



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:25 AM GMT

PDB ID : 2AC0
Title : Structural Basis of DNA Recognition by p53 Tetramers (complex I)
Authors : Kitayner, M.; Rozenberg, H.; Kessler, N.; Rabinovich, D.; Shakked, Z.
Deposited on : 2005-07-18
Resolution : 1.80 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

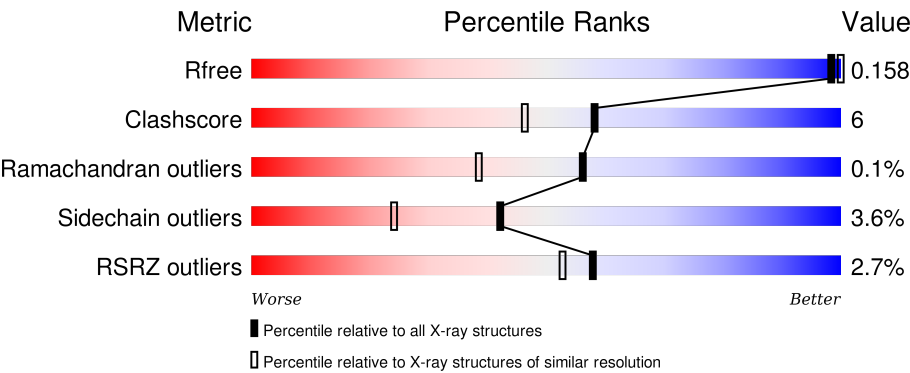
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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. 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	E	12	<div><div></div><div>67%33%</div></div>
1	F	12	<div><div></div><div>25%42%33%</div></div>
1	G	12	<div><div></div><div>42%50%8%</div></div>
1	H	12	<div><div></div><div>8%75%17%</div></div>
2	A	200	<div><div></div><div>3%92%7%..</div></div>

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Mol	Chain	Length	Quality of chain
2	B	200	<div><div></div><div>3%</div><div>88%</div><div>9%</div><div>••</div></div>
2	C	200	<div><div></div><div>2%</div><div>89%</div><div>9%</div><div>••</div></div>
2	D	200	<div><div></div><div>5%</div><div>85%</div><div>12%</div><div>••</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8247 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 5'-D(*CP*GP*GP*GP*CP*AP*TP*GP*CP*CP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	12	Total	C	N	O	P	0	0	0
			243	115	47	70	11			
1	F	12	Total	C	N	O	P	0	0	0
			243	115	47	70	11			
1	G	12	Total	C	N	O	P	0	0	0
			243	115	47	70	11			
1	H	12	Total	C	N	O	P	0	0	0
			243	115	47	70	11			

- Molecule 2 is a protein called Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	199	Total	C	N	O	S	0	2	1
			1557	957	289	294	17			
2	B	198	Total	C	N	O	S	0	4	0
			1557	957	287	296	17			
2	C	195	Total	C	N	O	S	0	5	0
			1544	954	282	290	18			
2	D	198	Total	C	N	O	S	0	2	1
			1559	961	290	291	17			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	255	Total 255	O 255	0	0
4	B	195	Total 195	O 195	0	0
4	C	253	Total 253	O 253	0	0
4	D	197	Total 197	O 197	0	0
4	E	51	Total 51	O 51	0	0
4	F	40	Total 40	O 40	0	0
4	G	31	Total 31	O 31	0	0
4	H	32	Total 32	O 32	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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 5'-D(*CP*GP*GP*GP*CP*AP*TP*GP*CP*CP*CP*G)-3'

Chain E: 



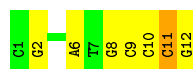
- Molecule 1: 5'-D(*CP*GP*GP*GP*CP*AP*TP*GP*CP*CP*CP*G)-3'

Chain F: 



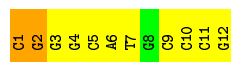
- Molecule 1: 5'-D(*CP*GP*GP*GP*CP*AP*TP*GP*CP*CP*CP*G)-3'

Chain G: 



- Molecule 1: 5'-D(*CP*GP*GP*GP*CP*AP*TP*GP*CP*CP*CP*G)-3'

Chain H: 




- Molecule 2: Cellular tumor antigen p53

Chain A: 

