



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:03 am BST

PDB ID : 1YPI  
Title : STRUCTURE OF YEAST TRIOSEPHOSPHATE ISOMERASE AT 1.9-  
ANGSTROMS RESOLUTION  
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Deposited on : 1990-01-12  
Resolution : 1.90 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

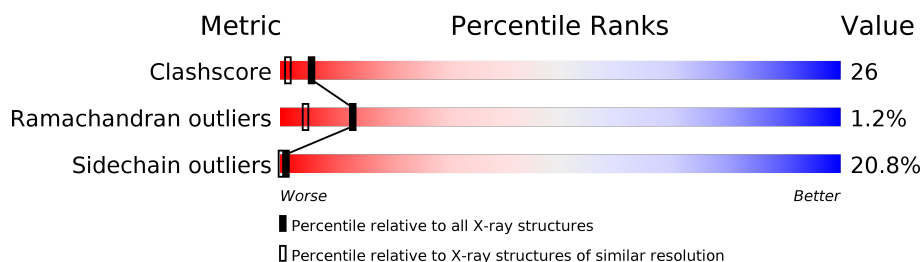
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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  $\geq 3$ , 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	247	
1	B	247	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3885 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 TRIOSEPHOSPHATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1883	1196	320	365	2			
1	B	247	Total	C	N	O	S	0	0	0
			1883	1196	320	365	2			

- Molecule 2 is water.

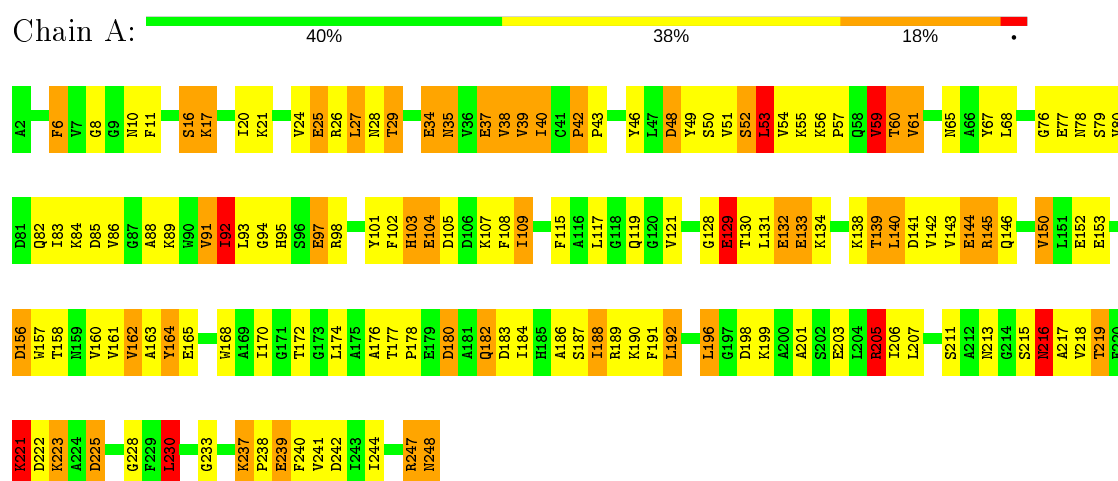
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	66	Total	O	0	0
			66	66		
2	B	53	Total	O	0	0
			53	53		

### 3 Residue-property plots

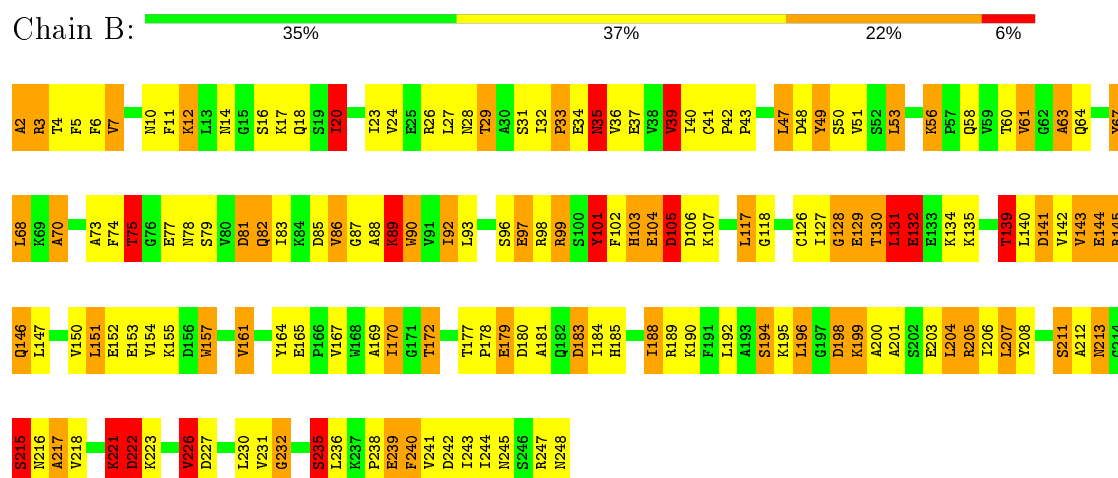
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



#### • Molecule 1: TRIOSEPHOSPHATE ISOMERASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.15Å 98.55Å 49.26Å 90.00° 91.20° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3885	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	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	2.03	41/1915 (2.1%)	2.42	98/2590 (3.8%)
1	B	2.12	46/1915 (2.4%)	2.49	115/2590 (4.4%)
All	All	2.07	87/3830 (2.3%)	2.45	213/5180 (4.1%)

