WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 10, 2020 – 08:58 AM BST

PDB ID	:	1ASO
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	:	2.20 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 (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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.

Percentile relative to all X-ray structures

Percentile relative to X-ray structures of similar resolution
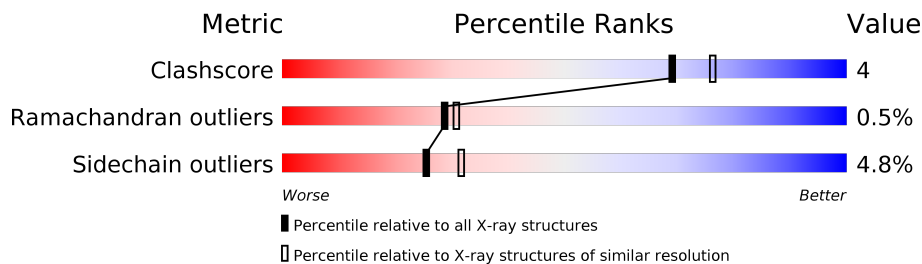
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 on 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 <=5%

Note EDS was not executed.

| Mol	Chain	Length	Quality of chain
1	A	552	84% 14% •
1	B	552	79% 18% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9740 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 4366	C 2803	N 746	O 801	S 16	0	0	0
1	B	552	Total 4366	C 2803	N 746	O 801	S 16	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
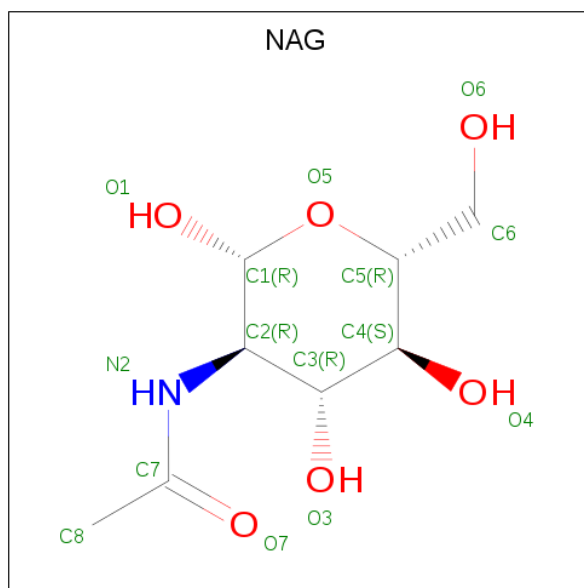
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 4 is HYDROXIDE ION (three-letter code: OH) (formula: HO).
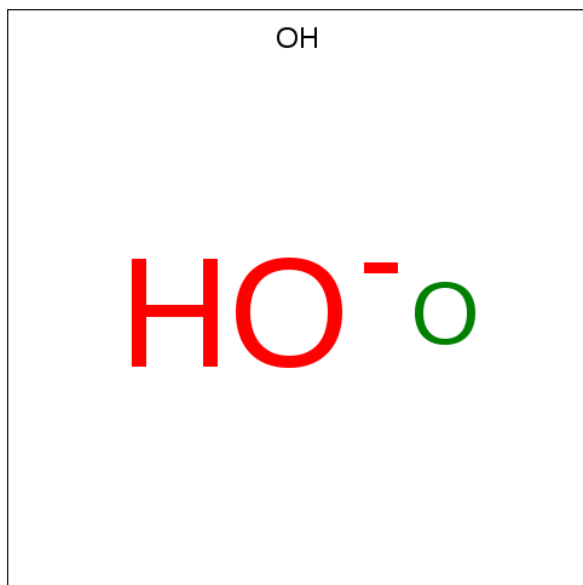
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	O 1	0	0
4	B	1	Total 1	O 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	514	Total 514	O 514	0	0
5	B	455	Total 455	O 455	0	0

