



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 08:30 pm BST

PDB ID : 2DUD  
Title : Crystal structure of human mitochondrial single-stranded DNA-binding protein(hmtSSB)  
Authors : Dong, X.; Bessho, Y.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2006-07-21  
Resolution : 2.70 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](mailto: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

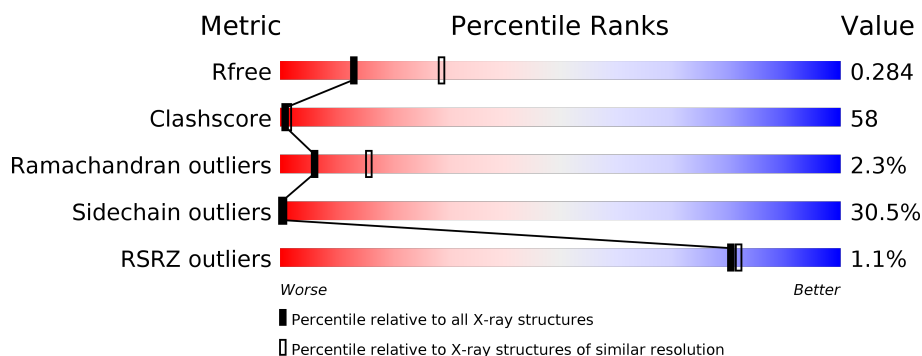
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	133	<div> <div>2%</div> <div>11% 23% 26% 13% 29%</div> </div>
1	B	133	<div> <div>11% 22% 20% 17% 31%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1539 atoms, of which 0 are hydrogens and 0 are deuteriums.

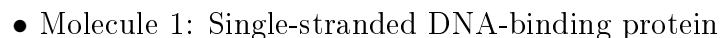
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Single-stranded DNA-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	95	Total	C	N	O	S	0	0	0
			783	498	146	137	2			
1	B	92	Total	C	N	O	S	0	0	0
			756	479	142	133	2			



- Molecule 1: Single-stranded DNA-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.90Å 106.90Å 90.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.99 – 2.70 34.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.99-2.70) 99.9 (34.99-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.34 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.259 , 0.287 0.258 , 0.284	Depositor DCC
$R_{free}$ test set	556 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.5	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	1539	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	3.17	85/797 (10.7%)	2.37	54/1074 (5.0%)
1	B	3.02	75/768 (9.8%)	2.57	52/1033 (5.0%)
All	All	3.09	160/1565 (10.2%)	2.47	106/2107 (5.0%)

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	3
1	B	0	4
All	All	0	7

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	GLU	CD-OE1	15.17	1.42	1.25
1	B	105	ASP	C-N	-15.06	0.99	1.34
1	A	70	ARG	CG-CD	13.06	1.84	1.51
1	B	123	PHE	N-CA	12.22	1.70	1.46
1	B	89	GLY	C-O	11.98	1.42	1.23
1	B	88	LYS	CD-CE	11.86	1.80	1.51
1	A	100	TYR	CE1-CZ	-11.50	1.23	1.38
1	A	46	ASN	CB-CG	-11.25	1.25	1.51
1	B	70	ARG	CB-CG	11.23	1.82	1.52
1	A	17	VAL	CB-CG2	-11.13	1.29	1.52
1	A	36	ASN	N-CA	10.99	1.68	1.46
1	A	93	TYR	CD1-CE1	10.80	1.55	1.39
1	A	112	GLN	CG-CD	10.70	1.75	1.51
1	A	96	GLY	C-O	10.54	1.40	1.23
1	A	111	ARG	NE-CZ	10.41	1.46	1.33
1	A	95	GLU	CD-OE1	10.40	1.37	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	PRO	CB-CG	10.19	2.00	1.50
1	B	118	ALA	CA-CB	10.01	1.73	1.52
1	B	64	GLN	CG-CD	10.00	1.74	1.51
1	B	36	ASN	C-O	9.91	1.42	1.23
1	A	66	THR	C-O	-9.88	1.04	1.23
1	A	62	VAL	CA-CB	9.63	1.75	1.54
1	A	79	ARG	CG-CD	9.57	1.75	1.51
