



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:16 PM UTC

PDB ID : 3KZ8 / pdb_00003kz8
Title : Diversity in DNA recognition by p53 revealed by crystal structures with Hoogsteen base pairs (p53-DNA complex 3)
Authors : Rozenberg, H.; Suad, O.; Shakked, Z.
Deposited on : 2009-12-08
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 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

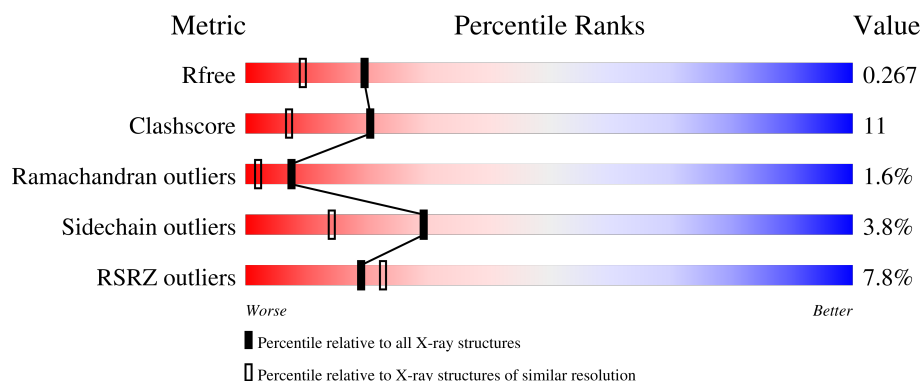
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

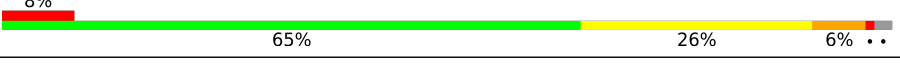
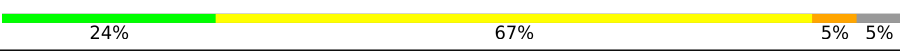
The reported resolution of this entry is 1.91 Å.

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))
R_{free}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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 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	A	200	
1	B	200	
2	C	21	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3784 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	195	Total	C	N	O	S	0	7	0
			1529	949	280	280	20			
1	B	195	Total	C	N	O	S	0	7	0
			1529	949	280	280	20			

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*GP*GP*CP*AP*TP*GP*CP*CP*CP*GP*GP*GP*CP*AP*TP*GP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			410	192	78	120	20			

- 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		

- Molecule 4 is IODIDE ION (CCD ID: IOD) (formula: I).

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

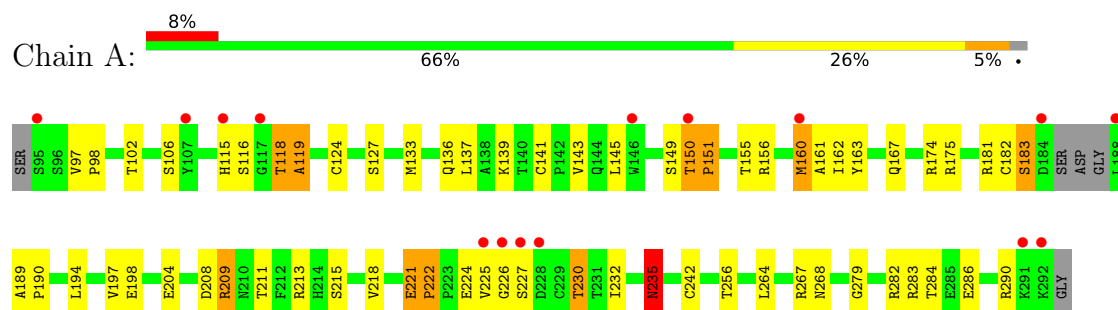
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	122	Total 122	O 122	0	0
5	B	123	Total 124	O 124	0	1
5	C	66	Total 66	O 66	0	0

