



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:32 AM UTC

PDB ID : 2AHI / pdb_00002ahi
Title : Structural Basis of DNA Recognition by p53 Tetramers (complex III)
Authors : Kitayner, M.; Rozenberg, H.; Kessler, N.; Rabinovich, D.; Shakked, Z.
Deposited on : 2005-07-28
Resolution : 1.85 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

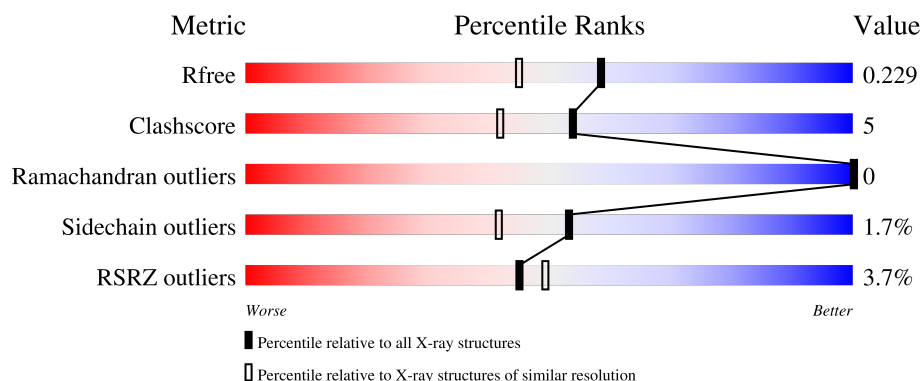
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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 $\leq 5\%$. 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	E	12	
1	F	12	
1	G	12	
1	H	12	
2	A	200	

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Mol	Chain	Length	Quality of chain
2	B	200	2% 90% 8% ••
2	C	200	4% 86% 10% •
2	D	200	7% 84% 14% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8058 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*AP*CP*AP*TP*GP*TP*CP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	10	Total	C	N	O	P	0	0	0
			202	97	38	58	9			
1	F	11	Total	C	N	O	P	0	0	0
			224	107	43	64	10			
1	G	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
1	H	12	Total	C	N	O	P	0	0	0
			243	116	46	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
			1555	957	289	292	17			
2	B	198	Total	C	N	O	S	0	0	1
			1538	946	284	292	16			
2	C	193	Total	C	N	O	S	0	2	0
			1514	935	279	283	17			
2	D	196	Total	C	N	O	S	0	3	1
			1537	946	282	292	17			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is water.

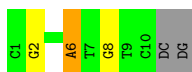
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	38	Total 38	O 38	0	0
4	F	24	Total 24	O 24	0	0
4	G	21	Total 21	O 21	0	0
4	H	27	Total 27	O 27	0	0
4	A	273	Total 273	O 273	0	0
4	B	211	Total 211	O 211	0	0
4	C	249	Total 249	O 249	0	0
4	D	155	Total 155	O 155	0	0

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

Chain E: 



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

Chain F: 



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

Chain G: 

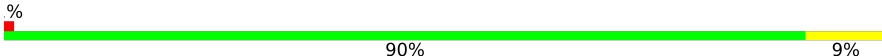


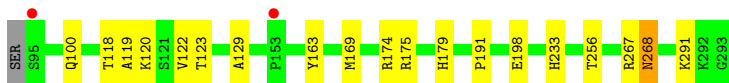
- Molecule 1: 5'-D(*CP*GP*GP*AP*CP*AP*TP*GP*TP*CP*CP*G)-3'

Chain H: 

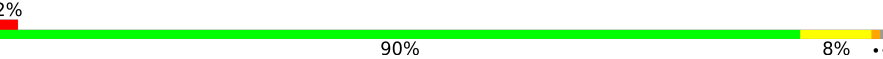


- Molecule 2: Cellular tumor antigen p53

Chain A: 



