



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:58 am BST

PDB ID : 4HJE
Title : Crystal structure of p53 core domain in complex with DNA
Authors : Chen, Y.; Chen, L.
Deposited on : 2012-10-12
Resolution : 1.91 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 ⓘ](#)) 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

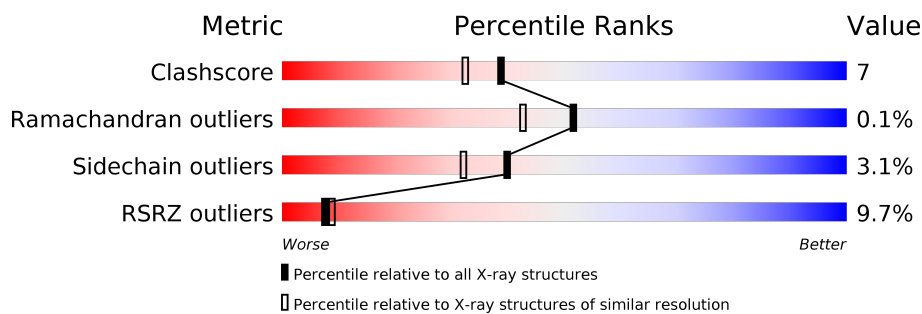
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	200	<div> <div>9%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	B	200	<div> <div>9%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	C	200	<div> <div>11%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	D	200	<div> <div>10%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
2	E	21	<div> <div>19%</div> <div>43%</div> <div>29%</div> <div>29%</div> </div>
3	F	21	<div> <div>10%</div> <div>24%</div> <div>57%</div> <div>19%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7975 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 Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1571	968	291	296	16			
1	B	200	Total	C	N	O	S	0	0	0
			1571	968	291	296	16			
1	C	200	Total	C	N	O	S	0	0	0
			1571	968	291	296	16			
1	D	200	Total	C	N	O	S	0	0	0
			1571	968	291	296	16			

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*CP*AP*CP*AP*AP*GP*TP*TP*AP*GP*AP*GP*AP*CP*AP*AP*GP*CP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	21	Total	C	N	O	P	0	0	0
			428	205	83	120	20			

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*GP*GP*CP*TP*TP*GP*TP*CP*TP*CP*TP*AP*AP*CP*TP*TP*GP*TP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	21	Total	C	N	O	P	0	0	0
			427	206	73	128	20			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Zn 1	0	0

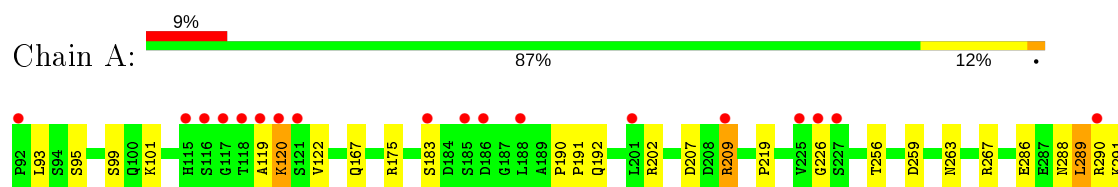
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	215	Total 215	O 215	0	0
5	B	163	Total 163	O 163	0	0
5	C	172	Total 172	O 172	0	0
5	D	210	Total 210	O 210	0	0
5	E	34	Total 34	O 34	0	0
5	F	38	Total 38	O 38	0	0

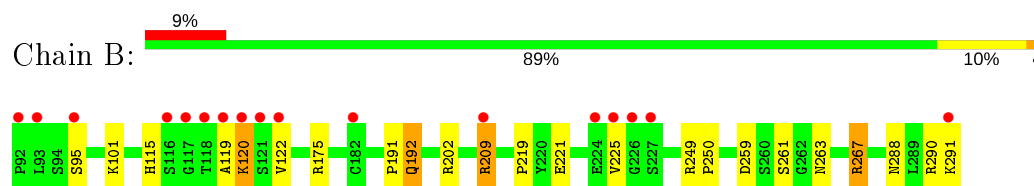
3 Residue-property plots [i](#)

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.

