



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:25 PM UTC

PDB ID : 2DUD / pdb_00002dud
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

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

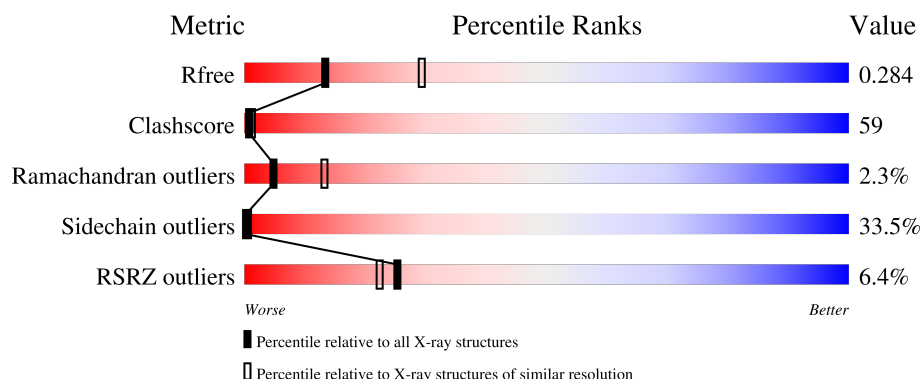
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	133	 3% 7% 17% 31% 29%
1	B	133	 6% 9% 21% 23% 16% 31%

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.

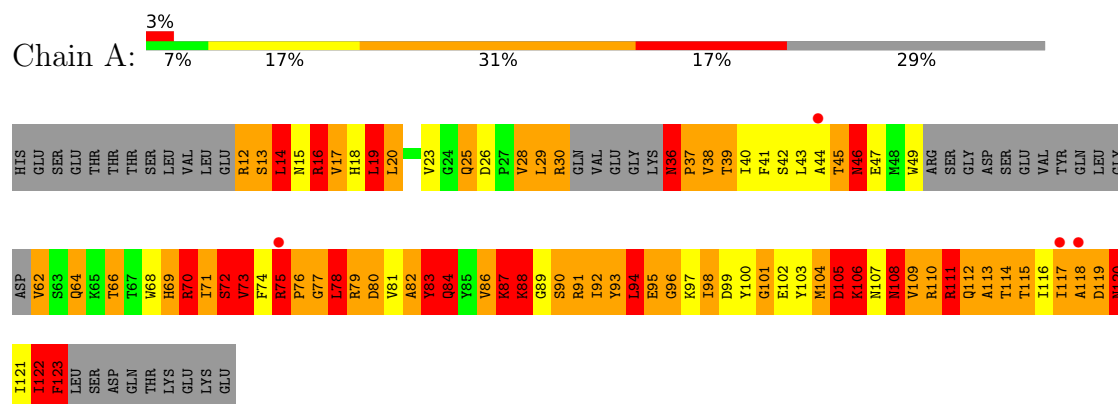
- Molecule 1 is a protein called Single-stranded DNA-binding protein.

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			

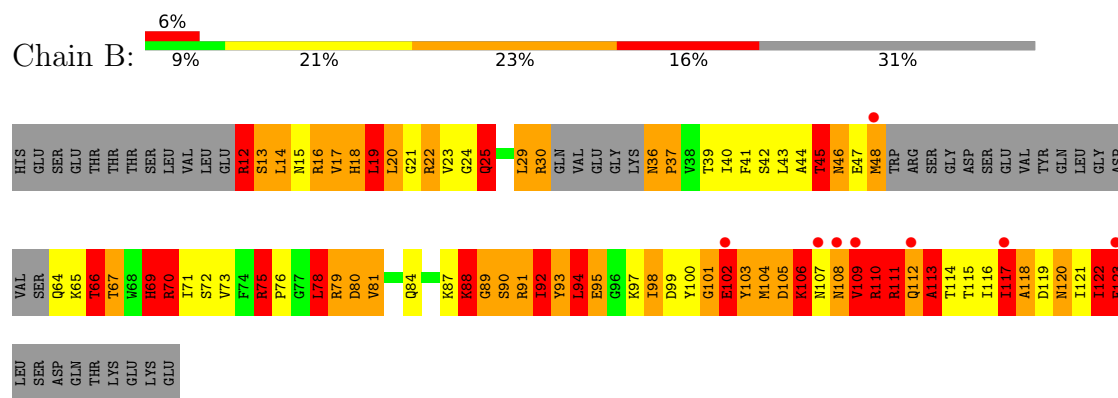
3 Residue-property plots

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: Single-stranded DNA-binding protein



• 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, α , β , γ	106.90Å 106.90Å 90.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.99 – 2.70 34.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.99-2.70) 99.9 (34.99-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	51.5	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	1539	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

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	3.89	143/797 (17.9%)	2.66	76/1074 (7.1%)
1	B	3.74	119/768 (15.5%)	2.83	76/1033 (7.4%)
All	All	3.82	262/1565 (16.7%)	2.75	152/2107 (7.2%)