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	235	SER	CB-OG	-11.36	1.27	1.42
1	B	165	GLU	CD-OE2	10.85	1.37	1.25
1	A	239	GLU	CD-OE1	-10.80	1.13	1.25
1	A	152	GLU	CD-OE2	10.26	1.36	1.25
1	A	144	GLU	CD-OE2	10.22	1.36	1.25
1	B	153	GLU	CD-OE2	9.84	1.36	1.25
1	A	165	GLU	CD-OE1	-9.62	1.15	1.25
1	A	165	GLU	CD-OE2	8.58	1.35	1.25
1	B	37	GLU	CD-OE2	8.28	1.34	1.25
1	B	215	SER	CB-OG	8.24	1.52	1.42
1	B	232	GLY	N-CA	-8.19	1.33	1.46
1	B	203	GLU	CD-OE2	7.96	1.34	1.25
1	A	132	GLU	CD-OE2	7.92	1.34	1.25
1	B	97	GLU	CD-OE1	-7.92	1.17	1.25
1	B	77	GLU	CD-OE2	7.82	1.34	1.25
1	B	165	GLU	CD-OE1	-7.77	1.17	1.25
1	A	46	TYR	CG-CD2	7.73	1.49	1.39
1	B	239	GLU	CD-OE1	-7.70	1.17	1.25
1	B	132	GLU	CD-OE2	7.64	1.34	1.25
1	B	87	GLY	C-O	7.62	1.35	1.23
1	B	144	GLU	CD-OE2	7.48	1.33	1.25
1	B	205	ARG	NE-CZ	7.43	1.42	1.33
1	A	216	ASN	CA-CB	7.24	1.72	1.53
1	B	34	GLU	CD-OE2	7.05	1.33	1.25
1	A	133	GLU	CD-OE2	7.00	1.33	1.25
1	A	52	SER	CA-CB	6.98	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	ARG	CZ-NH1	6.96	1.42	1.33
1	B	131	LEU	N-CA	6.88	1.60	1.46
1	B	199	LYS	N-CA	6.80	1.59	1.46
1	B	179	GLU	CD-OE2	6.74	1.33	1.25
1	B	144	GLU	CD-OE1	-6.68	1.18	1.25
1	A	129	GLU	CG-CD	-6.67	1.42	1.51
1	B	99	ARG	CZ-NH2	6.65	1.41	1.33
1	A	144	GLU	CG-CD	6.59	1.61	1.51
1	A	156	ASP	C-O	6.57	1.35	1.23
1	B	157	TRP	CE3-CZ3	6.57	1.49	1.38
1	B	194	SER	CA-CB	-6.49	1.43	1.52
1	A	42	PRO	N-CD	6.46	1.56	1.47
1	A	97	GLU	CD-OE2	6.44	1.32	1.25
1	A	34	GLU	N-CA	6.43	1.59	1.46
1	A	34	GLU	CD-OE2	6.41	1.32	1.25
1	A	153	GLU	CD-OE1	6.40	1.32	1.25
1	B	194	SER	CB-OG	6.36	1.50	1.42
1	B	128	GLY	CA-C	6.29	1.61	1.51
1	B	34	GLU	CG-CD	-6.19	1.42	1.51
1	B	29	THR	C-O	6.18	1.35	1.23
1	A	25	GLU	CD-OE2	6.09	1.32	1.25
1	B	31	SER	CB-OG	6.07	1.50	1.42
1	B	211	SER	CB-OG	6.05	1.50	1.42
1	B	157	TRP	CE2-CZ2	-5.99	1.29	1.39
1	B	230	LEU	CA-CB	-5.90	1.40	1.53
1	B	126	CYS	CB-SG	-5.90	1.72	1.81
1	B	43	PRO	C-O	5.85	1.34	1.23
1	B	5	PHE	CB-CG	-5.83	1.41	1.51
1	B	96	SER	CA-CB	-5.75	1.44	1.52
1	A	48	ASP	N-CA	5.65	1.57	1.46
1	B	29	THR	C-N	-5.61	1.21	1.34
1	A	187	SER	N-CA	-5.61	1.35	1.46
1	A	233	GLY	C-O	5.57	1.32	1.23
1	A	247	ARG	CD-NE	5.53	1.55	1.46
1	A	53	LEU	C-O	5.52	1.33	1.23
1	A	223	LYS	CD-CE	-5.50	1.37	1.51
1	B	70	ALA	CA-CB	-5.50	1.40	1.52
1	A	121	VAL	C-N	-5.50	1.23	1.33
1	B	130	THR	C-O	5.38	1.33	1.23
1	A	121	VAL	C-O	5.36	1.33	1.23
1	A	144	GLU	CD-OE1	-5.34	1.19	1.25
1	A	203	GLU	CD-OE2	5.33	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	GLU	CD-OE2	5.31	1.31	1.25
1	A	211	SER	N-CA	5.29	1.56	1.46
1	A	239	GLU	CD-OE2	5.28	1.31	1.25
1	B	231	VAL	C-N	-5.27	1.23	1.33
1	A	16	SER	CA-CB	-5.23	1.45	1.52
1	B	208	TYR	CG-CD2	5.20	1.46	1.39
1	B	63	ALA	C-N	-5.19	1.22	1.34
1	A	102	PHE	CD2-CE2	5.13	1.49	1.39
1	A	174	LEU	C-N	-5.11	1.22	1.34
1	B	5	PHE	CG-CD1	5.09	1.46	1.38
1	B	67	TYR	CE2-CZ	5.08	1.45	1.38
1	B	33	PRO	N-CD	5.07	1.54	1.47
1	B	248	ASN	N-CA	-5.07	1.36	1.46
1	B	104	GLU	CD-OE2	5.07	1.31	1.25
1	A	8	GLY	C-N	-5.06	1.24	1.33
1	A	230	LEU	CA-CB	-5.06	1.42	1.53
1	A	189	ARG	NE-CZ	5.06	1.39	1.33
1	A	40	ILE	CA-CB	-5.04	1.43	1.54
1	A	53	LEU	C-N	-5.03	1.22	1.34

