



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2026 – 06:02 PM EDT

PDB ID : 1AOZ / pdb_00001aoz
Title : REFINED CRYSTAL STRUCTURE OF ASCORBATE OXIDASE AT 1.9
ANGSTROMS RESOLUTION
Authors : Messerschmidt, A.; Ladenstein, R.; Huber, R.
Deposited on : 1992-01-08
Resolution : 1.90 Å(reported)

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

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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
Mogul	:	2022.3.0, CSD as543be (2022)
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

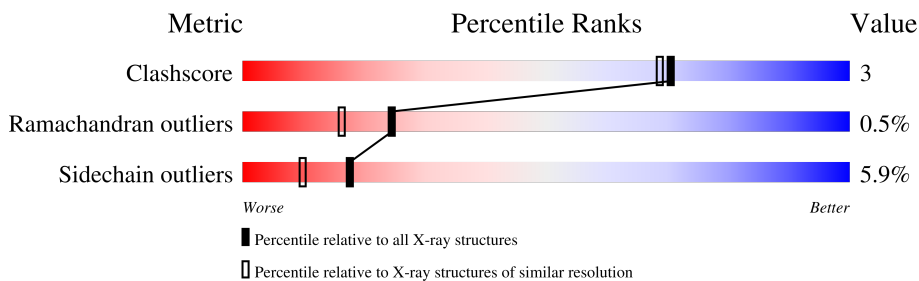
1 Overall quality at a glance

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	552	 78% 19% •
1	B	552	 76% 21% • •

2 Entry composition [i](#)

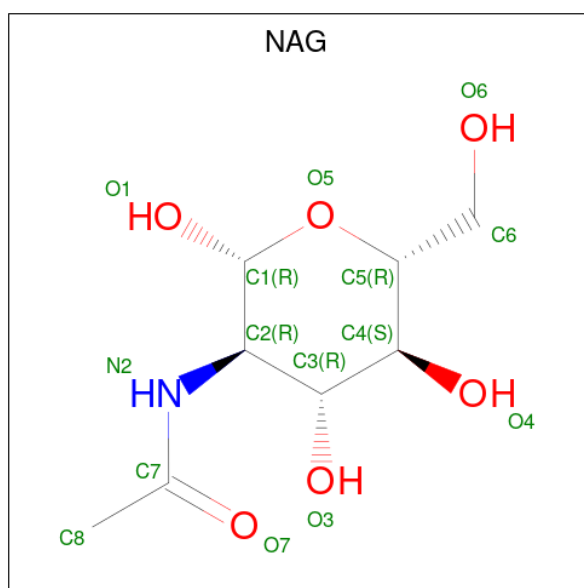
There are 5 unique types of molecules in this entry. The entry contains 9743 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ASCORBATE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4366	2803	746	801	16			
1	B	552	Total	C	N	O	S	0	0	0
			4366	2803	746	801	16			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

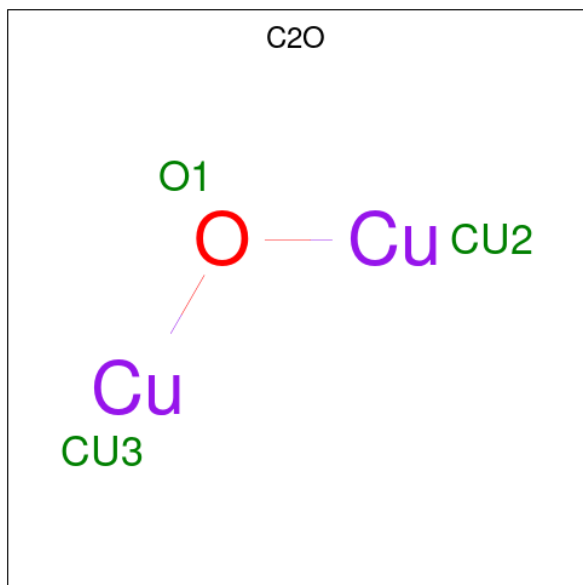


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Cu 3 3	0	0
3	B	2	Total Cu 2 2	0	0

- Molecule 4 is CU-O-CU LINKAGE (CCD ID: C2O) (formula: Cu_2O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cu O 3 2 1	0	0
4	B	1	Total Cu O 3 2 1	0	0

- Molecule 5 is water.

