



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:53 AM UTC

PDB ID : 1CHU / pdb_00001chu
Title : STRUCTURE OF L-ASPARTATE OXIDASE: IMPLICATIONS FOR THE
SUCCINATE DEHYDROGENASE/ FUMARATE REDUCATSE FAMILY
Authors : Mattevi, A.
Deposited on : 1999-03-29
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

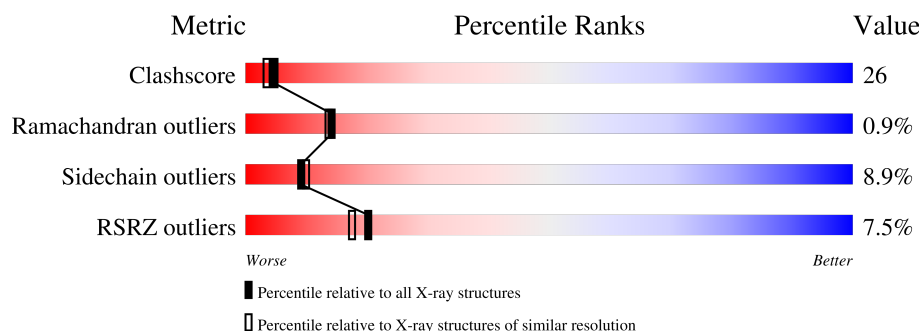
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	540	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3957 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROTEIN (L-ASPARTATE OXIDASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	88	0	0
			3761	2365	677	698	21			

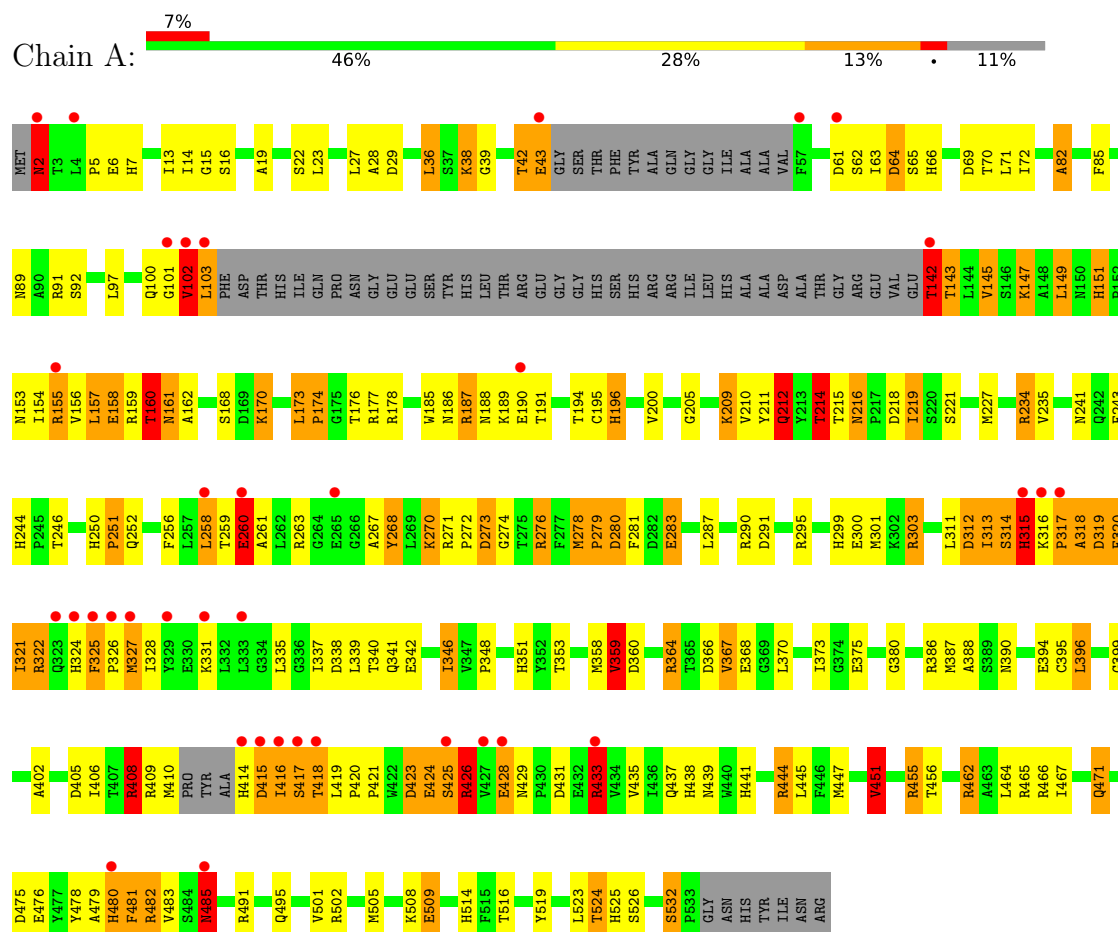
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	196	Total	O	2	0
			196	196		

3 Residue-property plots [i](#)

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

• Molecule 1: PROTEIN (L-ASPARTATE OXIDASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	84.75Å 84.75Å 159.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (20.00-2.20) 96.5 (20.00-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.281 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3957	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.23	7/3840 (0.2%)	2.48	220/5214 (4.2%)