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ARG	NE-CZ-NH1	21.15	130.87	120.30
1	A	205	ARG	NE-CZ-NH2	-19.66	110.47	120.30
1	B	205	ARG	NE-CZ-NH2	-19.34	110.63	120.30
1	B	203	GLU	CA-CB-CG	18.89	154.97	113.40
1	A	247	ARG	NE-CZ-NH1	-17.80	111.40	120.30
1	B	205	ARG	NE-CZ-NH1	16.89	128.75	120.30
1	B	3	ARG	NE-CZ-NH1	-16.51	112.05	120.30
1	B	144	GLU	CA-CB-CG	15.61	147.74	113.40
1	B	26	ARG	NE-CZ-NH1	-14.96	112.82	120.30
1	A	144	GLU	OE1-CD-OE2	13.25	139.19	123.30
1	B	205	ARG	CD-NE-CZ	-12.12	106.63	123.60
1	A	98	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	A	247	ARG	NE-CZ-NH2	10.83	125.71	120.30
1	A	221	LYS	CD-CE-NZ	10.74	136.41	111.70
1	A	46	TYR	CB-CG-CD1	10.74	127.45	121.00
1	B	29	THR	CA-CB-CG2	10.68	127.35	112.40
1	B	131	LEU	O-C-N	10.59	139.64	122.70
1	A	145	ARG	NE-CZ-NH1	-10.53	115.03	120.30
1	A	98	ARG	NE-CZ-NH1	10.45	125.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ASP	CB-CG-OD2	-10.42	108.92	118.30
1	B	247	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	B	26	ARG	CD-NE-CZ	10.28	137.99	123.60
1	A	105	ASP	CB-CG-OD1	10.08	127.37	118.30
1	A	222	ASP	CB-CG-OD1	9.97	127.27	118.30
1	B	161	VAL	CB-CA-C	9.81	130.03	111.40
1	B	221	LYS	CA-CB-CG	9.45	134.20	113.40
1	B	97	GLU	OE1-CD-OE2	9.39	134.57	123.30
1	A	37	GLU	CA-CB-CG	8.99	133.18	113.40
1	B	181	ALA	CB-CA-C	8.97	123.55	110.10
1	B	144	GLU	N-CA-CB	8.54	125.97	110.60
1	B	196	LEU	CA-CB-CG	8.16	134.06	115.30
1	A	216	ASN	CB-CA-C	-8.14	94.11	110.40
1	B	198	ASP	CB-CG-OD1	8.12	125.61	118.30
1	A	134	LYS	CB-CG-CD	7.64	131.47	111.60
1	A	156	ASP	CA-C-N	7.60	133.92	117.20
1	A	223	LYS	CB-CG-CD	7.60	131.37	111.60
1	A	191	PHE	CB-CG-CD2	7.59	126.11	120.80
1	B	37	GLU	OE1-CD-OE2	-7.59	114.19	123.30
1	A	183	ASP	CB-CG-OD1	-7.58	111.48	118.30
1	A	92	ILE	CA-CB-CG2	7.57	126.03	110.90
1	B	144	GLU	CB-CA-C	-7.47	95.46	110.40
1	B	104	GLU	CB-CA-C	7.38	125.16	110.40
1	A	101	TYR	CB-CG-CD2	7.36	125.42	121.00
1	A	230	LEU	CA-CB-CG	7.28	132.03	115.30
1	B	68	LEU	CA-CB-CG	7.17	131.80	115.30
1	A	139	THR	CA-CB-OG1	-7.14	94.00	109.00
1	B	105	ASP	CB-CG-OD2	-7.13	111.89	118.30
1	B	172	THR	CA-C-N	7.09	130.38	116.20
1	B	3	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	B	200	ALA	O-C-N	7.06	134.00	122.70
1	A	53	LEU	CA-CB-CG	7.04	131.48	115.30
1	A	109	ILE	CA-CB-CG1	-7.01	97.67	111.00
1	B	164	TYR	CG-CD1-CE1	-6.99	115.71	121.30
1	B	198	ASP	CA-CB-CG	6.95	128.68	113.40
1	B	49	TYR	CG-CD1-CE1	-6.93	115.76	121.30
1	B	152	GLU	OE1-CD-OE2	6.93	131.61	123.30
1	B	98	ARG	CG-CD-NE	6.91	126.32	111.80
1	B	144	GLU	CG-CD-OE2	-6.91	104.49	118.30
1	A	46	TYR	CB-CG-CD2	-6.90	116.86	121.00
1	A	216	ASN	CA-CB-CG	-6.87	98.28	113.40
1	A	78	ASN	CA-C-O	-6.84	105.72	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	B	227	ASP	CB-CG-OD1	-6.82	112.16	118.30
1	B	227	ASP	CB-CG-OD2	6.80	124.42	118.30
1	B	98	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	B	7	VAL	CB-CA-C	6.73	124.19	111.40
1	A	52	SER	CB-CA-C	-6.70	97.36	110.10
1	B	67	TYR	CB-CG-CD1	-6.70	116.98	121.00
1	A	186	ALA	C-N-CA	6.63	138.28	121.70
1	B	81	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	198	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	101	TYR	CB-CG-CD1	-6.59	117.05	121.00
1	B	153	GLU	OE1-CD-OE2	-6.59	115.39	123.30
1	A	129	GLU	CG-CD-OE1	6.57	131.44	118.30
1	A	86	VAL	CB-CA-C	6.55	123.85	111.40
1	B	117	LEU	CB-CA-C	6.55	122.64	110.20
1	A	219	THR	N-CA-CB	-6.52	97.91	110.30
1	A	221	LYS	CB-CG-CD	6.52	128.55	111.60
1	B	86	VAL	CA-CB-CG1	6.51	120.67	110.90
1	B	90	TRP	O-C-N	6.50	133.10	122.70
1	B	145	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	A	91	VAL	CB-CA-C	-6.46	99.13	111.40
1	B	35	ASN	CA-C-N	-6.44	103.04	117.20
1	A	196	LEU	CA-CB-CG	6.40	130.03	115.30
1	A	34	GLU	CA-CB-CG	6.40	127.48	113.40
1	B	145	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	A	161	VAL	N-CA-C	-6.36	93.83	111.00
1	B	153	GLU	CG-CD-OE1	6.35	131.00	118.30
1	B	180	ASP	O-C-N	6.34	132.85	122.70
1	B	183	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	B	3	ARG	N-CA-CB	6.28	121.90	110.60
1	B	222	ASP	CA-CB-CG	6.28	127.22	113.40
1	A	144	GLU	CB-CA-C	6.27	122.94	110.40
1	B	139	THR	O-C-N	6.23	132.67	122.70
1	A	108	PHE	CB-CG-CD1	-6.23	116.44	120.80
1	A	78	ASN	O-C-N	6.22	132.66	122.70
1	A	247	ARG	CB-CA-C	6.22	122.84	110.40
1	A	198	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	B	12	LYS	CA-C-O	-6.18	107.12	120.10
1	A	78	ASN	N-CA-CB	6.17	121.72	110.60
1	A	91	VAL	CA-CB-CG2	6.16	120.14	110.90
1	A	34	GLU	N-CA-C	-6.16	94.36	111.00
1	B	74	PHE	O-C-N	6.10	132.46	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	B	201	ALA	CB-CA-C	6.09	119.24	110.10
