



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:00 PM UTC

PDB ID : 1YPI / pdb_00001ypi
Title : STRUCTURE OF YEAST TRIOSEPHOSPHATE ISOMERASE AT 1.9-
ANGSTROMS RESOLUTION
Authors : Alber, T.; Lolis, E.; Petsko, G.A.
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

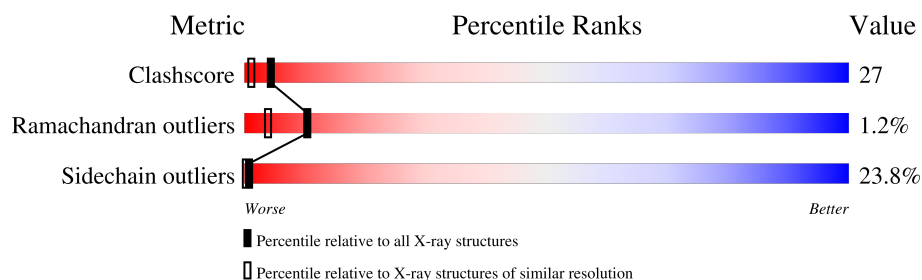
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	247	19% 45% 28% 8%
1	B	247	15% 40% 36% 9%

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.

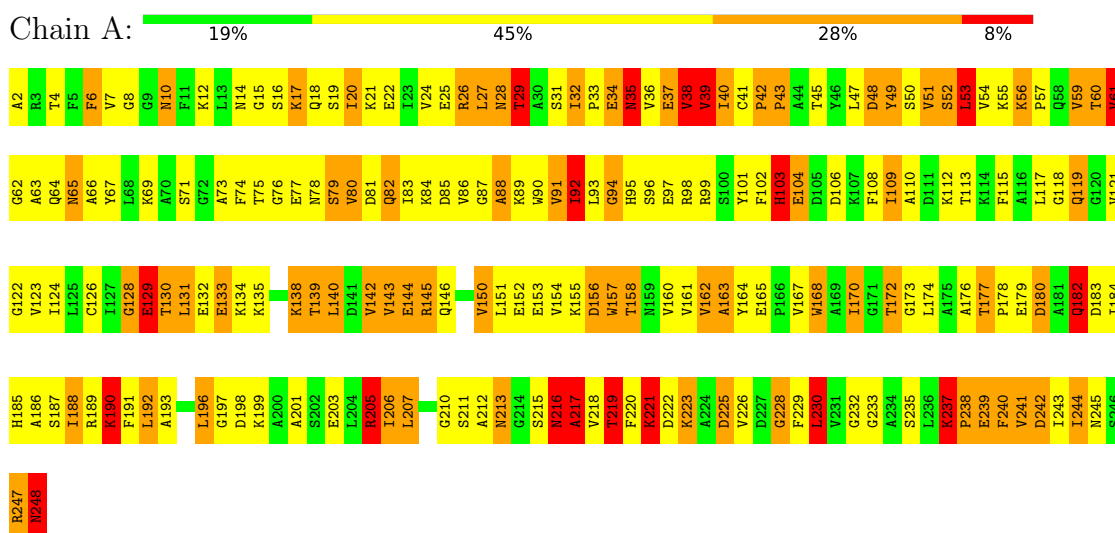
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	66	Total	O	0	0
			66	66		
2	B	53	Total	O	0	0
			53	53		

3 Residue-property plots

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

Note EDS was not executed.

• Molecule 1: 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, α , β , γ	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 ²)	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	2.65	136/1915 (7.1%)	2.99	250/2590 (9.7%)
1	B	2.67	131/1915 (6.8%)	3.11	244/2590 (9.4%)
All	All	2.66	267/3830 (7.0%)	3.05	494/5180 (9.5%)