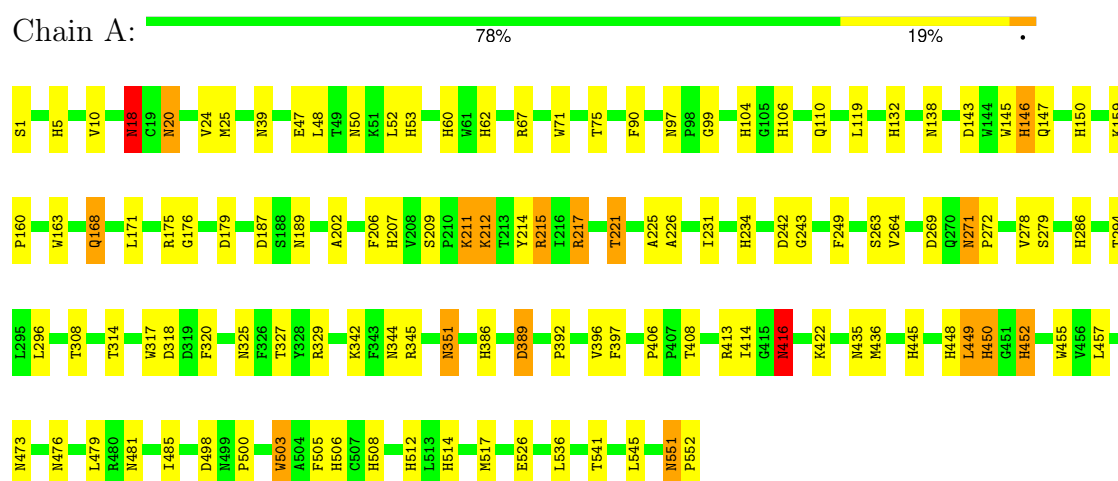
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	A	513	Total O 513 513	0	0
5	B	1	Total O 1 1	0	0
5	B	457	Total O 457 457	0	0

3 Residue-property plots

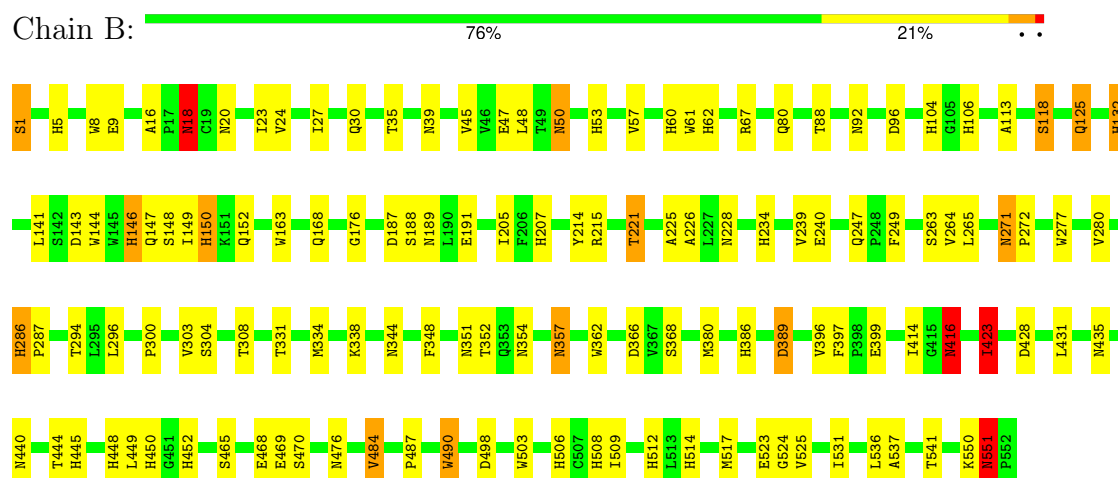
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: ASCORBATE OXIDASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.70Å 105.10Å 113.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9743	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, C2O, CU

