



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:03 PM UTC

PDB ID : 2GN5 / pdb_00002gn5
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 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

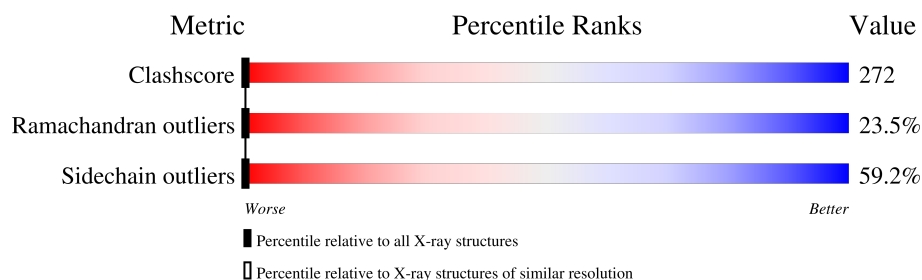
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 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 $\leq 5\%$.

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.

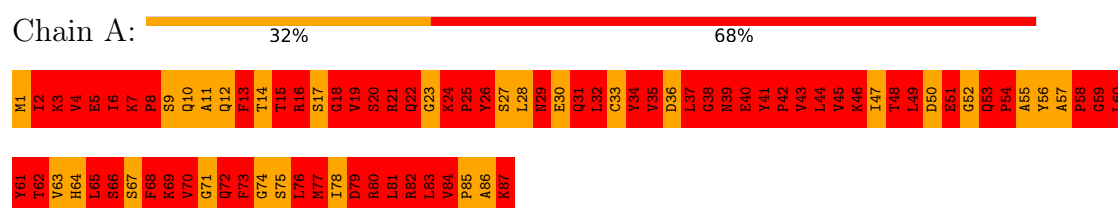
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		

3 Residue-property plots

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. 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. 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



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

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	2.82	60/696 (8.6%)	9.33	467/940 (49.7%)

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 (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	HIS	ND1-CE1	11.30	1.43	1.32
1	A	62	THR	CB-OG1	9.78	1.59	1.43
1	A	62	THR	C-O	9.39	1.34	1.23
1	A	8	PRO	CA-CB	9.18	1.66	1.53
1	A	11	ALA	C-O	8.60	1.34	1.24
1	A	16	ARG	CA-C	8.52	1.64	1.52
1	A	63	VAL	C-N	8.42	1.45	1.33
1	A	62	THR	N-CA	8.13	1.58	1.46
1	A	73	PHE	N-CA	7.95	1.56	1.46
1	A	36	ASP	C-N	-7.81	1.22	1.33
1	A	82	ARG	C-O	7.75	1.33	1.24
1	A	46	LYS	C-O	7.31	1.32	1.24
1	A	62	THR	CA-C	7.19	1.61	1.52
1	A	86	ALA	C-N	7.18	1.43	1.33
1	A	84	VAL	CA-CB	7.00	1.63	1.54
1	A	39	ASN	C-N	-6.99	1.24	1.33
1	A	59	GLY	C-O	6.96	1.33	1.23
1	A	82	ARG	N-CA	-6.93	1.38	1.46
1	A	78	ILE	CA-C	6.73	1.61	1.52
1	A	62	THR	CA-CB	6.68	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	ALA	N-CA	6.66	1.54	1.46
1	A	10	GLN	N-CA	6.61	1.54	1.45
1	A	31	GLN	N-CA	6.57	1.53	1.45
1	A	14	THR	N-CA	6.52	1.53	1.46
1	A	10	GLN	C-O	6.40	1.32	1.23
1	A	79	ASP	N-CA	-6.31	1.38	1.46
1	A	20	SER	N-CA	6.30	1.54	1.46
1	A	54	PRO	CA-C	6.30	1.60	1.52
1	A	16	ARG	NE-CZ	6.27	1.40	1.33
1	A	70	VAL	CA-CB	-6.19	1.46	1.54
1	A	12	GLN	C-N	6.14	1.41	1.33
1	A	75	SER	C-O	6.12	1.31	1.23
1	A	45	VAL	CA-C	6.10	1.60	1.52
1	A	70	VAL	C-O	6.08	1.31	1.24
1	A	71	GLY	N-CA	5.96	1.54	1.45
1	A	26	TYR	C-O	5.91	1.30	1.23
1	A	63	VAL	C-O	5.87	1.29	1.24
1	A	6	ILE	N-CA	5.84	1.53	1.46
1	A	12	GLN	N-CA	5.83	1.53	1.46
1	A	54	PRO	N-CA	-5.82	1.40	1.47
1	A	22	GLN	CA-C	5.79	1.59	1.52
1	A	41	TYR	CA-C	5.76	1.59	1.53
1	A	16	ARG	CZ-NH2	5.74	1.41	1.33
1	A	70	VAL	N-CA	5.66	1.53	1.46
1	A	72	GLN	C-O	5.62	1.31	1.24
1	A	59	GLY	C-N	-5.58	1.25	1.33
1	A	19	VAL	C-O	5.57	1.30	1.24
1	A	61	TYR	C-O	5.53	1.30	1.23
1	A	50	ASP	CA-C	-5.53	1.45	1.52
1	A	47	ILE	C-O	5.52	1.30	1.24
1	A	34	TYR	CA-C	5.50	1.60	1.53
1	A	28	LEU	CA-CB	5.44	1.60	1.52
1	A	86	ALA	C-O	5.40	1.30	1.23
1	A	52	GLY	C-O	-5.38	1.16	1.23
1	A	14	THR	CB-OG1	5.29	1.52	1.43
1	A	21	ARG	CA-C	5.23	1.59	1.52
1	A	63	VAL	CA-CB	5.16	1.59	1.54
1	A	29	ASN	CA-CB	5.12	1.59	1.52
1	A	9	SER	N-CA	-5.12	1.39	1.46
1	A	86	ALA	CA-C	5.11	1.59	1.52

