



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:25 PM GMT

PDB ID : 1AOZ
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.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

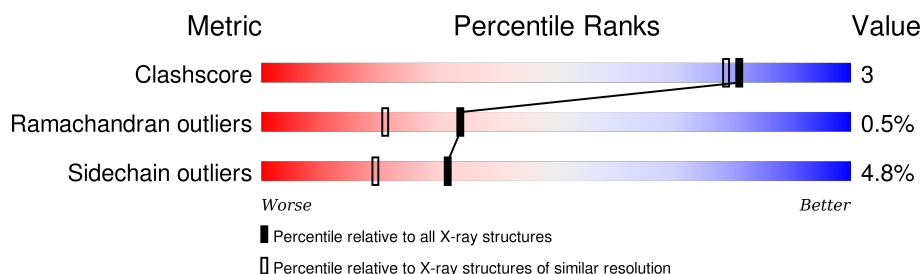
1 Overall quality at a glance

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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	552	
1	B	552	

2 Entry composition [i](#)

There are 6 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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

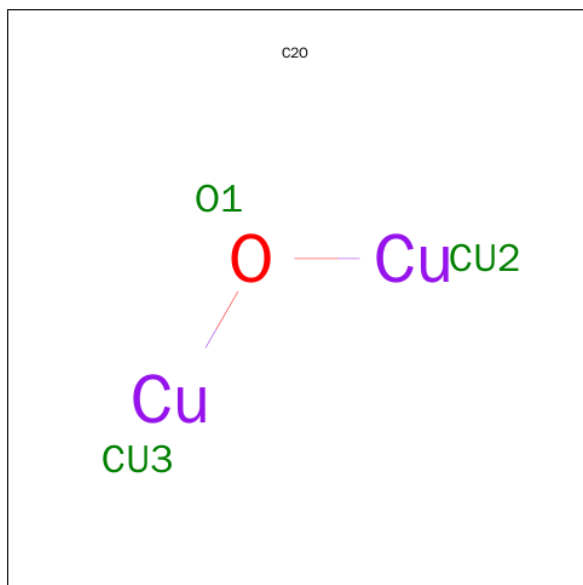


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

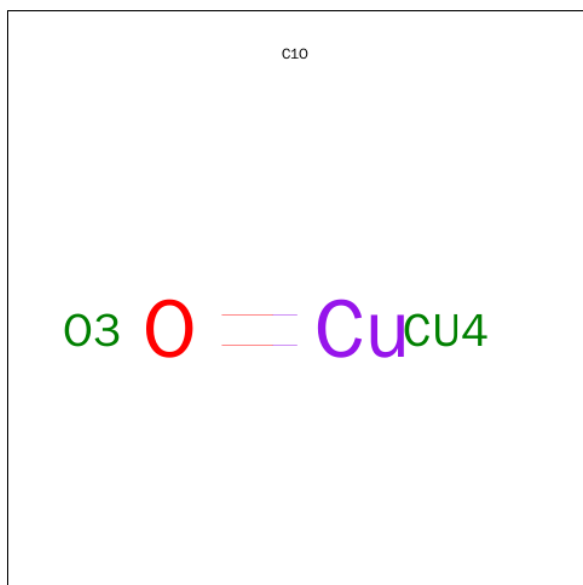
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cu	0	0
			1	1		
3	A	2	Total	Cu	0	0
			2	2		

- Molecule 4 is CU-O-CU LINKAGE (three-letter code: C2O) (formula: Cu_2O).



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

- Molecule 5 is CU-O LINKAGE (three-letter code: C1O) (formula: CuO).



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

- Molecule 6 is water.

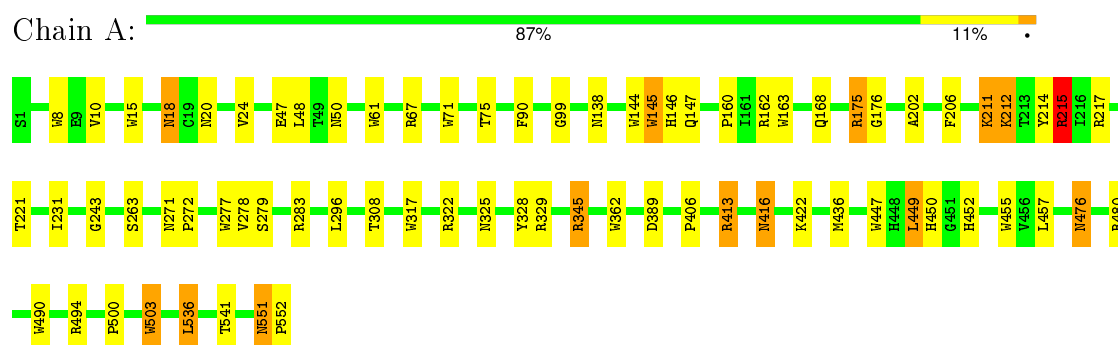
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	513	Total	O	0	0
			513	513		
6	B	457	Total	O	0	0
			457	457		