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. 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
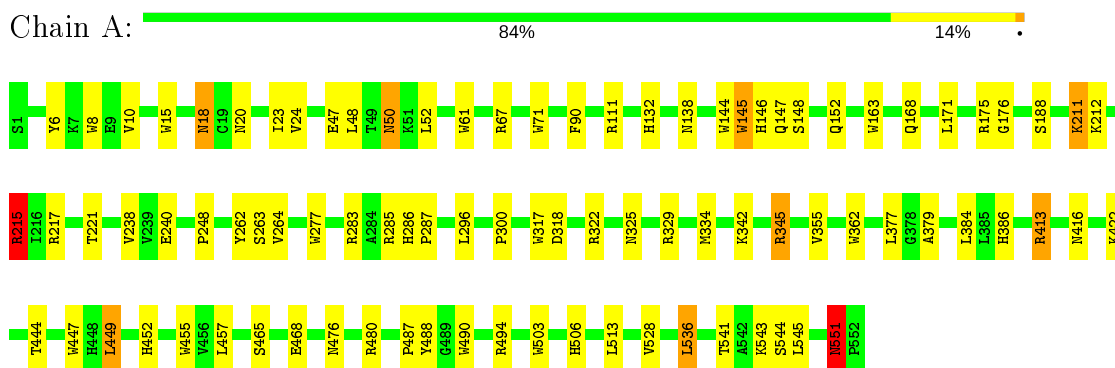
- Molecule 1: ASCORBATE OXIDASE
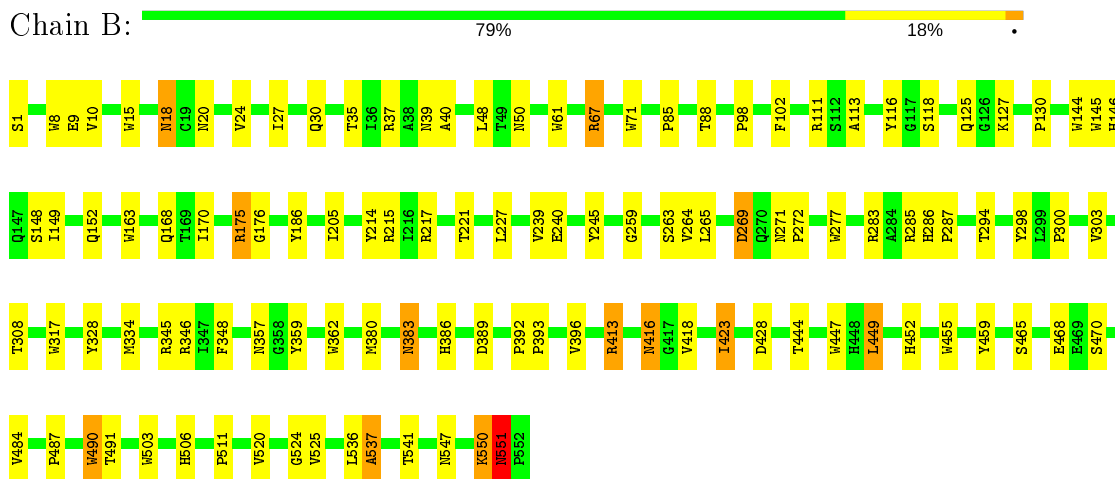
4 Data and refinement statistics (i)

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	106.09Å 105.21Å 112.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.196 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9740	wwPDB-VP
Average B, all atoms (Å²)	23.0	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: NAG, CU, 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	0.78	0/4508	1.49	77/6159 (1.3%)
1	B	0.76	0/4508	1.44	72/6159 (1.2%)
All	All	0.77	0/9016	1.46	149/12318 (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

There are no bond length outliers.

