



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:34 PM GMT

PDB ID : 1G6Q
Title : CRYSTAL STRUCTURE OF YEAST ARGININE METHYLTRANSFERASE, HMT1
Authors : Weiss, V.H.; McBride, A.E.; Soriano, M.A.; Filman, D.J.; Silver, P.A.; Hogle, J.M.
Deposited on : 2000-11-07
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

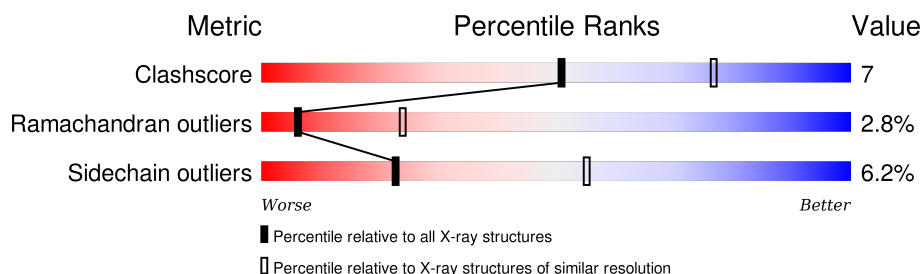
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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	1	328	
1	2	328	
1	3	328	
1	4	328	
1	5	328	
1	6	328	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15520 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 HNRNP ARGININE N-METHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	328	Total	C	N	O	S	0	0	0
			2656	1705	431	508	12			
1	2	320	Total	C	N	O	S	0	0	0
			2579	1654	423	490	12			
1	3	319	Total	C	N	O	S	0	0	0
			2562	1642	420	488	12			
1	4	318	Total	C	N	O	S	0	0	0
			2557	1639	419	487	12			
1	5	321	Total	C	N	O	S	0	0	0
			2587	1658	424	493	12			
1	6	320	Total	C	N	O	S	0	0	0
			2579	1654	423	490	12			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	21	ASP	GLN	ENGINEERED	UNP P38074
1	22	TYR	HIS	ENGINEERED	UNP P38074
1	25	ASP	ASN	ENGINEERED	UNP P38074
2	21	ASP	GLN	ENGINEERED	UNP P38074
2	22	TYR	HIS	ENGINEERED	UNP P38074
2	25	ASP	ASN	ENGINEERED	UNP P38074
3	21	ASP	GLN	ENGINEERED	UNP P38074
3	22	TYR	HIS	ENGINEERED	UNP P38074
3	25	ASP	ASN	ENGINEERED	UNP P38074
4	21	ASP	GLN	ENGINEERED	UNP P38074
4	22	TYR	HIS	ENGINEERED	UNP P38074
4	25	ASP	ASN	ENGINEERED	UNP P38074
5	21	ASP	GLN	ENGINEERED	UNP P38074
5	22	TYR	HIS	ENGINEERED	UNP P38074
5	25	ASP	ASN	ENGINEERED	UNP P38074
6	21	ASP	GLN	ENGINEERED	UNP P38074
6	22	TYR	HIS	ENGINEERED	UNP P38074

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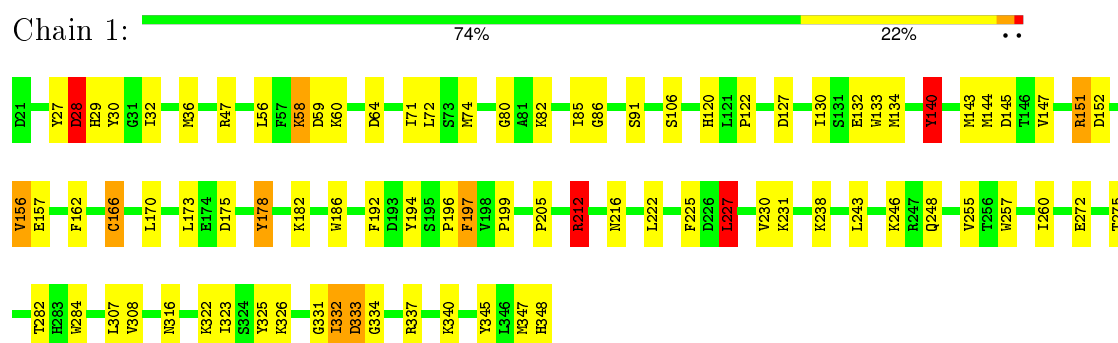
Chain	Residue	Modelled	Actual	Comment	Reference
6	25	ASP	ASN	ENGINEERED	UNP P38074

3 Residue-property plots

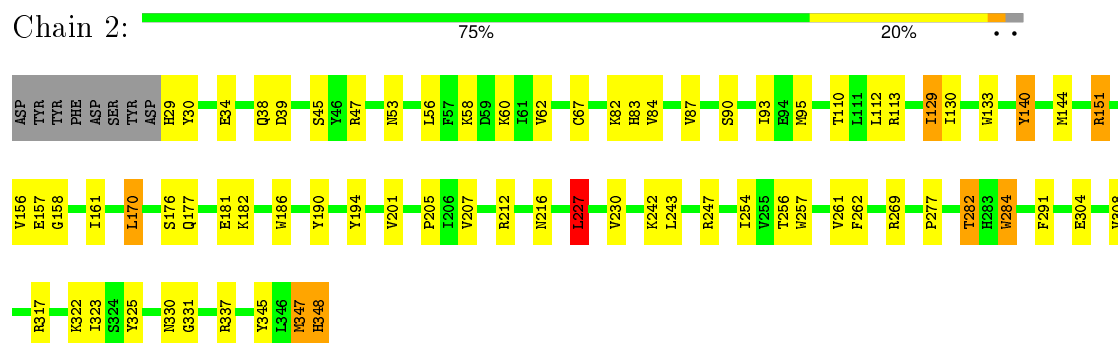
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

