



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:02 AM UTC

PDB ID : 1ASQ / pdb_00001asq
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 : 2.32 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

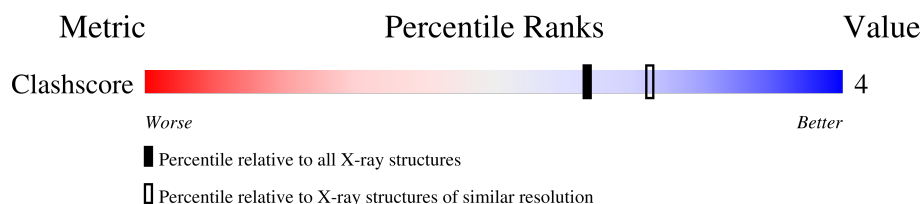
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	8383 (2.34-2.30)

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	 81% 16% .
1	B	552	 81% 17% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	AZI	A	559	-	X	-	-
5	AZI	A	560	-	X	-	-
5	AZI	B	559	-	X	-	-
5	AZI	B	560	-	X	-	-

2 Entry composition [i](#)

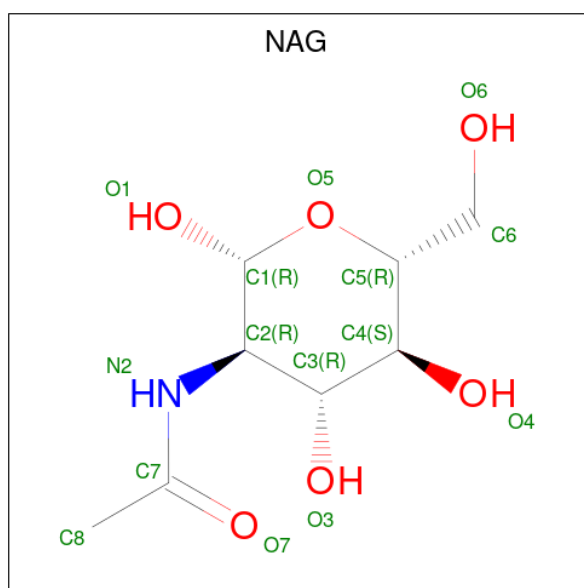
There are 6 unique types of molecules in this entry. The entry contains 9753 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: $C_8H_{15}NO_6$).

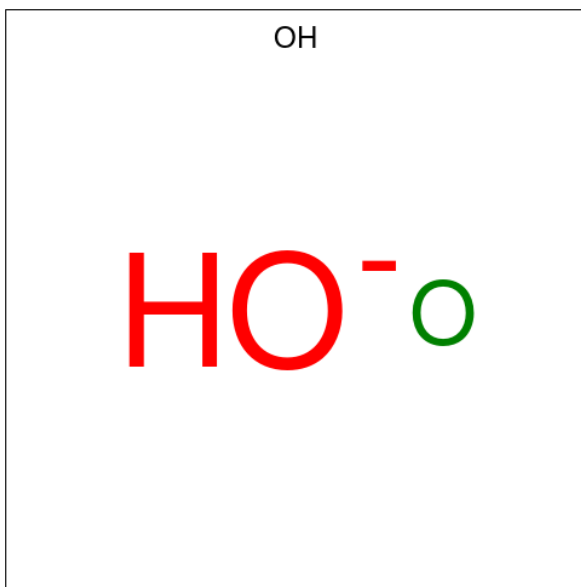


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

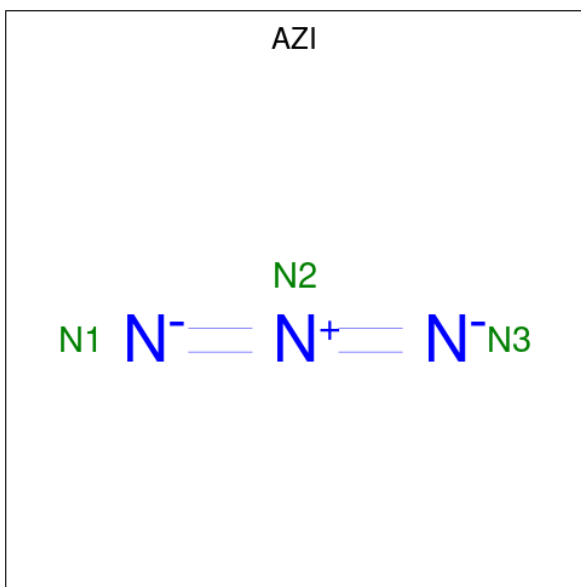
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Cu	0	0
			5	5		
3	B	4	Total	Cu	0	0
			4	4		

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



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

- Molecule 5 is AZIDE ION (CCD ID: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total N 3 3	0	0
5	A	1	Total N 3 3	0	0
5	B	1	Total N 3 3	0	0
5	B	1	Total N 3 3	0	0

- Molecule 6 is water.