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	15

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	414	HIS	CB-CG	10.59	1.65	1.50
1	A	61	ASP	CB-CG	-6.19	1.36	1.52
1	A	428	GLU	CG-CD	-6.00	1.37	1.52
1	A	71	LEU	C-N	-5.58	1.27	1.33
1	A	320	PHE	CB-CG	-5.56	1.37	1.50
1	A	2	ASN	CB-CG	5.50	1.65	1.52
1	A	319	ASP	CA-CB	-5.15	1.44	1.53

All (220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	ARG	CD-NE-CZ	34.51	172.72	124.40
1	A	187	ARG	CD-NE-CZ	25.36	159.91	124.40
1	A	428	GLU	CB-CG-CD	19.48	145.71	112.60
1	A	2	ASN	CA-CB-CG	18.62	131.22	112.60
1	A	428	GLU	CG-CD-OE1	-18.14	76.68	118.40
1	A	428	GLU	CG-CD-OE2	16.81	157.07	118.40
1	A	319	ASP	N-CA-CB	-14.65	85.41	110.32
1	A	386	ARG	CD-NE-CZ	12.96	142.55	124.40
1	A	317	PRO	O-C-N	11.93	138.75	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	502	ARG	CD-NE-CZ	11.50	140.51	124.40
1	A	61	ASP	CA-CB-CG	10.96	123.56	112.60
1	A	2	ASN	OD1-CG-ND2	-10.86	111.74	122.60
1	A	341	GLN	CA-CB-CG	10.83	135.76	114.10
1	A	319	ASP	CA-CB-CG	-10.25	102.35	112.60
1	A	161	ASN	OD1-CG-ND2	-10.24	112.36	122.60
1	A	466	ARG	NE-CZ-NH2	10.16	128.35	119.20
1	A	462	ARG	CD-NE-CZ	9.76	138.07	124.40
1	A	423	ASP	CA-CB-CG	9.69	122.29	112.60
1	A	462	ARG	NH1-CZ-NH2	-9.66	106.75	119.30
1	A	482	ARG	CB-CG-CD	9.61	133.40	111.30
1	A	341	GLN	OE1-CD-NE2	-9.58	113.02	122.60
1	A	219	ILE	N-CA-CB	-9.56	99.51	111.94
1	A	273	ASP	CB-CA-C	-9.52	90.23	110.32
1	A	43	GLU	CB-CG-CD	9.34	128.47	112.60
1	A	341	GLN	CB-CG-CD	9.30	128.41	112.60
1	A	170	LYS	N-CA-C	-9.25	102.57	114.04
1	A	143	THR	N-CA-C	9.22	124.17	110.52
1	A	187	ARG	NE-CZ-NH2	9.15	127.44	119.20
1	A	320	PHE	CB-CG-CD2	-8.94	105.50	120.70
1	A	227	MET	CA-C-N	8.82	132.82	120.29
1	A	227	MET	C-N-CA	8.82	132.82	120.29
1	A	64	ASP	CA-CB-CG	-8.73	103.87	112.60
1	A	188	ASN	CA-CB-CG	-8.68	103.92	112.60
1	A	462	ARG	NE-CZ-NH2	8.68	127.01	119.20
1	A	187	ARG	NE-CZ-NH1	-8.64	112.86	121.50
1	A	320	PHE	CA-CB-CG	-8.51	105.29	113.80
1	A	425	SER	N-CA-C	-8.44	96.86	110.20
1	A	476	GLU	CA-C-O	-8.42	111.98	120.82
1	A	66	HIS	CA-CB-CG	-8.41	105.39	113.80
1	A	61	ASP	CB-CG-OD1	-8.25	99.43	118.40
1	A	485	ASN	CA-CB-CG	-8.22	104.38	112.60
1	A	417	SER	CA-C-O	8.20	132.24	120.51
1	A	216	ASN	OD1-CG-ND2	-8.16	114.44	122.60
1	A	312	ASP	CA-CB-CG	7.99	120.59	112.60
1	A	321	ILE	CA-CB-CG2	7.87	123.88	110.50
1	A	196	HIS	CA-C-O	-7.78	112.17	120.80
1	A	320	PHE	CB-CG-CD1	7.77	133.91	120.70
1	A	303	ARG	CA-C-O	-7.76	111.33	120.10
1	A	502	ARG	NE-CZ-NH1	7.75	129.25	121.50
1	A	61	ASP	CB-CG-OD2	7.72	136.16	118.40
1	A	16	SER	CA-C-O	-7.55	114.22	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	SER	N-CA-C	7.49	126.75	110.80
1	A	429	ASN	CB-CG-ND2	-7.29	105.47	116.40
1	A	235	VAL	CA-C-O	-7.14	114.18	121.67
1	A	219	ILE	CA-CB-CG2	7.13	122.62	110.50
1	A	219	ILE	CB-CG1-CD1	-7.12	98.84	113.80
1	A	91	ARG	NE-CZ-NH1	7.09	128.59	121.50
1	A	475	ASP	CA-CB-CG	-7.08	105.53	112.60
1	A	290	ARG	CD-NE-CZ	-7.03	114.55	124.40
1	A	65	SER	CA-CB-OG	-7.03	97.04	111.10
1	A	178	ARG	NE-CZ-NH2	-6.96	112.93	119.20
1	A	317	PRO	CA-C-N	6.95	134.81	121.54
1	A	317	PRO	C-N-CA	6.95	134.81	121.54
1	A	465	ARG	NE-CZ-NH2	-6.94	112.96	119.20
1	A	390	ASN	OD1-CG-ND2	-6.84	115.76	122.60
1	A	466	ARG	NH1-CZ-NH2	-6.83	110.42	119.30
