



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2018 – 12:05 am GMT

PDB ID : 2GN5
Title : REFINED STRUCTURE OF THE GENE 5 DNA BINDING PROTEIN
FROM BACTERIOPHAGE FD
Authors : Brayer, G.D.; McPherson, A.
Deposited on : 1986-01-13
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

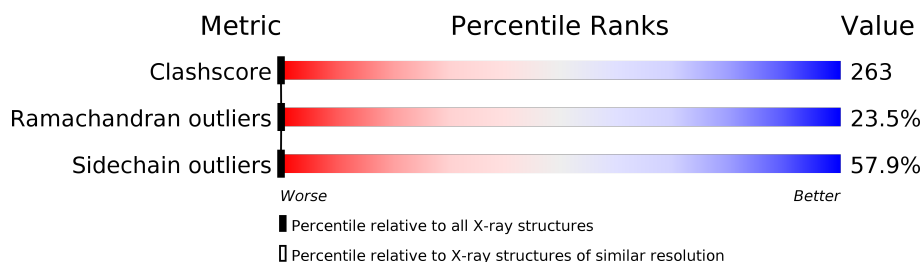
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	122078	5071 (2.30-2.30)
Ramachandran outliers	120005	5021 (2.30-2.30)
Sidechain outliers	119972	5020 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	87	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 694 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 GENE V PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	87	Total	C	N	O	S	0	0	0
			682	438	115	126	3			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		

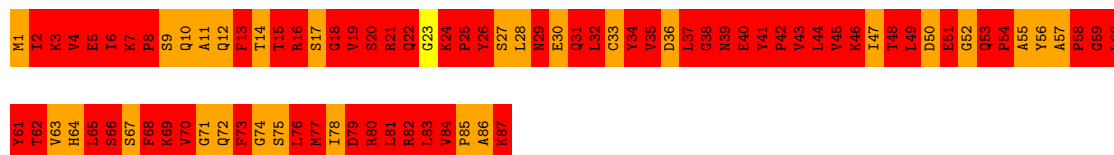
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

Note EDS was not executed.

• Molecule 1: GENE V PROTEIN

Chain A:  32% 67%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	76.08Å 27.78Å 42.00Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.217 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	694	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	2.11	15/696 (2.2%)	7.57	408/940 (43.4%)

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	15

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	THR	CB-OG1	8.07	1.59	1.43
1	A	34	TYR	CG-CD2	7.82	1.49	1.39
1	A	8	PRO	CA-CB	6.63	1.66	1.53
1	A	62	THR	N-CA	6.15	1.58	1.46
1	A	16	ARG	CZ-NH2	6.05	1.41	1.33
1	A	59	GLY	C-O	6.04	1.33	1.23
1	A	11	ALA	C-O	6.00	1.34	1.23
1	A	73	PHE	CG-CD2	5.88	1.47	1.38
1	A	26	TYR	CE2-CZ	5.68	1.46	1.38
1	A	62	THR	C-O	5.64	1.34	1.23
1	A	71	GLY	N-CA	5.31	1.54	1.46
1	A	16	ARG	NE-CZ	5.30	1.40	1.33
1	A	82	ARG	C-O	5.17	1.33	1.23
1	A	36	ASP	C-N	-5.06	1.22	1.34
1	A	73	PHE	N-CA	5.05	1.56	1.46