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	215	ARG	NE-CZ-NH1	12.81	126.70	120.30
1	A	283	ARG	NE-CZ-NH2	-10.46	115.07	120.30
1	A	494	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	A	494	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	A	345	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	A	413	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	B	144	TRP	CD1-CG-CD2	8.78	113.32	106.30
1	A	490	TRP	CD1-CG-CD2	8.74	113.29	106.30
1	A	455	TRP	CD1-CG-CD2	8.70	113.26	106.30
1	A	67	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	B	71	TRP	CD1-CG-CD2	8.55	113.14	106.30
1	A	317	TRP	CD1-CG-CD2	8.54	113.13	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	B	67	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	B	277	TRP	CD1-CG-CD2	8.46	113.07	106.30
1	A	345	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	A	144	TRP	CD1-CG-CD2	8.38	113.00	106.30
1	A	447	TRP	CD1-CG-CD2	8.33	112.97	106.30
1	A	163	TRP	CD1-CG-CD2	8.21	112.86	106.30
1	B	490	TRP	CD1-CG-CD2	8.18	112.84	106.30
1	A	145	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	A	144	TRP	CE2-CD2-CG	-8.14	100.79	107.30
1	B	163	TRP	CD1-CG-CD2	8.13	112.80	106.30
1	B	503	TRP	CE2-CD2-CG	-7.92	100.97	107.30
1	B	144	TRP	CE2-CD2-CG	-7.89	100.98	107.30
1	A	455	TRP	CE2-CD2-CG	-7.88	101.00	107.30
1	B	15	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	A	503	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	B	455	TRP	CD1-CG-CD2	7.74	112.50	106.30
1	B	71	TRP	CE2-CD2-CG	-7.72	101.13	107.30
1	A	71	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	B	503	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	B	245	TYR	CB-CG-CD2	-7.66	116.41	121.00
1	B	61	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	B	215	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	B	8	TRP	CD1-CG-CD2	7.56	112.35	106.30
1	B	163	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	B	15	TRP	CE2-CD2-CG	-7.52	101.28	107.30
1	A	362	TRP	CD1-CG-CD2	7.48	112.28	106.30
1	B	186	TYR	CB-CG-CD2	-7.47	116.52	121.00
1	A	145	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	A	71	TRP	CD1-CG-CD2	7.40	112.22	106.30
1	B	145	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	A	144	TRP	CG-CD2-CE3	7.40	140.56	133.90
1	A	15	TRP	CD1-CG-CD2	7.39	112.21	106.30
1	B	362	TRP	CE2-CD2-CG	-7.38	101.39	107.30
1	B	277	TRP	CE2-CD2-CG	-7.37	101.41	107.30
1	A	283	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	490	TRP	CE2-CD2-CG	-7.29	101.47	107.30
1	A	71	TRP	CG-CD2-CE3	7.28	140.45	133.90
1	A	322	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	285	ARG	NE-CZ-NH2	-7.27	116.66	120.30
1	B	145	TRP	CD1-CG-CD2	7.26	112.11	106.30
1	A	163	TRP	CE2-CD2-CG	-7.25	101.50	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	MET	CA-CB-CG	7.20	125.54	113.30
1	A	447	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	B	447	TRP	CD1-CG-CD2	7.10	111.98	106.30
1	B	8	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	A	175	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	490	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	B	298	TYR	CB-CG-CD2	-6.95	116.83	121.00
1	A	503	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	B	455	TRP	CE2-CD2-CG	-6.92	101.76	107.30
1	A	488	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	A	8	TRP	CE2-CD2-CG	-6.91	101.77	107.30
1	A	15	TRP	CE2-CD2-CG	-6.89	101.78	107.30
1	A	317	TRP	CE2-CD2-CG	-6.86	101.81	107.30
1	A	61	TRP	CD1-CG-CD2	6.84	111.77	106.30
1	B	317	TRP	CE2-CD2-CG	-6.83	101.83	107.30
1	A	362	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	B	61	TRP	CE2-CD2-CG	-6.76	101.89	107.30
1	B	362	TRP	CD1-CG-CD2	6.76	111.71	106.30
1	A	285	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	277	TRP	CD1-CG-CD2	6.67	111.64	106.30