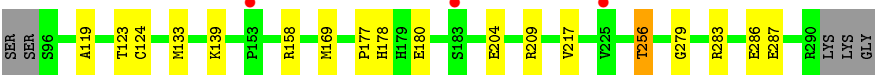
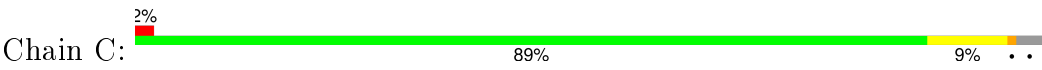


- Molecule 2: Cellular tumor antigen p53

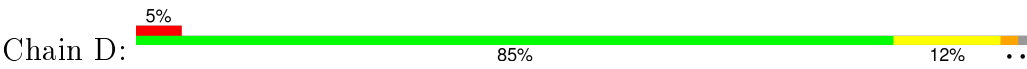
Chain B: 



● Molecule 2: Cellular tumor antigen p53



● Molecule 2: Cellular tumor antigen p53



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.44Å 58.15Å 77.54Å 82.93° 87.99° 73.60°	Depositor
Resolution (Å)	33.52 – 1.80 33.51 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (33.52-1.80) 88.5 (33.51-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.153 , 0.217 0.160 , 0.158	Depositor DCC
R_{free} test set	3993 reflections (5.44%)	DCC
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 79251 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8247	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	E	1.64	5/272 (1.8%)	2.25	15/418 (3.6%)
1	F	1.38	2/272 (0.7%)	2.14	12/418 (2.9%)
1	G	1.24	0/272	1.96	7/418 (1.7%)
1	H	1.14	0/272	2.06	15/418 (3.6%)
2	A	0.82	0/1599	0.83	1/2168 (0.0%)
2	B	0.74	0/1607	0.79	0/2179
2	C	0.82	0/1599	0.83	0/2169
2	D	0.69	0/1601	0.77	1/2168 (0.0%)
All	All	0.88	7/7494 (0.1%)	1.12	51/10356 (0.5%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	8	DG	C8-N7	6.84	1.35	1.30
1	E	7	DT	C5-C6	5.63	1.38	1.34
1	E	2	DG	C3'-O3'	-5.51	1.36	1.44
1	E	2	DG	N3-C4	5.32	1.39	1.35
1	E	2	DG	N7-C5	5.28	1.42	1.39
1	E	5	DC	C3'-O3'	-5.27	1.37	1.44
1	F	8	DG	C6-N1	5.25	1.43	1.39

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	10	DC	O4'-C1'-N1	-13.54	98.53	108.00
1	G	6	DA	O4'-C1'-N9	-13.34	98.66	108.00
1	E	3	DG	O4'-C1'-N9	-11.99	99.61	108.00
1	E	6	DA	O4'-C1'-N9	-11.81	99.73	108.00
1	H	6	DA	O4'-C1'-N9	-11.45	99.98	108.00
1	F	6	DA	O4'-C1'-N9	-11.10	100.23	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	2	DG	O4'-C1'-N9	-10.41	100.71	108.00
1	E	5	DC	P-O5'-C5'	-10.25	104.50	120.90
1	G	11	DC	O4'-C4'-C3'	-9.49	100.31	106.00
1	F	5	DC	O4'-C1'-N1	9.09	114.36	108.00
1	F	7	DT	C1'-O4'-C4'	-8.40	101.70	110.10
1	E	5	DC	C1'-O4'-C4'	-8.37	101.73	110.10
1	F	5	DC	P-O5'-C5'	-7.74	108.52	120.90
1	G	2	DG	O4'-C1'-N9	-7.04	103.08	108.00
1	H	1	DC	C2-N3-C4	7.00	123.40	119.90
1	F	12	DG	O4'-C1'-N9	6.87	112.81	108.00
1	F	5	DC	N3-C4-C5	-6.68	119.23	121.90
1	H	3	DG	P-O3'-C3'	6.66	127.69	119.70
1	E	7	DT	N3-C2-O2	-6.39	118.47	122.30
1	E	10	DC	O4'-C1'-N1	6.38	112.47	108.00
1	H	4	DG	C5-C6-O6	-6.32	124.81	128.60
1	H	7	DT	C3'-C2'-C1'	-6.15	95.12	102.50
1	H	1	DC	O4'-C1'-N1	-6.12	103.72	108.00
1	E	8	DG	O4'-C1'-C2'	6.01	110.70	105.90
1	E	5	DC	O4'-C1'-C2'	-5.94	101.15	105.90
1	E	7	DT	O4'-C1'-C2'	-5.91	101.17	105.90
2	D	264	LEU	CA-CB-CG	5.83	128.70	115.30
1	H	7	DT	C1'-O4'-C4'	-5.81	104.29	110.10
1	E	11	DC	O4'-C1'-N1	5.79	112.05	108.00
1	H	7	DT	P-O3'-C3'	5.73	126.57	119.70
1	F	5	DC	C5'-C4'-C3'	-5.60	104.02	114.10
1	F	1	DC	O4'-C1'-N1	-5.53	104.13	108.00
1	H	9	DC	N3-C4-C5	5.48	124.09	121.90
1	H	5	DC	O4'-C1'-N1	5.48	111.83	108.00
1	G	6	DA	N9-C1'-C2'	5.43	122.91	112.60
1	H	9	DC	O4'-C1'-N1	-5.40	104.22	108.00
1	F	9	DC	C2-N3-C4	5.34	122.57	119.90
1	G	9	DC	O5'-P-OP2	-5.29	100.94	105.70
1	F	7	DT	O4'-C1'-N1	5.26	111.68	108.00
1	E	11	DC	N1-C2-O2	5.24	122.05	118.90
1	E	11	DC	N3-C2-O2	-5.24	118.23	121.90
1	E	7	DT	C1'-O4'-C4'	-5.22	104.88	110.10
1	E	3	DG	N3-C2-N2	-5.17	116.28	119.90
1	E	4	DG	C5-C6-N1	5.13	114.07	111.50
1	H	2	DG	C8-N9-C4	5.10	108.44	106.40
1	F	3	DG	O4'-C1'-N9	-5.09	104.44	108.00
1	G	8	DG	O4'-C1'-N9	5.06	111.54	108.00
2	A	184	ASP	CB-CG-OD1	5.05	122.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	10	DC	O5'-P-OP1	-5.02	101.18	105.70
1	H	2	DG	P-O3'-C3'	5.01	125.72	119.70
1	H	4	DG	N3-C2-N2	-5.00	116.40	119.90