All (467) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ARG	CA-C-N	39.09	179.94	122.09
1	A	82	ARG	C-N-CA	39.09	179.94	122.09
1	A	10	GLN	OE1-CD-NE2	-35.94	86.66	122.60
1	A	16	ARG	CD-NE-CZ	33.78	171.69	124.40
1	A	82	ARG	O-C-N	-32.93	80.33	123.14
1	A	60	LEU	CA-C-O	31.92	166.16	120.51
1	A	73	PHE	CA-C-N	31.52	150.34	122.29
1	A	73	PHE	C-N-CA	31.52	150.34	122.29
1	A	39	ASN	CA-C-N	30.59	179.96	121.54
1	A	39	ASN	C-N-CA	30.59	179.96	121.54
1	A	15	THR	CA-C-N	30.59	179.96	121.54
1	A	15	THR	C-N-CA	30.59	179.96	121.54
1	A	59	GLY	O-C-N	-30.42	83.16	122.70
1	A	78	ILE	CA-C-N	29.83	178.51	121.54
1	A	78	ILE	C-N-CA	29.83	178.51	121.54
1	A	82	ARG	CA-C-O	29.43	157.34	120.25
1	A	62	THR	CA-C-N	28.44	159.73	120.49
1	A	62	THR	C-N-CA	28.44	159.73	120.49
1	A	10	GLN	CG-CD-NE2	28.07	158.51	116.40
1	A	37	LEU	CA-C-O	27.43	153.52	120.60
1	A	53	GLN	CB-CG-CD	27.32	159.05	112.60
1	A	26	TYR	CA-C-O	-25.82	88.09	120.89
1	A	10	GLN	CB-CG-CD	25.49	155.93	112.60
1	A	65	LEU	O-C-N	-25.43	88.77	122.59
1	A	21	ARG	CD-NE-CZ	25.03	159.45	124.40
1	A	81	LEU	CA-C-N	25.01	158.70	122.44
1	A	81	LEU	C-N-CA	25.01	158.70	122.44
1	A	60	LEU	CA-C-N	24.65	162.56	122.87
1	A	60	LEU	C-N-CA	24.65	162.56	122.87
1	A	65	LEU	CA-C-O	24.47	155.50	120.51
1	A	34	TYR	CA-CB-CG	24.35	157.74	113.90
1	A	31	GLN	OE1-CD-NE2	-24.11	98.49	122.60
1	A	83	LEU	CA-C-O	23.94	148.45	120.92
1	A	43	VAL	N-CA-C	22.91	140.29	107.75
1	A	66	SER	CA-CB-OG	22.52	156.14	111.10
1	A	60	LEU	O-C-N	-22.18	93.09	122.59
1	A	52	GLY	CA-C-O	22.16	159.13	120.57
1	A	16	ARG	NE-CZ-NH1	-21.96	99.54	121.50
1	A	62	THR	CA-C-O	21.70	143.49	121.14
1	A	12	GLN	OE1-CD-NE2	-21.61	100.99	122.60
1	A	8	PRO	N-CA-CB	-20.79	81.42	103.25
1	A	36	ASP	CA-CB-CG	20.58	133.18	112.60
1	A	77	MET	N-CA-CB	20.16	139.90	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	GLY	N-CA-C	20.08	150.89	111.34
1	A	6	ILE	O-C-N	-20.02	97.54	122.57
1	A	63	VAL	CA-C-O	19.97	144.65	121.28
1	A	64	HIS	CA-CB-CG	19.85	133.65	113.80
1	A	21	ARG	CA-C-N	19.13	155.17	121.89
1	A	21	ARG	C-N-CA	19.13	155.17	121.89
1	A	61	TYR	CA-C-O	-19.06	99.62	121.16
1	A	79	ASP	CB-CA-C	19.02	148.28	110.42
1	A	15	THR	CA-CB-OG1	18.71	137.67	109.60
1	A	78	ILE	CA-C-O	18.65	144.09	120.78
1	A	39	ASN	CB-CG-ND2	18.59	144.29	116.40
1	A	15	THR	O-C-N	-18.43	98.08	122.59
1	A	77	MET	N-CA-C	-18.12	91.31	113.41
1	A	62	THR	O-C-N	-18.09	99.39	122.73
1	A	40	GLU	N-CA-CB	-17.94	80.17	110.49
1	A	65	LEU	CA-C-N	17.65	155.26	121.54
1	A	65	LEU	C-N-CA	17.65	155.26	121.54
1	A	31	GLN	CB-CA-C	17.64	140.70	109.83
1	A	11	ALA	CB-CA-C	-17.29	76.92	110.46
1	A	82	ARG	CD-NE-CZ	17.28	148.59	124.40
1	A	68	PHE	CA-CB-CG	17.16	130.96	113.80
1	A	43	VAL	CA-C-O	17.10	135.11	121.09
1	A	50	ASP	CA-C-O	16.97	139.03	120.70
1	A	43	VAL	CA-C-N	16.83	153.68	121.54
1	A	43	VAL	C-N-CA	16.83	153.68	121.54
1	A	56	TYR	O-C-N	16.81	141.89	123.06
1	A	73	PHE	O-C-N	-16.64	100.46	122.59
1	A	29	ASN	OD1-CG-ND2	-16.59	106.01	122.60
1	A	39	ASN	O-C-N	-16.51	100.63	122.59
1	A	53	GLN	CG-CD-NE2	-16.46	91.71	116.40
1	A	19	VAL	CA-C-O	-16.42	100.25	120.78
1	A	28	LEU	N-CA-C	16.42	134.65	107.23
1	A	61	TYR	O-C-N	16.28	143.68	123.16
1	A	75	SER	CA-CB-OG	16.25	143.60	111.10
1	A	39	ASN	CB-CA-C	15.97	142.19	110.42
1	A	12	GLN	CG-CD-OE1	15.92	152.63	120.80
1	A	78	ILE	N-CA-CB	15.84	137.36	111.23
1	A	5	GLU	N-CA-C	15.83	144.52	110.80
1	A	15	THR	N-CA-CB	-15.79	83.81	110.49
1	A	22	GLN	CB-CG-CD	15.75	139.37	112.60
1	A	31	GLN	CG-CD-OE1	15.63	152.07	120.80
1	A	57	ALA	N-CA-CB	-15.56	87.41	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	PHE	N-CA-CB	-15.55	84.20	110.49
1	A	56	TYR	N-CA-C	-15.50	85.68	110.32
1	A	41	TYR	CA-C-O	15.32	133.67	119.72
1	A	8	PRO	N-CA-C	15.25	143.88	112.47
1	A	30	GLU	CA-C-O	-15.17	93.93	121.09
1	A	15	THR	CA-C-O	15.15	142.18	120.51
1	A	62	THR	CA-CB-CG2	15.08	136.14	110.50