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 (262) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	ASP	C-N	-24.48	0.99	1.33
1	B	117	ILE	CA-CB	-16.13	1.34	1.54
1	A	66	THR	C-O	-15.76	1.04	1.24
1	B	92	ILE	CA-CB	-14.71	1.35	1.54
1	A	94	LEU	C-O	-14.61	1.07	1.23
1	B	118	ALA	CA-CB	13.70	1.73	1.54
1	B	122	ILE	CA-CB	13.27	1.71	1.54
1	A	118	ALA	C-O	-13.00	1.06	1.24
1	B	123	PHE	N-CA	12.91	1.70	1.46
1	A	96	GLY	C-O	12.86	1.40	1.23
1	B	89	GLY	C-O	12.85	1.42	1.24
1	A	82	ALA	CA-C	-12.30	1.36	1.52
1	A	111	ARG	NE-CZ	12.30	1.46	1.33
1	A	43	LEU	C-O	12.30	1.39	1.24
1	A	40	ILE	N-CA	-12.26	1.31	1.46
1	A	92	ILE	C-O	-12.14	1.10	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	ILE	CA-C	-12.07	1.42	1.52
1	A	36	ASN	N-CA	11.62	1.68	1.46
1	A	122	ILE	N-CA	-11.60	1.33	1.46
1	B	44	ALA	N-CA	11.38	1.59	1.46
1	A	117	ILE	CA-CB	-11.21	1.41	1.54
1	A	46	ASN	CB-CG	-10.75	1.25	1.52
1	A	70	ARG	CG-CD	10.72	1.84	1.52
1	A	77	GLY	C-O	10.70	1.36	1.23
1	A	69	HIS	C-O	-10.64	1.10	1.24
1	A	103	TYR	C-O	-10.53	1.09	1.23
1	B	67	THR	CA-CB	-10.35	1.37	1.53
1	A	100	TYR	C-O	10.33	1.36	1.24
1	A	37	PRO	CB-CG	10.25	2.00	1.49
1	B	70	ARG	CA-C	-10.20	1.40	1.52
1	A	38	VAL	CA-C	-10.19	1.40	1.52
1	A	14	LEU	C-N	-10.16	1.20	1.33
1	B	70	ARG	CB-CG	10.14	1.82	1.52
1	A	70	ARG	NE-CZ	10.00	1.44	1.33
1	A	44	ALA	C-O	-9.97	1.12	1.23
1	B	14	LEU	C-O	-9.87	1.12	1.23
1	A	123	PHE	N-CA	9.83	1.65	1.46
1	A	113	ALA	CA-CB	9.52	1.67	1.53
1	B	88	LYS	CD-CE	9.48	1.80	1.52
1	A	112	GLN	CG-CD	9.44	1.75	1.52
1	A	23	VAL	CA-CB	-9.40	1.42	1.54
1	A	64	GLN	C-O	-9.32	1.12	1.23
1	B	36	ASN	C-O	9.31	1.42	1.23
1	A	13	SER	C-O	-9.28	1.12	1.24
1	A	70	ARG	C-O	9.23	1.35	1.24
1	B	70	ARG	N-CA	9.23	1.57	1.46
1	A	86	VAL	C-O	-9.23	1.15	1.24
1	A	13	SER	C-N	-9.21	1.20	1.33
1	A	118	ALA	CA-CB	9.19	1.68	1.53
1	A	111	ARG	CZ-NH2	9.18	1.45	1.33
1	B	79	ARG	N-CA	-9.09	1.35	1.46
1	B	29	LEU	CA-CB	-9.09	1.41	1.53
1	B	93	TYR	N-CA	9.04	1.57	1.46
1	B	25	GLN	N-CA	9.01	1.57	1.45
1	B	42	SER	N-CA	8.94	1.57	1.45
1	B	102	GLU	CD-OE1	8.94	1.42	1.25
1	B	37	PRO	CA-C	8.93	1.65	1.52
1	A	13	SER	N-CA	8.91	1.57	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	GLN	CG-CD	8.80	1.74	1.52
1	A	88	LYS	C-O	-8.76	1.12	1.24
1	B	78	LEU	C-O	-8.65	1.13	1.24
1	A	116	ILE	C-O	8.58	1.33	1.24
1	B	20	LEU	C-O	8.48	1.33	1.23
1	B	66	THR	CA-CB	-8.44	1.40	1.53
1	B	111	ARG	NE-CZ	8.44	1.42	1.33
1	A	66	THR	N-CA	-8.37	1.35	1.46
1	B	41	PHE	CA-CB	-8.36	1.39	1.53
1	A	19	LEU	CA-C	8.35	1.62	1.52
1	B	19	LEU	CG-CD1	-8.31	1.25	1.52
1	B	123	PHE	CA-C	8.30	1.70	1.52
1	A	122	ILE	C-O	-8.29	1.12	1.24
1	A	12	ARG	N-CA	8.28	1.61	1.46
1	B	112	GLN	CB-CG	8.28	1.77	1.52
1	B	116	ILE	C-O	8.27	1.33	1.24
1	A	26	ASP	CG-OD1	8.23	1.41	1.25
1	B	102	GLU	N-CA	-8.23	1.36	1.46
1	A	110	ARG	C-O	8.21	1.32	1.24
1	A	89	GLY	C-O	-8.21	1.12	1.24
1	A	91	ARG	NE-CZ	8.21	1.42	1.33
1	A	84	GLN	C-O	-8.11	1.13	1.24
1	A	45	THR	CA-C	-8.04	1.42	1.52
1	B	16	ARG	CB-CG	8.04	1.76	1.52
1	B	66	THR	C-O	-8.03	1.14	1.24
1	A	72	SER	CA-C	7.92	1.61	1.52
1	A	70	ARG	CZ-NH2	7.91	1.43	1.33