1	A	111	ARG	CZ-NH2	9.48	1.45	1.33
1	A	47	GLU	CD-OE2	9.41	1.35	1.25
1	B	95	GLU	CD-OE1	9.38	1.35	1.25
1	A	123	PHE	N-CA	9.29	1.65	1.46
1	B	112	GLN	CB-CG	9.16	1.77	1.52
1	B	117	ILE	CA-CB	-9.06	1.34	1.54
1	A	75	ARG	CG-CD	8.98	1.74	1.51
1	B	16	ARG	CB-CG	8.89	1.76	1.52
1	A	83	TYR	CD2-CE2	8.71	1.52	1.39
1	A	118	ALA	C-O	-8.64	1.06	1.23
1	A	43	LEU	C-O	8.61	1.39	1.23
1	A	42	SER	CB-OG	8.57	1.53	1.42
1	A	70	ARG	NE-CZ	8.46	1.44	1.33
1	B	25	GLN	CB-CG	8.43	1.75	1.52
1	B	17	VAL	CB-CG2	-8.42	1.35	1.52
1	B	92	ILE	CA-CB	-8.34	1.35	1.54
1	A	77	GLY	C-O	8.24	1.36	1.23
1	A	70	ARG	CZ-NH2	8.22	1.43	1.33
1	B	106	LYS	CB-CG	-8.20	1.30	1.52
1	A	94	LEU	C-O	-8.19	1.07	1.23
1	A	111	ARG	CZ-NH1	8.18	1.43	1.33
1	A	47	GLU	CD-OE1	-7.92	1.17	1.25
1	A	93	TYR	CG-CD2	7.87	1.49	1.39
1	A	12	ARG	N-CA	7.82	1.61	1.46
1	A	118	ALA	CA-CB	7.78	1.68	1.52
1	A	93	TYR	CE1-CZ	7.78	1.48	1.38
1	A	108	ASN	CB-CG	-7.77	1.33	1.51
1	A	100	TYR	CG-CD2	-7.76	1.29	1.39
1	A	111	ARG	CB-CG	7.75	1.73	1.52
1	A	68	TRP	CE3-CZ3	7.73	1.51	1.38
1	A	93	TYR	CD2-CE2	7.67	1.50	1.39
1	B	102	GLU	CG-CD	7.57	1.63	1.51
1	A	40	ILE	N-CA	-7.44	1.31	1.46
1	B	88	LYS	CB-CG	7.42	1.72	1.52
1	B	122	ILE	CA-CB	7.36	1.71	1.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	TYR	C-O	-7.23	1.09	1.23
1	B	19	LEU	CG-CD1	-7.22	1.25	1.51
1	A	100	TYR	C-O	7.18	1.36	1.23
1	A	113	ALA	CA-CB	7.16	1.67	1.52
1	B	111	ARG	NE-CZ	7.14	1.42	1.33
1	A	97	LYS	CE-NZ	7.11	1.66	1.49
1	A	89	GLY	C-O	-7.07	1.12	1.23
1	A	91	ARG	NE-CZ	6.95	1.42	1.33
1	A	119	ASP	CB-CG	6.91	1.66	1.51
1	B	123	PHE	CB-CG	-6.91	1.39	1.51
1	B	110	ARG	CB-CG	-6.86	1.34	1.52
1	A	92	ILE	C-O	-6.81	1.10	1.23
1	A	26	ASP	CG-OD1	6.80	1.41	1.25
1	B	44	ALA	N-CA	6.76	1.59	1.46
1	B	123	PHE	CA-C	6.71	1.70	1.52
1	A	62	VAL	N-CA	6.69	1.59	1.46
1	B	75	ARG	CG-CD	6.67	1.68	1.51
1	A	91	ARG	CZ-NH2	6.65	1.41	1.33
1	B	110	ARG	CZ-NH2	6.64	1.41	1.33
1	A	37	PRO	CG-CD	6.57	1.72	1.50
1	A	69	HIS	C-O	-6.56	1.10	1.23
1	A	112	GLN	CB-CG	6.54	1.70	1.52
1	B	90	SER	CB-OG	-6.54	1.33	1.42
1	A	122	ILE	N-CA	-6.54	1.33	1.46
1	B	16	ARG	NE-CZ	6.54	1.41	1.33
1	B	41	PHE	CA-CB	-6.50	1.39	1.53
1	B	64	GLN	CB-CG	6.40	1.69	1.52
1	B	120	ASN	CG-ND2	6.37	1.48	1.32
1	A	70	ARG	C-O	6.31	1.35	1.23
1	B	47	GLU	CD-OE1	6.29	1.32	1.25
1	B	16	ARG	CG-CD	6.26	1.67	1.51
1	A	82	ALA	CA-C	-6.16	1.36	1.52
1	B	37	PRO	CA-C	6.12	1.65	1.52
1	B	83	TYR	CD1-CE1	6.11	1.48	1.39
1	B	117	ILE	CB-CG2	-6.05	1.34	1.52
1	B	97	LYS	CD-CE	6.04	1.66	1.51
1	A	117	ILE	CA-CB	-6.03	1.41	1.54
1	B	13	SER	CB-OG	-6.00	1.34	1.42
1	B	70	ARG	NE-CZ	5.99	1.40	1.33
1	B	67	THR	CA-CB	-5.99	1.37	1.53
1	B	12	ARG	CB-CG	-5.98	1.36	1.52
1	B	12	ARG	CZ-NH1	-5.95	1.25	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	91	ARG	CZ-NH2	5.92	1.40	1.33
1	A	44	ALA	C-O	-5.90	1.12	1.23
