



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:09 PM UTC

PDB ID : 1F2J / pdb_00001f2j
Title : CRYSTAL STRUCTURE ANALYSIS OF ALDOLASE FROM T. BRUCEI
Authors : Chudzik, D.M.; Michels, P.A.; De Walque, S.; Hol, W.G.J.
Deposited on : 2000-05-25
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

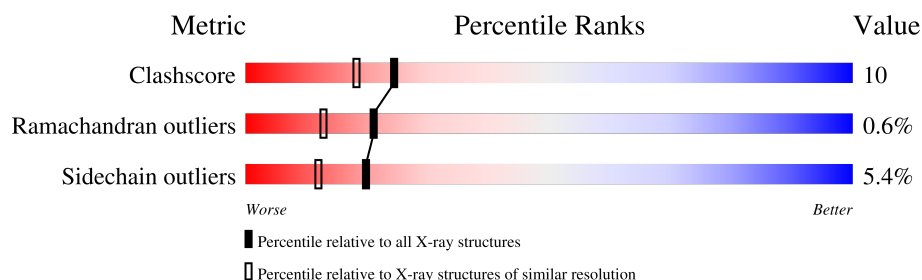
1 Overall quality at a glance

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	370	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2948 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 FRUCTOSE-BISPHOSPHATE ALDOLASE, GLYCOSOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2707	1709	478	501	19			

- Molecule 2 is water.

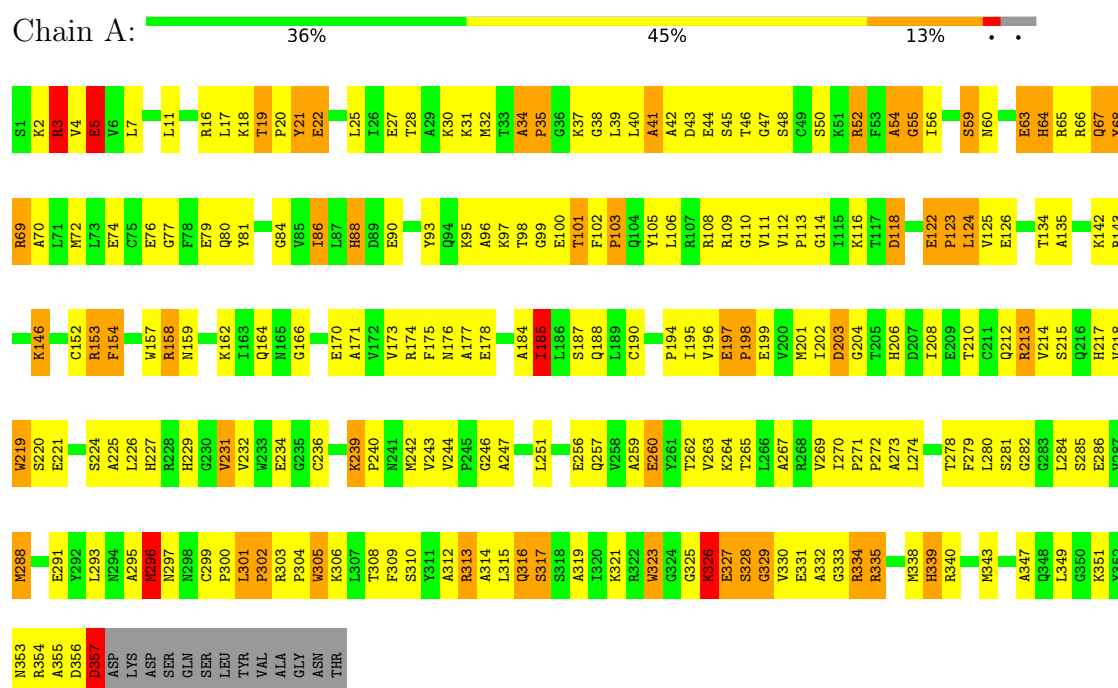
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	241	Total	O	0	0
			241	241		

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: FRUCTOSE-BISPHOSPHATE ALDOLASE, GLYCOSOMAL



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	209.66 Å 209.66 Å 209.66 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-1.90)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.199 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2948	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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	2.38	122/2762 (4.4%)	2.62	225/3745 (6.0%)