All (267) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	ASN	CA-CB	11.79	1.72	1.53
1	B	199	LYS	N-CA	11.40	1.59	1.46
1	B	131	LEU	N-CA	10.79	1.60	1.46
1	B	14	ASN	CA-C	10.39	1.65	1.52
1	B	43	PRO	C-O	10.16	1.34	1.23
1	A	34	GLU	N-CA	10.09	1.59	1.46
1	A	48	ASP	N-CA	9.78	1.57	1.46
1	A	187	SER	N-CA	-9.45	1.35	1.46
1	B	29	THR	C-N	-9.44	1.21	1.33
1	B	31	SER	C-N	-9.18	1.23	1.33
1	A	53	LEU	C-N	-9.13	1.22	1.33
1	A	40	ILE	CA-CB	-9.03	1.43	1.54
1	A	138	LYS	C-N	-9.03	1.22	1.33
1	B	198	ASP	C-N	-8.87	1.22	1.33
1	A	156	ASP	C-O	8.85	1.35	1.23
1	B	205	ARG	NE-CZ	8.78	1.42	1.33
1	B	205	ARG	CA-C	8.75	1.63	1.52
1	B	87	GLY	C-O	8.65	1.35	1.24
1	B	241	VAL	CA-C	-8.60	1.42	1.52
1	A	27	LEU	N-CA	8.51	1.56	1.46
1	B	230	LEU	CA-CB	-8.44	1.40	1.53
1	B	68	LEU	C-N	-8.41	1.23	1.33
1	B	29	THR	C-O	8.39	1.35	1.24
1	A	211	SER	N-CA	8.32	1.56	1.46
1	A	80	VAL	C-N	-8.24	1.23	1.33
1	B	109	ILE	CA-CB	-8.24	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	181	ALA	N-CA	8.23	1.55	1.46
1	B	187	SER	C-N	-8.20	1.24	1.33
1	A	82	GLN	C-N	-8.08	1.24	1.33
1	A	34	GLU	CA-C	-8.07	1.42	1.52
1	B	232	GLY	N-CA	-8.01	1.33	1.45
1	B	122	GLY	N-CA	7.91	1.53	1.44
1	B	63	ALA	C-N	-7.90	1.22	1.33
1	A	40	ILE	N-CA	7.89	1.55	1.46
1	B	210	GLY	N-CA	7.86	1.53	1.45
1	B	113	THR	N-CA	7.80	1.55	1.46
1	A	240	PHE	N-CA	-7.76	1.36	1.46
1	A	53	LEU	C-O	7.75	1.33	1.24
1	A	64	GLN	C-N	-7.72	1.24	1.33
1	B	70	ALA	CA-CB	-7.66	1.40	1.53
1	A	103	HIS	CE1-NE2	7.62	1.40	1.32
1	B	23	ILE	CA-CB	-7.59	1.43	1.54
1	A	210	GLY	C-O	7.59	1.31	1.23
1	A	73	ALA	CA-C	-7.57	1.45	1.53
1	B	121	VAL	C-O	7.53	1.31	1.23
1	A	233	GLY	C-O	7.52	1.32	1.23
1	A	156	ASP	C-N	-7.46	1.23	1.33
1	A	15	GLY	C-N	7.40	1.42	1.33
1	A	157	TRP	N-CA	7.36	1.54	1.46
1	A	18	GLN	CA-C	-7.35	1.43	1.52
1	B	235	SER	CB-OG	-7.33	1.27	1.42
1	A	65	ASN	C-O	7.28	1.32	1.23
1	A	174	LEU	C-N	-7.26	1.22	1.33
1	A	86	VAL	N-CA	7.23	1.55	1.46
1	A	126	CYS	CA-C	7.23	1.61	1.52
1	B	130	THR	C-O	7.23	1.33	1.24
1	A	223	LYS	C-O	-7.22	1.15	1.24
1	B	226	VAL	C-N	-7.13	1.23	1.33
1	A	161	VAL	CA-CB	-7.12	1.45	1.54
1	B	128	GLY	CA-C	7.11	1.61	1.51
1	A	19	SER	N-CA	7.11	1.55	1.46
1	A	237	LYS	N-CA	-7.10	1.41	1.46
1	B	84	LYS	C-N	-7.08	1.24	1.33
1	A	65	ASN	C-N	-7.08	1.24	1.33
1	A	32	ILE	CA-CB	-7.08	1.45	1.54
1	B	207	LEU	C-N	-7.07	1.23	1.33
1	B	18	GLN	C-O	7.07	1.32	1.24
1	B	161	VAL	N-CA	7.00	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	95	HIS	CE1-NE2	6.94	1.39	1.32
1	B	50	SER	CA-C	6.91	1.61	1.52
1	B	20	ILE	N-CA	6.90	1.55	1.46
1	B	139	THR	C-O	-6.89	1.16	1.24
1	B	212	ALA	N-CA	6.87	1.54	1.46
1	A	211	SER	C-N	-6.86	1.23	1.33
1	A	247	ARG	CD-NE	6.86	1.55	1.46
1	B	153	GLU	C-O	6.82	1.32	1.24
1	A	207	LEU	N-CA	-6.82	1.37	1.46
1	A	121	VAL	C-O	6.81	1.33	1.24
1	B	231	VAL	C-N	-6.80	1.23	1.33
1	A	189	ARG	C-N	-6.79	1.25	1.33
1	A	121	VAL	C-N	-6.79	1.23	1.33
1	A	27	LEU	C-O	6.76	1.31	1.23
1	B	41	CYS	C-N	-6.71	1.25	1.33
1	B	130	THR	N-CA	-6.70	1.37	1.46
1	A	144	GLU	C-O	6.68	1.32	1.24
1	A	145	ARG	CZ-NH1	6.68	1.42	1.32
1	A	12	LYS	C-O	6.67	1.32	1.24
1	A	183	ASP	CA-CB	6.65	1.64	1.53
1	A	140	LEU	CA-CB	-6.63	1.42	1.53
1	A	216	ASN	CA-C	-6.60	1.44	1.52
1	A	217	ALA	C-O	6.59	1.32	1.24
1	A	128	GLY	N-CA	6.56	1.52	1.45
1	A	152	GLU	C-O	-6.55	1.16	1.24
1	A	8	GLY	C-N	-6.54	1.24	1.33
1	A	215	SER	C-O	6.54	1.31	1.24
1	A	42	PRO	N-CD	6.53	1.56	1.47
1	B	178	PRO	CA-CB	-6.50	1.44	1.53
1	B	174	LEU	CA-C	6.50	1.61	1.52
1	B	108	PHE	N-CA	6.49	1.54	1.46
1	B	125	LEU	C-N	-6.48	1.24	1.33
1	A	61	VAL	CA-C	-6.47	1.44	1.52
1	A	153	GLU	N-CA	6.44	1.54	1.46
1	B	165	GLU	CD-OE2	6.44	1.37	1.25
1	A	144	GLU	N-CA	6.40	1.54	1.46
1	A	172	THR	N-CA	-6.39	1.37	1.46
1	B	26	ARG	C-O	6.35	1.31	1.24
1	B	99	ARG	CZ-NH2	6.34	1.41	1.33
1	B	193	ALA	CA-C	6.33	1.60	1.52
1	A	230	LEU	CA-CB	-6.29	1.42	1.53
1	B	240	PHE	N-CA	6.26	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	VAL	C-N	6.26	1.41	1.33
1	A	61	VAL	C-O	6.25	1.30	1.24
1	B	227	ASP	C-O	6.23	1.32	1.24
1	A	52	SER	CA-CB	6.22	1.63	1.53
1	B	223	LYS	N-CA	6.21	1.54	1.46
1	B	75	THR	N-CA	6.20	1.53	1.46
1	B	147	LEU	C-N	-6.19	1.25	1.33
1	B	194	SER	CA-CB	-6.17	1.43	1.53
1	A	197	GLY	C-O	6.16	1.30	1.24
1	B	203	GLU	CA-CB	-6.16	1.43	1.53
1	B	223	LYS	CA-CB	-6.14	1.45	1.53
1	B	154	VAL	N-CA	6.14	1.53	1.46
1	B	47	LEU	CB-CG	-6.13	1.41	1.53
1	B	177	THR	CA-C	6.12	1.61	1.52
1	A	79	SER	N-CA	6.12	1.53	1.45
1	B	228	GLY	CA-C	-6.12	1.44	1.52
1	A	179	GLU	C-O	6.12	1.31	1.24
1	A	223	LYS	N-CA	6.12	1.54	1.46
1	A	86	VAL	CA-C	-6.12	1.45	1.53
1	A	152	GLU	CD-OE2	6.10	1.36	1.25
1	B	78	ASN	N-CA	6.10	1.53	1.45
1	A	239	GLU	CD-OE1	-6.09	1.13	1.25
1	A	144	GLU	CD-OE2	6.08	1.36	1.25
1	B	153	GLU	CA-C	-6.07	1.44	1.52
1	B	169	ALA	N-CA	6.07	1.54	1.46
1	A	240	PHE	C-N	-6.07	1.26	1.33
1	B	113	THR	C-O	6.04	1.31	1.24
1	A	144	GLU	CA-CB	-6.01	1.43	1.53
1	A	73	ALA	C-O	6.00	1.30	1.23
1	B	103	HIS	CE1-NE2	5.98	1.38	1.32
1	A	189	ARG	NE-CZ	5.97	1.39	1.33
1	A	43	PRO	C-N	-5.96	1.25	1.34
1	A	228	GLY	N-CA	5.96	1.52	1.45
1	A	129	GLU	CA-CB	5.96	1.62	1.53
1	B	226	VAL	N-CA	5.94	1.53	1.46
1	B	199	LYS	C-N	-5.91	1.26	1.33
1	B	61	VAL	N-CA	5.91	1.52	1.46
1	A	201	ALA	CA-CB	-5.90	1.43	1.53
1	A	247	ARG	N-CA	5.90	1.53	1.46
1	B	32	ILE	C-O	-5.89	1.17	1.24
1	B	36	VAL	C-O	5.86	1.30	1.23
1	B	99	ARG	N-CA	-5.86	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	GLU	CD-OE2	5.86	1.36	1.25
1	A	63	ALA	C-O	-5.84	1.16	1.23
1	B	167	VAL	N-CA	5.84	1.53	1.46
1	B	59	VAL	CA-CB	5.84	1.61	1.54
1	B	172	THR	CB-OG1	-5.83	1.34	1.43
1	A	47	LEU	C-N	-5.82	1.26	1.33
1	B	164	TYR	CA-CB	-5.81	1.45	1.53
1	A	238	PRO	C-O	5.81	1.30	1.24
1	A	48	ASP	C-N	-5.77	1.26	1.33
1	B	147	LEU	C-O	5.77	1.30	1.24
1	B	63	ALA	CA-C	5.75	1.61	1.53
1	A	113	THR	C-O	5.74	1.30	1.24
1	B	96	SER	CA-CB	-5.74	1.44	1.53
1	B	229	PHE	C-N	5.73	1.43	1.33
1	B	36	VAL	C-N	-5.73	1.25	1.33
1	A	170	ILE	C-O	5.72	1.30	1.24
1	A	161	VAL	CA-C	5.69	1.59	1.52
1	A	28	ASN	N-CA	5.65	1.53	1.46
1	B	111	ASP	C-N	-5.62	1.26	1.33
1	B	156	ASP	CA-C	5.60	1.59	1.52
1	B	61	VAL	C-N	5.58	1.40	1.33
1	A	17	LYS	CA-CB	-5.58	1.44	1.53
1	A	115	PHE	N-CA	-5.58	1.39	1.46
1	A	130	THR	CA-C	-5.58	1.45	1.53
1	A	118	GLY	C-N	-5.57	1.25	1.33
1	A	51	VAL	CA-C	-5.56	1.46	1.52
1	A	217	ALA	C-N	-5.56	1.27	1.33
1	B	166	PRO	CA-CB	-5.56	1.46	1.53
1	A	152	GLU	C-N	5.55	1.41	1.33
1	B	61	VAL	CA-C	-5.53	1.46	1.52
1	B	200	ALA	C-N	-5.51	1.26	1.33
1	B	202	SER	N-CA	5.51	1.53	1.46
1	B	10	ASN	C-N	-5.51	1.25	1.33
1	A	222	ASP	N-CA	5.50	1.52	1.46
1	B	21	LYS	C-N	-5.49	1.26	1.34
1	A	90	TRP	C-N	5.49	1.41	1.33
1	B	120	GLY	C-N	5.49	1.38	1.33
1	B	217	ALA	N-CA	5.49	1.52	1.46
1	B	129	GLU	N-CA	5.48	1.52	1.45
1	A	91	VAL	N-CA	-5.48	1.39	1.46
1	B	27	LEU	CA-CB	-5.48	1.44	1.53
1	A	230	LEU	C-O	-5.45	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	ASN	C-N	-5.43	1.25	1.33
1	B	25	GLU	CA-CB	-5.43	1.45	1.53
1	B	186	ALA	CA-C	-5.42	1.45	1.52
1	B	95	HIS	CG-ND1	5.42	1.44	1.38
1	A	167	VAL	N-CA	5.42	1.53	1.46
1	B	54	VAL	CA-CB	-5.41	1.47	1.54
1	A	165	GLU	CD-OE1	-5.41	1.15	1.25
1	A	122	GLY	CA-C	5.41	1.58	1.52
1	B	215	SER	CB-OG	5.41	1.52	1.42
1	B	16	SER	C-N	-5.40	1.27	1.33
1	A	145	ARG	C-N	5.39	1.41	1.33
1	B	170	ILE	CB-CG1	-5.39	1.42	1.53
1	A	193	ALA	N-CA	5.39	1.53	1.46
1	A	223	LYS	CA-CB	-5.38	1.46	1.53
1	A	192	LEU	C-O	5.38	1.30	1.24
1	B	78	ASN	C-N	-5.37	1.26	1.33
1	A	155	LYS	C-N	5.36	1.40	1.33
1	A	182	GLN	N-CA	5.36	1.52	1.46
1	B	195	LYS	C-N	-5.36	1.26	1.33
1	A	106	ASP	C-N	-5.35	1.26	1.34
1	A	151	LEU	N-CA	5.35	1.53	1.46
1	A	144	GLU	CA-C	-5.34	1.45	1.52
1	A	61	VAL	CA-CB	5.34	1.63	1.55
1	B	23	ILE	C-N	-5.32	1.27	1.33
1	B	149	ALA	CA-C	5.30	1.59	1.52
1	A	123	VAL	N-CA	-5.29	1.40	1.46
1	A	34	GLU	CA-CB	-5.29	1.45	1.53
1	A	198	ASP	CA-C	5.29	1.59	1.52
1	B	248	ASN	N-CA	-5.28	1.36	1.46
1	B	170	ILE	C-N	5.28	1.41	1.33
1	B	241	VAL	CA-CB	5.28	1.60	1.54
1	A	168	TRP	CA-C	-5.26	1.45	1.52
1	B	157	TRP	NE1-CE2	5.22	1.43	1.37
1	A	20	ILE	C-N	5.22	1.40	1.33
1	A	242	ASP	C-O	-5.21	1.17	1.24
1	B	17	LYS	C-O	-5.21	1.18	1.24
1	B	37	GLU	N-CA	5.21	1.52	1.46
1	A	123	VAL	CA-C	5.21	1.59	1.52
1	A	233	GLY	C-N	-5.19	1.26	1.33
1	B	201	ALA	N-CA	5.19	1.52	1.46
1	B	238	PRO	C-O	5.16	1.30	1.24
1	A	131	LEU	C-N	-5.16	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	ALA	C-N	-5.16	1.25	1.33
1	B	219	THR	C-O	5.16	1.30	1.24
1	B	193	ALA	CA-CB	-5.15	1.45	1.53
1	A	22	GLU	CA-C	-5.15	1.46	1.52
1	B	33	PRO	N-CD	5.14	1.54	1.47
1	A	41	CYS	CA-CB	5.14	1.60	1.52
1	B	123	VAL	C-N	-5.13	1.26	1.33
1	A	27	LEU	C-N	-5.13	1.26	1.33
1	A	165	GLU	CD-OE2	5.12	1.35	1.25
1	A	225	ASP	C-O	5.12	1.31	1.24
1	A	244	ILE	C-O	5.12	1.30	1.24
1	B	161	VAL	CA-C	5.11	1.58	1.52
1	A	15	GLY	CA-C	-5.11	1.47	1.52
1	B	69	LYS	CA-C	5.10	1.58	1.52
1	B	16	SER	C-O	5.09	1.30	1.24
1	B	93	LEU	N-CA	5.09	1.52	1.46
1	B	12	LYS	C-N	-5.09	1.27	1.33
1	A	96	SER	C-N	5.09	1.41	1.33
1	B	86	VAL	C-O	5.09	1.30	1.24
1	A	69	LYS	C-O	5.08	1.30	1.23
1	B	24	VAL	N-CA	5.08	1.52	1.46
1	A	133	GLU	C-N	-5.07	1.27	1.33
1	A	65	ASN	CA-C	-5.06	1.46	1.52
1	A	77	GLU	CA-C	-5.06	1.46	1.53
1	A	156	ASP	CA-CB	5.06	1.61	1.53
1	B	234	ALA	N-CA	5.05	1.52	1.46
1	B	201	ALA	C-O	5.05	1.29	1.24
1	A	56	LYS	CA-C	5.04	1.59	1.52
1	A	212	ALA	C-O	5.03	1.29	1.23
1	A	88	ALA	C-O	5.03	1.30	1.23
1	B	150	VAL	C-N	-5.01	1.27	1.34

