



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:41 PM UTC

PDB ID : 1ASP / pdb_00001asp
Title : X-RAY STRUCTURES AND MECHANISTIC IMPLICATIONS OF THREE
FUNCTIONAL DERIVATIVES OF ASCORBATE OXIDASE FROM ZUC-
CHINI: REDUCED-, PEROXIDE-, AND AZIDE-FORMS
Authors : Messerschmidt, A.; Luecke, H.; Huber, R.
Deposited on : 1992-11-25
Resolution : 2.59 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
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

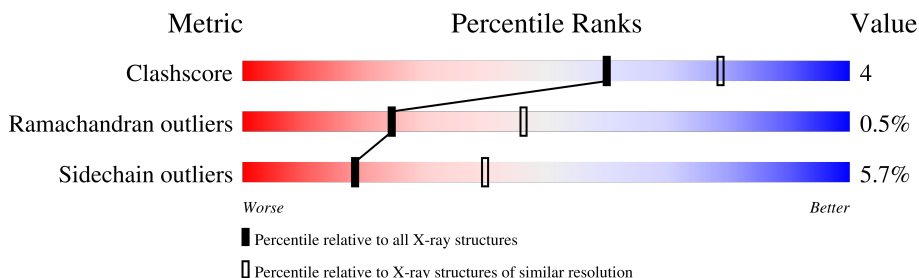
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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% 18% . .
1	B	552	 77% 18% . .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9742 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: $C_8H_{15}NO_6$).

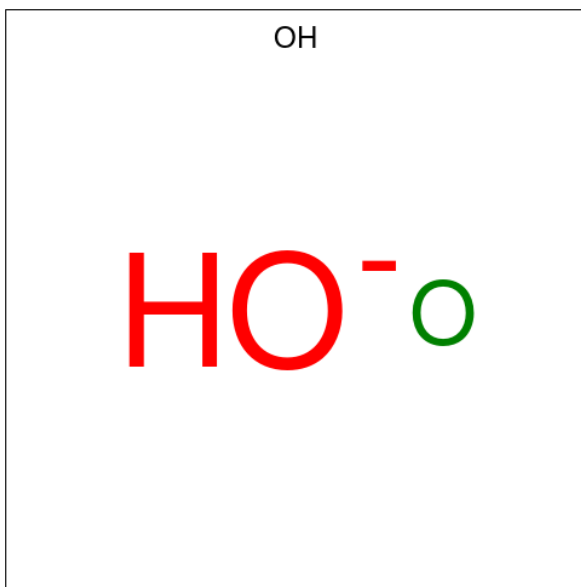


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

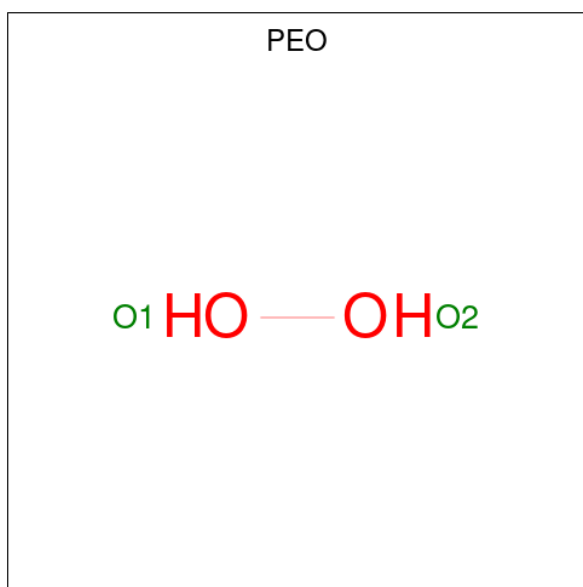
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total 5	Cu 5	0	0
3	B	4	Total 4	Cu 4	0	0

- Molecule 4 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



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

- Molecule 5 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H₂O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			2	2		
5	B	1	Total	O	0	0
			2	2		

- Molecule 6 is water.