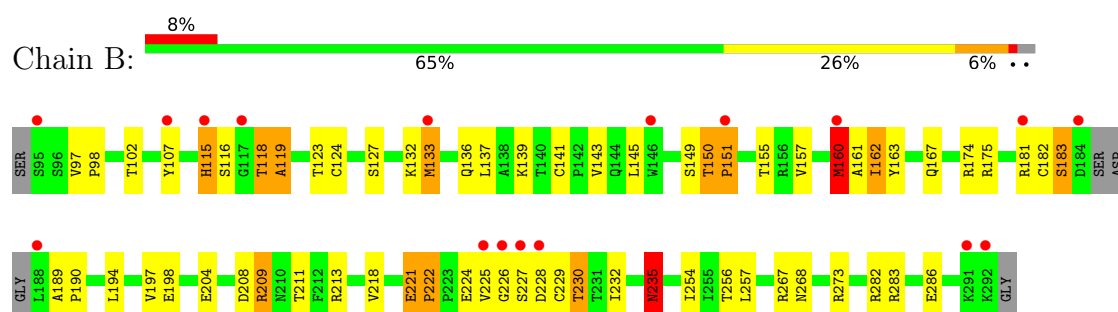
3 Residue-property plots [i](#)

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: Cellular tumor antigen p53



• Molecule 1: Cellular tumor antigen p53



• Molecule 2: DNA (5'-D(*TP*GP*GP*GP*CP*AP*TP*GP*CP*CP*CP*GP*GP*GP*CP*AP*TP*GP*CP*CP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.42Å 49.81Å 68.06Å 90.00° 93.48° 90.00°	Depositor
Resolution (Å)	34.54 – 1.91 34.54 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.6 (34.54-1.91) 99.6 (34.54-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.79 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.4.0078	Depositor
R, R_{free}	0.221 , 0.266 0.221 , 0.267	Depositor DCC
R_{free} test set	1916 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3784	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 96.92 % 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 3.1661e-10. 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, IOD

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	1.85	24/1572 (1.5%)	1.60	20/2134 (0.9%)
1	B	1.91	31/1572 (2.0%)	1.61	18/2134 (0.8%)
2	C	1.32	0/459	2.22	19/706 (2.7%)
All	All	1.82	55/3603 (1.5%)	1.70	57/4974 (1.1%)

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
1	A	0	1
1	B	0	2
All	All	0	3

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	ALA	CA-CB	11.23	1.70	1.53
1	B	181	ARG	CZ-NH2	-10.26	1.20	1.33
1	A	190	PRO	CA-C	9.09	1.56	1.51
1	B	190	PRO	CA-C	8.98	1.56	1.51
1	B	222	PRO	CA-C	8.42	1.57	1.52
1	B	227	SER	N-CA	7.89	1.55	1.46
1	B	132	LYS	C-O	7.59	1.32	1.23
1	B	197	VAL	CA-CB	7.44	1.63	1.54
1	B	155	THR	CA-C	7.21	1.62	1.52
1	A	155	THR	CA-C	6.86	1.61	1.52
1	A	222	PRO	CA-C	6.74	1.56	1.52
1	B	133[A]	MET	C-O	-6.69	1.15	1.23
1	B	133[B]	MET	C-O	-6.69	1.15	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	CYS	N-CA	6.62	1.54	1.46
1	A	227	SER	N-CA	6.62	1.53	1.46
1	A	151	PRO	CA-C	6.50	1.58	1.52
1	B	218	VAL	CA-C	-6.50	1.47	1.52
1	A	197	VAL	CA-CB	6.46	1.61	1.54
1	A	97	VAL	N-CA	6.43	1.51	1.46
1	B	204	GLU	N-CA	6.20	1.53	1.46
1	B	181	ARG	NE-CZ	-6.14	1.26	1.33
1	A	119	ALA	N-CA	6.13	1.53	1.45
1	B	119	ALA	N-CA	6.06	1.53	1.45
1	A	218	VAL	CA-C	-6.02	1.47	1.52
1	B	163	TYR	N-CA	6.01	1.53	1.46
1	A	115	HIS	CE1-NE2	5.96	1.38	1.32
1	A	215	SER	C-O	5.95	1.31	1.23
1	B	273	ARG	N-CA	5.90	1.53	1.46
1	B	161	ALA	C-O	5.89	1.30	1.23
1	B	97	VAL	N-CA	5.88	1.50	1.46
1	A	163	TYR	N-CA	5.76	1.53	1.46
1	A	204	GLU	N-CA	5.72	1.53	1.46
1	A	235	ASN	C-O	5.69	1.30	1.23
1	B	160[A]	MET	N-CA	5.67	1.53	1.45
1	B	160[B]	MET	N-CA	5.67	1.53	1.45
1	B	228	ASP	CA-C	5.64	1.59	1.52
1	A	161	ALA	N-CA	5.58	1.52	1.46
1	B	254	ILE	C-O	5.56	1.30	1.24
1	A	118	THR	CA-CB	5.51	1.60	1.53
1	B	157	VAL	C-O	5.51	1.30	1.24
1	B	118	THR	CA-CB	5.48	1.60	1.53
1	B	235	ASN	C-O	5.47	1.30	1.23
1	B	143	VAL	CA-CB	5.43	1.61	1.54
1	B	227	SER	CA-C	5.39	1.59	1.52
1	B	257	LEU	N-CA	-5.35	1.39	1.46
1	A	143	VAL	CA-CB	5.28	1.60	1.54
1	A	242	CYS	N-CA	5.22	1.52	1.46
1	B	115	HIS	C-O	5.20	1.30	1.23
1	A	161	ALA	C-O	5.19	1.30	1.24
1	B	162	ILE	C-O	-5.14	1.18	1.24
1	A	279	GLY	N-CA	5.12	1.52	1.45
1	A	156	ARG	N-CA	5.09	1.52	1.45
1	A	181	ARG	NE-CZ	5.08	1.38	1.33
1	A	106	SER	CA-C	-5.06	1.45	1.52
1	A	264	LEU	N-CA	5.02	1.52	1.46