All (494) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	GLU	CA-CB-CG	20.43	154.97	114.10
1	B	144	GLU	CA-CB-CG	16.82	147.74	114.10
1	B	198	ASP	CA-CB-CG	16.08	128.68	112.60
1	B	222	ASP	CA-CB-CG	14.62	127.22	112.60
1	A	216	ASN	CA-CB-CG	-14.32	98.28	112.60
1	A	78	ASN	CA-C-O	-14.14	105.72	120.71
1	B	11	PHE	CA-CB-CG	13.83	127.63	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ALA	CA-C-N	13.73	138.28	120.44
1	A	186	ALA	C-N-CA	13.73	138.28	120.44
1	B	131	LEU	O-C-N	12.82	139.64	122.59
1	B	205	ARG	CD-NE-CZ	-12.69	106.63	124.40
1	B	161	VAL	CB-CA-C	12.65	130.03	110.81
1	A	28	ASN	OD1-CG-ND2	-11.85	110.75	122.60
1	B	200	ALA	O-C-N	11.58	134.00	122.07
1	B	7	VAL	CB-CA-C	11.31	124.19	110.73
1	B	5	PHE	CA-CB-CG	11.02	124.82	113.80
1	B	144	GLU	N-CA-CB	11.01	125.97	110.01
1	A	216	ASN	CB-CA-C	-10.86	94.11	110.95
1	B	150	VAL	CA-C-O	-10.83	109.12	120.71
1	A	7	VAL	CA-C-N	-10.81	114.72	122.18
1	A	7	VAL	C-N-CA	-10.81	114.72	122.18
1	B	75	THR	CB-CA-C	10.66	127.42	109.72
1	A	215	SER	CA-C-N	10.62	135.07	120.63
1	A	215	SER	C-N-CA	10.62	135.07	120.63
1	A	139	THR	CA-CB-OG1	-10.40	94.00	109.60
1	B	139	THR	O-C-N	10.29	132.67	122.07
1	B	161	VAL	CA-C-O	-10.22	109.07	120.72
1	B	229	PHE	CA-CB-CG	10.21	124.01	113.80
1	A	161	VAL	N-CA-C	-10.17	93.83	108.48
1	A	247	ARG	NE-CZ-NH1	-10.10	111.40	121.50
1	A	40	ILE	CA-C-O	-10.06	109.25	120.72
1	B	148	ASN	CA-CB-CG	-10.05	102.55	112.60
1	B	221	LYS	CA-CB-CG	10.05	134.20	114.10
1	A	216	ASN	N-CA-C	10.04	122.18	111.03
1	B	89	LYS	CA-C-O	10.03	129.94	118.90
1	B	180	ASP	O-C-N	10.02	132.85	122.03
1	B	29	THR	CA-CB-CG2	9.91	127.35	110.50
1	A	102	PHE	CA-CB-CG	-9.84	103.96	113.80
1	B	92	ILE	CB-CA-C	9.83	123.10	110.91
1	B	144	GLU	CB-CA-C	-9.82	95.46	110.88
1	B	26	ARG	CD-NE-CZ	9.71	137.99	124.40
1	A	216	ASN	CA-C-O	9.70	130.89	120.90
1	A	205	ARG	NE-CZ-NH2	-9.70	110.47	119.20
1	A	86	VAL	N-CA-C	-9.65	103.22	112.29
1	B	121	VAL	CA-C-O	-9.63	114.07	121.68
1	B	217	ALA	CA-C-O	9.62	130.75	120.55
1	A	85	ASP	O-C-N	9.59	132.29	122.12
1	A	37	GLU	CA-CB-CG	9.54	133.18	114.10
1	B	205	ARG	NE-CZ-NH2	-9.52	110.63	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	ARG	NE-CZ-NH1	-9.45	112.05	121.50
1	B	130	THR	CA-C-O	-9.45	107.93	119.18
1	B	35	ASN	CA-CB-CG	-9.45	103.15	112.60
1	B	240	PHE	CA-C-O	9.40	130.51	120.55
1	B	132	GLU	N-CA-C	-9.38	101.03	111.07
1	A	205	ARG	NE-CZ-NH1	9.37	130.87	121.50
1	B	12	LYS	CA-C-O	-9.37	107.12	120.51
1	A	27	LEU	N-CA-C	-9.36	95.28	109.60
1	B	64	GLN	OE1-CD-NE2	-9.36	113.24	122.60
1	A	92	ILE	CA-CB-CG2	9.14	126.03	110.50
1	B	170	ILE	CA-C-O	9.13	130.30	120.53
1	A	129	GLU	CB-CG-CD	9.09	128.05	112.60
1	B	31	SER	CA-C-O	-9.03	111.92	122.13
1	B	104	GLU	CB-CA-C	8.94	125.16	110.22
1	A	40	ILE	O-C-N	8.94	132.26	123.14
1	A	65	ASN	O-C-N	-8.83	115.47	123.41
1	A	174	LEU	CA-C-O	-8.83	110.88	121.56
1	A	113	THR	N-CA-C	8.80	120.87	111.28
1	A	134	LYS	CB-CG-CD	8.77	131.47	111.30
1	A	86	VAL	CB-CA-C	8.74	123.85	111.88
1	B	79	SER	CA-C-O	-8.74	110.85	120.38
1	B	145	ARG	CA-C-O	-8.73	111.30	120.55
1	A	223	LYS	CB-CG-CD	8.72	131.37	111.30
1	B	26	ARG	NE-CZ-NH1	-8.68	112.82	121.50
1	B	39	VAL	CB-CA-C	8.59	122.87	110.33
1	B	109	ILE	N-CA-CB	8.53	120.53	110.55
1	B	226	VAL	CA-C-O	-8.51	110.71	120.66
1	A	28	ASN	CA-CB-CG	8.50	121.10	112.60
1	A	91	VAL	CA-C-N	-8.48	112.68	123.19
1	A	91	VAL	C-N-CA	-8.48	112.68	123.19
1	B	215	SER	CA-C-O	-8.36	111.56	120.42
1	B	14	ASN	CA-CB-CG	8.36	120.96	112.60
1	B	36	VAL	CA-C-O	-8.28	113.18	120.96
1	B	29	THR	CA-C-O	-8.26	109.07	119.31
1	B	109	ILE	O-C-N	8.24	129.99	121.91
1	A	232	GLY	CA-C-N	8.21	129.26	119.99
1	A	232	GLY	C-N-CA	8.21	129.26	119.99
1	B	90	TRP	O-C-N	8.21	133.10	123.17
1	B	243	ILE	N-CA-C	-8.14	102.88	110.53
1	B	241	VAL	CA-C-O	-8.13	112.81	121.27
1	B	105	ASP	O-C-N	8.13	132.19	122.68
1	A	52	SER	CB-CA-C	-8.06	97.36	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	VAL	N-CA-C	-8.04	97.77	108.06
1	A	245	ASN	CA-CB-CG	8.01	120.61	112.60
1	B	158	THR	CA-C-O	7.99	129.16	119.97
1	B	14	ASN	O-C-N	7.95	132.39	123.48
1	B	178	PRO	N-CA-C	-7.95	102.74	113.40
1	B	205	ARG	O-C-N	7.94	132.27	123.22
1	B	216	ASN	CA-CB-CG	-7.89	104.71	112.60
1	A	156	ASP	CA-CB-CG	-7.89	104.71	112.60
1	B	132	GLU	N-CA-CB	7.88	121.44	110.01
1	B	240	PHE	N-CA-C	-7.87	102.70	111.28
1	A	37	GLU	CA-C-O	-7.79	112.22	120.40
1	B	101	TYR	CA-C-O	-7.78	111.03	119.97
1	A	91	VAL	N-CA-CB	7.77	124.20	111.45
1	B	2	ALA	CA-C-N	7.76	136.37	121.54
1	B	2	ALA	C-N-CA	7.76	136.37	121.54
1	A	170	ILE	N-CA-C	7.75	117.85	106.85
1	A	219	THR	N-CA-CB	-7.74	97.91	110.14
1	A	34	GLU	N-CA-C	-7.70	94.36	107.99
1	A	221	LYS	CD-CE-NZ	7.66	136.41	111.90
1	B	181	ALA	CB-CA-C	7.66	123.55	110.84
1	B	120	GLY	CA-C-N	-7.61	114.12	122.27
1	B	120	GLY	C-N-CA	-7.61	114.12	122.27
1	B	159	ASN	CA-CB-CG	-7.59	105.01	112.60
1	B	151	LEU	CA-C-O	7.58	128.67	120.10
1	B	89	LYS	N-CA-CB	-7.56	100.44	110.88
1	B	180	ASP	N-CA-C	-7.55	102.64	111.03
1	B	58	GLN	CA-C-N	-7.53	113.44	122.93
1	B	58	GLN	C-N-CA	-7.53	113.44	122.93
1	A	8	GLY	O-C-N	7.51	130.01	123.25
1	A	124	ILE	CA-C-O	7.50	129.44	120.66
1	A	221	LYS	CB-CG-CD	7.50	128.55	111.30