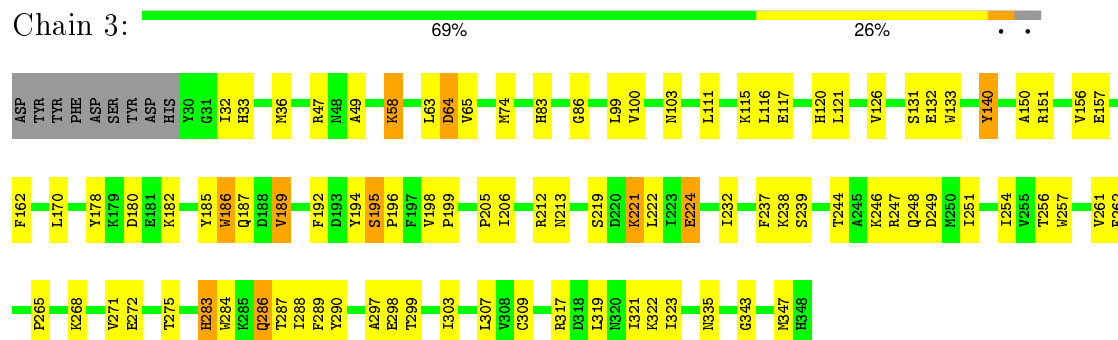
• Molecule 1: HNRNP ARGININE N-METHYLTRANSFERASE



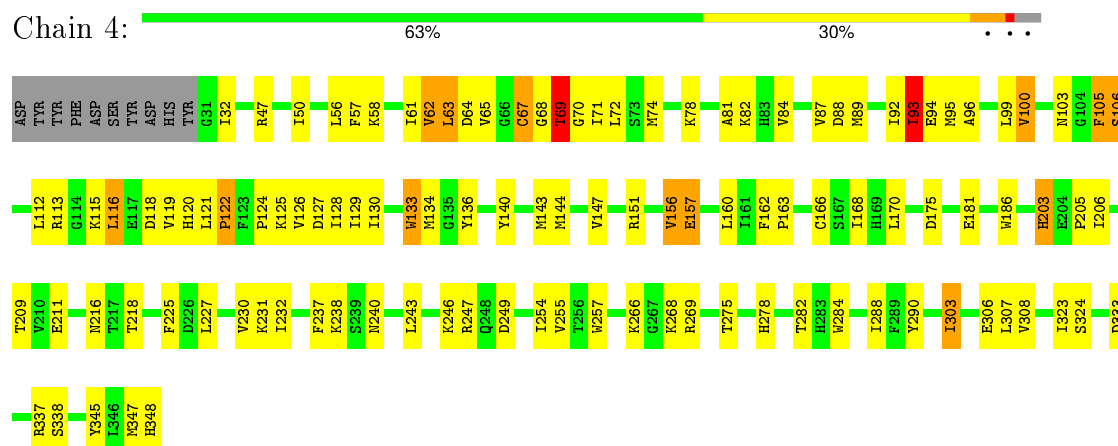
• Molecule 1: HNRNP ARGININE N-METHYLTRANSFERASE



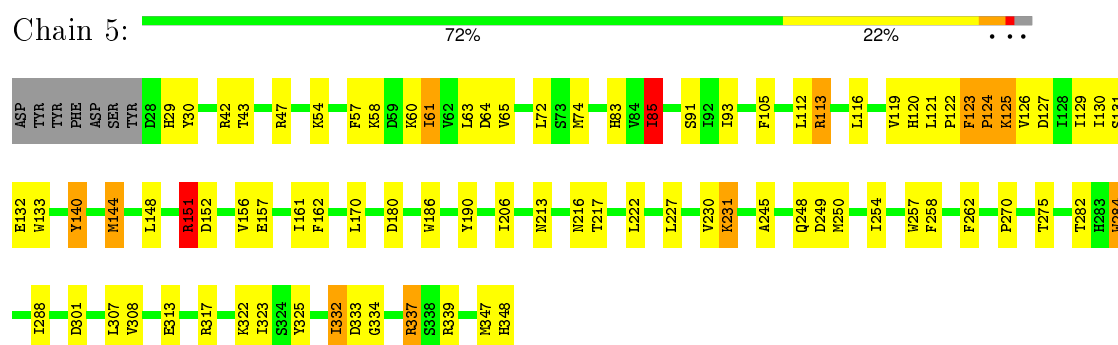
• Molecule 1: HNRNP ARGININE N-METHYLTRANSFERASE



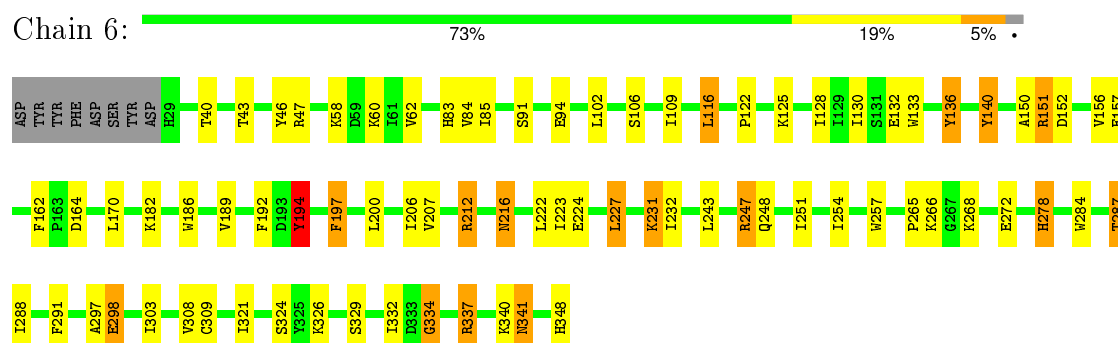
• Molecule 1: HNRNP ARGININE N-METHYLTRANSFERASE



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• Molecule 1: HNRNP ARGININE N-METHYLTRANSFERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.10 Å 129.43 Å 101.43 Å 90.00° 102.74° 90.00°	Depositor
Resolution (Å)	28.00 – 2.90	Depositor
% Data completeness (in resolution range)	99.1 (28.00-2.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.253 , 0.294	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15520	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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	1	0.84	0/2722	1.58	37/3684 (1.0%)
1	2	0.86	0/2641	1.61	41/3573 (1.1%)
1	3	0.80	0/2622	1.60	34/3547 (1.0%)
1	4	0.79	0/2617	1.61	24/3540 (0.7%)
1	5	0.81	0/2649	1.56	32/3584 (0.9%)
1	6	0.82	0/2641	1.53	25/3573 (0.7%)
All	All	0.82	0/15892	1.58	193/21501 (0.9%)

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	1	0	1
1	2	0	1
All	All	0	2

There are no bond length outliers.