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	DA	N9-C1'-C2'	9.99	128.49	113.50
2	C	15	DA	N9-C1'-C2'	9.91	128.37	113.50
1	B	181	ARG	NE-CZ-NH2	-7.14	112.78	119.20
2	C	15	DA	O4'-C1'-N9	-7.14	97.69	108.40
1	A	194	LEU	N-CA-C	6.94	118.49	111.07
2	C	18	DC	C4'-C3'-O3'	-6.76	99.86	110.00
2	C	5	DA	O4'-C1'-N9	-6.72	98.32	108.40
1	B	282	ARG	N-CA-C	-6.65	104.11	111.36
2	C	8	DC	C4'-C3'-O3'	-6.62	100.08	110.00
1	A	282	ARG	N-CA-C	-6.61	104.16	111.36
2	C	15	DA	C5'-C4'-O4'	6.53	119.20	109.40
1	B	194	LEU	N-CA-C	6.50	118.03	111.07
2	C	5	DA	C5'-C4'-O4'	6.45	119.08	109.40
1	A	209	ARG	CD-NE-CZ	-6.22	115.69	124.40
2	C	9	DC	C5'-C4'-O4'	6.06	118.49	109.40
2	C	2	DG	O3'-P-O5'	5.94	112.91	104.00
1	B	127	SER	CB-CA-C	-5.92	104.31	110.17
1	A	127	SER	CB-CA-C	-5.89	104.34	110.17
1	A	218	VAL	CA-C-N	-5.88	113.91	119.85
1	A	218	VAL	C-N-CA	-5.88	113.91	119.85
1	B	226	GLY	CA-C-N	5.88	131.85	121.80
1	B	226	GLY	C-N-CA	5.88	131.85	121.80
1	B	218	VAL	CA-C-N	-5.88	113.92	119.85
1	B	218	VAL	C-N-CA	-5.88	113.92	119.85
2	C	19	DC	C5'-C4'-O4'	5.81	118.12	109.40
1	B	189	ALA	CA-C-N	-5.80	115.43	119.66
1	B	189	ALA	C-N-CA	-5.80	115.43	119.66
1	B	116	SER	N-CA-C	-5.78	105.60	114.16
2	C	1	DG	P-O3'-C3'	5.66	128.69	120.20
1	A	106	SER	N-CA-C	5.63	120.02	113.20
2	C	12	DG	O3'-P-O5'	5.62	112.44	104.00
1	A	226	GLY	CA-C-N	5.58	131.35	121.80
1	A	226	GLY	C-N-CA	5.58	131.35	121.80
2	C	5	DA	C2-N3-C4	-5.54	102.50	110.80
1	B	286	GLU	N-CA-C	-5.46	105.41	111.36
1	B	97	VAL	N-CA-C	5.39	113.20	107.76
1	B	209	ARG	NE-CZ-NH1	-5.36	116.14	121.50
2	C	5	DA	C4'-C3'-O3'	-5.33	102.00	110.00
1	A	189	ALA	CA-C-N	-5.31	115.78	119.66
1	A	189	ALA	C-N-CA	-5.31	115.78	119.66
1	A	284	THR	N-CA-C	5.27	116.71	111.07
1	A	116	SER	N-CA-C	-5.26	106.38	114.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	ARG	CB-CA-C	-5.26	98.50	110.07
2	C	11	DG	P-O3'-C3'	5.25	128.08	120.20
2	C	16	DT	C4'-C3'-O3'	-5.25	102.13	110.00
1	A	221	GLU	CB-CA-C	5.22	115.63	109.47
1	A	116	SER	O-C-N	5.21	127.21	121.85
2	C	4	DC	C4'-C3'-O3'	-5.20	102.19	110.00
2	C	15	DA	C4'-C3'-O3'	-5.18	102.23	110.00
1	A	174	ARG	CB-CA-C	-5.17	98.70	110.07
1	A	209	ARG	NE-CZ-NH2	-5.16	114.55	119.20
1	B	151	PRO	CA-C-N	-5.13	115.10	120.38
1	B	151	PRO	C-N-CA	-5.13	115.10	120.38
1	A	97	VAL	N-CA-C	5.10	112.91	107.76
1	A	286	GLU	N-CA-C	-5.09	105.81	111.36
1	A	190	PRO	O-C-N	5.05	123.64	121.31
1	B	221	GLU	CB-CA-C	5.02	115.39	109.47