1	B	66	ALA	CA-C-O	-7.49	113.24	121.33
1	A	109	ILE	CA-CB-CG1	-7.49	97.67	110.40
1	A	78	ASN	O-C-N	7.44	132.66	123.21
1	A	89	LYS	CA-C-N	7.41	134.23	122.59
1	A	89	LYS	C-N-CA	7.41	134.23	122.59
1	B	98	ARG	CA-C-N	7.39	131.54	120.31
1	B	98	ARG	C-N-CA	7.39	131.54	120.31
1	A	161	VAL	N-CA-CB	7.36	124.20	111.39
1	A	92	ILE	CB-CG1-CD1	-7.28	98.50	113.80
1	B	162	VAL	O-C-N	7.27	130.55	123.14
1	B	4	THR	CB-CA-C	7.25	121.67	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	PHE	N-CA-C	-7.25	103.07	110.97
1	B	205	ARG	NE-CZ-NH1	7.25	128.75	121.50
1	A	10	ASN	OD1-CG-ND2	-7.24	115.36	122.60
1	A	247	ARG	NE-CZ-NH2	7.24	125.71	119.20
1	B	143	VAL	N-CA-CB	-7.24	102.08	110.55
1	A	176	ALA	CA-C-N	-7.23	110.71	124.01
1	A	176	ALA	C-N-CA	-7.23	110.71	124.01
1	B	161	VAL	N-CA-C	-7.23	98.05	108.53
1	A	216	ASN	CB-CG-ND2	-7.22	105.58	116.40
1	B	121	VAL	O-C-N	7.21	128.83	122.12
1	B	47	LEU	N-CA-CB	-7.18	99.65	110.07
1	A	38	VAL	CB-CA-C	7.17	121.70	110.81
1	B	29	THR	CA-CB-OG1	-7.17	98.85	109.60
1	A	8	GLY	CA-C-O	-7.14	114.69	121.11
1	B	125	LEU	CA-C-O	-7.14	112.94	120.58
1	A	109	ILE	CB-CG1-CD1	7.14	128.79	113.80
1	B	192	LEU	CA-C-N	7.11	130.38	120.29
1	B	192	LEU	C-N-CA	7.11	130.38	120.29
1	A	207	LEU	CA-C-O	-7.10	112.95	121.05
1	A	34	GLU	CA-C-O	-7.10	112.86	120.46
1	B	26	ARG	N-CA-C	-7.09	103.56	111.28
1	A	241	VAL	N-CA-CB	7.08	123.59	110.77
1	A	42	PRO	O-C-N	7.05	129.78	121.46
1	B	109	ILE	CA-C-O	-6.97	113.78	121.17
1	A	152	GLU	CB-CA-C	-6.97	99.22	110.79
1	A	67	TYR	O-C-N	6.95	131.19	122.43
1	A	182	GLN	CB-CG-CD	6.95	124.41	112.60
1	A	75	THR	CA-C-O	6.93	128.67	120.70
1	B	12	LYS	O-C-N	6.93	131.80	122.59
1	A	41	CYS	CA-C-N	6.91	127.50	120.38
1	A	41	CYS	C-N-CA	6.91	127.50	120.38
1	A	139	THR	CA-C-O	-6.91	113.75	121.00
1	B	20	ILE	CB-CA-C	6.91	123.45	112.26
1	A	56	LYS	CB-CA-C	-6.90	100.82	109.31
1	A	161	VAL	CA-C-O	-6.89	112.61	120.67
1	B	95	HIS	ND1-CE1-NE2	6.87	115.27	108.40
1	B	27	LEU	CA-C-N	6.86	129.36	120.44
1	B	27	LEU	C-N-CA	6.86	129.36	120.44
1	A	10	ASN	CA-CB-CG	6.86	119.46	112.60
1	A	78	ASN	N-CA-CB	6.85	121.72	110.69
1	A	237	LYS	O-C-N	6.84	127.13	121.32
1	A	216	ASN	OD1-CG-ND2	6.84	129.44	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	GLU	N-CA-C	-6.83	98.11	108.96
1	B	246	SER	CA-C-O	-6.82	112.12	119.97
1	B	132	GLU	O-C-N	6.80	129.08	122.07
1	A	53	LEU	N-CA-C	6.80	119.70	111.82
1	A	144	GLU	OE1-CD-OE2	6.79	139.19	122.90
1	B	139	THR	CA-C-O	-6.79	113.69	120.82
1	A	108	PHE	CB-CA-C	6.78	121.40	110.96
1	A	35	ASN	CA-CB-CG	6.76	119.36	112.60
1	B	3	ARG	N-CA-CB	6.75	121.90	110.49
1	A	230	LEU	N-CA-CB	6.70	121.75	110.69
1	B	234	ALA	CA-C-N	6.70	129.26	120.28
1	B	234	ALA	C-N-CA	6.70	129.26	120.28
1	A	161	VAL	O-C-N	6.70	130.41	123.18
1	A	91	VAL	CB-CA-C	-6.69	99.13	110.71
1	A	34	GLU	CA-CB-CG	6.69	127.48	114.10
1	A	144	GLU	CB-CA-C	6.69	122.94	110.70
1	A	77	GLU	CA-C-N	6.68	132.62	122.93
1	A	77	GLU	C-N-CA	6.68	132.62	122.93
1	B	118	GLY	CA-C-N	6.68	133.42	120.99
1	B	118	GLY	C-N-CA	6.68	133.42	120.99
1	A	110	ALA	N-CA-C	-6.68	103.61	111.03
1	A	62	GLY	O-C-N	6.67	129.79	123.65
1	B	184	ILE	O-C-N	6.67	128.81	121.94
1	A	36	VAL	N-CA-C	-6.66	98.00	108.86
1	A	156	ASP	CA-C-O	-6.66	110.81	120.13
1	B	153	GLU	CB-CG-CD	6.65	123.91	112.60
1	A	57	PRO	O-C-N	6.62	131.58	122.64
1	A	211	SER	CA-C-N	6.59	132.46	122.65
1	A	211	SER	C-N-CA	6.59	132.46	122.65
1	B	185	HIS	O-C-N	6.58	129.09	122.12
1	A	121	VAL	CA-C-O	-6.57	113.14	121.48
1	A	123	VAL	O-C-N	6.57	130.29	123.20
1	B	247	ARG	CA-C-N	6.56	133.51	121.70
1	B	247	ARG	C-N-CA	6.56	133.51	121.70
1	A	29	THR	CA-CB-OG1	-6.54	99.80	109.60
1	A	53	LEU	CA-C-O	-6.53	112.46	119.97
1	B	117	LEU	CB-CA-C	6.53	122.64	110.70
1	A	103	HIS	ND1-CG-CD2	6.52	112.62	106.10
1	A	15	GLY	CA-C-O	6.51	127.13	122.37
1	B	98	ARG	CG-CD-NE	6.51	126.32	112.00
1	B	198	ASP	O-C-N	6.50	129.82	122.22
1	B	78	ASN	OD1-CG-ND2	6.49	129.09	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	LEU	N-CA-CB	6.48	121.41	110.46
1	A	19	SER	CA-C-O	-6.47	113.56	120.42
1	B	140	LEU	CA-C-O	-6.47	113.69	120.55
1	A	31	SER	O-C-N	6.47	130.57	123.13
1	A	145	ARG	NE-CZ-NH1	-6.46	115.03	121.50
1	A	4	THR	CA-CB-OG1	-6.46	99.91	109.60
1	A	20	ILE	CB-CG1-CD1	6.46	127.36	113.80
1	B	140	LEU	O-C-N	6.46	128.97	122.12
1	B	226	VAL	O-C-N	6.43	131.31	122.88
1	B	174	LEU	CA-C-O	-6.42	113.83	121.66
1	A	18	GLN	N-CA-C	6.42	117.94	111.07
1	A	226	VAL	N-CA-C	-6.39	97.91	107.37
1	A	14	ASN	OD1-CG-ND2	-6.39	116.21	122.60
1	A	220	PHE	CB-CA-C	-6.37	100.43	110.94
1	B	240	PHE	O-C-N	-6.36	115.37	122.12
1	A	65	ASN	CA-C-N	6.36	133.26	121.62
1	A	65	ASN	C-N-CA	6.36	133.26	121.62
1	B	92	ILE	N-CA-C	-6.35	99.44	108.58
1	B	87	GLY	O-C-N	6.34	129.66	122.55
1	B	35	ASN	OD1-CG-ND2	6.32	128.92	122.60
1	B	77	GLU	CB-CG-CD	6.32	123.35	112.60
1	A	134	LYS	CA-CB-CG	6.32	126.74	114.10
1	A	65	ASN	OD1-CG-ND2	6.32	128.91	122.60
1	A	247	ARG	CB-CA-C	6.31	122.84	111.03
1	B	180	ASP	N-CA-CB	6.31	119.13	109.98
1	B	162	VAL	CA-C-O	-6.31	113.53	120.72
1	B	58	GLN	O-C-N	6.30	130.03	122.27
1	A	216	ASN	N-CA-CB	-6.29	100.86	109.98
1	A	193	ALA	O-C-N	-6.28	114.87	122.22
1	B	194	SER	N-CA-C	-6.28	104.49	111.71