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	3

All (122) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	ARG	NE-CZ	17.11	1.51	1.33
1	A	256	GLU	CD-OE2	10.09	1.44	1.25
1	A	40	LEU	C-O	9.86	1.36	1.24
1	A	213	ARG	CD-NE	9.64	1.59	1.46
1	A	313	ARG	CZ-NH2	9.57	1.45	1.33
1	A	112	VAL	CA-C	7.91	1.59	1.53
1	A	299	CYS	CA-C	7.90	1.61	1.52
1	A	3	ARG	NE-CZ	7.87	1.41	1.33
1	A	178	GLU	CD-OE2	7.75	1.40	1.25
1	A	335	ARG	CZ-NH1	7.68	1.43	1.32
1	A	204	GLY	N-CA	7.66	1.53	1.45
1	A	221	GLU	CD-OE2	7.62	1.39	1.25
1	A	229	HIS	CD2-NE2	7.62	1.46	1.37
1	A	56	ILE	CA-CB	7.61	1.63	1.54
1	A	356	ASP	CG-OD2	7.54	1.39	1.25
1	A	349	LEU	CA-C	-7.26	1.42	1.52
1	A	88	HIS	CE1-NE2	7.18	1.39	1.32
1	A	69	ARG	NE-CZ	7.11	1.40	1.33
1	A	353	ASN	C-N	-7.05	1.24	1.34
1	A	178	GLU	CA-C	6.98	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281	SER	CA-CB	6.88	1.64	1.53
1	A	185	ILE	CA-CB	6.78	1.62	1.54
1	A	217	HIS	CD2-NE2	6.75	1.45	1.37
1	A	297	ASN	C-N	-6.75	1.22	1.33
1	A	271	PRO	CA-C	6.74	1.58	1.52
1	A	126	GLU	CD-OE2	6.72	1.38	1.25
1	A	260	GLU	CD-OE2	6.70	1.38	1.25
1	A	272	PRO	C-O	-6.69	1.15	1.24
1	A	212	GLN	C-N	6.63	1.42	1.33
1	A	339	HIS	CA-C	6.63	1.61	1.52
1	A	327	GLU	CD-OE2	6.58	1.37	1.25
1	A	27	GLU	CD-OE2	6.55	1.37	1.25
1	A	251	LEU	CA-C	-6.48	1.45	1.52
1	A	175	PHE	CA-CB	6.48	1.63	1.53
1	A	219	TRP	C-N	6.45	1.42	1.34
1	A	84	GLY	CA-C	6.43	1.58	1.51
1	A	338	MET	CG-SD	6.42	1.96	1.80
1	A	41	ALA	C-O	6.42	1.32	1.24
1	A	32	MET	CA-C	-6.40	1.44	1.52
1	A	18	LYS	CA-CB	6.36	1.61	1.53
1	A	229	HIS	ND1-CE1	6.24	1.38	1.32
1	A	101	THR	C-O	6.23	1.32	1.23
1	A	269	VAL	CA-C	-6.22	1.44	1.52
1	A	114	GLY	C-O	6.18	1.31	1.23
1	A	178	GLU	CA-CB	6.18	1.62	1.53
1	A	246	GLY	CA-C	6.17	1.57	1.52
1	A	327	GLU	C-N	-6.16	1.25	1.33
1	A	76	GLU	CA-C	-6.15	1.44	1.52
1	A	329	GLY	N-CA	6.12	1.53	1.45
1	A	190	CYS	CA-C	6.11	1.62	1.52
1	A	213	ARG	CG-CD	6.06	1.70	1.52
1	A	31	LYS	CA-CB	6.02	1.62	1.53
1	A	206	HIS	ND1-CE1	6.01	1.38	1.32
1	A	70	ALA	CA-C	-6.00	1.44	1.52
1	A	19	THR	C-N	-5.99	1.28	1.34
1	A	326	LYS	CA-C	-5.96	1.45	1.52
1	A	347	ALA	CA-C	5.95	1.60	1.52
1	A	236	CYS	CA-CB	5.90	1.65	1.54
1	A	313	ARG	CZ-NH1	5.88	1.41	1.32
