Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2023 – 01:10 PM EDT

PDB ID	:	8SSR
Title	:	ZnFs 3-11 of CCCTC-binding factor (CTCF) Complexed with 35mer DNA 35-20
Authors	:	Horton, J.R.; Yang, J.; Cheng, X.
Deposited on	:	2023-05-08
Resolution	:	3.14 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

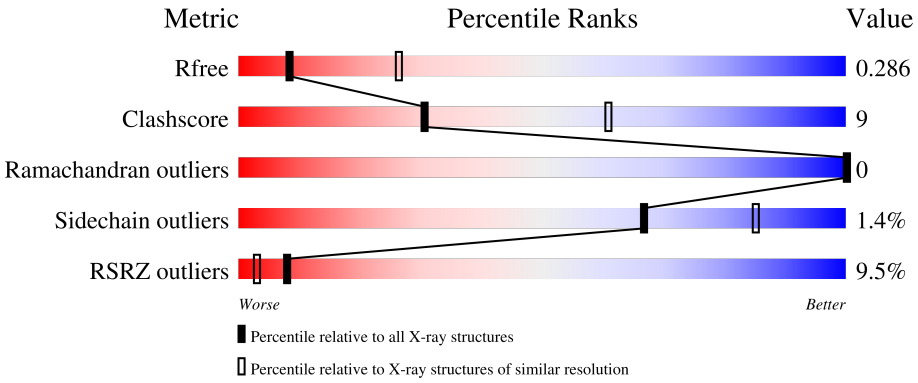
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.14 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	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	288	4% 69% 21% • 10%
1	D	288	16% 63% 17% 20%
2	B	35	54% 46%
2	E	35	3% 54% 46%
3	C	35	54% 46%

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Mol	Chain	Length	Quality of chain
3	F	35	40% 60%

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
5	NA	C	101	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6926 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	260	Total	C	N	O	S	0	0	0
			2152	1330	425	368	29			
1	D	230	Total	C	N	O	S	0	0	0
			1899	1175	372	326	26			

- Molecule 2 is a DNA chain called DNA (35-MER) Strand I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	35	Total	C	N	O	P	0	0	0
			713	341	127	211	34			
2	E	35	Total	C	N	O	P	0	0	0
			713	341	127	211	34			

- Molecule 3 is a DNA chain called DNA (35-MER) Strand II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	35	Total	C	N	O	P	0	0	0
			715	341	136	204	34			
3	F	35	Total	C	N	O	P	0	0	0
			715	341	136	204	34			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	Zn	0	0
			9	9		
4	D	8	Total	Zn	0	0
			8	8		

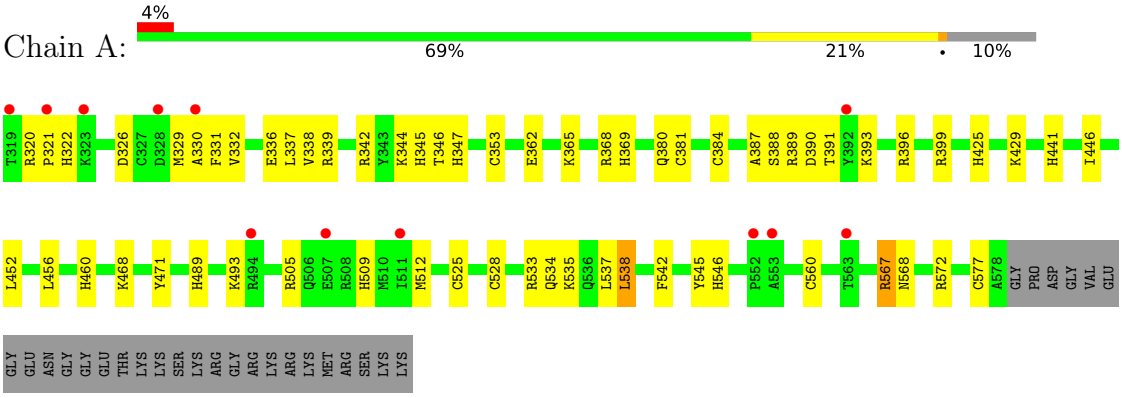
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0