1	A	99	ASP	C-O	7.88	1.32	1.23
1	A	111	ARG	CZ-NH1	7.81	1.43	1.32
1	A	79	ARG	CG-CD	7.81	1.75	1.52
1	A	69	HIS	CA-C	7.78	1.61	1.52
1	A	105	ASP	C-N	-7.78	1.22	1.33
1	A	91	ARG	C-O	-7.77	1.14	1.24
1	A	108	ASN	CA-C	7.74	1.61	1.52
1	A	122	ILE	CG1-CD1	7.73	1.81	1.51
1	B	16	ARG	NE-CZ	7.73	1.41	1.33
1	A	82	ALA	CA-CB	-7.65	1.41	1.53
1	A	83	TYR	N-CA	-7.65	1.36	1.46
1	B	25	GLN	CB-CG	7.62	1.75	1.52
1	B	106	LYS	N-CA	7.62	1.56	1.46
1	A	62	VAL	CA-CB	7.61	1.75	1.54
1	B	114	THR	N-CA	7.57	1.55	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	ASN	CB-CG	-7.55	1.33	1.52
1	B	119	ASP	N-CA	-7.52	1.36	1.46
1	B	22	ARG	N-CA	7.51	1.55	1.46
1	B	120	ASN	CG-ND2	7.40	1.48	1.33
1	B	106	LYS	CB-CG	-7.35	1.30	1.52
1	A	75	ARG	CG-CD	7.32	1.74	1.52
1	B	73	VAL	C-O	-7.22	1.16	1.24
1	A	86	VAL	CA-C	-7.22	1.44	1.52
1	B	41	PHE	N-CA	7.16	1.54	1.46
1	A	82	ALA	C-O	-7.11	1.15	1.24
1	B	69	HIS	CA-C	-7.11	1.44	1.52
1	B	29	LEU	CA-C	-7.10	1.43	1.52
1	A	62	VAL	N-CA	7.09	1.59	1.46
1	B	70	ARG	NE-CZ	7.08	1.40	1.33
1	B	75	ARG	C-O	-7.08	1.15	1.24
1	B	69	HIS	CA-CB	7.05	1.66	1.53
1	A	111	ARG	CB-CG	7.00	1.73	1.52
1	A	17	VAL	CB-CG2	-6.99	1.29	1.52
1	A	69	HIS	CB-CG	-6.94	1.40	1.50
1	B	105	ASP	CA-C	6.89	1.61	1.52
1	A	115	THR	N-CA	6.85	1.55	1.46
1	B	101	GLY	C-N	-6.84	1.24	1.33
1	A	120	ASN	CA-C	-6.82	1.44	1.52
1	B	120	ASN	C-N	-6.79	1.24	1.33
1	A	45	THR	CA-CB	6.78	1.66	1.53
1	B	88	LYS	CB-CG	6.71	1.72	1.52
1	B	119	ASP	CG-OD1	6.70	1.38	1.25
1	A	101	GLY	C-N	-6.63	1.24	1.33
1	B	65	LYS	CG-CD	6.63	1.72	1.52
1	A	100	TYR	CA-C	6.60	1.61	1.52
1	B	114	THR	C-O	6.59	1.32	1.23
1	A	78	LEU	N-CA	6.59	1.54	1.46
1	A	28	VAL	N-CA	-6.54	1.38	1.46
1	A	20	LEU	CA-C	6.53	1.60	1.52
1	B	115	THR	CB-OG1	6.53	1.54	1.43
1	B	110	ARG	C-O	6.53	1.32	1.23
1	B	91	ARG	CA-CB	-6.52	1.44	1.53
1	B	30	ARG	CD-NE	6.49	1.55	1.46
1	B	120	ASN	N-CA	6.45	1.54	1.46
1	B	88	LYS	CA-C	-6.44	1.44	1.52
1	A	68	TRP	C-O	6.43	1.31	1.24
1	A	39	THR	C-O	6.43	1.31	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	18	HIS	N-CA	6.43	1.54	1.46
1	A	107	ASN	CG-ND2	6.42	1.46	1.33
1	A	68	TRP	C-N	6.41	1.42	1.33
1	B	73	VAL	N-CA	-6.41	1.38	1.46
1	B	23	VAL	CA-C	6.36	1.59	1.52
1	B	65	LYS	C-O	6.36	1.31	1.24
1	A	37	PRO	CG-CD	6.35	1.72	1.50
1	A	91	ARG	CZ-NH2	6.34	1.41	1.33
1	A	96	GLY	N-CA	6.33	1.52	1.45
1	B	110	ARG	CZ-NH2	6.33	1.41	1.33
1	A	95	GLU	CA-C	-6.27	1.44	1.52
1	A	105	ASP	N-CA	6.26	1.50	1.46
1	B	106	LYS	CA-CB	-6.22	1.43	1.53
1	B	81	VAL	N-CA	-6.22	1.39	1.46
1	B	43	LEU	CA-CB	6.21	1.64	1.53
1	A	104	MET	C-N	-6.19	1.27	1.33
1	A	95	GLU	CD-OE1	6.18	1.37	1.25
1	B	94	LEU	N-CA	6.18	1.53	1.45
1	A	107	ASN	CA-C	-6.16	1.44	1.53
1	A	110	ARG	CA-CB	-6.16	1.44	1.53
1	B	110	ARG	CB-CG	-6.14	1.34	1.52
1	A	100	TYR	CE1-CZ	-6.11	1.23	1.38
1	A	117	ILE	CG1-CD1	6.07	1.75	1.51
1	B	89	GLY	C-N	6.06	1.41	1.33
1	A	16	ARG	CA-C	6.05	1.60	1.52
1	A	73	VAL	CA-C	6.00	1.59	1.52
1	B	93	TYR	CA-C	-6.00	1.45	1.52
1	B	111	ARG	CA-C	-5.99	1.45	1.52
1	A	119	ASP	CA-CB	5.97	1.63	1.53
1	B	79	ARG	NE-CZ	5.96	1.39	1.33
1	A	92	ILE	CB-CG1	-5.94	1.41	1.53
1	A	112	GLN	CB-CG	5.92	1.70	1.52