1	A	54	ALA	C-N	-5.86	1.26	1.33
1	A	99	GLY	CA-C	5.84	1.60	1.51
1	A	265	THR	CA-C	-5.80	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	ARG	CZ-NH2	5.79	1.41	1.33
1	A	16	ARG	NE-CZ	5.78	1.39	1.33
1	A	47	GLY	C-O	5.77	1.30	1.23
1	A	170	GLU	CA-C	5.71	1.60	1.52
1	A	243	VAL	CA-C	-5.71	1.45	1.52
1	A	64	HIS	C-N	5.71	1.41	1.33
1	A	114	GLY	N-CA	5.67	1.50	1.44
1	A	244	VAL	CA-C	-5.67	1.47	1.52
1	A	208	ILE	C-N	5.61	1.41	1.33
1	A	109	ARG	CZ-NH1	5.60	1.40	1.32
1	A	174	ARG	CZ-NH1	5.58	1.40	1.32
1	A	110	GLY	C-N	5.56	1.40	1.33
1	A	177	ALA	CA-C	-5.54	1.45	1.52
1	A	39	LEU	C-O	5.53	1.30	1.24
1	A	173	VAL	C-O	5.53	1.30	1.24
1	A	231	VAL	CA-CB	5.51	1.60	1.54
1	A	264	LYS	C-O	-5.50	1.17	1.24
1	A	351	LYS	C-N	-5.49	1.26	1.33
1	A	260	GLU	CA-CB	-5.45	1.44	1.53
1	A	74	GLU	C-O	-5.43	1.17	1.24
1	A	227	HIS	ND1-CE1	5.42	1.38	1.32
1	A	96	ALA	C-N	-5.42	1.26	1.33
1	A	231	VAL	CA-C	5.42	1.59	1.52
1	A	46	THR	C-N	-5.40	1.27	1.33
1	A	3	ARG	CZ-NH1	5.40	1.40	1.32
1	A	281	SER	CB-OG	5.39	1.52	1.42
1	A	54	ALA	N-CA	-5.38	1.40	1.46
1	A	174	ARG	C-N	-5.35	1.27	1.33
1	A	232	VAL	N-CA	5.34	1.52	1.46
1	A	95	LYS	CA-C	-5.33	1.46	1.52
1	A	321	LYS	C-N	-5.33	1.26	1.34
1	A	171	ALA	CA-CB	5.31	1.61	1.53
1	A	265	THR	C-N	-5.31	1.26	1.34
1	A	174	ARG	CA-C	-5.30	1.45	1.52
1	A	39	LEU	CA-C	5.29	1.58	1.52
1	A	178	GLU	C-N	5.29	1.41	1.33
1	A	217	HIS	ND1-CE1	5.26	1.37	1.32
1	A	257	GLN	N-CA	5.26	1.52	1.46
1	A	355	ALA	C-O	-5.25	1.17	1.24
1	A	304	PRO	N-CD	5.24	1.55	1.47
1	A	234	GLU	C-O	-5.23	1.17	1.24
1	A	106	LEU	CA-CB	5.23	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	MET	CA-C	-5.21	1.46	1.52
1	A	2	LYS	C-O	5.21	1.30	1.24
1	A	328	SER	N-CA	-5.21	1.39	1.46
1	A	162	LYS	C-O	5.20	1.30	1.24
1	A	103	PRO	CA-C	5.18	1.60	1.52
1	A	5	GLU	CD-OE2	5.17	1.35	1.25
1	A	224	SER	N-CA	5.16	1.52	1.46
1	A	55	GLY	C-O	-5.15	1.18	1.24
1	A	304	PRO	CA-CB	5.14	1.61	1.53
1	A	194	PRO	N-CA	-5.14	1.40	1.47
1	A	43	ASP	CG-OD1	-5.13	1.15	1.25
1	A	197	GLU	CD-OE2	5.12	1.35	1.25
1	A	88	HIS	CG-ND1	5.10	1.43	1.38
1	A	44	GLU	CD-OE1	-5.07	1.15	1.25
1	A	134	THR	N-CA	-5.05	1.39	1.46
1	A	185	ILE	CB-CG1	-5.04	1.43	1.53
1	A	273	ALA	CA-C	5.04	1.59	1.52
1	A	175	PHE	C-O	5.03	1.29	1.24

