



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:58 AM UTC

PDB ID : 1BVZ / pdb_00001bvz
Title : ALPHA-AMYLASE II (TVAII) FROM THERMOACTINOMYCES VULGARIS R-47
Authors : Kamitori, S.; Kondo, S.; Okuyama, K.; Yokota, T.; Shimura, Y.; Tonozuka, T.; Sakano, Y.
Deposited on : 1998-09-22
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

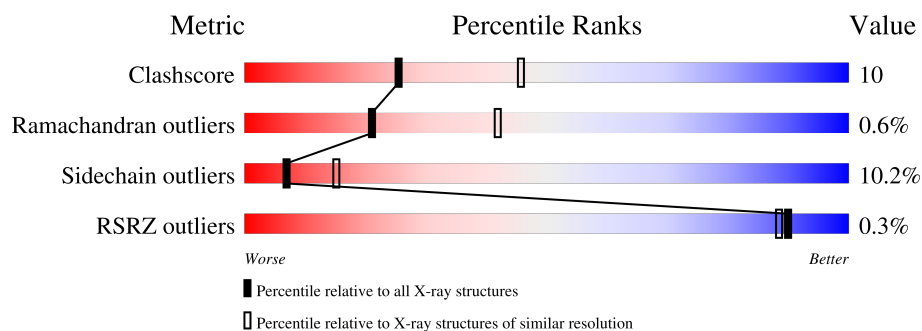
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	585	
1	B	585	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10030 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 PROTEIN (ALPHA-AMYLASE II).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4776	3056	831	874	15			
1	B	585	Total	C	N	O	S	0	0	0
			4776	3056	831	874	15			

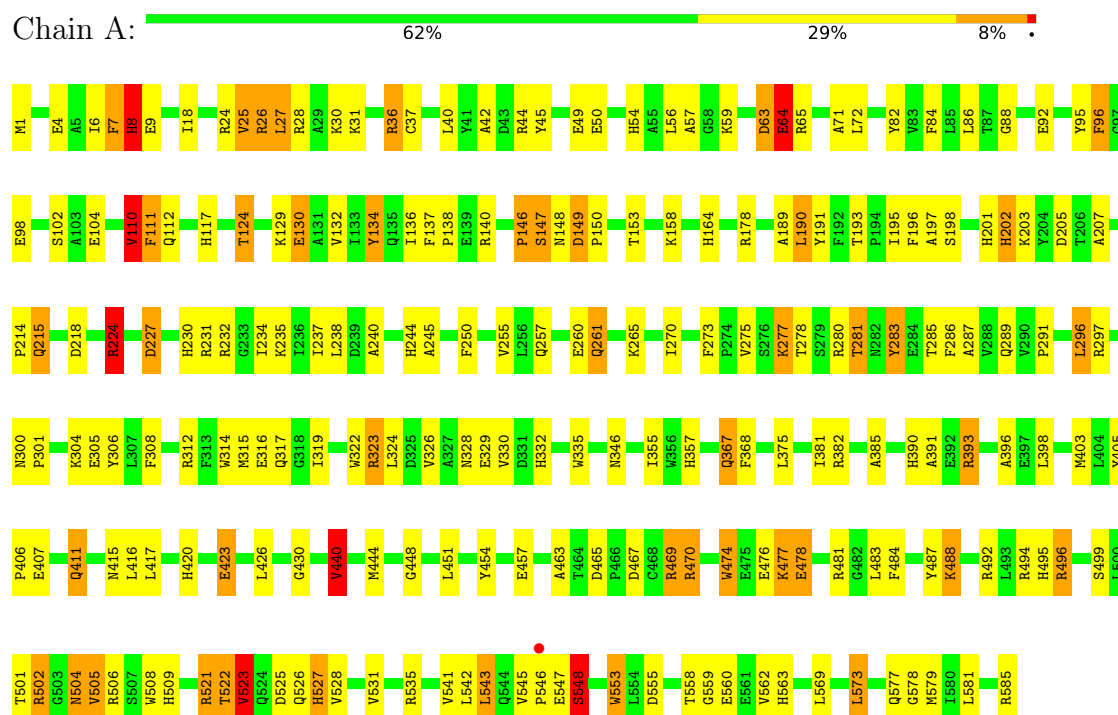
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	267	Total	O	0	0
			267	267		
2	B	211	Total	O	0	0
			211	211		

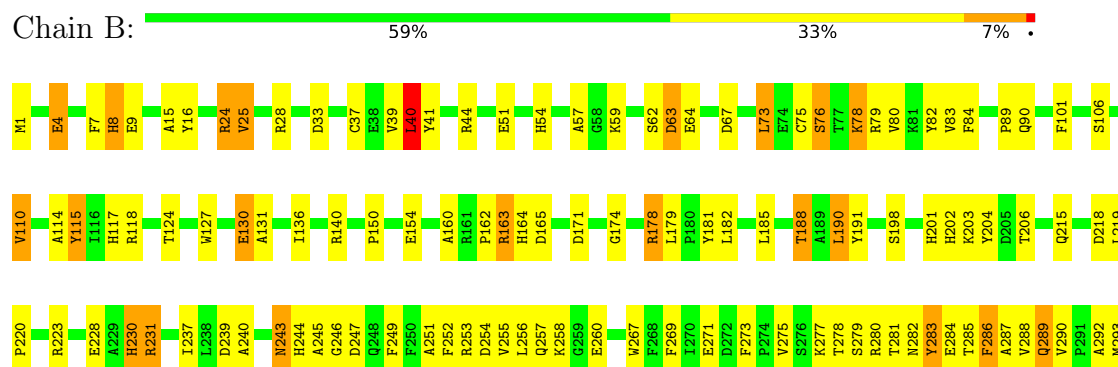
3 Residue-property plots [i](#)