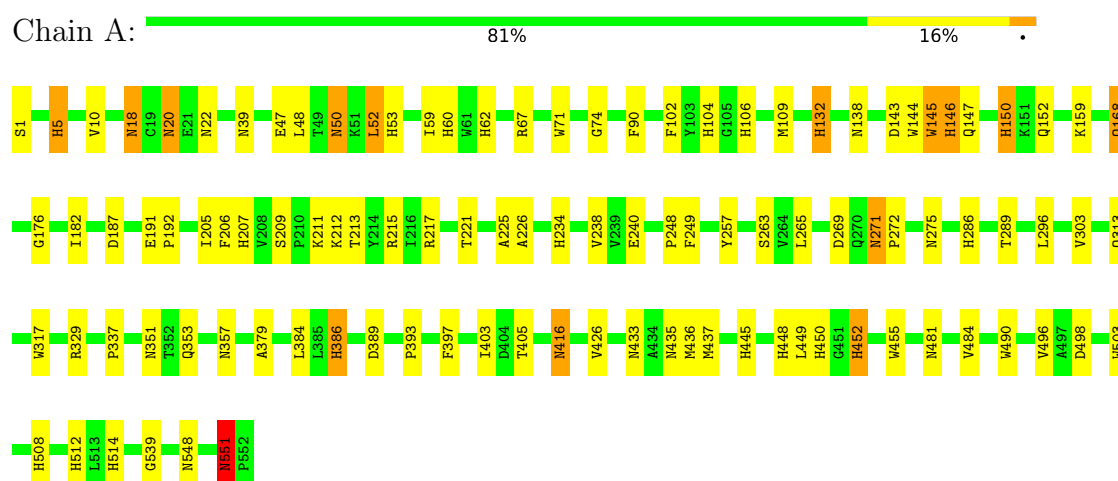
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	519	Total O 519 519	0	0
6	B	451	Total O 451 451	0	0