1	A	71	ILE	C-O	5.92	1.32	1.24
1	B	98	ILE	CA-C	-5.92	1.45	1.52
1	A	110	ARG	C-N	5.88	1.42	1.33
1	A	97	LYS	CE-NZ	5.83	1.66	1.49
1	B	80	ASP	C-N	-5.83	1.27	1.33
1	A	28	VAL	C-O	-5.81	1.18	1.24
1	A	110	ARG	CZ-NH2	-5.80	1.25	1.33
1	A	79	ARG	NE-CZ	5.80	1.39	1.33
1	B	64	GLN	CB-CG	5.80	1.69	1.52
1	A	19	LEU	CG-CD2	-5.78	1.33	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	71	ILE	C-O	-5.78	1.16	1.24
1	B	117	ILE	CA-C	5.77	1.59	1.52
1	B	65	LYS	N-CA	5.74	1.53	1.46
1	B	25	GLN	CA-CB	5.69	1.63	1.53
1	A	94	LEU	CG-CD1	-5.69	1.33	1.52
1	A	119	ASP	CB-CG	5.68	1.66	1.52
1	B	99	ASP	C-O	5.68	1.30	1.24
1	A	98	ILE	CA-C	5.65	1.58	1.52
1	A	93	TYR	CD1-CE1	5.63	1.55	1.38
1	A	42	SER	CB-OG	5.62	1.53	1.42
1	B	95	GLU	CA-CB	-5.62	1.43	1.53
1	B	91	ARG	CZ-NH2	5.61	1.40	1.33
1	A	47	GLU	CD-OE2	5.61	1.35	1.25
1	A	120	ASN	CG-OD1	5.60	1.34	1.23
1	B	117	ILE	CB-CG2	-5.59	1.34	1.52
1	B	95	GLU	CD-OE1	5.59	1.35	1.25
1	A	102	GLU	CA-CB	-5.59	1.45	1.53
1	B	23	VAL	N-CA	-5.58	1.39	1.46
1	A	97	LYS	C-N	-5.57	1.27	1.33
1	B	113	ALA	N-CA	5.55	1.52	1.46
1	A	80	ASP	N-CA	5.55	1.53	1.46
1	B	87	LYS	CG-CD	5.52	1.69	1.52
1	A	38	VAL	CA-CB	-5.52	1.47	1.55
1	B	73	VAL	CA-C	-5.50	1.45	1.52
1	B	91	ARG	CA-C	-5.49	1.45	1.52
1	B	42	SER	C-O	5.46	1.30	1.23
1	A	68	TRP	NE1-CE2	-5.45	1.31	1.37
1	A	91	ARG	CA-CB	-5.44	1.45	1.53
1	A	20	LEU	CG-CD2	-5.44	1.34	1.52
1	B	80	ASP	C-O	-5.43	1.17	1.24
1	B	12	ARG	CZ-NH2	-5.42	1.26	1.33
1	A	118	ALA	CA-C	5.42	1.60	1.52
1	A	17	VAL	CA-C	5.41	1.59	1.52
1	B	22	ARG	CA-C	5.41	1.59	1.52
1	A	71	ILE	CA-CB	5.40	1.61	1.54
1	B	75	ARG	CG-CD	5.39	1.68	1.52
1	B	67	THR	CA-C	-5.38	1.46	1.52
1	A	28	VAL	CA-C	-5.36	1.46	1.52
1	A	23	VAL	CA-C	-5.36	1.46	1.52
1	B	12	ARG	CB-CG	-5.35	1.36	1.52
1	B	14	LEU	CA-CB	-5.35	1.43	1.53
1	A	115	THR	CA-CB	5.33	1.60	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	THR	CA-CB	5.32	1.64	1.53
1	B	12	ARG	CZ-NH1	-5.31	1.25	1.32
1	A	87	LYS	CA-C	5.31	1.58	1.52
1	A	119	ASP	CG-OD1	5.31	1.35	1.25
1	B	112	GLN	C-O	5.30	1.30	1.24
1	A	115	THR	C-O	5.29	1.30	1.24
1	A	38	VAL	N-CA	5.28	1.52	1.46
1	A	40	ILE	C-O	5.27	1.29	1.24
1	B	17	VAL	CB-CG2	-5.27	1.35	1.52
1	A	64	GLN	CD-OE1	5.27	1.33	1.23
1	B	111	ARG	CZ-NH1	5.25	1.40	1.32
1	B	44	ALA	C-N	-5.25	1.27	1.33
1	B	66	THR	C-N	5.23	1.40	1.33
1	B	110	ARG	NE-CZ	-5.23	1.27	1.33
1	B	72	SER	N-CA	5.23	1.52	1.46
1	A	105	ASP	CA-C	-5.22	1.50	1.53
1	A	42	SER	CA-C	5.20	1.58	1.52
1	A	112	GLN	CA-C	5.19	1.58	1.52
1	A	78	LEU	C-O	5.19	1.30	1.24
1	B	69	HIS	ND1-CE1	5.18	1.37	1.32
1	A	122	ILE	CA-C	5.16	1.59	1.52
1	A	30	ARG	NE-CZ	5.16	1.38	1.33
1	A	117	ILE	CA-C	5.14	1.58	1.52
1	A	79	ARG	CD-NE	5.12	1.53	1.46
1	A	95	GLU	CA-CB	-5.11	1.44	1.53
1	B	30	ARG	NE-CZ	5.11	1.38	1.33
1	A	12	ARG	C-O	5.09	1.33	1.23
1	A	18	HIS	N-CA	-5.09	1.39	1.46
1	A	114	THR	CA-C	-5.09	1.46	1.52
1	B	20	LEU	C-N	5.07	1.38	1.33
1	A	37	PRO	C-O	5.06	1.30	1.23
1	B	29	LEU	CG-CD1	5.06	1.69	1.52
1	B	16	ARG	CG-CD	5.05	1.67	1.52
1	A	69	HIS	CA-CB	-5.04	1.44	1.53
1	B	97	LYS	CA-CB	-5.03	1.43	1.54
1	B	45	THR	CB-CG2	5.01	1.69	1.52