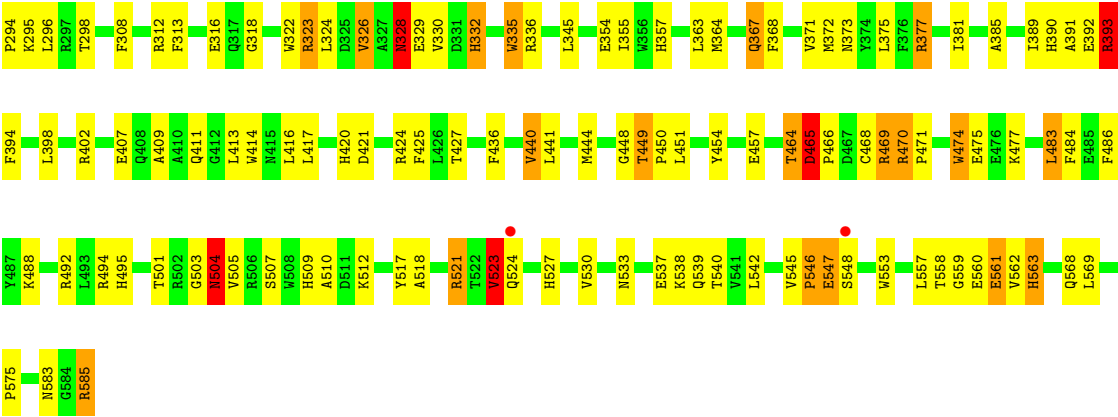
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PROTEIN (ALPHA-AMYLASE II)



• Molecule 1: PROTEIN (ALPHA-AMYLASE II)





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.60Å 117.90Å 114.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.60 7.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	85.0 (7.00-2.60) 80.3 (7.00-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.196 , 0.272 0.192 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.55 , 148.7	EDS
L-test for twinning ¹	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.038 for k,h,-l 0.042 for -h,-l,-k 0.036 for l,-k,h 0.025 for k,l,h 0.025 for l,h,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10030	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.04	19/4906 (0.4%)	1.76	96/6641 (1.4%)
1	B	1.01	18/4906 (0.4%)	1.72	77/6641 (1.2%)
All	All	1.02	37/9812 (0.4%)	1.74	173/13282 (1.3%)

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	24
1	B	0	26
All	All	0	50

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	HIS	CD2-NE2	-7.75	1.29	1.37
1	B	117	HIS	CD2-NE2	-7.34	1.29	1.37
1	B	527	HIS	CD2-NE2	-7.21	1.29	1.37
1	A	527	HIS	CD2-NE2	-7.20	1.29	1.37
1	B	230	HIS	CD2-NE2	-7.09	1.30	1.37
1	A	357	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	117	HIS	CD2-NE2	-6.81	1.30	1.37
1	A	563	HIS	CD2-NE2	-6.80	1.30	1.37
1	A	420	HIS	CD2-NE2	-6.71	1.30	1.37
1	B	8	HIS	CD2-NE2	-6.71	1.30	1.37
1	A	117	HIS	CG-ND1	-6.64	1.30	1.38
1	A	390	HIS	CD2-NE2	-6.57	1.30	1.37
1	B	201	HIS	CD2-NE2	-6.54	1.30	1.37
1	B	420	HIS	CD2-NE2	-6.53	1.30	1.37
1	B	390	HIS	CD2-NE2	-6.53	1.30	1.37
1	A	244	HIS	CD2-NE2	-6.52	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	HIS	CD2-NE2	-6.38	1.30	1.37
1	A	164	HIS	CD2-NE2	-6.26	1.30	1.37
1	B	244	HIS	CD2-NE2	-6.26	1.30	1.37
1	A	509	HIS	CD2-NE2	-6.22	1.31	1.37
1	B	357	HIS	CD2-NE2	-6.17	1.31	1.37
1	A	201	HIS	CD2-NE2	-6.17	1.31	1.37
1	B	54	HIS	CD2-NE2	-6.05	1.31	1.37
1	B	563	HIS	CD2-NE2	-5.97	1.31	1.37
1	B	202	HIS	CD2-NE2	-5.91	1.31	1.37
1	B	509	HIS	CD2-NE2	-5.90	1.31	1.37
1	B	332	HIS	CD2-NE2	-5.79	1.31	1.37
1	A	230	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	495	HIS	CD2-NE2	-5.74	1.31	1.37
1	B	164	HIS	CD2-NE2	-5.67	1.31	1.37
1	B	495	HIS	CD2-NE2	-5.66	1.31	1.37
1	A	332	HIS	CD2-NE2	-5.38	1.31	1.37
1	B	117	HIS	CG-ND1	-5.37	1.32	1.38
1	A	202	HIS	CD2-NE2	-5.24	1.32	1.37
1	A	244	HIS	CG-ND1	-5.12	1.32	1.38
1	B	8	HIS	CG-ND1	-5.11	1.32	1.38
1	A	357	HIS	CG-ND1	-5.03	1.32	1.38