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	0.99	33/4508 (0.7%)	1.69	88/6159 (1.4%)
1	B	0.96	25/4508 (0.6%)	1.67	85/6159 (1.4%)
All	All	0.97	58/9016 (0.6%)	1.68	173/12318 (1.4%)

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	1
1	B	0	1
All	All	0	2

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	386	HIS	CD2-NE2	-7.65	1.29	1.37
1	B	146	HIS	CD2-NE2	-7.30	1.29	1.37
1	A	386	HIS	CD2-NE2	-6.90	1.30	1.37
1	A	146	HIS	CD2-NE2	-6.76	1.30	1.37
1	A	62	HIS	CD2-NE2	-6.73	1.30	1.37
1	A	5	HIS	CD2-NE2	-6.70	1.30	1.37
1	B	60	HIS	CD2-NE2	-6.64	1.30	1.37
1	B	512	HIS	CD2-NE2	-6.61	1.30	1.37
1	A	132	HIS	CD2-NE2	-6.54	1.30	1.37
1	B	207	HIS	CD2-NE2	-6.50	1.30	1.37
1	B	62	HIS	CD2-NE2	-6.42	1.30	1.37
1	A	286	HIS	CD2-NE2	-6.37	1.30	1.37
1	B	106	HIS	CD2-NE2	-6.28	1.30	1.37
1	B	53	HIS	CD2-NE2	-6.23	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	HIS	CD2-NE2	-6.21	1.31	1.37
1	B	286	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	104	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	452	HIS	CD2-NE2	-6.12	1.31	1.37
1	A	234	HIS	CD2-NE2	-6.11	1.31	1.37
1	B	514	HIS	CD2-NE2	-6.09	1.31	1.37
1	B	234	HIS	CD2-NE2	-6.00	1.31	1.37
1	A	514	HIS	CG-ND1	-5.98	1.31	1.38
1	B	5	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	448	HIS	CD2-NE2	-5.89	1.31	1.37
1	A	445	HIS	CD2-NE2	-5.89	1.31	1.37
1	A	514	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	106	HIS	CD2-NE2	-5.82	1.31	1.37
1	B	445	HIS	CD2-NE2	-5.81	1.31	1.37
1	B	452	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	60	HIS	CD2-NE2	-5.74	1.31	1.37
1	A	512	HIS	CD2-NE2	-5.73	1.31	1.37
1	B	506	HIS	CD2-NE2	-5.72	1.31	1.37
1	B	104	HIS	CD2-NE2	-5.64	1.31	1.37
1	A	207	HIS	CD2-NE2	-5.64	1.31	1.37
1	B	448	HIS	CD2-NE2	-5.63	1.31	1.37
1	B	508	HIS	CD2-NE2	-5.63	1.31	1.37
1	B	132	HIS	CD2-NE2	-5.57	1.31	1.37
1	A	150	HIS	CD2-NE2	-5.55	1.31	1.37
1	B	450	HIS	CG-ND1	-5.53	1.32	1.38
1	B	512	HIS	CG-ND1	-5.49	1.32	1.38
1	A	445	HIS	CG-ND1	-5.48	1.32	1.38
1	B	150	HIS	CD2-NE2	-5.48	1.31	1.37
1	A	146	HIS	CG-ND1	-5.43	1.32	1.38
1	A	512	HIS	CG-ND1	-5.42	1.32	1.38
1	A	286	HIS	CG-ND1	-5.41	1.32	1.38
1	A	506	HIS	CG-ND1	-5.41	1.32	1.38
1	A	452	HIS	CG-ND1	-5.34	1.32	1.38
1	B	146	HIS	CG-ND1	-5.33	1.32	1.38
1	A	506	HIS	CD2-NE2	-5.29	1.32	1.37
1	A	207	HIS	CG-ND1	-5.19	1.32	1.38
1	B	104	HIS	CG-ND1	-5.19	1.32	1.38
1	A	508	HIS	CD2-NE2	-5.16	1.32	1.37
1	A	450	HIS	CG-ND1	-5.15	1.32	1.38
1	B	450	HIS	CD2-NE2	-5.06	1.32	1.37
1	A	106	HIS	CG-ND1	-5.04	1.32	1.38
1	A	5	HIS	CG-ND1	-5.03	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	HIS	CG-ND1	-5.02	1.32	1.38
1	A	234	HIS	CG-ND1	-5.02	1.32	1.38