1	A	509	GLU	CA-C-O	-6.80	113.62	121.10
1	A	317	PRO	N-CA-C	6.76	126.41	112.47
1	A	178	ARG	NH1-CZ-NH2	6.71	128.02	119.30
1	A	143	THR	CA-C-O	6.71	129.64	121.72
1	A	260	GLU	CB-CG-CD	6.69	123.97	112.60
1	A	89	ASN	CA-CB-CG	-6.67	105.93	112.60
1	A	157	LEU	CA-C-N	6.62	132.38	121.39
1	A	157	LEU	C-N-CA	6.62	132.38	121.39
1	A	71	LEU	N-CA-CB	6.59	119.80	110.12
1	A	478	TYR	CA-C-O	-6.58	111.48	119.32
1	A	27	LEU	CA-C-N	6.58	129.09	120.28
1	A	27	LEU	C-N-CA	6.58	129.09	120.28
1	A	416	ILE	CA-C-O	6.55	128.97	120.78
1	A	91	ARG	NE-CZ-NH2	-6.53	113.32	119.20
1	A	276	ARG	CD-NE-CZ	6.47	133.46	124.40
1	A	243	PHE	CA-C-O	-6.47	113.37	120.36
1	A	147	LYS	CA-C-O	-6.46	113.70	120.55
1	A	380	GLY	N-CA-C	-6.45	106.23	115.64
1	A	82	ALA	CA-C-O	-6.44	113.59	120.42
1	A	526	SER	CA-CB-OG	-6.42	98.26	111.10
1	A	341	GLN	CG-CD-NE2	6.42	126.03	116.40
1	A	324	HIS	CA-CB-CG	6.40	120.20	113.80
1	A	273	ASP	N-CA-CB	6.38	121.16	110.32
1	A	455	ARG	NE-CZ-NH2	-6.32	113.52	119.20
1	A	482	ARG	CG-CD-NE	6.31	125.89	112.00
1	A	160	THR	O-C-N	-6.29	115.05	123.23
1	A	441	HIS	CA-CB-CG	-6.29	107.51	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	ARG	CA-CB-CG	-6.25	101.59	114.10
1	A	270	LYS	N-CA-C	6.22	119.67	109.72
1	A	214	THR	CA-CB-OG1	-6.22	100.27	109.60
1	A	410	MET	CA-C-O	-6.21	110.25	120.80
1	A	483	VAL	CA-C-O	-6.18	114.56	121.36
1	A	359	VAL	N-CA-CB	-6.17	99.90	111.62
1	A	281	PHE	CA-C-O	6.15	126.19	119.24
1	A	519	TYR	O-C-N	-6.15	116.70	121.19
1	A	283	GLU	CB-CG-CD	6.15	123.05	112.60
1	A	418	THR	CA-C-O	-6.13	114.67	121.23
1	A	479	ALA	O-C-N	-6.11	116.26	123.11
1	A	416	ILE	O-C-N	-6.08	114.97	122.57
1	A	280	ASP	N-CA-C	-6.07	105.84	113.18
1	A	335	LEU	N-CA-CB	6.07	119.69	110.95
1	A	145	VAL	CA-C-O	-6.06	115.11	121.41
1	A	364	ARG	O-C-N	6.04	130.13	123.01
1	A	102	VAL	CB-CA-C	6.04	121.19	111.29
1	A	437	GLN	CB-CG-CD	6.03	122.85	112.60
1	A	162	ALA	N-CA-CB	6.02	118.82	109.97
1	A	214	THR	CA-CB-CG2	6.00	120.71	110.50
1	A	63	ILE	CA-C-O	5.98	127.17	120.95
1	A	281	PHE	CA-CB-CG	-5.97	107.83	113.80
1	A	160	THR	CA-CB-OG1	5.97	118.56	109.60
1	A	353	THR	O-C-N	-5.94	115.98	123.05
1	A	173	LEU	N-CA-CB	5.92	116.61	109.74
1	A	209	LYS	CA-CB-CG	5.92	125.94	114.10
1	A	451	VAL	CB-CA-C	-5.91	101.59	111.29
1	A	406	ILE	CA-C-N	5.87	128.42	120.38
1	A	406	ILE	C-N-CA	5.87	128.42	120.38
1	A	38	LYS	CA-C-O	-5.86	114.66	120.82
1	A	346	ILE	O-C-N	-5.85	116.57	123.00
1	A	2	ASN	CB-CG-ND2	5.83	125.14	116.40
1	A	431	ASP	CB-CG-OD2	5.83	131.80	118.40
1	A	157	LEU	CA-C-O	5.80	126.95	120.92
1	A	295	ARG	NE-CZ-NH1	-5.79	115.71	121.50
1	A	91	ARG	CA-C-O	-5.78	114.39	120.63
1	A	299	HIS	CB-CA-C	-5.76	102.09	110.96
1	A	43	GLU	CB-CA-C	5.74	121.01	110.10
1	A	278	MET	CA-C-N	5.74	125.42	119.56
1	A	278	MET	C-N-CA	5.74	125.42	119.56
1	A	188	ASN	OD1-CG-ND2	5.73	128.33	122.60
1	A	43	GLU	OE1-CD-OE2	-5.73	109.15	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ARG	CA-C-N	-5.71	110.97	120.68
1	A	91	ARG	C-N-CA	-5.71	110.97	120.68
1	A	162	ALA	N-CA-C	-5.69	101.86	110.28
1	A	312	ASP	N-CA-C	5.68	117.65	108.34
1	A	426	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	A	173	LEU	N-CA-C	-5.67	102.76	110.36
1	A	27	LEU	N-CA-CB	-5.67	101.60	110.44
1	A	186	ASN	N-CA-CB	-5.65	101.04	110.37