3 Residue-property plots

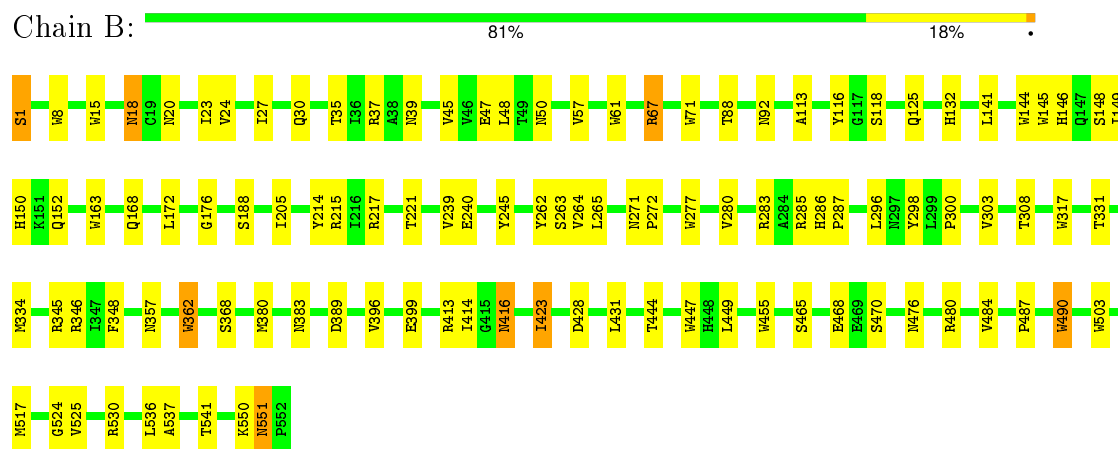
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

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 will therefore be 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: C1O, NAG, CU, C2O

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	1.46	67/6159 (1.1%)
1	B	0.76	0/4508	1.43	68/6159 (1.1%)
All	All	0.77	0/9016	1.45	135/12318 (1.1%)