3 Residue-property plots

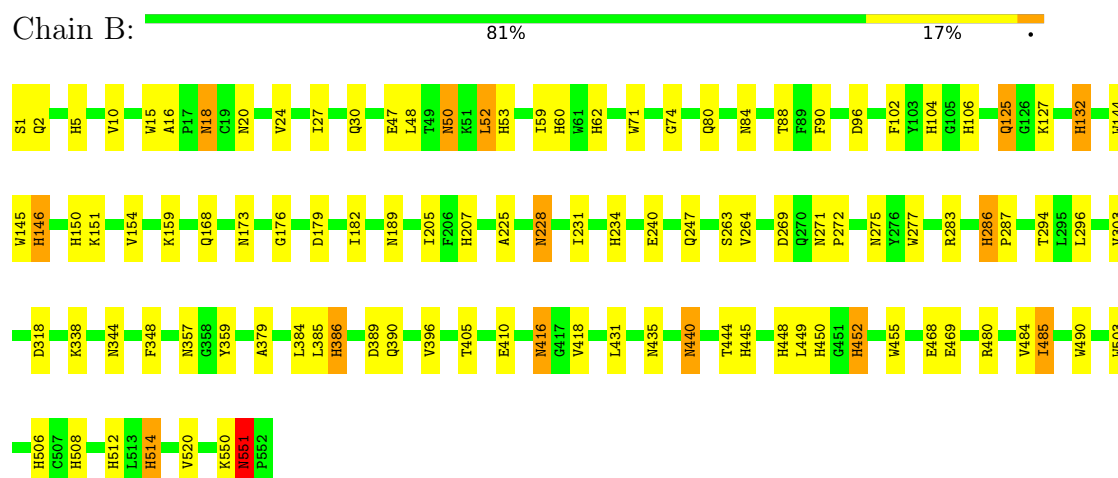
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	106.32Å 105.28Å 113.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.32	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.32)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9753	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, OH, NAG, 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	1.04	26/4508 (0.6%)	1.70	70/6159 (1.1%)
1	B	1.00	28/4508 (0.6%)	1.70	74/6159 (1.2%)
All	All	1.02	54/9016 (0.6%)	1.70	144/12318 (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 (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	HIS	CD2-NE2	-7.49	1.29	1.37
1	A	386	HIS	CD2-NE2	-7.10	1.30	1.37
1	A	53	HIS	CD2-NE2	-7.06	1.30	1.37
1	B	146	HIS	CD2-NE2	-6.98	1.30	1.37
1	A	207	HIS	CD2-NE2	-6.90	1.30	1.37
1	B	207	HIS	CE1-NE2	6.85	1.39	1.32
1	A	450	HIS	CG-ND1	-6.80	1.30	1.38
1	B	60	HIS	CD2-NE2	-6.76	1.30	1.37
1	A	146	HIS	CD2-NE2	-6.71	1.30	1.37
1	B	448	HIS	CD2-NE2	-6.64	1.30	1.37
1	B	386	HIS	CD2-NE2	-6.58	1.30	1.37
1	A	106	HIS	CD2-NE2	-6.55	1.30	1.37
1	A	234	HIS	CD2-NE2	-6.49	1.30	1.37
1	B	452	HIS	CD2-NE2	-6.48	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	452	HIS	CD2-NE2	-6.45	1.30	1.37
1	B	53	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	448	HIS	CD2-NE2	-6.42	1.30	1.37
1	B	512	HIS	CD2-NE2	-6.41	1.30	1.37
1	B	150	HIS	CD2-NE2	-6.38	1.30	1.37
1	A	5	HIS	CD2-NE2	-6.30	1.30	1.37
1	A	60	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	132	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	514	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	234	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	286	HIS	CG-ND1	-6.15	1.31	1.38
1	A	514	HIS	CD2-NE2	-6.12	1.31	1.37
1	B	450	HIS	CG-ND1	-6.09	1.31	1.38
1	B	5	HIS	CD2-NE2	-6.08	1.31	1.37
1	B	445	HIS	CD2-NE2	-6.04	1.31	1.37
1	A	445	HIS	CD2-NE2	-5.97	1.31	1.37
1	B	506	HIS	CD2-NE2	-5.77	1.31	1.37
1	A	512	HIS	CD2-NE2	-5.77	1.31	1.37
1	B	104	HIS	CD2-NE2	-5.72	1.31	1.37
1	B	512	HIS	CG-ND1	-5.71	1.31	1.38
1	A	104	HIS	CD2-NE2	-5.68	1.31	1.37
1	A	62	HIS	CD2-NE2	-5.65	1.31	1.37
1	B	450	HIS	CD2-NE2	-5.65	1.31	1.37
1	A	512	HIS	CG-ND1	-5.62	1.32	1.38
1	B	132	HIS	CD2-NE2	-5.52	1.31	1.37
1	B	207	HIS	CG-ND1	-5.52	1.32	1.38
1	A	514	HIS	CG-ND1	-5.47	1.32	1.38
1	B	508	HIS	CD2-NE2	-5.44	1.31	1.37
1	A	508	HIS	CD2-NE2	-5.38	1.31	1.37
1	B	286	HIS	CG-ND1	-5.37	1.32	1.38
1	B	15	TRP	CD1-NE1	-5.29	1.26	1.37
1	B	506	HIS	CG-ND1	-5.22	1.32	1.38
1	A	445	HIS	CG-ND1	-5.17	1.32	1.38
1	B	104	HIS	CG-ND1	-5.14	1.32	1.38
1	B	106	HIS	CD2-NE2	-5.12	1.32	1.37
1	A	182	ILE	CA-CB	5.11	1.60	1.54
1	A	403	ILE	CA-CB	5.06	1.60	1.54
1	B	62	HIS	CD2-NE2	-5.03	1.32	1.37
1	A	286	HIS	CD2-NE2	-5.03	1.32	1.37
1	B	5	HIS	CG-ND1	-5.01	1.32	1.38