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	551	ASN	CA-CB-CG	9.65	122.25	112.60
1	B	125	GLN	OE1-CD-NE2	-8.98	113.62	122.60
1	A	416	ASN	OD1-CG-ND2	-8.96	113.64	122.60
1	B	357	ASN	OD1-CG-ND2	-8.44	114.17	122.60
1	B	416	ASN	OD1-CG-ND2	-8.37	114.23	122.60
1	B	386	HIS	CB-CG-CD2	-7.97	120.84	131.20
1	A	416	ASN	CA-CB-CG	7.68	120.28	112.60
1	A	18	ASN	OD1-CG-ND2	-7.50	115.10	122.60
1	A	269	ASP	CA-CB-CG	7.44	120.04	112.60
1	B	18	ASN	OD1-CG-ND2	-7.40	115.20	122.60
1	A	50	ASN	OD1-CG-ND2	-7.38	115.22	122.60
1	A	242	ASP	CA-CB-CG	7.35	119.95	112.60
1	A	296	LEU	N-CA-C	-7.13	96.00	108.20
1	B	50	ASN	OD1-CG-ND2	-7.07	115.53	122.60
1	A	445	HIS	ND1-CG-CD2	7.05	113.15	106.10
1	B	60	HIS	CB-CG-CD2	-7.03	122.07	131.20
1	B	144	TRP	CG-CD2-CE3	6.96	140.86	133.90
1	B	20	ASN	N-CA-C	-6.86	97.10	108.34
1	A	481	ASN	CA-CB-CG	6.82	119.42	112.60
1	B	357	ASN	CB-CG-ND2	6.78	126.56	116.40
1	B	445	HIS	ND1-CG-CD2	6.56	112.66	106.10
1	B	484	VAL	CB-CA-C	-6.53	101.95	111.68
1	B	386	HIS	CB-CG-ND1	6.46	132.40	122.70
1	B	106	HIS	CB-CG-CD2	-6.44	122.82	131.20
1	B	338	LYS	CA-C-N	6.44	124.30	119.66
1	B	338	LYS	C-N-CA	6.44	124.30	119.66
1	B	144	TRP	CE2-CD2-CG	-6.41	99.51	107.20
1	B	508	HIS	CB-CG-CD2	-6.38	122.91	131.20
1	A	249	PHE	CA-CB-CG	6.36	120.16	113.80
1	B	118	SER	N-CA-C	6.34	120.40	110.32
1	B	469	GLU	N-CA-C	6.32	118.98	111.33
1	A	52	LEU	N-CA-C	-6.31	100.29	110.32
1	B	334	MET	CA-CB-CG	6.30	126.70	114.10
1	B	512	HIS	ND1-CG-CD2	6.30	112.40	106.10
1	A	211	LYS	CA-CB-CG	6.28	126.66	114.10
1	A	97	ASN	CA-CB-CG	6.22	118.82	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ALA	N-CA-C	6.22	119.25	110.23
1	A	505	PHE	N-CA-C	-6.20	98.18	108.34
1	B	351	ASN	CA-CB-CG	6.19	118.79	112.60
1	A	71	TRP	CG-CD2-CE3	6.18	140.09	133.90
1	A	221	THR	N-CA-C	-6.16	103.19	111.87
1	A	226	ALA	N-CA-C	-6.14	99.69	109.76
1	A	163	TRP	CB-CG-CD1	-6.13	117.71	126.90
1	B	357	ASN	CA-CB-CG	6.12	118.72	112.60
1	B	62	HIS	CB-CG-CD2	-6.08	123.30	131.20
1	B	366	ASP	N-CA-C	6.07	120.49	113.38
1	B	435	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	A	20	ASN	OD1-CG-ND2	-6.04	116.56	122.60
1	B	448	HIS	CB-CG-CD2	-6.01	123.38	131.20
1	A	50	ASN	CB-CG-ND2	5.99	125.39	116.40
1	B	225	ALA	N-CA-C	5.97	119.12	110.28
1	A	397	PHE	CA-C-N	5.92	125.68	119.76
1	A	397	PHE	C-N-CA	5.92	125.68	119.76
1	A	143	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	39	ASN	CA-CB-CG	5.90	118.50	112.60
1	A	189	ASN	CB-CG-ND2	5.89	125.24	116.40
1	A	517	MET	N-CA-C	5.89	119.30	108.58
1	B	351	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	A	397	PHE	CA-CB-CG	5.84	119.64	113.80
1	A	159	LYS	CB-CA-C	-5.83	101.55	109.42
1	B	50	ASN	CB-CG-ND2	5.83	125.14	116.40
