Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:01 am BST

PDB ID	:	5YEL
Title	:	Crystal structure of CTCF ZFs6-11-gb7CSE
Authors	:	Yin, M.; Wang, J.; Wang, M.; Li, X.; Wang, Y.
Deposited on	:	2017-09-18
Resolution	:	2.96 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:

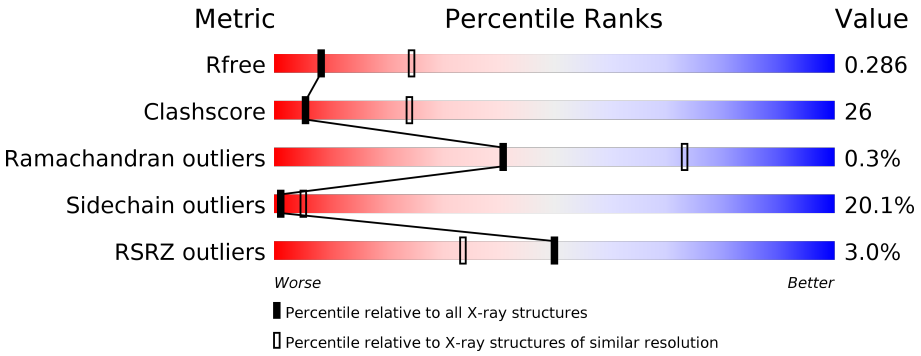
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.96 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	D	26	46% 54%
1	F	26	38% 62%
2	A	176	5% 47% 39% 9% • 6%
2	B	176	3% 44% 40% 10% • 5%
3	C	26	65% 35%
3	E	26	62% 38%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ZN	B	601	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4772 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 DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	26	Total	C	N	O	P	0	0	0
			526	253	98	150	25			
1	F	26	Total	C	N	O	P	0	0	0
			526	253	98	150	25			

- Molecule 2 is a protein called Transcriptional repressor CTCF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	166	Total	C	N	O	S	0	0	0
			1315	816	259	221	19			
2	B	168	Total	C	N	O	S	0	0	0
			1327	823	264	221	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	504	SER	CYS	engineered mutation	UNP P49711
B	504	SER	CYS	engineered mutation	UNP P49711

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	26	Total	C	N	O	P	0	0	0
			533	256	95	157	25			
3	E	26	Total	C	N	O	P	0	0	0
			533	256	95	157	25			

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

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

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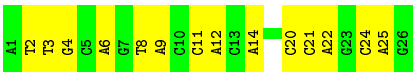
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	6	6	6	0	0

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.

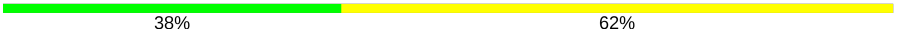
- Molecule 1: DNA (26-MER)

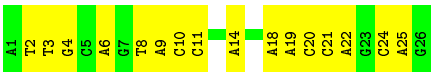
Chain D:



- Molecule 1: DNA (26-MER)

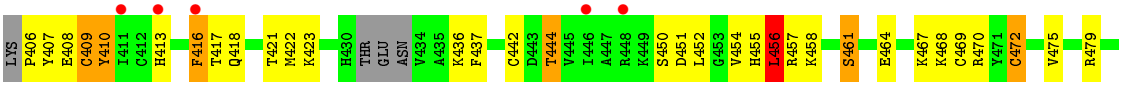
Chain F:

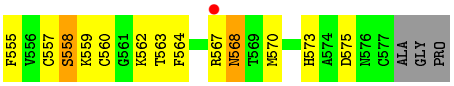




- Molecule 2: Transcriptional repressor CTCF

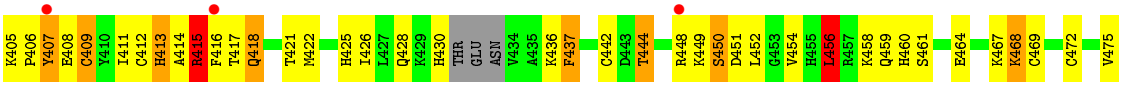
Chain A:

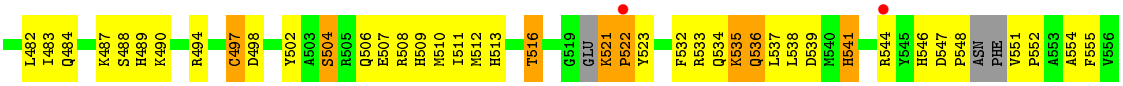




- Molecule 2: Transcriptional repressor CTCF

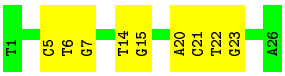
Chain B:





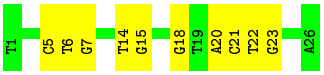
- Molecule 3: DNA (26-MER)

Chain C:



- Molecule 3: DNA (26-MER)

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	190.99Å 69.63Å 84.44Å 90.00° 116.25° 90.00°	Depositor
Resolution (Å)	37.87 – 2.96 37.87 – 2.96	Depositor EDS
% Data completeness (in resolution range)	98.1 (37.87-2.96) 98.0 (37.87-2.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.08 (at 2.95Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.268 , 0.286 0.268 , 0.286	Depositor DCC
R_{free} test set	1029 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	68.6	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 12.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.477 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4772	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% 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	D	0.57	0/590	0.97	0/906
1	F	0.58	0/590	0.95	0/906
2	A	0.51	2/1349 (0.1%)	0.71	2/1807 (0.1%)
2	B	0.61	3/1361 (0.2%)	0.75	5/1824 (0.3%)
3	C	0.68	0/597	1.04	0/921
3	E	0.68	0/597	1.03	0/921
All	All	0.60	5/5084 (0.1%)	0.88	7/7285 (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
2	A	0	1
2	B	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	472	CYS	CB-SG	-5.85	1.72	1.81
2	B	548	PRO	N-CD	5.78	1.55	1.47
2	A	548	PRO	N-CD	5.30	1.55	1.47
2	B	522	PRO	N-CD	5.26	1.55	1.47
2	B	552	PRO	N-CD	5.05	1.54	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	456	LEU	CA-CB-CG	6.63	130.54	115.30
2	B	456	LEU	CA-CB-CG	6.45	130.13	115.30
2	B	405	LYS	C-N-CD	5.80	140.59	128.40
2	B	551	VAL	C-N-CD	5.68	140.32	128.40
2	A	547	ASP	C-N-CD	5.66	140.28	128.40
2	B	521	LYS	C-N-CD	5.63	140.23	128.40
2	B	547	ASP	C-N-CD	5.29	139.50	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	546	HIS	Peptide
2	B	546	HIS	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	D	526	0	294	14	0
1	F	526	0	294	14	0
2	A	1315	0	1193	86	3
2	B	1327	0	1205	95	3
3	C	533	0	297	10	0
3	E	533	0	297	19	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
All	All	4772	0	3580	215	3

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 26.