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	151	ARG	NE-CZ-NH1	13.10	126.85	120.30
1	6	186	TRP	CD1-CG-CD2	10.59	114.77	106.30
1	5	284	TRP	CD1-CG-CD2	10.43	114.64	106.30
1	2	284	TRP	CD1-CG-CD2	9.82	114.16	106.30
1	2	257	TRP	CD1-CG-CD2	9.62	113.99	106.30
1	6	186	TRP	CE2-CD2-CG	-9.05	100.06	107.30
1	1	194	TYR	CB-CG-CD2	-8.79	115.73	121.00
1	5	339	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	5	317	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	2	151	ARG	NE-CZ-NH2	-8.59	116.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	284	TRP	CE2-CD2-CG	-8.53	100.48	107.30
1	5	257	TRP	CD1-CG-CD2	8.52	113.11	106.30
1	4	284	TRP	CD1-CG-CD2	8.48	113.09	106.30
1	5	186	TRP	CD1-CG-CD2	8.44	113.06	106.30
1	3	257	TRP	CD1-CG-CD2	8.41	113.03	106.30
1	2	257	TRP	CE2-CD2-CG	-8.39	100.59	107.30
1	6	133	TRP	CD1-CG-CD2	8.31	112.95	106.30
1	1	140	TYR	CA-C-N	8.30	135.46	117.20
1	4	133	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	5	284	TRP	CE2-CD2-CG	-8.23	100.72	107.30
1	5	186	TRP	CE2-CD2-CG	-8.14	100.79	107.30
1	4	284	TRP	CE2-CD2-CG	-8.13	100.79	107.30
1	1	133	TRP	CD1-CG-CD2	8.11	112.79	106.30
1	5	133	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	1	186	TRP	CE2-CD2-CG	-8.07	100.84	107.30
1	2	247	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	1	284	TRP	CD1-CG-CD2	7.87	112.59	106.30
1	4	203	HIS	CA-CB-CG	-7.86	100.24	113.60
1	3	257	TRP	CE2-CD2-CG	-7.85	101.02	107.30
1	5	257	TRP	CE2-CD2-CG	-7.83	101.04	107.30
1	1	186	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	3	186	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	5	337	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	5	133	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	3	120	HIS	CA-C-N	-7.76	100.13	117.20
1	3	186	TRP	CE2-CD2-CG	-7.68	101.15	107.30
1	2	337	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	3	151	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	6	133	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	4	290	TYR	CB-CG-CD1	-7.59	116.45	121.00
1	1	133	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	6	257	TRP	CD1-CG-CD2	7.57	112.36	106.30
1	2	186	TRP	CE2-CD2-CG	-7.53	101.28	107.30
1	6	284	TRP	CD1-CG-CD2	7.48	112.29	106.30
1	2	133	TRP	CD1-CG-CD2	7.47	112.27	106.30
1	3	186	TRP	CB-CG-CD1	-7.43	117.34	127.00
1	4	186	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	1	284	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	5	186	TRP	CG-CD2-CE3	7.34	140.50	133.90
1	4	125	LYS	CA-CB-CG	7.32	129.50	113.40
1	3	133	TRP	CD1-CG-CD2	7.31	112.15	106.30
1	3	284	TRP	CE2-CD2-CG	-7.28	101.48	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	186	TRP	CB-CG-CD1	-7.28	117.54	127.00
1	2	212	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	3	284	TRP	CD1-CG-CD2	7.26	112.11	106.30
1	2	133	TRP	CE2-CD2-CG	-7.24	101.51	107.30
1	6	257	TRP	CE2-CD2-CG	-7.22	101.53	107.30
1	4	186	TRP	CD1-CG-CD2	7.21	112.07	106.30
1	6	337	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	3	290	TYR	CB-CG-CD1	-7.20	116.68	121.00
1	1	257	TRP	CE2-CD2-CG	-7.18	101.55	107.30
1	6	284	TRP	CE2-CD2-CG	-7.17	101.57	107.30
1	2	47	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	2	186	TRP	CD1-CG-CD2	7.12	112.00	106.30
1	4	133	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	3	133	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	4	337	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	4	257	TRP	CD1-CG-CD2	6.97	111.87	106.30
1	6	194	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	2	269	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	6	186	TRP	CG-CD2-CE3	6.88	140.09	133.90
1	1	47	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	4	257	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	2	140	TYR	CA-C-N	6.81	132.19	117.20
1	3	140	TYR	CA-C-N	6.81	132.19	117.20
1	4	47	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	5	284	TRP	CG-CD1-NE1	-6.72	103.38	110.10
1	1	166	CYS	CA-CB-SG	-6.68	101.97	114.00
1	3	140	TYR	O-C-N	-6.67	112.02	122.70
1	1	74	MET	CG-SD-CE	-6.66	89.55	100.20
1	5	113	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	1	28	ASP	N-CA-C	6.54	128.66	111.00
1	1	140	TYR	O-C-N	-6.53	112.25	122.70
1	1	133	TRP	CG-CD2-CE3	6.46	139.72	133.90
1	2	284	TRP	CG-CD2-CE3	6.43	139.69	133.90
1	3	186	TRP	CG-CD2-CE3	6.42	139.68	133.90
1	1	326	LYS	CA-CB-CG	6.37	127.41	113.40
1	3	317	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	3	151	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	1	227	LEU	CA-CB-CG	6.35	129.90	115.30
1	1	257	TRP	CG-CD2-CE3	6.33	139.60	133.90
1	5	116	LEU	CA-CB-CG	6.31	129.82	115.30
1	5	47	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	6	247	ARG	NE-CZ-NH2	-6.27	117.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	257	TRP	CB-CG-CD1	-6.24	118.89	127.00
1	2	284	TRP	CG-CD1-NE1	-6.24	103.86	110.10
1	6	186	TRP	CG-CD1-NE1	-6.23	103.87	110.10
1	1	257	TRP	CD1-CG-CD2	6.20	111.26	106.30
1	5	186	TRP	CB-CG-CD1	-6.20	118.94	127.00
1	6	140	TYR	CA-C-N	6.20	130.84	117.20
1	1	28	ASP	CA-C-N	-6.19	103.57	117.20
1	1	58	LYS	N-CA-C	6.18	127.69	111.00
1	3	47	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	5	325	TYR	CB-CG-CD2	-6.16	117.31	121.00
1	5	85	ILE	CB-CG1-CD1	6.14	131.10	113.90
1	1	147	VAL	CG1-CB-CG2	-6.13	101.09	110.90
1	2	337	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	2	247	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	2	227	LEU	CA-CB-CG	5.99	129.08	115.30
1	1	143	MET	CA-CB-CG	-5.98	103.13	113.30
1	4	105	PHE	N-CA-C	5.98	127.15	111.00
1	1	47	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	2	151	ARG	CA-CB-CG	5.94	126.47	113.40
1	2	317	ARG	CA-CB-CG	-5.94	100.33	113.40
1	5	151	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	5	284	TRP	CG-CD2-CE3	5.92	139.23	133.90
1	6	272	GLU	CA-CB-CG	5.92	126.42	113.40
1	2	176	SER	CB-CA-C	-5.90	98.89	110.10
1	2	257	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	1	178	TYR	CB-CG-CD1	-5.86	117.48	121.00
1	1	186	TRP	CG-CD2-CE3	5.85	139.17	133.90
1	3	33	HIS	CA-CB-CG	-5.85	103.65	113.60
1	3	121	LEU	CB-CG-CD2	-5.82	101.10	111.00
1	1	284	TRP	CG-CD2-CE3	5.82	139.13	133.90
1	2	317	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	1	28	ASP	CA-C-O	5.78	132.23	120.10
1	1	272	GLU	CA-CB-CG	5.77	126.10	113.40
1	3	257	TRP	CG-CD2-CE3	5.74	139.07	133.90
1	5	248	GLN	CA-CB-CG	5.73	126.01	113.40
1	5	133	TRP	CB-CG-CD1	-5.72	119.56	127.00
1	1	212	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	2	325	TYR	CB-CG-CD2	-5.61	117.64	121.00
1	4	345	TYR	CB-CG-CD1	-5.61	117.64	121.00
1	6	140	TYR	O-C-N	-5.59	113.75	122.70
1	3	224	GLU	CA-CB-CG	5.59	125.69	113.40
1	2	95	MET	CG-SD-CE	-5.58	91.27	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	133	TRP	CB-CG-CD1	-5.57	119.76	127.00
1	6	136	TYR	N-CA-C	5.56	126.02	111.00
1	2	182	LYS	CD-CE-NZ	-5.56	98.92	111.70
1	3	212	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	3	195	SER	N-CA-C	5.54	125.94	111.00
1	3	185	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	6	47	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	1	140	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	2	186	TRP	CB-CG-CD1	-5.51	119.83	127.00
1	3	257	TRP	CG-CD1-NE1	-5.49	104.61	110.10
1	5	47	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	3	121	LEU	CA-CB-CG	5.48	127.90	115.30
1	5	60	LYS	N-CA-C	5.48	125.79	111.00
1	2	113	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	1	194	TYR	CB-CG-CD1	5.47	124.28	121.00
1	1	192	PHE	CB-CG-CD2	-5.47	116.97	120.80
1	2	194	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	3	283	HIS	CA-CB-CG	5.43	122.84	113.60
1	5	125	LYS	CA-CB-CG	5.42	125.31	113.40
1	2	39	ASP	CB-CG-OD2	5.40	123.16	118.30
1	1	325	TYR	CB-CG-CD2	-5.39	117.76	121.00
1	6	46	TYR	CB-CG-CD1	-5.39	117.76	121.00
1	2	347	MET	CG-SD-CE	-5.39	91.58	100.20
1	2	257	TRP	CG-CD2-CE3	5.38	138.75	133.90
1	2	330	ASN	CA-C-N	-5.37	105.45	116.20
1	4	69	THR	CB-CA-C	-5.37	97.09	111.60
1	2	113	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	1	151	ARG	CB-CG-CD	5.36	125.53	111.60
1	3	212	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	5	144	MET	CA-CB-CG	5.31	122.33	113.30
1	5	42	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	2	331	GLY	CA-C-N	5.23	128.71	117.20
1	4	133	TRP	N-CA-C	5.21	125.08	111.00
1	4	247	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	4	246	LYS	CA-CB-CG	5.20	124.85	113.40
1	4	186	TRP	CG-CD2-CE3	5.20	138.58	133.90
1	3	64	ASP	CB-CG-OD2	5.18	122.96	118.30
1	6	298	GLU	CA-CB-CG	5.18	124.79	113.40
1	4	133	TRP	CG-CD1-NE1	-5.17	104.93	110.10
1	6	133	TRP	CB-CG-CD1	-5.17	120.27	127.00
1	1	284	TRP	CB-CG-CD1	-5.14	120.31	127.00
1	2	284	TRP	CB-CG-CD1	-5.13	120.33	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	227	LEU	CA-CB-CG	5.13	127.10	115.30
1	3	58	LYS	N-CA-C	5.13	124.84	111.00
1	6	164	ASP	CA-CB-CG	5.11	124.64	113.40
1	2	207	VAL	CG1-CB-CG2	-5.11	102.73	110.90
1	4	47	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	3	284	TRP	CG-CD2-CE3	5.09	138.49	133.90
1	2	317	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	5	284	TRP	CB-CG-CD1	-5.09	120.38	127.00
1	5	301	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	4	93	ILE	CB-CA-C	-5.07	101.46	111.60
1	4	100	VAL	CA-CB-CG2	-5.05	103.33	110.90
1	6	337	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	5	124	PRO	N-CA-C	5.02	125.16	112.10
1	3	189	VAL	CG1-CB-CG2	-5.01	102.88	110.90
1	5	317	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	140	TYR	Sidechain
1	2	190	TYR	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	1	2656	0	2579	35	0
1	2	2579	0	2526	25	0
1	3	2562	0	2512	46	0
1	4	2557	0	2510	53	0
1	5	2587	0	2530	37	0
1	6	2579	0	2526	32	0
All	All	15520	0	15183	212	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 7.