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	558	THR	N-CA-C	15.05	133.71	112.04
1	B	558	THR	N-CA-C	13.65	131.69	112.04
1	B	547	GLU	N-CA-C	13.04	125.03	111.07
1	B	367	GLN	N-CA-C	11.02	128.42	111.56
1	B	287	ALA	N-CA-C	11.01	126.81	112.72
1	A	523	VAL	O-C-N	-10.92	111.47	122.94
1	B	546	PRO	N-CA-C	10.27	127.25	111.34
1	A	560	GLU	N-CA-C	10.17	125.25	110.10
1	A	63	ASP	CA-CB-CG	9.03	121.63	112.60
1	B	328	ASN	CA-CB-CG	8.80	121.40	112.60
1	B	286	PHE	CA-C-O	-8.62	111.83	120.70
1	A	8	HIS	CB-CG-CD2	-8.45	120.22	131.20
1	A	563	HIS	CB-CG-CD2	-8.45	120.22	131.20
1	A	54	HIS	CB-CG-CD2	-8.30	120.41	131.20
1	A	287	ALA	N-CA-C	8.15	123.05	112.12
1	B	523	VAL	O-C-N	-8.11	113.95	122.95
1	A	522	THR	CA-C-N	7.67	129.64	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	522	THR	C-N-CA	7.67	129.64	121.97
1	B	545	VAL	N-CA-C	7.66	117.39	108.96
1	A	548	SER	N-CA-C	7.60	121.81	112.23
1	A	527	HIS	CB-CG-CD2	-7.58	121.35	131.20
1	B	54	HIS	CB-CG-CD2	-7.45	121.51	131.20
1	A	148	ASN	CA-CB-CG	7.43	120.03	112.60
1	A	286	PHE	CA-C-O	-7.41	113.04	120.82
1	B	557	LEU	O-C-N	-7.22	114.02	122.32
1	A	558	THR	N-CA-CB	-7.17	99.07	110.19
1	A	357	HIS	CB-CG-CD2	-7.15	121.90	131.20
1	B	202	HIS	CB-CG-CD2	-7.05	122.03	131.20
1	A	54	HIS	CB-CG-ND1	7.04	133.25	122.70
1	A	164	HIS	CB-CG-CD2	-6.99	122.11	131.20
1	B	545	VAL	CA-C-N	6.99	127.40	119.92
1	B	545	VAL	C-N-CA	6.99	127.40	119.92
1	A	541	VAL	N-CA-C	6.93	118.10	108.12
1	B	560	GLU	N-CA-C	6.92	119.76	109.59
1	B	76	SER	N-CA-C	6.83	119.56	111.71
1	B	509	HIS	CB-CG-CD2	-6.79	122.37	131.20
1	A	286	PHE	CA-C-N	-6.73	111.80	122.17
1	A	286	PHE	C-N-CA	-6.73	111.80	122.17
1	B	117	HIS	CB-CG-CD2	-6.68	122.51	131.20
1	A	201	HIS	CB-CG-CD2	-6.67	122.54	131.20
1	A	509	HIS	CB-CG-CD2	-6.62	122.59	131.20
1	B	40	LEU	N-CA-C	-6.56	98.21	108.90
1	B	244	HIS	CB-CG-CD2	-6.54	122.69	131.20
1	A	289	GLN	N-CA-C	-6.50	97.47	108.26
1	A	205	ASP	CA-CB-CG	6.47	119.07	112.60
1	B	114	ALA	N-CA-C	6.46	118.87	111.11
1	B	54	HIS	CB-CG-ND1	6.45	132.37	122.70
1	B	63	ASP	CA-CB-CG	6.44	119.04	112.60
1	A	64	GLU	CA-CB-CG	-6.39	101.33	114.10
1	B	367	GLN	O-C-N	-6.38	114.99	122.32
1	A	504	ASN	CB-CG-ND2	6.37	125.96	116.40
1	A	367	GLN	N-CA-C	6.37	122.91	110.56
1	B	474	TRP	CG-CD1-NE1	-6.36	101.93	110.20
1	A	504	ASN	CA-CB-CG	6.34	118.94	112.60
1	A	277	LYS	CA-C-N	6.34	132.63	122.10
1	A	277	LYS	C-N-CA	6.34	132.63	122.10
1	B	243	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	B	465	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	357	HIS	CB-CG-CD2	-6.26	123.06	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	HIS	CB-CG-ND1	6.25	132.07	122.70
1	B	420	HIS	CB-CG-CD2	-6.23	123.10	131.20
1	B	79	ARG	N-CA-C	-6.22	97.28	108.48
1	A	391	ALA	N-CA-C	6.21	118.85	111.71
1	B	527	HIS	CB-CG-CD2	-6.14	123.22	131.20
1	B	539	GLN	OE1-CD-NE2	-6.12	116.48	122.60
1	A	111	PHE	N-CA-C	-6.10	100.25	109.95
1	A	148	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	B	218	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	525	ASP	CA-C-O	6.03	125.53	118.90
1	A	110	VAL	O-C-N	-6.00	116.16	123.00
1	A	411	GLN	OE1-CD-NE2	-6.00	116.60	122.60
1	B	164	HIS	CB-CG-CD2	-6.00	123.40	131.20
1	A	59	LYS	CB-CG-CD	-5.96	97.59	111.30
1	A	488	LYS	CB-CG-CD	-5.96	97.60	111.30
1	A	124	THR	CA-C-N	5.96	126.30	119.93
1	A	124	THR	C-N-CA	5.96	126.30	119.93
1	A	40	LEU	N-CA-C	-5.94	99.22	108.90
1	A	420	HIS	CB-CG-CD2	-5.89	123.54	131.20
1	A	543	LEU	N-CA-C	-5.89	99.80	109.40
1	B	244	HIS	CB-CG-ND1	5.86	131.49	122.70
1	B	495	HIS	CB-CG-CD2	-5.86	123.58	131.20
1	A	227	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	558	THR	O-C-N	-5.85	114.40	122.30
1	B	390	HIS	CB-CG-CD2	-5.83	123.62	131.20
1	B	523	VAL	N-CA-C	-5.81	100.22	108.65
1	A	215	GLN	CB-CA-C	-5.79	100.84	110.68
1	B	332	HIS	CB-CG-CD2	-5.79	123.68	131.20
1	B	90	GLN	OE1-CD-NE2	-5.75	116.84	122.60
1	B	288	VAL	N-CA-C	5.72	117.11	111.67
1	A	346	ASN	CA-C-N	5.71	125.39	119.05
1	A	346	ASN	C-N-CA	5.71	125.39	119.05
1	A	577	GLN	OE1-CD-NE2	-5.70	116.90	122.60
1	A	42	ALA	N-CA-C	5.70	116.61	108.74
1	A	164	HIS	CB-CG-ND1	5.68	131.22	122.70
1	B	188	THR	N-CA-CB	-5.66	103.38	110.90
1	B	474	TRP	CG-CD2-CE3	5.65	139.55	133.90
1	B	504	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	A	563	HIS	CB-CG-ND1	5.64	131.16	122.70
1	B	474	TRP	CD1-CG-CD2	5.63	115.32	106.30
1	B	8	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	A	111	PHE	CA-CB-CG	5.60	119.40	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	ASN	CB-CG-ND2	5.54	124.71	116.40
1	A	393	ARG	N-CA-C	-5.54	105.32	111.36
1	A	202	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	B	257	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	B	474	TRP	CE2-CD2-CG	-5.52	100.58	107.20
1	A	465	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	193	THR	CA-C-O	-5.50	114.48	120.87
1	A	96	PHE	CA-CB-CG	5.50	119.30	113.80
1	B	392	GLU	N-CA-C	5.48	117.96	111.33
1	A	278	THR	N-CA-C	-5.47	101.00	108.38
1	B	286	PHE	CA-C-N	-5.45	112.65	122.46
1	B	286	PHE	C-N-CA	-5.45	112.65	122.46
1	A	523	VAL	N-CA-C	-5.44	101.06	107.70
1	B	421	ASP	CA-CB-CG	5.43	118.03	112.60
1	B	110	VAL	CA-CB-CG1	5.38	119.55	110.40
1	B	449	THR	CB-CA-C	5.36	116.32	110.15
1	A	201	HIS	CB-CG-ND1	5.36	130.74	122.70
1	A	477	LYS	CA-CB-CG	-5.36	103.38	114.10
1	A	553	TRP	CG-CD2-CE3	5.35	139.25	133.90
1	A	545	VAL	CA-C-N	5.35	125.35	120.21
1	A	545	VAL	C-N-CA	5.35	125.35	120.21
1	B	377	ARG	N-CA-C	-5.35	105.35	111.07
1	A	390	HIS	CA-C-O	-5.34	114.95	121.78
1	B	267	TRP	CG-CD2-CE3	5.33	139.23	133.90
1	B	465	ASP	CA-C-O	5.33	124.19	119.71
1	A	202	HIS	O-C-N	-5.33	116.08	123.12
1	A	390	HIS	CB-CG-CD2	-5.31	124.30	131.20
1	A	25	VAL	N-CA-C	-5.30	99.93	107.77
1	B	188	THR	CA-CB-CG2	5.29	119.50	110.50
1	A	196	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	521	ARG	N-CA-C	-5.28	101.09	109.59
1	A	470	ARG	N-CA-C	-5.27	102.36	110.32
1	A	440	VAL	CA-CB-CG2	5.27	119.36	110.40
1	B	335	TRP	CE2-CD2-CG	-5.27	100.88	107.20
1	A	504	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	A	149	ASP	CA-C-N	5.25	123.44	119.66
1	A	149	ASP	C-N-CA	5.25	123.44	119.66
1	A	474	TRP	CG-CD1-NE1	-5.24	103.39	110.20
1	B	278	THR	N-CA-C	-5.23	101.33	108.38
1	A	244	HIS	CB-CG-CD2	-5.22	124.41	131.20
1	B	391	ALA	N-CA-C	5.21	117.38	111.02
1	A	305	GLU	N-CA-C	5.19	117.68	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	THR	N-CA-C	5.18	118.38	111.75
1	A	237	ILE	N-CA-C	-5.17	101.03	108.48
1	A	382	ARG	CA-CB-CG	-5.17	103.76	114.10
1	A	501	THR	N-CA-C	-5.16	105.82	112.68
1	A	508	TRP	CG-CD1-NE1	-5.15	103.50	110.20
1	A	218	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	504	ASN	CB-CG-ND2	5.15	124.12	116.40
1	A	478	GLU	CB-CG-CD	5.14	121.34	112.60
1	B	464	THR	CA-CB-CG2	5.14	119.24	110.50
1	B	202	HIS	CB-CG-ND1	5.14	130.41	122.70
1	A	147	SER	CA-C-N	5.13	127.58	120.29
1	A	147	SER	C-N-CA	5.13	127.58	120.29
1	B	510	ALA	N-CA-C	-5.12	99.94	108.34
1	A	315	MET	CA-CB-CG	-5.11	103.88	114.10
1	A	495	HIS	CB-CG-CD2	-5.10	124.56	131.20
1	A	304	LYS	CA-C-O	-5.10	115.46	121.07
1	A	132	VAL	N-CA-C	-5.09	100.24	107.77
1	B	474	TRP	CB-CG-CD1	-5.08	119.28	126.90
1	A	130	GLU	N-CA-C	5.08	118.97	112.26
1	B	289	GLN	N-CA-C	-5.07	99.72	108.69
1	B	160	ALA	N-CA-C	5.07	116.82	110.24
1	B	427	THR	CA-CB-OG1	-5.06	102.01	109.60
1	B	249	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	148	ASN	CB-CG-ND2	5.05	123.98	116.40
1	B	563	HIS	CA-CB-CG	5.04	118.84	113.80
1	B	561	GLU	CA-C-O	5.03	127.82	122.13
1	A	146	PRO	N-CA-C	5.03	120.47	113.98
1	B	533	ASN	CA-CB-CG	5.03	117.63	112.60
1	B	127	TRP	CE2-CD2-CG	-5.03	101.17	107.20
1	B	127	TRP	CG-CD1-NE1	-5.01	103.69	110.20