1	A	61	TRP	CE2-CD2-CG	-6.63	101.99	107.30
1	A	8	TRP	CD1-CG-CD2	6.59	111.57	106.30
1	A	277	TRP	CE2-CD2-CG	-6.54	102.06	107.30
1	A	71	TRP	CB-CG-CD1	-6.50	118.55	127.00
1	B	447	TRP	CE2-CD2-CG	-6.50	102.10	107.30
1	B	175	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	317	TRP	CD1-CG-CD2	6.31	111.34	106.30
1	B	346	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	283	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	A	503	TRP	CG-CD2-CE3	6.13	139.42	133.90
1	B	37	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	322	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	6	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	B	362	TRP	CG-CD2-CE3	5.94	139.25	133.90
1	B	116	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	B	71	TRP	CG-CD2-CE3	5.92	139.23	133.90
1	A	329	ARG	CA-CB-CG	5.86	126.29	113.40
1	A	145	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	B	328	TYR	CB-CG-CD2	-5.85	117.49	121.00
1	A	536	LEU	CA-CB-CG	5.84	128.74	115.30
1	A	317	TRP	CG-CD1-NE1	-5.79	104.31	110.10
1	B	503	TRP	CG-CD2-CE3	5.79	139.11	133.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	LYS	CA-CB-CG	5.77	126.09	113.40
1	A	455	TRP	CG-CD1-NE1	-5.77	104.33	110.10
1	B	71	TRP	CG-CD1-NE1	-5.76	104.34	110.10
1	B	413	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	B	71	TRP	CB-CG-CD1	-5.74	119.54	127.00
1	A	67	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	144	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	A	163	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	A	413	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	215	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	480	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	455	TRP	CG-CD2-CE3	5.59	138.93	133.90
1	A	455	TRP	CB-CG-CD1	-5.58	119.75	127.00
1	A	503	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	A	490	TRP	CG-CD1-NE1	-5.54	104.56	110.10
1	B	345	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	B	217	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	447	TRP	CG-CD1-NE1	-5.49	104.61	110.10
1	B	144	TRP	CG-CD1-NE1	-5.49	104.61	110.10
1	A	447	TRP	CG-CD2-CE3	5.48	138.83	133.90
1	B	145	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	B	490	TRP	CG-CD1-NE1	-5.41	104.69	110.10
1	B	163	TRP	CG-CD1-NE1	-5.39	104.71	110.10
1	B	111	ARG	CA-CB-CG	5.38	125.25	113.40
1	B	215	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	163	TRP	CB-CG-CD1	-5.36	120.03	127.00
1	A	329	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	503	TRP	CB-CG-CD1	-5.33	120.08	127.00
1	B	144	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	A	163	TRP	CB-CG-CD1	-5.29	120.12	127.00
1	B	359	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	A	111	ARG	CA-CB-CG	5.28	125.01	113.40
1	B	269	ASP	CB-CA-C	-5.27	99.86	110.40
1	B	20	ASN	N-CA-C	-5.26	96.79	111.00
1	B	285	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	15	TRP	CG-CD1-NE1	-5.25	104.84	110.10
1	A	144	TRP	CB-CG-CD1	-5.25	120.18	127.00
1	A	490	TRP	CB-CG-CD1	-5.23	120.20	127.00
1	B	503	TRP	CB-CG-CD1	-5.23	120.20	127.00
1	B	163	TRP	CG-CD2-CE3	5.22	138.60	133.90
1	B	455	TRP	CG-CD1-NE1	-5.21	104.89	110.10
1	B	413	ARG	NE-CZ-NH2	-5.20	117.70	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	B	67	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	8	TRP	CG-CD2-CE3	5.17	138.55	133.90
1	A	296	LEU	N-CA-C	-5.16	97.07	111.00
1	B	145	TRP	CG-CD2-CE3	5.08	138.47	133.90
1	B	144	TRP	CB-CG-CD1	-5.07	120.41	127.00
1	A	318	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	355	VAL	CG1-CB-CG2	-5.05	102.82	110.90
1	B	294	THR	CA-CB-CG2	5.04	119.45	112.40
1	A	262	TYR	CB-CG-CD1	-5.04	117.98	121.00
1	B	317	TRP	CG-CD2-CE3	5.02	138.42	133.90