1	A	64	HIS	O-C-N	-14.92	102.74	122.59
1	A	4	VAL	CA-C-O	-14.88	100.98	119.43
1	A	77	MET	O-C-N	14.79	143.37	122.36
1	A	63	VAL	N-CA-C	14.72	130.56	109.51
1	A	10	GLN	N-CA-C	-14.59	90.86	110.55
1	A	62	THR	N-CA-CB	14.50	136.57	110.76
1	A	32	LEU	CD1-CG-CD2	-14.49	78.93	110.80
1	A	44	LEU	CA-C-O	14.35	141.03	120.51
1	A	50	ASP	CB-CG-OD1	-14.24	85.64	118.40
1	A	79	ASP	CA-CB-CG	-14.15	98.45	112.60
1	A	77	MET	CA-CB-CG	-14.02	86.06	114.10
1	A	22	GLN	OE1-CD-NE2	-13.98	108.62	122.60
1	A	41	TYR	CA-CB-CG	13.93	138.97	113.90
1	A	53	GLN	CA-CB-CG	13.83	141.77	114.10
1	A	7	LYS	N-CA-C	-13.76	79.41	109.81
1	A	21	ARG	N-CA-CB	13.68	133.61	110.49
1	A	87	LYS	N-CA-CB	13.67	133.74	110.50
1	A	59	GLY	CA-C-O	-13.61	96.89	120.57
1	A	87	LYS	CB-CG-CD	13.53	142.41	111.30
1	A	75	SER	N-CA-C	-13.41	90.63	110.48
1	A	52	GLY	CA-C-N	13.37	154.42	121.80
1	A	52	GLY	C-N-CA	13.37	154.42	121.80
1	A	48	THR	CB-CA-C	13.25	131.24	111.76
1	A	16	ARG	NH1-CZ-NH2	13.22	136.49	119.30
1	A	40	GLU	O-C-N	-13.17	105.07	122.59
1	A	68	PHE	CB-CA-C	13.12	133.72	110.36
1	A	12	GLN	CB-CG-CD	13.07	134.82	112.60
1	A	46	LYS	O-C-N	13.03	138.38	123.27
1	A	28	LEU	N-CA-CB	-12.94	89.70	110.79
1	A	64	HIS	CB-CA-C	-12.92	84.70	110.42
1	A	53	GLN	CG-CD-OE1	12.90	146.60	120.80
1	A	22	GLN	N-CA-CB	12.85	132.04	110.71
1	A	28	LEU	CA-C-O	12.85	136.21	120.27
1	A	2	ILE	CA-C-N	12.83	146.04	121.54
1	A	2	ILE	C-N-CA	12.83	146.04	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	TYR	N-CA-CB	-12.82	90.34	110.85
1	A	57	ALA	CA-C-O	12.73	132.41	121.08
1	A	84	VAL	CA-C-N	12.67	132.82	119.90
1	A	84	VAL	C-N-CA	12.67	132.82	119.90
1	A	52	GLY	O-C-N	-12.60	106.32	122.70
1	A	78	ILE	N-CA-C	-12.54	83.25	109.34
1	A	48	THR	CA-C-N	12.52	145.45	121.54
1	A	48	THR	C-N-CA	12.52	145.45	121.54
1	A	39	ASN	CB-CG-OD1	-12.43	95.95	120.80
1	A	53	GLN	CA-C-N	12.41	134.01	120.11
1	A	53	GLN	C-N-CA	12.41	134.01	120.11
1	A	8	PRO	CA-C-N	12.38	141.09	122.77
1	A	8	PRO	C-N-CA	12.38	141.09	122.77
1	A	50	ASP	CB-CG-OD2	12.30	146.69	118.40
1	A	12	GLN	CB-CA-C	-12.26	90.44	110.79
1	A	84	VAL	N-CA-CB	-12.25	94.07	111.21
1	A	64	HIS	N-CA-CB	12.20	131.11	110.49
1	A	43	VAL	O-C-N	-12.19	110.00	122.67
1	A	22	GLN	O-C-N	12.11	138.34	123.44
1	A	22	GLN	CG-CD-OE1	12.08	144.96	120.80
1	A	76	LEU	CA-C-O	12.07	134.54	120.66
1	A	2	ILE	CA-C-O	12.04	135.83	120.78
1	A	37	LEU	N-CA-CB	-11.97	89.70	111.13
1	A	33	CYS	O-C-N	11.84	137.26	123.41
1	A	7	LYS	N-CA-CB	11.79	131.35	110.37
1	A	40	GLU	CB-CG-CD	11.76	132.59	112.60
1	A	37	LEU	O-C-N	-11.70	109.18	123.33
1	A	63	VAL	O-C-N	-11.68	110.25	122.75
1	A	66	SER	N-CA-C	-11.66	85.96	110.80
1	A	17	SER	N-CA-C	11.64	131.58	108.18
1	A	44	LEU	O-C-N	-11.64	107.11	122.59
1	A	59	GLY	N-CA-C	11.57	140.61	113.18
1	A	77	MET	CA-C-O	-11.50	106.42	119.41
1	A	3	LYS	CB-CG-CD	11.50	137.75	111.30
1	A	73	PHE	CA-C-O	11.49	136.94	120.51
1	A	39	ASN	N-CA-CB	-11.38	91.27	110.49
1	A	31	GLN	O-C-N	11.35	135.66	122.94
1	A	34	TYR	N-CA-C	-11.34	95.56	110.53
1	A	84	VAL	CA-CB-CG2	11.25	129.53	110.40
1	A	37	LEU	N-CA-C	11.21	128.12	109.06
1	A	79	ASP	CB-CG-OD1	11.16	144.08	118.40
1	A	65	LEU	CB-CA-C	11.15	132.60	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	LYS	O-C-N	11.11	134.09	121.32
1	A	2	ILE	N-CA-C	11.07	132.36	109.34
1	A	57	ALA	CA-C-N	11.03	133.63	119.84
1	A	57	ALA	C-N-CA	11.03	133.63	119.84
1	A	44	LEU	CA-C-N	11.00	138.76	122.92
1	A	44	LEU	C-N-CA	11.00	138.76	122.92
1	A	63	VAL	N-CA-CB	-10.91	92.57	110.14
1	A	80	ARG	N-CA-C	10.86	126.04	108.99
1	A	44	LEU	CD1-CG-CD2	-10.80	87.05	110.80
1	A	5	GLU	OE1-CD-OE2	10.74	148.69	122.90
1	A	27	SER	CB-CA-C	-10.73	91.89	110.45
1	A	80	ARG	NH1-CZ-NH2	10.72	133.24	119.30
1	A	4	VAL	CA-CB-CG2	10.57	128.37	110.40
1	A	51	GLU	CG-CD-OE1	10.57	142.71	118.40
1	A	64	HIS	CA-C-N	10.48	141.56	121.54
1	A	64	HIS	C-N-CA	10.48	141.56	121.54