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	TYR	Sidechain
1	A	140	ARG	Sidechain
1	A	191	TYR	Sidechain
1	A	224	ARG	Sidechain
1	A	231	ARG	Sidechain
1	A	24	ARG	Sidechain
1	A	26	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	28	ARG	Sidechain
1	A	283	TYR	Sidechain
1	A	323	ARG	Sidechain
1	A	367	GLN	Mainchain
1	A	405	TYR	Sidechain
1	A	45	TYR	Sidechain
1	A	469	ARG	Sidechain
1	A	481	ARG	Sidechain
1	A	487	TYR	Sidechain
1	A	492	ARG	Sidechain
1	A	496	ARG	Sidechain
1	A	502	ARG	Sidechain
1	A	506	ARG	Sidechain
1	A	523	VAL	Peptide
1	A	7	PHE	Sidechain
1	A	8	HIS	Peptide
1	A	96	PHE	Sidechain
1	B	115	TYR	Sidechain
1	B	16	TYR	Sidechain
1	B	163	ARG	Sidechain
1	B	178	ARG	Sidechain
1	B	181	TYR	Sidechain
1	B	191	TYR	Sidechain
1	B	204	TYR	Sidechain
1	B	24	ARG	Sidechain
1	B	28	ARG	Sidechain
1	B	280	ARG	Sidechain
1	B	283	TYR	Sidechain
1	B	323	ARG	Sidechain
1	B	377	ARG	Sidechain
1	B	393	ARG	Sidechain
1	B	394	PHE	Sidechain
1	B	402	ARG	Sidechain
1	B	454	TYR	Sidechain
1	B	469	ARG	Sidechain
1	B	470	ARG	Sidechain
1	B	492	ARG	Sidechain
1	B	517	TYR	Sidechain
1	B	521	ARG	Sidechain
1	B	523	VAL	Peptide
1	B	559	GLY	Peptide
1	B	63	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	B	82	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	A	4776	0	4607	86	0
1	B	4776	0	4607	96	0
2	A	267	0	0	2	0
2	B	211	0	0	0	0
All	All	10030	0	9214	180	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 10.