1	A	424	GLU	N-CA-CB	5.64	120.90	111.53
1	A	92	SER	CA-CB-OG	-5.63	99.84	111.10
1	A	28	ALA	CA-C-O	-5.62	114.59	120.55
1	A	156	VAL	N-CA-C	5.60	115.86	107.51
1	A	414	HIS	CB-CG-CD2	5.58	138.46	131.20
1	A	390	ASN	CB-CG-ND2	5.58	124.77	116.40
1	A	71	LEU	CA-C-N	5.58	127.67	120.70
1	A	71	LEU	C-N-CA	5.58	127.67	120.70
1	A	7	HIS	CA-C-O	-5.56	114.61	121.06
1	A	396	LEU	N-CA-C	5.55	117.01	111.07
1	A	439	ASN	CA-C-N	5.55	127.65	120.44
1	A	439	ASN	C-N-CA	5.55	127.65	120.44
1	A	85	PHE	CA-CB-CG	-5.53	108.27	113.80
1	A	325	PHE	N-CA-C	5.53	117.53	109.30
1	A	160	THR	CA-C-N	5.51	130.69	122.86
1	A	160	THR	C-N-CA	5.51	130.69	122.86
1	A	399	GLY	N-CA-C	-5.51	105.72	112.77
1	A	196	HIS	CA-CB-CG	-5.51	108.29	113.80
1	A	408	ARG	CD-NE-CZ	-5.49	116.72	124.40
1	A	532	SER	CA-C-O	-5.49	114.59	119.86
1	A	272	PRO	O-C-N	-5.46	115.96	122.24
1	A	15	GLY	O-C-N	-5.46	115.61	122.70
1	A	151	HIS	CA-C-O	5.45	124.13	119.66
1	A	145	VAL	N-CA-CB	5.43	116.33	110.62
1	A	322	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	A	160	THR	OG1-CB-CG2	-5.42	98.47	109.30
1	A	360	ASP	CB-CG-OD1	5.40	130.83	118.40
1	A	258	LEU	CA-C-N	5.40	128.52	120.90
1	A	258	LEU	C-N-CA	5.40	128.52	120.90
1	A	210	VAL	CA-C-N	5.40	130.76	122.93
1	A	210	VAL	C-N-CA	5.40	130.76	122.93
1	A	408	ARG	CA-CB-CG	5.37	124.84	114.10
1	A	268	TYR	CA-CB-CG	5.36	123.55	113.90
1	A	92	SER	CA-C-O	-5.35	113.48	119.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	THR	CA-CB-OG1	-5.34	101.60	109.60
1	A	200	VAL	CA-C-O	5.31	125.96	120.39
1	A	433	ARG	CA-C-O	-5.30	114.80	120.42
1	A	447	MET	CA-C-O	5.30	126.04	120.42
1	A	370	LEU	CA-C-O	-5.30	114.69	120.36
1	A	42	THR	O-C-N	-5.29	114.90	122.41
1	A	158	GLU	O-C-N	-5.29	116.99	122.96
1	A	61	ASP	N-CA-C	-5.28	105.53	111.28
1	A	471	GLN	CB-CG-CD	5.25	121.53	112.60
1	A	142	THR	N-CA-CB	5.25	120.42	111.50
1	A	388	ALA	CA-C-N	5.25	135.73	126.45
1	A	388	ALA	C-N-CA	5.25	135.73	126.45
1	A	101	GLY	N-CA-C	-5.23	108.05	115.43
1	A	5	PRO	CB-CA-C	5.22	118.22	110.85
1	A	303	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	525	HIS	CA-CB-CG	-5.21	108.59	113.80
1	A	335	LEU	N-CA-C	-5.21	105.67	113.89
1	A	65	SER	O-C-N	5.20	127.63	122.12
1	A	319	ASP	N-CA-C	-5.19	106.05	112.38
1	A	212	GLN	N-CA-CB	-5.18	102.51	110.12
1	A	444	ARG	CB-CG-CD	-5.18	99.39	111.30
1	A	394	GLU	O-C-N	-5.18	116.70	122.09
1	A	273	ASP	CA-C-N	-5.17	113.77	122.25
1	A	273	ASP	C-N-CA	-5.17	113.77	122.25
1	A	348	PRO	CA-C-O	-5.15	115.48	122.08
1	A	70	THR	CA-CB-CG2	5.15	119.25	110.50
1	A	402	ALA	N-CA-C	-5.12	105.78	111.36
1	A	438	HIS	N-CA-C	-5.11	105.60	111.07
1	A	368	GLU	CA-C-O	5.08	126.56	121.07
1	A	301	MET	N-CA-CB	5.08	117.67	110.06
1	A	72	ILE	CA-C-O	-5.07	115.87	121.29
1	A	456	THR	CA-CB-CG2	5.05	119.09	110.50
1	A	291	ASP	CA-C-N	5.05	127.03	120.56
1	A	291	ASP	C-N-CA	5.05	127.03	120.56
1	A	92	SER	N-CA-CB	5.05	118.08	110.30
1	A	147	LYS	N-CA-CB	5.04	117.53	110.12
1	A	279	PRO	N-CA-C	-5.04	107.29	113.84
1	A	421	PRO	CA-C-O	-5.03	115.22	122.31
1	A	367	VAL	O-C-N	-5.02	117.62	122.99
1	A	433	ARG	CA-CB-CG	5.02	124.14	114.10
1	A	481	PHE	CA-CB-CG	5.01	118.81	113.80
1	A	39	GLY	CA-C-N	5.01	125.24	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	39	GLY	C-N-CA	5.01	125.24	119.83