1	A	134	LYS	CA-CB-CG	6.06	126.74	113.40
1	B	99	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	67	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	B	39	VAL	CB-CA-C	6.04	122.87	111.40
1	B	132	GLU	N-CA-CB	6.02	121.44	110.60
1	A	85	ASP	O-C-N	5.99	132.29	122.70
1	A	176	ALA	CB-CA-C	5.99	119.08	110.10
1	B	205	ARG	O-C-N	5.98	132.27	122.70
1	A	40	ILE	O-C-N	5.97	132.26	122.70
1	B	49	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	B	181	ALA	N-CA-CB	-5.94	101.78	110.10
1	B	105	ASP	O-C-N	5.93	132.19	122.70
1	B	20	ILE	CB-CA-C	5.92	123.45	111.60
1	A	84	LYS	CA-CB-CG	5.91	126.41	113.40
1	B	67	TYR	CD1-CG-CD2	5.90	124.39	117.90
1	B	97	GLU	CG-CD-OE2	-5.88	106.55	118.30
1	B	2	ALA	C-N-CA	5.87	136.37	121.70
1	B	75	THR	CB-CA-C	5.86	127.42	111.60
1	A	141	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	81	ASP	CB-CG-OD1	-5.83	113.05	118.30
1	A	225	ASP	CB-CG-OD1	5.83	123.54	118.30
1	A	27	LEU	N-CA-C	-5.82	95.28	111.00
1	A	140	LEU	CA-CB-CG	5.82	128.69	115.30
1	B	130	THR	CA-C-O	-5.79	107.93	120.10
1	B	14	ASN	CB-CG-OD1	-5.79	110.03	121.60
1	A	161	VAL	N-CA-CB	5.77	124.20	111.50
1	A	91	VAL	N-CA-CB	5.77	124.20	111.50
1	B	35	ASN	CB-CG-OD1	-5.77	110.06	121.60
1	A	115	PHE	CG-CD1-CE1	5.75	127.13	120.80
1	B	92	ILE	CB-CA-C	5.75	123.10	111.60
1	B	235	SER	N-CA-CB	-5.74	101.90	110.50
1	B	207	LEU	CA-CB-CG	5.72	128.47	115.30
1	B	11	PHE	CA-CB-CG	5.72	127.63	113.90
1	B	143	VAL	CA-CB-CG1	5.72	119.48	110.90
1	B	12	LYS	O-C-N	5.69	131.80	122.70
1	B	37	GLU	CG-CD-OE1	5.68	129.67	118.30
1	A	230	LEU	N-CA-CB	5.67	121.75	110.40
1	B	106	ASP	CB-CG-OD1	-5.67	113.20	118.30
1	B	215	SER	CB-CA-C	5.65	120.84	110.10
1	A	216	ASN	CA-C-N	-5.64	104.78	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	LYS	N-CA-CB	-5.64	100.44	110.60
1	B	129	GLU	CA-CB-CG	5.60	125.73	113.40
1	B	146	GLN	CG-CD-OE1	-5.60	110.39	121.60
1	B	131	LEU	CB-CA-C	-5.59	99.58	110.20
1	A	152	GLU	CB-CA-C	-5.59	99.22	110.40
1	A	98	ARG	CG-CD-NE	5.59	123.53	111.80
1	A	104	GLU	CG-CD-OE1	5.59	129.47	118.30
1	A	59	VAL	CG1-CB-CG2	5.56	119.80	110.90
1	A	57	PRO	O-C-N	5.55	131.58	122.70
1	A	133	GLU	CG-CD-OE1	5.55	129.40	118.30
1	A	17	LYS	CA-CB-CG	5.53	125.57	113.40
1	B	247	ARG	NH1-CZ-NH2	-5.53	113.32	119.40
1	A	141	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	169	ALA	CB-CA-C	5.51	118.37	110.10
1	A	201	ALA	CB-CA-C	5.51	118.36	110.10
1	B	230	LEU	N-CA-CB	5.51	121.41	110.40
1	A	92	ILE	CB-CG1-CD1	-5.50	98.50	113.90
1	A	108	PHE	CB-CA-C	5.50	121.40	110.40
1	A	241	VAL	N-CA-CB	5.50	123.59	111.50
1	B	56	LYS	CA-CB-CG	5.48	125.45	113.40
1	A	219	THR	CA-CB-CG2	5.46	120.04	112.40
1	B	240	PHE	CB-CG-CD1	-5.45	116.99	120.80
1	A	38	VAL	CB-CA-C	5.42	121.70	111.40
1	B	5	PHE	CB-CG-CD2	5.42	124.59	120.80
1	A	216	ASN	N-CA-CB	-5.41	100.86	110.60
1	B	47	LEU	CA-CB-CG	5.41	127.75	115.30
1	B	218	VAL	CB-CA-C	5.41	121.68	111.40
1	B	14	ASN	O-C-N	5.41	132.39	123.20
1	A	165	GLU	CG-CD-OE1	5.39	129.08	118.30
1	B	49	TYR	CA-CB-CG	-5.39	103.16	113.40
1	B	226	VAL	O-C-N	5.38	131.31	122.70
1	B	47	LEU	N-CA-CB	-5.37	99.65	110.40
1	A	141	ASP	OD1-CG-OD2	-5.36	113.11	123.30
1	A	144	GLU	CG-CD-OE2	-5.36	107.58	118.30
1	A	215	SER	C-N-CA	5.35	135.07	121.70
1	A	97	GLU	CG-CD-OE2	-5.33	107.64	118.30
1	A	109	ILE	CB-CG1-CD1	5.32	128.79	113.90
1	A	67	TYR	O-C-N	5.30	131.19	122.70
1	B	26	ARG	NH1-CZ-NH2	5.30	125.23	119.40
1	B	205	ARG	CA-CB-CG	-5.29	101.77	113.40
1	B	199	LYS	CA-CB-CG	5.28	125.01	113.40
1	B	29	THR	CA-C-O	-5.25	109.07	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	VAL	CA-C-O	-5.25	109.07	120.10
1	A	102	PHE	CB-CG-CD2	-5.25	117.12	120.80
1	A	77	GLU	CG-CD-OE1	5.25	128.80	118.30
1	A	115	PHE	CZ-CE2-CD2	5.25	126.40	120.10
1	A	192	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	164	TYR	CB-CG-CD2	5.24	124.14	121.00
1	B	150	VAL	CA-C-O	-5.23	109.12	120.10
1	A	230	LEU	N-CA-C	-5.21	96.93	111.00
1	B	211	SER	O-C-N	5.19	131.00	122.70
1	B	78	ASN	O-C-N	5.18	130.99	122.70
1	A	40	ILE	CA-C-O	-5.17	109.25	120.10
1	B	101	TYR	CA-CB-CG	5.14	123.17	113.40
1	A	216	ASN	CA-C-O	5.14	130.89	120.10
1	B	199	LYS	CB-CG-CD	5.14	124.96	111.60
1	A	129	GLU	CB-CG-CD	5.13	128.05	114.20
1	B	213	ASN	CB-CG-OD1	5.13	131.85	121.60
1	B	131	LEU	CA-C-N	-5.11	105.96	117.20
1	B	67	TYR	CG-CD2-CE2	-5.11	117.21	121.30
1	B	20	ILE	CA-CB-CG2	5.08	121.06	110.90
1	B	217	ALA	CA-C-O	5.07	130.75	120.10
1	B	248	ASN	CA-C-O	-5.07	109.46	120.10
1	B	29	THR	CA-C-N	5.07	128.34	117.20
1	A	11	PHE	CB-CG-CD1	5.06	124.34	120.80
1	B	212	ALA	N-CA-CB	-5.03	103.06	110.10
1	A	89	LYS	C-N-CA	5.01	134.23	121.70
1	A	187	SER	N-CA-CB	5.01	118.02	110.50

