



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 07:15 AM EST

PDB ID : 2OXI
Title : REFINED CRYSTAL STRUCTURE OF CU-SUBSTITUTED ALCOHOL
DEHYDROGENASE AT 2.1 ANGSTROMS RESOLUTION
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Deposited on : unknown
Resolution : 2.10 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

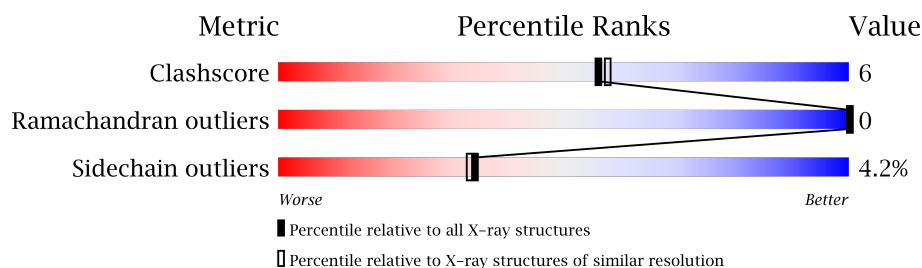
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)

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	374	
1	B	374	

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	DMS	A	378	-	-	X	-
5	DMS	B	378	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6125 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 ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	89	3	0
			2791	1772	472	521	26			
1	B	374	Total	C	N	O	S	64	2	0
			2789	1771	472	521	25			

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

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

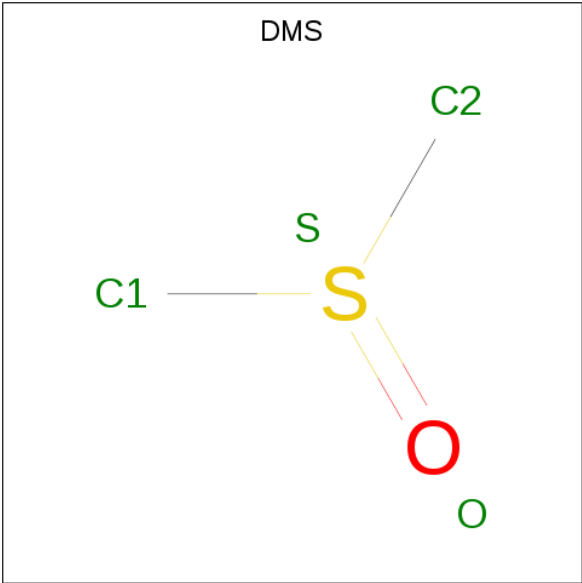
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is water.

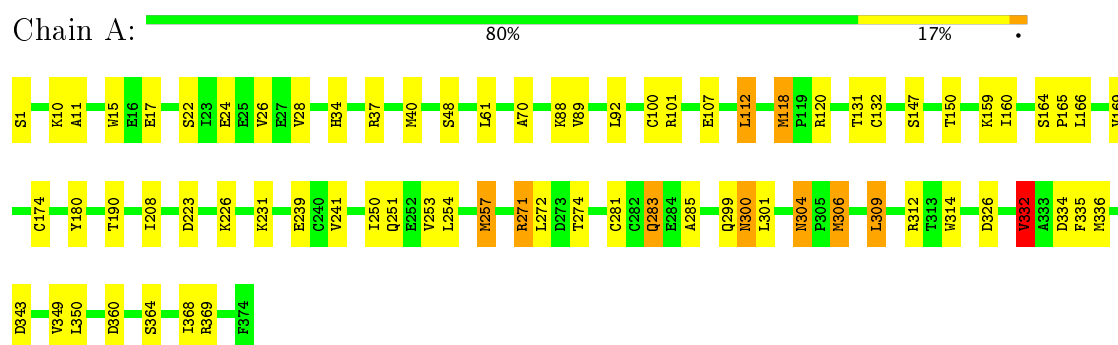
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	222	Total 222	O 222	0	0
6	B	223	Total 223	O 223	0	0