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ALA	N-CA-C	-13.02	97.08	113.23
1	B	117	ILE	N-CA-CB	-12.79	96.59	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ASP	CA-C-O	-12.36	110.77	117.94
1	A	106	LYS	O-C-N	12.26	138.90	122.59
1	B	92	ILE	CB-CA-C	-11.67	93.88	110.91
1	A	117	ILE	N-CA-CB	-11.61	97.05	110.99
1	A	117	ILE	N-CA-C	11.41	124.67	108.36
1	B	122	ILE	CB-CA-C	11.31	126.71	111.21
1	A	70	ARG	NE-CZ-NH2	11.18	129.26	119.20
1	B	101	GLY	CA-C-N	-10.91	106.61	122.44
1	B	101	GLY	C-N-CA	-10.91	106.61	122.44
1	B	117	ILE	N-CA-C	10.82	123.17	108.89
1	B	105	ASP	CA-C-N	10.33	141.26	121.54
1	B	105	ASP	C-N-CA	10.33	141.26	121.54
1	B	65	LYS	CA-C-N	-10.32	108.76	123.00
1	B	65	LYS	C-N-CA	-10.32	108.76	123.00
1	B	111	ARG	NE-CZ-NH1	9.97	131.47	121.50
1	B	110	ARG	NH1-CZ-NH2	9.71	131.93	119.30
1	B	91	ARG	NE-CZ-NH2	9.34	127.61	119.20
1	B	117	ILE	CB-CA-C	-9.18	99.22	111.15
1	A	70	ARG	NE-CZ-NH1	-9.04	112.46	121.50
1	B	123	PHE	N-CA-C	9.01	136.22	111.00
1	B	12	ARG	NE-CZ-NH2	9.00	127.30	119.20
1	B	110	ARG	NE-CZ-NH2	-8.91	111.18	119.20
1	A	29	LEU	CB-CA-C	8.78	126.63	109.33
1	A	89	GLY	N-CA-C	8.74	126.58	115.21
1	B	23	VAL	N-CA-C	8.73	120.22	109.30
1	A	98	ILE	CB-CG1-CD1	-8.64	95.66	113.80
1	B	91	ARG	NE-CZ-NH1	-8.52	112.98	121.50
1	B	23	VAL	N-CA-CB	-8.47	99.89	110.31
1	A	13	SER	O-C-N	-8.38	111.45	122.59
1	B	88	LYS	CA-CB-CG	8.32	130.73	114.10
1	B	122	ILE	N-CA-CB	-8.29	99.12	110.56
1	B	102	GLU	N-CA-C	8.15	121.91	107.80
1	B	88	LYS	CG-CD-CE	7.95	129.59	111.30
1	B	23	VAL	O-C-N	-7.59	114.40	122.67
1	B	113	ALA	CB-CA-C	7.54	123.52	109.71
1	A	90	SER	CB-CA-C	-7.45	96.94	109.53
1	B	118	ALA	N-CA-C	-7.40	104.50	113.97
1	A	73	VAL	CB-CA-C	-7.37	100.82	110.84
1	B	92	ILE	N-CA-C	7.36	117.51	108.53
1	B	103	TYR	N-CA-C	7.36	121.50	109.94
1	B	114	THR	OG1-CB-CG2	-7.35	94.60	109.30
1	B	112	GLN	CA-C-N	-7.14	112.92	122.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	GLN	C-N-CA	-7.14	112.92	122.99
1	A	17	VAL	CB-CA-C	-6.98	99.75	110.50
1	B	101	GLY	CA-C-O	6.95	128.03	121.64
1	A	117	ILE	CA-C-N	6.90	133.81	121.66
1	A	117	ILE	C-N-CA	6.90	133.81	121.66
1	B	89	GLY	N-CA-C	6.90	124.70	115.59
1	A	45	THR	CA-CB-CG2	6.88	122.19	110.50
1	B	41	PHE	CA-C-N	-6.85	111.32	122.82
1	B	41	PHE	C-N-CA	-6.85	111.32	122.82
1	A	23	VAL	CG1-CB-CG2	-6.75	95.94	110.80
1	A	123	PHE	CA-CB-CG	-6.73	107.07	113.80
1	B	106	LYS	CB-CA-C	-6.63	97.23	110.42
1	A	111	ARG	N-CA-C	6.60	120.29	109.06
1	B	123	PHE	CA-CB-CG	-6.58	107.22	113.80
1	A	14	LEU	O-C-N	-6.57	113.85	122.59
1	A	105	ASP	CA-C-N	6.57	134.09	121.54
1	A	105	ASP	C-N-CA	6.57	134.09	121.54
1	A	73	VAL	N-CA-C	6.55	117.73	108.36
1	B	46	ASN	N-CA-C	6.54	120.69	110.17
1	A	109	VAL	CB-CA-C	-6.54	102.65	111.15
1	B	89	GLY	O-C-N	6.53	130.00	122.23
1	A	45	THR	N-CA-CB	-6.48	99.58	110.80
1	B	113	ALA	CA-C-N	-6.47	111.93	122.81
1	B	113	ALA	C-N-CA	-6.47	111.93	122.81
1	B	102	GLU	CA-C-O	-6.35	112.25	120.25
1	B	109	VAL	N-CA-C	-6.33	97.21	107.28
1	A	101	GLY	O-C-N	-6.29	114.53	122.70
1	A	115	THR	CA-CB-CG2	-6.23	99.90	110.50
1	A	75	ARG	CB-CA-C	-6.20	97.96	110.17
1	A	25	GLN	N-CA-C	6.16	118.77	109.23
1	A	43	LEU	CB-CA-C	-6.14	97.65	109.37