1	B	87	LYS	CE-NZ	5.88	1.63	1.49
1	A	14	LEU	C-N	-5.87	1.20	1.34
1	A	103	TYR	CE2-CZ	5.86	1.46	1.38
1	A	23	VAL	CA-CB	-5.86	1.42	1.54
1	B	14	LEU	C-O	-5.85	1.12	1.23
1	B	65	LYS	CG-CD	5.85	1.72	1.52
1	A	13	SER	C-O	-5.82	1.12	1.23
1	A	13	SER	C-N	-5.76	1.20	1.34
1	A	64	GLN	C-O	-5.73	1.12	1.23
1	B	112	GLN	CG-CD	5.73	1.64	1.51
1	B	42	SER	N-CA	5.72	1.57	1.46
1	A	13	SER	N-CA	5.67	1.57	1.46
1	B	99	ASP	CB-CG	5.65	1.63	1.51
1	A	80	ASP	CB-CG	5.62	1.63	1.51
1	B	70	ARG	N-CA	5.59	1.57	1.46
1	A	107	ASN	CG-ND2	5.56	1.46	1.32
1	A	122	ILE	C-O	-5.54	1.12	1.23
1	B	119	ASP	CG-OD1	5.53	1.38	1.25
1	B	25	GLN	N-CA	5.51	1.57	1.46
1	A	110	ARG	CZ-NH2	-5.49	1.25	1.33
1	A	88	LYS	C-O	-5.48	1.12	1.23
1	B	97	LYS	CB-CG	-5.48	1.37	1.52
1	B	115	THR	CB-OG1	5.48	1.54	1.43
1	A	12	ARG	C-O	5.47	1.33	1.23
1	B	79	ARG	N-CA	-5.45	1.35	1.46
1	B	69	HIS	CA-CB	5.45	1.66	1.53
1	B	111	ARG	CZ-NH1	5.42	1.40	1.33
1	B	93	TYR	CE2-CZ	-5.42	1.31	1.38
1	A	82	ALA	CA-CB	-5.40	1.41	1.52
1	B	22	ARG	CG-CD	5.40	1.65	1.51
1	A	116	ILE	C-O	5.39	1.33	1.23
1	B	29	LEU	CA-CB	-5.39	1.41	1.53
1	B	85	TYR	CB-CG	-5.36	1.43	1.51
1	A	69	HIS	CB-CG	-5.34	1.40	1.50
1	B	20	LEU	C-O	5.34	1.33	1.23
1	B	93	TYR	N-CA	5.34	1.57	1.46
1	B	93	TYR	CB-CG	5.33	1.59	1.51
1	B	78	LEU	C-O	-5.30	1.13	1.23
1	B	123	PHE	CE1-CZ	5.28	1.47	1.37
1	A	66	THR	N-CA	-5.25	1.35	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	PHE	CB-CG	5.24	1.60	1.51
1	B	116	ILE	C-O	5.23	1.33	1.23
1	B	30	ARG	CD-NE	5.23	1.55	1.46
1	A	123	PHE	C-O	5.20	1.33	1.23
1	A	111	ARG	CG-CD	-5.19	1.39	1.51
1	A	102	GLU	CG-CD	5.16	1.59	1.51
1	A	84	GLN	C-O	-5.16	1.13	1.23
1	A	23	VAL	CB-CG2	5.14	1.63	1.52
1	B	12	ARG	CZ-NH2	-5.12	1.26	1.33
1	A	45	THR	CA-CB	5.11	1.66	1.53
1	A	83	TYR	CG-CD2	5.09	1.45	1.39
1	B	45	THR	CB-CG2	5.07	1.69	1.52
1	B	79	ARG	NE-CZ	5.04	1.39	1.33
1	A	68	TRP	CG-CD1	-5.04	1.29	1.36
1	A	110	ARG	C-O	5.03	1.32	1.23
1	B	70	ARG	CZ-NH2	5.02	1.39	1.33
1	B	93	TYR	CD2-CE2	-5.02	1.31	1.39
1	A	84	GLN	CG-CD	5.01	1.62	1.51

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	ARG	NE-CZ-NH1	22.34	131.47	120.30
1	B	110	ARG	NE-CZ-NH2	-18.24	111.18	120.30
1	A	70	ARG	NE-CZ-NH2	17.93	129.26	120.30
1	A	70	ARG	NE-CZ-NH1	-15.67	112.46	120.30
1	B	91	ARG	NE-CZ-NH1	-14.65	112.98	120.30
1	B	91	ARG	NE-CZ-NH2	14.62	127.61	120.30
1	B	12	ARG	NE-CZ-NH2	14.00	127.30	120.30
1	A	26	ASP	CB-CG-OD2	-13.03	106.57	118.30
1	A	26	ASP	CB-CG-OD1	12.31	129.38	118.30
1	B	111	ARG	NE-CZ-NH2	-12.16	114.22	120.30
1	B	110	ARG	NH1-CZ-NH2	11.39	131.93	119.40
1	B	105	ASP	CB-CG-OD2	10.91	128.12	118.30
1	A	106	LYS	O-C-N	10.12	138.90	122.70
1	B	43	LEU	CB-CG-CD1	-9.79	94.36	111.00
1	A	23	VAL	CG1-CB-CG2	-9.35	95.94	110.90
1	B	123	PHE	N-CA-C	9.34	136.22	111.00
1	B	113	ALA	CB-CA-C	8.94	123.52	110.10