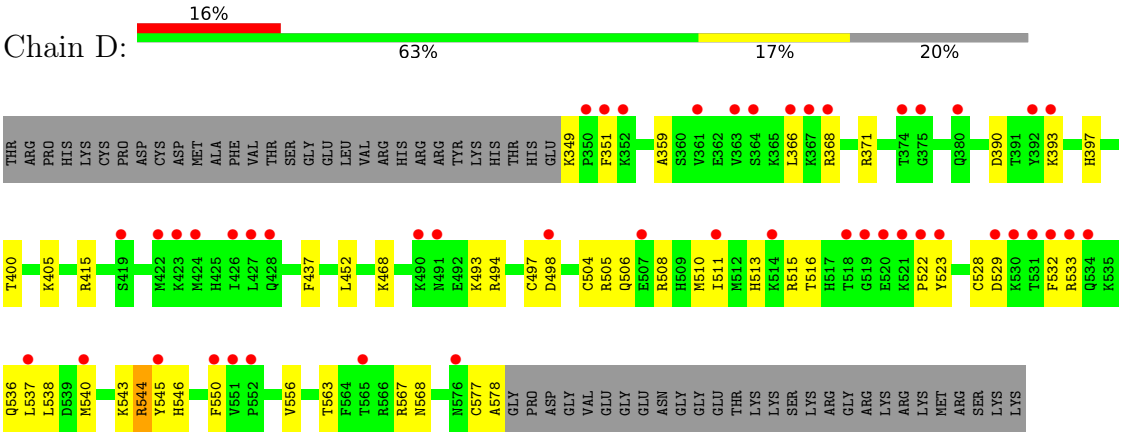
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Transcriptional repressor CTCF

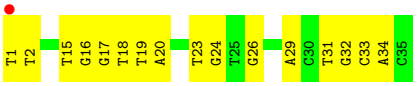


• Molecule 1: Transcriptional repressor CTCF



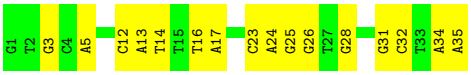
• Molecule 2: DNA (35-MER) Strand I

• Molecule 2: DNA (35-MER) Strand I



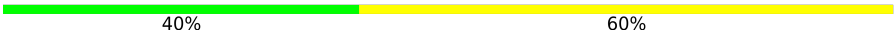
• Molecule 3: DNA (35-MER) Strand II

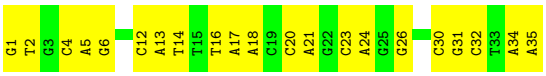
Chain C:



• Molecule 3: DNA (35-MER) Strand II

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	362.21Å 68.09Å 61.99Å 90.00° 94.87° 90.00°	Depositor
Resolution (Å)	37.59 – 3.14 49.53 – 3.14	Depositor EDS
% Data completeness (in resolution range)	90.6 (37.59-3.14) 81.0 (49.53-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.249 , 0.284 0.253 , 0.286	Depositor DCC
R_{free} test set	1215 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	85.6	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 107.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6926	wwPDB-VP
Average B, all atoms (Å^2)	203.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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: NA, 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	0.23	0/2209	0.48	0/2954
1	D	0.24	0/1948	0.49	0/2604
2	B	0.49	0/798	0.92	0/1230
2	E	0.48	0/798	0.91	0/1230
3	C	0.51	0/803	0.87	0/1236
3	F	0.48	0/803	0.84	0/1236
All	All	0.37	0/7359	0.70	0/10490

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2152	0	2078	43	0
1	D	1899	0	1834	35	0
2	B	713	0	397	13	0
2	E	713	0	397	13	0
3	C	715	0	394	12	0
3	F	715	0	394	15	0
4	A	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	8	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
All	All	6926	0	5494	114	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 9.