- Molecule 2: Cellular tumor antigen p53

Chain B:  90% 8% 2%



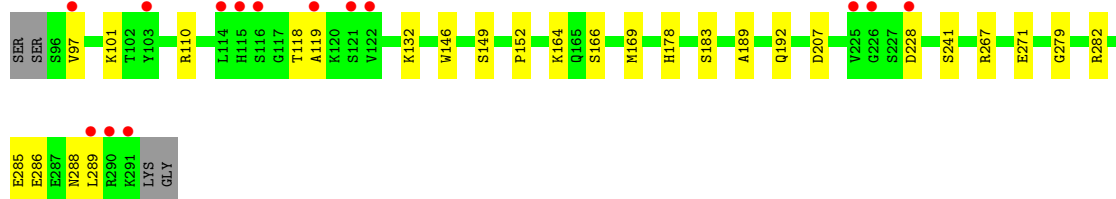
• Molecule 2: Cellular tumor antigen p53

Chain C:  86% 10% 4%



• Molecule 2: Cellular tumor antigen p53

Chain D:  84% 14% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.55Å 58.19Å 77.55Å 83.08° 87.94° 73.56°	Depositor
Resolution (Å)	38.49 – 1.85 38.49 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.49-1.85) 92.3 (38.49-1.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.162 , 0.225 0.169 , 0.229	Depositor DCC
R_{free} test set	3683 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.9	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	8058	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% 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, 0.333 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	E	0.64	0/226	1.39	2/347 (0.6%)
1	F	0.59	0/251	1.39	3/386 (0.8%)
1	G	0.48	0/272	1.25	2/418 (0.5%)
1	H	0.51	0/272	1.31	2/418 (0.5%)
2	A	0.97	2/1598 (0.1%)	1.00	0/2165
2	B	0.88	0/1573	1.00	2/2135 (0.1%)
2	C	1.00	0/1556	1.03	2/2111 (0.1%)
2	D	0.83	0/1580	0.94	4/2143 (0.2%)
All	All	0.88	2/7328 (0.0%)	1.05	17/10123 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	122	VAL	CA-CB	5.59	1.60	1.54
2	A	129	ALA	N-CA	5.35	1.52	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	6	DA	O4'-C1'-N9	-6.66	98.41	108.40
1	E	6	DA	O4'-C1'-N9	-6.55	98.58	108.40
1	E	8	DG	N9-C1'-C2'	-6.36	103.97	113.50
1	H	5	DC	C1'-O4'-C4'	-6.34	100.19	109.70
2	D	189	ALA	CA-C-N	-6.27	115.15	119.66
2	D	189	ALA	C-N-CA	-6.27	115.15	119.66
1	G	6	DA	O4'-C1'-N9	-6.18	99.14	108.40
2	D	166	SER	N-CA-C	6.12	118.73	111.33
2	D	241	SER	N-CA-C	5.86	119.69	112.54
2	C	118	THR	N-CA-C	5.62	119.32	111.56
2	C	287	GLU	N-CA-C	-5.59	106.81	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	6	DA	O4'-C1'-N9	-5.44	100.23	108.40
1	G	9	DT	N1-C1'-C2'	5.25	121.37	113.50
1	F	3	DG	P-O3'-C3'	5.25	128.07	120.20
2	B	189	ALA	CA-C-N	-5.22	115.90	119.66
2	B	189	ALA	C-N-CA	-5.22	115.90	119.66
1	F	11	DC	P-O3'-C3'	5.21	128.02	120.20

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	202	0	114	4	0
1	F	224	0	125	2	0
1	G	243	0	136	4	0
1	H	243	0	136	7	0
2	A	1555	0	1514	11	0
2	B	1538	0	1482	12	0
2	C	1514	0	1471	13	0
2	D	1537	0	1476	16	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	273	0	0	1	0
4	B	211	0	0	5	0
4	C	249	0	0	2	0
4	D	155	0	0	2	0
4	E	38	0	0	2	0
4	F	24	0	0	0	0
4	G	21	0	0	1	0
4	H	27	0	0	0	0
All	All	8058	0	6454	64	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 5.