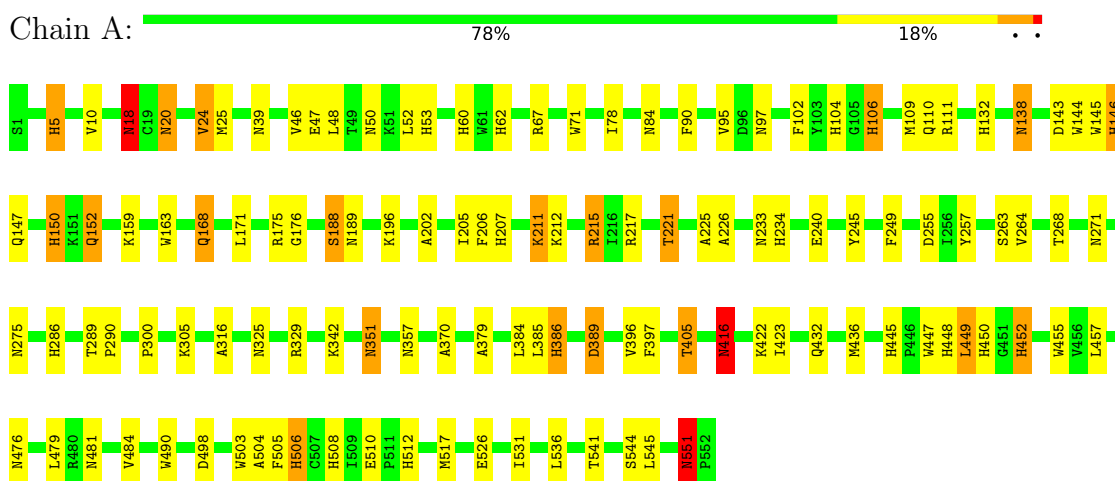
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	518	Total	O	0	0
			518	518		
6	B	449	Total	O	0	0
			449	449		

3 Residue-property plots

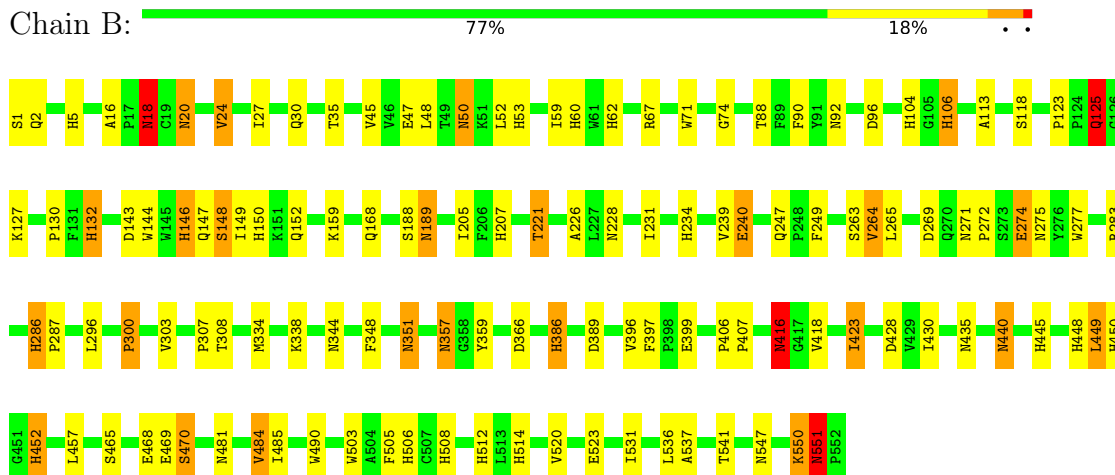
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	106.33Å 105.32Å 112.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.59	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.59)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9742	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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, CU, PEO, OH

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	1.10	33/4508 (0.7%)	1.78	87/6159 (1.4%)
1	B	1.06	31/4508 (0.7%)	1.66	66/6159 (1.1%)
All	All	1.08	64/9016 (0.7%)	1.72	153/12318 (1.2%)