All (114) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:523:TYR:HB3	1:D:538:LEU:HD22	1.66	0.77
1:A:322:HIS:HB3	1:A:337:LEU:HD22	1.69	0.74
1:D:537:LEU:HD11	3:F:4:DC:H2'	1.72	0.72
1:A:389:ARG:HH12	3:C:25:DG:H3'	1.55	0.70
1:A:389:ARG:NH1	3:C:26:DG:OP2	2.24	0.69
1:A:368:ARG:NH2	3:C:28:DG:N7	2.40	0.65
1:D:368:ARG:HA	1:D:371:ARG:HD2	1.80	0.64
1:D:511:ILE:HG22	1:D:515:ARG:HE	1.64	0.63
3:F:13:DA:H2"	3:F:14:DT:H5"	1.81	0.62
1:D:536:GLN:HE21	2:E:29:DA:N6	1.97	0.62
2:B:31:DT:H2"	2:B:32:DG:C8	2.36	0.61
1:D:536:GLN:NE2	3:F:6:DG:O6	2.33	0.61
2:E:15:DT:H2"	2:E:16:DG:C8	2.37	0.59
3:C:31:DG:H2"	3:C:32:DC:H5"	1.85	0.59
1:D:511:ILE:O	1:D:515:ARG:HG3	2.03	0.58
1:A:572:ARG:NH2	2:B:32:DG:OP2	2.36	0.58
1:A:533:ARG:NH1	3:C:5:DA:OP1	2.37	0.57
2:B:15:DT:H2"	2:B:16:DG:C8	2.40	0.57
1:A:326:ASP:HB2	1:A:345:HIS:CE1	2.39	0.57
1:D:506:GLN:OE1	1:D:508:ARG:NE	2.35	0.57
1:A:446:ILE:HD12	1:A:452:LEU:HA	1.89	0.55
1:D:493:LYS:HD3	1:D:504:CYS:HA	1.88	0.55
1:D:568:ASN:ND2	2:E:32:DG:OP2	2.39	0.55
1:A:338:VAL:O	1:A:342:ARG:HG2	2.07	0.54
1:A:388:SER:HB2	1:A:393:LYS:HB2	1.88	0.54
1:D:390:ASP:HB3	1:D:393:LYS:HG2	1.89	0.54
1:D:522:PRO:HD2	1:D:533:ARG:HA	1.90	0.53
2:B:5:DC:H2"	2:B:6:DG:H8	1.73	0.53
1:D:497:CYS:HA	1:D:510:MET:HE3	1.91	0.53
1:D:556:VAL:HG22	1:D:563:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:30:DC:H2"	3:F:31:DG:N7	2.24	0.53
2:B:16:DG:H2"	2:B:17:DG:C8	2.44	0.52
1:A:339:ARG:NH2	3:C:31:DG:N7	2.48	0.52
2:E:33:DC:H2"	2:E:34:DA:C8	2.46	0.51
1:A:320:ARG:NH1	1:A:330:ALA:O	2.43	0.51
2:E:31:DT:H2"	2:E:32:DG:C8	2.46	0.51
2:B:19:DT:H2"	2:B:20:DA:C8	2.46	0.51
1:A:456:LEU:HD23	1:A:460:HIS:HD2	1.77	0.50
1:A:471:TYR:HB2	1:A:489:HIS:HD2	1.77	0.50
2:B:17:DG:H1'	2:B:18:DT:H5'	1.93	0.50
1:A:396:ARG:HG3	1:A:399:ARG:HH21	1.76	0.50
2:B:33:DC:H2"	2:B:34:DA:C8	2.47	0.50
1:A:525:CYS:CB	1:A:528:CYS:SG	2.97	0.50
1:D:493:LYS:HG2	1:D:505:ARG:HG3	1.94	0.49
3:C:23:DC:H2'	3:C:24:DA:C8	2.47	0.49
1:D:351:PHE:HB3	1:D:366:LEU:HD22	1.94	0.49
3:C:16:DT:H2"	3:C:17:DA:C8	2.48	0.49
1:D:532:PHE:CG	1:D:533:ARG:N	2.80	0.49
2:E:16:DG:H2"	2:E:17:DG:C8	2.48	0.48
1:D:405:LYS:O	1:D:415:ARG:NH2	2.42	0.48
1:D:544:ARG:HG3	1:D:545:TYR:HD1	1.78	0.48
1:A:471:TYR:HB2	1:A:489:HIS:CD2	2.49	0.48
1:D:437:PHE:HB3	1:D:452:LEU:HD22	1.96	0.47
1:D:532:PHE:HZ	3:F:5:DA:OP2	1.96	0.47
3:F:16:DT:H2"	3:F:17:DA:C8	2.49	0.47
1:D:529:ASP:N	1:D:529:ASP:OD1	2.41	0.47
2:B:5:DC:H2"	2:B:6:DG:C8	2.50	0.47
1:D:567:ARG:HB3	2:E:31:DT:OP2	2.14	0.47
2:E:19:DT:H2"	2:E:20:DA:C8	2.49	0.47
2:B:23:DT:H2"	2:B:24:DG:C8	2.50	0.47
1:A:362:GLU:HB2	1:A:365:LYS:HG2	1.97	0.47
1:D:513:HIS:O	1:D:516:THR:OG1	2.23	0.47
1:A:493:LYS:HG2	1:A:505:ARG:HG3	1.97	0.46