1	B	114	LYS	CA-C-O	6.27	128.36	121.02
1	A	48	ASP	O-C-N	6.26	128.78	122.08
1	B	130	THR	N-CA-C	6.26	120.92	113.28
1	B	32	ILE	CA-C-N	6.25	127.66	119.84
1	B	32	ILE	C-N-CA	6.25	127.66	119.84
1	B	84	LYS	CG-CD-CE	6.24	125.65	111.30
1	B	110	ALA	N-CA-C	-6.23	104.41	111.07
1	B	211	SER	O-C-N	6.23	131.00	122.41
1	B	78	ASN	O-C-N	6.21	130.99	123.16
1	B	20	ILE	CA-CB-CG2	6.21	121.06	110.50
1	A	108	PHE	CA-CB-CG	6.18	119.98	113.80
1	B	198	ASP	CA-C-O	-6.18	113.12	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	THR	CA-C-N	6.17	125.85	119.56
1	A	177	THR	C-N-CA	6.17	125.85	119.56
1	B	205	ARG	CA-CB-CG	-6.17	101.77	114.10
1	A	81	ASP	O-C-N	6.16	128.65	122.12
1	A	145	ARG	CB-CA-C	-6.15	100.58	110.79
1	A	66	ALA	CA-C-O	-6.15	114.65	121.23
1	A	84	LYS	CA-CB-CG	6.15	126.41	114.10
1	B	200	ALA	CA-C-O	-6.15	114.36	120.82
1	B	78	ASN	CA-C-O	-6.15	114.21	121.16
1	B	218	VAL	CB-CA-C	6.14	121.68	112.16
1	A	240	PHE	N-CA-CB	6.12	119.24	110.06
1	B	191	PHE	CA-C-O	-6.11	112.55	120.00
1	A	161	VAL	CA-C-N	-6.09	114.65	123.06
1	A	161	VAL	C-N-CA	-6.09	114.65	123.06
1	A	104	GLU	CB-CG-CD	6.08	122.94	112.60
1	A	221	LYS	CG-CD-CE	6.08	125.28	111.30
1	B	185	HIS	CA-CB-CG	6.08	119.88	113.80
1	A	73	ALA	CA-C-O	-6.08	115.05	122.64
1	A	10	ASN	CA-C-O	-6.07	114.08	120.58
1	B	91	VAL	CA-C-N	-6.07	114.55	122.37
1	B	91	VAL	C-N-CA	-6.07	114.55	122.37
1	A	42	PRO	CA-C-O	-6.06	111.78	120.56
1	B	94	GLY	N-CA-C	6.05	124.40	115.08
1	B	211	SER	CA-C-N	-6.05	114.37	122.72
1	B	211	SER	C-N-CA	-6.05	114.37	122.72
1	A	158	THR	N-CA-C	-6.05	105.39	112.89
1	B	144	GLU	CG-CD-OE2	-6.05	104.49	118.40
1	B	92	ILE	CA-CB-CG2	6.05	120.78	110.50
1	B	86	VAL	CA-CB-CG1	6.04	120.67	110.40
1	A	179	GLU	CA-C-N	6.04	128.29	120.44
1	A	179	GLU	C-N-CA	6.04	128.29	120.44
1	B	14	ASN	OD1-CG-ND2	6.02	128.62	122.60
1	B	186	ALA	CA-C-O	6.01	126.93	120.55
1	A	165	GLU	CB-CA-C	-6.01	103.50	110.17
1	B	134	LYS	N-CA-C	-6.01	104.07	111.40
1	B	46	TYR	CB-CA-C	-6.01	101.29	111.02
1	B	10	ASN	OD1-CG-ND2	6.00	128.60	122.60
1	A	154	VAL	N-CA-CB	-5.99	104.35	111.90
1	B	182	GLN	CB-CA-C	5.98	120.38	110.81
1	B	221	LYS	CA-C-O	-5.98	115.29	121.87
1	B	49	TYR	CA-CB-CG	-5.97	103.16	113.90
1	B	10	ASN	CA-C-O	-5.97	114.20	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	LYS	N-CA-C	5.94	117.76	111.28
1	B	199	LYS	CB-CG-CD	5.94	124.96	111.30
1	A	129	GLU	CA-C-O	-5.94	114.18	121.78
1	A	173	GLY	O-C-N	5.93	129.44	122.38
1	B	233	GLY	O-C-N	5.93	128.53	122.24
1	B	69	LYS	O-C-N	5.93	130.03	123.33
1	A	52	SER	O-C-N	5.92	128.92	122.11
1	A	71	SER	N-CA-C	5.92	117.78	108.96
1	B	173	GLY	CA-C-O	5.91	126.34	119.13
1	A	28	ASN	CA-C-N	5.90	132.05	121.66
1	A	28	ASN	C-N-CA	5.90	132.05	121.66
1	A	33	PRO	CA-C-N	-5.88	114.75	123.11
1	A	33	PRO	C-N-CA	-5.88	114.75	123.11
1	B	215	SER	CB-CA-C	5.88	120.84	110.85
1	B	14	ASN	CA-C-O	-5.87	114.43	120.89
1	A	31	SER	CA-C-O	-5.87	113.86	120.43
1	B	102	PHE	CA-C-O	5.87	126.30	119.32
1	B	215	SER	CA-CB-OG	-5.85	99.40	111.10
1	A	32	ILE	N-CA-CB	5.84	119.39	111.21
1	A	85	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	161	VAL	CB-CA-C	5.84	119.32	110.62
1	B	60	THR	CA-CB-OG1	-5.83	100.86	109.60
1	A	28	ASN	CB-CG-ND2	5.82	125.14	116.40
1	B	129	GLU	CA-CB-CG	5.81	125.73	114.10
1	B	148	ASN	N-CA-C	5.81	117.61	111.28
1	B	223	LYS	N-CA-C	-5.81	99.06	108.41
1	B	172	THR	CA-C-O	-5.80	112.21	120.51
1	B	54	VAL	N-CA-CB	5.80	118.21	110.26
1	B	92	ILE	N-CA-CB	5.80	117.04	110.72
1	A	176	ALA	CB-CA-C	5.79	119.08	109.53
1	A	222	ASP	CA-C-O	-5.78	112.77	119.59
1	A	69	LYS	CA-C-N	5.77	130.44	120.58
1	A	69	LYS	C-N-CA	5.77	130.44	120.58
1	A	80	VAL	CA-C-O	-5.77	112.70	119.85
1	B	95	HIS	CE1-NE2-CD2	-5.76	103.24	109.00
1	A	112	LYS	N-CA-CB	5.74	118.33	110.01
1	B	171	GLY	CA-C-N	5.74	132.51	121.54
1	B	171	GLY	C-N-CA	5.74	132.51	121.54
1	A	17	LYS	CA-CB-CG	5.74	125.57	114.10
1	A	119	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	A	91	VAL	CA-CB-CG2	5.73	120.14	110.40
1	B	169	ALA	N-CA-C	-5.73	105.95	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	LYS	CA-C-N	5.73	128.21	120.65
1	A	138	LYS	C-N-CA	5.73	128.21	120.65
1	A	67	TYR	N-CA-C	-5.73	101.52	110.17
1	B	75	THR	CA-C-N	5.72	131.29	122.20
1	B	75	THR	C-N-CA	5.72	131.29	122.20
1	A	39	VAL	CB-CA-C	5.71	118.66	110.33
1	B	103	HIS	CA-C-O	5.70	128.65	120.51
1	A	163	ALA	O-C-N	5.69	130.07	123.30
1	A	102	PHE	CA-C-N	5.69	132.41	121.54
1	A	102	PHE	C-N-CA	5.69	132.41	121.54
1	A	212	ALA	CA-C-O	-5.69	114.49	120.80
1	A	138	LYS	CA-CB-CG	-5.67	102.75	114.10
1	B	56	LYS	CA-CB-CG	5.67	125.45	114.10
1	A	129	GLU	CG-CD-OE1	5.67	131.44	118.40
1	B	3	ARG	CA-CB-CG	-5.64	102.81	114.10
1	A	240	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	144	GLU	O-C-N	5.63	127.87	122.07
1	A	213	ASN	O-C-N	5.62	129.97	122.73
1	A	219	THR	CA-CB-CG2	5.61	120.04	110.50
1	B	82	GLN	OE1-CD-NE2	5.60	128.20	122.60
1	B	235	SER	N-CA-CB	-5.59	101.90	110.12
1	A	103	HIS	CA-C-N	5.59	129.49	121.50
1	A	103	HIS	C-N-CA	5.59	129.49	121.50
1	B	152	GLU	CB-CG-CD	-5.58	103.12	112.60
1	A	206	ILE	CA-C-N	5.57	129.39	121.42
1	A	206	ILE	C-N-CA	5.57	129.39	121.42
1	A	84	LYS	N-CA-C	-5.57	105.60	112.90
1	B	146	GLN	OE1-CD-NE2	5.57	128.17	122.60