1	A	16	ARG	CB-CG-CD	10.46	135.36	111.30
1	A	35	VAL	CA-C-O	10.45	133.84	120.78
1	A	78	ILE	O-C-N	-10.40	109.57	122.57
1	A	58	PRO	N-CA-CB	-10.31	92.42	103.25
1	A	80	ARG	CA-C-N	-10.24	106.39	120.82
1	A	80	ARG	C-N-CA	-10.24	106.39	120.82
1	A	81	LEU	N-CA-CB	10.12	125.17	109.69
1	A	80	ARG	NE-CZ-NH1	-10.08	111.42	121.50
1	A	6	ILE	CA-CB-CG2	-10.06	93.40	110.50
1	A	20	SER	O-C-N	-9.96	109.35	122.59
1	A	38	GLY	O-C-N	9.93	135.61	122.70
1	A	51	GLU	CB-CA-C	9.92	127.98	111.31
1	A	70	VAL	CA-C-N	-9.78	102.24	121.41
1	A	70	VAL	C-N-CA	-9.78	102.24	121.41
1	A	12	GLN	CA-C-N	-9.74	107.55	122.16
1	A	12	GLN	C-N-CA	-9.74	107.55	122.16
1	A	78	ILE	CB-CA-C	-9.71	95.36	111.29
1	A	5	GLU	CA-C-N	9.68	139.40	121.97
1	A	5	GLU	C-N-CA	9.68	139.40	121.97
1	A	12	GLN	CA-C-O	9.68	130.81	120.55
1	A	76	LEU	CB-CA-C	9.68	128.52	109.35
1	A	73	PHE	CA-CB-CG	-9.66	104.14	113.80
1	A	6	ILE	CA-C-N	9.64	145.32	121.80
1	A	6	ILE	C-N-CA	9.64	145.32	121.80
1	A	30	GLU	CA-CB-CG	-9.62	94.86	114.10
1	A	43	VAL	CA-CB-CG1	9.61	126.74	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	THR	OG1-CB-CG2	-9.54	90.22	109.30
1	A	24	LYS	CG-CD-CE	9.51	133.17	111.30
1	A	4	VAL	CA-CB-CG1	-9.49	94.27	110.40
1	A	39	ASN	CA-CB-CG	9.45	122.05	112.60
1	A	43	VAL	CA-CB-CG2	-9.41	94.40	110.40
1	A	37	LEU	CA-CB-CG	9.40	149.21	116.30
1	A	14	THR	CB-CA-C	9.40	125.78	110.37
1	A	12	GLN	CA-CB-CG	9.39	132.88	114.10
1	A	18	GLY	N-CA-C	9.39	135.44	113.18
1	A	74	GLY	CA-C-O	-9.34	112.78	120.81
1	A	32	LEU	O-C-N	-9.33	112.04	123.33
1	A	55	ALA	CA-C-O	9.30	132.79	121.81
1	A	13	PHE	N-CA-CB	9.30	123.12	110.57
1	A	29	ASN	O-C-N	-9.29	110.36	122.43
1	A	71	GLY	O-C-N	9.29	134.77	122.70
1	A	58	PRO	CB-CG-CD	-9.28	76.42	106.10
1	A	30	GLU	CG-CD-OE2	-9.27	97.07	118.40
1	A	85	PRO	CA-C-N	-9.15	107.92	120.82
1	A	85	PRO	C-N-CA	-9.15	107.92	120.82
1	A	29	ASN	CB-CG-ND2	9.13	130.09	116.40
1	A	45	VAL	CA-CB-CG1	9.12	125.89	110.40
1	A	84	VAL	CG1-CB-CG2	-9.09	90.81	110.80
1	A	34	TYR	CB-CA-C	9.08	128.30	109.68
1	A	65	LEU	N-CA-C	-9.06	91.49	110.80
1	A	10	GLN	CB-CA-C	9.03	127.72	109.76
1	A	48	THR	CA-CB-CG2	8.91	125.65	110.50
1	A	9	SER	CA-CB-OG	-8.89	93.32	111.10
1	A	19	VAL	N-CA-CB	8.89	125.90	111.23
1	A	1	MET	N-CA-CB	8.86	125.57	110.50
1	A	35	VAL	N-CA-CB	8.86	125.85	111.23
1	A	75	SER	CB-CA-C	8.85	125.74	109.46
1	A	85	PRO	CB-CA-C	-8.84	100.34	111.56
1	A	70	VAL	CB-CA-C	8.80	125.72	111.29
1	A	80	ARG	O-C-N	8.75	133.21	123.33
1	A	17	SER	CA-CB-OG	8.73	128.57	111.10
1	A	41	TYR	N-CA-CB	8.72	136.12	110.48
1	A	64	HIS	CA-C-O	8.72	132.98	120.51
1	A	37	LEU	CD1-CG-CD2	8.68	129.89	110.80
1	A	2	ILE	O-C-N	-8.68	111.73	122.57
1	A	7	LYS	CA-C-N	-8.65	109.03	119.84
1	A	7	LYS	C-N-CA	-8.65	109.03	119.84
1	A	57	ALA	O-C-N	-8.64	114.92	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ILE	O-C-N	-8.64	113.22	122.81
1	A	6	ILE	CA-CB-CG1	8.63	125.07	110.40
1	A	22	GLN	CA-C-N	8.63	138.32	121.41
1	A	22	GLN	C-N-CA	8.63	138.32	121.41
1	A	86	ALA	N-CA-CB	8.61	122.86	109.69
1	A	7	LYS	CA-CB-CG	8.59	131.28	114.10
1	A	33	CYS	CA-CB-SG	8.59	134.15	114.40
1	A	36	ASP	OD1-CG-OD2	8.57	143.47	122.90
1	A	5	GLU	N-CA-CB	-8.56	96.02	110.49
1	A	86	ALA	CB-CA-C	8.55	123.24	109.90
1	A	30	GLU	CB-CG-CD	-8.53	98.11	112.60
1	A	37	LEU	CA-C-N	8.46	138.00	121.41
1	A	37	LEU	C-N-CA	8.46	138.00	121.41
1	A	31	GLN	N-CA-C	-8.42	98.05	110.52
1	A	7	LYS	CB-CA-C	8.38	126.67	110.17
1	A	38	GLY	CA-C-N	-8.34	105.61	121.54
1	A	38	GLY	C-N-CA	-8.34	105.61	121.54
1	A	40	GLU	CB-CA-C	8.34	127.01	110.42
1	A	3	LYS	CG-CD-CE	8.30	130.39	111.30
1	A	69	LYS	N-CA-C	8.30	128.47	110.80
1	A	74	GLY	CA-C-N	-8.30	107.62	121.39
1	A	74	GLY	C-N-CA	-8.30	107.62	121.39
1	A	21	ARG	CA-C-O	8.29	132.36	120.51
1	A	3	LYS	CD-CE-NZ	8.27	138.37	111.90
1	A	69	LYS	N-CA-CB	-8.27	96.52	110.49
1	A	9	SER	CA-C-O	8.25	130.63	121.39