1	B	509	ILE	N-CA-C	-5.83	98.83	107.51
1	A	211	LYS	N-CA-CB	-5.81	103.31	112.08
1	B	296	LEU	N-CA-C	-5.80	96.96	107.75
1	A	351	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	A	106	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	A	351	ASN	CB-CG-ND2	5.71	124.97	116.40
1	B	344	ASN	OD1-CG-ND2	-5.70	116.90	122.60
1	A	71	TRP	CB-CG-CD1	-5.69	118.37	126.90
1	B	354	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	B	143	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	187	ASP	CA-CB-CG	5.67	118.28	112.60
1	A	416	ASN	CB-CG-ND2	5.67	124.90	116.40
1	A	271	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	B	277	TRP	CE2-CD2-CG	-5.66	100.41	107.20
1	B	514	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	B	277	TRP	CG-CD2-CE3	5.62	139.53	133.90
1	A	39	ASN	N-CA-C	-5.62	101.01	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	HIS	ND1-CG-CD2	5.59	111.69	106.10
1	B	221	THR	N-CA-C	-5.57	103.76	110.88
1	B	144	TRP	CB-CG-CD1	-5.56	118.56	126.90
1	A	351	ASN	CA-CB-CG	5.56	118.16	112.60
1	A	508	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	B	397	PHE	CA-CB-CG	5.56	119.36	113.80
1	A	18	ASN	CA-CB-CG	5.55	118.15	112.60
1	A	209	SER	CA-C-N	5.55	125.55	119.89
1	A	209	SER	C-N-CA	5.55	125.55	119.89
1	B	96	ASP	N-CA-C	5.54	118.50	111.69
1	B	147	GLN	OE1-CD-NE2	-5.53	117.07	122.60
1	B	490	TRP	CE2-CD2-CG	-5.53	100.56	107.20
1	A	448	HIS	CB-CG-CD2	-5.52	124.03	131.20
1	A	179	ASP	N-CA-C	5.51	119.83	113.38
1	A	206	PHE	CA-CB-CG	5.51	119.31	113.80
1	A	317	TRP	N-CA-C	5.51	118.80	111.75
1	B	226	ALA	N-CA-C	-5.51	100.27	109.24
1	A	481	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	B	249	PHE	CA-CB-CG	5.47	119.27	113.80
1	B	294	THR	CA-CB-OG1	-5.47	101.39	109.60
1	B	187	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	423	ILE	N-CA-CB	-5.46	102.22	111.23
1	B	234	HIS	CB-CG-CD2	-5.45	124.11	131.20
1	A	294	THR	CA-CB-OG1	-5.43	101.45	109.60
1	B	271	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	B	351	ASN	CB-CG-ND2	5.43	124.54	116.40
1	A	168	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	A	327	THR	N-CA-C	5.41	117.88	111.33
1	B	247	GLN	CA-C-N	5.41	125.35	119.78
1	B	247	GLN	C-N-CA	5.41	125.35	119.78
1	A	62	HIS	CB-CG-CD2	-5.40	124.17	131.20
1	B	514	HIS	CB-CG-ND1	5.39	130.79	122.70
1	A	189	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	B	498	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	318	ASP	CA-CB-CG	5.38	117.97	112.60
1	A	163	TRP	CG-CD2-CE3	5.37	139.27	133.90
1	A	320	PHE	CA-CB-CG	-5.36	108.44	113.80
1	A	344	ASN	N-CA-C	-5.33	107.15	113.97
1	A	503	TRP	CG-CD2-CE3	5.31	139.21	133.90
1	A	314	THR	CA-C-N	5.30	125.30	119.89