1	A	115	THR	CA-CB-CG2	-8.93	99.90	112.40
1	B	92	ILE	CB-CA-C	-8.86	93.88	111.60
1	B	16	ARG	NE-CZ-NH1	8.83	124.71	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	LEU	CB-CA-C	8.65	126.63	110.20
1	A	106	LYS	CA-C-N	-8.55	98.39	117.20
1	B	19	LEU	CB-CG-CD1	8.01	124.61	111.00
1	B	88	LYS	CA-CB-CG	7.88	130.73	113.40
1	B	105	ASP	C-N-CA	7.83	141.26	121.70
1	B	26	ASP	CB-CG-OD1	-7.81	111.27	118.30
1	A	87	LYS	CD-CE-NZ	-7.75	93.88	111.70
1	A	83	TYR	CB-CG-CD2	7.62	125.57	121.00
1	B	122	ILE	CB-CA-C	7.55	126.71	111.60
1	B	78	LEU	CB-CG-CD1	-7.54	98.18	111.00
1	B	78	LEU	CB-CG-CD2	7.31	123.42	111.00
1	A	13	SER	O-C-N	-7.03	111.45	122.70
1	A	45	THR	CA-CB-CG2	6.99	122.19	112.40
1	A	90	SER	CB-CA-C	-6.93	96.94	110.10
1	B	110	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	B	113	ALA	N-CA-CB	6.82	119.65	110.10
1	A	43	LEU	CB-CG-CD2	6.76	122.50	111.00
1	B	114	THR	OG1-CB-CG2	-6.70	94.60	110.00
1	B	12	ARG	NE-CZ-NH1	-6.67	116.97	120.30
1	B	102	GLU	CG-CD-OE2	-6.62	105.06	118.30
1	A	43	LEU	CB-CA-C	-6.61	97.65	110.20
1	B	106	LYS	CB-CA-C	-6.59	97.23	110.40
1	B	105	ASP	OD1-CG-OD2	-6.57	110.81	123.30
1	B	111	ARG	CD-NE-CZ	6.52	132.72	123.60
1	A	98	ILE	CB-CG1-CD1	-6.51	95.66	113.90
1	A	120	ASN	CB-CA-C	-6.30	97.80	110.40
1	A	75	ARG	CB-CA-C	-6.22	97.96	110.40
1	A	113	ALA	N-CA-CB	6.21	118.80	110.10
1	B	117	ILE	CB-CA-C	-6.19	99.22	111.60
1	B	117	ILE	N-CA-CB	-6.18	96.59	110.80
1	A	47	GLU	CG-CD-OE1	-6.14	106.01	118.30
1	A	17	VAL	CB-CA-C	-6.13	99.75	111.40
1	B	29	LEU	CB-CG-CD1	6.11	121.38	111.00
1	B	75	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	B	101	GLY	C-N-CA	-6.04	106.61	121.70
1	A	106	LYS	CB-CA-C	-6.00	98.40	110.40
1	A	117	ILE	N-CA-CB	-5.98	97.05	110.80
1	A	75	ARG	N-CA-CB	5.92	121.27	110.60
1	B	88	LYS	CG-CD-CE	5.90	129.59	111.90
1	A	72	SER	N-CA-CB	-5.88	101.68	110.50
1	A	99	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	17	VAL	CG1-CB-CG2	-5.86	101.52	110.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	VAL	CG1-CB-CG2	-5.82	101.59	110.90
1	B	120	ASN	CB-CA-C	-5.77	98.85	110.40
1	A	75	ARG	CG-CD-NE	-5.71	99.82	111.80
1	B	80	ASP	CB-CG-OD2	5.68	123.42	118.30
1	A	45	THR	N-CA-CB	-5.64	99.58	110.30
1	A	118	ALA	CA-C-N	5.63	129.58	117.20
1	B	20	LEU	CB-CG-CD2	-5.62	101.44	111.00
1	A	73	VAL	CB-CA-C	-5.57	100.82	111.40
1	A	29	LEU	CB-CG-CD1	5.56	120.46	111.00
1	A	83	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	A	14	LEU	O-C-N	-5.53	113.85	122.70
1	A	105	ASP	CA-C-N	5.52	129.34	117.20
1	A	12	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	A	40	ILE	CG1-CB-CG2	-5.45	99.42	111.40
1	B	70	ARG	CG-CD-NE	-5.43	100.40	111.80
1	B	43	LEU	CB-CG-CD2	5.42	120.22	111.00