1:D:528:CYS:HB3	1:D:546:HIS:CE1	2.50	0.46
1:A:321:PRO:HD2	1:A:332:VAL:HA	1.97	0.46
1:A:441:HIS:HB2	1:A:460:HIS:CD2	2.50	0.46
1:A:567:ARG:HD2	2:B:31:DT:OP2	2.15	0.46
3:F:23:DC:H2'	3:F:24:DA:C8	2.51	0.46
1:D:497:CYS:SG	1:D:498:ASP:N	2.89	0.46
3:F:31:DG:H2"	3:F:32:DC:C5	2.52	0.45
1:A:542:PHE:HA	1:A:546:HIS:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:23:DT:H2"	2:E:24:DG:C8	2.51	0.45
3:F:20:DC:H2"	3:F:21:DA:C8	2.52	0.45
1:A:525:CYS:HB3	1:A:528:CYS:SG	2.57	0.45
1:A:329:MET:HB3	1:A:331:PHE:HE1	1.81	0.45
3:C:34:DA:H4'	3:C:35:DA:OP1	2.16	0.45
1:A:535:LYS:HA	1:A:538:LEU:HD23	1.99	0.44
1:D:508:ARG:NH2	2:E:26:DG:N7	2.64	0.44
3:F:1:DG:H2"	3:F:2:DT:H5'	1.98	0.44
3:F:12:DC:H2"	3:F:13:DA:C8	2.53	0.44
1:A:390:ASP:OD1	1:A:391:THR:N	2.51	0.44
1:D:349:LYS:HB3	1:D:359:ALA:HB1	2.00	0.44
3:C:13:DA:H2"	3:C:14:DT:H5"	2.00	0.44
1:A:381:CYS:CB	1:A:384:CYS:SG	3.06	0.43
1:A:381:CYS:HB3	1:A:384:CYS:SG	2.58	0.43
2:E:17:DG:H1'	2:E:18:DT:H5'	2.00	0.43
1:A:353:CYS:HB3	1:A:369:HIS:CD2	2.53	0.43
2:E:16:DG:H2"	2:E:17:DG:H8	1.84	0.43
3:C:12:DC:H2"	3:C:13:DA:C8	2.54	0.43
1:D:397:HIS:O	1:D:400:THR:HG22	2.18	0.43
3:F:34:DA:H2"	3:F:35:DA:O5'	2.18	0.43
3:F:30:DC:H2"	3:F:31:DG:C8	2.54	0.43
1:A:342:ARG:HA	1:A:346:THR:OG1	2.19	0.42
1:A:441:HIS:HB2	1:A:460:HIS:NE2	2.34	0.42
1:A:331:PHE:HD2	1:A:336:GLU:HB3	1.85	0.42
1:D:544:ARG:HG3	1:D:545:TYR:CD1	2.55	0.42
1:A:342:ARG:HD2	1:A:346:THR:HG21	2.00	0.42
1:A:425:HIS:O	1:A:429:LYS:HB2	2.20	0.42
1:D:577:CYS:SG	1:D:578:ALA:N	2.93	0.42
1:A:509:HIS:HA	1:A:512:MET:HE2	2.01	0.42
1:A:380:GLN:HA	1:A:387:ALA:HA	2.02	0.42
1:A:468:LYS:HD3	1:D:468:LYS:H	1.85	0.42
1:D:393:LYS:NZ	3:F:26:DG:N7	2.47	0.41
3:F:17:DA:H2"	3:F:18:DA:C8	2.54	0.41
1:A:344:LYS:O	1:A:347:HIS:NE2	2.53	0.41
1:A:320:ARG:HD3	1:A:330:ALA:HB3	2.01	0.41
1:D:543:LYS:HD2	1:D:550:PHE:CD1	2.55	0.41
1:D:515:ARG:HB3	1:D:533:ARG:HB3	2.03	0.41
1:A:534:GLN:HB2	1:A:537:LEU:HG	2.03	0.40
2:B:28:DT:H2"	2:B:29:DA:C8	2.56	0.40
2:E:1:DT:H2"	2:E:2:DT:H5'	2.03	0.40
1:A:545:TYR:OH	3:C:3:DG:OP1	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:DG:H2"	2:B:17:DG:H8	1.86	0.40
1:A:560:CYS:HB3	1:A:577:CYS:SG	2.62	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	258/288 (90%)	250 (97%)	8 (3%)	0	100	100
1	D	228/288 (79%)	224 (98%)	4 (2%)	0	100	100
All	All	486/576 (84%)	474 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	236/259 (91%)	233 (99%)	3 (1%)	69	86
1	D	208/259 (80%)	205 (99%)	3 (1%)	67	85
All	All	444/518 (86%)	438 (99%)	6 (1%)	67	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	538	LEU
1	A	567	ARG
1	A	568	ASN
1	D	494	ARG
1	D	540	MET
1	D	544	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	568	ASN