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	1
1	B	0	1
All	All	0	2

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	506	HIS	ND1-CE1	-18.14	1.14	1.32
1	A	506	HIS	ND1-CE1	-16.59	1.16	1.32
1	A	506	HIS	CG-ND1	-11.35	1.25	1.38
1	A	106	HIS	CE1-NE2	-10.87	1.21	1.32
1	A	106	HIS	CG-ND1	-10.12	1.27	1.38
1	B	506	HIS	CG-ND1	-8.30	1.29	1.38
1	B	146	HIS	CD2-NE2	-7.69	1.29	1.37
1	B	506	HIS	CD2-NE2	-7.31	1.29	1.37
1	B	106	HIS	N-CA	-7.16	1.38	1.46
1	A	234	HIS	CD2-NE2	-6.97	1.30	1.37
1	B	448	HIS	CD2-NE2	-6.95	1.30	1.37
1	A	452	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	386	HIS	CD2-NE2	-6.81	1.30	1.37
1	B	53	HIS	CD2-NE2	-6.81	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	HIS	CD2-NE2	-6.81	1.30	1.37
1	B	512	HIS	CD2-NE2	-6.75	1.30	1.37
1	A	53	HIS	CD2-NE2	-6.74	1.30	1.37
1	B	207	HIS	CD2-NE2	-6.69	1.30	1.37
1	A	5	HIS	CD2-NE2	-6.68	1.30	1.37
1	B	60	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	62	HIS	CD2-NE2	-6.51	1.30	1.37
1	B	445	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	512	HIS	CD2-NE2	-6.45	1.30	1.37
1	B	452	HIS	CD2-NE2	-6.37	1.30	1.37
1	B	386	HIS	CD2-NE2	-6.34	1.30	1.37
1	A	448	HIS	CD2-NE2	-6.30	1.30	1.37
1	A	132	HIS	CD2-NE2	-6.27	1.30	1.37
1	B	5	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	106	HIS	CG-CD2	6.23	1.42	1.35
1	A	450	HIS	CG-ND1	-6.21	1.31	1.38
1	B	150	HIS	CD2-NE2	-6.17	1.31	1.37
1	B	450	HIS	CD2-NE2	-6.07	1.31	1.37
1	B	450	HIS	CG-ND1	-5.99	1.31	1.38
1	A	60	HIS	CD2-NE2	-5.92	1.31	1.37
1	B	286	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	445	HIS	CD2-NE2	-5.89	1.31	1.37
1	A	286	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	207	HIS	CD2-NE2	-5.86	1.31	1.37
1	A	512	HIS	CG-ND1	-5.81	1.31	1.38
1	A	286	HIS	CG-ND1	-5.81	1.31	1.38
1	B	514	HIS	CD2-NE2	-5.81	1.31	1.37
1	B	508	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	104	HIS	CD2-NE2	-5.73	1.31	1.37
1	B	234	HIS	CD2-NE2	-5.73	1.31	1.37
1	B	5	HIS	CG-ND1	-5.69	1.31	1.38
1	B	146	HIS	CG-ND1	-5.64	1.32	1.38
1	B	62	HIS	CD2-NE2	-5.63	1.31	1.37
1	B	104	HIS	CD2-NE2	-5.61	1.31	1.37
1	B	512	HIS	CG-ND1	-5.59	1.32	1.38
1	A	5	HIS	CG-ND1	-5.57	1.32	1.38
1	B	132	HIS	CD2-NE2	-5.47	1.31	1.37
1	B	430	ILE	CA-CB	5.45	1.60	1.54
1	A	506	HIS	CD2-NE2	-5.45	1.31	1.37
1	A	508	HIS	CD2-NE2	-5.44	1.31	1.37
1	B	150	HIS	CG-ND1	-5.41	1.32	1.38
1	B	386	HIS	CG-ND1	-5.31	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	HIS	CD2-NE2	-5.27	1.32	1.37
1	A	508	HIS	CG-ND1	-5.23	1.32	1.38
1	A	450	HIS	CD2-NE2	-5.20	1.32	1.37
1	A	386	HIS	CG-ND1	-5.17	1.32	1.38
1	A	290	PRO	CA-CB	-5.16	1.49	1.53
1	A	46	VAL	CA-CB	5.12	1.60	1.54
1	B	448	HIS	CG-ND1	-5.11	1.32	1.38
1	A	448	HIS	CG-ND1	-5.01	1.32	1.38