All (215) 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:B:497:CYS:HB2	2:B:510:MET:CE	1.39	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:497:CYS:CB	2:B:510:MET:HE1	1.68	1.22
2:A:568:ASN:ND2	3:E:22:DT:OP2	1.78	1.16
2:A:516:THR:HA	2:A:533:ARG:NH1	1.62	1.12
2:B:497:CYS:HB2	2:B:510:MET:HE1	1.15	1.11
2:B:497:CYS:HB2	2:B:510:MET:HE3	1.17	1.10
2:B:414:ALA:CA	2:B:415:ARG:HB2	1.82	1.09
2:A:534:GLN:HB3	2:A:538:LEU:HD12	1.27	1.08
2:B:497:CYS:CB	2:B:510:MET:CE	2.26	1.08
2:A:495:PHE:CE2	2:A:507:GLU:HG3	1.89	1.07
2:A:516:THR:HA	2:A:533:ARG:HH11	1.14	1.05
2:B:536:GLN:O	2:B:539:ASP:N	1.91	1.02
1:D:3:DT:H3'	2:B:544:ARG:NH2	1.74	1.02
2:A:534:GLN:CB	2:A:538:LEU:HD12	1.90	1.01
2:B:414:ALA:HA	2:B:415:ARG:HB2	1.02	1.00
2:B:411:ILE:HD12	2:B:430:HIS:CD2	1.97	0.99
2:B:534:GLN:HB3	2:B:538:LEU:CD1	1.95	0.97
2:B:414:ALA:HA	2:B:415:ARG:CB	1.96	0.92
2:A:500:CYS:HB3	2:A:517:HIS:CE1	2.04	0.92
2:B:534:GLN:HB3	2:B:538:LEU:HD13	1.51	0.91
2:B:408:GLU:HA	2:B:414:ALA:O	1.73	0.88
2:B:497:CYS:CA	2:B:510:MET:HE1	2.06	0.86
1:D:3:DT:H3'	2:B:544:ARG:HH21	1.36	0.86
2:A:513:HIS:O	2:A:516:THR:HG22	1.74	0.86
2:B:436:LYS:CB	2:B:437:PHE:HA	2.06	0.86
2:A:510:MET:HE3	2:A:510:MET:O	1.78	0.83
2:A:500:CYS:HB3	2:A:517:HIS:NE2	1.94	0.81
2:A:568:ASN:HD22	3:E:22:DT:P	2.03	0.80
2:A:555:PHE:HB2	2:A:564:PHE:O	1.82	0.80
2:B:437:PHE:HE1	2:B:449:LYS:N	1.81	0.79
2:B:412:CYS:SG	2:B:425:HIS:CE1	2.76	0.79
2:A:442:CYS:SG	2:A:444:THR:OG1	2.41	0.79
2:A:535:LYS:NZ	3:E:18:DG:OP1	2.15	0.78
2:A:535:LYS:NZ	3:E:18:DG:P	2.56	0.78
2:B:409:CYS:N	2:B:414:ALA:O	2.18	0.76
2:B:416:PHE:CD1	2:B:422:MET:HA	2.21	0.76
2:A:490:LYS:HA	2:A:491:ASN:C	2.05	0.75
2:B:416:PHE:HD1	2:B:422:MET:HB2	1.52	0.74
2:B:437:PHE:CE1	2:B:449:LYS:N	2.56	0.73
2:B:567:ARG:NH1	3:C:21:DC:OP2	2.22	0.73
2:B:555:PHE:HB2	2:B:564:PHE:O	1.91	0.71
2:B:513:HIS:O	2:B:516:THR:HG23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:516:THR:CA	2:A:533:ARG:HH11	2.00	0.69
2:B:406:PRO:HB2	2:B:407:TYR:CD2	2.27	0.69
2:B:534:GLN:HG2	2:B:535:LYS:H	1.57	0.69
2:A:562:LYS:HZ3	2:A:573:HIS:HE1	1.40	0.69
2:A:507:GLU:O	2:A:511:ILE:HD12	1.93	0.68
2:B:507:GLU:O	2:B:511:ILE:HD12	1.94	0.67
2:B:534:GLN:CG	2:B:535:LYS:H	2.07	0.67
2:B:568:ASN:OD1	3:C:22:DT:OP2	2.14	0.66
2:B:442:CYS:SG	2:B:444:THR:OG1	2.54	0.65
2:A:436:LYS:CB	2:A:437:PHE:HA	2.26	0.65