All (408) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ARG	NE-CZ-NH1	-41.52	99.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	ASP	CB-CG-OD1	-36.29	85.64	118.30
1	A	16	ARG	CD-NE-CZ	34.35	171.69	123.60
1	A	50	ASP	CB-CG-OD2	31.55	146.69	118.30
1	A	79	ASP	CB-CG-OD1	28.64	144.08	118.30
1	A	59	GLY	CA-C-N	28.52	179.95	117.20
1	A	82	ARG	O-C-N	-26.48	80.33	122.70
1	A	21	ARG	CD-NE-CZ	25.60	159.45	123.60
1	A	59	GLY	O-C-N	-24.71	83.16	122.70
1	A	34	TYR	CA-CB-CG	23.34	157.74	113.40
1	A	15	THR	C-N-CA	23.30	179.96	121.70
1	A	39	ASN	C-N-CA	23.30	179.96	121.70
1	A	82	ARG	C-N-CA	23.30	179.94	121.70
1	A	78	ILE	C-N-CA	22.72	178.51	121.70
1	A	11	ALA	CB-CA-C	-22.12	76.92	110.10
1	A	60	LEU	CA-C-O	21.93	166.16	120.10
1	A	52	GLY	CA-C-O	21.41	159.13	120.60
1	A	65	LEU	O-C-N	-21.21	88.77	122.70
1	A	5	GLU	OE1-CD-OE2	21.16	148.69	123.30
1	A	79	ASP	CB-CA-C	18.94	148.28	110.40
1	A	73	PHE	CB-CG-CD1	18.57	133.80	120.80
1	A	60	LEU	O-C-N	-18.51	93.09	122.70
1	A	53	GLN	CB-CG-CD	18.25	159.05	111.60
1	A	8	PRO	N-CA-CB	-18.23	81.42	103.30
1	A	82	ARG	CD-NE-CZ	17.85	148.59	123.60
1	A	80	ARG	NE-CZ-NH1	-17.77	111.42	120.30
1	A	82	ARG	CA-C-O	17.73	157.34	120.10
1	A	10	GLN	CG-CD-NE2	17.42	158.51	116.70
1	A	10	GLN	CB-CG-CD	17.05	155.93	111.60
1	A	62	THR	CA-CB-CG2	16.96	136.14	112.40
1	A	40	GLU	N-CA-CB	-16.90	80.17	110.60
1	A	65	LEU	CA-C-O	16.86	155.50	120.10
1	A	66	SER	CA-CB-OG	16.64	156.14	111.20
1	A	60	LEU	C-N-CA	16.34	162.56	121.70
1	A	26	TYR	CB-CG-CD1	16.31	130.78	121.00
1	A	77	MET	N-CA-CB	16.28	139.90	110.60
1	A	57	ALA	N-CA-CB	-16.21	87.41	110.10
1	A	77	MET	CA-CB-CG	-16.02	86.06	113.30
1	A	37	LEU	CA-C-O	15.91	153.52	120.10
1	A	39	ASN	CB-CA-C	15.90	142.19	110.40
1	A	6	ILE	O-C-N	-15.72	97.54	122.70
1	A	16	ARG	NH1-CZ-NH2	15.53	136.49	119.40
1	A	12	GLN	CG-CD-OE1	15.52	152.63	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	THR	O-C-N	-15.39	98.08	122.70
1	A	10	GLN	OE1-CD-NE2	-15.32	86.66	121.90
1	A	26	TYR	CA-C-O	-15.24	88.09	120.10
1	A	31	GLN	CG-CD-OE1	15.23	152.07	121.60
1	A	62	THR	C-N-CA	15.21	159.73	121.70
1	A	31	GLN	CB-CA-C	15.15	140.70	110.40
1	A	21	ARG	NE-CZ-NH1	15.13	127.87	120.30
1	A	74	GLY	N-CA-C	15.12	150.89	113.10
1	A	81	LEU	C-N-CA	14.80	158.70	121.70
1	A	37	LEU	CA-CB-CG	14.74	149.21	115.30
1	A	73	PHE	N-CA-CB	-14.66	84.20	110.60
1	A	62	THR	O-C-N	-14.57	99.39	122.70
1	A	83	LEU	CA-C-N	-14.21	85.93	117.20
1	A	41	TYR	N-CA-CB	14.18	136.12	110.60
1	A	73	PHE	CB-CG-CD2	-14.18	110.88	120.80
1	A	15	THR	N-CA-CB	-13.94	83.81	110.30
1	A	62	THR	N-CA-CB	13.83	136.57	110.30
1	A	39	ASN	O-C-N	-13.80	100.63	122.70
1	A	82	ARG	NE-CZ-NH1	-13.66	113.47	120.30
1	A	15	THR	CA-CB-OG1	13.65	137.67	109.00
1	A	36	ASP	CB-CG-OD2	-13.51	106.14	118.30
1	A	83	LEU	CA-C-O	13.50	148.45	120.10
1	A	41	TYR	CA-CB-CG	13.46	138.97	113.40
1	A	65	LEU	C-N-CA	13.42	155.26	121.70
1	A	21	ARG	C-N-CA	13.39	155.17	121.70
1	A	73	PHE	O-C-N	-13.37	100.46	123.20
1	A	73	PHE	C-N-CA	13.35	150.34	122.30
1	A	59	GLY	CA-C-O	-13.17	96.89	120.60
1	A	61	TYR	O-C-N	13.11	143.68	122.70
1	A	44	LEU	CB-CG-CD2	13.10	133.27	111.00
1	A	52	GLY	C-N-CA	13.09	154.42	121.70
1	A	77	MET	O-C-N	12.92	143.37	122.70
1	A	65	LEU	CA-CB-CG	12.90	144.96	115.30
1	A	53	GLN	CA-CB-CG	12.89	141.77	113.40
1	A	87	LYS	N-CA-CB	12.85	133.74	110.60
1	A	64	HIS	CB-CA-C	-12.85	84.70	110.40
1	A	39	ASN	CB-CG-OD1	-12.83	95.95	121.60
1	A	43	VAL	C-N-CA	12.79	153.68	121.70
1	A	21	ARG	N-CA-CB	12.78	133.61	110.60
1	A	80	ARG	NH1-CZ-NH2	12.58	133.24	119.40
1	A	84	VAL	CG1-CB-CG2	-12.56	90.81	110.90
1	A	60	LEU	CB-CG-CD1	12.55	132.33	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	GLN	CG-CD-OE1	12.50	146.60	121.60
1	A	64	HIS	O-C-N	-12.47	102.74	122.70
1	A	30	GLU	CA-C-O	-12.46	93.93	120.10
1	A	84	VAL	CA-CB-CG2	12.42	129.53	110.90
1	A	5	GLU	N-CA-C	12.41	144.52	111.00
1	A	32	LEU	CA-CB-CG	12.31	143.62	115.30
1	A	8	PRO	N-CA-C	12.22	143.88	112.10
1	A	51	GLU	CG-CD-OE1	12.21	142.71	118.30
1	A	75	SER	CA-CB-OG	12.00	143.60	111.20
1	A	56	TYR	O-C-N	11.99	141.89	122.70
1	A	22	GLN	N-CA-CB	11.91	132.04	110.60
1	A	87	LYS	CB-CG-CD	11.85	142.41	111.60
1	A	64	HIS	CA-CB-CG	11.79	133.65	113.60
1	A	65	LEU	CB-CA-C	11.79	132.60	110.20
1	A	7	LYS	N-CA-C	-11.70	79.41	111.00
1	A	63	VAL	CA-C-O	11.69	144.65	120.10
1	A	22	GLN	CG-CD-OE1	11.68	144.96	121.60
1	A	68	PHE	CB-CA-C	11.66	133.72	110.40
1	A	4	VAL	CA-CB-CG2	11.65	128.37	110.90
1	A	3	LYS	CD-CE-NZ	11.60	138.37	111.70
1	A	78	ILE	N-CA-CB	11.55	137.36	110.80
1	A	7	LYS	N-CA-CB	11.53	131.35	110.60
1	A	39	ASN	CB-CG-ND2	11.50	144.29	116.70
1	A	26	TYR	CG-CD1-CE1	11.43	130.44	121.30
1	A	78	ILE	CA-C-O	11.42	144.09	120.10
1	A	64	HIS	N-CA-CB	11.39	131.11	110.60
1	A	61	TYR	N-CA-CB	-11.26	90.34	110.60
1	A	33	CYS	CA-CB-SG	11.19	134.15	114.00
1	A	62	THR	CA-C-O	11.14	143.49	120.10
1	A	4	VAL	CA-CB-CG1	-11.09	94.27	110.90
1	A	40	GLU	O-C-N	-11.02	105.07	122.70
1	A	52	GLY	CA-C-N	-11.01	92.98	117.20
1	A	59	GLY	N-CA-C	11.01	140.61	113.10
1	A	43	VAL	CA-CB-CG2	-11.00	94.40	110.90
1	A	63	VAL	CG1-CB-CG2	-10.99	93.32	110.90
1	A	43	VAL	N-CA-C	10.85	140.29	111.00
1	A	39	ASN	N-CA-CB	-10.74	91.27	110.60
1	A	22	GLN	CB-CG-CD	10.68	139.37	111.60
1	A	30	GLU	CG-CD-OE2	-10.61	97.07	118.30
1	A	36	ASP	OD1-CG-OD2	10.61	143.47	123.30
1	A	30	GLU	OE1-CD-OE2	10.61	136.03	123.30
1	A	43	VAL	CA-CB-CG1	10.56	126.74	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	LEU	CD1-CG-CD2	-10.52	78.93	110.50
1	A	15	THR	CA-C-O	10.51	142.18	120.10
1	A	79	ASP	OD1-CG-OD2	-10.51	103.33	123.30
1	A	60	LEU	CA-CB-CG	10.47	139.39	115.30
1	A	53	GLN	CG-CD-NE2	-10.41	91.71	116.70