1	A	314	THR	C-N-CA	5.30	125.30	119.89
1	A	18	ASN	CB-CG-ND2	5.28	124.32	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	LYS	N-CA-C	-5.28	100.96	109.40
1	B	16	ALA	CA-C-N	5.28	126.44	119.84
1	B	16	ALA	C-N-CA	5.28	126.44	119.84
1	A	53	HIS	N-CA-C	5.27	117.10	111.36
1	A	408	THR	N-CA-C	-5.27	107.02	113.50
1	B	47	GLU	CA-CB-CG	5.25	124.60	114.10
1	A	104	HIS	CA-CB-CG	5.25	119.05	113.80
1	B	144	TRP	CG-CD1-NE1	-5.25	103.38	110.20
1	B	189	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	A	445	HIS	CG-CD2-NE2	-5.23	101.97	107.20
1	B	191	GLU	CA-C-N	5.22	124.98	119.76
1	B	191	GLU	C-N-CA	5.22	124.98	119.76
1	B	47	GLU	CA-C-O	5.22	126.05	120.46
1	A	386	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	B	8	TRP	CE2-CD2-CG	-5.20	100.96	107.20
1	A	163	TRP	CG-CD1-NE1	-5.19	103.45	110.20
1	A	294	THR	CA-CB-CG2	5.18	119.31	110.50
1	A	455	TRP	CB-CG-CD1	-5.18	119.12	126.90
1	A	159	LYS	N-CA-CB	5.18	119.40	110.23
1	B	144	TRP	CD1-CG-CD2	5.18	114.59	106.30
1	B	277	TRP	CB-CG-CD1	-5.17	119.14	126.90
1	A	53	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	B	416	ASN	CB-CG-ND2	5.16	124.14	116.40
1	A	389	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	132	HIS	CB-CG-CD2	-5.15	124.51	131.20
1	A	20	ASN	N-CA-C	-5.15	99.90	108.34
1	B	286	HIS	CA-C-N	5.14	124.90	119.76
1	B	286	HIS	C-N-CA	5.14	124.90	119.76
1	B	389	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	435	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	B	452	HIS	CA-CB-CG	5.12	118.92	113.80
1	A	217	ARG	N-CA-C	-5.10	100.99	109.46
1	A	150	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	B	163	TRP	CB-CG-CD1	-5.10	119.25	126.90
1	B	189	ASN	CB-CG-ND2	5.10	124.05	116.40
1	A	455	TRP	CG-CD2-CE3	5.09	138.99	133.90
1	B	207	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	B	503	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	A	329	ARG	CA-CB-CG	5.08	124.25	114.10
1	A	392	PRO	CA-C-N	5.08	123.37	119.66
1	A	392	PRO	C-N-CA	5.08	123.37	119.66
1	A	119	LEU	N-CA-C	-5.07	99.04	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	TRP	CE2-CD2-CG	-5.07	101.12	107.20
1	B	440	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	B	228	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	A	473	ASN	CA-CB-CG	5.06	117.66	112.60
1	A	414	ILE	N-CA-C	-5.04	101.15	109.12
1	B	80	GLN	N-CA-C	5.01	116.69	109.07
1	B	531	ILE	CA-C-N	5.01	125.29	119.93
1	B	531	ILE	C-N-CA	5.01	125.29	119.93
1	A	503	TRP	CB-CG-CD1	-5.01	119.39	126.90
1	B	352	THR	N-CA-C	5.01	117.29	109.52
1	A	392	PRO	N-CA-C	5.00	116.80	110.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	551	ASN	Peptide
1	B	551	ASN	Peptide