All (180) 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:B:281:THR:H	1:B:289:GLN:HE22	1.28	0.79
1:A:136:ILE:HD12	1:A:190:LEU:HG	1.67	0.76
1:B:136:ILE:HD12	1:B:190:LEU:HG	1.66	0.76
1:B:75:CYS:SG	1:B:80:VAL:HB	2.27	0.75
1:B:290:VAL:HG11	1:B:293:MET:SD	2.29	0.73
1:B:185:LEU:HA	1:B:488:LYS:HG2	1.71	0.73
1:A:297:ARG:HG2	1:A:300:ASN:HB2	1.73	0.71
1:A:27:LEU:HD22	1:A:37:CYS:SG	2.33	0.69
1:B:363:LEU:HD21	1:B:371:VAL:HG13	1.75	0.69
1:A:417:LEU:HD11	1:A:440:VAL:HG12	1.75	0.67
1:A:328:ASN:ND2	1:A:355:ILE:HG23	2.10	0.67
1:A:7:PHE:HZ	1:A:9:GLU:HG3	1.60	0.67
1:A:484:PHE:CE2	1:A:488:LYS:HE3	2.30	0.66
1:B:583:ASN:ND2	1:B:585:ARG:HB2	2.10	0.66
1:A:224:ARG:NH2	1:A:227:ASP:HB3	2.10	0.66
1:B:256:LEU:HD21	1:B:277:LYS:HD3	1.78	0.65
1:A:6:ILE:HD13	1:A:86:LEU:HD13	1.78	0.65
1:B:131:ALA:HA	1:B:188:THR:HG21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LEU:HD12	1:B:83:VAL:HG13	1.77	0.64
1:A:328:ASN:HD22	1:A:355:ILE:HG23	1.64	0.62
1:B:363:LEU:HD12	1:B:409:ALA:HB1	1.81	0.62
1:B:484:PHE:CE2	1:B:488:LYS:HD2	2.34	0.62
1:A:523:VAL:O	1:A:526:GLN:HB3	2.00	0.61
1:B:245:ALA:HB2	1:B:296:LEU:HD13	1.83	0.60
1:A:423:GLU:HB3	1:A:463:ALA:HA	1.84	0.60
1:B:178:ARG:HG3	1:B:474:TRP:CZ2	2.37	0.59
1:B:140:ARG:HH21	1:B:162:PRO:HB3	1.66	0.59
1:A:7:PHE:CZ	1:A:9:GLU:HG3	2.37	0.59
1:A:261:GLN:H	1:A:261:GLN:HE21	1.50	0.59
1:A:44:ARG:HG2	1:A:112:GLN:HE21	1.68	0.58
1:B:198:SER:HB3	1:B:203:LYS:HD2	1.85	0.58
1:B:503:GLY:HA2	1:B:523:VAL:HG23	1.86	0.57
1:B:8:HIS:HE1	1:B:25:VAL:HG23	1.69	0.57
1:A:546:PRO:HG3	1:A:553:TRP:CH2	2.39	0.57
1:A:407:GLU:O	1:A:411:GLN:HG3	2.05	0.57
1:B:8:HIS:CE1	1:B:25:VAL:HG23	2.39	0.57
1:B:323:ARG:HH12	1:B:354:GLU:CD	2.13	0.56
1:B:253:ARG:HA	1:B:256:LEU:HD12	1.86	0.56
1:A:98:GLU:HB2	1:A:110:VAL:O	2.04	0.56
1:B:542:LEU:HD22	1:B:568:GLN:HB3	1.86	0.56
1:B:583:ASN:HD21	1:B:585:ARG:HB2	1.71	0.56
1:B:163:ARG:NH2	1:B:165:ASP:HB2	2.22	0.55
1:A:314:TRP:HB3	1:A:319:ILE:HD13	1.89	0.55
1:A:1:MET:HE3	1:A:92:GLU:HB2	1.89	0.55
1:A:36:ARG:HG2	1:A:56:LEU:HD11	1.89	0.55
1:A:30:LYS:HG3	1:B:4:GLU:HG3	1.88	0.55
1:A:260:GLU:HA	1:A:265:LYS:HD3	1.89	0.54
1:A:499:SER:OG	1:A:526:GLN:HG2	2.07	0.54
1:B:389:ILE:HB	1:B:393:ARG:HB3	1.89	0.54
1:B:1:MET:HA	1:B:33:ASP:HB3	1.90	0.53
1:A:573:LEU:HD13	1:A:579:MET:SD	2.48	0.53
1:B:130:GLU:HB3	1:B:501:THR:HG21	1.91	0.52
1:B:174:GLY:O	1:B:178:ARG:HG2	2.09	0.52
1:B:7:PHE:CZ	1:B:9:GLU:HG3	2.45	0.52
1:B:256:LEU:CD2	1:B:277:LYS:HD3	2.40	0.52
1:B:269:PHE:HB2	1:B:284:GLU:HB2	1.92	0.52
1:A:281:THR:HG21	1:A:285:THR:HG23	1.91	0.52
1:A:178:ARG:HG3	1:A:474:TRP:CZ2	2.45	0.51
1:B:416:LEU:H	1:B:416:LEU:HD23	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LYS:NZ	2:A:751:HOH:O	2.44	0.51
1:B:444:MET:O	1:B:494:ARG:HD2	2.09	0.51
1:A:543:LEU:HD12	1:A:569:LEU:HD23	1.93	0.51
1:B:246:GLY:HA2	1:B:292:ALA:O	2.12	0.50
1:B:230:HIS:HE1	1:B:318:GLY:O	1.93	0.50
1:B:332:HIS:O	1:B:336:ARG:HB2	2.12	0.50
1:B:78:LYS:O	1:B:115:TYR:HA	2.12	0.50
1:A:57:ALA:HA	1:A:71:ALA:HB2	1.94	0.50
1:A:82:TYR:CE2	1:A:111:PHE:HB2	2.47	0.49
1:A:281:THR:HG22	1:A:283:TYR:H	1.76	0.49
1:A:542:LEU:HA	1:A:569:LEU:O	2.11	0.49
1:B:546:PRO:HD2	1:B:553:TRP:CZ2	2.47	0.49
1:B:243:ASN:OD1	1:B:295:LYS:NZ	2.45	0.49
1:B:483:LEU:O	1:B:486:PHE:HB3	2.13	0.49
1:A:261:GLN:H	1:A:261:GLN:NE2	2.11	0.48
1:A:484:PHE:HE2	1:A:488:LYS:HE3	1.77	0.48
1:A:415:ASN:ND2	1:A:448:GLY:HA3	2.28	0.48
1:B:37:CYS:HB3	1:B:57:ALA:HB3	1.94	0.48
1:B:324:LEU:HD13	1:B:335:TRP:CZ3	2.48	0.48
1:B:281:THR:N	1:B:289:GLN:HE22	2.05	0.48
1:A:281:THR:HG21	1:A:285:THR:CG2	2.43	0.48
1:A:240:ALA:HB2	1:A:322:TRP:CE3	2.49	0.48
1:B:470:ARG:HG3	1:B:471:PRO:HD2	1.94	0.48
1:B:372:MET:HE1	1:B:451:LEU:CD2	2.44	0.47
1:B:372:MET:SD	1:B:414:TRP:HE3	2.37	0.47
1:A:505:VAL:HG13	1:A:521:ARG:HD3	1.95	0.47
1:B:332:HIS:HD2	1:B:367:GLN:OE1	1.97	0.47
1:B:150:PRO:HD3	1:B:215:GLN:HG3	1.96	0.47
1:A:324:LEU:HD13	1:A:335:TRP:CZ3	2.50	0.47
1:B:468:CYS:SG	1:B:469:ARG:HG3	2.55	0.47
1:A:138:PRO:HG2	1:A:195:ILE:HG22	1.97	0.47
1:B:24:ARG:HD2	1:B:407:GLU:OE1	2.15	0.47
1:A:1:MET:HE2	1:A:88:GLY:N	2.29	0.47
1:A:527:HIS:HE1	1:A:548:SER:HB3	1.80	0.47
1:A:30:LYS:HG2	1:A:31:LYS:N	2.30	0.46
1:B:256:LEU:HD23	1:B:275:VAL:HG23	1.97	0.46