1	A	28	LEU	N-CA-CB	-10.35	89.70	110.40
1	A	37	LEU	N-CA-CB	-10.35	89.70	110.40
1	A	4	VAL	N-CA-CB	10.31	134.19	111.50
1	A	26	TYR	CA-C-N	10.31	139.89	117.20
1	A	60	LEU	CB-CG-CD2	-10.28	93.53	111.00
1	A	78	ILE	N-CA-C	-10.28	83.25	111.00
1	A	52	GLY	O-C-N	-10.24	106.32	122.70
1	A	31	GLN	OE1-CD-NE2	-10.18	98.49	121.90
1	A	3	LYS	CB-CG-CD	10.06	137.75	111.60
1	A	55	ALA	CB-CA-C	10.04	125.15	110.10
1	A	45	VAL	CA-CB-CG1	10.00	125.89	110.90
1	A	80	ARG	NE-CZ-NH2	-9.99	115.31	120.30
1	A	12	GLN	CB-CA-C	-9.98	90.44	110.40
1	A	44	LEU	CA-C-O	9.97	141.03	120.10
1	A	46	LYS	O-C-N	9.80	138.38	122.70
1	A	61	TYR	CA-C-O	-9.75	99.62	120.10
1	A	44	LEU	O-C-N	-9.74	107.11	122.70
1	A	2	ILE	C-N-CA	9.74	146.04	121.70
1	A	56	TYR	CA-C-N	-9.70	95.86	117.20
1	A	76	LEU	CB-CA-C	9.64	128.52	110.20
1	A	30	GLU	CA-C-N	9.60	138.31	117.20
1	A	27	SER	CB-CA-C	-9.58	91.89	110.10
1	A	68	PHE	CB-CG-CD1	9.57	127.50	120.80
1	A	70	VAL	C-N-CA	-9.55	102.24	122.30
1	A	48	THR	C-N-CA	9.50	145.45	121.70
1	A	34	TYR	CB-CG-CD2	9.49	126.69	121.00
1	A	48	THR	CA-CB-CG2	9.47	125.65	112.40
1	A	37	LEU	CA-C-N	-9.46	97.28	116.20
1	A	6	ILE	C-N-CA	9.45	145.32	121.70
1	A	19	VAL	CA-C-O	-9.45	100.25	120.10
1	A	56	TYR	N-CA-C	-9.38	85.68	111.00
1	A	55	ALA	CA-C-N	-9.31	96.71	117.20
1	A	66	SER	N-CA-C	-9.27	85.96	111.00
1	A	26	TYR	CB-CG-CD2	-9.14	115.52	121.00
1	A	16	ARG	CB-CG-CD	9.14	135.36	111.60
1	A	86	ALA	N-CA-CB	9.12	122.86	110.10
1	A	4	VAL	CA-C-O	-9.10	100.98	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	CYS	O-C-N	9.10	137.26	122.70
1	A	12	GLN	OE1-CD-NE2	-9.09	100.99	121.90
1	A	15	THR	CA-CB-CG2	-9.07	99.71	112.40
1	A	58	PRO	N-CA-CB	-9.06	92.42	103.30
1	A	51	GLU	OE1-CD-OE2	-9.05	112.44	123.30
1	A	50	ASP	CA-C-O	9.02	139.03	120.10
1	A	36	ASP	CA-CB-CG	8.99	133.18	113.40
1	A	34	TYR	CB-CA-C	8.95	128.30	110.40
1	A	18	GLY	N-CA-C	8.94	135.44	113.10
1	A	12	GLN	CB-CG-CD	8.93	134.82	111.60
1	A	36	ASP	CB-CG-OD1	-8.91	110.28	118.30
1	A	22	GLN	O-C-N	8.90	138.34	123.20
1	A	12	GLN	CA-CB-CG	8.86	132.88	113.40
1	A	13	PHE	CD1-CE1-CZ	8.80	130.67	120.10
1	A	51	GLU	CB-CA-C	8.79	127.98	110.40
1	A	86	ALA	CB-CA-C	8.76	123.24	110.10
1	A	28	LEU	N-CA-C	8.76	134.65	111.00
1	A	6	ILE	CA-CB-CG2	-8.75	93.40	110.90
1	A	10	GLN	CB-CA-C	8.66	127.72	110.40
1	A	63	VAL	N-CA-CB	-8.60	92.57	111.50
1	A	62	THR	OG1-CB-CG2	-8.60	90.22	110.00
1	A	82	ARG	NE-CZ-NH2	8.53	124.56	120.30
1	A	13	PHE	CG-CD1-CE1	-8.52	111.43	120.80
1	A	37	LEU	CB-CG-CD1	-8.51	96.53	111.00
1	A	30	GLU	CA-CB-CG	-8.43	94.86	113.40
1	A	20	SER	O-C-N	-8.35	109.35	122.70
1	A	1	MET	N-CA-CB	8.31	125.57	110.60
1	A	40	GLU	CB-CA-C	8.30	127.01	110.40
1	A	80	ARG	CB-CA-C	-8.27	93.86	110.40
1	A	37	LEU	O-C-N	-8.25	109.18	123.20
1	A	75	SER	CB-CA-C	8.23	125.74	110.10
1	A	78	ILE	O-C-N	-8.21	109.57	122.70
1	A	17	SER	CA-C-O	8.17	137.25	120.10
1	A	38	GLY	CA-C-N	-8.14	99.28	117.20
1	A	7	LYS	CB-CA-C	8.14	126.67	110.40
1	A	7	LYS	CA-CB-CG	8.13	131.28	113.40
1	A	78	ILE	CB-CA-C	-8.12	95.36	111.60
1	A	5	GLU	N-CA-CB	-8.10	96.02	110.60
1	A	31	GLN	O-C-N	8.10	135.66	122.70
1	A	70	VAL	CA-C-N	-8.09	100.03	116.20
1	A	38	GLY	O-C-N	8.07	135.61	122.70
1	A	73	PHE	CA-C-O	8.02	136.94	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	HIS	C-N-CA	7.95	141.56	121.70
1	A	43	VAL	O-C-N	-7.94	110.00	122.70
1	A	84	VAL	N-CA-CB	-7.92	94.07	111.50
1	A	2	ILE	N-CA-C	7.91	132.36	111.00
1	A	8	PRO	CA-C-N	-7.88	99.87	117.20
1	A	13	PHE	CB-CG-CD2	-7.84	115.31	120.80
1	A	69	LYS	N-CA-CB	-7.82	96.52	110.60
1	A	44	LEU	CD1-CG-CD2	-7.82	87.05	110.50
1	A	60	LEU	CA-C-N	-7.79	100.07	117.20
1	A	63	VAL	O-C-N	-7.78	110.25	122.70
1	A	8	PRO	C-N-CA	7.76	141.09	121.70
1	A	29	ASN	O-C-N	-7.71	110.36	122.70
1	A	58	PRO	CB-CG-CD	-7.71	76.42	106.50
1	A	28	LEU	CA-C-O	7.67	136.21	120.10
1	A	22	GLN	C-N-CA	7.63	138.32	122.30
1	A	17	SER	N-CA-C	7.62	131.58	111.00
1	A	19	VAL	CA-CB-CG2	7.61	122.31	110.90
1	A	52	GLY	N-CA-C	-7.60	94.09	113.10
1	A	47	ILE	CG1-CB-CG2	-7.56	94.76	111.40
1	A	75	SER	N-CA-C	-7.55	90.63	111.00
1	A	71	GLY	O-C-N	7.54	134.77	122.70
1	A	61	TYR	CB-CG-CD2	-7.54	116.48	121.00
1	A	70	VAL	CB-CA-C	7.54	125.72	111.40
1	A	2	ILE	CA-C-O	7.49	135.83	120.10
1	A	26	TYR	CZ-CE2-CD2	7.48	126.53	119.80
1	A	37	LEU	C-N-CA	7.47	138.00	122.30
1	A	66	SER	N-CA-CB	7.47	121.71	110.50
1	A	10	GLN	N-CA-C	-7.46	90.86	111.00
1	A	2	ILE	CA-CB-CG1	-7.46	96.83	111.00
1	A	51	GLU	CA-CB-CG	7.45	129.79	113.40
1	A	5	GLU	CG-CD-OE2	-7.43	103.43	118.30
1	A	7	LYS	CD-CE-NZ	-7.41	94.66	111.70
1	A	6	ILE	CA-CB-CG1	7.41	125.07	111.00
1	A	81	LEU	N-CA-CB	7.39	125.17	110.40
1	A	24	LYS	CB-CA-C	7.38	125.17	110.40
1	A	9	SER	N-CA-CB	7.36	121.54	110.50
1	A	56	TYR	CB-CG-CD2	-7.30	116.62	121.00
1	A	77	MET	N-CA-C	-7.29	91.31	111.00
1	A	83	LEU	CB-CG-CD2	-7.28	98.62	111.00
1	A	48	THR	CB-CA-C	7.27	131.24	111.60
1	A	63	VAL	N-CA-C	7.24	130.56	111.00
1	A	56	TYR	N-CA-CB	7.23	123.62	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	LEU	N-CA-C	-7.22	91.49	111.00
1	A	43	VAL	CA-C-O	7.15	135.11	120.10
1	A	31	GLN	N-CA-CB	-7.14	97.74	110.60
1	A	61	TYR	CD1-CE1-CZ	7.14	126.23	119.80
1	A	34	TYR	CG-CD2-CE2	7.14	127.01	121.30
1	A	84	VAL	CB-CA-C	7.13	124.95	111.40
1	A	79	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	A	68	PHE	CA-CB-CG	7.11	130.96	113.90
1	A	24	LYS	CG-CD-CE	7.09	133.17	111.90
1	A	5	GLU	C-N-CA	7.08	139.40	121.70
1	A	63	VAL	CB-CA-C	7.07	124.84	111.40
1	A	72	GLN	CA-CB-CG	7.07	128.96	113.40
1	A	71	GLY	N-CA-C	-7.07	95.43	113.10
1	A	84	VAL	CA-CB-CG1	7.04	121.46	110.90
1	A	41	TYR	CG-CD1-CE1	-7.00	115.70	121.30
1	A	85	PRO	CA-N-CD	-7.00	101.70	111.50
1	A	24	LYS	CA-CB-CG	6.98	128.76	113.40