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	ARG	Mainchain
1	A	195	CYS	Mainchain
1	A	205	GLY	Mainchain
1	A	22	SER	Mainchain
1	A	234	ARG	Mainchain
1	A	251	PRO	Mainchain
1	A	273	ASP	Mainchain
1	A	29	ASP	Mainchain
1	A	303	ARG	Mainchain
1	A	375	GLU	Sidechain
1	A	395	CYS	Mainchain
1	A	396	LEU	Mainchain
1	A	408	ARG	Mainchain
1	A	415	ASP	Sidechain
1	A	82	ALA	Mainchain

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	3761	0	3709	186	2
2	A	196	0	0	23	1
All	All	3957	0	3709	186	3

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 (186) 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:187:ARG:NH1	2:A:633:HOH:O	1.60	1.32
1:A:69:ASP:CB	1:A:387:MET:HE1	1.62	1.28
1:A:234:ARG:HB3	1:A:358:MET:CE	1.60	1.28
1:A:317:PRO:O	1:A:320:PHE:HB2	1.18	1.27
1:A:69:ASP:HB3	1:A:387:MET:CE	1.72	1.20
1:A:317:PRO:O	1:A:320:PHE:CB	1.91	1.18
1:A:462:ARG:CZ	2:A:735:HOH:O	1.91	1.17
1:A:234:ARG:CB	1:A:358:MET:CE	2.23	1.16
1:A:364:ARG:NH1	1:A:409:ARG:NH2	1.97	1.13
1:A:425:SER:HB2	1:A:480:HIS:O	1.46	1.12
1:A:256:PHE:CD1	1:A:331:LYS:HE3	1.83	1.12
1:A:259:THR:HG22	1:A:261:ALA:H	1.01	1.10
1:A:256:PHE:CD1	1:A:331:LYS:CE	2.34	1.09
1:A:256:PHE:CE1	1:A:331:LYS:CE	2.36	1.07
1:A:69:ASP:HB3	1:A:387:MET:HE1	1.10	1.05
1:A:425:SER:CB	1:A:480:HIS:HB3	1.85	1.05
1:A:234:ARG:HD2	1:A:358:MET:HE1	1.38	1.05
1:A:256:PHE:CD1	1:A:331:LYS:NZ	2.25	1.04
1:A:234:ARG:HB3	1:A:358:MET:HE2	1.03	1.02
1:A:433:ARG:HH22	1:A:482:ARG:HG2	1.24	1.01
1:A:69:ASP:C	1:A:387:MET:HE1	1.85	1.01
1:A:317:PRO:C	1:A:320:PHE:HB2	1.85	1.01
1:A:234:ARG:CB	1:A:358:MET:HE3	1.91	1.00
1:A:455:ARG:HH11	1:A:514:HIS:HD2	1.07	0.99
1:A:462:ARG:NE	2:A:735:HOH:O	1.93	0.97
1:A:258:LEU:HD13	1:A:311:LEU:HD23	1.47	0.96
1:A:258:LEU:CD1	1:A:311:LEU:HD23	1.96	0.95
1:A:234:ARG:HB2	1:A:358:MET:HE3	1.48	0.95
1:A:524:THR:HG22	2:A:556:HOH:O	1.65	0.95
1:A:268:TYR:CD1	1:A:276:ARG:NE	2.38	0.92
1:A:259:THR:HG22	1:A:261:ALA:N	1.85	0.92
1:A:69:ASP:C	1:A:387:MET:CE	2.43	0.91
1:A:424:GLU:HG3	2:A:575:HOH:O	1.69	0.91
1:A:250:HIS:HD2	1:A:252:GLN:H	1.19	0.90
1:A:69:ASP:CA	1:A:387:MET:HE1	2.01	0.90
1:A:313:ILE:HD11	1:A:339:LEU:HG	1.54	0.89
1:A:319:ASP:HA	1:A:322:ARG:HB2	1.52	0.88
1:A:364:ARG:NH1	1:A:409:ARG:HH22	1.70	0.85
1:A:69:ASP:O	1:A:387:MET:HE3	1.77	0.85
1:A:256:PHE:HD1	1:A:331:LYS:HZ1	1.22	0.84
1:A:312:ASP:OD1	1:A:314:SER:HB2	1.77	0.83
1:A:256:PHE:CE1	1:A:331:LYS:HE2	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ARG:HH11	1:A:409:ARG:NH2	1.75	0.82
1:A:256:PHE:CE1	1:A:331:LYS:HE3	2.08	0.81
1:A:425:SER:CB	1:A:480:HIS:CB	2.51	0.81
1:A:250:HIS:CD2	1:A:251:PRO:HD2	2.14	0.81
1:A:185:TRP:CZ2	2:A:658:HOH:O	2.33	0.80
1:A:433:ARG:NH2	1:A:482:ARG:HG2	1.97	0.80
1:A:313:ILE:HD11	1:A:339:LEU:CG	2.11	0.80
1:A:234:ARG:CD	1:A:358:MET:HE1	2.10	0.79
1:A:234:ARG:CB	1:A:358:MET:HE2	1.95	0.78
1:A:451:VAL:HG21	1:A:501:VAL:HG22	1.66	0.77