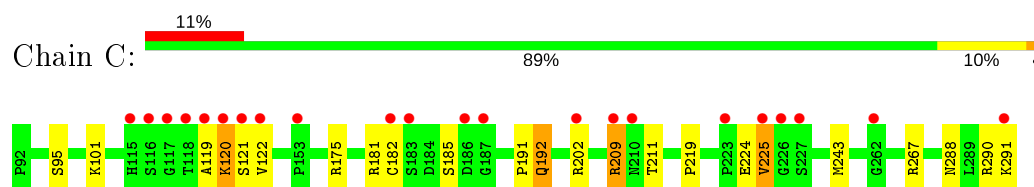
• Molecule 1: Cellular tumor antigen p53



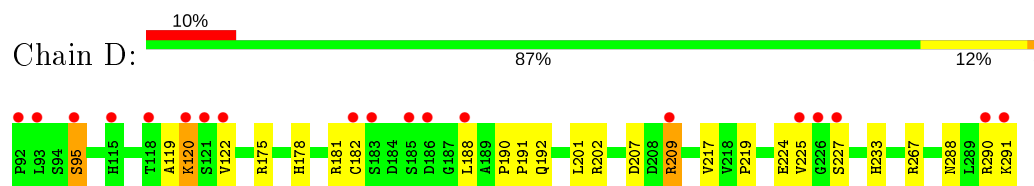
• Molecule 1: Cellular tumor antigen p53



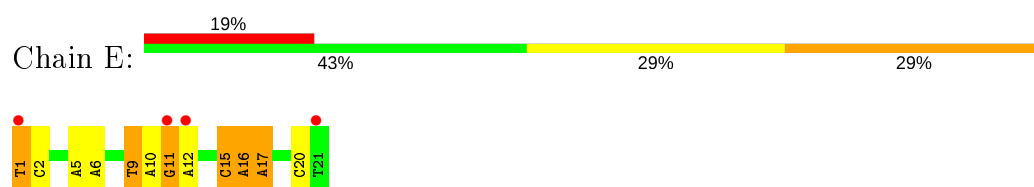
• Molecule 1: Cellular tumor antigen p53



• Molecule 1: Cellular tumor antigen p53



• Molecule 2: DNA (5'-D(*TP*CP*AP*CP*AP*AP*GP*TP*TP*AP*GP*AP*GP*AP*CP*AP*AP*GP*CP*CP*T)-3')



- Molecule 3: DNA (5'-D(*AP*GP*GP*CP*TP*TP*GP*TP*CP*TP*CP*TP*AP*AP*CP*TP*TP*GP*TP*GP*A)-3')

