Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:28 pm BST

PDB ID	:	2IWK
Title	:	Inhibitor-bound form of nitrous oxide reductase from Achromobacter Cycloclastes at 1.7 Angstrom resolution
Authors	:	Paraskevopoulos, K.; Antonyuk, S.V.; Sawers, R.G.; Eady, R.R.; Hasnain, S.S.
Deposited on	:	2006-06-30
Resolution	:	1.70 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 following versions of software and data (see references ⓘ) were used in the production of this report:

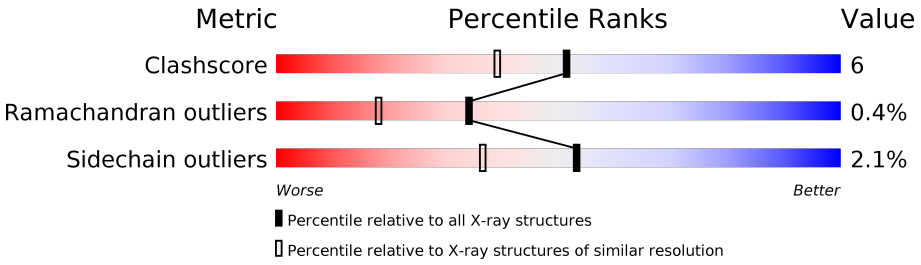
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.70 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	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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	642	84% 7% • 8%
1	B	642	84% 7% • 8%

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
4	IOD	B	1636	-	-	X	-
6	CL	A	1624	-	-	X	-
6	CL	B	1617	-	-	X	-
6	CL	B	1618	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10214 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 NITROUS OXIDE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	2	0
			4636	2917	799	888	32			
1	B	590	Total	C	N	O	S	0	1	0
			4630	2913	798	887	32			

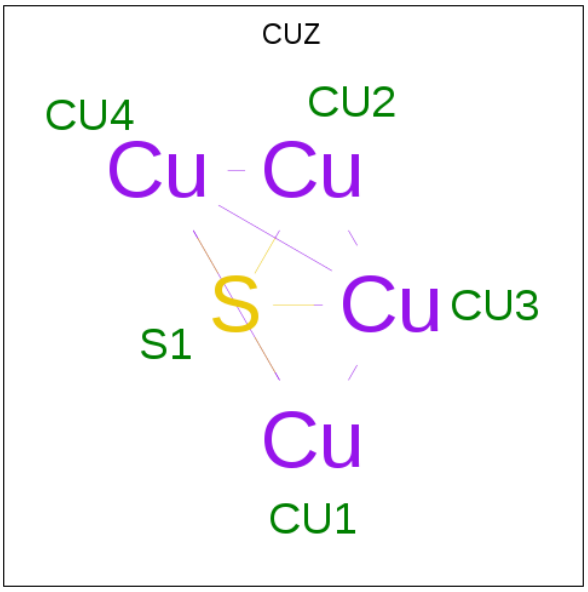
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	472	ASN	LYS	conflict	UNP P94127
B	472	ASN	LYS	conflict	UNP P94127

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 3 is (MU-4-SULFIDO)-TETRA-NUCLEAR COPPER ION (three-letter code: CUZ) (formula: Cu_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu S 5 4 1	0	0
3	B	1	Total Cu S 5 4 1	0	0

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	10	Total I 10 10	0	0
4	A	5	Total I 5 5	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	11	Total Ca 11 11	0	0
5	A	17	Total Ca 17 17	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	5	Total Cl 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total Cl 3 3	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	16	Total Na 16 16	0	0
7	A	14	Total Na 14 14	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	431	Total O 431 431	0	0
8	B	422	Total O 422 422	0	0

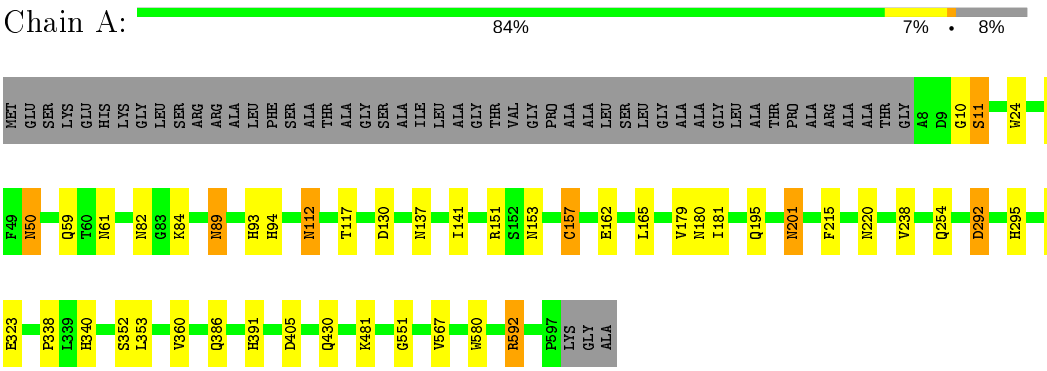
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