All (212) 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)
1:4:87:VAL:HG11	1:4:116:LEU:HB2	1.53	0.88
1:4:170:LEU:HD12	1:4:254:ILE:HG21	1.53	0.87
1:2:242:LYS:HG3	1:2:304:GLU:HG2	1.60	0.82
1:4:89:MET:SD	1:4:115:LYS:HG2	2.20	0.81
1:4:112:LEU:HD23	1:4:121:LEU:HG	1.62	0.79
1:4:96:ALA:HA	1:4:99:LEU:HD12	1.69	0.75
1:1:308:VAL:HG22	1:1:322:LYS:HB3	1.70	0.72
1:5:170:LEU:HD22	1:5:222:LEU:HG	1.73	0.70
1:1:332:ILE:HD13	1:3:246:LYS:HA	1.74	0.69
1:6:130:ILE:HG22	1:6:162:PHE:HB2	1.74	0.69
1:5:93:ILE:HG21	1:5:113:ARG:HB2	1.73	0.69
1:1:205:PRO:HG2	1:1:347:MET:HG3	1.76	0.67
1:2:205:PRO:HG2	1:2:347:MET:HG3	1.76	0.67
1:2:170:LEU:HD13	1:2:243:LEU:HD21	1.77	0.67
1:3:192:PHE:CE2	1:4:74:MET:HB3	2.30	0.67
1:3:195:SER:O	1:3:198:VAL:HG22	1.97	0.65
1:5:222:LEU:HD11	1:5:307:LEU:HD13	1.80	0.64
1:5:130:ILE:HG22	1:5:162:PHE:HB2	1.80	0.64
1:1:248:GLN:HE21	1:3:247:ARG:NH2	1.96	0.63
1:4:62:VAL:HG12	1:4:128:ILE:HB	1.79	0.63
1:3:261:VAL:HG13	1:3:272:GLU:HB3	1.80	0.62
1:5:74:MET:HB3	1:6:192:PHE:CE2	2.34	0.61
1:3:186:TRP:HA	1:3:189:VAL:HG23	1.82	0.61
1:3:49:ALA:HA	1:3:271:VAL:HG21	1.82	0.61
1:2:87:VAL:HG22	1:2:112:LEU:HB2	1.83	0.60
1:4:128:ILE:HG12	1:4:160:LEU:HB2	1.83	0.59
1:4:67:CYS:SG	1:4:70:GLY:N	2.75	0.59
1:4:127:ASP:HA	1:4:156:VAL:HG22	1.85	0.59
1:6:116:LEU:HD21	1:6:150:ALA:HB2	1.84	0.58
1:4:87:VAL:HG21	1:4:116:LEU:HD13	1.85	0.58
1:3:65:VAL:HB	1:3:131:SER:HB2	1.86	0.58
1:6:298:GLU:HG2	1:6:337:ARG:NH2	2.20	0.57
1:5:65:VAL:HB	1:5:131:SER:HB2	1.87	0.57
1:4:168:ILE:HD11	1:4:237:PHE:CZ	2.40	0.56
1:3:256:THR:HG22	1:3:287:THR:O	2.05	0.56
1:6:206:ILE:HG13	1:6:288:ILE:HB	1.87	0.56
1:2:83:HIS:HE1	1:2:110:THR:OG1	1.90	0.55
1:3:198:VAL:HG23	1:3:199:PRO:HD3	1.88	0.55
1:3:116:LEU:HD21	1:3:150:ALA:HB2	1.89	0.55
1:4:72:LEU:HD13	1:4:130:ILE:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:254:ILE:HD11	1:5:323:ILE:HD13	1.89	0.54
1:1:27:TYR:HB3	1:1:91:SER:OG	2.08	0.54
1:2:34:GLU:HG2	1:2:38:GLN:NE2	2.23	0.54
1:1:151:ARG:HG3	1:1:152:ASP:N	2.24	0.53
1:5:217:THR:HG22	1:5:245:ALA:HA	1.90	0.53
1:3:251:ILE:HG21	1:3:303:ILE:HD11	1.91	0.53
1:2:177:GLN:O	1:2:181:GLU:HG2	2.08	0.53
1:4:62:VAL:CG1	1:4:128:ILE:HB	2.39	0.53
1:4:307:LEU:HD12	1:4:323:ILE:HG12	1.89	0.52
1:6:85:ILE:HD12	1:6:122:PRO:HG2	1.91	0.52
1:1:173:LEU:HD22	1:1:175:ASP:HB2	1.92	0.52
1:3:222:LEU:HD21	1:3:307:LEU:HD23	1.91	0.52
1:3:170:LEU:HD12	1:3:254:ILE:HD13	1.91	0.52
1:1:56:LEU:O	1:1:60:LYS:HD2	2.10	0.52
1:3:206:ILE:HG23	1:3:288:ILE:HB	1.91	0.52
1:4:112:LEU:CD2	1:4:121:LEU:HG	2.38	0.52
1:3:205:PRO:HG2	1:3:347:MET:HG3	1.91	0.52
1:1:166:CYS:SG	1:1:225:PHE:HB2	2.50	0.52
1:4:227:LEU:HA	1:4:230:VAL:HG12	1.92	0.52
1:4:206:ILE:HG13	1:4:288:ILE:HB	1.91	0.52
1:1:173:LEU:HD12	1:1:255:VAL:HB	1.93	0.51
1:4:116:LEU:HA	1:4:119:VAL:HG12	1.92	0.51
1:3:63:LEU:HB2	1:3:126:VAL:HG21	1.91	0.51
1:4:93:ILE:HG12	1:4:112:LEU:O	2.11	0.51
1:4:128:ILE:HG23	1:4:160:LEU:HB2	1.92	0.51
1:4:64:ASP:HA	1:4:130:ILE:O	2.11	0.51
1:4:61:ILE:HG23	1:4:126:VAL:HA	1.92	0.51
1:1:130:ILE:HG22	1:1:162:PHE:HB2	1.93	0.51
1:4:166:CYS:SG	1:4:225:PHE:HB2	2.50	0.50
1:3:74:MET:HE2	1:3:103:ASN:HB2	1.93	0.50
1:3:32:ILE:O	1:3:36:MET:HG2	2.11	0.50
1:2:67:CYS:SG	1:2:93:ILE:HD11	2.52	0.50
1:3:196:PRO:O	1:3:199:PRO:HD2	2.11	0.50