2:B:498:ASP:N	2:B:498:ASP:OD1	2.25	0.65
1:F:3:DT:H2"	1:F:4:DG:C8	2.32	0.64
2:A:568:ASN:ND2	3:E:22:DT:P	2.68	0.64
2:B:414:ALA:CA	2:B:415:ARG:CB	2.63	0.64
3:C:22:DT:H2"	3:C:23:DG:C8	2.33	0.64
2:A:535:LYS:HZ1	3:E:18:DG:P	2.18	0.63
2:B:409:CYS:O	2:B:413:HIS:HA	1.98	0.63
3:C:14:DT:H2"	3:C:15:DG:C8	2.33	0.62
1:D:3:DT:H2"	1:D:4:DG:C8	2.35	0.62
2:A:534:GLN:HB2	2:A:538:LEU:HD12	1.82	0.61
2:B:504:SER:OG	2:B:506:GLN:O	2.16	0.61
2:B:523:TYR:OH	2:B:535:LYS:HG2	1.99	0.61
1:F:2:DT:H2'	1:F:3:DT:C6	2.35	0.61
1:D:2:DT:H2'	1:D:3:DT:C6	2.36	0.61
3:E:22:DT:H2"	3:E:23:DG:C8	2.35	0.61
2:A:406:PRO:HB2	2:A:407:TYR:CD1	2.37	0.60
2:B:497:CYS:CA	2:B:510:MET:CE	2.73	0.59
2:A:535:LYS:NZ	3:E:18:DG:OP2	2.36	0.59
2:A:534:GLN:NE2	2:A:537:LEU:HD23	2.18	0.59
2:A:557:CYS:SG	2:A:558:SER:N	2.76	0.59
2:A:502:TYR:CD1	2:A:513:HIS:CG	2.91	0.58
2:A:562:LYS:HZ3	2:A:573:HIS:CE1	2.22	0.58
3:E:20:DA:H2"	3:E:21:DC:O5'	2.04	0.57
2:B:406:PRO:HB2	2:B:407:TYR:CG	2.39	0.57
1:F:8:DT:H1'	1:F:9:DA:H5'	1.86	0.57
2:B:557:CYS:SG	2:B:558:SER:N	2.78	0.57
2:B:407:TYR:N	2:B:407:TYR:CD1	2.72	0.57
2:A:545:TYR:N	2:A:545:TYR:CD2	2.73	0.57
2:B:482:LEU:HD12	2:B:482:LEU:O	2.05	0.56
3:E:14:DT:H2"	3:E:15:DG:C8	2.39	0.56
2:A:567:ARG:HH21	2:A:567:ARG:HG3	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:455:HIS:HD2	1:F:19:DA:OP1	1.88	0.56
2:A:500:CYS:CB	2:A:517:HIS:HE2	2.12	0.56
2:B:534:GLN:OE1	2:B:537:LEU:HD23	2.05	0.56
3:C:20:DA:H2"	3:C:21:DC:O5'	2.06	0.56
2:A:450:SER:CB	3:E:5:DC:H5	2.19	0.56
2:B:507:GLU:HG2	2:B:511:ILE:HD11	1.88	0.56
1:D:20:DC:H6	1:D:20:DC:H5'	1.70	0.55
2:A:523:TYR:CZ	2:A:535:LYS:HA	2.42	0.55
2:B:416:PHE:HD1	2:B:422:MET:CB	2.20	0.55
2:A:491:ASN:CB	2:A:492:GLU:CB	2.85	0.55
2:A:491:ASN:CB	2:A:492:GLU:CA	2.84	0.55
2:A:508:ARG:HG3	2:A:509:HIS:N	2.22	0.55
1:F:2:DT:H2"	1:F:3:DT:H5'	1.88	0.55
2:B:416:PHE:CD1	2:B:422:MET:HB2	2.37	0.55
2:B:502:TYR:CD1	2:B:513:HIS:CG	2.95	0.54
2:B:523:TYR:CZ	2:B:535:LYS:HA	2.42	0.54
2:A:534:GLN:CG	2:A:535:LYS:H	2.20	0.54
1:F:21:DC:H2"	1:F:22:DA:C8	2.42	0.54
1:D:24:DC:H2"	1:D:25:DA:C8	2.43	0.54
2:A:498:ASP:OD1	2:A:498:ASP:N	2.40	0.53
2:A:554:ALA:O	2:A:563:THR:HG23	2.08	0.53
2:A:568:ASN:ND2	2:A:568:ASN:H	2.05	0.53
2:B:436:LYS:CB	2:B:437:PHE:CA	2.85	0.53
2:B:483:ILE:HG13	2:B:484:GLN:N	2.24	0.53
1:D:6:DA:C8	1:D:6:DA:H5'	2.44	0.53
2:B:468:LYS:HD2	2:B:469:CYS:O	2.09	0.53