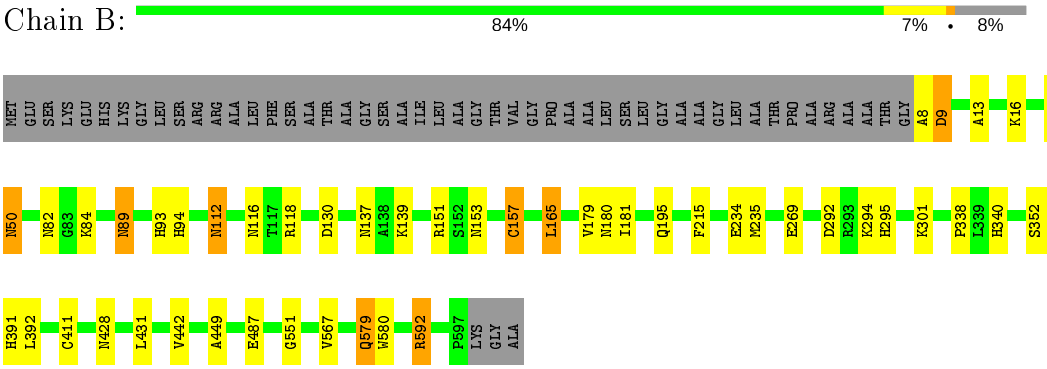
- Molecule 1: NITROUS OXIDE REDUCTASE

Chain A:



- Molecule 1: NITROUS OXIDE REDUCTASE

Chain B:



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 21	Depositor
Cell constants a, b, c, α, β, γ	71.11Å 120.91Å 137.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70	Depositor
% Data completeness (in resolution range)	98.3 (50.00-1.70)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.168 , 0.207	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10214	wwPDB-VP
Average B, all atoms (Å^2)	23.0	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: CL, NA, CA, CUZ, IOD, CU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.75	1/4749 (0.0%)	0.85	4/6446 (0.1%)
1	B	0.76	1/4740 (0.0%)	0.82	3/6434 (0.0%)
All	All	0.76	2/9489 (0.0%)	0.84	7/12880 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	157	CYS	CB-SG	-7.88	1.68	1.82
1	A	157	CYS	CB-SG	-6.18	1.71	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	592	ARG	NE-CZ-NH1	15.59	128.09	120.30
1	A	592	ARG	NE-CZ-NH2	-15.01	112.80	120.30
1	B	592	ARG	NE-CZ-NH1	11.68	126.14	120.30
1	B	592	ARG	NE-CZ-NH2	-11.66	114.47	120.30
1	B	118	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	592	ARG	CD-NE-CZ	5.52	131.33	123.60
1	A	292	ASP	CB-CG-OD1	5.23	123.01	118.30

There are no chirality outliers.

There are no planarity outliers.

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	4636	0	4477	52	0
1	B	4630	0	4468	56	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	5	0	0	0	0
4	B	10	0	0	2	0
5	A	17	0	0	0	0
5	B	11	0	0	0	0
6	A	3	0	0	3	0
6	B	5	0	0	5	0
7	A	14	0	0	0	0
7	B	16	0	0	0	0
8	A	431	0	0	7	0
8	B	422	0	0	12	0
All	All	10214	0	8945	101	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 6.