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	4366	0	4211	25	0
1	B	4366	0	4211	33	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	514	0	0	4	0
5	B	458	0	0	4	0
All	All	9743	0	8448	58	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (58) 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:240:GLU:HB3	1:B:263:SER:HB2	1.78	0.66
1:A:10:VAL:HG23	1:A:48:LEU:HD11	1.77	0.65
1:A:138:ASN:HD22	1:A:217:ARG:HB2	1.62	0.64
1:A:436:MET:HA	5:A:1129:HOH:O	1.98	0.62
1:A:18:ASN:ND2	1:A:20:ASN:HB2	2.18	0.59
1:B:146:HIS:H	1:B:168:GLN:HE21	1.51	0.58
1:A:231:ILE:HG12	1:A:278:VAL:HG22	1.85	0.58
1:B:146:HIS:H	1:B:168:GLN:NE2	2.02	0.57
1:B:389:ASP:H	1:B:416:ASN:ND2	2.04	0.56
1:A:160:PRO:HB2	5:A:1307:HOH:O	2.06	0.55
1:B:27:ILE:O	1:B:30:GLN:HG2	2.08	0.54
1:B:205:ILE:HD13	1:B:303:VAL:HG21	1.90	0.54
1:B:23:ILE:HD11	5:B:1160:HOH:O	2.07	0.53
1:B:1:SER:N	1:B:125:GLN:OE1	2.42	0.52
1:B:113:ALA:HB2	1:B:149:ILE:HG13	1.91	0.52
1:B:39:ASN:HB2	1:B:125:GLN:HE21	1.75	0.51
1:B:380:MET:HB3	1:B:525:VAL:HG11	1.93	0.51
1:A:18:ASN:HD21	1:A:20:ASN:HB2	1.75	0.51
1:A:75:THR:HG21	1:A:450:HIS:CE1	2.45	0.50
1:B:148:SER:O	1:B:152:GLN:HG3	2.13	0.49
1:A:18:ASN:HA	1:A:176:GLY:O	2.13	0.48
1:B:286:HIS:HA	1:B:287:PRO:HD3	1.74	0.47
1:B:45:VAL:HG13	1:B:92:ASN:OD1	2.15	0.47
1:A:449:LEU:HD13	1:A:452:HIS:HB2	1.96	0.47
1:A:99:GLY:HA3	1:A:243:GLY:HA2	1.97	0.47
1:B:150:HIS:HD2	5:B:832:HOH:O	1.97	0.47
1:A:146:HIS:H	1:A:168:GLN:HE21	1.62	0.46
1:A:146:HIS:H	1:A:168:GLN:NE2	2.14	0.46
1:A:175:ARG:HD3	1:A:202:ALA:O	2.16	0.46
1:A:389:ASP:H	1:A:416:ASN:ND2	2.14	0.45
1:A:10:VAL:CG2	1:A:48:LEU:HD11	2.46	0.45
1:B:423:ILE:HD13	1:B:524:GLY:HA3	1.98	0.45
1:A:212:LYS:HB2	1:A:214:TYR:CE1	2.52	0.45
1:B:271:ASN:HA	1:B:272:PRO:HD3	1.74	0.45
1:B:141:LEU:HD22	1:B:280:VAL:HG11	1.99	0.45
1:A:47:GLU:HB3	1:A:90:PHE:CE1	2.52	0.45
1:B:362:TRP:HB3	1:B:517:MET:HB2	1.99	0.45
1:A:67:ARG:HH22	1:A:498:ASP:CG	2.25	0.44
1:B:348:PHE:HD2	1:B:396:VAL:HG12	1.82	0.44
1:A:145:TRP:HA	1:A:168:GLN:HE21	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:HIS:N	1:B:168:GLN:HE21	2.15	0.43
1:A:215:ARG:HD2	1:A:263:SER:HB3	1.99	0.43
1:B:35:THR:HG23	1:B:118:SER:HB2	2.00	0.43
1:A:147:GLN:HA	5:A:1171:HOH:O	2.18	0.43
1:B:239:VAL:HG21	1:B:265:LEU:HD13	2.01	0.43
1:B:214:TYR:O	1:B:265:LEU:HA	2.19	0.42
1:A:271:ASN:HA	1:A:272:PRO:HD3	1.86	0.42
1:B:465:SER:O	1:B:468:GLU:HB2	2.19	0.42
1:B:132:HIS:HA	5:B:939:HOH:O	2.20	0.42
1:B:48:LEU:O	1:B:88:THR:HA	2.21	0.41
1:B:444:THR:HG22	1:B:487:PRO:HD3	2.02	0.41
1:A:25:MET:HE1	1:A:110:GLN:HG2	2.03	0.41
1:A:503:TRP:HA	5:A:988:HOH:O	2.20	0.41
1:B:205:ILE:HD13	1:B:303:VAL:CG2	2.51	0.41
1:B:150:HIS:CG	5:B:946:HOH:O	2.74	0.40
1:B:431:LEU:O	1:B:490:TRP:HA	2.21	0.40
1:B:18:ASN:HA	1:B:176:GLY:O	2.22	0.40
1:B:368:SER:HB3	1:B:414:ILE:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/552 (100%)	534 (97%)	14 (2%)	2 (0%)	30	22
1	B	550/552 (100%)	527 (96%)	19 (4%)	4 (1%)	18	10
All	All	1100/1104 (100%)	1061 (96%)	33 (3%)	6 (0%)	24	16