1:A:161:ASN:ND2	1:A:485:ASN:OD1	2.17	0.77
1:A:268:TYR:CD1	1:A:276:ARG:HD2	2.21	0.76
1:A:209:LYS:HA	1:A:214:THR:HG21	1.67	0.76
1:A:337:ILE:HA	1:A:342:GLU:OE2	1.85	0.75
1:A:6:GLU:OE1	1:A:194:THR:N	2.19	0.75
1:A:212:GLN:NE2	1:A:445:LEU:HD23	2.04	0.72
1:A:417:SER:O	1:A:418:THR:HG23	1.89	0.72
1:A:267:ALA:HB2	1:A:313:ILE:HG23	1.71	0.71
1:A:215:THR:OG1	1:A:351:HIS:HD2	1.74	0.71
1:A:268:TYR:CD1	1:A:276:ARG:CD	2.73	0.71
1:A:250:HIS:CD2	1:A:252:GLN:H	2.07	0.71
1:A:256:PHE:CG	1:A:331:LYS:HE3	2.25	0.70
1:A:185:TRP:CZ3	1:A:187:ARG:HG2	2.26	0.69
1:A:417:SER:O	1:A:418:THR:CG2	2.40	0.69
1:A:185:TRP:HZ2	2:A:658:HOH:O	1.74	0.69
1:A:338:ASP:OD1	1:A:340:THR:HB	1.92	0.68
1:A:69:ASP:HB3	1:A:387:MET:HE2	1.73	0.68
1:A:234:ARG:CD	1:A:358:MET:CE	2.72	0.68
1:A:268:TYR:HD1	1:A:276:ARG:HE	1.40	0.68
1:A:268:TYR:CG	1:A:276:ARG:HD2	2.29	0.67
1:A:69:ASP:O	1:A:387:MET:CE	2.40	0.67
1:A:158:GLU:OE1	2:A:674:HOH:O	2.14	0.65
1:A:185:TRP:CE3	1:A:187:ARG:HG2	2.31	0.65
1:A:212:GLN:NE2	1:A:445:LEU:CD2	2.60	0.65
1:A:258:LEU:HD12	1:A:311:LEU:HD23	1.75	0.65
1:A:250:HIS:CD2	1:A:251:PRO:CD	2.80	0.64
1:A:455:ARG:HH11	1:A:514:HIS:CD2	2.00	0.63
1:A:256:PHE:HD1	1:A:331:LYS:NZ	1.78	0.61
1:A:13:ILE:CD1	1:A:23:LEU:HD23	2.31	0.61
1:A:313:ILE:CD1	1:A:339:LEU:HG	2.30	0.60
1:A:185:TRP:HZ2	1:A:190:GLU:OE1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ILE:HD13	1:A:23:LEU:HD23	1.84	0.59
1:A:154:ILE:O	2:A:628:HOH:O	2.17	0.59
1:A:102:VAL:O	1:A:103:LEU:C	2.47	0.58
1:A:270:LYS:HD3	1:A:274:GLY:O	2.03	0.58
1:A:364:ARG:HH12	1:A:409:ARG:NH2	1.96	0.58
1:A:19:ALA:HB1	1:A:373:ILE:HD12	1.85	0.58
1:A:259:THR:CG2	1:A:261:ALA:H	1.94	0.58
1:A:417:SER:C	1:A:418:THR:HG23	2.28	0.58
1:A:501:VAL:O	1:A:505:MET:HG3	2.03	0.58
1:A:256:PHE:CE1	1:A:331:LYS:NZ	2.64	0.57
1:A:102:VAL:HG21	1:A:143:THR:O	2.05	0.57
1:A:100:GLN:O	1:A:147:LYS:HE3	2.04	0.57
1:A:185:TRP:NE1	2:A:658:HOH:O	2.37	0.57
1:A:313:ILE:HD11	1:A:339:LEU:CD1	2.35	0.57
1:A:314:SER:O	1:A:316:LYS:N	2.38	0.56
1:A:451:VAL:CG2	1:A:501:VAL:HG22	2.35	0.56
1:A:455:ARG:NH1	1:A:514:HIS:HD2	1.90	0.55
1:A:234:ARG:HD2	1:A:358:MET:CE	2.22	0.55
1:A:322:ARG:O	1:A:326:PRO:HG3	2.07	0.55
1:A:315:HIS:H	1:A:315:HIS:CD2	2.24	0.54
1:A:405:ASP:OD1	1:A:408:ARG:NH2	2.40	0.54
1:A:270:LYS:NZ	1:A:312:ASP:OD2	2.41	0.54
1:A:185:TRP:CZ2	1:A:190:GLU:OE1	2.60	0.53
1:A:491:ARG:HG2	2:A:705:HOH:O	2.08	0.53
1:A:151:HIS:CE1	1:A:153:ASN:HB2	2.44	0.52
1:A:387:MET:CE	2:A:719:HOH:O	2.58	0.52
1:A:462:ARG:NH2	2:A:735:HOH:O	2.24	0.52
1:A:425:SER:CB	1:A:480:HIS:HB2	2.36	0.52
1:A:524:THR:CG2	2:A:556:HOH:O	2.37	0.52
1:A:168:SER:C	1:A:170:LYS:H	2.17	0.52
1:A:38:LYS:NZ	1:A:218:ASP:HA	2.25	0.51
1:A:185:TRP:CE2	2:A:658:HOH:O	2.57	0.51
1:A:177:ARG:NH2	1:A:366:ASP:O	2.44	0.51
1:A:509:GLU:HB3	1:A:523:LEU:HG	1.93	0.51
1:A:267:ALA:CB	1:A:313:ILE:HG23	2.40	0.50
1:A:480:HIS:O	1:A:481:PHE:C	2.50	0.50