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 (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	TRP	CD1-CG-CD2	10.36	114.59	106.30
1	A	215	ARG	NE-CZ-NH1	9.97	125.29	120.30
1	B	144	TRP	CE2-CD2-CG	-9.73	99.51	107.30
1	B	490	TRP	CD1-CG-CD2	9.29	113.73	106.30
1	B	277	TRP	CD1-CG-CD2	8.77	113.32	106.30
1	B	8	TRP	CD1-CG-CD2	8.73	113.28	106.30
1	A	455	TRP	CD1-CG-CD2	8.62	113.20	106.30
1	B	277	TRP	CE2-CD2-CG	-8.61	100.41	107.30
1	A	317	TRP	CD1-CG-CD2	8.50	113.10	106.30
1	B	490	TRP	CE2-CD2-CG	-8.42	100.56	107.30
1	A	163	TRP	CD1-CG-CD2	8.36	112.99	106.30
1	B	61	TRP	CD1-CG-CD2	8.20	112.86	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ARG	NE-CZ-NH2	-8.17	116.21	120.30
1	B	245	TYR	CB-CG-CD2	-8.17	116.10	121.00
1	A	145	TRP	CD1-CG-CD2	8.11	112.79	106.30
1	B	455	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	A	490	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	A	413	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	A	362	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	B	8	TRP	CE2-CD2-CG	-7.93	100.96	107.30
1	B	503	TRP	CD1-CG-CD2	7.88	112.61	106.30
1	B	334	MET	CA-CB-CG	7.88	126.70	113.30
1	B	145	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	A	494	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	B	503	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	B	144	TRP	CG-CD2-CE3	7.74	140.86	133.90
1	A	447	TRP	CD1-CG-CD2	7.73	112.49	106.30
1	B	61	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	A	71	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	B	447	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	B	71	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	B	67	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	A	71	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	B	317	TRP	CD1-CG-CD2	7.57	112.36	106.30
1	A	277	TRP	CD1-CG-CD2	7.57	112.36	106.30
1	A	277	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	A	163	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	A	8	TRP	CD1-CG-CD2	7.46	112.27	106.30
1	B	145	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	B	362	TRP	CD1-CG-CD2	7.41	112.23	106.30
1	A	15	TRP	CD1-CG-CD2	7.36	112.19	106.30
1	B	317	TRP	CE2-CD2-CG	-7.33	101.43	107.30
1	A	144	TRP	CD1-CG-CD2	7.33	112.16	106.30
1	A	317	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	A	145	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	A	162	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	B	455	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	B	71	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	B	15	TRP	CD1-CG-CD2	7.23	112.08	106.30
1	B	15	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	A	455	TRP	CE2-CD2-CG	-7.18	101.55	107.30
1	A	163	TRP	CB-CG-CD1	-7.15	117.71	127.00
1	A	144	TRP	CE2-CD2-CG	-7.12	101.61	107.30
1	A	447	TRP	CE2-CD2-CG	-7.08	101.63	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	8	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	A	503	TRP	CD1-CG-CD2	7.02	111.92	106.30
1	A	490	TRP	CE2-CD2-CG	-6.98	101.72	107.30
1	B	362	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	B	447	TRP	CE2-CD2-CG	-6.93	101.76	107.30
1	A	15	TRP	CE2-CD2-CG	-6.89	101.78	107.30
1	B	298	TYR	CB-CG-CD2	-6.89	116.87	121.00
1	B	283	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	503	TRP	CE2-CD2-CG	-6.87	101.80	107.30
1	A	71	TRP	CG-CD2-CE3	6.87	140.09	133.90
1	B	163	TRP	CD1-CG-CD2	6.84	111.77	106.30
1	A	362	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	A	61	TRP	CD1-CG-CD2	6.77	111.71	106.30
1	B	144	TRP	CG-CD1-NE1	-6.72	103.38	110.10
1	A	328	TYR	CB-CG-CD2	-6.69	116.99	121.00
1	A	163	TRP	CG-CD1-NE1	-6.65	103.45	110.10
1	A	71	TRP	CB-CG-CD1	-6.64	118.37	127.00
1	A	67	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	494	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	B	163	TRP	CE2-CD2-CG	-6.50	102.10	107.30
1	B	144	TRP	CB-CG-CD1	-6.49	118.56	127.00
1	A	61	TRP	CE2-CD2-CG	-6.46	102.13	107.30
1	A	175	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	283	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	277	TRP	CG-CD2-CE3	6.25	139.53	133.90
1	B	285	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	455	TRP	CB-CG-CD1	-6.06	119.12	127.00
1	B	277	TRP	CB-CG-CD1	-6.05	119.14	127.00
1	A	211	LYS	CA-CB-CG	6.03	126.66	113.40
1	B	262	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	B	345	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	163	TRP	CG-CD2-CE3	5.97	139.27	133.90
1	B	163	TRP	CB-CG-CD1	-5.96	119.25	127.00
1	A	503	TRP	CG-CD2-CE3	5.91	139.21	133.90
1	A	503	TRP	CB-CG-CD1	-5.86	119.39	127.00
1	A	536	LEU	CA-CB-CG	5.79	128.61	115.30
1	A	480	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	345	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	455	TRP	CG-CD1-NE1	-5.73	104.37	110.10
1	A	455	TRP	CG-CD2-CE3	5.66	138.99	133.90
1	A	317	TRP	CG-CD1-NE1	-5.64	104.46	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	TRP	CB-CG-CD1	-5.64	119.66	127.00
1	B	285	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	145	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	B	116	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	B	490	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	A	296	LEU	N-CA-C	-5.55	96.00	111.00
1	B	283	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	B	67	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	B	8	TRP	CG-CD1-NE1	-5.51	104.59	110.10
1	A	447	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	B	480	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	322	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	413	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	345	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	217	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	490	TRP	CG-CD1-NE1	-5.27	104.83	110.10
1	B	8	TRP	CG-CD2-CE3	5.27	138.64	133.90
1	B	61	TRP	CB-CG-CD1	-5.24	120.18	127.00
1	A	329	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	145	TRP	CB-CG-CD1	-5.22	120.22	127.00
1	B	215	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	490	TRP	CG-CD2-CE3	5.21	138.59	133.90
1	A	206	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	B	447	TRP	CG-CD1-NE1	-5.20	104.90	110.10
1	A	277	TRP	CB-CG-CD1	-5.20	120.24	127.00
1	B	296	LEU	N-CA-C	-5.20	96.96	111.00
1	A	447	TRP	CG-CD1-NE1	-5.19	104.91	110.10
1	B	317	TRP	CG-CD2-CE3	5.16	138.54	133.90
1	B	20	ASN	N-CA-C	-5.15	97.10	111.00
1	A	362	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	B	346	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	37	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	47	GLU	CA-CB-CG	5.09	124.60	113.40
1	B	530	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	175	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	B	71	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	B	145	TRP	CG-CD1-NE1	-5.01	105.09	110.10
1	B	172	LEU	CA-CB-CG	5.01	126.82	115.30
1	B	455	TRP	CG-CD1-NE1	-5.01	105.09	110.10