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	E	243	0	135	8	0
1	F	243	0	135	5	0
1	G	243	0	135	2	0
1	H	243	0	135	6	0
2	A	1557	0	1511	9	0
2	B	1557	0	1503	25	0
2	C	1544	0	1505	16	0
2	D	1559	0	1526	21	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	255	0	0	4	2
4	B	195	0	0	4	0
4	C	253	0	0	4	2
4	D	197	0	0	6	0
4	E	51	0	0	2	0
4	F	40	0	0	0	0
4	G	31	0	0	0	0
4	H	32	0	0	0	0
All	All	8247	0	6585	81	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 6.

All (81) 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:102:THR:HG23	2:B:268:ASN:HD21	1.18	1.02
2:B:102:THR:HG23	2:B:268:ASN:ND2	1.84	0.92
2:D:207:ASP:HB3	4:D:426:HOH:O	1.82	0.78
1:E:11:DC:H5	4:E:919:HOH:O	1.67	0.78
2:C:256[A]:THR:HG22	4:C:317:HOH:O	1.86	0.76
2:D:174:ARG:HD3	4:D:424:HOH:O	1.88	0.74
1:E:1:DC:H5'	1:G:12:DG:H2'	1.68	0.73
1:E:12:DG:OP1	4:E:982:HOH:O	2.08	0.71
2:D:166:SER:HA	2:D:169:MET:HG3	1.73	0.69
2:B:119:ALA:O	2:B:279:GLY:HA3	1.92	0.69
1:F:1:DC:O5'	2:B:283:ARG:HD3	1.94	0.67
1:F:5:DC:H2''	1:F:6:DA:C8	2.30	0.66
2:C:286:GLU:OE1	4:C:475:HOH:O	2.13	0.65
2:C:124:CYS:SG	2:C:133[B]:MET:SD	2.94	0.65
2:C:178:HIS:CD2	2:D:243:MET:HG3	2.33	0.63
2:B:247:ASN:ND2	4:B:450:HOH:O	2.31	0.63
2:C:123[B]:THR:CG2	2:C:139:LYS:HB3	2.31	0.61
2:A:100:GLN:HG2	4:A:377:HOH:O	2.03	0.59
2:B:110:ARG:HB2	4:B:383:HOH:O	2.01	0.59
1:E:5:DC:H2''	1:E:6:DA:C8	2.40	0.57
1:H:1:DC:H5''	2:C:119:ALA:HB1	1.86	0.57
2:A:268:ASN:HD22	2:A:269:SER:N	2.02	0.56
1:H:11:DC:H2''	1:H:12:DG:C8	2.41	0.56
2:D:288:ASN:ND2	4:D:463:HOH:O	2.39	0.55
2:C:123[B]:THR:HG23	2:C:139:LYS:HB3	1.88	0.55
2:A:175:ARG:HD3	2:A:191:PRO:O	2.07	0.55
2:C:204:GLU:HB3	2:C:217[A]:VAL:HG13	1.90	0.54
2:B:192:GLN:HB3	4:B:341:HOH:O	2.07	0.54
1:H:11:DC:C2'	1:H:12:DG:C8	2.91	0.53
2:C:123[B]:THR:HG23	2:C:139:LYS:CB	2.38	0.53
2:D:259:ASP:HA	4:D:354:HOH:O	2.09	0.52
4:A:435:HOH:O	2:B:243:MET:HE1	2.09	0.52
1:H:1:DC:H2'	1:H:2:DG:C8	2.44	0.52
2:A:287:GLU:O	2:A:290:ARG:HG2	2.10	0.52
2:B:243:MET:HA	2:B:247:ASN:HD22	1.75	0.51
2:D:158:ARG:NH1	2:D:217:VAL:CG2	2.73	0.51