1	A	105	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	91	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	83	TYR	CE1-CZ-OH	-5.41	105.49	120.10
1	A	14	LEU	CB-CA-C	5.41	120.48	110.20
1	A	89	GLY	N-CA-C	5.39	126.58	113.10
1	B	39	THR	OG1-CB-CG2	-5.33	97.73	110.00
1	B	70	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	23	VAL	N-CA-CB	-5.28	99.89	111.50
1	A	13	SER	CA-C-N	5.26	128.78	117.20
1	A	123	PHE	CB-CG-CD2	5.25	124.47	120.80
1	A	75	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	B	28	VAL	CG1-CB-CG2	-5.21	102.56	110.90
1	A	83	TYR	OH-CZ-CE2	5.20	134.13	120.10
1	B	23	VAL	O-C-N	-5.17	114.40	123.20
1	B	65	LYS	C-N-CA	-5.17	108.76	121.70
1	A	118	ALA	N-CA-C	-5.16	97.08	111.00
1	B	94	LEU	CB-CG-CD2	5.12	119.70	111.00
1	A	101	GLY	O-C-N	-5.11	114.53	122.70
1	A	12	ARG	CB-CA-C	-5.11	100.19	110.40
1	B	109	VAL	N-CA-C	-5.11	97.21	111.00
1	B	111	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
1	A	37	PRO	CB-CG-CD	-5.10	86.60	106.50
1	A	91	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	B	122	ILE	N-CA-CB	-5.08	99.12	110.80
1	A	112	GLN	CA-CB-CG	5.07	124.55	113.40
1	A	117	ILE	N-CA-C	5.07	124.67	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	ILE	CG1-CB-CG2	-5.04	100.30	111.40
1	B	80	ASP	CB-CG-OD1	-5.01	113.79	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ASP	Mainchain,Peptide
1	A	36	ASN	Peptide
1	B	102	GLU	Mainchain
1	B	108	ASN	Peptide
1	B	113	ALA	Mainchain
1	B	69	HIS	Sidechain

## 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	783	0	791	101	0
1	B	756	0	769	89	0
All	All	1539	0	1560	179	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 58.

All (179) 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:62:VAL:CB	1:A:62:VAL:CA	1.75	1.64
1:A:117:ILE:CG1	1:A:117:ILE:CD1	1.75	1.62
1:B:16:ARG:CB	1:B:16:ARG:CG	1.76	1.62
1:A:36:ASN:CA	1:A:36:ASN:N	1.68	1.57
1:B:112:GLN:CG	1:B:112:GLN:CB	1.77	1.56
1:B:25:GLN:CB	1:B:25:GLN:CG	1.75	1.56
1:B:88:LYS:CD	1:B:88:LYS:CE	1.80	1.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ILE:CD1	1:A:122:ILE:CG1	1.81	1.55
1:B:70:ARG:CG	1:B:70:ARG:CB	1.82	1.55
1:A:79:ARG:CG	1:A:79:ARG:CD	1.75	1.55
1:A:112:GLN:CD	1:A:112:GLN:CG	1.75	1.54
1:B:123:PHE:CA	1:B:123:PHE:N	1.70	1.51
1:A:70:ARG:CD	1:A:70:ARG:CG	1.84	1.49
1:A:37:PRO:CB	1:A:37:PRO:CG	2.00	1.37
1:B:123:PHE:CD1	1:B:123:PHE:N	2.19	1.10
1:B:117:ILE:HG22	1:B:117:ILE:O	1.37	1.07
1:A:106:LYS:HB2	1:A:106:LYS:NZ	1.66	1.06
1:B:37:PRO:HD2	1:B:79:ARG:NH1	1.76	1.00
1:A:106:LYS:HB2	1:A:106:LYS:HZ3	1.30	0.97
1:B:92:ILE:HG22	1:B:121:ILE:O	1.63	0.97
1:B:94:LEU:HD23	1:B:117:ILE:HD11	1.47	0.97
1:A:94:LEU:HD22	1:A:117:ILE:HD12	1.47	0.96
1:A:13:SER:O	1:A:14:LEU:HB2	1.66	0.94
1:B:16:ARG:HH22	1:B:118:ALA:HB3	1.28	0.94
1:A:120:ASN:HD22	1:A:120:ASN:N	1.66	0.93
1:A:109:VAL:O	1:A:109:VAL:HG23	1.67	0.93