There are no chirality outliers.

There are no planarity outliers.

## 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	1883	0	1888	94	1
1	B	1883	0	1886	112	1
2	A	66	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	0	11	0
All	All	3885	0	3774	194	1

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 26.

All (194) 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:232:GLY:O	1:B:235:SER:HB2	1.55	1.06
1:A:130:THR:OG1	1:A:133:GLU:HG3	1.55	1.04
1:B:151:LEU:HD12	1:B:157:TRP:CZ2	1.98	0.99
1:B:130:THR:O	1:B:131:LEU:HB2	1.58	0.98
1:A:216:ASN:O	1:A:219:THR:HB	1.65	0.97
1:B:161:VAL:HG23	1:B:205:ARG:HB2	1.47	0.96
1:B:102:PHE:HB3	2:B:755:HOH:O	1.67	0.95
1:A:140:LEU:O	1:A:144:GLU:HG2	1.69	0.92
1:B:151:LEU:HD12	1:B:157:TRP:HZ2	1.32	0.92
1:B:118:GLY:HA3	2:B:631:HOH:O	1.68	0.91
1:A:218:VAL:HG22	1:A:221:LYS:HE3	1.53	0.90
1:B:79:SER:HB3	1:B:82:GLN:CG	2.02	0.90
1:A:27:LEU:O	1:A:28:ASN:HB2	1.75	0.85
1:A:184:ILE:O	1:A:188:ILE:HG13	1.77	0.84
1:B:20:ILE:HD13	1:B:50:SER:OG	1.78	0.84
1:B:35:ASN:OD1	1:B:35:ASN:N	2.05	0.83
1:B:147:LEU:O	1:B:151:LEU:HD13	1.79	0.83
1:A:82:GLN:OE1	2:A:705:HOH:O	1.97	0.82
1:B:130:THR:O	1:B:131:LEU:CB	2.27	0.82
1:B:132:GLU:OE2	1:B:132:GLU:N	2.14	0.81
1:B:102:PHE:O	2:B:755:HOH:O	1.99	0.80
1:B:131:LEU:HB3	1:B:132:GLU:OE2	1.81	0.80
1:A:38:VAL:HG22	1:A:59:VAL:HB	1.63	0.79
1:B:128:GLY:H	1:B:146:GLN:HE22	1.30	0.77
1:B:60:THR:HG22	2:B:680:HOH:O	1.85	0.76
1:B:131:LEU:O	1:B:135:LYS:N	2.18	0.76
1:B:16:SER:O	1:B:20:ILE:HG23	1.85	0.76
1:B:33:PRO:HD3	1:B:245:ASN:ND2	2.01	0.75
1:A:97:GLU:OE2	1:B:75:THR:HG23	1.86	0.75
1:B:20:ILE:CD1	1:B:50:SER:OG	2.34	0.75
1:B:189:ARG:NH1	1:B:204:LEU:O	2.19	0.74
1:A:184:ILE:CD1	2:A:644:HOH:O	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLY:HA2	1:A:109:ILE:HD13	1.71	0.72
1:A:10:ASN:HD21	1:B:75:THR:HG21	1.55	0.72
1:A:6:PHE:CD2	1:A:37:GLU:HG2	2.25	0.71
1:A:184:ILE:HD13	2:A:644:HOH:O	1.90	0.71
1:B:32:ILE:O	1:B:32:ILE:HG13	1.91	0.71
1:A:97:GLU:OE2	1:B:75:THR:CG2	2.38	0.70
1:B:79:SER:HB3	1:B:82:GLN:HG2	1.71	0.70
1:B:221:LYS:O	1:B:222:ASP:HB2	1.92	0.69
1:B:79:SER:HB3	1:B:82:GLN:HG3	1.74	0.69
1:A:128:GLY:H	1:A:146:GLN:HE22	1.39	0.69
1:B:194:SER:C	1:B:195:LYS:HD3	2.13	0.69
1:B:178:PRO:HD2	1:B:179:GLU:OE1	1.92	0.68
1:B:131:LEU:CA	1:B:134:LYS:HB3	2.24	0.68
1:A:156:ASP:OD2	1:A:158:THR:HG23	1.93	0.68
1:B:151:LEU:CD1	1:B:157:TRP:CZ2	2.74	0.68
1:B:24:VAL:HG11	1:B:53:LEU:HB3	1.76	0.67
1:A:130:THR:HG1	1:A:133:GLU:HG3	1.59	0.66
1:A:218:VAL:O	1:A:221:LYS:HE3	1.95	0.66
1:A:76:GLY:H	1:B:64:GLN:HE21	1.45	0.65
1:B:32:ILE:HA	1:B:245:ASN:HD21	1.61	0.64
1:B:128:GLY:N	1:B:146:GLN:HE22	1.94	0.64
1:B:33:PRO:CD	1:B:245:ASN:ND2	2.61	0.64
1:A:138:LYS:O	1:A:142:VAL:HG13	1.98	0.64
1:A:132:GLU:CD	1:A:132:GLU:H	2.01	0.64
1:B:131:LEU:HA	1:B:134:LYS:HB3	1.80	0.64
1:B:32:ILE:O	1:B:32:ILE:CG1	2.47	0.62