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	ALA	Peptide
1	B	119	ALA	Peptide
1	B	160[A]	MET	Mainchain

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	A	1529	0	1459	36	1
1	B	1529	0	1459	37	0
2	C	410	0	223	2	1
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	122	0	0	3	0
5	B	124	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	66	0	0	2	0
All	All	3784	0	3141	74	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 11.

All (74) 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:A:98:PRO:HG2	1:A:160[A]:MET:CE	1.58	1.32
1:B:98:PRO:HG2	1:B:160[A]:MET:CE	1.74	1.17
1:B:98:PRO:HG2	1:B:160[A]:MET:HE2	1.16	1.11
1:A:98:PRO:HG2	1:A:160[A]:MET:HE2	1.09	1.08
1:A:98:PRO:CG	1:A:160[A]:MET:CE	2.39	1.01
1:A:98:PRO:CG	1:A:160[A]:MET:HE1	2.02	0.90
1:A:221:GLU:O	1:A:230:THR:HG21	1.74	0.84
1:B:98:PRO:CG	1:B:160[A]:MET:CE	2.54	0.84
1:A:98:PRO:HG2	1:A:160[A]:MET:HE1	1.58	0.84
1:B:221:GLU:O	1:B:230:THR:HG21	1.74	0.84
1:B:124[A]:CYS:SG	1:B:133[A]:MET:SD	2.81	0.79
1:B:182:CYS:O	1:B:183:SER:O	2.02	0.78
1:A:124[A]:CYS:SG	1:A:133[A]:MET:SD	2.81	0.78
1:B:150[A]:THR:HG23	5:B:335:HOH:O	1.82	0.77
1:A:182:CYS:O	1:A:183:SER:O	2.08	0.72
1:A:98:PRO:CG	1:A:160[A]:MET:HE2	2.05	0.70
1:A:150[A]:THR:HG23	5:A:331:HOH:O	1.93	0.69
1:B:145:LEU:HD11	1:B:232:ILE:HD11	1.75	0.66
1:A:145:LEU:HD11	1:A:232:ILE:HD11	1.76	0.66
1:B:98:PRO:CG	1:B:160[A]:MET:HE1	2.26	0.64
1:A:198:GLU:OE1	1:A:235:ASN:ND2	2.33	0.58
1:B:198:GLU:OE1	1:B:235:ASN:ND2	2.34	0.58
1:B:160[A]:MET:HE1	1:B:213:ARG:CD	2.33	0.57
1:A:141[B]:CYS:SG	1:A:141[B]:CYS:O	2.64	0.56
1:B:182:CYS:C	1:B:183:SER:O	2.48	0.56
1:B:209:ARG:HG2	5:B:334:HOH:O	2.06	0.55
1:B:136[B]:GLN:NE2	1:B:139:LYS:HZ2	2.05	0.54
1:A:182:CYS:C	1:A:183:SER:O	2.51	0.53
1:B:160[A]:MET:HE1	1:B:213:ARG:HD3	1.91	0.53
1:A:137:LEU:N	1:A:137:LEU:HD23	2.24	0.52
1:A:145:LEU:HD11	1:A:232:ILE:CD1	2.38	0.52
1:A:256:THR:HG22	1:A:267:ARG:HG3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LEU:N	1:B:137:LEU:HD23	2.23	0.52