1:A:202:HIS:O	1:A:202:HIS:ND1	2.48	0.46
1:B:162:PRO:HG2	1:B:470:ARG:HA	1.97	0.46
1:B:275:VAL:HA	1:B:282:ASN:HD21	1.80	0.46
1:B:363:LEU:HD12	1:B:409:ALA:CB	2.43	0.46
1:B:240:ALA:HB2	1:B:322:TRP:CE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:HB2	1:A:234:ILE:HD12	1.98	0.46
1:B:33:ASP:O	1:B:89:PRO:HD3	2.15	0.46
1:A:197:ALA:O	1:A:207:ALA:HB3	2.15	0.46
1:A:326:VAL:HG12	1:A:329:GLU:HB2	1.98	0.46
1:A:416:LEU:HB3	1:A:451:LEU:HD23	1.97	0.46
1:A:553:TRP:HB3	1:A:581:LEU:HB3	1.98	0.46
1:B:449:THR:HA	1:B:450:PRO:HD3	1.86	0.46
1:A:198:SER:HB3	1:A:203:LYS:HD2	1.98	0.45
1:B:39:VAL:HG22	1:B:84:PHE:CD1	2.51	0.45
1:A:265:LYS:HB2	1:A:273:PHE:HZ	1.81	0.45
1:A:312:ARG:O	1:A:316:GLU:HG2	2.16	0.45
1:B:283:TYR:CE1	1:B:294:PRO:HB3	2.51	0.45
1:B:286:PHE:HE1	1:B:326:VAL:HG21	1.82	0.45
1:B:381:ILE:O	1:B:385:ALA:HB3	2.16	0.45
1:A:245:ALA:HB2	1:A:296:LEU:HD11	1.99	0.45
1:A:444:MET:C	1:A:494:ARG:HH11	2.24	0.45
1:B:59:LYS:NZ	1:B:67:ASP:CG	2.74	0.45
1:A:189:ALA:HA	1:A:235:LYS:H	1.82	0.44
1:B:417:LEU:HD11	1:B:440:VAL:HG12	1.99	0.44
1:B:371:VAL:H	1:B:413:LEU:HD23	1.83	0.44
1:A:300:ASN:HA	1:A:301:PRO:HD3	1.90	0.44
1:A:308:PHE:O	1:A:312:ARG:HG3	2.18	0.44
1:B:328:ASN:HB3	1:B:355:ILE:CG1	2.48	0.44
1:B:15:ALA:HA	1:B:24:ARG:O	2.17	0.44
1:B:328:ASN:HB3	1:B:355:ILE:HG13	2.00	0.44
1:B:355:ILE:HD11	1:B:368:PHE:HE2	1.83	0.43
1:B:372:MET:SD	1:B:414:TRP:CE3	3.11	0.43
1:B:163:ARG:HH22	1:B:165:ASP:HB2	1.83	0.43
1:B:219:LEU:HD21	1:B:313:PHE:HZ	1.82	0.43
1:B:425:PHE:HB3	1:B:436:PHE:HE1	1.82	0.43
1:A:124:THR:HB	2:A:706:HOH:O	2.18	0.43
1:B:260:GLU:HB3	1:B:273:PHE:CD2	2.54	0.43
1:A:64:GLU:H	1:A:396:ALA:HB1	1.83	0.43
1:A:467:ASP:O	1:A:470:ARG:HG3	2.18	0.43
1:B:41:TYR:CD1	1:B:73:LEU:HG	2.54	0.43
1:B:179:LEU:HD23	1:B:182:LEU:HD12	1.98	0.43
1:B:465:ASP:HA	1:B:466:PRO:HA	1.66	0.43
1:B:448:GLY:O	1:B:494:ARG:NH2	2.52	0.43
1:A:158:LYS:CD	1:A:478:GLU:HG3	2.49	0.42
1:A:149:ASP:HB3	1:A:153:THR:OG1	2.19	0.42
1:A:240:ALA:HB2	1:A:322:TRP:HE3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:HB2	1:A:502:ARG:HH21	1.84	0.42
1:B:424:ARG:HH11	1:B:424:ARG:HD3	1.65	0.42
1:A:137:PHE:CZ	1:A:469:ARG:HD3	2.55	0.42
1:A:527:HIS:CE1	1:A:548:SER:HB3	2.54	0.42
1:B:75:CYS:SG	1:B:80:VAL:CB	3.02	0.42
1:A:250:PHE:HE2	1:A:306:TYR:CE2	2.38	0.42
1:B:285:THR:HB	1:B:290:VAL:O	2.19	0.42
1:B:518:ALA:HA	1:B:530:VAL:O	2.19	0.42
1:A:26:ARG:HD2	1:A:403:MET:SD	2.60	0.41
1:A:65:ARG:HH12	1:B:101:PHE:HD2	1.67	0.41
1:A:150:PRO:HG3	1:A:215:GLN:HG2	2.02	0.41
1:A:297:ARG:HG2	1:A:300:ASN:CB	2.48	0.41
1:A:526:GLN:HA	1:A:585:ARG:HB2	2.02	0.41
1:B:251:ALA:O	1:B:255:VAL:HG23	2.21	0.41
1:A:8:HIS:CD2	1:A:26:ARG:O	2.73	0.41
1:A:102:SER:HB3	1:A:104:GLU:O	2.20	0.41
1:B:504:ASN:O	1:B:521:ARG:HA	2.21	0.41
1:B:373:ASN:HB2	1:B:413:LEU:HB3	2.03	0.41
1:A:531:VAL:O	1:A:578:GLY:HA2	2.20	0.41
1:B:247:ASP:HA	1:B:252:PHE:CD2	2.55	0.41
1:A:522:THR:HA	1:A:526:GLN:O	2.21	0.41
1:B:381:ILE:HD13	1:B:425:PHE:HE1	1.85	0.41
1:A:476:GLU:HB2	1:A:477:LYS:HE2	2.03	0.41
1:B:308:PHE:O	1:B:312:ARG:HG3	2.21	0.41
1:B:381:ILE:HD13	1:B:425:PHE:CE1	2.56	0.41
1:B:563:HIS:O	1:B:569:LEU:HA	2.20	0.41
1:A:84:PHE:O	1:A:95:TYR:HA	2.21	0.41
1:A:134:TYR:OH	1:A:454:TYR:HA	2.21	0.41
1:A:381:ILE:O	1:A:385:ALA:HB3	2.20	0.41
1:A:555:ASP:HB3	1:A:559:GLY:H	1.86	0.41
1:B:230:HIS:CE1	1:B:318:GLY:O	2.72	0.41
1:B:505:VAL:HG22	1:B:521:ARG:CD	2.51	0.41
1:A:146:PRO:HA	1:A:149:ASP:OD1	2.21	0.41
1:B:44:ARG:HH11	1:B:44:ARG:HD3	1.73	0.41
1:B:228:GLU:CD	1:B:231:ARG:HH21	2.29	0.40
1:A:190:LEU:HD13	1:A:234:ILE:HG21	2.02	0.40
1:B:240:ALA:HB3	1:B:324:LEU:HD23	2.04	0.40
1:A:149:ASP:HA	1:A:150:PRO:HD3	1.86	0.40
1:A:355:ILE:HD11	1:A:368:PHE:HE2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	583/585 (100%)	534 (92%)	45 (8%)	4 (1%)	18	38
1	B	583/585 (100%)	534 (92%)	46 (8%)	3 (0%)	24	46
All	All	1166/1170 (100%)	1068 (92%)	91 (8%)	7 (1%)	21	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	562	VAL
1	A	64	GLU
1	B	562	VAL
1	A	430	GLY
1	B	118	ARG
1	B	345	LEU
1	A	275	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	493/493 (100%)	449 (91%)	44 (9%)	9	20
1	B	493/493 (100%)	436 (88%)	57 (12%)	5	11
All	All	986/986 (100%)	885 (90%)	101 (10%)	7	15