3 Residue-property plots

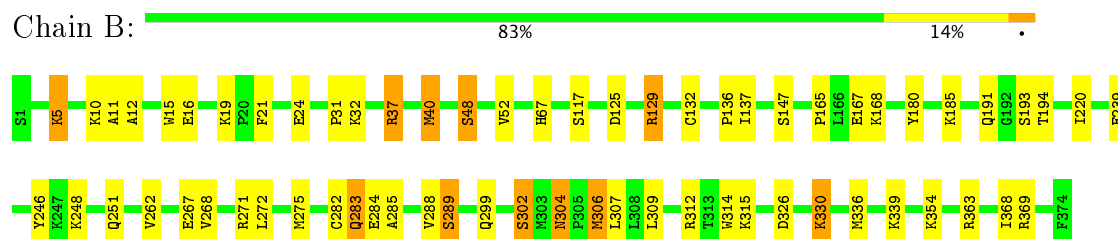
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($RSRZ > 2$). 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: ALCOHOL DEHYDROGENASE



• Molecule 1: ALCOHOL DEHYDROGENASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.40Å 180.60Å 50.80Å 90.00° 108.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	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	6125	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: ZN, DMS, NAD, 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	0.97	1/2855 (0.0%)	1.62	36/3858 (0.9%)
1	B	1.01	4/2849 (0.1%)	1.62	34/3850 (0.9%)
All	All	0.99	5/5704 (0.1%)	1.62	70/7708 (0.9%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	SER	CA-CB	-6.27	1.43	1.52
1	B	284	GLU	CD-OE2	-5.62	1.19	1.25
1	B	48	SER	CA-CB	-5.49	1.44	1.52
1	B	302	SER	CA-CB	-5.38	1.44	1.52
1	A	190	THR	C-O	-5.07	1.13	1.23