1	A	66	SER	CA-C-N	8.24	137.28	121.54
1	A	66	SER	C-N-CA	8.24	137.28	121.54
1	A	8	PRO	CB-CA-C	-8.23	97.98	111.56
1	A	17	SER	CB-CA-C	-8.22	98.13	111.86
1	A	4	VAL	N-CA-CB	8.22	134.19	111.75
1	A	27	SER	O-C-N	-8.20	113.33	122.84
1	A	65	LEU	CA-CB-CG	8.19	144.96	116.30
1	A	25	PRO	CA-C-N	8.19	136.85	121.87
1	A	25	PRO	C-N-CA	8.19	136.85	121.87
1	A	36	ASP	CA-C-O	8.16	129.86	120.89
1	A	79	ASP	OD1-CG-OD2	-8.15	103.33	122.90
1	A	33	CYS	CA-C-O	-8.13	110.54	120.54
1	A	56	TYR	N-CA-CB	8.11	123.62	110.41
1	A	63	VAL	CB-CA-C	8.08	124.84	111.51
1	A	83	LEU	CD1-CG-CD2	8.06	128.53	110.80
1	A	52	GLY	N-CA-C	-8.05	94.09	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ARG	NE-CZ-NH1	-8.03	113.47	121.50
1	A	47	ILE	CA-CB-CG1	8.00	123.99	110.40
1	A	2	ILE	N-CA-CB	-7.99	98.05	111.23
1	A	2	ILE	CA-CB-CG1	-7.98	96.83	110.40
1	A	85	PRO	CA-C-O	-7.96	112.37	121.36
1	A	31	GLN	N-CA-CB	-7.95	97.74	110.46
1	A	63	VAL	CG1-CB-CG2	-7.95	93.32	110.80
1	A	64	HIS	ND1-CG-CD2	7.85	113.95	106.10
1	A	51	GLU	CA-CB-CG	7.84	129.79	114.10
1	A	17	SER	CA-C-O	7.82	137.25	122.62
1	A	32	LEU	CA-CB-CG	7.80	143.62	116.30
1	A	27	SER	CA-CB-OG	7.80	126.70	111.10
1	A	55	ALA	CB-CA-C	7.74	125.15	109.76
1	A	68	PHE	N-CA-C	-7.73	98.78	110.14
1	A	73	PHE	CB-CG-CD1	7.70	133.80	120.70
1	A	85	PRO	O-C-N	7.70	132.66	122.89
1	A	17	SER	CA-C-N	7.69	136.48	121.41
1	A	17	SER	C-N-CA	7.69	136.48	121.41
1	A	24	LYS	CB-CA-C	7.61	125.17	110.17
1	A	80	ARG	CA-C-O	-7.60	112.48	120.99
1	A	27	SER	N-CA-C	7.57	121.66	110.46
1	A	80	ARG	CB-CA-C	-7.55	93.86	109.94
1	A	82	ARG	N-CA-CB	7.54	122.66	110.90
1	A	44	LEU	CB-CG-CD2	7.52	133.27	110.70
1	A	32	LEU	N-CA-C	7.52	121.84	109.06
1	A	59	GLY	CA-C-N	7.49	135.85	121.54
1	A	59	GLY	C-N-CA	7.49	135.85	121.54
1	A	71	GLY	N-CA-C	-7.49	95.43	113.18
1	A	84	VAL	CB-CA-C	7.46	124.95	111.36
1	A	72	GLN	CA-CB-CG	7.43	128.96	114.10
1	A	26	TYR	O-C-N	7.42	131.89	123.28
1	A	72	GLN	O-C-N	7.42	132.46	122.59
1	A	36	ASP	CB-CA-C	7.42	123.73	110.16
1	A	12	GLN	N-CA-CB	7.38	120.97	110.12
1	A	85	PRO	CA-N-CD	-7.36	101.70	112.00
1	A	34	TYR	N-CA-CB	7.35	120.87	110.36
1	A	9	SER	CA-C-N	-7.34	105.91	121.32
1	A	9	SER	C-N-CA	-7.34	105.91	121.32
1	A	24	LYS	CA-CB-CG	7.33	128.76	114.10
1	A	76	LEU	O-C-N	-7.30	114.36	123.27
1	A	70	VAL	CA-C-O	7.29	129.89	120.78
1	A	60	LEU	CB-CG-CD1	7.21	132.33	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	ALA	CA-C-N	-7.20	108.74	121.70
1	A	86	ALA	C-N-CA	-7.20	108.74	121.70
1	A	27	SER	CA-C-O	7.19	131.02	121.89
1	A	48	THR	CA-CB-OG1	-7.15	98.87	109.60
1	A	5	GLU	O-C-N	-7.04	113.23	122.59
1	A	82	ARG	CB-CA-C	-7.02	100.37	110.62
1	A	19	VAL	CA-CB-CG2	7.01	122.31	110.40
1	A	16	ARG	O-C-N	-6.96	113.33	122.59
1	A	24	LYS	N-CA-C	-6.94	94.47	109.81
1	A	58	PRO	CB-CA-C	6.92	122.99	111.56
1	A	7	LYS	CA-C-O	-6.92	110.69	120.16
1	A	32	LEU	CA-C-O	6.87	128.84	120.60
1	A	18	GLY	CA-C-O	6.83	132.46	120.57
1	A	24	LYS	CA-C-O	-6.83	110.81	120.16
1	A	20	SER	CA-C-N	6.82	134.57	121.54
1	A	20	SER	C-N-CA	6.82	134.57	121.54
1	A	6	ILE	CB-CA-C	-6.81	100.12	111.29
1	A	43	VAL	CB-CA-C	-6.80	101.81	111.40
1	A	54	PRO	CA-C-O	6.74	132.02	122.31
1	A	73	PHE	CB-CA-C	6.73	123.81	110.42
1	A	79	ASP	CA-C-O	-6.70	110.92	120.51
1	A	47	ILE	N-CA-CB	-6.70	103.23	110.53
1	A	10	GLN	O-C-N	6.68	130.47	122.85
1	A	58	PRO	CA-N-CD	-6.68	102.64	112.00
1	A	12	GLN	CG-CD-NE2	-6.68	106.38	116.40
1	A	22	GLN	CG-CD-NE2	-6.66	106.41	116.40
1	A	26	TYR	CB-CG-CD1	6.66	130.78	120.80
1	A	66	SER	N-CA-CB	6.64	121.71	110.49
1	A	9	SER	N-CA-CB	6.63	121.54	110.53
1	A	58	PRO	N-CA-C	6.63	126.12	112.47
1	A	42	PRO	CA-C-N	-6.62	114.70	122.11
1	A	42	PRO	C-N-CA	-6.62	114.70	122.11
1	A	60	LEU	CA-CB-CG	6.60	139.39	116.30
1	A	29	ASN	CA-CB-CG	-6.59	106.01	112.60
1	A	62	THR	CA-CB-OG1	6.57	119.46	109.60
1	A	75	SER	O-C-N	6.53	130.34	122.96
1	A	5	GLU	CG-CD-OE2	-6.51	103.43	118.40