1:3:115:LYS:HG3	1:3:117:GLU:HG2	1.93	0.50
1:5:61:ILE:HD13	1:5:126:VAL:HA	1.93	0.50
1:2:308:VAL:HG22	1:2:322:LYS:HB3	1.94	0.50
1:4:254:ILE:HG22	1:4:255:VAL:N	2.27	0.50
1:1:127:ASP:HA	1:1:156:VAL:HG22	1.93	0.50
1:1:323:ILE:HD12	1:1:345:TYR:CE1	2.47	0.50
1:5:112:LEU:HD13	1:5:119:VAL:HG12	1.94	0.50
1:4:133:TRP:HB3	1:4:147:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:133:TRP:CZ3	1:4:144:MET:SD	3.05	0.49
1:1:197:PHE:HE2	1:2:30:TYR:HB2	1.77	0.49
1:2:254:ILE:HG23	1:2:291:PHE:CZ	2.47	0.49
1:6:212:ARG:HD3	1:6:278:HIS:HB3	1.94	0.49
1:2:62:VAL:HB	1:2:84:VAL:HG13	1.95	0.49
1:4:50:ILE:HG23	1:4:57:PHE:CZ	2.48	0.49
1:4:306:GLU:HB3	1:4:324:SER:OG	2.13	0.49
1:4:56:LEU:HG	1:4:160:LEU:HD11	1.95	0.49
1:6:254:ILE:HG23	1:6:291:PHE:CZ	2.48	0.48
1:3:63:LEU:HD21	1:3:116:LEU:HD11	1.95	0.48
1:3:162:PHE:HD1	1:3:262:PHE:HD1	1.61	0.48
1:6:265:PRO:HG2	1:6:268:LYS:HD2	1.94	0.48
1:3:192:PHE:HE1	1:4:78:LYS:HD2	1.77	0.48
1:5:127:ASP:HA	1:5:156:VAL:HG22	1.96	0.48
1:6:340:LYS:HD3	1:6:341:ASN:N	2.28	0.48
1:5:151:ARG:HG3	1:5:152:ASP:N	2.29	0.48
1:6:248:GLN:HA	1:6:297:ALA:O	2.14	0.47
1:5:112:LEU:HD11	1:5:122:PRO:HD3	1.96	0.47
1:6:223:ILE:HG13	1:6:224:GLU:N	2.30	0.47
1:4:275:THR:CA	1:4:282:THR:HG21	2.44	0.47
1:4:88:ASP:HB3	1:4:93:ILE:HG23	1.96	0.47
1:6:298:GLU:HG2	1:6:337:ARG:HH22	1.79	0.47
1:4:203:HIS:O	1:4:205:PRO:HD3	2.14	0.47
1:3:178:TYR:O	1:3:182:LYS:HG2	2.14	0.47
1:3:307:LEU:HD11	1:3:321:ILE:HG23	1.97	0.47
1:1:27:TYR:O	1:2:348:HIS:NE2	2.48	0.47
1:2:282:THR:OG1	1:2:284:TRP:HE3	1.98	0.47
1:4:275:THR:HA	1:4:282:THR:HG21	1.96	0.47
1:1:196:PRO:O	1:1:199:PRO:HD2	2.15	0.47
1:5:72:LEU:HB3	1:5:130:ILE:HD12	1.97	0.46
1:4:68:GLY:O	1:4:69:THR:HG23	2.15	0.46
1:2:170:LEU:HB3	1:2:256:THR:HG22	1.96	0.46
1:4:100:VAL:HG12	1:4:106:SER:HA	1.96	0.46
1:5:227:LEU:HA	1:5:230:VAL:HG12	1.96	0.46
1:1:178:TYR:CE1	1:1:182:LYS:HD2	2.51	0.46
1:2:323:ILE:HD12	1:2:345:TYR:CE1	2.51	0.46
1:3:162:PHE:HD1	1:3:262:PHE:CD1	2.34	0.46
1:4:205:PRO:HG2	1:4:347:MET:HG2	1.97	0.46
1:3:198:VAL:CG2	1:3:199:PRO:HD3	2.46	0.45
1:6:170:LEU:HD23	1:6:222:LEU:HD11	1.96	0.45
1:5:333:ASP:HB3	1:5:337:ARG:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:63:LEU:HD22	1:4:65:VAL:HG22	1.97	0.45
1:1:64:ASP:HB3	1:1:86:GLY:HA2	1.99	0.45
1:2:53:ASN:OD1	1:2:56:LEU:HD12	2.17	0.45
1:6:243:LEU:HB2	1:6:303:ILE:HB	1.99	0.45
1:5:105:PHE:HE2	1:6:192:PHE:HE2	1.64	0.45
1:3:256:THR:HG21	1:3:289:PHE:HE2	1.81	0.45
1:1:246:LYS:HA	1:5:332:ILE:HG13	1.99	0.45
1:6:329:SER:HB3	1:6:334:GLY:HA2	1.99	0.44
1:4:143:MET:O	1:4:147:VAL:HG23	2.17	0.44
1:2:156:VAL:O	1:2:158:GLY:N	2.51	0.44
1:3:265:PRO:HG2	1:3:268:LYS:HG3	1.98	0.44
1:2:129:ILE:HG23	1:2:161:ILE:HG12	1.99	0.44
1:1:222:LEU:HD11	1:1:307:LEU:HD13	1.99	0.44
1:4:93:ILE:HD11	1:4:113:ARG:HE	1.83	0.44
1:3:309:CYS:SG	1:3:319:LEU:HD22	2.57	0.44
1:1:85:ILE:HD13	1:1:122:PRO:HD2	2.00	0.44
1:4:92:ILE:O	1:4:95:MET:HB3	2.18	0.44
1:4:121:LEU:HB3	1:4:122:PRO:HD2	1.98	0.44
1:3:275:THR:O	1:3:286:GLN:NE2	2.50	0.44
1:6:216:ASN:ND2	1:6:251:ILE:HG12	2.33	0.44
1:1:59:ASP:O	1:1:82:LYS:HE2	2.18	0.44
1:5:140:TYR:CE2	1:5:347:MET:HB3	2.53	0.44
1:6:189:VAL:HG21	1:6:194:TYR:CD1	2.53	0.44
1:6:329:SER:OG	1:6:337:ARG:NH2	2.52	0.43
1:2:62:VAL:HB	1:2:84:VAL:HG22	1.99	0.43