1:D:8:DT:H1'	1:D:9:DA:H5'	1.90	0.53
1:D:11:DC:H2"	1:D:12:DA:OP2	2.09	0.53
2:B:408:GLU:CA	2:B:414:ALA:O	2.52	0.53
2:B:534:GLN:HG2	2:B:535:LYS:N	2.24	0.53
2:B:450:SER:CB	3:C:5:DC:H5	2.23	0.52
2:A:500:CYS:CB	2:A:517:HIS:NE2	2.64	0.52
2:A:532:PHE:HZ	2:A:541:HIS:ND1	2.07	0.52
2:B:409:CYS:SG	2:B:426:ILE:HD11	2.50	0.52
2:B:534:GLN:CG	2:B:535:LYS:N	2.73	0.52
2:B:472:CYS:HB2	2:B:489:HIS:CE1	2.43	0.52
2:A:534:GLN:NE2	2:A:537:LEU:CD2	2.73	0.52
2:A:560:CYS:SG	2:A:562:LYS:NZ	2.79	0.52
2:B:407:TYR:HE1	2:B:418:GLN:HA	1.75	0.52
2:A:410:TYR:HD1	2:A:410:TYR:H	1.58	0.51
2:B:411:ILE:HD12	2:B:430:HIS:HD2	1.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:DC:H5'	1:F:20:DC:H6	1.74	0.51
1:F:6:DA:C8	1:F:6:DA:H5'	2.46	0.51
2:B:554:ALA:O	2:B:563:THR:HG23	2.11	0.51
2:A:535:LYS:HG2	2:A:536:GLN:H	1.76	0.51
1:D:2:DT:H2"	1:D:3:DT:H5'	1.91	0.51
1:F:24:DC:H2"	1:F:25:DA:C8	2.46	0.50
2:A:508:ARG:O	2:A:512:MET:HG3	2.11	0.50
2:A:525:CYS:SG	2:A:546:HIS:HD2	2.35	0.50
2:B:437:PHE:CE1	2:B:449:LYS:CA	2.94	0.50
2:A:406:PRO:HB2	2:A:407:TYR:CG	2.47	0.49
2:A:497:CYS:HB2	2:A:510:MET:CE	2.42	0.49
2:A:516:THR:HG23	2:A:517:HIS:N	2.27	0.49
1:D:21:DC:H2"	1:D:22:DA:C8	2.48	0.49
2:B:459:GLN:HB2	2:B:460:HIS:CD2	2.47	0.49
2:B:484:GLN:O	2:B:487:LYS:HB3	2.13	0.49
2:B:534:GLN:HB3	2:B:538:LEU:HD12	1.89	0.49
2:B:467:LYS:HB2	2:B:482:LEU:HD22	1.95	0.49
1:D:3:DT:H3'	2:B:544:ARG:HH22	1.69	0.49
2:B:413:HIS:N	2:B:413:HIS:ND1	2.60	0.49
2:B:425:HIS:HD2	2:B:426:ILE:HD12	1.76	0.49
2:A:452:LEU:O	2:A:456:LEU:HD22	2.13	0.49
2:A:507:GLU:O	2:A:510:MET:N	2.46	0.48
2:B:497:CYS:HA	2:B:510:MET:CE	2.43	0.48
2:B:425:HIS:CD2	2:B:426:ILE:HD12	2.48	0.48
2:B:428:GLN:NE2	2:B:448:ARG:HE	2.11	0.48
2:A:416:PHE:CD1	2:A:422:MET:HB2	2.49	0.48
2:A:495:PHE:N	2:A:495:PHE:CD1	2.81	0.48
2:B:414:ALA:CB	2:B:416:PHE:CZ	2.97	0.48
2:A:467:LYS:O	2:A:475:VAL:HA	2.13	0.47
3:C:14:DT:H2"	3:C:15:DG:H8	1.78	0.47
2:A:502:TYR:HD1	2:A:513:HIS:CG	2.32	0.47
2:A:558:SER:HA	2:A:559:LYS:HA	1.68	0.47
2:A:468:LYS:HE3	2:A:469:CYS:O	2.15	0.47
2:B:467:LYS:O	2:B:475:VAL:HA	2.14	0.47
2:B:532:PHE:CZ	2:B:541:HIS:CG	3.03	0.47
2:A:545:TYR:N	2:A:545:TYR:HD2	2.13	0.47
2:A:409:CYS:O	2:A:413:HIS:HA	2.14	0.46
2:B:451:ASP:O	2:B:454:VAL:HG12	2.15	0.46
2:A:500:CYS:SG	2:A:513:HIS:CE1	3.01	0.46
2:A:567:ARG:NH2	2:A:567:ARG:HG3	2.29	0.46