Chain F: 10% 24% 57% 19%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.42Å 93.88Å 145.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.66 – 1.91 48.66 – 1.91	Depositor EDS
% Data completeness (in resolution range)	96.1 (48.66-1.91) 96.2 (48.66-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.188 , 0.228 0.187 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7975	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3108e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/1607	0.61	2/2176 (0.1%)
1	B	0.32	0/1607	0.77	3/2176 (0.1%)
1	C	0.32	0/1607	0.61	2/2176 (0.1%)
1	D	0.36	0/1607	0.65	2/2176 (0.1%)
2	E	0.73	0/481	1.69	15/740 (2.0%)
3	F	0.79	0/477	1.87	16/735 (2.2%)
All	All	0.41	0/7386	0.92	40/10179 (0.4%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	ARG	NE-CZ-NH1	-16.94	111.83	120.30
1	B	267	ARG	NE-CZ-NH2	16.94	128.77	120.30
3	F	11	DC	O4'-C1'-N1	13.30	117.31	108.00
2	E	16	DA	O4'-C1'-N9	-12.22	99.44	108.00
3	F	11	DC	P-O3'-C3'	11.27	133.22	119.70
3	F	5	DT	N3-C2-O2	-9.09	116.84	122.30
2	E	15	DC	P-O5'-C5'	-8.83	106.77	120.90
1	D	267	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	B	267	ARG	CD-NE-CZ	8.42	135.39	123.60
3	F	15	DC	C1'-O4'-C4'	-8.13	101.97	110.10
1	D	267	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	267	ARG	NE-CZ-NH2	-7.56	116.52	120.30
2	E	17	DA	N1-C6-N6	7.51	123.10	118.60
2	E	11	DG	O4'-C1'-N9	7.48	113.23	108.00
3	F	16	DT	N3-C2-O2	-7.47	117.82	122.30
3	F	17	DT	O4'-C1'-N1	7.19	113.03	108.00
1	C	267	ARG	NE-CZ-NH2	-7.19	116.71	120.30
2	E	5	DA	O4'-C1'-N9	-7.15	103.00	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	6	DT	N3-C2-O2	-6.91	118.15	122.30
1	C	267	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	A	267	ARG	NE-CZ-NH1	6.81	123.70	120.30
2	E	15	DC	C1'-O4'-C4'	-6.08	104.02	110.10
3	F	12	DT	P-O3'-C3'	6.04	126.94	119.70
3	F	20	DG	O4'-C1'-N9	-5.88	103.89	108.00
2	E	20	DC	C3'-C2'-C1'	-5.87	95.46	102.50
3	F	17	DT	C1'-O4'-C4'	-5.86	104.24	110.10
2	E	16	DA	N1-C6-N6	5.85	122.11	118.60
3	F	5	DT	O4'-C1'-N1	-5.84	103.91	108.00
2	E	17	DA	O4'-C1'-N9	5.80	112.06	108.00
3	F	6	DT	O4'-C1'-N1	5.62	111.93	108.00
2	E	9	DT	N3-C4-O4	5.42	123.15	119.90
3	F	10	DT	C3'-C2'-C1'	-5.40	96.02	102.50
2	E	1	DT	N3-C4-O4	5.38	123.13	119.90
3	F	21	DA	O4'-C1'-N9	-5.34	104.26	108.00
2	E	6	DA	O4'-C1'-N9	5.30	111.71	108.00
3	F	4	DC	C1'-O4'-C4'	-5.25	104.85	110.10
3	F	12	DT	C5'-C4'-C3'	5.20	123.46	114.10
2	E	20	DC	O4'-C1'-N1	5.19	111.63	108.00
2	E	17	DA	C1'-O4'-C4'	-5.09	105.01	110.10
2	E	5	DA	N1-C6-N6	5.06	121.63	118.60

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	1571	0	1535	21	1
1	B	1571	0	1535	16	1
1	C	1571	0	1535	22	0
1	D	1571	0	1535	25	2
2	E	428	0	237	26	0
3	F	427	0	241	15	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	215	0	0	4	0
5	B	163	0	0	4	0
5	C	172	0	0	5	0
5	D	210	0	0	6	0
5	E	34	0	0	3	0
5	F	38	0	0	2	0
All	All	7975	0	6618	101	2

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 7.