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	551	ASN	CA-CB-CG	10.55	123.15	112.60
1	B	207	HIS	CB-CG-CD2	-9.76	118.52	131.20
1	A	18	ASN	OD1-CG-ND2	-9.46	113.14	122.60
1	B	357	ASN	OD1-CG-ND2	-9.06	113.54	122.60
1	B	18	ASN	OD1-CG-ND2	-9.00	113.60	122.60
1	B	416	ASN	OD1-CG-ND2	-8.93	113.67	122.60
1	B	84	ASN	OD1-CG-ND2	-8.92	113.68	122.60
1	B	50	ASN	OD1-CG-ND2	-8.84	113.76	122.60
1	B	189	ASN	OD1-CG-ND2	-8.36	114.24	122.60
1	B	228	ASN	OD1-CG-ND2	-7.58	115.02	122.60
1	B	125	GLN	OE1-CD-NE2	-7.56	115.04	122.60
1	A	435	ASN	OD1-CG-ND2	-7.40	115.20	122.60
1	B	357	ASN	CB-CG-ND2	7.34	127.41	116.40
1	A	71	TRP	CG-CD2-CE3	7.21	141.11	133.90
1	A	416	ASN	CA-CB-CG	7.14	119.74	112.60
1	B	275	ASN	OD1-CG-ND2	-7.14	115.46	122.60
1	A	452	HIS	CB-CG-CD2	-7.10	121.98	131.20
1	B	15	TRP	CG-CD2-CE3	7.06	140.96	133.90
1	B	514	HIS	CB-CG-ND1	7.05	133.27	122.70
1	B	225	ALA	N-CA-C	6.98	120.50	110.10
1	A	271	ASN	OD1-CG-ND2	-6.94	115.66	122.60
1	B	514	HIS	CB-CG-CD2	-6.93	122.19	131.20
1	B	469	GLU	N-CA-C	6.88	119.66	111.33
1	B	207	HIS	CB-CG-ND1	6.80	132.91	122.70
1	A	211	LYS	N-CA-CB	-6.71	101.94	112.08
1	A	1	SER	CA-CB-OG	-6.70	97.70	111.10
1	B	189	ASN	CB-CG-ND2	6.69	126.43	116.40
1	A	225	ALA	N-CA-C	6.68	120.16	110.28
1	A	433	ASN	OD1-CG-ND2	-6.60	116.00	122.60
1	B	445	HIS	ND1-CG-CD2	6.57	112.67	106.10
1	A	159	LYS	CB-CA-C	-6.55	101.35	110.13
1	A	249	PHE	CA-CB-CG	6.55	120.35	113.80
1	B	512	HIS	ND1-CG-CD2	6.54	112.64	106.10
1	A	187	ASP	CA-CB-CG	6.50	119.10	112.60
1	A	481	ASN	OD1-CG-ND2	-6.43	116.17	122.60
1	A	50	ASN	OD1-CG-ND2	-6.42	116.18	122.60
1	B	80	GLN	OE1-CD-NE2	-6.40	116.20	122.60
1	A	357	ASN	CA-CB-CG	-6.38	106.22	112.60
1	A	397	PHE	CA-C-N	6.38	126.14	119.76
1	A	397	PHE	C-N-CA	6.38	126.14	119.76
1	B	448	HIS	CB-CG-CD2	-6.36	122.94	131.20
1	B	247	GLN	OE1-CD-NE2	-6.34	116.26	122.60
1	B	294	THR	CA-CB-OG1	-6.34	100.09	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	B	484	VAL	CB-CA-C	-6.31	102.28	111.68
1	B	390	GLN	OE1-CD-NE2	-6.29	116.31	122.60
1	A	71	TRP	CB-CG-CD1	-6.27	117.49	126.90
1	A	22	ASN	O-C-N	-6.26	116.29	122.99
1	B	60	HIS	CB-CG-CD2	-6.22	123.11	131.20
1	B	50	ASN	CB-CG-ND2	6.21	125.72	116.40
1	B	435	ASN	OD1-CG-ND2	-6.14	116.46	122.60
1	A	386	HIS	CB-CG-CD2	-6.14	123.22	131.20
1	B	264	VAL	N-CA-CB	-6.13	101.39	111.44
1	B	20	ASN	N-CA-C	-6.12	98.44	108.41
1	B	96	ASP	N-CA-C	6.10	118.84	111.40
1	A	207	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	A	275	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	B	16	ALA	CA-C-N	6.08	125.80	119.05
1	B	16	ALA	C-N-CA	6.08	125.80	119.05
1	B	338	LYS	CA-C-N	6.06	124.08	119.66
1	B	338	LYS	C-N-CA	6.06	124.08	119.66
1	A	313	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	A	289	THR	CA-C-N	6.02	124.06	119.66
1	A	289	THR	C-N-CA	6.02	124.06	119.66
1	A	329	ARG	CA-CB-CG	5.97	126.04	114.10
1	A	405	THR	CB-CA-C	5.93	117.80	108.84
1	B	452	HIS	CB-CG-CD2	-5.85	123.60	131.20
1	A	211	LYS	CA-CB-CG	5.84	125.77	114.10
1	A	503	TRP	CG-CD2-CE3	5.82	139.72	133.90
1	B	144	TRP	CG-CD2-CE3	5.79	139.69	133.90
1	B	440	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	B	15	TRP	CE2-CD2-CG	-5.70	100.36	107.20
1	B	173	ASN	OD1-CG-ND2	-5.70	116.90	122.60
1	B	405	THR	CA-CB-OG1	-5.70	101.05	109.60