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	HIS	ND1-CE1-NE2	20.13	128.53	108.40
1	A	106	HIS	CE1-NE2-CD2	-15.38	93.62	109.00
1	A	506	HIS	ND1-CE1-NE2	14.11	122.51	108.40
1	A	506	HIS	CE1-NE2-CD2	-12.11	96.89	109.00
1	B	50	ASN	OD1-CG-ND2	-9.22	113.38	122.60
1	A	53	HIS	CB-CG-CD2	-9.16	119.29	131.20
1	A	143	ASP	CA-CB-CG	8.80	121.41	112.60
1	B	189	ASN	OD1-CG-ND2	-8.70	113.90	122.60
1	A	18	ASN	OD1-CG-ND2	-8.59	114.01	122.60
1	B	357	ASN	OD1-CG-ND2	-8.57	114.03	122.60
1	B	551	ASN	CA-CB-CG	8.29	120.89	112.60
1	B	416	ASN	OD1-CG-ND2	-8.07	114.53	122.60
1	B	344	ASN	OD1-CG-ND2	-7.98	114.62	122.60
1	B	481	ASN	OD1-CG-ND2	-7.97	114.63	122.60
1	A	50	ASN	OD1-CG-ND2	-7.84	114.75	122.60
1	B	125	GLN	OE1-CD-NE2	-7.69	114.91	122.60
1	A	289	THR	CA-C-N	7.66	125.25	119.66
1	A	289	THR	C-N-CA	7.66	125.25	119.66
1	A	357	ASN	CA-CB-CG	-7.58	105.02	112.60
1	A	53	HIS	CB-CG-ND1	7.57	134.05	122.70
1	A	249	PHE	CA-CB-CG	7.55	121.35	113.80
1	A	168	GLN	OE1-CD-NE2	-7.48	115.12	122.60
1	B	144	TRP	CG-CD2-CE3	7.41	141.31	133.90
1	B	445	HIS	ND1-CG-CD2	7.32	113.42	106.10
1	A	481	ASN	OD1-CG-ND2	-7.22	115.38	122.60
1	A	503	TRP	CG-CD2-CE3	6.78	140.68	133.90
1	B	469	GLU	N-CA-C	6.72	119.18	111.11
1	B	512	HIS	ND1-CG-CD2	6.72	112.83	106.10
1	B	50	ASN	CB-CG-ND2	6.71	126.46	116.40
1	A	159	LYS	CB-CA-C	-6.65	100.44	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ASN	CB-CG-ND2	6.63	126.35	116.40
1	B	143	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	255	ASP	CA-CB-CG	6.57	119.17	112.60
1	B	440	ASN	OD1-CG-ND2	-6.51	116.09	122.60
1	B	448	HIS	CB-CG-CD2	-6.46	122.80	131.20
1	A	452	HIS	CB-CG-CD2	-6.43	122.84	131.20
1	B	357	ASN	CB-CG-ND2	6.40	126.00	116.40
1	B	450	HIS	CA-CB-CG	6.38	120.18	113.80
1	A	416	ASN	CA-CB-CG	6.32	118.92	112.60
1	A	52	LEU	N-CA-C	-6.31	100.28	110.32
1	B	435	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	A	397	PHE	CA-C-N	6.27	126.48	119.90
1	A	397	PHE	C-N-CA	6.27	126.48	119.90
1	A	234	HIS	CB-CG-CD2	-6.25	123.08	131.20
1	A	405	THR	CB-CA-C	6.25	118.55	108.87
1	A	20	ASN	N-CA-C	-6.21	98.16	108.34
1	A	211	LYS	N-CA-CB	-6.18	102.75	112.08
1	A	152	GLN	OE1-CD-NE2	-6.17	116.43	122.60
1	B	18	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	B	60	HIS	CB-CG-CD2	-6.14	123.22	131.20
1	A	39	ASN	CA-CB-CG	6.13	118.73	112.60