1:E:1:DC:H3'	2:A:121:SER:HB2	1.93	0.51
1:G:11:DC:H2'	1:G:12:DG:C8	2.46	0.51
2:B:198:GLU:CG	2:B:233:HIS:HB3	2.41	0.51
2:B:198:GLU:CG	2:B:233:HIS:CB	2.89	0.50
2:D:158:ARG:CZ	2:D:217:VAL:HG21	2.41	0.50
2:C:177:PRO:HB2	2:D:177:PRO:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:102:THR:HG23	2:D:268:ASN:HD21	1.76	0.49
2:D:99:SER:OG	2:D:101:LYS:HG2	2.12	0.49
2:B:174:ARG:HD3	4:B:426:HOH:O	2.13	0.49
2:C:158:ARG:HB3	2:C:256[A]:THR:HG23	1.95	0.49
2:C:119:ALA:O	2:C:279:GLY:HA3	2.13	0.49
2:B:198:GLU:HG2	2:B:233:HIS:HB3	1.95	0.49
1:E:1:DC:H2''	1:E:2:DG:C8	2.48	0.48
2:B:167:GLN:HB3	4:C:380:HOH:O	2.13	0.48
2:C:178:HIS:CD2	2:D:243:MET:CG	2.97	0.48
1:F:1:DC:O5'	2:B:283:ARG:CD	2.63	0.47
2:B:198:GLU:HG3	2:B:233:HIS:HB2	1.97	0.47
1:F:12:DG:H2''	1:H:1:DC:H5'	1.98	0.46
2:D:259:ASP:OD2	2:D:263:ASN:HB2	2.16	0.46
2:B:198:GLU:HG2	2:B:233:HIS:CB	2.45	0.45
2:B:192:GLN:CD	2:B:192:GLN:H	2.20	0.45
2:D:102:THR:HG23	2:D:268:ASN:ND2	2.32	0.45
1:H:10:DC:H2''	1:H:11:DC:C6	2.52	0.45
2:C:158:ARG:NH1	2:C:217[B]:VAL:CG2	2.80	0.45
4:A:435:HOH:O	2:B:243:MET:CE	2.63	0.45
2:D:158:ARG:NH1	2:D:217:VAL:HG21	2.30	0.45
2:C:209:ARG:HD3	4:C:428:HOH:O	2.17	0.45
2:A:198:GLU:CD	4:A:488:HOH:O	2.54	0.45
2:B:198:GLU:CG	2:B:233:HIS:HB2	2.47	0.44
2:C:158:ARG:CZ	2:C:217[B]:VAL:HG21	2.47	0.44
2:A:178:HIS:HD2	2:B:243:MET:HE3	1.83	0.43
2:D:118:THR:HG22	2:D:282:ARG:HD3	1.99	0.43
2:B:175:ARG:HD3	2:B:191:PRO:O	2.19	0.43
2:D:202:ARG:NH1	2:D:221:GLU:OE2	2.53	0.42
2:B:151:PRO:HD2	2:B:220:TYR:CE2	2.54	0.42
1:E:1:DC:C2'	1:E:2:DG:C8	3.03	0.41
2:D:145:LEU:HD11	2:D:232:ILE:HD11	2.02	0.41
2:D:97:VAL:HG21	2:D:169:MET:HB3	2.03	0.41
2:B:267:ARG:O	2:B:268:ASN:ND2	2.46	0.41
1:F:1:DC:C5'	2:B:283:ARG:HD3	2.50	0.41
2:A:100:GLN:HG2	2:A:100:GLN:H	1.30	0.41
2:D:152:PRO:HG2	4:D:354:HOH:O	2.21	0.41
1:E:9:DC:O2	1:E:12:DG:H2'	2.21	0.40
2:D:128:PRO:HD2	4:D:407:HOH:O	2.21	0.40
2:A:204:GLU:HB3	2:A:217:VAL:HG13	2.03	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)
4:A:344:HOH:O	4:C:537:HOH:O[1_665]	2.04	0.16
4:A:516:HOH:O	4:C:535:HOH:O[1_655]	2.12	0.08