All (101) 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:A:157:CYS:SG	8:A:2124:HOH:O	1.95	1.22
1:B:157:CYS:SG	8:B:2104:HOH:O	2.09	1.06
1:A:567:VAL:H	1:B:82:ASN:HD21	1.16	0.93
1:A:82:ASN:HD21	1:B:567:VAL:H	1.10	0.91
1:B:157:CYS:HB3	8:B:2104:HOH:O	1.73	0.88
1:A:157:CYS:CB	8:A:2124:HOH:O	2.16	0.88
1:A:157:CYS:HB3	8:A:2124:HOH:O	1.73	0.87
1:B:157:CYS:CB	8:B:2104:HOH:O	2.23	0.87
1:B:8:ALA:C	1:B:9:ASP:OD1	2.15	0.85
1:B:179:VAL:HG11	4:B:1636:IOD:I	2.47	0.84
1:A:180:ASN:C	1:A:181:ILE:HD12	2.02	0.80
1:A:50:ASN:H	1:A:50:ASN:HD22	1.35	0.75
1:A:84:LYS:NZ	6:A:1623:CL:CL	2.56	0.74
1:A:137:ASN:HD22	1:A:195:GLN:HE22	1.35	0.73
1:B:50:ASN:HD22	1:B:50:ASN:H	1.36	0.72
1:A:10:GLY:HA3	1:A:11:SER:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:ARG:HD3	8:B:2144:HOH:O	1.90	0.70
1:A:254[B]:GLN:HE21	1:A:254[B]:GLN:HA	1.58	0.68
1:B:137:ASN:HD22	1:B:195:GLN:HE22	1.41	0.67
1:A:592:ARG:CD	8:B:2144:HOH:O	2.43	0.66
1:B:8:ALA:O	1:B:9:ASP:CB	2.45	0.64
1:A:386:GLN:H	1:A:430:GLN:HE22	1.46	0.64
1:B:353:LEU:HD11	1:B:360:VAL:CG2	2.29	0.63
1:A:10:GLY:HA3	1:A:11:SER:CB	2.28	0.62
1:A:353:LEU:HD11	1:A:360:VAL:HG21	1.80	0.62
1:B:93:HIS:H	1:B:112:ASN:HD21	1.46	0.60
1:B:139:LYS:NZ	6:B:1617:CL:CL	2.69	0.60
1:A:181:ILE:HD12	1:A:181:ILE:N	2.15	0.60
1:A:47:PRO:HA	1:A:50:ASN:HD21	1.65	0.60
1:A:151:ARG:HH11	1:A:153:ASN:ND2	2.00	0.59
1:B:487:GLU:CA	8:B:2341:HOH:O	2.50	0.59
1:B:8:ALA:O	1:B:9:ASP:CG	2.42	0.58
1:A:82:ASN:ND2	1:B:567:VAL:H	1.92	0.58
1:B:9:ASP:OD1	1:B:9:ASP:N	2.37	0.58
1:A:292:ASP:OD2	1:A:295:HIS:HD2	1.87	0.57
1:B:592:ARG:HD3	8:B:2371:HOH:O	2.04	0.57
8:A:2417:HOH:O	6:B:1641:CL:CL	2.54	0.57
1:A:567:VAL:H	1:B:82:ASN:ND2	1.96	0.56
1:A:93:HIS:H	1:A:112:ASN:HD21	1.52	0.56
1:B:47:PRO:HA	1:B:50:ASN:HD21	1.70	0.55
1:B:292:ASP:OD2	1:B:295:HIS:HD2	1.88	0.55
1:A:551:GLY:HA2	1:B:89:ASN:HD21	1.72	0.55
1:B:8:ALA:O	1:B:9:ASP:OD1	2.25	0.55
1:B:89:ASN:ND2	6:B:1618:CL:CL	2.77	0.55
1:B:165:LEU:HD13	1:B:179:VAL:CG2	2.37	0.55
1:B:137:ASN:HD22	1:B:195:GLN:NE2	2.05	0.54
1:A:567:VAL:N	1:B:82:ASN:HD21	1.96	0.54
1:A:353:LEU:HD11	1:A:360:VAL:CG2	2.39	0.53
1:A:61:ASN:ND2	6:A:1624:CL:CL	2.79	0.53
1:A:338:PRO:HA	1:A:352:SER:O	2.08	0.52
1:B:295:HIS:HE1	8:B:2205:HOH:O	1.91	0.52
1:A:137:ASN:HD22	1:A:195:GLN:NE2	2.05	0.52
1:A:10:GLY:O	1:A:38:PRO:HB2	2.10	0.52
1:B:84:LYS:NZ	6:B:1618:CL:CL	2.79	0.51
1:B:269:GLU:HG2	8:B:2182:HOH:O	2.11	0.51
1:A:162:GLU:HG3	1:A:180:ASN:HD21	1.75	0.51
1:A:89:ASN:HD21	1:B:551:GLY:HA2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:LEU:O	1:B:442:VAL:HG22	2.10	0.51
1:B:353:LEU:HD11	1:B:360:VAL:HG21	1.93	0.51
1:A:82:ASN:HD21	1:B:567:VAL:N	1.93	0.50
1:A:112:ASN:HD22	1:A:112:ASN:H	1.59	0.50
1:A:201:ASN:ND2	1:A:220:ASN:H	2.09	0.50
1:B:151:ARG:HH11	1:B:153:ASN:ND2	2.08	0.50
1:A:10:GLY:CA	1:A:11:SER:CB	2.89	0.49
1:A:165:LEU:HD21	1:A:181:ILE:HD11	1.95	0.49
1:A:238:VAL:HG21	1:A:298:VAL:HG21	1.95	0.49
1:B:8:ALA:O	1:B:9:ASP:HB3	2.13	0.48
1:B:338:PRO:HA	1:B:352:SER:O	2.14	0.48
1:B:13:ALA:HB3	1:B:16:LYS:HD3	1.96	0.48
1:B:592:ARG:CD	8:B:2371:HOH:O	2.58	0.48
1:A:50:ASN:H	1:A:50:ASN:ND2	2.07	0.47
1:A:151:ARG:HH11	1:A:153:ASN:HD22	1.63	0.47
1:B:340:HIS:CE1	1:B:391:HIS:CE1	3.02	0.47
1:B:269:GLU:CD	1:B:269:GLU:H	2.18	0.47
1:B:89:ASN:HD21	1:B:116:ASN:HD21	1.62	0.46
1:A:405:ASP:HB3	8:A:2295:HOH:O	2.16	0.46
1:B:234:GLU:HG2	1:B:235:MET:HG3	1.98	0.46
1:A:59:GLN:O	6:A:1624:CL:CL	2.72	0.45
1:A:94:HIS:CD2	8:A:2083:HOH:O	2.69	0.45
1:B:89:ASN:ND2	1:B:116:ASN:HD21	2.15	0.45
1:B:579:GLN:H	1:B:579:GLN:HE21	1.62	0.44
1:B:165:LEU:HD11	1:B:181:ILE:CD1	2.47	0.44
1:A:181:ILE:N	1:A:181:ILE:CD1	2.78	0.44
1:A:592:ARG:HD2	8:B:2144:HOH:O	2.13	0.44
1:B:112:ASN:HD22	1:B:112:ASN:H	1.66	0.44
1:B:151:ARG:HH11	1:B:153:ASN:HD22	1.66	0.44
1:B:94:HIS:CD2	8:B:2315:HOH:O	2.71	0.44
1:A:179:VAL:HG12	8:A:2137:HOH:O	2.18	0.43
1:A:117:THR:HG23	1:A:141:ILE:HG12	2.00	0.43
1:A:254[B]:GLN:NE2	1:A:254[B]:GLN:HA	2.29	0.43
1:B:8:ALA:C	1:B:9:ASP:CG	2.75	0.43
1:A:386:GLN:H	1:A:430:GLN:NE2	2.14	0.43
1:B:411:CYS:HB2	1:B:428:ASN:O	2.18	0.43
1:B:139:LYS:CE	6:B:1617:CL:CL	3.03	0.43
1:B:180:ASN:C	1:B:181:ILE:HD12	2.38	0.42
1:B:50:ASN:ND2	1:B:50:ASN:H	2.08	0.42
1:A:340:HIS:CE1	1:A:391:HIS:CE1	3.08	0.42
1:A:48:VAL:H	1:A:50:ASN:ND2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:VAL:HG23	1:A:181:ILE:HD11	2.02	0.41
1:B:353:LEU:CD1	1:B:360:VAL:CG2	2.99	0.41
1:B:179:VAL:CG1	4:B:1636:IOD:I	3.32	0.41

