323	LYS	2.8
1	G	322	HIS	2.8
1	B	473	ASP	2.6
1	B	323	LYS	2.6
1	J	438	HIS	2.5
1	B	322	HIS	2.3
1	J	323	LYS	2.3
1	J	321	PRO	2.3
1	G	387	ALA	2.2
1	G	351	PHE	2.2
1	A	403	GLY	2.2
1	J	395	LYS	2.1
1	J	342	ARG	2.1

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 carbohydrates 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, 95^{th} 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(Å^2)	Q<0.9
4	ZN	G	502	1/1	0.84	0.18	272,272,272,272	0
4	ZN	B	506	1/1	0.85	0.19	98,98,98,98	0
4	ZN	J	501	1/1	0.86	0.22	147,147,147,147	0
4	ZN	J	505	1/1	0.92	0.17	60,60,60,60	0
4	ZN	A	502	1/1	0.94	0.20	257,257,257,257	0
4	ZN	B	502	1/1	0.95	0.18	163,163,163,163	0
4	ZN	B	501	1/1	0.95	0.12	151,151,151,151	0
4	ZN	G	505	1/1	0.96	0.17	64,64,64,64	0
4	ZN	A	503	1/1	0.96	0.09	84,84,84,84	0
4	ZN	A	505	1/1	0.96	0.18	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	G	503	1/1	0.96	0.12	87,87,87,87	0
4	ZN	B	504	1/1	0.97	0.21	57,57,57,57	0
4	ZN	J	506	1/1	0.97	0.15	83,83,83,83	0
4	ZN	B	505	1/1	0.97	0.15	59,59,59,59	0
4	ZN	J	502	1/1	0.97	0.20	106,106,106,106	0
4	ZN	J	503	1/1	0.97	0.17	89,89,89,89	0
4	ZN	G	501	1/1	0.98	0.16	78,78,78,78	0
4	ZN	B	503	1/1	0.98	0.16	71,71,71,71	0
4	ZN	A	506	1/1	0.98	0.18	83,83,83,83	0
4	ZN	G	504	1/1	0.99	0.28	88,88,88,88	0
4	ZN	A	504	1/1	0.99	0.20	59,59,59,59	0
4	ZN	A	501	1/1	0.99	0.20	94,94,94,94	0
4	ZN	J	504	1/1	0.99	0.20	56,56,56,56	0
4	ZN	G	506	1/1	0.99	0.12	85,85,85,85	0

6.5 Other polymers (i)

There are no such residues in this entry.