1:A:94:LEU:HD22	1:A:117:ILE:CD1	1.99	0.92
1:A:119:ASP:C	1:A:120:ASN:HD22	1.72	0.92
1:A:77:GLY:O	1:A:81:VAL:HG23	1.71	0.91
1:B:67:THR:HG22	1:B:69:HIS:CE1	2.06	0.90
1:A:46:ASN:ND2	1:A:64:GLN:HE21	1.69	0.90
1:B:105:ASP:O	1:B:106:LYS:NZ	2.04	0.89
1:B:75:ARG:O	1:B:79:ARG:HB2	1.74	0.88
1:B:123:PHE:CG	1:B:123:PHE:N	2.45	0.84
1:B:110:ARG:HH21	1:B:110:ARG:HB2	1.41	0.84
1:B:94:LEU:CD2	1:B:117:ILE:HD11	2.07	0.83
1:B:19:LEU:HD21	1:B:69:HIS:CD2	2.15	0.82
1:A:117:ILE:CB	1:A:117:ILE:CD1	2.58	0.81
1:A:117:ILE:O	1:A:117:ILE:HG23	1.81	0.80
1:B:37:PRO:HD2	1:B:79:ARG:HH12	1.43	0.80
1:B:105:ASP:O	1:B:106:LYS:CE	2.31	0.79
1:B:16:ARG:CA	1:B:16:ARG:CG	2.61	0.78
1:A:123:PHE:CD1	1:A:123:PHE:N	2.51	0.77
1:B:94:LEU:HD23	1:B:117:ILE:CD1	2.14	0.77
1:B:110:ARG:HH21	1:B:110:ARG:CB	1.99	0.76
1:B:18:HIS:HD2	1:B:95:GLU:HG2	1.51	0.76
1:A:13:SER:O	1:A:14:LEU:CB	2.31	0.75
1:B:67:THR:HG22	1:B:69:HIS:HE1	1.51	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:O	1:A:109:VAL:CG2	2.32	0.75
1:B:122:ILE:C	1:B:123:PHE:CD1	2.59	0.75
1:A:16:ARG:HH12	1:A:118:ALA:HB3	1.53	0.74
1:B:67:THR:CG2	1:B:69:HIS:HE1	2.02	0.73
1:B:123:PHE:CB	1:B:123:PHE:N	2.51	0.73
1:A:82:ALA:O	1:A:86:VAL:HG23	1.86	0.73
1:B:123:PHE:HA	1:B:123:PHE:N	2.01	0.73
1:A:69:HIS:HD2	1:B:100:TYR:OH	1.71	0.73
1:A:62:VAL:CG1	1:A:62:VAL:CA	2.67	0.72
1:A:38:VAL:HG11	1:A:74:PHE:CE1	2.24	0.72
1:A:74:PHE:O	1:A:75:ARG:C	2.28	0.72
1:B:24:GLY:O	1:B:88:LYS:HD3	1.91	0.71
1:A:62:VAL:CB	1:A:62:VAL:C	2.57	0.70
1:B:117:ILE:O	1:B:117:ILE:CG2	2.17	0.70
1:A:101:GLY:N	1:A:112:GLN:O	2.23	0.69
1:A:106:LYS:CB	1:A:106:LYS:NZ	2.42	0.69
1:B:12:ARG:HH21	1:B:12:ARG:HB3	1.58	0.69
1:A:62:VAL:CG2	1:A:62:VAL:CA	2.70	0.68
1:B:67:THR:CG2	1:B:69:HIS:CE1	2.75	0.68
1:B:123:PHE:HD1	1:B:123:PHE:N	1.88	0.67
1:B:94:LEU:N	1:B:94:LEU:HD13	2.08	0.67
1:A:120:ASN:N	1:A:120:ASN:ND2	2.40	0.66
1:A:78:LEU:HD11	1:A:119:ASP:HA	1.76	0.66
1:A:105:ASP:OD1	1:A:108:ASN:ND2	2.28	0.66
1:B:88:LYS:CD	1:B:88:LYS:NZ	2.57	0.66
1:B:109:VAL:O	1:B:109:VAL:HG12	1.95	0.65
1:B:94:LEU:H	1:B:94:LEU:HD13	1.61	0.65
1:B:122:ILE:O	1:B:123:PHE:HD1	1.81	0.64
1:A:117:ILE:O	1:A:117:ILE:CG2	2.45	0.64
1:A:74:PHE:O	1:A:75:ARG:O	2.15	0.64
1:A:83:TYR:CD2	1:A:83:TYR:C	2.70	0.63
1:B:101:GLY:C	1:B:102:GLU:HG3	2.19	0.62
1:B:80:ASP:O	1:B:81:VAL:C	2.33	0.62
1:A:83:TYR:HD2	1:A:83:TYR:C	2.03	0.62
1:B:122:ILE:C	1:B:123:PHE:HD1	2.02	0.61
1:B:78:LEU:HD21	1:B:120:ASN:HB2	1.81	0.61
1:A:16:ARG:HH12	1:A:118:ALA:CB	2.14	0.60
1:A:117:ILE:HD13	1:A:117:ILE:HG21	1.83	0.59
1:A:122:ILE:C	1:A:123:PHE:CD1	2.76	0.59
1:A:83:TYR:HD2	1:A:83:TYR:O	1.86	0.59
1:A:69:HIS:CD2	1:B:100:TYR:OH	2.54	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ARG:NH1	1:B:113:ALA:H	2.01	0.58