1	B	151	LYS	N-CA-C	-5.70	105.05	112.23
1	A	269	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	551	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	A	20	ASN	N-CA-C	-5.68	99.16	108.41
1	A	53	HIS	CB-CG-CD2	-5.68	123.82	131.20
1	A	20	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	B	318	ASP	CA-CB-CG	5.60	118.20	112.60
1	B	450	HIS	CG-CD2-NE2	-5.57	101.63	107.20
1	A	152	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	B	2	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	B	503	TRP	CG-CD2-CE3	5.54	139.44	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	HIS	ND1-CG-CD2	5.48	111.58	106.10
1	A	512	HIS	ND1-CG-CD2	5.48	111.58	106.10
1	A	39	ASN	CA-CB-CG	5.48	118.08	112.60
1	A	455	TRP	CG-CD2-CE3	5.47	139.38	133.90
1	B	179	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	39	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	A	416	ASN	OD1-CG-ND2	-5.45	117.16	122.60
1	A	448	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	A	393	PRO	CB-CA-C	5.42	117.54	110.92
1	A	271	ASN	CA-C-N	5.40	125.49	119.87
1	A	271	ASN	C-N-CA	5.40	125.49	119.87
1	A	143	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	234	HIS	CB-CG-CD2	-5.32	124.28	131.20
1	B	144	TRP	CB-CG-CD1	-5.32	118.92	126.90
1	B	24	VAL	N-CA-CB	-5.32	103.51	112.44
1	A	548	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	B	125	GLN	CG-CD-NE2	5.31	124.36	116.40
1	B	154	VAL	N-CA-C	-5.27	105.40	110.72
1	A	206	PHE	CA-CB-CG	5.25	119.05	113.80
1	B	144	TRP	CG-CD1-NE1	-5.25	103.38	110.20
1	A	145	TRP	CE2-CD2-CG	-5.25	100.91	107.20
1	B	277	TRP	CE2-CD2-CG	-5.23	100.93	107.20
1	A	168	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	A	539	GLY	CA-C-N	5.21	126.84	120.22
1	A	539	GLY	C-N-CA	5.21	126.84	120.22
1	A	52	LEU	N-CA-C	-5.21	102.77	110.48
1	A	296	LEU	N-CA-C	-5.20	98.83	107.99
1	B	71	TRP	CG-CD2-CE3	5.20	139.10	133.90
1	B	416	ASN	CB-CG-ND2	5.19	124.19	116.40
1	A	490	TRP	CE2-CD2-CG	-5.19	100.97	107.20
1	A	144	TRP	CG-CD1-NE1	-5.18	103.46	110.20
1	B	247	GLN	CA-C-N	5.18	125.18	119.90
1	B	247	GLN	C-N-CA	5.18	125.18	119.90
1	B	145	TRP	CE2-CD2-CG	-5.18	100.99	107.20
1	A	146	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	B	410	GLU	N-CA-C	5.16	116.59	111.07
1	B	182	ILE	N-CA-C	-5.15	106.06	113.07
1	B	52	LEU	N-CA-C	-5.15	103.59	110.55
1	B	15	TRP	CB-CG-CD1	-5.15	119.18	126.90
1	B	264	VAL	CB-CA-C	5.15	118.43	110.50
1	A	226	ALA	N-CA-C	-5.14	100.86	109.24
1	A	132	HIS	CB-CG-CD2	-5.14	124.52	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	HIS	CB-CG-CD2	-5.14	124.52	131.20
1	A	455	TRP	CE2-CD2-CG	-5.13	101.04	107.20
1	B	506	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	B	102	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	150	HIS	CB-CG-CD2	-5.12	124.55	131.20
1	B	269	ASP	CB-CA-C	-5.12	101.34	110.70
1	A	213	THR	CA-CB-OG1	-5.10	101.95	109.60
1	A	18	ASN	CB-CG-ND2	5.09	124.03	116.40
1	B	503	TRP	CE2-CD2-CG	-5.08	101.11	107.20
1	A	503	TRP	CB-CG-CD1	-5.07	119.29	126.90
1	B	485	ILE	N-CA-C	-5.06	101.08	108.17
1	A	176	GLY	O-C-N	-5.05	118.10	123.45
1	A	146	HIS	CB-CG-ND1	5.04	130.27	122.70
1	B	480	ARG	CA-CB-CG	-5.03	104.05	114.10
1	A	317	TRP	CE2-CD2-CG	-5.02	101.17	107.20
1	B	455	TRP	CE2-CD2-CG	-5.02	101.18	107.20
1	A	351	ASN	CB-CG-ND2	5.01	123.91	116.40