1:4:93:ILE:HD12	1:4:94:GLU:N	2.32	0.43
1:1:248:GLN:OE1	1:3:213:ASN:HB3	2.19	0.43
1:3:170:LEU:HD22	1:3:222:LEU:HD13	2.00	0.43
1:6:309:CYS:SG	1:6:321:ILE:CD1	3.07	0.43
1:5:144:MET:SD	1:5:227:LEU:HD11	2.58	0.43
1:4:62:VAL:HG23	1:4:84:VAL:HB	2.00	0.43
1:2:82:LYS:HE2	1:2:82:LYS:HB2	1.87	0.43
1:4:162:PHE:HA	1:4:163:PRO:HA	1.84	0.43
1:3:64:ASP:HB3	1:3:86:GLY:HA2	2.00	0.43
1:4:93:ILE:HG12	1:4:113:ARG:HA	2.01	0.43
1:1:134:MET:HG2	1:1:260:ILE:HD11	2.00	0.43
1:4:63:LEU:HB3	1:4:129:ILE:HG22	2.00	0.43
1:3:74:MET:HE1	1:3:99:LEU:O	2.19	0.43
1:5:151:ARG:HG3	1:5:152:ASP:H	1.84	0.43
1:1:333:ASP:HB2	1:1:337:ARG:HE	1.83	0.43
1:6:207:VAL:HG22	1:6:287:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:197:PHE:O	1:6:200:LEU:HB3	2.18	0.43
1:3:254:ILE:HG13	1:3:289:PHE:HB2	2.01	0.43
1:1:58:LYS:HA	1:1:58:LYS:HD3	1.85	0.42
1:4:63:LEU:HB2	1:4:126:VAL:HG21	2.02	0.42
1:6:326:LYS:HB3	1:6:326:LYS:HE2	1.78	0.42
1:1:30:TYR:CD2	1:2:201:VAL:HG22	2.54	0.42
1:5:64:ASP:HA	1:5:130:ILE:O	2.19	0.42
1:4:218:THR:O	1:4:243:LEU:HD22	2.19	0.42
1:1:32:ILE:O	1:1:36:MET:HG2	2.20	0.42
1:5:206:ILE:HG13	1:5:288:ILE:HB	2.02	0.42
1:5:151:ARG:HH21	1:5:231:LYS:NZ	2.18	0.42
1:3:248:GLN:HA	1:3:297:ALA:O	2.20	0.42
1:2:130:ILE:HD13	1:2:130:ILE:HG21	1.90	0.42
1:5:262:PHE:O	1:5:270:PRO:HB3	2.18	0.42
1:5:105:PHE:HE2	1:6:192:PHE:CE2	2.38	0.42
1:1:71:ILE:HG23	1:1:72:LEU:N	2.34	0.42
1:6:84:VAL:HB	1:6:109:ILE:HG23	2.02	0.41
1:5:54:LYS:HA	1:5:57:PHE:HB2	2.01	0.41
1:1:231:LYS:HA	1:1:231:LYS:HD3	1.84	0.41
1:6:182:LYS:HA	1:6:182:LYS:HD3	1.74	0.41
1:5:129:ILE:HG23	1:5:161:ILE:HG12	2.02	0.41
1:3:36:MET:SD	1:3:283:HIS:CE1	3.14	0.41
1:3:100:VAL:HG21	1:3:111:LEU:HD11	2.01	0.41
1:5:30:TYR:HB2	1:6:197:PHE:HE2	1.85	0.41
1:2:227:LEU:HA	1:2:230:VAL:HG12	2.02	0.41
1:1:212:ARG:CZ	1:5:250:MET:SD	3.08	0.41
1:3:237:PHE:HD1	1:3:239:SER:HG	1.69	0.41
1:5:151:ARG:HH21	1:5:231:LYS:HZ2	1.69	0.41
1:5:308:VAL:HG22	1:5:322:LYS:HB3	2.02	0.41
1:3:221:LYS:HB3	1:3:221:LYS:NZ	2.36	0.41
1:1:248:GLN:NE2	1:3:247:ARG:NH2	2.67	0.41
1:3:307:LEU:HD13	1:3:323:ILE:HG12	2.02	0.41
1:4:63:LEU:HD22	1:4:65:VAL:CG2	2.50	0.41
1:1:170:LEU:CD1	1:1:243:LEU:HD21	2.51	0.41
1:4:238:LYS:HG3	1:4:308:VAL:HB	2.02	0.41
1:5:258:PHE:CE1	1:5:275:THR:HG21	2.56	0.41
1:1:227:LEU:HA	1:1:230:VAL:HG12	2.03	0.41
1:5:63:LEU:HD12	1:5:85:ILE:O	2.21	0.41
1:6:151:ARG:HH21	1:6:231:LYS:NZ	2.19	0.41
1:1:275:THR:HG22	1:1:282:THR:HG21	2.02	0.41
1:5:148:LEU:O	1:5:151:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:62:VAL:HA	1:6:128:ILE:O	2.20	0.40
1:4:243:LEU:HB2	1:4:303:ILE:CG2	2.51	0.40
1:2:261:VAL:HG12	1:2:262:PHE:N	2.36	0.40
1:3:205:PRO:HB3	1:3:289:PHE:CE1	2.55	0.40
1:6:151:ARG:HG3	1:6:152:ASP:N	2.37	0.40
1:5:282:THR:OG1	1:5:284:TRP:HE3	2.04	0.40
1:5:190:TYR:OH	1:6:40:THR:HA	2.21	0.40
1:3:322:LYS:HA	1:3:343:GLY:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	326/328 (99%)	304 (93%)	14 (4%)	8 (2%)	7	27
1	2	318/328 (97%)	295 (93%)	20 (6%)	3 (1%)	21	57
1	3	317/328 (97%)	275 (87%)	35 (11%)	7 (2%)	8	31
1	4	316/328 (96%)	273 (86%)	26 (8%)	17 (5%)	2	7
1	5	319/328 (97%)	284 (89%)	25 (8%)	10 (3%)	5	21
1	6	318/328 (97%)	290 (91%)	19 (6%)	9 (3%)	6	24
All	All	1914/1968 (97%)	1721 (90%)	139 (7%)	54 (3%)	6	24