1:B:145:LEU:HD11	1:B:232:ILE:CD1	2.39	0.52
1:B:102:THR:HG23	1:B:268:ASN:ND2	2.24	0.51
1:B:256:THR:HG22	1:B:267:ARG:HG3	1.92	0.51
1:A:102:THR:HG23	1:A:268:ASN:ND2	2.25	0.51
1:B:141[B]:CYS:SG	1:B:141[B]:CYS:O	2.69	0.51
1:B:136[A]:GLN:OE1	1:B:139:LYS:NZ	2.35	0.50
1:A:98:PRO:HG3	1:A:160[A]:MET:HE1	1.87	0.50
1:B:136[B]:GLN:NE2	1:B:139:LYS:NZ	2.59	0.50
1:A:118:THR:O	1:A:283:ARG:NH2	2.45	0.49
1:A:136[B]:GLN:NE2	1:A:139:LYS:HZ2	2.10	0.49
1:A:136[B]:GLN:NE2	1:A:139:LYS:NZ	2.62	0.47
1:A:124[B]:CYS:O	1:A:124[B]:CYS:SG	2.71	0.47
1:A:136[A]:GLN:OE1	1:A:139:LYS:NZ	2.40	0.47
1:A:167:GLN:OE1	1:B:123:THR:HG21	2.14	0.47
1:A:118:THR:O	1:A:283:ARG:NE	2.45	0.46
1:A:160[B]:MET:HE1	5:A:365:HOH:O	2.15	0.46
1:B:118:THR:O	1:B:283:ARG:NE	2.46	0.46
1:A:167:GLN:NE2	5:A:55:HOH:O	2.38	0.45
1:B:118:THR:O	1:B:283:ARG:NH2	2.45	0.43
1:A:160[A]:MET:HE2	1:A:162:ILE:CG2	2.49	0.43
1:B:136[B]:GLN:HE21	1:B:136[B]:GLN:HB3	1.48	0.43
1:A:160[A]:MET:HE1	1:A:213:ARG:CD	2.49	0.43
1:A:150[B]:THR:HA	1:A:151:PRO:HD3	1.94	0.43
1:B:208:ASP:HB3	1:B:211:THR:OG1	2.19	0.43
2:C:13:DG:H8	5:C:274:HOH:O	2.01	0.42
1:B:137:LEU:HD23	1:B:137:LEU:H	1.84	0.42
1:B:160[A]:MET:CE	1:B:162:ILE:CG2	2.97	0.42
1:A:137:LEU:HD23	1:A:137:LEU:H	1.84	0.42
1:A:208:ASP:HB3	1:A:211:THR:OG1	2.20	0.42
1:B:167:GLN:NE2	5:B:45:HOH:O	2.40	0.42
1:B:150[B]:THR:HA	1:B:151:PRO:HD3	1.93	0.41
1:B:160[A]:MET:HE3	1:B:162:ILE:HG22	2.03	0.41
1:B:107:TYR:CE1	1:B:151:PRO:HA	2.56	0.41
1:A:150[A]:THR:H	1:A:150[A]:THR:HG22	1.59	0.41
1:A:160[A]:MET:CE	1:A:162:ILE:CG2	2.99	0.40
1:B:115:HIS:CD2	5:B:378:HOH:O	2.73	0.40
1:B:160[A]:MET:CE	1:B:213:ARG:HD3	2.51	0.40
2:C:3:DG:H8	5:C:277:HOH:O	2.03	0.40
1:A:221:GLU:HA	1:A:222:PRO:HD3	2.00	0.40
1:B:150[A]:THR:H	1:B:150[A]:THR:HG22	1.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:GLU:HA	1:B:222:PRO:HD3	2.00	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:209:ARG:NH1	1:A:290:ARG:O[1_545]	1.83	0.37
2:C:1:DG:P	2:C:20:DC:O3'[1_554]	2.01	0.19