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	18	ILE
1	A	25	VAL
1	A	27	LEU
1	A	36	ARG
1	A	49	GLU
1	A	50	GLU
1	A	63	ASP
1	A	72	LEU
1	A	110	VAL
1	A	130	GLU
1	A	147	SER
1	A	190	LEU
1	A	214	PRO
1	A	224	ARG
1	A	238	LEU
1	A	255	VAL
1	A	257	GLN
1	A	261	GLN
1	A	270	ILE
1	A	280	ARG
1	A	281	THR
1	A	291	PRO
1	A	296	LEU
1	A	317	GLN
1	A	323	ARG
1	A	330	VAL
1	A	375	LEU
1	A	393	ARG
1	A	398	LEU
1	A	406	PRO
1	A	423	GLU
1	A	426	LEU
1	A	440	VAL
1	A	457	GLU
1	A	483	LEU
1	A	496	ARG
1	A	504	ASN
1	A	505	VAL
1	A	528	VAL
1	A	535	ARG
1	A	547	GLU
1	A	548	SER

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Mol	Chain	Res	Type
1	A	573	LEU
1	B	4	GLU
1	B	25	VAL
1	B	40	LEU
1	B	51	GLU
1	B	62	SER
1	B	64	GLU
1	B	73	LEU
1	B	76	SER
1	B	78	LYS
1	B	106	SER
1	B	110	VAL
1	B	124	THR
1	B	130	GLU
1	B	154	GLU
1	B	171	ASP
1	B	190	LEU
1	B	206	THR
1	B	220	PRO
1	B	223	ARG
1	B	231	ARG
1	B	237	ILE
1	B	239	ASP
1	B	254	ASP
1	B	258	LYS
1	B	271	GLU
1	B	279	SER
1	B	316	GLU
1	B	326	VAL
1	B	328	ASN
1	B	329	GLU
1	B	330	VAL
1	B	364	MET
1	B	375	LEU
1	B	393	ARG
1	B	398	LEU
1	B	411	GLN
1	B	440	VAL
1	B	441	LEU
1	B	457	GLU
1	B	464	THR
1	B	465	ASP