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	GLU	CB-CG-CD	-18.08	81.86	112.60
1	A	213	ARG	CB-CG-CD	13.93	143.34	111.30
1	A	185	ILE	CA-CB-CG1	-12.72	88.78	110.40
1	A	269	VAL	CA-C-N	-12.59	113.52	122.59
1	A	269	VAL	C-N-CA	-12.59	113.52	122.59
1	A	59	SER	N-CA-CB	-11.42	93.72	110.17
1	A	185	ILE	CA-CB-CG2	10.93	129.09	110.50
1	A	213	ARG	NH1-CZ-NH2	-10.70	105.39	119.30
1	A	213	ARG	NE-CZ-NH2	10.64	128.78	119.20
1	A	112	VAL	CB-CA-C	-10.59	101.09	110.94
1	A	5	GLU	CB-CG-CD	-9.63	96.22	112.60
1	A	219	TRP	CA-C-N	-9.38	106.06	120.31
1	A	219	TRP	C-N-CA	-9.38	106.06	120.31
1	A	153	ARG	NE-CZ-NH2	9.35	127.62	119.20
1	A	31	LYS	CB-CA-C	9.28	126.19	110.79
1	A	221	GLU	CG-CD-OE2	-9.18	97.30	118.40
1	A	229	HIS	CA-C-N	-8.70	110.25	122.00
1	A	229	HIS	C-N-CA	-8.70	110.25	122.00
1	A	16	ARG	NE-CZ-NH1	8.63	130.13	121.50
1	A	213	ARG	CD-NE-CZ	8.59	136.43	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ALA	CA-C-N	-8.57	102.08	121.19
1	A	54	ALA	C-N-CA	-8.57	102.08	121.19
1	A	327	GLU	CA-C-O	8.55	129.86	120.63
1	A	212	GLN	N-CA-CB	-8.51	97.56	110.16
1	A	18	LYS	CB-CA-C	8.43	124.26	110.78
1	A	88	HIS	CA-CB-CG	-8.27	105.53	113.80
1	A	259	ALA	CA-C-N	-8.27	108.55	120.29
1	A	259	ALA	C-N-CA	-8.27	108.55	120.29
1	A	213	ARG	CB-CA-C	8.24	123.81	110.88
1	A	109	ARG	NE-CZ-NH2	-8.06	111.94	119.20
1	A	22	GLU	N-CA-C	7.86	120.55	111.11
1	A	314	ALA	CA-C-N	-7.83	109.27	122.11
1	A	314	ALA	C-N-CA	-7.83	109.27	122.11
1	A	21	TYR	CA-C-N	-7.72	110.12	120.54
1	A	21	TYR	C-N-CA	-7.72	110.12	120.54
1	A	50	SER	CA-C-O	7.59	128.59	120.55
1	A	338	MET	CA-C-N	-7.47	109.68	120.29
1	A	338	MET	C-N-CA	-7.47	109.68	120.29
1	A	176	ASN	CA-CB-CG	-7.43	105.17	112.60
1	A	40	LEU	CA-C-N	-7.39	112.33	122.30
1	A	40	LEU	C-N-CA	-7.39	112.33	122.30
1	A	263	VAL	CA-C-N	-7.34	109.71	120.28
1	A	263	VAL	C-N-CA	-7.34	109.71	120.28
1	A	229	HIS	CA-CB-CG	-7.23	106.57	113.80
1	A	56	ILE	N-CA-C	-7.20	105.99	112.90
1	A	46	THR	CA-C-O	7.17	128.57	120.90
1	A	313	ARG	NE-CZ-NH2	-7.11	112.80	119.20
1	A	313	ARG	CA-C-O	7.11	128.13	120.10
1	A	313	ARG	CD-NE-CZ	7.08	134.31	124.40
1	A	221	GLU	OE1-CD-OE2	7.05	139.83	122.90
1	A	296	MET	CA-CB-CG	7.05	128.20	114.10
1	A	46	THR	O-C-N	-6.98	114.83	122.09
1	A	316	GLN	OE1-CD-NE2	-6.82	115.78	122.60
1	A	80	GLN	CA-C-N	-6.80	111.44	122.26
1	A	80	GLN	C-N-CA	-6.80	111.44	122.26
1	A	16	ARG	NE-CZ-NH2	-6.79	113.08	119.20
1	A	313	ARG	CB-CG-CD	6.79	126.92	111.30