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%)	191 (96%)	4 (2%)	3 (2%)	8	2
1	B	198/200 (99%)	191 (96%)	4 (2%)	3 (2%)	8	2
All	All	396/400 (99%)	382 (96%)	8 (2%)	6 (2%)	7	2

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	SER
1	A	225	VAL
1	B	183	SER
1	B	225	VAL
1	A	224	GLU
1	B	224	GLU

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	167/179 (93%)	159 (95%)	8 (5%)	23	8
1	B	167/179 (93%)	159 (95%)	8 (5%)	23	8
All	All	334/358 (93%)	318 (95%)	16 (5%)	29	8

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	SER
1	A	150[A]	THR
1	A	150[B]	THR
1	A	160[A]	MET
1	A	160[B]	MET
1	A	175	ARG
1	A	230	THR
1	A	235	ASN
1	B	149	SER
1	B	150[A]	THR
1	B	150[B]	THR
1	B	160[A]	MET
1	B	160[B]	MET
1	B	175	ARG
1	B	230	THR
1	B	235	ASN

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

Mol	Chain	Res	Type
1	A	115	HIS
1	A	247	ASN
1	A	263	ASN
1	A	268	ASN
1	B	115	HIS
1	B	247	ASN
1	B	263	ASN
1	B	268	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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, 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	195/200 (97%)	0.17	15 (7%)	19 23	10, 26, 46, 70	7 (3%)
1	B	195/200 (97%)	0.18	17 (8%)	16 19	9, 26, 47, 73	7 (3%)
2	C	20/21 (95%)	-0.74	0	100 100	18, 27, 33, 33	0
All	All	410/421 (97%)	0.13	32 (7%)	19 22	9, 26, 46, 73	14 (3%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	SER	5.1
1	A	160[A]	MET	4.0
1	A	225	VAL	3.9
1	B	107	TYR	3.8
1	A	228	ASP	3.8
1	B	225	VAL	3.7
1	B	188	LEU	3.6
1	A	188	LEU	3.4
1	B	160[A]	MET	3.4
1	B	228	ASP	3.2
1	A	292	LYS	3.2
1	A	291	LYS	3.2
1	B	227	SER	3.1
1	A	107	TYR	3.0
1	B	292	LYS	2.8
1	B	181	ARG	2.7
1	B	115	HIS	2.7
1	B	184	ASP	2.6
1	B	151	PRO	2.5
1	A	226	GLY	2.5
1	A	95	SER	2.4
1	B	291	LYS	2.4
1	B	226	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	184	ASP	2.4
1	B	95	SER	2.4
1	B	133[A]	MET	2.3
1	A	117	GLY	2.3
1	B	117	GLY	2.2
1	A	146	TRP	2.2
1	B	146	TRP	2.2
1	A	150[A]	THR	2.2
1	A	115	HIS	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 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
4	IOD	A	2	1/1	0.94	0.11	43,43,43,43	1
4	IOD	B	2	1/1	0.95	0.11	42,42,42,42	1
3	ZN	A	1	1/1	1.00	0.01	19,19,19,19	0
3	ZN	B	1	1/1	1.00	0.01	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.