1	A	211	LYS	CA-CB-CG	6.12	126.34	114.10
1	A	445	HIS	ND1-CG-CD2	6.11	112.21	106.10
1	A	97	ASN	CA-CB-CG	6.09	118.69	112.60
1	A	71	TRP	CB-CG-CD1	-6.06	117.81	126.90
1	A	138	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	A	71	TRP	CG-CD2-CE3	5.96	139.87	133.90
1	A	102	PHE	CA-CB-CG	5.96	119.76	113.80
1	B	481	ASN	CA-CB-CG	5.94	118.54	112.60
1	A	405	THR	N-CA-CB	-5.88	100.38	110.72
1	A	225	ALA	N-CA-C	5.88	118.34	110.35
1	A	448	HIS	CB-CG-CD2	-5.86	123.58	131.20
1	A	226	ALA	N-CA-C	-5.85	99.70	109.24
1	A	385	LEU	N-CA-C	5.84	121.44	113.37
1	A	189	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	B	144	TRP	CE2-CD2-CG	-5.83	100.20	107.20
1	A	207	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	B	16	ALA	CA-C-N	5.79	125.92	119.32
1	B	16	ALA	C-N-CA	5.79	125.92	119.32
1	B	416	ASN	CB-CG-ND2	5.79	125.08	116.40
1	B	189	ASN	CB-CG-ND2	5.76	125.05	116.40
1	B	207	HIS	CB-CG-CD2	-5.70	123.79	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	HIS	CB-CG-CD2	-5.70	123.79	131.20
1	A	508	HIS	CB-CG-CD2	-5.69	123.80	131.20
1	A	106	HIS	CG-ND1-CE1	-5.67	99.66	109.30
1	B	24	VAL	N-CA-CB	-5.67	102.92	112.44
1	A	503	TRP	CB-CG-CD1	-5.66	118.41	126.90
1	B	452	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	A	351	ASN	CB-CG-ND2	5.65	124.88	116.40
1	A	18	ASN	CA-CB-CG	5.65	118.25	112.60
1	A	505	PHE	N-CA-C	-5.63	99.11	108.34
1	B	484	VAL	CB-CA-C	-5.63	102.81	111.31
1	A	106	HIS	CG-CD2-NE2	5.60	112.80	107.20
1	B	264	VAL	N-CA-CB	-5.60	102.26	111.44
1	A	163	TRP	CE2-CD2-CG	-5.59	100.49	107.20
1	B	269	ASP	CB-CA-C	-5.59	101.39	110.79
1	B	338	LYS	CA-C-N	5.58	123.73	119.66
1	B	338	LYS	C-N-CA	5.58	123.73	119.66
1	B	485	ILE	N-CA-C	-5.57	100.39	108.36
1	A	233	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	B	20	ASN	N-CA-C	-5.56	99.21	108.34
1	A	221	THR	N-CA-C	-5.56	103.35	111.30
1	A	386	HIS	CB-CG-CD2	-5.55	123.99	131.20
1	A	24	VAL	N-CA-CB	-5.54	103.14	112.44
1	A	163	TRP	CG-CD2-CE3	5.53	139.43	133.90
1	A	50	ASN	CB-CG-ND2	5.53	124.69	116.40
1	B	514	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	B	249	PHE	CA-CB-CG	5.47	119.27	113.80
1	B	221	THR	N-CA-C	-5.43	104.07	111.56
1	A	389	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	329	ARG	CA-CB-CG	5.41	124.91	114.10
1	B	503	TRP	CG-CD2-CE3	5.39	139.29	133.90
1	B	351	ASN	CB-CG-ND2	5.38	124.46	116.40