1	A	143	ARG	NE-CZ-NH2	-6.78	113.10	119.20
1	A	297	ASN	CA-CB-CG	-6.70	105.90	112.60
1	A	3	ARG	NE-CZ-NH1	6.69	128.19	121.50
1	A	338	MET	CA-CB-CG	-6.69	100.71	114.10
1	A	101	THR	N-CA-C	-6.67	101.73	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	GLU	CA-CB-CG	-6.58	100.93	114.10
1	A	327	GLU	CB-CG-CD	-6.56	101.44	112.60
1	A	109	ARG	CA-C-N	-6.55	111.56	121.51
1	A	109	ARG	C-N-CA	-6.55	111.56	121.51
1	A	323	TRP	O-C-N	-6.54	115.03	122.09
1	A	64	HIS	O-C-N	6.52	130.28	122.27
1	A	63	GLU	CA-C-O	6.51	127.33	120.42
1	A	314	ALA	N-CA-C	-6.41	105.42	113.18
1	A	77	GLY	N-CA-C	-6.40	106.31	114.37
1	A	355	ALA	N-CA-C	-6.39	104.59	112.38
1	A	95	LYS	CB-CG-CD	6.37	125.96	111.30
1	A	334	ARG	CA-C-N	-6.34	111.78	120.28
1	A	334	ARG	C-N-CA	-6.34	111.78	120.28
1	A	16	ARG	CA-C-O	-6.33	113.29	120.32
1	A	35	PRO	N-CA-CB	6.33	108.94	103.31
1	A	47	GLY	CA-C-N	-6.31	111.20	120.28
1	A	47	GLY	C-N-CA	-6.31	111.20	120.28
1	A	79	GLU	CG-CD-OE2	-6.29	103.93	118.40
1	A	334	ARG	NE-CZ-NH2	-6.29	113.54	119.20
1	A	247	ALA	CA-C-N	-6.26	112.67	122.49
1	A	247	ALA	C-N-CA	-6.26	112.67	122.49
1	A	330	VAL	N-CA-C	6.22	116.89	110.36
1	A	226	LEU	CA-C-N	-6.20	112.38	120.44
1	A	226	LEU	C-N-CA	-6.20	112.38	120.44
1	A	242	MET	N-CA-C	-6.17	101.39	110.52
1	A	50	SER	N-CA-CB	6.15	119.16	110.12
1	A	60	ASN	N-CA-C	6.12	119.32	108.24
1	A	215	SER	CA-C-N	-6.09	112.12	120.28
1	A	215	SER	C-N-CA	-6.09	112.12	120.28
1	A	331	GLU	N-CA-CB	6.08	119.06	110.12
1	A	220	SER	CA-C-N	-6.08	111.07	120.31
1	A	220	SER	C-N-CA	-6.08	111.07	120.31
1	A	2	LYS	CB-CA-C	6.06	120.23	110.29
1	A	332	ALA	O-C-N	6.04	129.70	122.27
1	A	225	ALA	CA-C-N	-6.03	112.20	120.28
1	A	225	ALA	C-N-CA	-6.03	112.20	120.28
1	A	353	ASN	CA-CB-CG	6.03	118.63	112.60
1	A	308	THR	N-CA-C	6.01	116.37	108.07
1	A	95	LYS	CA-CB-CG	-6.01	102.07	114.10
1	A	105	TYR	O-C-N	-6.00	115.89	122.07
1	A	325	GLY	N-CA-C	-5.99	106.98	115.30
1	A	102	PHE	CA-C-O	5.99	124.14	118.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ALA	N-CA-CB	-5.97	100.90	110.46
1	A	81	TYR	CA-C-N	-5.97	115.79	123.19
1	A	81	TYR	C-N-CA	-5.97	115.79	123.19
1	A	19	THR	CA-C-O	5.95	125.57	119.86
1	A	333	GLY	N-CA-C	-5.94	105.61	112.50
1	A	262	THR	CA-C-N	-5.94	111.99	120.42
1	A	262	THR	C-N-CA	-5.94	111.99	120.42
1	A	274	LEU	N-CA-C	-5.94	100.77	109.50
1	A	299	CYS	CB-CA-C	-5.93	99.80	109.41
1	A	72	MET	CA-CB-CG	-5.91	102.28	114.10
1	A	195	ILE	CA-CB-CG1	-5.91	100.36	110.40