1:A:425:SER:HB2	1:A:480:HIS:CB	2.40	0.50
1:A:426:ARG:O	1:A:428:GLU:HG2	2.12	0.50
1:A:212:GLN:HE22	1:A:445:LEU:CD2	2.25	0.49
1:A:314:SER:C	1:A:316:LYS:N	2.71	0.49
1:A:314:SER:C	1:A:316:LYS:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:HIS:HD2	1:A:252:GLN:N	1.99	0.48
1:A:338:ASP:C	1:A:340:THR:H	2.22	0.48
1:A:338:ASP:C	1:A:340:THR:N	2.70	0.48
1:A:271:ARG:NE	1:A:300:GLU:OE2	2.47	0.48
1:A:196:HIS:HD2	1:A:419:LEU:HD11	1.79	0.48
1:A:142:THR:HB	1:A:143:THR:H	1.65	0.48
1:A:359:VAL:HA	1:A:364:ARG:O	2.14	0.48
1:A:417:SER:OG	1:A:418:THR:N	2.46	0.47
1:A:495:GLN:NE2	2:A:608:HOH:O	2.38	0.47
1:A:173:LEU:HD23	1:A:174:PRO:HD3	1.96	0.47
1:A:318:ALA:O	1:A:321:ILE:N	2.46	0.47
1:A:338:ASP:OD1	1:A:340:THR:CB	2.63	0.47
1:A:433:ARG:HH22	1:A:482:ARG:CG	2.13	0.47
1:A:313:ILE:HD12	1:A:321:ILE:HG12	1.97	0.47
1:A:318:ALA:O	1:A:321:ILE:HB	2.14	0.47
1:A:161:ASN:CG	1:A:485:ASN:OD1	2.58	0.46
1:A:268:TYR:CE1	1:A:276:ARG:NE	2.81	0.46
1:A:433:ARG:NE	2:A:606:HOH:O	2.21	0.46
1:A:417:SER:O	1:A:418:THR:HG22	2.16	0.46
1:A:157:LEU:O	1:A:160:THR:OG1	2.34	0.45
1:A:244:HIS:HE1	2:A:629:HOH:O	2.00	0.45
1:A:419:LEU:HB3	1:A:420:PRO:HD2	1.98	0.45
1:A:467:ILE:O	1:A:471:GLN:HG3	2.17	0.45
1:A:14:ILE:HG12	1:A:36:LEU:HD22	1.99	0.45
1:A:250:HIS:CG	1:A:251:PRO:CD	2.99	0.45
1:A:338:ASP:N	1:A:342:GLU:OE2	2.46	0.45
1:A:408:ARG:NH2	2:A:626:HOH:O	2.50	0.45
1:A:185:TRP:CZ3	1:A:187:ARG:CD	3.00	0.44
1:A:244:HIS:CD2	1:A:246:THR:H	2.34	0.44
1:A:215:THR:OG1	1:A:216:ASN:ND2	2.48	0.44
1:A:325:PHE:N	1:A:326:PRO:HD3	2.32	0.44
1:A:364:ARG:NH1	1:A:409:ARG:HH21	2.06	0.44
1:A:464:LEU:HD22	1:A:505:MET:HE1	1.99	0.44
1:A:318:ALA:C	1:A:320:PHE:N	2.74	0.44
1:A:158:GLU:O	1:A:159:ARG:C	2.60	0.44
1:A:211:TYR:O	1:A:214:THR:HG22	2.18	0.43
1:A:244:HIS:HD2	1:A:246:THR:H	1.66	0.43
1:A:256:PHE:CZ	1:A:328:ILE:HG12	2.52	0.43
1:A:278:MET:N	1:A:279:PRO:CD	2.81	0.43
1:A:185:TRP:CZ3	1:A:187:ARG:CG	2.99	0.43
1:A:313:ILE:HD11	1:A:339:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:MET:H	1:A:327:MET:HG2	1.60	0.42
1:A:145:VAL:HG22	1:A:149:LEU:HD22	2.01	0.42
1:A:6:GLU:H	1:A:6:GLU:CD	2.28	0.42
1:A:176:THR:HG22	1:A:177:ARG:O	2.19	0.42
1:A:451:VAL:HG21	1:A:501:VAL:CG2	2.44	0.42
1:A:214:THR:HG23	1:A:444:ARG:NH2	2.35	0.42
1:A:189:LYS:O	1:A:191:THR:HG23	2.19	0.42
1:A:418:THR:C	1:A:419:LEU:HG	2.45	0.42
1:A:250:HIS:CG	1:A:251:PRO:HD2	2.54	0.42
1:A:42:THR:OG1	1:A:43:GLU:OE1	2.34	0.41
1:A:189:LYS:O	1:A:190:GLU:HB2	2.19	0.41
1:A:194:THR:HG21	1:A:419:LEU:HB2	2.01	0.41
1:A:241:ASN:HB3	2:A:612:HOH:O	2.21	0.41
1:A:387:MET:HE2	2:A:719:HOH:O	2.21	0.41
1:A:142:THR:N	2:A:709:HOH:O	2.53	0.41
1:A:260:GLU:HG3	1:A:263:ARG:NH2	2.35	0.41
1:A:508:LYS:NZ	2:A:732:HOH:O	2.46	0.41
1:A:69:ASP:C	1:A:387:MET:HE3	2.24	0.40
1:A:177:ARG:CZ	1:A:367:VAL:HG22	2.51	0.40
1:A:267:ALA:CA	1:A:313:ILE:HG23	2.51	0.40
1:A:313:ILE:H	1:A:313:ILE:HG13	1.68	0.40