1:B:18:HIS:CD2	1:B:95:GLU:HG2	2.36	0.58
1:A:117:ILE:CD1	1:A:117:ILE:HG21	2.34	0.57
1:B:37:PRO:HD2	1:B:79:ARG:HH11	1.64	0.57
1:B:25:GLN:CB	1:B:25:GLN:CD	2.68	0.57
1:A:37:PRO:O	1:A:38:VAL:HG13	2.05	0.57
1:A:106:LYS:HB2	1:A:106:LYS:HZ2	1.66	0.57
1:B:46:ASN:ND2	1:B:66:THR:HB	2.19	0.56
1:A:117:ILE:CD1	1:A:117:ILE:CG2	2.83	0.56
1:B:19:LEU:HD21	1:B:69:HIS:HD2	1.69	0.56
1:A:82:ALA:HB1	1:A:86:VAL:HG21	1.88	0.56
1:B:25:GLN:CA	1:B:25:GLN:CG	2.80	0.55
1:A:82:ALA:HA	1:A:86:VAL:HG23	1.87	0.55
1:A:46:ASN:HD21	1:A:64:GLN:HE21	1.51	0.55
1:A:87:LYS:HB2	1:A:87:LYS:HZ2	1.72	0.54
1:B:12:ARG:HB3	1:B:12:ARG:NH2	2.21	0.54
1:B:94:LEU:N	1:B:94:LEU:CD1	2.69	0.54
1:A:17:VAL:O	1:A:95:GLU:HA	2.07	0.54
1:B:103:TYR:C	1:B:104:MET:HE2	2.27	0.54
1:A:82:ALA:CA	1:A:86:VAL:HG23	2.37	0.53
1:A:122:ILE:O	1:A:123:PHE:CD1	2.62	0.53
1:B:105:ASP:O	1:B:106:LYS:HE3	2.08	0.53
1:B:122:ILE:O	1:B:123:PHE:CD1	2.59	0.53
1:A:94:LEU:HD13	1:A:117:ILE:HG13	1.89	0.52
1:B:20:LEU:HD12	1:B:93:TYR:HB2	1.91	0.52
1:A:80:ASP:O	1:A:84:GLN:HB2	2.08	0.52
1:A:105:ASP:OD2	1:A:108:ASN:ND2	2.42	0.52
1:A:94:LEU:HD22	1:A:117:ILE:HD11	1.90	0.52
1:B:110:ARG:HH21	1:B:110:ARG:CG	2.14	0.52
1:A:111:ARG:HH11	1:B:113:ALA:H	1.58	0.52
1:A:83:TYR:CD2	1:A:83:TYR:O	2.63	0.51
1:A:38:VAL:HG11	1:A:74:PHE:CD1	2.46	0.50
1:A:91:ARG:O	1:A:92:ILE:HG12	2.11	0.50
1:A:119:ASP:C	1:A:120:ASN:ND2	2.54	0.49
1:A:82:ALA:O	1:A:86:VAL:CG2	2.60	0.49
1:B:88:LYS:HD2	1:B:89:GLY:N	2.28	0.49
1:A:112:GLN:CG	1:A:112:GLN:NE2	2.63	0.49
1:A:16:ARG:HA	1:A:96:GLY:O	2.13	0.48
1:A:122:ILE:O	1:A:123:PHE:HD1	1.97	0.48
1:B:20:LEU:HD23	1:B:20:LEU:C	2.34	0.48
1:A:16:ARG:HH22	1:A:118:ALA:HB2	1.79	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:TYR:CE2	1:A:95:GLU:HG3	2.49	0.47
1:B:108:ASN:OD1	1:B:110:ARG:NH2	2.47	0.47
1:B:22:ARG:HA	1:B:90:SER:O	2.15	0.47
1:B:103:TYR:O	1:B:104:MET:HE2	2.14	0.47
1:A:69:HIS:CD2	1:B:100:TYR:CE1	3.03	0.47
1:A:38:VAL:CG1	1:A:74:PHE:CD1	2.98	0.47
1:B:45:THR:HG22	1:B:45:THR:O	2.14	0.47
1:B:47:GLU:C	1:B:48:MET:HG2	2.35	0.47
1:A:76:PRO:HB3	1:A:79:ARG:HH21	1.80	0.46
1:A:108:ASN:HD21	1:A:110:ARG:NH2	2.14	0.46
1:B:104:MET:CA	1:B:104:MET:HE2	2.46	0.46
1:A:69:HIS:CD2	1:B:100:TYR:HE1	2.33	0.46
1:B:122:ILE:C	1:B:123:PHE:CA	2.72	0.46
1:A:46:ASN:O	1:B:13:SER:HB2	2.16	0.46
1:A:70:ARG:HG2	1:A:114:THR:CB	2.46	0.46
1:B:121:ILE:HG22	1:B:123:PHE:HE1	1.80	0.46
1:A:73:VAL:HG13	1:A:117:ILE:CG2	2.46	0.46
1:A:15:ASN:HB2	1:B:45:THR:HG21	1.97	0.45
1:A:94:LEU:C	1:A:94:LEU:HD12	2.36	0.45
1:B:45:THR:HG22	1:B:67:THR:HB	1.98	0.45
1:B:98:ILE:HG21	1:B:98:ILE:HD13	1.77	0.45
1:A:108:ASN:HD21	1:A:110:ARG:CZ	2.31	0.44
1:B:75:ARG:HA	1:B:76:PRO:HD3	1.48	0.44
1:A:92:ILE:CD1	1:A:122:ILE:HA	2.48	0.44
1:A:91:ARG:HB3	1:A:123:PHE:HD2	1.83	0.44