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Mol	Chain	Res	Type
1	B	475	GLU
1	B	477	LYS
1	B	483	LEU
1	B	504	ASN
1	B	507	SER
1	B	512	LYS
1	B	523	VAL
1	B	524	GLN
1	B	537	GLU
1	B	538	LYS
1	B	540	THR
1	B	547	GLU
1	B	548	SER
1	B	561	GLU
1	B	575	PRO
1	B	585	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	54	HIS
1	A	112	GLN
1	A	148	ASN
1	A	244	HIS
1	A	261	GLN
1	A	328	ASN
1	A	332	HIS
1	A	443	GLN
1	A	479	GLN
1	A	504	ASN
1	A	527	HIS
1	A	534	ASN
1	B	54	HIS
1	B	244	HIS
1	B	289	GLN
1	B	332	HIS
1	B	346	ASN
1	B	504	ASN
1	B	509	HIS
1	B	534	ASN
1	B	539	GLN

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Mol	Chain	Res	Type
1	B	544	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 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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	585/585 (100%)	-0.74	1 (0%) 91 90	8, 26, 45, 55	0
1	B	585/585 (100%)	-0.65	2 (0%) 90 88	7, 29, 47, 60	0
All	All	1170/1170 (100%)	-0.69	3 (0%) 90 88	7, 28, 46, 60	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	546	PRO	3.9
1	B	548	SER	3.5
1	B	524	GLN	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.