1	A	4	VAL	CA-C-N	6.97	132.54	117.20
1	A	13	PHE	N-CA-CB	6.96	123.12	110.60
1	A	51	GLU	CG-CD-OE2	-6.92	104.45	118.30
1	A	29	ASN	OD1-CG-ND2	-6.91	106.01	121.90
1	A	32	LEU	CB-CG-CD2	6.90	122.73	111.00
1	A	19	VAL	CA-C-N	6.88	132.32	117.20
1	A	76	LEU	CA-C-O	6.88	134.54	120.10
1	A	2	ILE	O-C-N	-6.86	111.73	122.70
1	A	24	LYS	O-C-N	6.84	134.09	121.10
1	A	47	ILE	CA-CB-CG1	6.84	123.99	111.00
1	A	44	LEU	C-N-CA	6.83	138.76	121.70
1	A	20	SER	N-CA-CB	-6.82	100.27	110.50
1	A	49	LEU	CA-C-N	-6.82	102.19	117.20
1	A	40	GLU	CB-CG-CD	6.81	132.59	114.20
1	A	19	VAL	CG1-CB-CG2	6.80	121.78	110.90
1	A	79	ASP	CA-CB-CG	-6.80	98.45	113.40
1	A	28	LEU	CB-CG-CD2	-6.76	99.51	111.00
1	A	17	SER	C-N-CA	6.75	136.48	122.30
1	A	68	PHE	CD1-CG-CD2	-6.72	109.56	118.30
1	A	73	PHE	CB-CA-C	6.71	123.81	110.40
1	A	82	ARG	N-CA-CB	6.70	122.66	110.60
1	A	36	ASP	CB-CA-C	6.67	123.73	110.40
1	A	32	LEU	O-C-N	-6.66	112.04	122.70
1	A	6	ILE	CG1-CB-CG2	-6.64	96.80	111.40
1	A	5	GLU	CG-CD-OE1	-6.62	105.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	SER	CA-CB-OG	-6.62	93.32	111.20
1	A	16	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	A	18	GLY	CA-C-O	6.59	132.46	120.60
1	A	80	ARG	O-C-N	6.57	133.21	122.70
1	A	19	VAL	N-CA-CB	6.55	125.90	111.50
1	A	35	VAL	CA-C-O	6.54	133.84	120.10
1	A	35	VAL	N-CA-CB	6.52	125.85	111.50
1	A	77	MET	CA-C-O	-6.52	106.42	120.10
1	A	69	LYS	N-CA-C	6.47	128.47	111.00
1	A	37	LEU	CD1-CG-CD2	6.46	129.89	110.50
1	A	41	TYR	CA-C-O	6.46	133.67	120.10
1	A	49	LEU	CA-CB-CG	6.44	130.12	115.30
1	A	42	PRO	CA-C-N	6.44	131.36	117.20
1	A	38	GLY	C-N-CA	-6.44	105.61	121.70
1	A	17	SER	CA-CB-OG	6.43	128.57	111.20
1	A	66	SER	CA-C-N	-6.40	103.11	117.20
1	A	37	LEU	N-CA-C	6.34	128.12	111.00
1	A	58	PRO	CA-N-CD	-6.33	102.64	111.50
1	A	21	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	9	SER	C-N-CA	-6.32	105.91	121.70
1	A	17	SER	CB-CA-C	-6.30	98.13	110.10
1	A	86	ALA	CA-C-N	-6.24	103.47	117.20
1	A	66	SER	C-N-CA	6.23	137.28	121.70
1	A	85	PRO	O-C-N	6.23	132.66	122.70
1	A	3	LYS	CG-CD-CE	6.16	130.39	111.90
1	A	53	GLN	CB-CA-C	6.15	122.70	110.40
1	A	64	HIS	CA-C-O	6.13	132.98	120.10
1	A	80	ARG	C-N-CA	-6.13	106.39	121.70
1	A	12	GLN	CA-C-N	-6.12	103.73	117.20
1	A	24	LYS	N-CA-C	-6.12	94.47	111.00
1	A	75	SER	CA-C-N	-6.11	103.77	117.20
1	A	72	GLN	O-C-N	6.10	132.46	122.70
1	A	50	ASP	CA-C-N	-6.08	103.81	117.20
1	A	25	PRO	C-N-CA	6.06	136.85	121.70
1	A	55	ALA	CA-C-O	6.04	132.79	120.10
1	A	83	LEU	CD1-CG-CD2	6.01	128.53	110.50
1	A	32	LEU	CB-CA-C	5.99	121.58	110.20
1	A	37	LEU	CB-CA-C	5.99	121.58	110.20
1	A	44	LEU	CB-CA-C	-5.98	98.84	110.20
1	A	30	GLU	CB-CG-CD	-5.96	98.11	114.20
1	A	27	SER	N-CA-CB	5.96	119.44	110.50
1	A	41	TYR	CB-CG-CD2	-5.95	117.43	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	GLU	CB-CA-C	-5.93	98.53	110.40
1	A	47	ILE	O-C-N	-5.92	113.22	122.70
1	A	5	GLU	O-C-N	-5.92	113.23	122.70
1	A	63	VAL	CA-C-N	-5.87	104.29	117.20
1	A	57	ALA	CA-C-O	5.86	132.41	120.10
1	A	27	SER	O-C-N	-5.86	113.33	122.70
1	A	16	ARG	O-C-N	-5.85	113.33	122.70
1	A	21	ARG	CA-C-O	5.84	132.36	120.10
1	A	31	GLN	CA-C-N	-5.82	104.39	117.20
1	A	39	ASN	CA-C-N	5.81	129.98	117.20
1	A	68	PHE	CG-CD2-CE2	5.80	127.19	120.80
1	A	44	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	22	GLN	OE1-CD-NE2	-5.77	108.62	121.90
1	A	34	TYR	CD1-CE1-CZ	5.77	124.99	119.80
1	A	12	GLN	N-CA-CB	5.76	120.97	110.60
1	A	26	TYR	O-C-N	5.75	131.89	122.70
1	A	6	ILE	CB-CA-C	-5.74	100.12	111.60
1	A	27	SER	CA-CB-OG	5.74	126.70	111.20
1	A	34	TYR	N-CA-C	-5.72	95.56	111.00
1	A	63	VAL	CA-CB-CG2	5.72	119.48	110.90
1	A	34	TYR	N-CA-CB	5.71	120.87	110.60
1	A	48	THR	N-CA-C	-5.69	95.64	111.00
1	A	20	SER	CA-C-N	5.67	129.68	117.20
1	A	59	GLY	C-N-CA	5.66	135.85	121.70
1	A	12	GLN	C-N-CA	-5.66	107.55	121.70
1	A	5	GLU	CA-CB-CG	5.64	125.81	113.40
1	A	74	GLY	C-N-CA	-5.63	107.62	121.70
1	A	8	PRO	CB-CA-C	-5.61	97.98	112.00
1	A	11	ALA	N-CA-CB	5.61	117.95	110.10
1	A	29	ASN	CB-CG-ND2	5.58	130.09	116.70
1	A	51	GLU	N-CA-C	-5.58	95.93	111.00
1	A	45	VAL	CA-CB-CG2	-5.57	102.55	110.90
1	A	80	ARG	N-CA-C	5.57	126.04	111.00
1	A	40	GLU	CA-C-N	5.56	129.43	117.20
1	A	2	ILE	N-CA-CB	-5.54	98.05	110.80
1	A	67	SER	CB-CA-C	-5.53	99.59	110.10
1	A	68	PHE	CG-CD1-CE1	5.53	126.88	120.80
1	A	56	TYR	CB-CG-CD1	5.52	124.31	121.00
1	A	85	PRO	C-N-CA	-5.51	107.92	121.70
1	A	35	VAL	CA-C-N	-5.50	105.11	117.20
1	A	80	ARG	CD-NE-CZ	5.49	131.28	123.60
1	A	61	TYR	CG-CD1-CE1	-5.46	116.93	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	LYS	CA-C-O	5.44	131.52	120.10
1	A	54	PRO	CA-C-N	-5.40	105.33	117.20
1	A	9	SER	CA-C-N	-5.39	105.33	117.20
1	A	58	PRO	N-CA-C	5.39	126.12	112.10
1	A	46	LYS	N-CA-CB	5.38	120.29	110.60
1	A	28	LEU	CA-C-N	-5.37	105.38	117.20
1	A	85	PRO	CA-CB-CG	5.34	114.95	104.80
1	A	26	TYR	CE1-CZ-OH	5.34	134.51	120.10
1	A	1	MET	CA-CB-CG	-5.31	104.27	113.30
1	A	21	ARG	CB-CA-C	-5.31	99.78	110.40
1	A	14	THR	CB-CA-C	5.25	125.78	111.60
1	A	50	ASP	N-CA-CB	-5.23	101.19	110.60
1	A	76	LEU	O-C-N	-5.21	114.36	122.70
1	A	27	SER	CA-C-O	5.20	131.02	120.10
1	A	46	LYS	CA-C-N	-5.20	105.77	117.20
1	A	68	PHE	N-CA-CB	5.19	119.95	110.60
1	A	86	ALA	C-N-CA	-5.18	108.74	121.70
1	A	40	GLU	CA-CB-CG	5.17	124.77	113.40
1	A	20	SER	C-N-CA	5.15	134.57	121.70
1	A	16	ARG	CG-CD-NE	5.14	122.60	111.80
1	A	61	TYR	CB-CG-CD1	5.13	124.08	121.00
1	A	69	LYS	CA-CB-CG	-5.13	102.11	113.40
1	A	44	LEU	N-CA-CB	5.13	120.66	110.40
1	A	66	SER	O-C-N	5.13	130.91	122.70
1	A	12	GLN	CA-C-O	5.10	130.81	120.10
1	A	64	HIS	N-CA-C	-5.07	97.33	111.00
1	A	43	VAL	CB-CA-C	-5.05	101.81	111.40
1	A	82	ARG	CB-CA-C	-5.02	100.37	110.40
1	A	9	SER	CA-C-O	5.01	130.63	120.10