1	A	490	TRP	CE2-CD2-CG	-5.37	100.76	107.20
1	B	366	ASP	N-CA-C	5.36	119.65	113.38
1	A	144	TRP	CG-CD2-CE3	5.35	139.25	133.90
1	A	206	PHE	CA-CB-CG	5.33	119.13	113.80
1	B	445	HIS	CB-CG-CD2	-5.32	124.29	131.20
1	B	96	ASP	N-CA-C	5.32	118.23	111.69
1	A	104	HIS	CB-CG-CD2	-5.31	124.30	131.20
1	B	52	LEU	N-CA-C	-5.31	103.39	110.55
1	B	386	HIS	CB-CG-CD2	-5.31	124.30	131.20
1	B	505	PHE	N-CA-C	-5.30	98.58	108.02
1	A	18	ASN	CB-CG-ND2	5.30	124.34	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	531	ILE	CA-C-N	5.30	126.46	119.84
1	B	531	ILE	C-N-CA	5.30	126.46	119.84
1	B	226	ALA	N-CA-C	-5.29	100.11	108.73
1	A	275	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	B	334	MET	CA-CB-CG	5.27	124.64	114.10
1	A	268	THR	N-CA-CB	-5.27	104.11	110.53
1	B	470	SER	CA-CB-OG	5.25	121.61	111.10
1	A	455	TRP	CE2-CD2-CG	-5.24	100.92	107.20
1	B	277	TRP	CE2-CD2-CG	-5.23	100.93	107.20
1	A	517	MET	N-CA-C	5.23	117.70	109.39
1	A	159	LYS	CA-CB-CG	5.22	124.55	114.10
1	A	512	HIS	ND1-CG-CD2	5.21	111.31	106.10
1	A	144	TRP	CE2-CD2-CG	-5.20	100.96	107.20
1	A	351	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	B	24	VAL	CB-CA-C	5.18	118.42	110.55
1	A	271	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	A	503	TRP	CE2-CD2-CG	-5.17	101.00	107.20
1	A	447	TRP	CG-CD2-CE3	5.17	139.07	133.90
1	A	455	TRP	CB-CG-CD1	-5.14	119.19	126.90
1	B	53	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	B	125	GLN	CG-CD-NE2	5.12	124.08	116.40
1	B	514	HIS	CB-CG-ND1	5.11	130.36	122.70
1	A	39	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	432	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	B	397	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	450	HIS	CA-CB-CG	5.08	118.89	113.80
1	A	305	LYS	CA-C-O	5.08	126.21	120.92
1	B	2	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	B	423	ILE	N-CA-CB	-5.08	102.84	111.23
1	A	455	TRP	CG-CD1-NE1	-5.08	103.60	110.20
1	A	531	ILE	CA-C-N	5.08	125.08	119.90
1	A	531	ILE	C-N-CA	5.08	125.08	119.90
1	A	111	ARG	CA-CB-CG	5.05	124.20	114.10
1	B	386	HIS	CB-CG-ND1	5.05	130.28	122.70
1	A	202	ALA	CA-C-N	5.04	125.04	119.90
1	A	202	ALA	C-N-CA	5.04	125.04	119.90
1	B	247	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	B	71	TRP	CG-CD2-CE3	5.01	138.91	133.90
1	B	274	GLU	O-C-N	5.01	128.96	123.25