All (64) 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:C:119:ALA:O	2:C:279:GLY:HA3	1.74	0.87
1:G:12:DG:OP2	4:G:545:HOH:O	2.04	0.76
1:H:11:DC:H2''	1:H:12:DG:C8	2.23	0.74
2:D:192:GLN:NE2	2:D:207[A]:ASP:OD1	2.21	0.72
2:B:283:ARG:O	2:B:287:GLU:HG2	1.91	0.71
2:B:283:ARG:HH11	2:B:283:ARG:HB3	1.57	0.70
2:D:118:THR:HG22	2:D:282:ARG:HD3	1.75	0.68
1:E:6:DA:OP1	4:E:824:HOH:O	2.12	0.66
2:D:97:VAL:CG1	2:D:169:MET:HB3	2.26	0.66
2:A:175:ARG:HD3	2:A:191:PRO:O	1.97	0.65
2:C:178:HIS:ND1	4:C:542:HOH:O	2.30	0.64
1:E:2:DG:H2''	2:A:120:LYS:HD3	1.84	0.60
2:D:97:VAL:HG11	2:D:169:MET:HB3	1.84	0.59
1:E:2:DG:N3	4:E:823:HOH:O	2.31	0.58
2:C:158:ARG:HB3	2:C:256[B]:THR:CG2	2.35	0.57
2:C:283:ARG:O	2:C:286:GLU:N	2.38	0.57
2:B:258:GLU:OE1	4:B:460:HOH:O	2.18	0.56
2:D:152:PRO:HG2	4:D:395:HOH:O	2.06	0.55
2:C:283:ARG:O	2:C:287:GLU:N	2.38	0.54
2:C:120:LYS:HG3	2:C:280:ARG:HB2	1.91	0.53
2:D:119:ALA:O	2:D:279:GLY:HA3	2.09	0.52
1:E:2:DG:C2'	2:A:120:LYS:HD3	2.40	0.52
2:A:256:THR:HG22	2:A:267:ARG:HG3	1.93	0.51
1:H:1:DC:H2'	1:H:2:DG:N7	2.26	0.51
2:C:248:ARG:NH1	4:C:467:HOH:O	2.44	0.50
2:D:132:LYS:HD2	2:D:271:GLU:CD	2.36	0.50
1:F:5:DC:H2''	1:F:6:DA:C8	2.47	0.50
2:B:283:ARG:NH1	4:B:431:HOH:O	2.44	0.48
1:H:3:DG:H4'	1:H:3:DG:OP1	2.13	0.48
1:G:1:DC:H2'	1:G:2:DG:C8	2.49	0.47
2:A:163:TYR:O	2:A:169:MET:HG2	2.14	0.47
1:G:10:DC:H2''	1:G:11:DC:C5	2.50	0.47
2:B:174:ARG:HD3	4:B:397:HOH:O	2.14	0.47
2:C:136:GLN:OE1	2:C:139:LYS:NZ	2.46	0.47
2:D:110:ARG:NH2	2:D:146:TRP:HB3	2.30	0.47
1:H:5:DC:H2''	1:H:6:DA:C8	2.50	0.46
1:F:12:DG:OP2	2:C:123:THR:HG23	2.16	0.46
2:B:145:LEU:HD11	2:B:232:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:101:LYS:O	2:D:267:ARG:HD2	2.15	0.46
2:A:175:ARG:NH2	2:A:179:HIS:HB3	2.30	0.46
1:H:1:DC:C2'	1:H:2:DG:C8	2.98	0.46
2:D:164:LYS:O	2:D:169:MET:HE3	2.16	0.45
2:A:198:GLU:HG2	2:A:233:HIS:HB3	1.99	0.44
1:H:11:DC:H2''	1:H:12:DG:H8	1.76	0.44
2:B:150:THR:HA	2:B:151:PRO:HD3	1.84	0.44
2:B:110:ARG:HB2	4:B:385:HOH:O	2.16	0.44
1:H:1:DC:H2''	1:H:2:DG:C8	2.53	0.43
2:C:158:ARG:HB3	2:C:256[B]:THR:HG22	2.00	0.43
2:D:97:VAL:HG11	2:D:169:MET:SD	2.59	0.43
2:C:175:ARG:HD3	2:C:191:PRO:O	2.19	0.42
2:D:288:ASN:ND2	4:D:426:HOH:O	2.53	0.42
2:A:118:THR:O	2:A:119:ALA:C	2.63	0.42
2:C:108:GLY:O	2:C:110:ARG:HD3	2.20	0.42
2:C:243:MET:HG2	2:D:178:HIS:CD2	2.55	0.41
2:A:100:GLN:HG2	4:A:540:HOH:O	2.18	0.41
2:D:132:LYS:NZ	2:D:285:GLU:OE1	2.34	0.41
2:B:105:GLY:O	4:B:477:HOH:O	2.21	0.41
2:D:286:GLU:O	2:D:289:LEU:HB3	2.21	0.41
2:B:193:HIS:CE1	2:B:214:HIS:HB3	2.56	0.41
1:G:12:DG:C8	2:A:123:THR:HG21	2.55	0.40
2:B:283:ARG:HB3	2:B:283:ARG:NH1	2.30	0.40
2:B:101:LYS:O	2:B:267:ARG:HD2	2.21	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
2	A	199/200 (100%)	198 (100%)	1 (0%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	196/200 (98%)	192 (98%)	4 (2%)	0	100	100
2	C	193/200 (96%)	191 (99%)	2 (1%)	0	100	100
2	D	197/200 (98%)	193 (98%)	4 (2%)	0	100	100
All	All	785/800 (98%)	774 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	178/179 (99%)	175 (98%)	3 (2%)	53	42
2	B	175/179 (98%)	170 (97%)	5 (3%)	37	22
2	C	173/179 (97%)	171 (99%)	2 (1%)	63	55
2	D	176/179 (98%)	174 (99%)	2 (1%)	65	57
All	All	702/716 (98%)	690 (98%)	12 (2%)	53	42