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	MET	CG-SD-CE	-18.33	70.87	100.20
1	B	15	TRP	CD1-CG-CD2	11.12	115.20	106.30
1	B	40	MET	CG-SD-CE	-10.01	84.19	100.20
1	A	306	MET	CG-SD-CE	9.94	116.10	100.20
1	A	15	TRP	CD1-CG-CD2	9.17	113.64	106.30
1	A	118	MET	CA-CB-CG	9.05	128.69	113.30
1	B	246	TYR	CB-CG-CD2	-8.88	115.67	121.00
1	B	314	TRP	CD1-CG-CD2	8.80	113.34	106.30
1	B	15	TRP	CG-CD1-NE1	-8.43	101.67	110.10
1	A	1	SER	CA-C-N	7.77	134.29	117.20
1	B	15	TRP	CE2-CD2-CG	-7.69	101.14	107.30
1	A	37	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	B	180	TYR	CB-CG-CD1	-7.51	116.50	121.00
1	B	369	ARG	NE-CZ-NH1	7.41	124.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	VAL	CG1-CB-CG2	-7.37	99.11	110.90
1	A	314	TRP	CD1-CG-CD2	7.28	112.12	106.30
1	A	15	TRP	CE2-CD2-CG	-7.24	101.51	107.30
1	A	1	SER	CA-C-O	-7.17	105.03	120.10
1	B	167	GLU	CA-CB-CG	7.13	129.10	113.40
1	B	193	SER	N-CA-CB	-7.12	99.83	110.50
1	A	112	LEU	CB-CG-CD1	-6.87	99.32	111.00
1	A	312	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	B	314	TRP	CE2-CD2-CG	-6.69	101.95	107.30
1	B	129	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	B	363	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	B	15	TRP	CB-CG-CD1	-6.55	118.49	127.00
1	B	314	TRP	CG-CD1-NE1	-6.54	103.56	110.10
1	B	5	LYS	CB-CG-CD	-6.31	95.20	111.60
1	B	330	LYS	N-CA-CB	-6.27	99.31	110.60
1	A	271	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	271	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	101	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	28	VAL	CA-CB-CG1	-6.02	101.86	110.90
1	A	309	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	120	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	107	GLU	CA-C-N	5.76	127.72	116.20
1	A	314	TRP	CE2-CD2-CG	-5.72	102.73	107.30
1	B	15	TRP	CG-CD2-CE3	5.70	139.03	133.90
1	B	67	HIS	CA-C-N	5.68	129.69	117.20
1	B	168	LYS	CB-CG-CD	-5.64	96.92	111.60
1	A	1	SER	CA-CB-OG	-5.60	96.07	111.20
1	A	301	LEU	CA-CB-CG	5.60	128.18	115.30
1	B	363	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	257	MET	CG-SD-CE	5.58	109.14	100.20
1	B	180	TYR	CD1-CG-CD2	5.58	124.03	117.90
1	A	332	VAL	CA-CB-CG2	-5.57	102.55	110.90
1	A	314	TRP	CG-CD1-NE1	-5.55	104.55	110.10
1	B	125	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	368	ILE	N-CA-C	-5.52	96.09	111.00
1	A	368	ILE	N-CA-C	-5.49	96.17	111.00
1	A	101	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	37	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	223	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	117	SER	CB-CA-C	-5.39	99.85	110.10
1	B	246	TYR	CD1-CG-CD2	5.35	123.79	117.90
1	A	326	ASP	CB-CG-OD1	5.30	123.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	220	ILE	CA-C-N	5.29	126.79	116.20
1	A	364	SER	O-C-N	-5.28	114.22	123.20
1	A	15	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	B	268	VAL	CG1-CB-CG2	-5.21	102.57	110.90
1	B	251	GLN	CA-CB-CG	5.21	124.85	113.40
1	B	15	TRP	CD1-NE1-CE2	5.19	113.67	109.00
1	A	226	LYS	CA-CB-CG	5.18	124.81	113.40
1	A	300	ASN	CB-CG-ND2	5.11	128.97	116.70
1	A	180	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	A	369	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	271	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	17	GLU	CA-CB-CG	5.03	124.47	113.40
1	A	334	ASP	CB-CG-OD1	5.00	122.80	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	2791	0	2851	36	0