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	32	4
1	B	4366	0	4211	42	4
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	5	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	1	0
5	B	2	0	0	0	0
6	A	518	0	0	10	0
6	B	449	0	0	9	0
All	All	9742	0	8448	74	4

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 4.

All (74) 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	1.65	0.78
1:A:436:MET:HA	6:A:878:HOH:O	1.92	0.69
1:B:205:ILE:HD13	1:B:303:VAL:HG21	1.76	0.67
1:A:146:HIS:H	1:A:168:GLN:NE2	1.96	0.63
1:A:147:GLN:HE21	1:A:152:GLN:HG2	1.63	0.63
1:A:449:LEU:HD13	1:A:452:HIS:HB2	1.83	0.59
1:A:18:ASN:ND2	1:A:20:ASN:HB2	2.19	0.58
1:B:389:ASP:H	1:B:416:ASN:ND2	2.03	0.57
1:A:138:ASN:HD22	1:A:217:ARG:HB2	1.71	0.55
1:B:146:HIS:H	1:B:168:GLN:HE21	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ILE:HD13	1:B:303:VAL:CG2	2.37	0.54
1:B:147:GLN:HE21	1:B:152:GLN:HG2	1.73	0.54
1:A:379:ALA:HA	1:A:384:LEU:HD12	1.91	0.53
1:B:113:ALA:HB2	1:B:149:ILE:HG13	1.90	0.53
1:B:47:GLU:HB3	1:B:90:PHE:CE1	2.44	0.53
1:B:449:LEU:HD13	1:B:452:HIS:HB2	1.91	0.53
1:A:145:TRP:HA	1:A:168:GLN:HE21	1.74	0.52
1:B:440:ASN:HA	6:B:869:HOH:O	2.09	0.52
1:A:145:TRP:HA	1:A:168:GLN:NE2	2.25	0.52
1:B:146:HIS:H	1:B:168:GLN:NE2	2.07	0.52
1:B:1:SER:N	1:B:125:GLN:OE1	2.40	0.51
1:B:27:ILE:O	1:B:30:GLN:HG2	2.10	0.51
1:A:5:HIS:HB2	6:A:782:HOH:O	2.10	0.51
1:B:300:PRO:HD2	6:B:893:HOH:O	2.10	0.51
1:B:468:GLU:HG2	1:B:490:TRP:CZ2	2.45	0.51
1:A:506:HIS:HE1	5:A:560:PEO:O2	1.93	0.51
1:A:240:GLU:HB3	1:A:263:SER:HB2	1.93	0.50
1:A:215:ARG:HD2	1:A:263:SER:HB3	1.93	0.49
1:A:510:GLU:HB3	6:A:738:HOH:O	2.12	0.49
1:B:123:PRO:HB3	6:B:822:HOH:O	2.13	0.48
1:A:245:TYR:HD2	6:A:750:HOH:O	1.97	0.47
1:B:418:VAL:HG22	1:B:520:VAL:HB	1.96	0.47
1:B:228:ASN:HB2	1:B:283:ARG:HG3	1.97	0.46
1:A:257:TYR:CD2	1:A:484:VAL:HG21	2.51	0.46
1:A:188:SER:HB2	6:A:1072:HOH:O	2.15	0.46
1:B:127:LYS:HB3	1:B:127:LYS:HE2	1.71	0.46
1:A:47:GLU:HB3	1:A:90:PHE:CE1	2.50	0.46
1:B:148:SER:HB3	6:B:999:HOH:O	2.15	0.46
1:B:132:HIS:HA	6:B:786:HOH:O	2.16	0.45
1:B:189:ASN:ND2	6:B:569:HOH:O	2.49	0.45
1:B:48:LEU:O	1:B:88:THR:HA	2.17	0.45
1:A:67:ARG:HH22	1:A:498:ASP:CG	2.24	0.45
1:B:106:HIS:HE1	6:B:718:HOH:O	2.00	0.45
1:B:159:LYS:HB2	1:B:359:TYR:CE1	2.51	0.44
1:B:399:GLU:HB3	6:B:813:HOH:O	2.17	0.44
1:A:106:HIS:HE1	6:A:812:HOH:O	2.01	0.44
1:A:25:MET:HE1	1:A:110:GLN:HG2	2.00	0.43
1:B:275:ASN:O	1:B:307:PRO:HG3	2.18	0.43
1:A:370:ALA:O	1:A:416:ASN:HB3	2.18	0.43
1:B:550:LYS:N	1:B:550:LYS:HD3	2.34	0.43
1:A:10:VAL:CG2	1:A:48:LEU:HD11	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:HIS:N	1:B:168:GLN:HE21	2.16	0.42
1:B:231:ILE:HG21	1:B:296:LEU:HD22	2.01	0.42
1:B:286:HIS:HA	1:B:287:PRO:HD3	1.70	0.42
1:B:348:PHE:HD2	1:B:396:VAL:HG12	1.83	0.42
1:A:84:ASN:ND2	6:A:869:HOH:O	2.53	0.42
1:B:18:ASN:HD21	1:B:20:ASN:HB2	1.85	0.42
1:B:271:ASN:HA	1:B:272:PRO:HD3	1.75	0.42
1:A:196:LYS:HE3	1:A:196:LYS:HB2	1.91	0.42
1:A:18:ASN:HD21	1:A:20:ASN:HB2	1.85	0.42
1:A:150:HIS:CE1	6:A:660:HOH:O	2.72	0.42
1:A:389:ASP:H	1:A:416:ASN:ND2	2.17	0.42
1:B:18:ASN:ND2	6:B:665:HOH:O	2.51	0.42
1:A:109:MET:HE2	6:A:738:HOH:O	2.19	0.42
1:B:465:SER:O	1:B:468:GLU:HB2	2.20	0.42
1:A:18:ASN:HA	1:A:176:GLY:O	2.21	0.41
1:B:35:THR:HG23	1:B:118:SER:HB2	2.02	0.41
1:B:239:VAL:HG21	1:B:265:LEU:HD13	2.02	0.41
1:B:348:PHE:CD2	1:B:396:VAL:HG12	2.56	0.41
1:B:45:VAL:HG13	1:B:92:ASN:OD1	2.21	0.41
1:B:406:PRO:HA	1:B:407:PRO:HD3	2.00	0.40
1:A:78:ILE:HD13	1:A:504:ALA:HB2	2.02	0.40
1:B:59:ILE:O	1:B:74:GLY:HA3	2.21	0.40
1:A:316:ALA:HA	6:A:671:HOH:O	2.21	0.40