1	A	27	LEU	CA-C-O	-5.56	115.69	121.98
1	A	103	HIS	CA-C-O	5.56	128.46	120.51
1	A	121	VAL	CA-C-N	5.55	126.80	120.53
1	A	121	VAL	C-N-CA	5.55	126.80	120.53
1	A	243	ILE	O-C-N	5.55	127.67	121.90
1	A	140	LEU	N-CA-CB	5.54	118.87	110.28
1	B	82	GLN	CA-C-N	5.54	129.38	120.30
1	B	82	GLN	C-N-CA	5.54	129.38	120.30
1	B	123	VAL	O-C-N	5.53	129.02	123.10
1	A	172	THR	CA-CB-OG1	-5.53	101.31	109.60
1	B	61	VAL	CA-C-O	5.53	127.69	121.28
1	B	213	ASN	CB-CG-OD1	5.53	131.85	120.80
1	A	187	SER	N-CA-CB	5.52	118.02	110.01
1	A	198	ASP	O-C-N	5.51	129.05	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	ILE	O-C-N	5.51	127.63	121.90
1	A	193	ALA	CA-C-N	5.51	130.04	120.68
1	A	193	ALA	C-N-CA	5.51	130.04	120.68
1	B	111	ASP	CA-C-O	-5.49	115.02	120.90
1	A	113	THR	CA-CB-OG1	-5.49	101.37	109.60
1	A	36	VAL	O-C-N	5.49	128.87	123.00
1	A	155	LYS	CG-CD-CE	5.49	123.92	111.30
1	B	35	ASN	CA-C-O	5.48	126.95	120.70
1	B	153	GLU	CG-CD-OE1	5.48	131.00	118.40
1	A	74	PHE	CA-CB-CG	-5.48	108.32	113.80
1	A	104	GLU	CA-C-O	-5.47	114.45	120.69
1	A	144	GLU	N-CA-C	-5.47	104.96	111.69
1	A	203	GLU	CB-CG-CD	5.47	121.90	112.60
1	A	63	ALA	N-CA-C	-5.46	101.96	110.42
1	B	199	LYS	CA-CB-CG	5.46	125.01	114.10
1	A	211	SER	CA-C-O	-5.45	112.71	120.51
1	B	131	LEU	CB-CA-C	-5.45	99.58	110.42
1	A	101	TYR	N-CA-C	5.44	117.21	111.28
1	A	201	ALA	CA-C-O	-5.43	113.73	119.97
1	B	45	THR	O-C-N	5.43	128.39	122.20
1	B	68	LEU	CA-C-O	-5.42	113.33	119.78
1	B	56	LYS	CG-CD-CE	5.42	123.77	111.30
1	A	182	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	B	106	ASP	CA-C-O	-5.39	114.88	120.92
1	B	14	ASN	CB-CG-OD1	-5.39	110.03	120.80
1	A	87	GLY	O-C-N	5.38	128.74	122.45
1	B	124	ILE	CA-C-O	5.38	127.37	120.97
1	B	35	ASN	CB-CG-OD1	-5.37	110.06	120.80
1	A	240	PHE	CA-C-N	5.36	129.09	120.30
1	A	240	PHE	C-N-CA	5.36	129.09	120.30
1	B	174	LEU	O-C-N	5.36	129.09	123.03
1	A	230	LEU	N-CA-C	-5.36	96.93	107.69
1	B	78	ASN	CA-CB-CG	5.35	117.95	112.60
1	A	98	ARG	NE-CZ-NH2	-5.35	114.39	119.20
1	B	35	ASN	O-C-N	5.35	129.96	123.01
1	B	143	VAL	CA-CB-CG1	5.34	119.48	110.40
1	A	64	GLN	OE1-CD-NE2	5.34	127.94	122.60
1	A	20	ILE	CA-C-O	5.33	126.50	120.85
1	B	201	ALA	CB-CA-C	5.33	119.24	110.88
1	B	83	ILE	CA-C-O	5.31	126.21	120.47
1	A	26	ARG	N-CA-C	-5.31	105.41	111.14
1	A	99	ARG	N-CA-C	-5.30	105.41	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	PHE	CA-CB-CG	5.30	119.10	113.80
1	A	165	GLU	CA-C-N	5.30	126.47	119.84
1	A	165	GLU	C-N-CA	5.30	126.47	119.84
1	A	156	ASP	O-C-N	-5.30	115.25	122.19
1	B	28	ASN	CA-C-O	-5.30	115.26	120.82
1	B	143	VAL	CA-C-O	-5.29	115.56	121.17
1	A	245	ASN	CB-CG-ND2	-5.29	108.46	116.40
1	B	58	GLN	N-CA-C	5.28	117.95	111.82
1	B	62	GLY	O-C-N	-5.28	118.61	123.42
1	A	87	GLY	N-CA-C	5.28	122.87	115.43
1	B	170	ILE	N-CA-C	5.27	115.45	107.80
1	A	56	LYS	N-CA-CB	5.25	117.99	109.90
1	A	98	ARG	CG-CD-NE	5.24	123.53	112.00
1	B	200	ALA	CB-CA-C	-5.24	102.65	110.88
1	B	222	ASP	CA-C-O	-5.23	113.03	120.51
1	B	28	ASN	N-CA-CB	5.23	117.59	110.01
1	B	130	THR	CA-C-N	-5.21	111.58	121.54
1	B	130	THR	C-N-CA	-5.21	111.58	121.54
1	B	19	SER	CA-C-O	-5.21	113.98	119.97
1	B	143	VAL	CB-CA-C	5.21	118.64	111.97
1	B	124	ILE	N-CA-CB	5.21	117.85	111.60
1	A	109	ILE	CA-C-O	5.20	126.14	120.57
1	B	146	GLN	CG-CD-OE1	-5.20	110.39	120.80
1	A	53	LEU	CB-CA-C	-5.19	100.71	110.67
1	A	196	LEU	CA-C-O	-5.18	113.42	118.97
1	B	193	ALA	CA-C-O	-5.18	114.93	120.42
1	A	185	HIS	N-CA-C	-5.18	105.32	111.69
1	B	133	GLU	CB-CG-CD	5.17	121.38	112.60
1	B	28	ASN	O-C-N	5.16	127.39	122.07
1	A	49	TYR	CB-CA-C	5.16	119.06	110.81
1	B	3	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	B	97	GLU	CG-CD-OE2	-5.15	106.55	118.40
1	B	101	TYR	CA-CB-CG	5.15	123.17	113.90
1	A	213	ASN	CA-C-O	-5.15	115.84	121.14
1	A	215	SER	O-C-N	-5.14	116.67	122.12
1	A	2	ALA	CA-C-O	5.14	129.54	120.80
1	A	40	ILE	CB-CA-C	5.14	118.63	110.81
1	A	56	LYS	CA-CB-CG	-5.14	103.82	114.10
1	A	235	SER	CA-C-O	5.13	125.67	119.31
1	A	45	THR	OG1-CB-CG2	-5.13	99.04	109.30
1	A	43	PRO	CA-C-O	-5.12	111.28	120.60
1	A	134	LYS	CA-C-O	5.11	125.84	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	SER	CA-C-N	-5.11	113.78	122.56
1	B	235	SER	C-N-CA	-5.11	113.78	122.56
1	A	90	TRP	CD2-CE2-CZ2	-5.10	117.30	122.40
1	A	94	GLY	O-C-N	-5.10	116.00	122.32
1	A	158	THR	CB-CA-C	5.10	120.64	109.99
1	B	58	GLN	OE1-CD-NE2	5.08	127.69	122.60
1	A	190	LYS	CA-C-N	-5.08	113.94	120.65
1	A	190	LYS	C-N-CA	-5.08	113.94	120.65
1	B	119	GLN	O-C-N	5.08	129.19	122.43
1	B	115	PHE	CA-CB-CG	-5.08	108.72	113.80
1	B	196	LEU	CA-CB-CG	5.08	134.06	116.30
1	A	248	ASN	N-CA-CB	5.07	119.11	110.50
1	A	85	ASP	CA-C-O	-5.07	115.18	120.55
1	A	77	GLU	CA-C-O	-5.06	115.97	121.89
1	B	184	ILE	CA-CB-CG1	-5.03	101.84	110.40
1	A	79	SER	CA-C-N	-5.03	112.29	120.64
1	A	79	SER	C-N-CA	-5.03	112.29	120.64
1	A	85	ASP	CA-C-N	-5.03	115.14	122.28
1	A	85	ASP	C-N-CA	-5.03	115.14	122.28
1	B	12	LYS	CA-CB-CG	-5.02	104.06	114.10
1	B	49	TYR	O-C-N	-5.02	116.71	122.08
1	B	230	LEU	N-CA-C	-5.01	97.75	107.62
1	A	145	ARG	O-C-N	5.01	127.43	122.12
1	B	102	PHE	CA-CB-CG	-5.01	108.79	113.80
1	A	71	SER	CA-C-O	-5.00	116.10	121.45