1	A	52	ARG	NE-CZ-NH2	-5.90	113.89	119.20
1	A	76	GLU	CA-C-N	-5.89	115.13	123.08
1	A	76	GLU	C-N-CA	-5.89	115.13	123.08
1	A	159	ASN	CA-CB-CG	-5.87	106.73	112.60
1	A	316	GLN	CG-CD-NE2	5.85	125.18	116.40
1	A	173	VAL	CA-C-N	-5.84	110.59	120.58
1	A	173	VAL	C-N-CA	-5.84	110.59	120.58
1	A	319	ALA	CA-C-O	5.84	126.74	120.55
1	A	256	GLU	CB-CA-C	-5.79	101.00	110.85
1	A	210	THR	CA-C-O	5.79	126.69	120.55
1	A	122	GLU	CB-CA-C	-5.78	99.44	109.32
1	A	334	ARG	CA-C-O	5.78	126.54	120.42
1	A	124	LEU	N-CA-CB	-5.77	100.81	110.39
1	A	301	LEU	CA-C-O	5.77	127.82	121.01
1	A	214	VAL	CA-C-N	-5.76	112.11	120.29
1	A	214	VAL	C-N-CA	-5.76	112.11	120.29
1	A	280	LEU	O-C-N	-5.76	116.61	123.06
1	A	239	LYS	O-C-N	5.75	126.55	121.32
1	A	323	TRP	CA-C-O	5.73	126.60	120.70
1	A	154	PHE	N-CA-CB	5.72	120.89	111.62
1	A	42	ALA	N-CA-CB	-5.72	103.25	111.54
1	A	213	ARG	N-CA-C	-5.72	104.95	111.07
1	A	68	TYR	N-CA-C	-5.71	105.05	111.28
1	A	267	ALA	N-CA-C	-5.69	105.60	112.54
1	A	315	LEU	N-CA-C	-5.67	106.70	113.97
1	A	330	VAL	N-CA-CB	5.67	116.80	110.51
1	A	260	GLU	CB-CA-C	-5.66	101.24	110.85
1	A	202	ILE	CA-C-O	5.65	126.44	119.43
1	A	199	GLU	N-CA-C	5.63	117.39	108.67
1	A	299	CYS	CA-C-O	5.62	124.76	119.76
1	A	339	HIS	N-CA-CB	-5.62	101.85	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	ILE	CB-CA-C	-5.61	104.12	111.25
1	A	260	GLU	N-CA-C	5.61	117.47	111.36
1	A	37	LYS	CA-CB-CG	-5.60	102.90	114.10
1	A	264	LYS	CG-CD-CE	5.55	124.06	111.30
1	A	296	MET	N-CA-C	-5.52	105.17	111.07
1	A	357	ASP	N-CA-CB	-5.51	101.14	110.50
1	A	11	LEU	CA-C-O	5.49	126.28	120.63
1	A	188	GLN	CA-C-O	5.48	126.30	120.10
1	A	323	TRP	N-CA-CB	-5.48	102.12	110.07
1	A	67	GLN	CA-CB-CG	-5.47	103.16	114.10
1	A	265	THR	CA-CB-OG1	-5.46	101.41	109.60
1	A	177	ALA	CA-C-O	5.45	126.54	120.82
1	A	142	LYS	CA-C-N	-5.45	113.03	120.44
1	A	142	LYS	C-N-CA	-5.45	113.03	120.44
1	A	66	ARG	CA-C-O	5.43	126.71	120.90
1	A	335	ARG	CA-C-N	-5.43	112.58	120.29
1	A	335	ARG	C-N-CA	-5.43	112.58	120.29
1	A	272	PRO	N-CA-CB	5.43	108.72	103.51
1	A	279	PHE	CB-CA-C	-5.43	100.71	109.72
1	A	304	PRO	CB-CA-C	-5.41	103.78	111.68
1	A	260	GLU	CA-CB-CG	-5.41	103.28	114.10
1	A	201	MET	N-CA-CB	-5.41	102.39	110.17
1	A	288	MET	N-CA-CB	-5.39	102.19	110.12
1	A	68	TYR	N-CA-CB	-5.38	102.21	110.12
1	A	313	ARG	N-CA-C	5.34	117.85	111.71
1	A	317	SER	CA-CB-OG	-5.33	100.43	111.10
1	A	270	ILE	CB-CA-C	-5.32	105.01	110.71