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	TYR	Sidechain
1	A	34	TYR	Mainchain
1	A	45	VAL	Mainchain
1	A	48	THR	Mainchain
1	A	5	GLU	Mainchain
1	A	55	ALA	Mainchain
1	A	59	GLY	Mainchain,Peptide
1	A	6	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	A	61	TYR	Sidechain
1	A	62	THR	Mainchain
1	A	7	LYS	Mainchain
1	A	76	LEU	Mainchain
1	A	81	LEU	Mainchain
1	A	82	ARG	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	682	0	685	360	2
2	A	12	0	0	1	0
All	All	694	0	685	360	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 263.

All (360) 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:50:ASP:CB	1:A:53:GLN:HG2	1.22	1.57
1:A:50:ASP:HB2	1:A:53:GLN:CG	1.41	1.47
1:A:46:LYS:HE2	1:A:48:THR:CG2	1.44	1.45
1:A:72:GLN:HG3	1:A:73:PHE:CE2	1.52	1.44
1:A:6:ILE:CG2	1:A:35:VAL:HG21	1.58	1.34
1:A:61:TYR:CB	1:A:83:LEU:HD11	1.55	1.33
1:A:62:THR:CG2	1:A:63:VAL:HG12	1.60	1.30
1:A:14:THR:O	1:A:15:THR:HG22	1.19	1.28
1:A:46:LYS:CE	1:A:48:THR:CG2	2.15	1.23
1:A:69:LYS:CD	1:A:78:ILE:HG23	1.70	1.22
1:A:72:GLN:CG	1:A:73:PHE:CE2	2.21	1.22
1:A:72:GLN:HB3	1:A:73:PHE:CE2	1.74	1.22
1:A:72:GLN:HB3	1:A:73:PHE:CD2	1.75	1.21
1:A:62:THR:HG23	1:A:63:VAL:CG1	1.69	1.21
1:A:46:LYS:CE	1:A:48:THR:HG21	1.73	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LYS:NZ	1:A:48:THR:HG21	1.57	1.17
1:A:68:PHE:HA	1:A:76:LEU:O	1.44	1.14
1:A:69:LYS:HD3	1:A:78:ILE:CG2	1.77	1.14
1:A:87:LYS:CA	1:A:87:LYS:HZ1	1.58	1.14
1:A:14:THR:C	1:A:15:THR:HG22	1.63	1.14
1:A:46:LYS:HE2	1:A:48:THR:HB	1.19	1.13
1:A:18:GLY:O	1:A:20:SER:N	1.81	1.12
1:A:23:GLY:HA3	1:A:27:SER:HA	1.15	1.12
1:A:35:VAL:CG2	1:A:36:ASP:H	1.59	1.12
1:A:87:LYS:N	1:A:87:LYS:HZ1	1.47	1.12
1:A:29:ASN:HB2	1:A:51:GLU:HG2	1.27	1.12
1:A:69:LYS:HD3	1:A:78:ILE:HG23	1.12	1.11
1:A:14:THR:O	1:A:15:THR:CG2	2.00	1.10
1:A:50:ASP:HB2	1:A:53:GLN:CD	1.70	1.10
1:A:1:MET:HE2	1:A:2:ILE:HG13	1.23	1.09
1:A:35:VAL:HG22	1:A:36:ASP:N	1.58	1.09
1:A:39:ASN:C	1:A:40:GLU:HG2	1.70	1.09
1:A:25:PRO:O	1:A:26:TYR:HD2	1.36	1.08
1:A:6:ILE:HG22	1:A:35:VAL:HG21	1.23	1.08
1:A:61:TYR:HA	1:A:84:VAL:O	1.51	1.08
1:A:46:LYS:HE2	1:A:48:THR:CB	1.81	1.08
1:A:46:LYS:HE2	1:A:48:THR:HG22	1.34	1.08
1:A:72:GLN:CB	1:A:73:PHE:CE2	2.36	1.08
1:A:52:GLY:O	1:A:54:PRO:HD3	1.53	1.06
1:A:29:ASN:HB2	1:A:51:GLU:CG	1.85	1.06
1:A:87:LYS:HZ1	1:A:87:LYS:HA	1.19	1.05
1:A:69:LYS:HD2	1:A:79:ASP:HB2	1.35	1.04
1:A:62:THR:N	1:A:84:VAL:O	1.89	1.04
1:A:24:LYS:CD	1:A:25:PRO:HD2	1.87	1.04
1:A:35:VAL:HG22	1:A:36:ASP:H	0.90	1.04
1:A:50:ASP:O	1:A:53:GLN:HB2	1.57	1.04
1:A:6:ILE:HG22	1:A:35:VAL:CG2	1.88	1.03
1:A:21:ARG:HH21	1:A:21:ARG:HB2	1.22	1.03
1:A:60:LEU:HD13	1:A:86:ALA:HB3	1.40	1.03
1:A:61:TYR:HB3	1:A:83:LEU:CD1	1.90	1.01
1:A:25:PRO:O	1:A:26:TYR:CD2	2.14	1.01
1:A:73:PHE:N	1:A:73:PHE:CD2	2.25	1.00
1:A:46:LYS:CE	1:A:48:THR:HB	1.91	1.00
1:A:61:TYR:HB3	1:A:83:LEU:HD11	0.99	0.99
1:A:24:LYS:HD3	1:A:25:PRO:CD	1.92	0.98
1:A:18:GLY:HA2	1:A:30:GLU:O	1.62	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:THR:HG21	1:A:33:CYS:SG	2.03	0.98
1:A:50:ASP:CG	1:A:53:GLN:HG2	1.83	0.98
1:A:65:LEU:O	1:A:82:ARG:HG3	1.64	0.97
1:A:21:ARG:HB2	1:A:21:ARG:NH2	1.80	0.97
1:A:23:GLY:CA	1:A:27:SER:HA	1.95	0.96
1:A:83:LEU:CD1	1:A:84:VAL:H	1.78	0.96
1:A:6:ILE:CD1	1:A:83:LEU:HD22	1.95	0.96
1:A:50:ASP:CB	1:A:53:GLN:CG	2.14	0.95
1:A:24:LYS:HD3	1:A:25:PRO:HD2	0.97	0.95
1:A:25:PRO:C	1:A:26:TYR:HD2	1.69	0.95
1:A:30:GLU:OE2	1:A:30:GLU:HA	1.54	0.95
1:A:85:PRO:O	1:A:87:LYS:NZ	2.00	0.95
1:A:72:GLN:HB3	1:A:73:PHE:CZ	2.00	0.95
1:A:70:VAL:HA	1:A:74:GLY:O	1.66	0.94
1:A:87:LYS:N	1:A:87:LYS:NZ	2.16	0.94
1:A:34:TYR:CE2	1:A:44:LEU:HD21	2.03	0.93
1:A:7:LYS:HB3	1:A:60:LEU:HD23	1.50	0.93
1:A:69:LYS:N	1:A:76:LEU:O	2.02	0.93
1:A:72:GLN:CB	1:A:73:PHE:CZ	2.52	0.93
1:A:70:VAL:CA	1:A:74:GLY:O	2.17	0.92
1:A:46:LYS:HZ1	1:A:48:THR:HG21	1.22	0.92
1:A:1:MET:CE	1:A:2:ILE:HG13	1.99	0.91
1:A:23:GLY:HA3	1:A:27:SER:CA	1.99	0.91
1:A:39:ASN:C	1:A:40:GLU:CG	2.39	0.91
1:A:68:PHE:CA	1:A:76:LEU:O	2.19	0.91
1:A:72:GLN:HG3	1:A:73:PHE:HE2	1.19	0.90
1:A:36:ASP:HB2	1:A:44:LEU:N	1.87	0.90
1:A:7:LYS:O	1:A:60:LEU:N	2.05	0.90
1:A:87:LYS:CA	1:A:87:LYS:NZ	2.34	0.89
1:A:87:LYS:NZ	1:A:87:LYS:HA	1.87	0.88
1:A:72:GLN:HG3	1:A:73:PHE:CZ	2.07	0.87
1:A:80:ARG:HH12	1:A:82:ARG:HH21	1.23	0.87
1:A:83:LEU:HD13	1:A:84:VAL:H	1.36	0.87
1:A:50:ASP:O	1:A:53:GLN:CB	2.22	0.86
1:A:9:SER:CB	1:A:58:PRO:HA	2.05	0.86
1:A:7:LYS:HB3	1:A:60:LEU:CD2	2.06	0.86
1:A:69:LYS:HD2	1:A:79:ASP:CB	2.05	0.85
1:A:37:LEU:O	1:A:39:ASN:HB2	1.76	0.85
1:A:31:GLN:HG2	1:A:51:GLU:HB3	1.60	0.84
1:A:4:VAL:C	1:A:5:GLU:HG3	1.97	0.84
1:A:75:SER:O	1:A:76:LEU:HD23	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:TYR:CG	1:A:83:LEU:HD11	2.13	0.84
1:A:56:TYR:HB3	1:A:61:TYR:CE1	2.13	0.84
1:A:9:SER:HB2	1:A:58:PRO:C	1.98	0.83
1:A:19:VAL:HG13	1:A:32:LEU:CD1	2.07	0.83
1:A:21:ARG:HH21	1:A:21:ARG:CB	1.92	0.83
1:A:83:LEU:HD12	1:A:84:VAL:N	1.92	0.83
1:A:7:LYS:HA	1:A:60:LEU:HB2	1.59	0.83
1:A:6:ILE:HD13	1:A:83:LEU:HD22	1.60	0.83
1:A:21:ARG:HG2	1:A:22:GLN:N	1.93	0.82
1:A:72:GLN:CG	1:A:73:PHE:CZ	2.62	0.82
1:A:46:LYS:NZ	1:A:48:THR:CG2	2.37	0.82
1:A:83:LEU:CD1	1:A:84:VAL:N	2.43	0.82
1:A:24:LYS:HB2	1:A:25:PRO:HD3	1.61	0.81