1:A:218:VAL:HG22	1:A:221:LYS:CE	2.28	0.62
1:A:26:ARG:C	1:A:27:LEU:O	2.36	0.61
1:A:49:TYR:O	1:A:52:SER:HB2	2.00	0.61
1:A:131:LEU:HB3	1:A:132:GLU:OE1	2.00	0.61
1:A:34:GLU:O	1:A:35:ASN:HB3	2.00	0.61
1:A:25:GLU:O	1:A:27:LEU:O	2.19	0.61
1:B:102:PHE:CB	2:B:755:HOH:O	2.38	0.61
1:B:129:GLU:OE2	1:B:139:THR:HB	2.01	0.60
1:A:92:ILE:O	1:A:92:ILE:HG13	2.00	0.60
1:A:237:LYS:HB3	1:A:238:PRO:HD2	1.83	0.60
1:A:216:ASN:O	1:A:219:THR:CB	2.47	0.60
1:B:47:LEU:O	1:B:51:VAL:HG23	2.01	0.60
1:A:205:ARG:NH2	2:A:660:HOH:O	2.33	0.60
1:B:167:VAL:O	1:B:170:ILE:HG23	2.01	0.60
1:A:83:ILE:HG23	1:A:88:ALA:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:VAL:O	1:B:88:ALA:HB1	2.00	0.60
1:B:79:SER:O	1:B:83:ILE:HG13	2.02	0.60
1:A:168:TRP:O	1:A:172:THR:HG21	2.02	0.59
1:B:89:LYS:HD3	1:B:90:TRP:NE1	2.18	0.59
1:B:89:LYS:HB3	1:B:90:TRP:CD1	2.39	0.58
1:B:42:PRO:HG2	1:B:47:LEU:HD23	1.84	0.58
1:B:33:PRO:HD3	1:B:245:ASN:HD22	1.68	0.58
1:B:63:ALA:HB2	1:B:83:ILE:HD13	1.86	0.58
1:A:34:GLU:O	1:A:35:ASN:ND2	2.37	0.58
1:B:185:HIS:CD2	1:B:226:VAL:HA	2.39	0.57
1:B:188:ILE:HD13	1:B:206:ILE:HD13	1.86	0.57
1:B:104:GLU:OE1	2:B:754:HOH:O	2.17	0.57
1:A:51:VAL:HG22	1:A:61:VAL:HG11	1.87	0.57
1:A:129:GLU:OE1	1:A:139:THR:HB	2.05	0.57
1:A:43:PRO:CB	1:B:82:GLN:HE22	2.18	0.56
1:A:16:SER:O	1:A:20:ILE:HG12	2.06	0.56
1:B:127:ILE:HB	1:B:146:GLN:NE2	2.20	0.56
1:A:104:GLU:OE1	2:A:718:HOH:O	2.17	0.56
1:A:34:GLU:O	1:A:35:ASN:CB	2.53	0.56
1:A:40:ILE:O	1:A:61:VAL:HA	2.06	0.56
1:A:230:LEU:HD13	2:A:602:HOH:O	2.06	0.55
1:A:92:ILE:HD11	1:A:95:HIS:HB2	1.88	0.55
1:B:12:LYS:NZ	1:B:97:GLU:OE2	2.40	0.55
1:A:48:ASP:OD1	1:B:17:LYS:NZ	2.37	0.55
1:B:49:TYR:HB2	2:B:706:HOH:O	2.06	0.55
1:A:239:GLU:O	1:A:242:ASP:HB2	2.08	0.54
1:A:237:LYS:HB3	1:A:238:PRO:CD	2.37	0.54
1:B:39:VAL:HA	1:B:60:THR:O	2.07	0.54
1:A:20:ILE:O	1:A:24:VAL:HG23	2.08	0.53
1:A:133:GLU:OE2	1:A:142:VAL:HG11	2.08	0.53
1:B:188:ILE:CD1	1:B:206:ILE:HD13	2.38	0.53
1:A:43:PRO:CG	1:B:82:GLN:HE22	2.21	0.53
1:B:67:TYR:OH	2:B:662:HOH:O	2.15	0.53
1:B:216:ASN:OD1	1:B:216:ASN:C	2.47	0.53
1:B:63:ALA:CB	1:B:83:ILE:HD13	2.39	0.53
1:B:195:LYS:HD3	1:B:195:LYS:N	2.24	0.52
1:B:28:ASN:O	1:B:56:LYS:NZ	2.42	0.52
1:A:177:THR:O	1:A:180:ASP:HB2	2.10	0.52
1:A:6:PHE:HD2	1:A:37:GLU:HG2	1.73	0.52
1:A:240:PHE:O	1:A:244:ILE:HG13	2.10	0.52
1:B:132:GLU:OE2	1:B:132:GLU:CA	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLN:HE22	1:A:225:ASP:HB2	1.75	0.51
1:B:188:ILE:HD13	1:B:206:ILE:HG21	1.92	0.51
1:A:142:VAL:HG22	1:A:143:VAL:N	2.26	0.50
1:B:129:GLU:OE2	1:B:139:THR:CG2	2.59	0.50
1:A:142:VAL:CG2	1:A:143:VAL:N	2.73	0.50
1:B:141:ASP:OD1	1:B:141:ASP:N	2.44	0.50
1:A:80:VAL:CG2	1:A:119:GLN:HG3	2.42	0.50
1:B:102:PHE:O	1:B:103:HIS:C	2.50	0.50
1:B:105:ASP:OD2	1:B:105:ASP:N	2.42	0.49
1:B:117:LEU:O	1:B:118:GLY:C	2.49	0.49
1:B:101:TYR:H	1:B:101:TYR:HD2	1.61	0.49
1:A:213:ASN:H	1:A:216:ASN:HB2	1.78	0.49