1	A	101	THR	CA-CB-CG2	-5.32	101.46	110.50
1	A	153	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	A	34	ALA	CA-C-O	5.30	125.16	120.02
1	A	152	CYS	CA-C-N	-5.30	113.73	121.99
1	A	152	CYS	C-N-CA	-5.30	113.73	121.99
1	A	4	VAL	CA-C-N	-5.28	114.75	122.19
1	A	4	VAL	C-N-CA	-5.28	114.75	122.19
1	A	184	ALA	CA-C-O	5.28	126.36	120.82
1	A	22	GLU	CA-C-O	5.27	126.54	120.90
1	A	203	ASP	O-C-N	-5.26	116.55	122.97
1	A	300	PRO	CB-CA-C	-5.26	103.50	111.44
1	A	113	PRO	CA-C-N	-5.25	116.89	122.67
1	A	113	PRO	C-N-CA	-5.25	116.89	122.67
1	A	306	LYS	CB-CA-C	-5.25	100.68	109.65
1	A	302	PRO	CB-CA-C	-5.25	105.11	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	GLU	CB-CA-C	-5.24	102.65	110.88
1	A	66	ARG	NE-CZ-NH2	-5.24	114.48	119.20
1	A	270	ILE	N-CA-C	5.24	113.05	107.76
1	A	288	MET	CA-CB-CG	5.24	124.58	114.10
1	A	7	LEU	CA-C-N	-5.22	112.77	120.28
1	A	7	LEU	C-N-CA	-5.22	112.77	120.28
1	A	37	LYS	CB-CG-CD	-5.20	99.33	111.30
1	A	39	LEU	CA-C-O	5.20	126.22	120.71
1	A	333	GLY	O-C-N	-5.19	117.20	122.18
1	A	274	LEU	CB-CA-C	-5.18	101.12	109.67
1	A	18	LYS	O-C-N	-5.17	116.90	123.05
1	A	100	GLU	N-CA-C	-5.17	103.57	110.55
1	A	25	LEU	CA-C-O	5.17	126.25	120.82
1	A	316	GLN	CA-C-O	5.14	124.48	118.97
1	A	201	MET	N-CA-C	5.14	117.74	110.50
1	A	158	ARG	CB-CG-CD	-5.13	99.49	111.30
1	A	116	LYS	CG-CD-CE	5.10	123.04	111.30
1	A	170	GLU	CA-C-O	5.10	125.84	119.97
1	A	260	GLU	N-CA-CB	-5.09	102.62	110.16
1	A	164	GLN	CB-CA-C	-5.08	100.76	109.65
1	A	30	LYS	CB-CA-C	-5.08	102.36	110.79
1	A	328	SER	N-CA-CB	-5.08	101.96	110.39
1	A	260	GLU	CG-CD-OE1	-5.06	106.75	118.40
1	A	197	GLU	N-CA-CB	-5.06	101.45	110.05
1	A	123	PRO	CB-CA-C	-5.06	104.94	111.46
1	A	274	LEU	CA-C-O	5.05	124.86	119.80
1	A	105	TYR	N-CA-CB	-5.05	102.68	110.01
1	A	166	GLY	CA-C-N	-5.03	113.54	122.20
1	A	166	GLY	C-N-CA	-5.03	113.54	122.20
1	A	111	VAL	CA-C-N	-5.03	114.29	121.23
1	A	111	VAL	C-N-CA	-5.03	114.29	121.23
1	A	28	THR	CA-C-O	5.03	125.88	120.55
1	A	187	SER	CA-CB-OG	-5.02	101.05	111.10
1	A	218	VAL	CB-CA-C	-5.02	105.54	111.97
1	A	55	GLY	O-C-N	-5.02	117.02	122.84
1	A	30	LYS	N-CA-C	-5.01	105.82	111.28
1	A	340	ARG	NE-CZ-NH1	-5.01	116.49	121.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ASP	Sidechain
1	A	260	GLU	Sidechain
1	A	5	GLU	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	2707	0	2668	53	0
2	A	241	0	0	1	1
All	All	2948	0	2668	53	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 10.