1:A:47:ILE:HG22	1:A:49:LEU:HD23	1.59	0.81
1:A:69:LYS:HB2	1:A:78:ILE:O	1.82	0.80
1:A:31:GLN:OE1	1:A:50:ASP:O	1.99	0.80
1:A:72:GLN:NE2	1:A:72:GLN:HA	1.95	0.80
1:A:70:VAL:O	1:A:72:GLN:N	2.13	0.80
1:A:6:ILE:HD12	1:A:83:LEU:HD22	1.63	0.79
1:A:62:THR:O	1:A:83:LEU:HA	1.81	0.79
1:A:65:LEU:O	1:A:82:ARG:CG	2.30	0.79
1:A:61:TYR:CD2	1:A:83:LEU:HD12	2.18	0.78
1:A:61:TYR:CD2	1:A:83:LEU:CD1	2.66	0.78
1:A:64:HIS:HA	1:A:67:SER:HB2	1.66	0.78
1:A:3:LYS:NZ	1:A:87:LYS:HB2	1.99	0.78
1:A:69:LYS:HE3	1:A:79:ASP:OD2	1.84	0.77
1:A:35:VAL:O	1:A:36:ASP:HB3	1.84	0.77
1:A:30:GLU:OE2	1:A:30:GLU:CA	2.29	0.77
1:A:69:LYS:O	1:A:70:VAL:HB	1.82	0.77
1:A:6:ILE:HD11	1:A:81:LEU:CD1	2.14	0.77
1:A:7:LYS:O	1:A:60:LEU:CA	2.34	0.76
1:A:83:LEU:C	1:A:84:VAL:HG12	2.04	0.76
1:A:27:SER:O	1:A:28:LEU:HD23	1.86	0.76
1:A:6:ILE:HG21	1:A:35:VAL:HG21	1.66	0.76
1:A:70:VAL:HG22	1:A:72:GLN:O	1.85	0.75
1:A:66:SER:HB3	1:A:82:ARG:HH11	1.51	0.75
1:A:50:ASP:C	1:A:53:GLN:HB2	2.07	0.75
1:A:41:TYR:CB	1:A:42:PRO:HD2	2.16	0.75
1:A:76:LEU:HB3	1:A:78:ILE:HG22	1.68	0.75
1:A:41:TYR:HD2	1:A:42:PRO:HG2	1.51	0.74
1:A:50:ASP:CG	1:A:53:GLN:CB	2.55	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:HG23	1:A:19:VAL:O	1.86	0.74
1:A:61:TYR:CB	1:A:83:LEU:CD1	2.51	0.74
1:A:14:THR:C	1:A:15:THR:CG2	2.38	0.74
1:A:29:ASN:C	1:A:51:GLU:HG3	2.08	0.74
1:A:5:GLU:HB3	1:A:7:LYS:HE2	1.68	0.74
1:A:47:ILE:CG2	1:A:49:LEU:HD23	2.18	0.74
1:A:41:TYR:CD2	1:A:42:PRO:HD2	2.22	0.73
1:A:72:GLN:CB	1:A:73:PHE:CD2	2.62	0.73
1:A:61:TYR:CA	1:A:83:LEU:HD11	2.18	0.73
1:A:78:ILE:HG12	1:A:79:ASP:CG	2.09	0.73
1:A:80:ARG:HG3	1:A:81:LEU:N	2.01	0.73
1:A:6:ILE:HD13	1:A:83:LEU:CD2	2.19	0.73
1:A:78:ILE:HG12	1:A:79:ASP:OD1	1.87	0.73
1:A:69:LYS:HD2	1:A:78:ILE:HG23	1.70	0.72
1:A:49:LEU:O	1:A:51:GLU:OE1	2.07	0.71
1:A:50:ASP:CA	1:A:53:GLN:HG2	2.17	0.71
1:A:66:SER:HB3	1:A:82:ARG:NH1	2.06	0.71
1:A:15:THR:CG2	1:A:33:CYS:SG	2.79	0.71
1:A:50:ASP:C	1:A:53:GLN:CG	2.58	0.71
1:A:50:ASP:O	1:A:53:GLN:O	2.08	0.70
1:A:77:MET:O	1:A:78:ILE:C	2.22	0.70
1:A:6:ILE:CG2	1:A:35:VAL:CG2	2.48	0.70
1:A:7:LYS:CB	1:A:60:LEU:HD23	2.21	0.70
1:A:60:LEU:O	1:A:86:ALA:N	2.24	0.70
1:A:50:ASP:CG	1:A:53:GLN:HB2	2.12	0.70
1:A:9:SER:HB3	1:A:58:PRO:HA	1.74	0.69
1:A:9:SER:CB	1:A:58:PRO:CA	2.71	0.69
1:A:19:VAL:HG13	1:A:32:LEU:HD13	1.74	0.69
1:A:4:VAL:C	1:A:5:GLU:CG	2.61	0.69
1:A:19:VAL:CG2	1:A:19:VAL:O	2.41	0.69
1:A:80:ARG:O	1:A:82:ARG:HG2	1.91	0.69
1:A:31:GLN:OE1	1:A:53:GLN:O	2.12	0.68
1:A:50:ASP:OD2	1:A:53:GLN:CB	2.42	0.68
1:A:31:GLN:NE2	1:A:53:GLN:O	2.23	0.68
1:A:50:ASP:OD2	1:A:53:GLN:HB2	1.92	0.68
1:A:11:ALA:O	1:A:14:THR:OG1	2.08	0.68
1:A:62:THR:O	1:A:82:ARG:O	2.12	0.68
1:A:9:SER:HB2	1:A:58:PRO:CA	2.23	0.68
1:A:16:ARG:HA	1:A:32:LEU:O	1.92	0.68
1:A:86:ALA:C	1:A:87:LYS:HZ1	1.96	0.68
1:A:69:LYS:CD	1:A:79:ASP:HB2	2.18	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ILE:CD1	1:A:83:LEU:CD2	2.70	0.68
1:A:70:VAL:C	1:A:72:GLN:N	2.46	0.68
1:A:18:GLY:O	1:A:19:VAL:C	2.31	0.67
1:A:41:TYR:CG	1:A:42:PRO:HD2	2.30	0.67
1:A:65:LEU:HG	1:A:84:VAL:HG11	1.75	0.67
1:A:76:LEU:CB	1:A:78:ILE:HG22	2.25	0.67
1:A:80:ARG:HB2	1:A:80:ARG:CZ	2.24	0.67
1:A:31:GLN:NE2	1:A:50:ASP:O	2.28	0.67
1:A:7:LYS:O	1:A:60:LEU:HA	1.95	0.67
1:A:70:VAL:CG1	1:A:71:GLY:N	2.58	0.66
1:A:56:TYR:HB3	1:A:61:TYR:CZ	2.29	0.66
1:A:61:TYR:CA	1:A:84:VAL:O	2.36	0.66
1:A:7:LYS:CA	1:A:60:LEU:HB2	2.25	0.66
1:A:80:ARG:CG	1:A:80:ARG:HH11	2.08	0.66
1:A:50:ASP:HB2	1:A:53:GLN:HG2	0.67	0.66
1:A:24:LYS:HB2	1:A:25:PRO:CD	2.26	0.66
1:A:34:TYR:CD2	1:A:44:LEU:HD21	2.31	0.66
1:A:62:THR:HG23	1:A:63:VAL:HG12	0.74	0.65
1:A:6:ILE:O	1:A:7:LYS:O	2.14	0.65
1:A:14:THR:O	1:A:15:THR:C	2.35	0.65
1:A:48:THR:O	1:A:80:ARG:CD	2.44	0.65
1:A:5:GLU:HB3	1:A:7:LYS:CE	2.26	0.65
1:A:80:ARG:HH12	1:A:82:ARG:NH2	1.93	0.65
1:A:50:ASP:CA	1:A:53:GLN:CG	2.74	0.64
1:A:64:HIS:HB3	1:A:66:SER:O	1.97	0.64
1:A:36:ASP:HB3	1:A:44:LEU:HA	1.80	0.64
1:A:25:PRO:C	1:A:26:TYR:CD2	2.61	0.64
1:A:62:THR:CG2	1:A:63:VAL:CG1	2.47	0.64
1:A:75:SER:O	1:A:76:LEU:CD2	2.46	0.63
1:A:70:VAL:CG1	1:A:71:GLY:H	2.11	0.63
1:A:24:LYS:CB	1:A:25:PRO:CD	2.76	0.63
1:A:87:LYS:CE	1:A:87:LYS:HA	2.28	0.63
1:A:9:SER:HB2	1:A:58:PRO:HA	1.80	0.63
1:A:83:LEU:C	1:A:84:VAL:CG1	2.67	0.63
1:A:6:ILE:O	1:A:7:LYS:C	2.35	0.63
1:A:41:TYR:O	1:A:43:VAL:HG13	1.99	0.63
1:A:29:ASN:O	1:A:51:GLU:HG3	1.99	0.62
1:A:31:GLN:CD	1:A:50:ASP:O	2.38	0.62
1:A:1:MET:CE	1:A:2:ILE:CG1	2.74	0.62
1:A:36:ASP:CB	1:A:44:LEU:HA	2.30	0.61
1:A:19:VAL:HG13	1:A:32:LEU:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:TYR:CD2	1:A:42:PRO:HG2	2.32	0.61
1:A:10:GLN:HB2	1:A:13:PHE:CE2	2.34	0.61
1:A:3:LYS:HZ3	1:A:87:LYS:HB2	1.66	0.61
1:A:3:LYS:HZ2	1:A:87:LYS:HB2	1.64	0.60
1:A:64:HIS:CA	1:A:67:SER:HB2	2.31	0.60
1:A:68:PHE:C	1:A:76:LEU:O	2.40	0.60
1:A:13:PHE:CD2	1:A:13:PHE:N	2.69	0.60
1:A:16:ARG:O	1:A:16:ARG:HG2	1.96	0.60
1:A:70:VAL:HG13	1:A:71:GLY:N	2.17	0.60
1:A:46:LYS:CE	1:A:48:THR:CB	2.60	0.60
1:A:50:ASP:C	1:A:53:GLN:CB	2.68	0.60
1:A:80:ARG:HB2	1:A:80:ARG:NH1	2.17	0.59
1:A:14:THR:O	1:A:15:THR:O	2.19	0.59
1:A:10:GLN:HG3	1:A:13:PHE:CE1	2.38	0.59
1:A:68:PHE:CB	1:A:76:LEU:O	2.49	0.59
1:A:50:ASP:CB	1:A:53:GLN:CD	2.57	0.58
1:A:9:SER:HB2	1:A:59:GLY:N	2.17	0.58