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	174	ARG
2	A	268	ASN
2	A	291	LYS
2	B	110	ARG
2	B	149	SER
2	B	225	VAL
2	B	247	ASN
2	B	283	ARG
2	C	96	SER
2	C	174	ARG
2	D	149	SER
2	D	228	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	100	GLN
2	A	136	GLN
2	A	178	HIS
2	A	268	ASN
2	A	288	ASN
2	B	100	GLN
2	B	178	HIS
2	B	210	ASN
2	B	235	ASN
2	B	288	ASN
2	C	178	HIS
2	C	239	ASN
2	D	100	GLN
2	D	168	HIS
2	D	178	HIS
2	D	239	ASN
2	D	263	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 oligosaccharides 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	10/12 (83%)	-0.03	0 100 100	29, 41, 47, 58	0
1	F	11/12 (91%)	0.27	1 (9%) 15 15	29, 41, 79, 101	0
1	G	12/12 (100%)	0.25	1 (8%) 17 18	31, 48, 77, 98	0
1	H	12/12 (100%)	0.57	1 (8%) 17 18	33, 49, 97, 108	0
2	A	199/200 (99%)	-0.16	2 (1%) 79 83	21, 30, 47, 67	2 (1%)
2	B	198/200 (99%)	0.17	3 (1%) 72 76	25, 35, 56, 70	0
2	C	193/200 (96%)	-0.06	9 (4%) 36 39	18, 30, 49, 68	2 (1%)
2	D	196/200 (98%)	0.52	14 (7%) 22 24	18, 41, 69, 76	3 (1%)
All	All	831/848 (97%)	0.13	31 (3%) 45 49	18, 34, 61, 108	7 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	288	ASN	5.1
2	D	291	LYS	5.0
2	B	291	LYS	4.7
2	C	119	ALA	4.2
2	D	119	ALA	4.0
2	C	284	THR	3.8
2	C	287	GLU	3.4
2	C	121	SER	3.2
2	D	225	VAL	3.2
2	D	122	VAL	3.1
2	A	153	PRO	3.0
2	D	115	HIS	2.8
2	D	97	VAL	2.8
2	D	103	TYR	2.6
2	A	95	SER	2.6
2	D	121	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	2	DG	2.6
2	B	210	ASN	2.6
2	D	290	ARG	2.4
2	D	114	LEU	2.3
2	D	289	LEU	2.3
2	D	116	SER	2.2
1	G	1	DC	2.2
2	C	226	GLY	2.1
2	D	226	GLY	2.1
2	C	183	SER	2.1
2	C	283	ARG	2.1
2	C	286	GLU	2.1
2	D	228	ASP	2.1
1	H	12	DG	2.0
2	B	225	VAL	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 oligosaccharides 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, 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(Å ²)	Q<0.9
3	ZN	A	1	1/1	0.99	0.04	30,30,30,30	0
3	ZN	B	1	1/1	1.00	0.04	31,31,31,31	0
3	ZN	C	1	1/1	1.00	0.03	29,29,29,29	0
3	ZN	D	1	1/1	1.00	0.03	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.