All (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:HD2	1:A:90:GLU:H	1.24	0.84
1:A:88:HIS:CD2	1:A:90:GLU:H	1.97	0.81
1:A:63:GLU:HG3	1:A:67:GLN:NE2	1.97	0.78
1:A:284:LEU:HB3	1:A:288:MET:HG2	1.71	0.72
1:A:326:LYS:O	1:A:329:GLY:N	2.26	0.65
1:A:285:SER:H	1:A:288:MET:HE3	1.60	0.64
1:A:3:ARG:HH11	1:A:3:ARG:HG3	1.61	0.64
1:A:323:TRP:O	1:A:326:LYS:HE2	2.00	0.61
1:A:122:GLU:HB3	1:A:123:PRO:HD2	1.87	0.56
1:A:293:LEU:O	1:A:296:MET:HB2	2.06	0.56
1:A:19:THR:OG1	1:A:20:PRO:HD2	2.06	0.56
1:A:339:HIS:O	1:A:343:MET:HG2	2.06	0.55
1:A:339:HIS:HE1	1:A:357:ASP:OD1	1.90	0.55
1:A:301:LEU:HB3	1:A:302:PRO:HD2	1.88	0.54
1:A:88:HIS:HD2	1:A:90:GLU:N	2.01	0.54
1:A:54:ALA:O	1:A:55:GLY:C	2.50	0.52
1:A:286:GLU:OE2	1:A:317:SER:HB3	2.11	0.51
1:A:278:THR:HB	1:A:310:SER:HB2	1.94	0.50
1:A:21:TYR:O	1:A:22:GLU:C	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLU:HG3	1:A:67:GLN:HE22	1.73	0.49
1:A:97:LYS:HG3	1:A:98:THR:N	2.26	0.48
1:A:219:TRP:CZ2	1:A:240:PRO:HB2	2.49	0.48
1:A:196:VAL:O	1:A:198:PRO:HD3	2.14	0.47
1:A:197:GLU:HG3	1:A:239:LYS:O	2.15	0.47
1:A:285:SER:H	1:A:288:MET:CE	2.24	0.47
1:A:101:THR:HB	1:A:103:PRO:HD2	1.97	0.46
1:A:59:SER:HB3	1:A:64:HIS:CE1	2.51	0.46
1:A:158:ARG:HA	1:A:197:GLU:HB3	1.98	0.46
1:A:118:ASP:HA	1:A:157:TRP:CE3	2.51	0.45
1:A:52:ARG:HA	1:A:52:ARG:HD3	1.79	0.45
1:A:313:ARG:O	1:A:317:SER:HB2	2.17	0.45
1:A:295:ALA:O	1:A:296:MET:C	2.60	0.45
1:A:93:TYR:OH	1:A:146:LYS:HE2	2.17	0.44
1:A:334:ARG:O	1:A:335:ARG:C	2.56	0.44
1:A:52:ARG:NH1	1:A:316:GLN:OE1	2.52	0.43
1:A:185:ILE:HD11	1:A:231:VAL:HA	2.00	0.43
1:A:41:ALA:HB3	1:A:312:ALA:HB2	2.01	0.42
1:A:86:ILE:HG12	1:A:154:PHE:HE1	1.84	0.42
1:A:108:ARG:NH1	1:A:108:ARG:HG2	2.34	0.42
1:A:301:LEU:HB3	1:A:302:PRO:CD	2.49	0.42
1:A:124:LEU:O	1:A:125:VAL:HB	2.20	0.41
1:A:65:ARG:O	1:A:68:TYR:HB3	2.20	0.41
1:A:34:ALA:HA	1:A:35:PRO:HD3	1.93	0.41
1:A:153:ARG:HD3	1:A:153:ARG:HA	1.82	0.41
1:A:122:GLU:HB3	1:A:123:PRO:CD	2.50	0.41
1:A:101:THR:CB	1:A:103:PRO:HD2	2.51	0.41
1:A:34:ALA:HA	2:A:575:HOH:O	2.21	0.41
1:A:38:GLY:HA3	1:A:309:PHE:CZ	2.56	0.41
1:A:45:SER:N	1:A:48:SER:HG	2.19	0.41
1:A:45:SER:N	1:A:48:SER:OG	2.54	0.41
1:A:303:ARG:HA	1:A:305:TRP:CZ3	2.56	0.41
1:A:197:GLU:HA	1:A:239:LYS:O	2.22	0.40
1:A:339:HIS:CE1	1:A:357:ASP:OD1	2.73	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)
2:A:593:HOH:O	2:A:593:HOH:O[38_556]	1.92	0.28

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	355/370 (96%)	343 (97%)	10 (3%)	2 (1%)	21	13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	PRO
1	A	282	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/302 (91%)	261 (95%)	15 (5%)	20	12

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	5	GLU
1	A	17	LEU
1	A	69	ARG
1	A	146	LYS
1	A	185	ILE
1	A	203	ASP
1	A	213	ARG
1	A	296	MET

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Mol	Chain	Res	Type
1	A	305	TRP
1	A	326	LYS
1	A	327	GLU
1	A	328	SER
1	A	354	ARG
1	A	357	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	88	HIS
1	A	339	HIS

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.