1	B	2789	0	2850	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	44	0	26	1	0
4	B	44	0	26	0	0
5	A	4	0	6	6	0
5	B	4	0	6	6	0
6	A	222	0	0	2	0
6	B	223	0	0	0	0
All	All	6125	0	5765	64	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 (64) 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:48:SER:OG	5:B:378:DMS:H11	1.59	1.01
1:B:48:SER:OG	5:B:378:DMS:C1	2.13	0.94
1:A:48:SER:HB3	5:A:378:DMS:H12	1.48	0.92
1:B:48:SER:CB	5:B:378:DMS:H12	2.04	0.87
1:B:48:SER:HB3	5:B:378:DMS:H12	1.57	0.85
1:A:48:SER:CB	5:A:378:DMS:H12	2.16	0.75
1:A:251:GLN:HA	1:A:281[B]:CYS:SG	2.27	0.75
1:B:48:SER:OG	5:B:378:DMS:H12	1.93	0.68
1:A:283:GLN:HE22	1:A:285:ALA:HB3	1.64	0.63
1:B:165:PRO:HD3	1:B:336:MET:HE1	1.83	0.61
1:A:160:ILE:HB	1:A:332:VAL:HG11	1.82	0.60
1:B:48:SER:CB	5:B:378:DMS:C1	2.70	0.59
1:A:100:CYS:HB2	1:A:112:LEU:HD12	1.86	0.58
1:A:40:MET:CE	1:A:150:THR:HG22	2.35	0.57
1:A:283:GLN:NE2	1:A:285:ALA:H	2.05	0.54
1:A:26:VAL:HG12	1:A:132:CYS:HB2	1.90	0.54
1:B:304:ASN:HD22	1:B:306:MET:H	1.56	0.54
1:A:48:SER:CB	5:A:378:DMS:C1	2.84	0.53
1:B:282[B]:CYS:SG	1:B:288:VAL:O	2.66	0.53
1:A:48:SER:OG	5:A:378:DMS:H11	2.09	0.52
1:A:254:LEU:HD12	1:A:281[B]:CYS:SG	2.49	0.52
1:B:31:PRO:HD3	1:B:37:ARG:HB2	1.91	0.52
1:B:283:GLN:HE22	1:B:285:ALA:HB3	1.75	0.52
1:B:272:LEU:HD11	1:B:299:GLN:HE21	1.74	0.52
1:A:34:HIS:HE1	6:A:542:HOH:O	1.93	0.52
1:A:48:SER:HB3	5:A:378:DMS:C1	2.31	0.51
1:A:165:PRO:HD3	1:A:336:MET:HE1	1.91	0.51
1:A:166:LEU:HA	1:A:169:VAL:HG22	1.92	0.50
1:A:336:MET:HA	1:A:336:MET:HE2	1.92	0.50
1:B:283:GLN:NE2	1:B:285:ALA:H	2.09	0.50
1:B:132:CYS:HB3	1:B:137:ILE:HD11	1.94	0.50
1:A:304:ASN:ND2	1:A:306:MET:H	2.10	0.49
1:B:194:THR:HG22	1:B:262:VAL:HG12	1.96	0.48
1:A:253:VAL:O	1:A:257:MET:HG3	2.12	0.48
1:B:304:ASN:ND2	1:B:306:MET:H	2.12	0.48
1:A:89:VAL:HG12	1:A:159:LYS:HA	1.96	0.47
1:A:241:VAL:HG21	1:A:250:ILE:HD11	1.97	0.46
1:B:326:ASP:O	1:B:330:LYS:HE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:SER:OG	5:A:378:DMS:C1	2.64	0.45
1:A:174:CYS:SG	4:A:377:NAD:H5N	2.57	0.45
1:A:92:LEU:HA	6:A:443:HOH:O	2.16	0.45
1:A:304:ASN:HD22	1:A:306:MET:H	1.65	0.45
1:A:165:PRO:HG2	1:A:335:PHE:HE2	1.82	0.45
1:A:40:MET:HE3	1:A:150:THR:HG22	2.00	0.44
1:B:16:GLU:HG3	1:B:19:LYS:HG2	1.98	0.44
1:A:283:GLN:HE22	1:A:285:ALA:H	1.64	0.44
1:B:267:GLU:HG3	1:B:275:MET:HA	2.00	0.44
1:B:16:GLU:HG3	1:B:19:LYS:CG	2.48	0.43
1:A:70:ALA:HB1	1:A:166:LEU:HD22	2.00	0.42
1:B:32:LYS:HD2	1:B:129:ARG:NH2	2.33	0.42
1:A:271:ARG:HB2	1:A:274:THR:OG1	2.20	0.42
1:B:272:LEU:HD11	1:B:299:GLN:HB3	2.02	0.42
1:A:272:LEU:HD11	1:A:299:GLN:HB3	2.00	0.42
1:A:88:LYS:HE2	1:A:166:LEU:HG	2.02	0.42
1:B:12:ALA:HB1	1:B:21:PHE:HB3	2.01	0.41
1:A:11:ALA:HA	1:A:147:SER:HA	2.01	0.41
1:A:208:ILE:HG21	1:A:208:ILE:HD13	1.92	0.41
1:B:10:LYS:HA	1:B:24:GLU:O	2.21	0.41
1:A:349:VAL:O	1:A:350:LEU:HD23	2.21	0.41
1:B:307:LEU:O	1:B:312:ARG:HD2	2.22	0.40
1:B:11:ALA:HA	1:B:147:SER:HA	2.02	0.40
1:B:282[B]:CYS:SG	1:B:289:SER:HB2	2.61	0.40
1:B:40:MET:HE2	1:B:40:MET:HB2	1.78	0.40
1:A:10:LYS:HA	1:A:24:GLU: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	375/374 (100%)	359 (96%)	16 (4%)	0	100	100
1	B	374/374 (100%)	358 (96%)	16 (4%)	0	100	100
All	All	749/748 (100%)	717 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	311/308 (101%)	298 (96%)	13 (4%)	34	33
1	B	310/308 (101%)	297 (96%)	13 (4%)	34	33
All	All	621/616 (101%)	595 (96%)	26 (4%)	34	33