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	1892	99	1
1	B	1883	0	1892	116	1
2	A	66	0	0	7	0
2	B	53	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3885	0	3784	202	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 27.

All (202) 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:A:216:ASN:O	1:A:219:THR:HB	1.65	0.97
1:B:130:THR:O	1:B:131:LEU:HB2	1.58	0.96
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:N	1:B:35:ASN:OD1	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:N	1:B:132:GLU:OE2	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:A:97:GLU:OE2	1:B:75:THR:HG23	1.86	0.75
1:B:33:PRO:HD3	1:B:245:ASN:ND2	2.01	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:B:194:SER:C	1:B:195:LYS:HD3	2.13	0.73
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:HG13	1:B:32:ILE:O	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:A:132:GLU:H	1:A:132:GLU:CD	2.01	0.69
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: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:218:VAL:O	1:A:221:LYS:HE3	1.95	0.66
1:A:26:ARG:C	1:A:27:LEU:O	2.36	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:B:131:LEU:HA	1:B:134:LYS:HB3	1.80	0.64
1:A:168:TRP:CD1	1:A:168:TRP:H	2.17	0.63
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:49:TYR:O	1:A:52:SER:HB2	2.00	0.61
1:A:34:GLU:O	1:A:35:ASN:HB3	2.00	0.61
1:A:131:LEU:HB3	1:A:132:GLU:OE1	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:92:ILE:HG13	1:A:92:ILE:O	2.00	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:216:ASN:OD1	1:B:216:ASN:C	2.47	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:34:GLU:O	1:A:35:ASN:CB	2.53	0.56
1:A:104:GLU:OE1	2:A:718:HOH:O	2.17	0.56
1:A:40:ILE:O	1:A:61:VAL:HA	2.06	0.56
1:A:92:ILE:HD11	1:A:95:HIS:HB2	1.88	0.55
1:A:230:LEU:HD13	2:A:602:HOH:O	2.06	0.55
1:B:12:LYS:NZ	1:B:97:GLU:OE2	2.40	0.55
1:B:49:TYR:HB2	2:B:706:HOH:O	2.06	0.55
1:B:102:PHE:O	1:B:103:HIS:C	2.50	0.54
1:B:117:LEU:O	1:B:118:GLY:C	2.49	0.54
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: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:129:GLU:CD	1:B:139:THR:HB	2.35	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:48:ASP:OD1	1:B:17:LYS:NZ	2.37	0.50
1:A:142:VAL:CG2	1:A:143:VAL:N	2.73	0.50
1:B:141:ASP:N	1:B:141:ASP:OD1	2.44	0.50
1:A:80:VAL:CG2	1:A:119:GLN:HG3	2.42	0.50
1:B:105:ASP:OD2	1:B:105:ASP:N	2.42	0.49
1:B:101:TYR:HD2	1:B:101:TYR:H	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:20:ILE:HD11	1:B:50:SER:OG	2.13	0.48
1:B:33:PRO:CD	1:B:245:ASN:HD22	2.23	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:49:TYR:O	1:A:53:LEU:HD22	2.15	0.47
1:A:50:SER:O	1:A:54:VAL:HG23	2.15	0.47
1:B:131:LEU:HD22	1:B:135:LYS:HG3	1.96	0.47
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:38:VAL:O	1:A:59:VAL:HA	2.16	0.45
1:A:104:GLU:HB3	1:A:109:ILE:HD11	1.99	0.45
1:A:28:ASN:O	1:A:56:LYS:HD3	2.17	0.45
1:A:139:THR:OG1	1:A:140:LEU:N	2.49	0.45
1:B:102:PHE:CA	2:B:755:HOH:O	2.63	0.45
1:B:102:PHE:C	2:B:755:HOH:O	2.52	0.45
1:A:17:LYS:HE3	1:B:48:ASP:OD1	2.16	0.45
1:A:129:GLU:H	1:A:129:GLU:HG3	1.38	0.45
1:A:216:ASN:O	1:A:217:ALA:C	2.59	0.45
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:33:PRO:HD3	1:B:245:ASN:HD21	1.82	0.44
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:A:27:LEU:C	1:A:29:THR:H	2.24	0.44
1:A:6:PHE:C	1:A:6:PHE:CD1	2.96	0.43
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:28:ASN:HD22	1:B:28:ASN:HA	1.52	0.43
1:B:211:SER:HA	2:B:637:HOH:O	2.18	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:A:190:LYS:O	1:A:191:PHE:C	2.58	0.42
1:B:241:VAL:O	1:B:244:ILE:HB	2.19	0.42
1:A:43:PRO:HG2	1:B:82:GLN:HE22	1.84	0.42
1:A:182:GLN:NE2	1:A:225:ASP:H	2.17	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:B:113:THR:O	1:B:114:LYS:C	2.63	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:11:PHE:C	1:B:12:LYS:O	2.61	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:A:48:ASP:CG	1:B:17:LYS:HZ2	2.24	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:CD2	1:B:101:TYR:N	2.88	0.41
1:A:6:PHE:O	1:A:228:GLY:HA3	2.20	0.41
1:B:205:ARG:HH21	1:B:205:ARG:HD2	1.44	0.41
1:A:128:GLY:HA2	1:A:164:TYR:CE1	2.56	0.41
1:B:237:LYS:O	1:B:238:PRO:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	245/247 (99%)	230 (94%)	12 (5%)	3 (1%)	10	4
1	B	245/247 (99%)	229 (94%)	13 (5%)	3 (1%)	10	4
All	All	490/494 (99%)	459 (94%)	25 (5%)	6 (1%)	10	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 ⓘ