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	140	TYR
1	1	157	GLU
1	1	334	GLY
1	2	140	TYR

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Mol	Chain	Res	Type
1	2	157	GLU
1	3	58	LYS
1	3	140	TYR
1	4	32	ILE
1	4	58	LYS
1	4	105	PHE
1	4	136	TYR
1	4	232	ILE
1	5	58	LYS
1	5	120	HIS
1	5	123	PHE
1	5	140	TYR
1	5	157	GLU
1	5	332	ILE
1	5	334	GLY
1	6	58	LYS
1	6	116	LEU
1	6	140	TYR
1	1	28	ASP
1	2	58	LYS
1	3	157	GLU
1	3	219	SER
1	3	232	ILE
1	4	67	CYS
1	4	69	THR
1	4	81	ALA
1	4	124	PRO
1	4	157	GLU
1	6	157	GLU
1	1	332	ILE
1	4	106	SER
1	4	116	LEU
1	4	122	PRO
1	4	140	TYR
1	4	156	VAL
1	4	266	LYS
1	5	91	SER
1	5	124	PRO
1	6	136	TYR
1	6	332	ILE
1	3	156	VAL
1	3	299	THR

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Mol	Chain	Res	Type
1	4	82	LYS
1	6	91	SER
1	1	156	VAL
1	5	29	HIS
1	6	156	VAL
1	6	334	GLY
1	1	80	GLY
1	1	331	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	1	295/295 (100%)	279 (95%)	16 (5%)	27	62
1	2	287/295 (97%)	274 (96%)	13 (4%)	34	70
1	3	285/295 (97%)	272 (95%)	13 (5%)	33	69
1	4	285/295 (97%)	260 (91%)	25 (9%)	12	35
1	5	288/295 (98%)	272 (94%)	16 (6%)	26	60
1	6	287/295 (97%)	263 (92%)	24 (8%)	14	37
All	All	1727/1770 (98%)	1620 (94%)	107 (6%)	23	55