All (4) 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:551:ASN:OD1	1:B:386:HIS:NE2[2_654]	1.94	0.26
1:A:386:HIS:NE2	1:B:551:ASN:O[2_654]	2.11	0.09
1:A:386:HIS:NE2	1:B:551:ASN:OD1[2_654]	2.16	0.04
1:A:544:SER:O	1:B:547:ASN:ND2[2_654]	2.19	0.01

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	550/552 (100%)	535 (97%)	13 (2%)	2 (0%)	30	51
1	B	550/552 (100%)	531 (96%)	15 (3%)	4 (1%)	18	38
All	All	1100/1104 (100%)	1066 (97%)	28 (2%)	6 (0%)	24	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	551	ASN
1	B	551	ASN
1	B	537	ALA
1	B	130	PRO
1	A	476	ASN
1	B	423	ILE

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%)	447 (94%)	28 (6%)	18	38
1	B	475/475 (100%)	449 (94%)	26 (6%)	19	41
All	All	950/950 (100%)	896 (94%)	54 (6%)	18	40

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	24	VAL
1	A	95	VAL
1	A	171	LEU
1	A	175	ARG
1	A	188	SER
1	A	205	ILE

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Mol	Chain	Res	Type
1	A	211	LYS
1	A	212	LYS
1	A	215	ARG
1	A	221	THR
1	A	264	VAL
1	A	300	PRO
1	A	325	ASN
1	A	342	LYS
1	A	351	ASN
1	A	396	VAL
1	A	405	THR
1	A	416	ASN
1	A	422	LYS
1	A	423	ILE
1	A	449	LEU
1	A	457	LEU
1	A	479	LEU
1	A	526	GLU
1	A	536	LEU
1	A	541	THR
1	A	545	LEU
1	B	18	ASN
1	B	24	VAL
1	B	50	ASN
1	B	67	ARG
1	B	125	GLN
1	B	148	SER
1	B	188	SER
1	B	221	THR
1	B	240	GLU
1	B	264	VAL
1	B	274	GLU
1	B	300	PRO
1	B	308	THR
1	B	351	ASN
1	B	357	ASN
1	B	416	ASN
1	B	428	ASP
1	B	449	LEU
1	B	457	LEU
1	B	470	SER
1	B	484	VAL

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Mol	Chain	Res	Type
1	B	523	GLU
1	B	536	LEU
1	B	541	THR
1	B	550	LYS
1	B	551	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	39	ASN
1	A	50	ASN
1	A	80	GLN
1	A	84	ASN
1	A	97	ASN
1	A	138	ASN
1	A	147	GLN
1	A	168	GLN
1	A	233	ASN
1	A	247	GLN
1	A	297	ASN
1	A	354	ASN
1	A	390	GLN
1	A	409	ASN
1	A	416	ASN
1	A	476	ASN
1	B	18	ASN
1	B	39	ASN
1	B	50	ASN
1	B	97	ASN
1	B	138	ASN
1	B	147	GLN
1	B	168	GLN
1	B	228	ASN
1	B	235	GLN
1	B	247	GLN
1	B	297	ASN
1	B	386	HIS
1	B	390	GLN
1	B	416	ASN
1	B	476	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 15 ligands modelled in this entry, 9 are monoatomic and 2 are modelled with single atom - 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
5	PEO	B	559	3	1,1,1	0.68	0	-		
2	NAG	A	553	1	14,14,15	0.94	1 (7%)	17,19,21	0.90	1 (5%)
5	PEO	A	560	3	1,1,1	0.49	0	-		
2	NAG	B	553	1	14,14,15	1.33	2 (14%)	17,19,21	1.41	3 (17%)

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	553	1	-	0/6/23/26	0/1/1/1
2	NAG	B	553	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	553	NAG	O5-C5	2.70	1.48	1.43
2	B	553	NAG	C1-C2	-2.25	1.49	1.52
2	A	553	NAG	C1-C2	-2.15	1.49	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	553	NAG	C2-N2-C7	-3.70	117.94	122.90
2	B	553	NAG	C4-C3-C2	-2.99	106.63	111.02
2	A	553	NAG	C2-N2-C7	-2.17	120.00	122.90
2	B	553	NAG	O5-C5-C4	-2.09	105.74	110.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	560	PEO	1	0

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.