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%)	160 (80%)	40 (20%)	1	0
1	B	200/200 (100%)	145 (72%)	55 (28%)	0	0
All	All	400/400 (100%)	305 (76%)	95 (24%)	1	0

All (95) 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	32	ILE
1	A	38	VAL
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	79	SER
1	A	91	VAL
1	A	92	ILE
1	A	93	LEU
1	A	103	HIS
1	A	129	GLU
1	A	135	LYS
1	A	142	VAL
1	A	143	VAL
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

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Mol	Chain	Res	Type
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	219	THR
1	A	221	LYS
1	A	223	LYS
1	A	230	LEU
1	A	237	LYS
1	A	241	VAL
1	A	248	ASN
1	B	4	THR
1	B	7	VAL
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	54	VAL
1	B	59	VAL
1	B	61	VAL
1	B	68	LEU
1	B	69	LYS
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	123	VAL
1	B	131	LEU
1	B	132	GLU
1	B	139	THR

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Mol	Chain	Res	Type
1	B	140	LEU
1	B	141	ASP
1	B	143	VAL
1	B	144	GLU
1	B	151	LEU
1	B	154	VAL
1	B	155	LYS
1	B	160	VAL
1	B	170	ILE
1	B	183	ASP
1	B	188	ILE
1	B	190	LYS
1	B	196	LEU
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	223	LYS
1	B	226	VAL
1	B	231	VAL
1	B	235	SER
1	B	236	LEU
1	B	238	PRO
1	B	239	GLU

Sometimes 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	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	103	HIS
1	B	146	GLN
1	B	185	HIS

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Mol	Chain	Res	Type
1	B	245	ASN

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

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.