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	23	0
1	B	4366	0	4211	33	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	513	0	0	4	0
6	B	457	0	0	4	0
All	All	9743	0	8448	56	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 (56) 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	6: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	6:A:1307:HOH:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	6: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:B:150:HIS:HD2	6:B:832:HOH:O	1.97	0.47
1:A:99:GLY:HA3	1:A:243:GLY:HA2	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:B:362:TRP:HB3	1:B:517:MET:HB2	1.99	0.45
1:A:47:GLU:HB3	1:A:90:PHE:CE1	2.52	0.45
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
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	6: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	6: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:B:205:ILE:HD13	1:B:303:VAL:CG2	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:TRP:HA	6:A:988:HOH:O	2.20	0.41
1:B:150:HIS:CG	6:B:946:HOH:O	2.74	0.40
1:B:431:LEU:O	1:B:490:TRP:HA	2.21	0.40
1:B:368:SER:HB3	1:B:414:ILE:HG12	2.02	0.40
1:B:18:ASN:HA	1:B:176:GLY:O	2.22	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%)	39	27
1	B	550/552 (100%)	527 (96%)	19 (4%)	4 (1%)	26	14
All	All	1100/1104 (100%)	1061 (96%)	33 (3%)	6 (0%)	34	21

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 [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%)	453 (95%)	22 (5%)	33	21
1	B	475/475 (100%)	451 (95%)	24 (5%)	29	17
All	All	950/950 (100%)	904 (95%)	46 (5%)	31	19

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	211	LYS
1	A	212	LYS
1	A	215	ARG
1	A	221	THR
1	A	279	SER
1	A	308	THR
1	A	325	ASN
1	A	345	ARG
1	A	406	PRO
1	A	413	ARG
1	A	416	ASN
1	A	422	LYS
1	A	449	LEU
1	A	457	LEU
1	A	476	ASN
1	A	500	PRO
1	A	536	LEU
1	A	541	THR
1	A	552	PRO
1	B	1	SER
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	221	THR
1	B	264	VAL
1	B	300	PRO
1	B	308	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	331	THR
1	B	357	ASN
1	B	383	ASN
1	B	399	GLU
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 (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	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	B	2	GLN
1	B	18	ASN
1	B	39	ASN
1	B	50	ASN
1	B	138	ASN
1	B	147	GLN
1	B	168	GLN
1	B	189	ASN
1	B	390	GLN
1	B	416	ASN
1	B	440	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 3 are monoatomic - 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	601	1	14,14,15	1.03	1 (7%)	15,19,21	0.50	0
4	C2O	A	702	1	0,2,2	0.00	-	0,1,1	0.00	-
5	C1O	A	703	1	0,1,1	0.00	-	0,0,0	0.00	-
2	NAG	B	601	1	14,14,15	0.67	0	15,19,21	0.60	0
4	C2O	B	702	1	0,2,2	0.00	-	0,1,1	0.00	-
5	C1O	B	703	1	0,1,1	0.00	-	0,0,0	0.00	-

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
4	C2O	A	702	1	-	0/0/0/0	0/0/0/0
5	C1O	A	703	1	-	0/0/0/0	0/0/0/0
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1
4	C2O	B	702	1	-	0/0/0/0	0/0/0/0
5	C1O	B	703	1	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAG	C2-N2	-2.09	1.42	1.46

There are no bond angle outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.