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	24	7
1	B	4366	0	4211	39	10
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	514	0	0	3	3
5	B	455	0	0	2	4
All	All	9740	0	8448	63	14

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 (63) 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	1.71	0.70
1:A:23:ILE:HD11	5:A:788:HOH:O	1.97	0.64
1:A:10:VAL:HG23	1:A:48:LEU:HD11	1.79	0.64
1:A:138:ASN:HD22	1:A:217:ARG:HB2	1.65	0.61
1:A:146:HIS:H	1:A:168:GLN:NE2	2.00	0.59
1:B:449:LEU:HD13	1:B:452:HIS:HB2	1.87	0.56
1:B:146:HIS:H	1:B:168:GLN:NE2	2.04	0.56
1:B:146:HIS:H	1:B:168:GLN:HE21	1.53	0.54
1:B:205:ILE:HD13	1:B:303:VAL:HG21	1.88	0.54
1:B:389:ASP:H	1:B:416:ASN:ND2	2.06	0.53
1:B:40:ALA:HB2	1:B:98:PRO:HD3	1.92	0.51
1:A:444:THR:HG22	1:A:487:PRO:HD3	1.93	0.51
1:A:18:ASN:ND2	1:A:20:ASN:HB2	2.27	0.49
1:B:444:THR:HG22	1:B:487:PRO:HD3	1.94	0.49
1:B:1:SER:N	1:B:125:GLN:OE1	2.42	0.49
1:B:146:HIS:N	1:B:168:GLN:HE21	2.10	0.48
1:A:506:HIS:HB2	1:A:513:LEU:HD13	1.96	0.48
1:B:468:GLU:HG2	1:B:490:TRP:CZ2	2.48	0.48
1:B:113:ALA:HB2	1:B:149:ILE:HG13	1.96	0.47
1:A:10:VAL:CG2	1:A:48:LEU:HD11	2.43	0.47
1:A:132:HIS:HA	5:A:769:HOH:O	2.14	0.47
1:A:379:ALA:HA	1:A:384:LEU:HD12	1.96	0.47
1:A:50:ASN:ND2	1:A:52:LEU:H	2.12	0.47
1:B:348:PHE:HD2	1:B:396:VAL:HG12	1.79	0.46
1:A:240:GLU:HB3	1:A:263:SER:HB2	1.98	0.46
1:A:145:TRP:HA	1:A:168:GLN:HE21	1.80	0.46
1:B:286:HIS:HA	1:B:287:PRO:HD3	1.81	0.45
1:A:146:HIS:H	1:A:168:GLN:HE21	1.65	0.45
1:B:239:VAL:HG21	1:B:265:LEU:HD13	1.99	0.45
1:B:271:ASN:HA	1:B:272:PRO:HD3	1.77	0.44
1:B:380:MET:HB3	1:B:525:VAL:HG11	1.98	0.44
1:B:148:SER:O	1:B:152:GLN:HG3	2.18	0.44
1:A:215:ARG:HD2	1:A:263:SER:HB3	1.99	0.43
1:B:550:LYS:N	1:B:550:LYS:HD3	2.33	0.43
1:A:449:LEU:HD13	1:A:452:HIS:HB2	2.00	0.43
1:A:465:SER:H	1:A:468:GLU:HG3	1.83	0.43
1:B:18:ASN:HA	1:B:176:GLY:O	2.19	0.43
1:B:465:SER:O	1:B:468:GLU:HB2	2.19	0.43
1:B:423:ILE:HD13	1:B:524:GLY:HA3	2.00	0.43
1:B:170:ILE:HD12	1:B:227:LEU:HD21	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:PHE:HZ	1:B:259:GLY:HA2	1.83	0.43
1:B:27:ILE:O	1:B:30:GLN:HG2	2.20	0.42
1:B:127:LYS:HB3	1:B:127:LYS:HE2	1.78	0.42
1:B:39:ASN:HB2	1:B:125:GLN:HE21	1.84	0.42
1:B:205:ILE:HD13	1:B:303:VAL:CG2	2.50	0.41
1:B:511:PRO:HD3	5:B:759:HOH:O	2.19	0.41
1:A:334:MET:N	5:A:697:HOH:O	2.54	0.41
1:B:48:LEU:O	1:B:88:THR:HA	2.20	0.41
1:B:10:VAL:HG23	1:B:48:LEU:HD11	2.02	0.41
1:A:238:VAL:O	1:A:248:PRO:HA	2.20	0.41
1:A:377:LEU:HD11	1:A:528:VAL:HG11	2.03	0.41
1:B:392:PRO:HA	1:B:393:PRO:HD2	2.00	0.41
1:B:506:HIS:HB3	5:B:725:HOH:O	2.19	0.41
1:A:147:GLN:HE21	1:A:152:GLN:HG2	1.86	0.41
1:A:47:GLU:HB3	1:A:90:PHE:CE2	2.56	0.41
1:B:418:VAL:HG22	1:B:520:VAL:HB	2.01	0.41
1:A:18:ASN:HA	1:A:176:GLY:O	2.21	0.40
1:B:214:TYR:O	1:B:265:LEU:HA	2.21	0.40
1:B:389:ASP:H	1:B:416:ASN:HD22	1.69	0.40
1:B:348:PHE:CD2	1:B:396:VAL:HG12	2.56	0.40
1:B:459:TYR:HD2	1:B:491:THR:HG1	1.67	0.40
1:A:286:HIS:HA	1:A:287:PRO:HD3	1.92	0.40
1:B:35:THR:HG23	1:B:118:SER:HB2	2.03	0.40