All (101) 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:E:11:DG:H2''	2:E:12:DA:H5'	1.43	1.01
1:A:101:LYS:NZ	1:D:225:VAL:HG22	1.79	0.97
2:E:11:DG:H8	2:E:11:DG:H5''	1.36	0.91
1:A:101:LYS:HZ3	1:D:225:VAL:HG22	1.31	0.89
2:E:10:DA:H2''	2:E:11:DG:H5''	1.57	0.84
2:E:11:DG:C8	2:E:11:DG:H5''	2.19	0.76
3:F:12:DT:OP2	3:F:12:DT:H2'	1.87	0.74
1:B:202:ARG:HE	1:B:219:PRO:HG2	1.52	0.73
5:C:429:HOH:O	1:D:181:ARG:HG3	1.87	0.73
1:D:202:ARG:HE	1:D:219:PRO:HG2	1.52	0.73
1:C:121:SER:HB3	2:E:1:DT:C7	2.19	0.73
1:C:202:ARG:HE	1:C:219:PRO:HG2	1.53	0.72
1:A:202:ARG:HE	1:A:219:PRO:HG2	1.54	0.72
1:C:122:VAL:HA	5:C:485:HOH:O	1.88	0.72
2:E:10:DA:H2''	2:E:11:DG:C8	2.27	0.70
2:E:10:DA:H2''	2:E:11:DG:H8	1.58	0.69
1:C:120:LYS:HZ3	2:E:2:DC:H5	1.38	0.67
1:A:207:ASP:HB2	5:A:609:HOH:O	1.94	0.66
1:A:122:VAL:HA	5:A:493:HOH:O	1.97	0.65
2:E:10:DA:N1	3:F:12:DT:O4	2.30	0.64
1:B:119:ALA:HB1	2:E:11:DG:O5'	1.98	0.63
5:E:130:HOH:O	3:F:21:DA:N1	2.30	0.63
1:C:181:ARG:NH2	5:C:429:HOH:O	2.30	0.63
1:A:167:GLN:HA	1:D:233:HIS:CE1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:ARG:HG3	5:D:550:HOH:O	1.99	0.62
1:A:209:ARG:H	1:A:209:ARG:NE	1.99	0.61
1:D:209:ARG:H	1:D:209:ARG:NE	1.99	0.61
3:F:10:DT:H73	5:F:113:HOH:O	2.01	0.60
2:E:11:DG:H8	2:E:11:DG:C5'	2.12	0.60
1:A:99:SER:OG	1:D:224:GLU:OE2	2.14	0.59
1:C:209:ARG:NE	1:C:209:ARG:H	1.99	0.59
1:B:209:ARG:H	1:B:209:ARG:NE	2.00	0.58
1:A:101:LYS:HZ2	1:D:225:VAL:HG22	1.67	0.58
1:A:256:THR:HG21	5:A:552:HOH:O	2.03	0.58
1:C:121:SER:CB	2:E:1:DT:H71	2.34	0.57
1:C:121:SER:HB3	2:E:1:DT:H71	1.87	0.57
3:F:21:DA:C8	3:F:21:DA:OP2	2.57	0.57
2:E:11:DG:C8	2:E:11:DG:C5'	2.88	0.56
3:F:11:DC:H3'	3:F:11:DC:OP2	2.06	0.56
1:A:101:LYS:HZ3	1:D:225:VAL:CG2	2.13	0.54
1:C:121:SER:CB	2:E:1:DT:C7	2.86	0.53
3:F:1:DA:H2''	3:F:2:DG:C8	2.43	0.53
5:E:130:HOH:O	3:F:21:DA:C2	2.62	0.52
2:E:11:DG:H2''	2:E:12:DA:C5'	2.26	0.52
1:D:207:ASP:HB2	5:D:545:HOH:O	2.07	0.52
1:D:202:ARG:NH1	5:D:573:HOH:O	2.42	0.51
3:F:14:DA:H5''	5:F:138:HOH:O	2.11	0.51
1:A:93:LEU:HB2	1:D:201:LEU:HG	1.93	0.50
1:B:175:ARG:HD3	1:B:191:PRO:O	2.12	0.50
1:B:221:GLU:HG3	5:B:516:HOH:O	2.11	0.50
1:C:120:LYS:NZ	2:E:2:DC:H5	2.07	0.50
1:C:175:ARG:HD3	1:C:191:PRO:O	2.12	0.49
1:D:175:ARG:HD3	1:D:191:PRO:O	2.12	0.48
1:C:211:THR:HA	5:C:569:HOH:O	2.13	0.48
1:A:175:ARG:HD3	1:A:191:PRO:O	2.13	0.47
3:F:2:DG:H2''	3:F:3:DG:O5'	2.14	0.47
1:C:121:SER:HB3	2:E:1:DT:H73	1.96	0.47
1:A:167:GLN:CA	1:D:233:HIS:CE1	2.98	0.47
1:C:243:MET:CG	1:D:178:HIS:CD2	2.98	0.46
1:D:119:ALA:HB1	3:F:11:DC:OP2	2.14	0.46
2:E:9:DT:H2''	2:E:10:DA:C8	2.50	0.46
1:C:185:SER:HB2	5:C:517:HOH:O	2.15	0.46
2:E:12:DA:H2	3:F:10:DT:H3	1.63	0.46
2:E:10:DA:N1	3:F:12:DT:C4	2.84	0.45
1:C:192:GLN:H	1:C:192:GLN:HG3	1.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:O	1:D:201:LEU:HD11	2.16	0.45
1:B:225:VAL:HB	1:C:101:LYS:NZ	2.31	0.45
1:B:192:GLN:H	1:B:192:GLN:HG3	1.48	0.45
1:B:122:VAL:HG12	5:B:554:HOH:O	2.17	0.44
1:C:121:SER:OG	2:E:1:DT:H71	2.18	0.44
3:F:12:DT:H1'	3:F:13:DA:H5'	2.00	0.44
1:A:226:GLY:N	5:A:602:HOH:O	2.44	0.43
1:B:122:VAL:N	5:B:554:HOH:O	2.40	0.43
1:A:259:ASP:OD2	1:A:263:ASN:HB2	2.18	0.43
1:D:288:ASN:HD22	1:D:291:LYS:HD3	1.83	0.43
1:C:119:ALA:O	1:C:120:LYS:C	2.56	0.43
1:D:227:SER:HB3	5:D:558:HOH:O	2.18	0.43
1:A:119:ALA:O	1:A:120:LYS:C	2.57	0.43
2:E:9:DT:H2''	2:E:10:DA:O5'	2.19	0.43
1:D:119:ALA:O	1:D:120:LYS:C	2.58	0.42
1:B:101:LYS:O	1:B:267:ARG:HD2	2.19	0.42
1:D:202:ARG:NH2	5:D:566:HOH:O	2.52	0.42
1:A:288:ASN:HD22	1:A:291:LYS:HD3	1.85	0.42
1:A:286:GLU:O	1:A:289:LEU:HB2	2.20	0.42
1:B:225:VAL:HG12	1:B:225:VAL:O	2.20	0.42
1:D:122:VAL:HA	5:D:603:HOH:O	2.18	0.42
1:B:288:ASN:HD22	1:B:291:LYS:HD3	1.85	0.42
1:A:190:PRO:HA	1:A:191:PRO:HD3	1.93	0.41
1:C:182:CYS:O	1:C:182:CYS:SG	2.78	0.41
1:B:115:HIS:HD2	5:B:530:HOH:O	2.04	0.41
1:B:119:ALA:O	1:B:120:LYS:C	2.58	0.41
1:B:249:ARG:HA	1:B:250:PRO:HD3	1.97	0.41
2:E:17:DA:N7	5:E:122:HOH:O	2.37	0.41
1:C:224:GLU:O	1:C:225:VAL:C	2.59	0.41
3:F:11:DC:H3'	3:F:11:DC:P	2.59	0.41
2:E:15:DC:H2''	2:E:16:DA:C8	2.55	0.40
2:E:9:DT:H2''	2:E:10:DA:H8	1.86	0.40
1:D:190:PRO:HA	1:D:191:PRO:HD3	1.93	0.40
1:B:259:ASP:OD2	1:B:263:ASN:HB2	2.20	0.40
1:D:182:CYS:O	1:D:182:CYS:SG	2.80	0.40
1:C:288:ASN:HD22	1:C:291:LYS:HD3	1.87	0.40