1:B:142:VAL:HG22	1:B:145:ARG:HH11	1.78	0.49
1:B:192:LEU:O	1:B:196:LEU:N	2.44	0.49
1:B:33:PRO:CD	1:B:245:ASN:HD22	2.23	0.48
1:B:20:ILE:HD11	1:B:50:SER:OG	2.13	0.48
1:A:178:PRO:HG3	1:A:219:THR:HG22	1.94	0.48
1:B:33:PRO:O	1:B:58:GLN:NE2	2.40	0.48
1:B:177:THR:HB	1:B:178:PRO:CD	2.43	0.48
1:A:143:VAL:HG11	1:A:188:ILE:CD1	2.44	0.48
1:A:117:LEU:HD11	1:A:160:VAL:CG2	2.45	0.47
1:A:150:VAL:CG2	1:A:157:TRP:CZ2	2.98	0.47
1:A:163:ALA:HA	1:A:207:LEU:HB2	1.97	0.47
1:B:70:ALA:HB1	1:B:81:ASP:OD1	2.14	0.47
1:A:50:SER:O	1:A:54:VAL:HG23	2.15	0.47
1:A:49:TYR:O	1:A:53:LEU:HD22	2.15	0.47
1:B:131:LEU:HD22	1:B:135:LYS:HG3	1.96	0.47
1:B:129:GLU:CD	1:B:139:THR:HB	2.35	0.46
1:B:20:ILE:HD11	1:B:50:SER:HA	1.98	0.46
1:A:43:PRO:CB	1:B:82:GLN:NE2	2.79	0.46
1:B:6:PHE:CZ	1:B:39:VAL:CG1	2.99	0.46
1:B:10:ASN:HA	1:B:41:CYS:HB2	1.97	0.45
1:A:104:GLU:HB3	1:A:109:ILE:HD11	1.99	0.45
1:A:38:VAL:O	1:A:59:VAL:HA	2.16	0.45
1:A:139:THR:OG1	1:A:140:LEU:N	2.49	0.45
1:A:28:ASN:O	1:A:56:LYS:HD3	2.17	0.45
1:B:102:PHE:CA	2:B:755:HOH:O	2.63	0.45
1:A:129:GLU:HG3	1:A:129:GLU:H	1.38	0.45
1:A:17:LYS:HE3	1:B:48:ASP:OD1	2.16	0.45
1:B:33:PRO:HD3	1:B:245:ASN:HD21	1.82	0.44
1:B:2:ALA:HB1	1:B:3:ARG:H	1.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ARG:O	1:B:103:HIS:HA	2.17	0.44
1:A:178:PRO:HG3	1:A:219:THR:CG2	2.47	0.44
1:A:138:LYS:O	1:A:142:VAL:CG1	2.63	0.44
1:A:162:VAL:O	1:A:206:ILE:HA	2.17	0.44
1:A:39:VAL:HA	1:A:60:THR:O	2.17	0.44
1:B:79:SER:CB	1:B:82:GLN:HG2	2.44	0.43
1:A:182:GLN:HE22	1:A:225:ASP:H	1.65	0.43
1:A:182:GLN:NE2	1:A:182:GLN:HA	2.33	0.43
1:B:211:SER:HA	2:B:637:HOH:O	2.18	0.43
1:B:28:ASN:HA	1:B:28:ASN:HD22	1.52	0.43
1:A:53:LEU:O	1:A:55:LYS:HD2	2.19	0.43
1:B:240:PHE:O	1:B:243:ILE:HB	2.18	0.43
1:B:241:VAL:O	1:B:244:ILE:HB	2.19	0.42
1:A:182:GLN:NE2	1:A:225:ASP:H	2.17	0.42
1:A:43:PRO:HG2	1:B:82:GLN:HE22	1.84	0.42
1:A:25:GLU:O	1:A:29:THR:HB	2.19	0.42
1:A:28:ASN:H	1:A:56:LYS:HG3	1.85	0.42
1:A:54:VAL:HG11	1:A:59:VAL:HG22	2.00	0.42
1:A:247:ARG:NH1	2:A:682:HOH:O	2.31	0.42
1:A:97:GLU:OE2	1:B:75:THR:HG22	2.15	0.42
1:A:178:PRO:HG2	1:A:219:THR:HG23	2.02	0.41
1:A:218:VAL:CG2	1:A:221:LYS:HE3	2.35	0.41
1:A:65:ASN:HD22	1:A:65:ASN:HA	1.70	0.41
1:B:235:SER:HB3	1:B:236:LEU:HG	2.02	0.41
1:A:97:GLU:OE1	1:B:73:ALA:HB1	2.21	0.41
1:B:154:VAL:HG23	1:B:157:TRP:NE1	2.36	0.41
1:B:184:ILE:H	1:B:184:ILE:HG13	1.50	0.41
1:B:61:VAL:HG22	1:B:88:ALA:HB2	2.02	0.41
1:A:248:ASN:HD22	1:A:248:ASN:HA	1.31	0.41
1:B:101:TYR:N	1:B:101:TYR:CD2	2.88	0.41
1:A:6:PHE:O	1:A:228:GLY:HA3	2.20	0.41
1:B:205:ARG:HD2	1:B:205:ARG:HH21	1.44	0.41
1:B:102:PHE:C	2:B:755:HOH:O	2.52	0.41
1:A:128:GLY:HA2	1:A:164:TYR:CE1	2.56	0.41
1:B:213:ASN:O	1:B:217:ALA:HB2	2.21	0.40
1:B:6:PHE:CZ	1:B:39:VAL:HG11	2.55	0.40
1:B:170:ILE:O	1:B:170:ILE:HD13	2.22	0.40
1:A:178:PRO:CG	1:A:219:THR:CG2	3.00	0.40
1:B:33:PRO:HD2	1:B:245:ASN:ND2	2.35	0.40