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 [i](#)

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	35	2
1	B	4366	0	4211	34	2
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	6	0	0	0	0
5	B	6	0	0	0	0
6	A	519	0	0	8	0
6	B	451	0	0	4	0
All	All	9753	0	8448	69	2

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 (69) 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	1.67	0.76
1:B:146:HIS:H	1:B:168:GLN:HE21	1.38	0.70
1:B:449:LEU:HD13	1:B:452:HIS:HB2	1.79	0.64
1:B:389:ASP:H	1:B:416:ASN:ND2	1.96	0.63
1:B:205:ILE:HD13	1:B:303:VAL:HG21	1.81	0.62
1:B:146:HIS:H	1:B:168:GLN:NE2	1.97	0.60
1:A:449:LEU:HD13	1:A:452:HIS:HB2	1.83	0.60
1:A:10:VAL:HG23	1:A:48:LEU:HD11	1.86	0.57
1:B:1:SER:N	1:B:125:GLN:OE1	2.38	0.56
1:A:132:HIS:HA	6:A:771:HOH:O	2.06	0.56
1:A:205:ILE:HG12	1:A:303:VAL:HG21	1.87	0.56
1:A:146:HIS:H	1:A:168:GLN:NE2	2.03	0.56
1:B:132:HIS:HA	6:B:789:HOH:O	2.07	0.54
1:A:138:ASN:HD22	1:A:217:ARG:HB2	1.72	0.53
1:A:145:TRP:HA	1:A:168:GLN:HE21	1.72	0.53
1:B:48:LEU:O	1:B:88:THR:HA	2.09	0.52
1:A:145:TRP:HA	1:A:168:GLN:NE2	2.25	0.52
1:A:436:MET:HA	6:A:882:HOH:O	2.10	0.51
1:B:146:HIS:N	1:B:168:GLN:HE21	2.08	0.50
1:B:468:GLU:HG2	1:B:490:TRP:CZ2	2.46	0.50
1:A:240:GLU:HB3	1:A:263:SER:HB2	1.93	0.49
1:B:27:ILE:O	1:B:30:GLN:HG2	2.12	0.49
1:A:389:ASP:H	1:A:416:ASN:ND2	2.12	0.48
1:B:127:LYS:HB3	1:B:127:LYS:HE2	1.71	0.47
1:A:379:ALA:HA	1:A:384:LEU:HD12	1.98	0.46
1:B:47:GLU:HB3	1:B:90:PHE:CE2	2.51	0.46
1:B:379:ALA:HA	1:B:384:LEU:HD12	1.98	0.45
1:B:514:HIS:CD2	6:B:829:HOH:O	2.68	0.45
1:B:440:ASN:HA	6:B:872:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PHE:CE2	1:A:221:THR:HG23	2.52	0.45
1:B:271:ASN:HA	1:B:272:PRO:HD3	1.73	0.45
1:B:286:HIS:HA	1:B:287:PRO:HD3	1.71	0.45
1:B:59:ILE:O	1:B:74:GLY:HA3	2.17	0.45
1:B:18:ASN:HA	1:B:176:GLY:O	2.17	0.44
1:A:215:ARG:HD2	1:A:263:SER:HB3	1.98	0.44
1:B:228:ASN:HB2	1:B:283:ARG:HG3	2.00	0.44
1:B:418:VAL:HG22	1:B:520:VAL:HB	1.98	0.44
1:A:109:MET:HE2	6:A:741:HOH:O	2.18	0.44
1:A:337:PRO:HA	6:A:1053:HOH:O	2.16	0.43
1:A:150:HIS:HD2	6:A:663:HOH:O	2.00	0.43
1:B:159:LYS:HB2	1:B:359:TYR:CE1	2.52	0.43
1:A:10:VAL:CG2	1:A:48:LEU:HD11	2.47	0.43
1:A:257:TYR:CD2	1:A:484:VAL:HG21	2.54	0.42
1:B:348:PHE:HD2	1:B:396:VAL:HG12	1.84	0.42
1:A:146:HIS:H	1:A:168:GLN:HE21	1.67	0.42
1:B:389:ASP:H	1:B:416:ASN:HD21	1.67	0.42
1:B:550:LYS:N	1:B:550:LYS:HD3	2.34	0.42
1:B:385:LEU:HD23	6:B:960:HOH:O	2.19	0.42
1:A:59:ILE:O	1:A:74:GLY:HA3	2.20	0.42
1:A:353:GLN:HE21	1:A:437:MET:H	1.68	0.42
1:B:231:ILE:HG21	1:B:296:LEU:HD22	2.01	0.42
1:B:444:THR:HA	1:B:485:ILE:O	2.20	0.42
1:A:67:ARG:HH22	1:A:498:ASP:CG	2.29	0.41
1:A:147:GLN:HA	6:A:924:HOH:O	2.19	0.41
1:A:238:VAL:O	1:A:248:PRO:HA	2.21	0.41
1:A:209:SER:HB2	1:A:212:LYS:HG3	2.02	0.41
1:A:191:GLU:HA	1:A:192:PRO:HD3	1.89	0.41
1:A:271:ASN:HA	1:A:272:PRO:HD3	1.77	0.41
1:A:426:VAL:HG22	1:A:496:VAL:HG22	2.03	0.41
1:A:5:HIS:HB2	6:A:785:HOH:O	2.21	0.41
1:A:150:HIS:CD2	6:A:663:HOH:O	2.74	0.41
1:A:50:ASN:ND2	1:A:52:LEU:H	2.18	0.41
1:A:215:ARG:HA	1:A:265:LEU:HD12	2.02	0.41
1:B:10:VAL:HG23	1:B:48:LEU:HD11	2.02	0.41
1:B:125:GLN:NE2	1:B:125:GLN:H	2.19	0.41
1:A:18:ASN:ND2	1:A:20:ASN:HB2	2.37	0.40
1:B:50:ASN:HD22	1:B:52:LEU:H	1.69	0.40
1:A:47:GLU:HB3	1:A:90:PHE:CE2	2.56	0.40
1:B:431:LEU:O	1:B:490:TRP:HA	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry 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]	2.11	0.09
1:A:386:HIS:NE2	1:B:551:ASN:O[2_654]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