All (2) 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)
1:A:183:SER:OG	1:D:95:SER:O[1_455]	1.97	0.23
1:B:261:SER:OG	1:D:188:LEU:O[4_445]	2.10	0.10

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	198/200 (99%)	195 (98%)	3 (2%)	0	100	100
1	B	198/200 (99%)	195 (98%)	3 (2%)	0	100	100
1	C	198/200 (99%)	195 (98%)	2 (1%)	1 (0%)	29	18
1	D	198/200 (99%)	194 (98%)	4 (2%)	0	100	100
All	All	792/800 (99%)	779 (98%)	12 (2%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	225	VAL

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	180/180 (100%)	174 (97%)	6 (3%)	38	29
1	B	180/180 (100%)	175 (97%)	5 (3%)	43	36
1	C	180/180 (100%)	175 (97%)	5 (3%)	43	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	180/180 (100%)	174 (97%)	6 (3%)	38	29
All	All	720/720 (100%)	698 (97%)	22 (3%)	40	32

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	SER
1	A	120	LYS
1	A	192	GLN
1	A	209	ARG
1	A	289	LEU
1	A	290	ARG
1	B	95	SER
1	B	120	LYS
1	B	192	GLN
1	B	209	ARG
1	B	290	ARG
1	C	95	SER
1	C	120	LYS
1	C	192	GLN
1	C	209	ARG
1	C	290	ARG
1	D	95	SER
1	D	120	LYS
1	D	192	GLN
1	D	209	ARG
1	D	217	VAL
1	D	290	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	247	ASN
1	A	288	ASN
1	B	247	ASN
1	B	288	ASN
1	C	247	ASN
1	C	288	ASN
1	D	100	GLN
1	D	178	HIS