1:A:1:MET:HE2	1:A:2:ILE:CG1	2.15	0.58
1:A:62:THR:O	1:A:83:LEU:CA	2.49	0.58
1:A:31:GLN:CD	1:A:51:GLU:HA	2.24	0.58
1:A:61:TYR:CG	1:A:83:LEU:CD1	2.84	0.58
1:A:18:GLY:C	1:A:30:GLU:HB3	2.24	0.58
1:A:6:ILE:CD1	1:A:81:LEU:CD1	2.82	0.58
1:A:50:ASP:CG	1:A:53:GLN:CG	2.64	0.58
1:A:69:LYS:HB3	1:A:76:LEU:HB2	1.86	0.58
1:A:20:SER:HB3	1:A:28:LEU:HB3	1.86	0.57
1:A:35:VAL:CG2	1:A:36:ASP:N	2.29	0.57
1:A:65:LEU:HG	1:A:84:VAL:CG1	2.34	0.57
1:A:68:PHE:HB3	1:A:76:LEU:O	2.05	0.57
1:A:80:ARG:HG3	1:A:81:LEU:O	2.04	0.57
1:A:5:GLU:CB	1:A:7:LYS:HE2	2.35	0.56
1:A:30:GLU:HG3	1:A:32:LEU:HD12	1.87	0.56
1:A:80:ARG:NH1	1:A:80:ARG:CB	2.68	0.56
1:A:61:TYR:CD2	1:A:83:LEU:HD11	2.37	0.56
1:A:12:GLN:HB3	1:A:13:PHE:CD2	2.40	0.56
1:A:29:ASN:HB2	1:A:51:GLU:HG3	1.81	0.56
1:A:4:VAL:HG22	1:A:63:VAL:HG21	1.87	0.56
1:A:6:ILE:HG23	1:A:35:VAL:HG21	1.76	0.56
1:A:9:SER:CB	1:A:57:ALA:O	2.53	0.56
1:A:39:ASN:O	1:A:40:GLU:HG2	2.05	0.56
1:A:9:SER:HB3	1:A:58:PRO:CA	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:TYR:C	1:A:84:VAL:O	2.44	0.55
1:A:9:SER:O	1:A:58:PRO:O	2.25	0.55
1:A:6:ILE:C	1:A:8:PRO:N	2.50	0.55
1:A:70:VAL:N	1:A:74:GLY:O	2.40	0.54
1:A:41:TYR:CD2	1:A:42:PRO:CD	2.91	0.54
1:A:36:ASP:HB2	1:A:43:VAL:HA	1.89	0.54
1:A:70:VAL:HG12	1:A:71:GLY:H	1.73	0.53
1:A:72:GLN:HB3	1:A:73:PHE:CG	2.42	0.53
1:A:56:TYR:CZ	1:A:83:LEU:HB3	2.43	0.53
1:A:68:PHE:CD1	1:A:77:MET:CE	2.91	0.53
1:A:50:ASP:OD2	1:A:53:GLN:HB3	2.08	0.53
1:A:6:ILE:HD11	1:A:81:LEU:HD13	1.91	0.53
1:A:69:LYS:CE	1:A:79:ASP:OD2	2.55	0.53
1:A:41:TYR:HD2	1:A:42:PRO:CG	2.21	0.52
1:A:34:TYR:CD2	1:A:44:LEU:CD2	2.93	0.52
1:A:50:ASP:O	1:A:53:GLN:CA	2.57	0.52
1:A:69:LYS:CB	1:A:78:ILE:O	2.55	0.52
1:A:65:LEU:O	1:A:82:ARG:CD	2.58	0.51
1:A:9:SER:HB2	1:A:57:ALA:O	2.11	0.51
1:A:69:LYS:O	1:A:70:VAL:CB	2.56	0.51
1:A:77:MET:C	1:A:78:ILE:O	2.38	0.51
1:A:72:GLN:HE21	1:A:73:PHE:HD2	1.58	0.50
1:A:62:THR:O	1:A:83:LEU:N	2.44	0.50
1:A:61:TYR:HA	1:A:84:VAL:C	2.29	0.50
1:A:75:SER:C	1:A:76:LEU:HD23	2.32	0.50
1:A:10:GLN:O	1:A:13:PHE:N	2.45	0.50
1:A:46:LYS:CE	1:A:48:THR:HG22	2.10	0.49
1:A:31:GLN:OE1	1:A:51:GLU:HA	2.13	0.49
1:A:5:GLU:OE2	1:A:38:GLY:O	2.30	0.49
1:A:27:SER:O	1:A:28:LEU:CD2	2.59	0.49
1:A:29:ASN:CB	1:A:51:GLU:HG2	2.20	0.49
1:A:69:LYS:HD3	1:A:78:ILE:HG21	1.84	0.49
1:A:80:ARG:HH11	1:A:80:ARG:HG2	1.77	0.49
1:A:60:LEU:HD13	1:A:86:ALA:CB	2.27	0.48
1:A:35:VAL:HG13	1:A:45:VAL:CG2	2.44	0.48
1:A:69:LYS:HB2	1:A:76:LEU:C	2.34	0.48
1:A:20:SER:OG	1:A:28:LEU:CD1	2.62	0.48
1:A:26:TYR:CD2	1:A:26:TYR:N	2.80	0.48
1:A:12:GLN:HB3	1:A:13:PHE:HD2	1.78	0.48
1:A:36:ASP:HB2	1:A:43:VAL:C	2.33	0.48
1:A:61:TYR:CA	1:A:83:LEU:CD1	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:VAL:HG11	2:A:91:HOH:O	2.14	0.47
1:A:72:GLN:HB3	1:A:73:PHE:CD1	2.50	0.47
1:A:63:VAL:O	1:A:64:HIS:HB2	2.15	0.47
1:A:16:ARG:O	1:A:16:ARG:CG	2.62	0.47
1:A:20:SER:OG	1:A:28:LEU:HD13	2.14	0.46
1:A:6:ILE:CD1	1:A:81:LEU:HD12	2.46	0.46
1:A:80:ARG:NH1	1:A:82:ARG:HH21	2.04	0.46
1:A:35:VAL:HG12	1:A:47:ILE:HG13	1.97	0.46
1:A:83:LEU:HA	1:A:83:LEU:HD13	1.63	0.46
1:A:31:GLN:HG3	1:A:31:GLN:H	1.19	0.46
1:A:68:PHE:CD1	1:A:77:MET:HE3	2.50	0.46
1:A:6:ILE:HD12	1:A:83:LEU:CD2	2.39	0.46
1:A:5:GLU:HB3	1:A:7:LYS:NZ	2.31	0.46
1:A:10:GLN:HG3	1:A:13:PHE:CZ	2.51	0.46
1:A:42:PRO:O	1:A:43:VAL:HG12	2.15	0.46
1:A:72:GLN:HB3	1:A:73:PHE:CE1	2.48	0.46
1:A:42:PRO:C	1:A:43:VAL:CG1	2.83	0.46
1:A:29:ASN:O	1:A:51:GLU:CG	2.64	0.45
1:A:80:ARG:HG3	1:A:81:LEU:C	2.37	0.45
1:A:62:THR:N	1:A:83:LEU:HD13	2.31	0.45
1:A:7:LYS:HA	1:A:60:LEU:CD2	2.47	0.45
1:A:34:TYR:CZ	1:A:44:LEU:HD21	2.49	0.45
1:A:64:HIS:CB	1:A:66:SER:O	2.63	0.45
1:A:7:LYS:HA	1:A:60:LEU:HD22	1.99	0.45
1:A:39:ASN:CA	1:A:40:GLU:CG	2.95	0.44
1:A:84:VAL:HA	1:A:85:PRO:HD2	1.55	0.44
1:A:37:LEU:H	1:A:43:VAL:C	2.21	0.44
1:A:21:ARG:HG2	1:A:22:GLN:CA	2.46	0.44
1:A:26:TYR:N	1:A:26:TYR:HD2	2.09	0.44
1:A:69:LYS:N	1:A:76:LEU:C	2.69	0.44
1:A:65:LEU:O	1:A:82:ARG:HD2	2.18	0.44
1:A:35:VAL:CG1	1:A:47:ILE:HG13	2.47	0.44
1:A:39:ASN:CA	1:A:40:GLU:HG3	2.48	0.44
1:A:4:VAL:O	1:A:5:GLU:HG3	2.16	0.43
1:A:50:ASP:CB	1:A:53:GLN:CB	2.86	0.43
1:A:21:ARG:CZ	1:A:21:ARG:HB2	2.40	0.43
1:A:86:ALA:C	1:A:87:LYS:NZ	2.66	0.43
1:A:37:LEU:C	1:A:43:VAL:H	2.23	0.43
1:A:80:ARG:O	1:A:81:LEU:C	2.56	0.43
1:A:48:THR:O	1:A:80:ARG:HD2	2.17	0.42
1:A:3:LYS:CB	1:A:62:THR:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:CD	1:A:51:GLU:CA	2.88	0.42
1:A:87:LYS:NZ	1:A:87:LYS:CB	2.77	0.42
1:A:30:GLU:OE2	1:A:30:GLU:C	2.58	0.42
1:A:35:VAL:O	1:A:44:LEU:HA	2.20	0.42
1:A:50:ASP:CG	1:A:53:GLN:HB3	2.35	0.42
1:A:61:TYR:HD2	1:A:83:LEU:HD12	1.77	0.42
1:A:23:GLY:CA	1:A:27:SER:CA	2.76	0.42
1:A:7:LYS:HB3	1:A:60:LEU:HD22	1.96	0.42
1:A:41:TYR:C	1:A:43:VAL:HG13	2.40	0.41
1:A:64:HIS:HB3	1:A:65:LEU:H	1.28	0.41
1:A:48:THR:O	1:A:80:ARG:HD3	2.19	0.41
1:A:57:ALA:HA	1:A:58:PRO:HD3	1.62	0.41
1:A:35:VAL:HG13	1:A:45:VAL:HG22	2.03	0.41
1:A:81:LEU:HA	1:A:81:LEU:HD22	1.48	0.41
1:A:13:PHE:HD2	1:A:13:PHE:N	2.17	0.41
1:A:80:ARG:CB	1:A:80:ARG:HH11	2.31	0.40
1:A:1:MET:HE1	1:A:2:ILE:CG1	2.52	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:1:MET:CA	1:A:76:LEU:CD1[2_565]	1.69	0.51
1:A:2:ILE:CD1	1:A:72:GLN:CG[2_565]	2.04	0.16