Of 17 ligands modelled in this entry, 9 are monoatomic and 2 are modelled with single atom - leaving 6 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	553	1	14,14,15	1.26	1 (7%)	17,19,21	1.24	1 (5%)
5	AZI	A	560	3	2,2,2	2.31	2 (100%)	0,1,1	-	-
5	AZI	B	559	3	2,2,2	3.86	2 (100%)	0,1,1	-	-
5	AZI	B	560	3	2,2,2	2.30	2 (100%)	0,1,1	-	-
2	NAG	B	553	1	14,14,15	0.91	0	17,19,21	0.97	1 (5%)
5	AZI	A	559	3	2,2,2	3.96	2 (100%)	0,1,1	-	-

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	559	AZI	N3-N2	-4.30	1.14	1.23
5	B	559	AZI	N3-N2	-3.98	1.15	1.23
5	B	559	AZI	N1-N2	-3.74	1.15	1.23
5	A	559	AZI	N1-N2	-3.58	1.15	1.23
2	A	553	NAG	C1-C2	2.59	1.55	1.52
5	A	560	AZI	N1-N2	-2.38	1.18	1.23
5	B	560	AZI	N1-N2	-2.34	1.18	1.23
5	B	560	AZI	N3-N2	-2.25	1.18	1.23
5	A	560	AZI	N3-N2	-2.24	1.18	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	553	NAG	C4-C3-C2	-2.61	107.19	111.02
2	B	553	NAG	C1-O5-C5	2.31	115.29	112.19

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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.