1	A	75	ARG	N-CA-CB	6.12	121.27	110.37
1	A	92	ILE	N-CA-CB	-6.10	101.36	111.36
1	A	37	PRO	CB-CG-CD	-6.09	86.60	106.10
1	A	68	TRP	O-C-N	6.04	130.11	123.22
1	A	106	LYS	CB-CA-C	-6.04	98.40	110.42
1	A	94	LEU	N-CA-C	6.03	116.52	108.38
1	B	105	ASP	N-CA-C	6.01	121.53	113.72
1	B	120	ASN	CB-CA-C	-5.99	98.85	109.70
1	A	76	PRO	CA-C-N	-5.98	113.42	119.94
1	A	76	PRO	C-N-CA	-5.98	113.42	119.94
1	B	111	ARG	CD-NE-CZ	5.95	132.72	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ARG	CA-C-N	-5.93	110.21	121.54
1	A	12	ARG	C-N-CA	-5.93	110.21	121.54
1	B	87	LYS	CA-C-N	5.87	130.71	121.56
1	B	87	LYS	C-N-CA	5.87	130.71	121.56
1	B	66	THR	CA-C-O	-5.87	113.99	120.38
1	A	116	ILE	CA-C-O	5.84	126.95	120.59
1	A	95	GLU	CA-C-N	-5.80	113.00	120.72
1	A	95	GLU	C-N-CA	-5.80	113.00	120.72
1	B	102	GLU	CG-CD-OE2	-5.80	105.06	118.40
1	B	90	SER	CA-CB-OG	5.79	122.68	111.10
1	B	39	THR	OG1-CB-CG2	-5.79	97.73	109.30
1	B	70	ARG	CB-CG-CD	5.77	124.56	111.30
1	B	113	ALA	N-CA-C	-5.74	99.55	108.90
1	A	98	ILE	N-CA-C	5.72	116.45	109.30
1	A	113	ALA	N-CA-CB	5.71	118.80	109.95
1	A	106	LYS	N-CA-C	5.68	122.90	110.80
1	A	89	GLY	CA-C-N	5.64	129.48	121.42
1	A	89	GLY	C-N-CA	5.64	129.48	121.42
1	A	87	LYS	CD-CE-NZ	-5.63	93.88	111.90
1	B	122	ILE	CA-C-O	-5.57	113.94	121.02
1	A	112	GLN	CB-CG-CD	5.57	122.06	112.60
1	A	75	ARG	CG-CD-NE	-5.54	99.82	112.00
1	B	111	ARG	NE-CZ-NH2	-5.53	114.22	119.20
1	A	108	ASN	N-CA-C	5.51	117.88	108.90
1	A	122	ILE	CA-C-N	5.46	131.52	121.70
1	A	122	ILE	C-N-CA	5.46	131.52	121.70
1	B	43	LEU	CB-CG-CD1	-5.45	94.36	110.70
1	A	72	SER	N-CA-CB	-5.43	101.68	110.81
1	B	17	VAL	CA-C-N	-5.42	113.96	122.73
1	B	17	VAL	C-N-CA	-5.42	113.96	122.73
1	A	47	GLU	CG-CD-OE1	-5.39	106.01	118.40
1	A	122	ILE	CA-C-O	-5.34	114.08	121.51
1	A	118	ALA	O-C-N	-5.34	115.14	122.46
1	B	113	ALA	N-CA-CB	5.34	119.65	110.68
1	B	21	GLY	CA-C-O	-5.31	116.36	121.41
1	A	120	ASN	CB-CA-C	-5.30	97.80	109.56
1	A	101	GLY	CA-C-N	-5.28	115.18	122.30
1	A	101	GLY	C-N-CA	-5.28	115.18	122.30
1	B	70	ARG	CG-CD-NE	-5.28	100.40	112.00
1	B	66	THR	CB-CA-C	5.25	118.81	109.72
1	A	14	LEU	CA-C-N	5.24	131.29	123.23
1	A	14	LEU	C-N-CA	5.24	131.29	123.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	GLN	CA-CB-CG	5.23	124.55	114.10
1	A	12	ARG	CB-CA-C	-5.22	100.19	110.10
1	B	90	SER	N-CA-C	5.20	117.43	110.35
1	B	69	HIS	CA-C-N	-5.20	115.86	122.77
1	B	69	HIS	C-N-CA	-5.20	115.86	122.77
1	A	72	SER	CB-CA-C	5.19	118.74	109.65
1	A	119	ASP	CA-C-O	-5.19	113.09	120.51
1	A	36	ASN	CA-C-N	-5.18	114.30	120.11
1	A	36	ASN	C-N-CA	-5.18	114.30	120.11
1	A	68	TRP	CA-C-O	-5.15	114.85	120.36
1	A	26	ASP	CB-CG-OD2	-5.14	106.57	118.40
1	B	41	PHE	N-CA-C	5.13	116.09	108.60
1	B	94	LEU	CA-C-O	-5.12	115.11	121.11
1	B	15	ASN	CB-CA-C	-5.12	104.53	111.95
1	A	13	SER	CA-CB-OG	-5.10	100.90	111.10
1	B	120	ASN	N-CA-CB	-5.10	101.98	110.80
1	B	120	ASN	N-CA-C	5.08	117.35	108.76
1	A	92	ILE	CB-CG1-CD1	-5.06	103.18	113.80
1	A	14	LEU	CB-CA-C	5.06	120.48	110.42
1	A	121	ILE	CA-C-O	-5.05	115.00	120.36
1	B	114	THR	CA-C-N	-5.04	115.96	123.11
1	B	114	THR	C-N-CA	-5.04	115.96	123.11
1	B	105	ASP	OD1-CG-OD2	-5.04	110.81	122.90
1	B	14	LEU	N-CA-CB	-5.03	102.12	111.13