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	61	LEU
1	A	118	MET
1	A	131	THR
1	A	164	SER
1	A	231	LYS
1	A	239	GLU
1	A	283	GLN
1	A	300	ASN
1	A	304	ASN
1	A	309	LEU
1	A	332	VAL
1	A	343	ASP
1	B	5	LYS
1	B	136	PRO
1	B	185	LYS
1	B	191	GLN
1	B	239	GLU

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Mol	Chain	Res	Type
1	B	248	LYS
1	B	283	GLN
1	B	302	SER
1	B	304	ASN
1	B	309	LEU
1	B	315	LYS
1	B	339	LYS
1	B	354	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	304	ASN
1	B	283	GLN
1	B	299	GLN
1	B	300	ASN
1	B	304	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - 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	$\# Z > 2$
4	NAD	A	377	-	41,48,48	0.94	2 (4%)	43,73,73	1.62	7 (16%)
5	DMS	A	378	-	3,3,3	0.09	0	3,3,3	1.14	0
4	NAD	B	377	-	41,48,48	0.95	1 (2%)	43,73,73	1.78	10 (23%)
5	DMS	B	378	-	3,3,3	0.50	0	3,3,3	2.47	2 (66%)

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
4	NAD	A	377	-	-	0/22/62/62	0/5/5/5
5	DMS	A	378	-	-	0/0/0/0	0/0/0/0
4	NAD	B	377	-	-	0/22/62/62	0/5/5/5
5	DMS	B	378	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	377	NAD	O4B-C1B	2.45	1.44	1.41
4	B	377	NAD	O4D-C1D	2.71	1.45	1.41
4	A	377	NAD	O4D-C1D	2.92	1.45	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	377	NAD	N3A-C2A-N1A	-6.55	123.15	128.86
4	A	377	NAD	N3A-C2A-N1A	-6.07	123.57	128.86
4	B	377	NAD	O7N-C7N-C3N	-3.61	115.41	119.62
4	B	377	NAD	O4B-C4B-C5B	-3.13	98.82	109.40
4	B	377	NAD	C4D-O4D-C1D	-2.72	106.87	109.77
4	B	377	NAD	C3N-C2N-N1N	-2.63	117.78	120.43
5	B	378	DMS	C2-S-C1	-2.57	85.14	98.44
4	A	377	NAD	O3D-C3D-C4D	-2.40	104.08	111.09
4	A	377	NAD	O5B-C5B-C4B	-2.39	100.52	109.00
4	B	377	NAD	O4D-C4D-C5D	-2.18	102.03	109.40
4	A	377	NAD	C4B-O4B-C1B	-2.10	107.53	109.77
4	B	377	NAD	C3N-C7N-N7N	2.02	120.08	117.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
4	B	377	NAD	N6A-C6A-N1A	2.16	123.06	118.77
4	A	377	NAD	N6A-C6A-N1A	2.73	124.17	118.77
4	B	377	NAD	C4A-C5A-N7A	2.74	112.06	109.41
4	A	377	NAD	C2N-C3N-C4N	2.80	121.45	118.26
4	B	377	NAD	C2N-C3N-C4N	2.90	121.57	118.26
5	B	378	DMS	O-S-C2	3.17	123.25	106.54
4	A	377	NAD	C4A-C5A-N7A	4.06	113.33	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	377	NAD	1	0
5	A	378	DMS	6	0
5	B	378	DMS	6	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.