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	199/200 (100%)	196 (98%)	3 (2%)	0	100	100
2	B	199/200 (100%)	196 (98%)	3 (2%)	0	100	100
2	C	198/200 (99%)	196 (99%)	2 (1%)	0	100	100
2	D	198/200 (99%)	192 (97%)	5 (2%)	1 (0%)	34	17
All	All	794/800 (99%)	780 (98%)	13 (2%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	290	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	179/179 (100%)	174 (97%)	5 (3%)	51	35
2	B	180/179 (101%)	171 (95%)	9 (5%)	30	13
2	C	179/179 (100%)	173 (97%)	6 (3%)	44	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	179/179 (100%)	173 (97%)	6 (3%)	44	26
All	All	717/716 (100%)	691 (96%)	26 (4%)	42	24

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	100	GLN
2	A	110	ARG
2	A	224	GLU
2	A	264	LEU
2	A	268	ASN
2	B	110	ARG
2	B	149	SER
2	B	192	GLN
2	B	209	ARG
2	B	224	GLU
2	B	243	MET
2	B	268	ASN
2	B	283	ARG
2	B	290	ARG
2	C	169	MET
2	C	180	GLU
2	C	256[A]	THR
2	C	256[B]	THR
2	C	283	ARG
2	C	287	GLU
2	D	96	SER
2	D	174	ARG
2	D	228	ASP
2	D	243	MET
2	D	264	LEU
2	D	268	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	268	ASN
2	A	288	ASN
2	B	247	ASN
2	B	268	ASN
2	C	104	GLN

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Mol	Chain	Res	Type
2	D	100	GLN
2	D	247	ASN
2	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	E	12/12 (100%)	-0.49	0	100	100	19, 25, 42, 49	0
1	F	12/12 (100%)	-0.23	0	100	100	18, 24, 45, 50	0
1	G	12/12 (100%)	-0.45	0	100	100	19, 27, 44, 46	0
1	H	12/12 (100%)	-0.22	0	100	100	20, 32, 64, 66	0
2	A	199/200 (99%)	-0.32	5 (2%)	61	56	11, 19, 39, 54	0
2	B	198/200 (99%)	-0.20	5 (2%)	61	56	13, 26, 48, 65	0
2	C	195/200 (97%)	-0.40	3 (1%)	76	72	10, 20, 39, 57	0
2	D	198/200 (99%)	0.02	10 (5%)	32	26	15, 28, 55, 77	0
All	All	838/848 (98%)	-0.23	23 (2%)	58	53	10, 24, 48, 77	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	226	GLY	6.7
2	D	225	VAL	6.4
2	D	293	GLY	5.9
2	A	225	VAL	5.6
2	A	94	SER	5.0
2	B	225	VAL	4.9
2	B	226	GLY	4.2
2	D	289	LEU	4.0
2	D	292	LYS	3.7
2	A	183	SER	3.4
2	B	228	ASP	3.0
2	D	228	ASP	2.9
2	D	227	SER	2.9
2	C	153	PRO	2.9
2	B	146	TRP	2.9
2	A	226	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	225	VAL	2.7
2	B	115	HIS	2.6
2	D	224	GLU	2.4
2	A	96	SER	2.3
2	C	183	SER	2.3
2	D	290	ARG	2.2
2	D	222	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ZN	B	1	1/1	1.00	0.05	-0.78	20,20,20,20	0
3	ZN	C	1	1/1	1.00	0.05	-0.84	17,17,17,17	0
3	ZN	A	1	1/1	1.00	0.04	-1.02	17,17,17,17	0
3	ZN	D	1	1/1	1.00	0.04	-2.30	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.