All (14) 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]	1.77	0.43
1:B:383:ASN:O	5:A:946:HOH:O[2_656]	1.82	0.38
5:B:1004:HOH:O	5:B:1004:HOH:O[2_655]	1.91	0.29
1:A:386:HIS:NE2	1:B:551:ASN:O[2_654]	1.92	0.28
1:A:386:HIS:NE2	1:B:551:ASN:OD1[2_654]	1.99	0.21
1:A:544:SER:O	1:B:547:ASN:ND2[2_654]	2.06	0.14
1:A:386:HIS:CE1	1:B:551:ASN:OD1[2_654]	2.07	0.13
1:A:551:ASN:OD1	1:B:386:HIS:CE1[2_654]	2.08	0.12
5:A:801:HOH:O	5:A:958:HOH:O[2_655]	2.09	0.11
1:B:85:PRO:O	5:B:648:HOH:O[2_655]	2.09	0.11
1:B:537:ALA:O	5:B:982:HOH:O[2_655]	2.12	0.08
5:B:767:HOH:O	5:B:778:HOH:O[2_655]	2.17	0.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:563:HOH:O	5:A:563:HOH:O[2_655]	2.19	0.01
1:A:544:SER:O	1:B:547:ASN:OD1[2_654]	2.19	0.01

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%)	538 (98%)	10 (2%)	2 (0%)	34	37
1	B	550/552 (100%)	529 (96%)	17 (3%)	4 (1%)	22	22
All	All	1100/1104 (100%)	1067 (97%)	27 (2%)	6 (0%)	29	31

All (6) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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%)	451 (95%)	24 (5%)	24	29

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	475/475 (100%)	453 (95%)	22 (5%)	27	34
All	All	950/950 (100%)	904 (95%)	46 (5%)	25	32

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	24	VAL
1	A	50	ASN
1	A	148	SER
1	A	171	LEU
1	A	188	SER
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	345	ARG
1	A	413	ARG
1	A	416	ASN
1	A	422	LYS
1	A	449	LEU
1	A	457	LEU
1	A	536	LEU
1	A	541	THR
1	A	543	LYS
1	A	545	LEU
1	B	9	GLU
1	B	18	ASN
1	B	24	VAL
1	B	50	ASN
1	B	67	ARG
1	B	175	ARG
1	B	221	THR
1	B	264	VAL
1	B	269	ASP
1	B	300	PRO
1	B	308	THR
1	B	357	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	383	ASN
1	B	413	ARG
1	B	416	ASN
1	B	428	ASP
1	B	449	LEU
1	B	470	SER
1	B	484	VAL
1	B	536	LEU
1	B	541	THR
1	B	550	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	39	ASN
1	A	50	ASN
1	A	138	ASN
1	A	147	GLN
1	A	168	GLN
1	A	189	ASN
1	A	353	GLN
1	A	416	ASN
1	A	420	GLN
1	A	476	ASN
1	B	2	GLN
1	B	18	ASN
1	B	138	ASN
1	B	147	GLN
1	B	150	HIS
1	B	168	GLN
1	B	416	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 2 are modelled with single atom and 9 are monoatomic - leaving 2 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	B	553	1	14,14,15	0.64	0	17,19,21	0.89	1 (5%)
2	NAG	A	553	1	14,14,15	0.68	0	17,19,21	1.07	2 (11%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	553	NAG	C1-O5-C5	2.42	115.47	112.19
2	A	553	NAG	O5-C5-C6	2.40	110.97	107.20
2	B	553	NAG	C4-C3-C2	-2.13	107.89	111.02

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.