1	A	84	VAL	CA-CB-CG1	6.51	121.46	110.40
1	A	86	ALA	CA-C-O	6.46	128.29	120.92
1	A	21	ARG	NE-CZ-NH1	6.37	127.87	121.50
1	A	53	GLN	CB-CA-C	6.36	122.70	110.17
1	A	81	LEU	CA-C-O	-6.36	113.67	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	GLU	N-CA-C	-6.35	95.93	107.75
1	A	48	THR	N-CA-C	-6.35	95.64	107.71
1	A	15	THR	CA-CB-CG2	-6.35	99.71	110.50
1	A	64	HIS	N-CA-C	-6.33	97.33	110.80
1	A	72	GLN	CA-C-N	-6.30	109.50	121.54
1	A	72	GLN	C-N-CA	-6.30	109.50	121.54
1	A	56	TYR	CA-C-N	-6.30	112.42	124.01
1	A	56	TYR	C-N-CA	-6.30	112.42	124.01
1	A	67	SER	N-CA-C	6.30	124.21	110.80
1	A	47	ILE	CB-CG1-CD1	6.29	127.02	113.80
1	A	66	SER	O-C-N	6.25	130.91	122.59
1	A	8	PRO	CA-C-O	6.24	131.95	120.60
1	A	20	SER	N-CA-C	6.22	124.05	110.80
1	A	68	PHE	N-CA-CB	6.21	119.95	110.70
1	A	46	LYS	N-CA-CB	6.18	120.29	110.65
1	A	11	ALA	O-C-N	6.18	129.24	122.20
1	A	26	TYR	CG-CD1-CE1	6.16	130.44	121.20
1	A	47	ILE	N-CA-C	-6.16	100.76	108.89
1	A	5	GLU	CA-C-O	6.13	129.28	120.51
1	A	39	ASN	CA-C-O	6.12	129.26	120.51
1	A	48	THR	O-C-N	-6.07	114.92	122.82
1	A	51	GLU	CG-CD-OE2	-6.06	104.45	118.40
1	A	20	SER	N-CA-CB	-6.05	100.27	110.49
1	A	16	ARG	N-CA-C	6.03	123.64	110.80
1	A	68	PHE	CD1-CG-CD2	-6.03	109.56	118.60
1	A	44	LEU	N-CA-CB	6.02	120.66	110.49
1	A	37	LEU	CB-CA-C	6.01	121.58	109.38
1	A	32	LEU	CB-CA-C	6.01	121.58	109.38
1	A	69	LYS	CA-CB-CG	-6.00	102.11	114.10
1	A	14	THR	N-CA-C	-5.99	105.05	112.72
1	A	5	GLU	CB-CA-C	-5.97	98.53	110.42
1	A	32	LEU	N-CA-CB	-5.96	100.46	111.13
1	A	82	ARG	NE-CZ-NH2	5.96	124.56	119.20
1	A	13	PHE	CD1-CE1-CZ	5.93	130.67	120.00
1	A	77	MET	CA-C-N	-5.90	111.35	121.97
1	A	77	MET	C-N-CA	-5.90	111.35	121.97
1	A	64	HIS	CG-ND1-CE1	-5.88	99.30	109.30
1	A	33	CYS	CA-C-N	5.88	131.66	120.97
1	A	33	CYS	C-N-CA	5.88	131.66	120.97
1	A	5	GLU	CA-CB-CG	5.86	125.81	114.10
1	A	14	THR	CA-C-N	-5.84	110.39	121.54
1	A	14	THR	C-N-CA	-5.84	110.39	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	LEU	CB-CA-C	-5.82	98.84	110.42
1	A	5	GLU	CG-CD-OE1	-5.80	105.05	118.40
1	A	27	SER	N-CA-CB	5.79	119.44	110.46
1	A	25	PRO	CA-C-O	5.79	131.13	120.60
1	A	36	ASP	N-CA-C	5.79	117.90	108.76
1	A	73	PHE	CB-CG-CD2	-5.78	110.88	120.70
1	A	60	LEU	CB-CG-CD2	-5.72	93.53	110.70
1	A	3	LYS	CA-C-N	5.70	130.49	121.09
1	A	3	LYS	C-N-CA	5.70	130.49	121.09
1	A	43	VAL	N-CA-CB	-5.68	101.58	110.96
1	A	28	LEU	CA-C-N	5.68	131.43	122.34
1	A	28	LEU	C-N-CA	5.68	131.43	122.34
1	A	54	PRO	CA-C-N	-5.66	109.44	121.32
1	A	54	PRO	C-N-CA	-5.66	109.44	121.32
1	A	50	ASP	O-C-N	-5.65	115.88	123.23
1	A	46	LYS	CB-CA-C	-5.63	100.82	110.16
1	A	50	ASP	N-CA-CB	-5.54	101.19	110.83
1	A	45	VAL	CA-C-N	5.52	130.78	123.00
1	A	45	VAL	C-N-CA	5.52	130.78	123.00
1	A	85	PRO	CA-CB-CG	5.50	114.95	104.50
1	A	30	GLU	OE1-CD-OE2	5.47	136.03	122.90
1	A	13	PHE	CG-CD1-CE1	-5.45	111.43	120.70
1	A	49	LEU	CA-C-O	5.45	128.30	120.51
1	A	67	SER	CB-CA-C	-5.44	99.59	110.42
1	A	22	GLN	CA-C-O	-5.40	112.92	120.21
1	A	7	LYS	CD-CE-NZ	-5.39	94.66	111.90
1	A	18	GLY	O-C-N	-5.38	115.70	122.70
1	A	21	ARG	CB-CA-C	-5.35	99.78	110.42
1	A	63	VAL	CA-CB-CG2	5.34	119.48	110.40
1	A	21	ARG	CB-CG-CD	5.34	123.58	111.30
1	A	40	GLU	CA-CB-CG	5.33	124.77	114.10
1	A	36	ASP	CB-CG-OD2	-5.33	106.14	118.40
1	A	47	ILE	CG1-CB-CG2	-5.31	94.76	110.70
1	A	2	ILE	CA-CB-CG2	5.30	119.51	110.50
1	A	6	ILE	CB-CG1-CD1	5.29	124.91	113.80
1	A	10	GLN	N-CA-CB	5.28	118.47	110.45
1	A	2	ILE	CB-CA-C	5.27	119.94	111.29
1	A	21	ARG	O-C-N	-5.21	115.66	122.59
1	A	29	ASN	N-CA-CB	5.18	118.16	110.49
1	A	62	THR	N-CA-C	-5.18	101.92	108.45
1	A	64	HIS	ND1-CE1-NE2	5.17	113.56	108.40
1	A	23	GLY	O-C-N	5.16	129.41	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	LYS	CG-CD-CE	-5.13	99.49	111.30
1	A	38	GLY	N-CA-C	-5.12	101.04	113.18
1	A	61	TYR	N-CA-C	5.06	118.00	109.95
1	A	79	ASP	N-CA-CB	-5.01	102.03	110.49