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ASP	Peptide,Mainchain
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	794	103	0
1	B	756	0	769	90	0
All	All	1539	0	1563	182	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 59.

All (182) 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:CA	1:A:62:VAL:CB	1.75	1.64
1:A:117:ILE:CD1	1:A:117:ILE:CG1	1.75	1.62
1:B:16:ARG:CB	1:B:16:ARG:CG	1.76	1.62
1:A:112:GLN:CD	1:A:112:GLN:CG	1.75	1.59
1:A:36:ASN:N	1:A:36:ASN:CA	1.68	1.57
1:B:25:GLN:CB	1:B:25:GLN:CG	1.75	1.56
1:B:112:GLN:CG	1:B:112:GLN:CB	1.77	1.56
1:B:88:LYS:CD	1:B:88:LYS:CE	1.80	1.56
1:A:122:ILE:CD1	1:A:122:ILE:CG1	1.81	1.55
1:A:79:ARG:CD	1:A:79:ARG:CG	1.75	1.55
1:B:70:ARG:CB	1:B:70:ARG:CG	1.82	1.55
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:N	1:B:123:PHE:CD1	2.19	1.10
1:B:117:ILE:O	1:B:117:ILE:HG22	1.37	1.07
1:A:106:LYS:NZ	1:A:106:LYS:HB2	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:119:ASP:C	1:A:120:ASN:HD22	1.72	0.96
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:HG23	1:A:109:VAL:O	1.67	0.93
1:A:94:LEU:HD22	1:A:117:ILE:CD1	1.99	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:123:PHE:CG	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:CD1	1:A:117:ILE:CB	2.58	0.81
1:A:117:ILE:O	1:A:117:ILE:HG23	1.81	0.80
1:B:122:ILE:C	1:B:123:PHE:CD1	2.59	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:CG	1:B:16:ARG:CA	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:A:74:PHE:O	1:A:75:ARG:C	2.28	0.76
1:A:62:VAL:CB	1:A:62:VAL:C	2.57	0.76
1:B:18:HIS:HD2	1:B:95:GLU:HG2	1.51	0.76
1:B:110:ARG:HH21	1:B:110:ARG:CB	1.99	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
1:A:109:VAL:O	1:A:109:VAL:CG2	2.32	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:N	1:B:123:PHE:CB	2.51	0.73
1:A:82:ALA:O	1:A:86:VAL:HG23	1.86	0.73
1:B:123:PHE:N	1:B:123:PHE:HA	2.01	0.73
1:A:69:HIS:HD2	1:B:100:TYR:OH	1.71	0.73
1:A:62:VAL:CA	1:A:62:VAL:CG1	2.67	0.72
1:A:38:VAL:HG11	1:A:74:PHE:CE1	2.24	0.72
1:B:24:GLY:O	1:B:88:LYS:HD3	1.91	0.71
1:A:101:GLY:N	1:A:112:GLN:O	2.23	0.69
1:A:106:LYS:NZ	1:A:106:LYS:CB	2.42	0.69
1:B:12:ARG:HH21	1:B:12:ARG:HB3	1.58	0.69
1:A:62:VAL:CA	1:A:62:VAL:CG2	2.70	0.68
1:B:67:THR:CG2	1:B:69:HIS:CE1	2.75	0.68
1:A:83:TYR:CD2	1:A:83:TYR:C	2.70	0.68
1:B:101:GLY:C	1:B:102:GLU:HG3	2.19	0.68
1:B:123:PHE:N	1:B:123:PHE:HD1	1.88	0.67
1:B:94:LEU:HD13	1:B:94:LEU:N	2.08	0.67
1:B:80:ASP:O	1:B:81:VAL:C	2.33	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:TYR:C	1:A:83:TYR:HD2	2.03	0.66
1:A:78:LEU:HD11	1:A:119:ASP:HA	1.76	0.66
1:B:122:ILE:C	1:B:123:PHE:HD1	2.02	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:HG12	1:B:109:VAL:O	1.95	0.65
1:B:94:LEU:HD13	1:B:94:LEU:H	1.61	0.65
1:B:122:ILE:O	1:B:123:PHE:HD1	1.81	0.64
1:A:122:ILE:C	1:A:123:PHE:CD1	2.76	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:B:25:GLN:CB	1:B:25:GLN:CD	2.68	0.62
1:A:120:ASN:N	1:A:120:ASN:ND2	2.40	0.62
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:HG21	1:A:117:ILE:HD13	1.83	0.59
1:A:83:TYR:HD2	1:A:83:TYR:O	1.86	0.59
1:B:103:TYR:C	1:B:104:MET:HE2	2.27	0.58
1:A:69:HIS:CD2	1:B:100:TYR:OH	2.54	0.58
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: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:A:119:ASP:C	1:A:120:ASN:ND2	2.54	0.56
1:B:25:GLN:CG	1:B:25:GLN:CA	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LEU:HD13	1:A:117:ILE:HG13	1.89	0.52
1:B:20:LEU:C	1:B:20:LEU:HD23	2.34	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:94:LEU:HD22	1:A:117:ILE:HD11	1.90	0.52
1:A:105:ASP:OD2	1:A:108:ASN:ND2	2.42	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:B:47:GLU:C	1:B:48:MET:HG2	2.35	0.51
1:A:83:TYR:CD2	1:A:83:TYR:O	2.63	0.51
1:B:122:ILE:C	1:B:123:PHE:CA	2.72	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:94:LEU:C	1:A:94:LEU:HD12	2.36	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: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:A:16:ARG:HH22	1:A:118:ALA:HB2	1.79	0.47
1:A:93:TYR:CE2	1:A:95:GLU:HG3	2.49	0.47
1:B:22:ARG:HA	1:B:90:SER:O	2.15	0.47
1:B:108:ASN:OD1	1:B:110:ARG:NH2	2.47	0.47
1:B:103:TYR:O	1:B:104:MET:HE2	2.14	0.47
1:B:117:ILE:O	1:B:117:ILE:CG2	2.17	0.47
1:B:101:GLY:C	1:B:102:GLU:CG	2.87	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:A:76:PRO:HB3	1:A:79:ARG:HH21	1.80	0.46
1:A:87:LYS:O	1:A:88:LYS:C	2.58	0.46
1:A:108:ASN:HD21	1:A:110:ARG:NH2	2.14	0.46
1:B:104:MET:HE2	1:B:104:MET:CA	2.46	0.46
1:A:46:ASN:O	1:B:13:SER:HB2	2.16	0.46
1:A:69:HIS:CD2	1:B:100:TYR:HE1	2.33	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:105:ASP:CG	1:A:108:ASN:ND2	2.73	0.45
1:B:45:THR:HG22	1:B:67:THR:HB	1.98	0.45
1:B:98:ILE:HD13	1:B:98:ILE:HG21	1.77	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:91:ARG:HB3	1:A:123:PHE:HD2	1.83	0.44
1:A:92:ILE:CD1	1:A:122:ILE:HA	2.48	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:20:LEU:C	1:A:20:LEU:HD23	2.43	0.43
1:B:92:ILE:HG22	1:B:121:ILE:C	2.37	0.43
1:A:94:LEU:HB2	1:A:117:ILE:HD11	2.01	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:HD12	1:B:92:ILE:HG21	1.59	0.42
1:A:12:ARG:N	1:B:91:ARG:NH2	2.68	0.41
1:A:41:PHE:CD1	1:A:41:PHE:N	2.88	0.41
1:A:49:TRP:CD1	1:A:49:TRP:C	2.97	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:N	1:A:36:ASN:CB	2.71	0.41
1:A:71:ILE:HD13	1:A:115:THR:HB	2.02	0.41
1:A:92:ILE:HD13	1:A:92:ILE:HA	1.69	0.41
1:A:93:TYR:CD2	1:A:93:TYR:C	2.99	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:98:ILE:HD13	1:A:98:ILE:HG23	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 ⓘ