2:A:451:ASP:O	2:A:454:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:457:ARG:O	2:A:461:SER:OG	2.31	0.46
2:B:532:PHE:HZ	2:B:541:HIS:CG	2.33	0.45
2:A:490:LYS:HE2	3:E:15:DG:OP2	2.16	0.45
2:B:521:LYS:HA	2:B:533:ARG:HA	1.98	0.45
1:D:14:DA:C2	3:C:15:DG:C2	3.05	0.45
2:B:508:ARG:HG3	2:B:509:HIS:N	2.31	0.45
2:A:541:HIS:C	2:A:541:HIS:CD2	2.90	0.45
2:B:416:PHE:CD1	2:B:422:MET:CA	2.96	0.45
2:B:536:GLN:O	2:B:538:LEU:N	2.50	0.45
2:B:416:PHE:CD1	2:B:422:MET:CB	3.00	0.44
2:A:494:ARG:HH22	3:E:15:DG:P	2.40	0.44
1:F:14:DA:C2	3:E:15:DG:C2	3.05	0.44
2:A:502:TYR:CD1	2:A:513:HIS:ND1	2.86	0.44
3:E:6:DT:H2"	3:E:7:DG:C8	2.53	0.44
2:A:458:LYS:HB3	2:A:458:LYS:HE2	1.53	0.44
2:B:558:SER:HA	2:B:559:LYS:HA	1.68	0.44
3:C:6:DT:C2'	3:C:7:DG:C8	3.01	0.44
2:B:406:PRO:O	2:B:416:PHE:O	2.36	0.43
2:B:458:LYS:HB3	2:B:458:LYS:HE2	1.63	0.43
2:A:450:SER:HB2	3:E:5:DC:H5	1.82	0.43
2:B:452:LEU:O	2:B:456:LEU:HD22	2.17	0.43
3:C:6:DT:H2"	3:C:7:DG:C8	2.54	0.43
2:B:416:PHE:CZ	2:B:425:HIS:CG	3.07	0.43
2:B:414:ALA:HB3	2:B:416:PHE:CE1	2.54	0.43
2:A:545:TYR:OH	1:F:4:DG:OP1	2.18	0.43
2:A:491:ASN:CB	2:A:492:GLU:HA	2.49	0.42
2:B:406:PRO:CB	2:B:407:TYR:HA	2.49	0.42
2:B:409:CYS:SG	2:B:426:ILE:CD1	3.07	0.42
2:A:507:GLU:O	2:A:508:ARG:C	2.57	0.42
1:D:20:DC:C6	1:D:20:DC:H5'	2.51	0.42
2:B:407:TYR:N	2:B:416:PHE:O	2.53	0.42
3:E:6:DT:C2'	3:E:7:DG:C8	3.02	0.42
2:A:472:CYS:HB2	2:A:489:HIS:CE1	2.54	0.42
1:F:10:DC:H2"	1:F:11:DC:C6	2.55	0.42
2:B:559:LYS:O	2:B:561:GLY:N	2.53	0.42
2:A:467:LYS:HB2	2:A:482:LEU:HD22	2.02	0.41
2:B:523:TYR:HB2	2:B:532:PHE:O	2.20	0.41
2:B:412:CYS:O	2:B:412:CYS:SG	2.79	0.41
1:F:20:DC:H5'	1:F:20:DC:C6	2.53	0.41
2:A:455:HIS:ND1	2:A:455:HIS:C	2.74	0.41
2:A:534:GLN:CG	2:A:535:LYS:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:428:GLN:HE21	2:B:448:ARG:HE	1.67	0.41
2:A:479:ARG:HH21	1:F:18:DA:P	2.44	0.41
2:A:497:CYS:HB2	2:A:510:MET:HE1	2.03	0.41
2:A:407:TYR:HE1	2:A:417:THR:O	2.04	0.40
2:A:495:PHE:CD2	2:A:507:GLU:HG3	2.47	0.40
2:A:535:LYS:HZ3	3:E:18:DG:P	2.42	0.40
2:B:416:PHE:CZ	2:B:425:HIS:CB	3.04	0.40
3:E:21:DC:H2'	3:E:22:DT:H72	2.03	0.40
2:A:487:LYS:C	2:A:489:HIS:H	2.24	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:413:HIS:NE2	2:B:413:HIS:NE2[1_566]	2.01	0.19
2:A:413:HIS:CE1	2:B:413:HIS:CE1[1_566]	2.05	0.15
2:A:413:HIS:CE1	2:B:413:HIS:NE2[1_566]	2.19	0.01