All (3) 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:650:HOH:O	2:A:650:HOH:O[4_555]	1.20	1.00
1:A:2:ASN:ND2	1:A:480:HIS:NE2[5_675]	1.60	0.60
1:A:435:VAL:CG1	1:A:462:ARG:NH1[4_555]	1.98	0.22

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	470/540 (87%)	446 (95%)	20 (4%)	4 (1%)	14 14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	HIS
1	A	416	ILE
1	A	318	ALA
1	A	174	PRO

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	405/452 (90%)	369 (91%)	36 (9%)	9 10

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	36	LEU
1	A	62	SER
1	A	64	ASP
1	A	97	LEU
1	A	102	VAL
1	A	103	LEU
1	A	142	THR
1	A	149	LEU
1	A	155	ARG
1	A	160	THR
1	A	212	GLN
1	A	214	THR
1	A	219	ILE
1	A	221	SER
1	A	260	GLU
1	A	280	ASP

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Mol	Chain	Res	Type
1	A	283	GLU
1	A	287	LEU
1	A	313	ILE
1	A	314	SER
1	A	315	HIS
1	A	327	MET
1	A	346	ILE
1	A	359	VAL
1	A	408	ARG
1	A	415	ASP
1	A	423	ASP
1	A	426	ARG
1	A	433	ARG
1	A	451	VAL
1	A	480	HIS
1	A	485	ASN
1	A	516	THR
1	A	524	THR
1	A	532	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	66	HIS
1	A	196	HIS
1	A	212	GLN
1	A	216	ASN
1	A	242	GLN
1	A	244	HIS
1	A	250	HIS
1	A	351	HIS
1	A	362	HIS
1	A	437	GLN
1	A	439	ASN
1	A	495	GLN
1	A	514	HIS

5.3.3 RNA ⓘ

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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	478/540 (88%)	0.23	36 (7%) 20 17	22, 37, 68, 85	23 (4%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	415	ASP	5.7
1	A	315	HIS	4.3
1	A	425	SER	4.0
1	A	325	PHE	4.0
1	A	326	PRO	3.9
1	A	103	LEU	3.6
1	A	2	ASN	3.6
1	A	427	VAL	3.6
1	A	485	ASN	3.6
1	A	414	HIS	3.5
1	A	329	TYR	3.2
1	A	480	HIS	3.0
1	A	333	LEU	3.0
1	A	327	MET	2.9
1	A	260	GLU	2.9
1	A	416	ILE	2.8
1	A	323	GLN	2.7
1	A	142	THR	2.7
1	A	316	LYS	2.6
1	A	57	PHE	2.6
1	A	331	LYS	2.6
1	A	101	GLY	2.5
1	A	102	VAL	2.5
1	A	417	SER	2.5
1	A	43	GLU	2.5
1	A	324	HIS	2.5
1	A	317	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	258	LEU	2.3
1	A	61	ASP	2.2
1	A	190	GLU	2.2
1	A	4	LEU	2.2
1	A	433	ARG	2.2
1	A	418	THR	2.1
1	A	265	GLU	2.1
1	A	155	ARG	2.1
1	A	428	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.