All (1) 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:239:GLU:OE1	1:B:215:SER:OG[1_455]	2.11	0.09

## 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	245/247 (99%)	230 (94%)	12 (5%)	3 (1%)	13	4
1	B	245/247 (99%)	229 (94%)	13 (5%)	3 (1%)	13	4
All	All	490/494 (99%)	459 (94%)	25 (5%)	6 (1%)	13	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	B	131	LEU
1	B	103	HIS
1	B	172	THR
1	A	103	HIS
1	A	217	ALA

### 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	200/200 (100%)	165 (82%)	35 (18%)	2	0
1	B	200/200 (100%)	152 (76%)	48 (24%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	400/400 (100%)	317 (79%)	83 (21%)	<b>1</b> <b>0</b>

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PHE
1	A	21	LYS
1	A	29	THR
1	A	39	VAL
1	A	42	PRO
1	A	53	LEU
1	A	59	VAL
1	A	60	THR
1	A	61	VAL
1	A	68	LEU
1	A	79	SER
1	A	91	VAL
1	A	92	ILE
1	A	93	LEU
1	A	103	HIS
1	A	107	LYS
1	A	129	GLU
1	A	145	ARG
1	A	150	VAL
1	A	162	VAL
1	A	170	ILE
1	A	180	ASP
1	A	182	GLN
1	A	188	ILE
1	A	190	LYS
1	A	192	LEU
1	A	196	LEU
1	A	199	LYS
1	A	205	ARG
1	A	216	ASN
1	A	221	LYS
1	A	223	LYS
1	A	230	LEU
1	A	237	LYS
1	A	248	ASN
1	B	4	THR
1	B	7	VAL

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Mol	Chain	Res	Type
1	B	18	GLN
1	B	20	ILE
1	B	23	ILE
1	B	27	LEU
1	B	29	THR
1	B	35	ASN
1	B	36	VAL
1	B	39	VAL
1	B	40	ILE
1	B	53	LEU
1	B	61	VAL
1	B	68	LEU
1	B	75	THR
1	B	82	GLN
1	B	86	VAL
1	B	89	LYS
1	B	92	ILE
1	B	93	LEU
1	B	101	TYR
1	B	105	ASP
1	B	107	LYS
1	B	131	LEU
1	B	132	GLU
1	B	139	THR
1	B	140	LEU
1	B	141	ASP
1	B	143	VAL
1	B	144	GLU
1	B	151	LEU
1	B	155	LYS
1	B	170	ILE
1	B	183	ASP
1	B	188	ILE
1	B	190	LYS
1	B	198	ASP
1	B	199	LYS
1	B	204	LEU
1	B	207	LEU
1	B	215	SER
1	B	221	LYS
1	B	222	ASP
1	B	223	LYS

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Mol	Chain	Res	Type
1	B	226	VAL
1	B	235	SER
1	B	238	PRO
1	B	239	GLU

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

Mol	Chain	Res	Type
1	A	10	ASN
1	A	65	ASN
1	A	78	ASN
1	A	146	GLN
1	A	182	GLN
1	A	216	ASN
1	A	248	ASN
1	B	28	ASN
1	B	64	GLN
1	B	82	GLN
1	B	146	GLN
1	B	185	HIS
1	B	245	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.