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	
2	A	158/176 (90%)	149 (94%)	9 (6%)	0	100	100
2	B	160/176 (91%)	150 (94%)	9 (6%)	1 (1%)	25	60
All	All	318/352 (90%)	299 (94%)	18 (6%)	1 (0%)	41	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	415	ARG

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
2	A	132/158 (84%)	108 (82%)	24 (18%)	1 7
2	B	132/158 (84%)	103 (78%)	29 (22%)	1 4
All	All	264/316 (84%)	211 (80%)	53 (20%)	1 5

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	408	GLU
2	A	409	CYS
2	A	410	TYR
2	A	416	PHE
2	A	418	GLN
2	A	421	THR
2	A	423	LYS
2	A	444	THR
2	A	456	LEU
2	A	461	SER
2	A	464	GLU
2	A	470	ARG
2	A	490	LYS
2	A	497	CYS
2	A	500	CYS
2	A	512	MET
2	A	515	ARG
2	A	539	ASP
2	A	541	HIS
2	A	545	TYR
2	A	558	SER
2	A	568	ASN
2	A	570	MET
2	A	575	ASP
2	B	407	TYR
2	B	409	CYS
2	B	413	HIS

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Mol	Chain	Res	Type
2	B	415	ARG
2	B	417	THR
2	B	418	GLN
2	B	421	THR
2	B	437	PHE
2	B	444	THR
2	B	450	SER
2	B	456	LEU
2	B	461	SER
2	B	464	GLU
2	B	468	LYS
2	B	488	SER
2	B	490	LYS
2	B	494	ARG
2	B	497	CYS
2	B	504	SER
2	B	512	MET
2	B	516	THR
2	B	522	PRO
2	B	535	LYS
2	B	536	GLN
2	B	541	HIS
2	B	558	SER
2	B	568	ASN
2	B	569	THR
2	B	570	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	568	ASN
2	B	465	GLN

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 12 ligands modelled in this entry, 12 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	D	26/26 (100%)	-0.43	0 100 100	44, 79, 101, 105	0
1	F	26/26 (100%)	-0.51	0 100 100	47, 80, 95, 98	0
2	A	166/176 (94%)	0.26	8 (4%) 30 19	35, 75, 103, 128	0
2	B	168/176 (95%)	0.22	5 (2%) 50 34	15, 78, 110, 137	0
3	C	26/26 (100%)	-0.36	0 100 100	53, 70, 102, 107	0
3	E	26/26 (100%)	-0.51	0 100 100	53, 68, 101, 109	0
All	All	438/456 (96%)	0.08	13 (2%) 50 34	15, 76, 107, 137	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	448	ARG	4.1
2	A	503	ALA	3.6
2	A	448	ARG	3.3
2	A	416	PHE	3.2
2	A	446	ILE	2.9
2	A	413	HIS	2.7
2	A	537	LEU	2.6
2	B	544	ARG	2.3
2	A	567	ARG	2.3
2	B	416	PHE	2.2
2	A	411	ILE	2.0
2	B	407	TYR	2.0
2	B	522	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no 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	B	601	1/1	0.59	0.80	248,248,248,248	0
4	ZN	B	606	1/1	0.79	0.06	61,61,61,61	0
4	ZN	B	604	1/1	0.85	0.15	110,110,110,110	0
4	ZN	B	603	1/1	0.85	0.13	82,82,82,82	0
4	ZN	A	605	1/1	0.86	0.06	37,37,37,37	0
4	ZN	B	602	1/1	0.92	0.05	68,68,68,68	0
4	ZN	B	605	1/1	0.92	0.05	60,60,60,60	0
4	ZN	A	606	1/1	0.94	0.05	31,31,31,31	0
4	ZN	A	604	1/1	0.95	0.05	42,42,42,42	0
4	ZN	A	601	1/1	0.97	0.10	50,50,50,50	0
4	ZN	A	603	1/1	0.98	0.04	23,23,23,23	0
4	ZN	A	602	1/1	0.99	0.02	9,9,9,9	0

6.5 Other polymers (i)

There are no such residues in this entry.