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	85/87 (98%)	45 (53%)	20 (24%)	20 (24%)	<div><div>0</div><div>0</div></div>

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	PRO
1	A	15	THR
1	A	16	ARG
1	A	18	GLY
1	A	19	VAL
1	A	24	LYS
1	A	42	PRO
1	A	49	LEU
1	A	53	GLN
1	A	58	PRO
1	A	65	LEU
1	A	66	SER
1	A	70	VAL
1	A	79	ASP
1	A	2	ILE
1	A	44	LEU
1	A	73	PHE
1	A	5	GLU
1	A	35	VAL
1	A	38	GLY

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	76/76 (100%)	32 (42%)	44 (58%)	0 0

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	4	VAL
1	A	5	GLU
1	A	7	LYS
1	A	8	PRO
1	A	13	PHE
1	A	15	THR

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Mol	Chain	Res	Type
1	A	16	ARG
1	A	17	SER
1	A	20	SER
1	A	21	ARG
1	A	22	GLN
1	A	24	LYS
1	A	25	PRO
1	A	29	ASN
1	A	31	GLN
1	A	32	LEU
1	A	37	LEU
1	A	39	ASN
1	A	40	GLU
1	A	41	TYR
1	A	43	VAL
1	A	44	LEU
1	A	46	LYS
1	A	48	THR
1	A	49	LEU
1	A	51	GLU
1	A	53	GLN
1	A	54	PRO
1	A	58	PRO
1	A	60	LEU
1	A	62	THR
1	A	65	LEU
1	A	66	SER
1	A	68	PHE
1	A	69	LYS
1	A	73	PHE
1	A	77	MET
1	A	80	ARG
1	A	81	LEU
1	A	82	ARG
1	A	83	LEU
1	A	84	VAL
1	A	87	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN

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 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](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.