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Mol	Chain	Res	Type
1	D	233	HIS
1	D	247	ASN
1	D	288	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	200/200 (100%)	0.29	18 (9%) 9 10	13, 24, 70, 152	0
1	B	200/200 (100%)	0.53	17 (8%) 10 12	16, 27, 74, 153	0
1	C	200/200 (100%)	0.51	22 (11%) 5 6	15, 28, 70, 153	0
1	D	200/200 (100%)	0.48	19 (9%) 8 9	12, 25, 71, 153	0
2	E	21/21 (100%)	0.53	4 (19%) 1 1	22, 41, 83, 122	0
3	F	21/21 (100%)	0.42	2 (9%) 8 9	21, 38, 81, 109	0
All	All	842/842 (100%)	0.45	82 (9%) 7 9	12, 27, 74, 153	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	226	GLY	19.8
1	B	121	SER	18.0
1	D	226	GLY	17.9
1	D	121	SER	17.6
1	C	121	SER	13.5
1	A	121	SER	10.8
1	C	226	GLY	10.1
1	A	226	GLY	8.3
1	B	92	PRO	7.3
1	B	118	THR	7.3
1	C	120	LYS	7.1
1	C	118	THR	6.9
1	B	227	SER	6.9
1	C	119	ALA	6.5
1	A	119	ALA	6.5
1	C	225	VAL	6.2
1	B	117	GLY	6.2
1	B	120	LYS	6.0
1	D	95	SER	5.8

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Mol	Chain	Res	Type	RSRZ
1	D	120	LYS	5.5
1	D	225	VAL	5.5
1	A	115	HIS	5.1
1	C	116	SER	4.9
1	D	92	PRO	4.8
1	B	291	LYS	4.6
1	B	225	VAL	4.4
1	A	120	LYS	4.4
1	B	116	SER	4.4
2	E	21	DT	4.2
1	B	95	SER	4.1
1	A	116	SER	4.1
1	B	119	ALA	4.1
1	C	291	LYS	4.0
1	C	115	HIS	4.0
1	D	122	VAL	4.0
1	D	227	SER	3.8
1	D	183	SER	3.7
3	F	21	DA	3.7
1	D	118	THR	3.7
1	D	209	ARG	3.6
1	C	117	GLY	3.5
1	B	224	GLU	3.5
1	C	227	SER	3.3
1	C	210	ASN	3.2
1	A	227	SER	3.1
1	C	262	GLY	2.9
1	A	118	THR	2.9
2	E	11	DG	2.9
1	D	182	CYS	2.9
1	A	188	LEU	2.8
1	D	291	LYS	2.8
1	D	290	ARG	2.8
2	E	1	DT	2.7
1	C	209	ARG	2.7
1	A	117	GLY	2.7
1	B	122	VAL	2.7
1	C	122	VAL	2.7
1	B	209	ARG	2.7
1	C	202	ARG	2.7
1	A	92	PRO	2.6
1	D	188	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	186	ASP	2.6
1	A	209	ARG	2.5
1	A	290	ARG	2.5
1	B	182	CYS	2.5
1	C	182	CYS	2.5
3	F	1	DA	2.4
1	C	153	PRO	2.4
1	C	183	SER	2.4
1	C	223	PRO	2.4
1	C	187	GLY	2.4
1	D	185	SER	2.4
1	D	186	ASP	2.4
1	B	93	LEU	2.3
1	A	183	SER	2.2
1	A	185	SER	2.2
2	E	12	DA	2.2
1	A	186	ASP	2.2
1	A	201	LEU	2.1
1	D	115	HIS	2.1
1	A	225	VAL	2.1
1	D	93	LEU	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 ⓘ

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ZN	A	301	1/1	1.00	0.10	20,20,20,20	0
4	ZN	C	301	1/1	1.00	0.07	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ZN	B	301	1/1	1.00	0.09	20,20,20,20	0
4	ZN	D	301	1/1	1.00	0.09	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.