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
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

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	692	374	2
2	A	12	0	0	1	0
All	All	694	0	692	374	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 272.

All (374) 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:14:THR:C	1:A:15:THR:HG22	1.63	1.19
1:A:46:LYS:CE	1:A:48:THR:HG21	1.73	1.19
1:A:46:LYS:NZ	1:A:48:THR:HG21	1.57	1.17
1:A:50:ASP:HB2	1:A:53:GLN:CD	1.70	1.15
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:HZ1	1:A:87:LYS:CA	1.58	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:HZ1	1:A:87:LYS:N	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:39:ASN:C	1:A:40:GLU:HG2	1.70	1.11
1:A:1:MET:HE2	1:A:2:ILE:CG1	1.81	1.10
1:A:14:THR:O	1:A:15:THR:CG2	2.00	1.10
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: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:61:TYR:HA	1:A:84:VAL:O	1.51	1.08
1:A:72:GLN:CB	1:A:73:PHE:CE2	2.36	1.08
1:A:35:VAL:HG22	1:A:36:ASP:N	1.58	1.07
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:62:THR:N	1:A:84:VAL:O	1.89	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:50:ASP:CG	1:A:53:GLN:HG2	1.83	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:CD2	1:A:73:PHE:N	2.25	1.00
1:A:1:MET:HE2	1:A:2:ILE:HG13	1.03	1.00
1:A:25:PRO:C	1:A:26:TYR:HD2	1.69	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:15:THR:HG21	1:A:33:CYS:SG	2.03	0.98
1:A:18:GLY:HA2	1:A:30:GLU:O	1.62	0.98
1:A:24:LYS:HD3	1:A:25:PRO:CD	1.92	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:39:ASN:C	1:A:40:GLU:CG	2.39	0.95
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: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:68:PHE:CD1	1:A:77:MET:HE3	2.03	0.93
1:A:7:LYS:HB3	1:A:60:LEU:HD23	1.50	0.93
1:A:34:TYR:CE2	1:A:44:LEU:HD21	2.03	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:23:GLY:HA3	1:A:27:SER:CA	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4:VAL:C	1:A:5:GLU:HG3	1.97	0.89
1:A:9:SER:HB2	1:A:58:PRO:C	1.98	0.89
1:A:87:LYS:HA	1:A:87:LYS:NZ	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:7:LYS:HB3	1:A:60:LEU:CD2	2.06	0.86
1:A:9:SER:CB	1:A:58:PRO:HA	2.05	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:61:TYR:CG	1:A:83:LEU:HD11	2.13	0.84
1:A:75:SER:O	1:A:76:LEU:HD23	1.77	0.84
1:A:56:TYR:HB3	1:A:61:TYR:CE1	2.13	0.84
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:72:GLN:CG	1:A:73:PHE:CZ	2.62	0.82
1:A:1:MET:CE	1:A:2:ILE:HG13	1.99	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:21:ARG:HG2	1:A:22:GLN:N	1.93	0.81
1:A:83:LEU:C	1:A:84:VAL:HG12	2.04	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:HA	1:A:72:GLN:NE2	1.95	0.80
1:A:50:ASP:C	1:A:53:GLN:HB2	2.07	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:50:ASP:CG	1:A:53:GLN:CB	2.55	0.79
1:A:65:LEU:O	1:A:82:ARG:CG	2.30	0.79
1:A:29:ASN:C	1:A:51:GLU:HG3	2.08	0.79
1:A:61:TYR:CD2	1:A:83:LEU:HD12	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:HG12	1:A:79:ASP:CG	2.09	0.78
1:A:3:LYS:NZ	1:A:87:LYS:HB2	1.99	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:69:LYS:HE3	1:A:79:ASP:OD2	1.84	0.77
1:A:14:THR:C	1:A:15:THR:CG2	2.38	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:46:LYS:HZ1	1:A:48:THR:HG21	1.45	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: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:50:ASP:C	1:A:53:GLN:CG	2.58	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:25:PRO:C	1:A:26:TYR:CD2	2.61	0.75
1:A:77:MET:O	1:A:78:ILE:C	2.22	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:HB2	2.12	0.74
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: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:80:ARG:HG3	1:A:81:LEU:N	2.01	0.73
1:A:4:VAL:C	1:A:5:GLU:CG	2.61	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:86:ALA:C	1:A:87:LYS:HZ1	1.96	0.72
1:A:69:LYS:HD2	1:A:78:ILE:HG23	1.70	0.72
1:A:18:GLY:O	1:A:19:VAL:C	2.31	0.72
1:A:70:VAL:C	1:A:72:GLN:N	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:THR:CG2	1:A:33:CYS:SG	2.79	0.71
1:A:50:ASP:O	1:A:53:GLN:O	2.08	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: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:14:THR:O	1:A:15:THR:C	2.35	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:9:SER:HB2	1:A:58:PRO:CA	2.23	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:16:ARG:HA	1:A:32:LEU:O	1.92	0.68
1:A:6:ILE:O	1:A:7:LYS:C	2.35	0.68
1:A:69:LYS:CD	1:A:79:ASP:HB2	2.18	0.68
1:A:6:ILE:CD1	1:A:83:LEU:CD2	2.70	0.68
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:CZ	1:A:80:ARG:HB2	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:31:GLN:CD	1:A:50:ASP:O	2.38	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:HH11	1:A:80:ARG:CG	2.08	0.66
1:A:19:VAL:O	1:A:19:VAL:CG2	2.41	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:50:ASP:HB2	1:A:53:GLN:HG2	0.67	0.65
1:A:6:ILE:O	1:A:7:LYS:O	2.14	0.65
1:A:68:PHE:CE1	1:A:77:MET:HE3	2.30	0.65
1:A:48:THR:O	1:A:80:ARG:CD	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:68:PHE:C	1:A:76:LEU:O	2.40	0.65