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	28	ASP
1	1	29	HIS
1	1	106	SER
1	1	120	HIS
1	1	132	GLU
1	1	144	MET
1	1	145	ASP
1	1	197	PHE
1	1	212	ARG
1	1	216	ASN

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Mol	Chain	Res	Type
1	1	227	LEU
1	1	238	LYS
1	1	316	ASN
1	1	333	ASP
1	1	340	LYS
1	1	348	HIS
1	2	29	HIS
1	2	45	SER
1	2	60	LYS
1	2	90	SER
1	2	129	ILE
1	2	144	MET
1	2	151	ARG
1	2	170	LEU
1	2	216	ASN
1	2	227	LEU
1	2	277	PRO
1	2	282	THR
1	2	348	HIS
1	3	83	HIS
1	3	132	GLU
1	3	180	ASP
1	3	187	GLN
1	3	194	TYR
1	3	221	LYS
1	3	224	GLU
1	3	238	LYS
1	3	244	THR
1	3	249	ASP
1	3	286	GLN
1	3	298	GLU
1	3	335	ASN
1	4	62	VAL
1	4	63	LEU
1	4	71	ILE
1	4	93	ILE
1	4	103	ASN
1	4	118	ASP
1	4	120	HIS
1	4	134	MET
1	4	151	ARG
1	4	157	GLU

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Mol	Chain	Res	Type
1	4	175	ASP
1	4	181	GLU
1	4	209	THR
1	4	211	GLU
1	4	216	ASN
1	4	231	LYS
1	4	240	ASN
1	4	249	ASP
1	4	268	LYS
1	4	269	ARG
1	4	278	HIS
1	4	303	ILE
1	4	333	ASP
1	4	338	SER
1	4	348	HIS
1	5	43	THR
1	5	61	ILE
1	5	83	HIS
1	5	85	ILE
1	5	121	LEU
1	5	123	PHE
1	5	125	LYS
1	5	132	GLU
1	5	151	ARG
1	5	180	ASP
1	5	213	ASN
1	5	216	ASN
1	5	231	LYS
1	5	249	ASP
1	5	313	GLU
1	5	348	HIS
1	6	43	THR
1	6	60	LYS
1	6	83	HIS
1	6	94	GLU
1	6	102	LEU
1	6	106	SER
1	6	125	LYS
1	6	132	GLU
1	6	151	ARG
1	6	194	TYR
1	6	197	PHE

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Mol	Chain	Res	Type
1	6	212	ARG
1	6	216	ASN
1	6	227	LEU
1	6	231	LYS
1	6	232	ILE
1	6	247	ARG
1	6	266	LYS
1	6	278	HIS
1	6	287	THR
1	6	308	VAL
1	6	324	SER
1	6	341	ASN
1	6	348	HIS

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

Mol	Chain	Res	Type
1	2	33	HIS
1	2	38	GLN
1	2	83	HIS
1	2	169	HIS
1	2	187	GLN
1	2	216	ASN
1	3	83	HIS
1	3	169	HIS
1	3	283	HIS
1	4	169	HIS
1	5	216	ASN
1	5	312	ASN
1	6	169	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 [i](#)

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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.