5.3.1 Protein backbone ⓘ

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	7
1	B	86/133 (65%)	79 (92%)	6 (7%)	1 (1%)	10	27
All	All	175/266 (66%)	156 (89%)	15 (9%)	4 (2%)	5	13

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 ⓘ

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%)	57 (67%)	28 (33%)	0	1
1	B	82/120 (68%)	54 (66%)	28 (34%)	0	0
All	All	167/240 (70%)	111 (66%)	56 (34%)	0	0

All (56) 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	28	VAL
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	94	LEU
1	A	104	MET
1	A	106	LYS
1	A	108	ASN
1	A	111	ARG
1	A	120	ASN
1	A	122	ILE
1	A	123	PHE
1	B	12	ARG
1	B	13	SER
1	B	14	LEU
1	B	19	LEU
1	B	25	GLN
1	B	29	LEU
1	B	30	ARG
1	B	40	ILE
1	B	45	THR
1	B	48	MET
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	107	ASN
1	B	109	VAL
1	B	110	ARG
1	B	111	ARG
1	B	117	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	122	ILE
1	B	123	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	25	GLN
1	A	36	ASN
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
1	B	120	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](#)

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, 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	95/133 (71%)	0.30	4 (4%)	40 37	16, 41, 63, 71	0
1	B	92/133 (69%)	0.32	8 (8%)	16 13	19, 41, 68, 72	0
All	All	187/266 (70%)	0.31	12 (6%)	25 22	16, 41, 66, 72	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	ILE	6.0
1	B	123	PHE	3.6
1	B	48	MET	3.1
1	B	102	GLU	3.0
1	B	112	GLN	2.9
1	B	107	ASN	2.9
1	A	118	ALA	2.6
1	B	109	VAL	2.3
1	B	117	ILE	2.3
1	A	75	ARG	2.2
1	A	44	ALA	2.1
1	B	108	ASN	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.