1	D	534	GLN
1	D	536	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 19 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	A	260/288 (90%)	0.09	12 (4%) 32 15	94, 175, 300, 384	0
1	D	230/288 (79%)	1.09	47 (20%) 1 0	94, 220, 365, 477	0
2	B	35/35 (100%)	-0.15	0 100 100	114, 170, 288, 305	0
2	E	35/35 (100%)	-0.30	1 (2%) 51 30	157, 197, 341, 371	0
3	C	35/35 (100%)	-0.24	0 100 100	105, 158, 259, 309	0
3	F	35/35 (100%)	-0.30	0 100 100	138, 215, 393, 446	0
All	All	630/716 (87%)	0.38	60 (9%) 8 3	94, 194, 341, 477	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	350	PRO	16.5
1	D	534	GLN	9.4
1	D	363	VAL	9.1
1	D	361	VAL	8.8
1	D	351	PHE	8.5
1	D	532	PHE	8.5
1	A	328	ASP	8.3
1	D	520	GLU	8.3
1	D	392	TYR	8.0
1	D	519	GLY	7.7
1	D	374	THR	6.5
1	A	319	THR	6.4
1	D	537	LEU	5.9
1	A	323	LYS	5.5
1	D	364	SER	5.3
1	D	531	THR	5.1
1	D	367	LYS	4.6
1	D	522	PRO	4.5
1	D	426	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	530	LYS	4.4
1	D	552	PRO	4.3
1	D	533	ARG	4.2
1	D	428	GLN	4.2
1	D	551	VAL	4.2
2	E	1	DT	4.2
1	D	518	THR	4.2
1	D	366	LEU	4.1
1	D	523	TYR	4.1
1	D	514	LYS	4.0
1	D	540	MET	3.9
1	D	507	GLU	3.6
1	D	419	SER	3.6
1	D	550	PHE	3.5
1	A	330	ALA	3.2
1	D	368	ARG	3.2
1	D	423	LYS	3.1
1	D	529	ASP	3.1
1	D	380	GLN	3.1
1	D	576	ASN	2.9
1	D	375	GLY	2.8
1	A	392	TYR	2.8
1	A	321	PRO	2.6
1	A	563	THR	2.6
1	D	490	LYS	2.6
1	D	491	ASN	2.6
1	D	393	LYS	2.6
1	A	552	PRO	2.6
1	D	545	TYR	2.6
1	D	427	LEU	2.5
1	A	511	ILE	2.4
1	D	511	ILE	2.4
1	D	424	MET	2.3
1	D	498	ASP	2.3
1	A	507	GLU	2.2
1	D	422	MET	2.2
1	A	494	ARG	2.2
1	D	565	THR	2.1
1	D	352	LYS	2.1
1	A	553	ALA	2.1
1	D	521	LYS	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 monosaccharides 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	D	701	1/1	-0.67	0.13	401,401,401,401	0
5	NA	C	101	1/1	0.21	0.81	122,122,122,122	0
4	ZN	A	709	1/1	0.69	0.09	318,318,318,318	0
4	ZN	A	702	1/1	0.77	0.10	265,265,265,265	0
4	ZN	A	706	1/1	0.83	0.44	230,230,230,230	0
4	ZN	D	708	1/1	0.84	0.08	269,269,269,269	0
4	ZN	D	707	1/1	0.85	0.13	367,367,367,367	0
4	ZN	D	703	1/1	0.86	0.18	184,184,184,184	0
4	ZN	A	705	1/1	0.92	0.32	232,232,232,232	0
4	ZN	A	701	1/1	0.92	0.07	305,305,305,305	0
5	NA	A	710	1/1	0.94	1.45	182,182,182,182	0
4	ZN	D	706	1/1	0.94	0.07	276,276,276,276	0
4	ZN	A	707	1/1	0.95	0.18	146,146,146,146	0
4	ZN	A	708	1/1	0.95	0.20	234,234,234,234	0
4	ZN	D	704	1/1	0.95	0.36	271,271,271,271	0
4	ZN	A	704	1/1	0.95	0.18	156,156,156,156	0
4	ZN	D	705	1/1	0.96	0.35	225,225,225,225	0
4	ZN	D	702	1/1	0.98	0.17	224,224,224,224	0
4	ZN	A	703	1/1	0.99	0.25	120,120,120,120	0

6.5 Other polymers (i)

There are no such residues in this entry.