1:A:83:LEU:C	1:A:84:VAL:CG1	2.67	0.65
1:A:50:ASP:C	1:A:53:GLN:CB	2.68	0.64
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: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:HA	1:A:87:LYS:CE	2.28	0.63
1:A:9:SER:HB2	1:A:58:PRO:HA	1.80	0.63
1:A:31:GLN:CD	1:A:51:GLU:HA	2.24	0.63
1:A:18:GLY:C	1:A:30:GLU:HB3	2.24	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:36:ASP:HB2	1:A:44:LEU:H	1.61	0.62
1:A:50:ASP:CG	1:A:53:GLN:CG	2.64	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
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:13:PHE:CD2	1:A:13:PHE:N	2.69	0.60
1:A:61:TYR:C	1:A:84:VAL:O	2.44	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: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:6:ILE:C	1:A:8:PRO:N	2.50	0.58
1:A:9:SER:HB2	1:A:59:GLY:N	2.17	0.58
1:A:62:THR:O	1:A:83:LEU:CA	2.49	0.58
1:A:61:TYR:CG	1:A:83:LEU:CD1	2.84	0.58
1:A:6:ILE:CD1	1:A:81:LEU:CD1	2.82	0.58
1:A:50:ASP:CB	1:A:53:GLN:CD	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4:VAL:HG22	1:A:63:VAL:HG21	1.87	0.56
1:A:29:ASN:HB2	1:A:51:GLU:HG3	1.81	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
1:A:9:SER:O	1:A:58:PRO:O	2.25	0.55
1:A:61:TYR:HA	1:A:84:VAL:C	2.29	0.55
1:A:75:SER:C	1:A:76:LEU:HD23	2.32	0.54
1:A:46:LYS:HZ3	1:A:48:THR:CG2	2.20	0.54
1:A:70:VAL:N	1:A:74:GLY:O	2.40	0.54
1:A:77:MET:C	1:A:78:ILE:O	2.38	0.54
1:A:36:ASP:HB2	1:A:43:VAL:HA	1.89	0.54
1:A:41:TYR:CD2	1:A:42:PRO:CD	2.91	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:50:ASP:OD2	1:A:53:GLN:HB3	2.08	0.53
1:A:69:LYS:HB2	1:A:76:LEU:C	2.34	0.53
1:A:6:ILE:HD11	1:A:81:LEU:HD13	1.91	0.53
1:A:36:ASP:HB2	1:A:43:VAL:C	2.33	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:72:GLN:C	1:A:74:GLY:H	2.18	0.51
1:A:69:LYS:O	1:A:70:VAL:CB	2.56	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:46:LYS:HZ3	1:A:48:THR:HG21	1.65	0.50
1:A:80:ARG:HG3	1:A:81:LEU:C	2.37	0.50
1:A:9:SER:CB	1:A:58:PRO:C	2.79	0.50
1:A:42:PRO:C	1:A:43:VAL:CG1	2.83	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:37:LEU:H	1:A:43:VAL:C	2.21	0.49
1:A:69:LYS:HD3	1:A:78:ILE:HG21	1.84	0.49
1:A:69:LYS:N	1:A:76:LEU:C	2.69	0.49
1:A:80:ARG:HH11	1:A:80:ARG:HG2	1.77	0.49
1:A:50:ASP:CG	1:A:53:GLN:HB3	2.35	0.48
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:20:SER:OG	1:A:28:LEU:CD1	2.62	0.48
1:A:12:GLN:HB3	1:A:13:PHE:HD2	1.78	0.48
1:A:61:TYR:CA	1:A:83:LEU:CD1	2.92	0.47
1:A:37:LEU:C	1:A:43:VAL:H	2.23	0.47
1:A:80:ARG:O	1:A:81:LEU:C	2.56	0.47
1:A:43:VAL:HG11	2:A:91:HOH:O	2.14	0.47
1:A:31:GLN:CD	1:A:51:GLU:CA	2.88	0.47
1:A:86:ALA:C	1:A:87:LYS:NZ	2.66	0.47
1:A:1:MET:HE2	1:A:2:ILE:CD1	2.41	0.47
1:A:72:GLN:HB3	1:A:73:PHE:CD1	2.50	0.47
1:A:30:GLU:OE2	1:A:30:GLU:C	2.58	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:41:TYR:C	1:A:43:VAL:HG13	2.40	0.46
1:A:83:LEU:HD13	1:A:83:LEU:HA	1.63	0.46
1:A:31:GLN:H	1:A:31:GLN:HG3	1.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:29:ASN:O	1:A:51:GLU:CG	2.64	0.45
1:A:68:PHE:HD1	1:A:77:MET:HE3	1.68	0.45
1:A:7:LYS:HA	1:A:60:LEU:CD2	2.47	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:HD22	1.99	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:24:LYS:C	1:A:26:TYR:H	2.25	0.44
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:7:LYS:H	1:A:7:LYS:HD2	1.82	0.44
1:A:21:ARG:HG2	1:A:22:GLN:CA	2.46	0.44
1:A:27:SER:C	1:A:28:LEU:CG	2.90	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:24:LYS:C	1:A:26:TYR:N	2.75	0.43
1:A:69:LYS:HD2	1:A:79:ASP:CG	2.42	0.43
1:A:26:TYR:CD2	1:A:26:TYR:N	2.80	0.43
1:A:50:ASP:CB	1:A:53:GLN:CB	2.86	0.43
1:A:21:ARG:HB2	1:A:21:ARG:CZ	2.40	0.43
1:A:16:ARG:O	1:A:16:ARG:HG2	1.96	0.43
1:A:23:GLY:C	1:A:27:SER:HA	2.42	0.42
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
1:A:87:LYS:NZ	1:A:87:LYS:CB	2.77	0.42
1:A:35:VAL:O	1:A:44:LEU:HA	2.20	0.42
1:A:61:TYR:HD2	1:A:83:LEU:HD12	1.77	0.42
1:A:7:LYS:HB3	1:A:60:LEU:HD22	1.96	0.42
1:A:23:GLY:CA	1:A:27:SER:CA	2.76	0.42
1:A:69:LYS:H	1:A:76:LEU:C	2.26	0.42
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:68:PHE:CD1	1:A:77:MET:CE	2.91	0.41
1:A:35:VAL:HG13	1:A:45:VAL:HG22	2.03	0.41
1:A:81:LEU:HD22	1:A:81:LEU:HA	1.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PHE:N	1:A:13:PHE:HD2	2.17	0.41
1:A:50:ASP:CA	1:A:53:GLN:CD	2.94	0.41
1:A:80:ARG:HH11	1:A:80:ARG:CB	2.31	0.40
1:A:59:GLY:O	1:A:60:LEU:C	2.57	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%)	0 0

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

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Mol	Chain	Res	Type
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%)	31 (41%)	45 (59%)	0 0

All (45) 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
1	A	16	ARG
1	A	17	SER
1	A	19	VAL
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

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Mol	Chain	Res	Type
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	72	GLN
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

Sometimes 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 ⓘ

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](#)

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.