1:A:113:ALA:H	1:B:111:ARG:HD3	1.81	0.44
1:B:36:ASN:N	1:B:37:PRO:HD3	2.33	0.43
1:A:94:LEU:HB2	1:A:117:ILE:HD11	2.01	0.43
1:B:101:GLY:C	1:B:102:GLU:CG	2.87	0.43
1:B:92:ILE:HG23	1:B:92:ILE:HD13	1.67	0.43
1:B:75:ARG:O	1:B:79:ARG:CB	2.58	0.42
1:B:92:ILE:HG21	1:B:92:ILE:HD12	1.59	0.42
1:A:12:ARG:N	1:B:91:ARG:NH2	2.68	0.41
1:A:87:LYS:O	1:A:88:LYS:C	2.58	0.41
1:A:41:PHE:CD1	1:A:41:PHE:N	2.88	0.41
1:A:92:ILE:HD13	1:A:122:ILE:HA	2.02	0.41
1:A:36:ASN:N	1:A:36:ASN:HA	2.05	0.41
1:A:39:THR:O	1:A:72:SER:HA	2.21	0.41
1:B:105:ASP:OD1	1:B:106:LYS:N	2.53	0.41
1:A:36:ASN:CB	1:A:36:ASN:N	2.71	0.41
1:A:92:ILE:HD13	1:A:92:ILE:HA	1.69	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ILE:HD13	1:A:115:THR:HB	2.02	0.41
1:B:17:VAL:HG12	1:B:19:LEU:HD13	2.03	0.41
1:A:12:ARG:O	1:B:91:ARG:NH2	2.53	0.41
1:A:105:ASP:CG	1:A:108:ASN:ND2	2.73	0.40
1:A:98:ILE:HG23	1:A:98:ILE:HD13	1.52	0.40
1:A:46:ASN:HD21	1:A:64:GLN:NE2	2.18	0.40
1:A:17:VAL:HG12	1:A:19:LEU:HD13	2.03	0.40
1:B:104:MET:HE3	1:B:104:MET:HB2	1.77	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	89/133 (67%)	77 (86%)	9 (10%)	3 (3%)	3	8
1	B	86/133 (65%)	79 (92%)	6 (7%)	1 (1%)	13	32
All	All	175/266 (66%)	156 (89%)	15 (9%)	4 (2%)	6	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	106	LYS
1	B	106	LYS
1	A	75	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	
1	A	85/120 (71%)	60 (71%)	25 (29%)	0	1
1	B	82/120 (68%)	56 (68%)	26 (32%)	0	0
All	All	167/240 (70%)	116 (70%)	51 (30%)	0	0

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	16	ARG
1	A	19	LEU
1	A	25	GLN
1	A	29	LEU
1	A	30	ARG
1	A	36	ASN
1	A	45	THR
1	A	46	ASN
1	A	66	THR
1	A	70	ARG
1	A	72	SER
1	A	73	VAL
1	A	78	LEU
1	A	83	TYR
1	A	84	GLN
1	A	87	LYS
1	A	88	LYS
1	A	90	SER
1	A	104	MET
1	A	106	LYS
1	A	108	ASN
1	A	111	ARG
1	A	120	ASN
1	A	123	PHE
1	B	12	ARG
1	B	13	SER
1	B	14	LEU
1	B	25	GLN
1	B	29	LEU
1	B	37	PRO
1	B	45	THR
1	B	48	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	66	THR
1	B	70	ARG
1	B	75	ARG
1	B	78	LEU
1	B	84	GLN
1	B	88	LYS
1	B	92	ILE
1	B	94	LEU
1	B	102	GLU
1	B	104	MET
1	B	106	LYS
1	B	109	VAL
1	B	110	ARG
1	B	111	ARG
1	B	117	ILE
1	B	120	ASN
1	B	122	ILE
1	B	123	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	25	GLN
1	A	46	ASN
1	A	69	HIS
1	A	84	GLN
1	A	108	ASN
1	A	120	ASN
1	B	18	HIS
1	B	46	ASN
1	B	69	HIS
1	B	107	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	105:ASP	C	106:LYS	N	0.99

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	95/133 (71%)	-0.32	2 (2%) 63 65	16, 41, 63, 71	0
1	B	92/133 (69%)	-0.38	0 100 100	19, 41, 68, 72	0
All	All	187/266 (70%)	-0.35	2 (1%) 80 82	16, 41, 66, 72	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	ILE	2.7
1	A	29	LEU	2.6

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.