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	551	ASN
1	B	551	ASN
1	B	537	ALA
1	A	476	ASN
1	B	423	ILE
1	B	476	ASN

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	475/475 (100%)	445 (94%)	30 (6%)	16	8
1	B	475/475 (100%)	449 (94%)	26 (6%)	19	11
All	All	950/950 (100%)	894 (94%)	56 (6%)	18	10

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	18	ASN
1	A	24	VAL
1	A	171	LEU
1	A	211	LYS
1	A	212	LYS
1	A	215	ARG
1	A	221	THR
1	A	264	VAL
1	A	279	SER
1	A	308	THR
1	A	325	ASN
1	A	342	LYS
1	A	345	ARG
1	A	351	ASN
1	A	396	VAL
1	A	406	PRO
1	A	413	ARG

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Mol	Chain	Res	Type
1	A	416	ASN
1	A	422	LYS
1	A	449	LEU
1	A	457	LEU
1	A	479	LEU
1	A	485	ILE
1	A	500	PRO
1	A	526	GLU
1	A	536	LEU
1	A	541	THR
1	A	545	LEU
1	A	552	PRO
1	B	1	SER
1	B	9	GLU
1	B	18	ASN
1	B	24	VAL
1	B	50	ASN
1	B	57	VAL
1	B	67	ARG
1	B	188	SER
1	B	215	ARG
1	B	221	THR
1	B	264	VAL
1	B	300	PRO
1	B	304	SER
1	B	308	THR
1	B	331	THR
1	B	357	ASN
1	B	399	GLU
1	B	416	ASN
1	B	428	ASP
1	B	449	LEU
1	B	470	SER
1	B	484	VAL
1	B	523	GLU
1	B	536	LEU
1	B	541	THR
1	B	550	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	84	ASN
1	A	97	ASN
1	A	138	ASN
1	A	147	GLN
1	A	168	GLN
1	A	228	ASN
1	A	233	ASN
1	A	270	GLN
1	A	297	ASN
1	A	313	GLN
1	A	390	GLN
1	A	416	ASN
1	B	2	GLN
1	B	5	HIS
1	B	18	ASN
1	B	39	ASN
1	B	50	ASN
1	B	147	GLN
1	B	168	GLN
1	B	228	ASN
1	B	235	GLN
1	B	297	ASN
1	B	354	ASN
1	B	357	ASN
1	B	390	GLN
1	B	416	ASN
1	B	551	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	601	1	14,14,15	1.07	1 (7%)	17,19,21	0.71	0
4	C2O	B	702	1	0,2,2	-	-	-		
2	NAG	B	601	1	14,14,15	0.70	0	17,19,21	0.79	1 (5%)
4	C2O	A	702	1	0,2,2	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAG	C2-N2	-2.21	1.42	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAG	C1-C2-N2	2.04	113.65	110.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.