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	589/642 (92%)	565 (96%)	22 (4%)	2 (0%)	41	24
1	B	588/642 (92%)	568 (97%)	17 (3%)	3 (0%)	29	13
All	All	1177/1284 (92%)	1133 (96%)	39 (3%)	5 (0%)	34	18

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	B	9	ASP
1	A	301	LYS
1	B	301	LYS
1	B	449	ALA

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	502/532 (94%)	492 (98%)	10 (2%)	55 38
1	B	501/532 (94%)	490 (98%)	11 (2%)	52 34
All	All	1003/1064 (94%)	982 (98%)	21 (2%)	53 36

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	50	ASN
1	A	89	ASN
1	A	112	ASN
1	A	130	ASP
1	A	201	ASN
1	A	215	PHE
1	A	323	GLU
1	A	481	LYS
1	A	580	TRP
1	B	24	TRP
1	B	50	ASN
1	B	89	ASN
1	B	112	ASN
1	B	130	ASP
1	B	165	LEU
1	B	215	PHE
1	B	294	LYS
1	B	392	LEU
1	B	579	GLN
1	B	580	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	61	ASN
1	A	82	ASN
1	A	89	ASN
1	A	112	ASN
1	A	153	ASN
1	A	180	ASN
1	A	195	GLN
1	A	201	ASN

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Mol	Chain	Res	Type
1	A	295	HIS
1	A	388	GLN
1	A	430	GLN
1	A	443	HIS
1	B	50	ASN
1	B	61	ASN
1	B	82	ASN
1	B	89	ASN
1	B	94	HIS
1	B	112	ASN
1	B	153	ASN
1	B	158	ASN
1	B	195	GLN
1	B	295	HIS
1	B	388	GLN
1	B	472	ASN
1	B	559	GLN
1	B	579	GLN

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 87 ligands modelled in this entry, 85 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	$\#\|Z\| > 2$
3	CUZ	B	1600	1,4	0,9,9	0.00	-	-		
3	CUZ	A	1600	1,4	0,9,9	0.00	-	-		

There are no bond length outliers.

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 (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.