



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:05 pm GMT

PDB ID : 4GLO  
Title : Crystal structure of a short chain dehydrogenase homolog (target EFI-505321) from burkholderia multivorans, with bound NAD  
Authors : Vetting, M.W.; Hobbs, M.E.; Morisco, L.L.; Wasserman, S.R.; Sojitra, S.; Imker, H.J.; Raushel, F.M.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)  
Deposited on : 2012-08-14  
Resolution : 1.80 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](mailto: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.

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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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

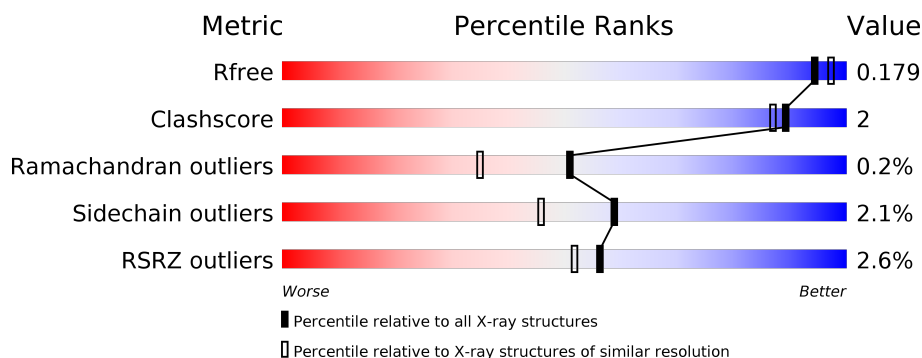
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	258	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
1	B	258	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	C	258	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>7%</div> </div> </div>
1	D	258	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>• • •</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	D	302	-	-	-	X
5	EDO	A	306	-	-	-	X
5	EDO	A	307	-	-	-	X
5	EDO	B	305	-	-	-	X
5	EDO	C	305	-	-	-	X
5	EDO	C	306	-	-	-	X
5	EDO	C	307	-	-	-	X
5	EDO	D	306	-	-	-	X

## 2 Entry composition [i](#)

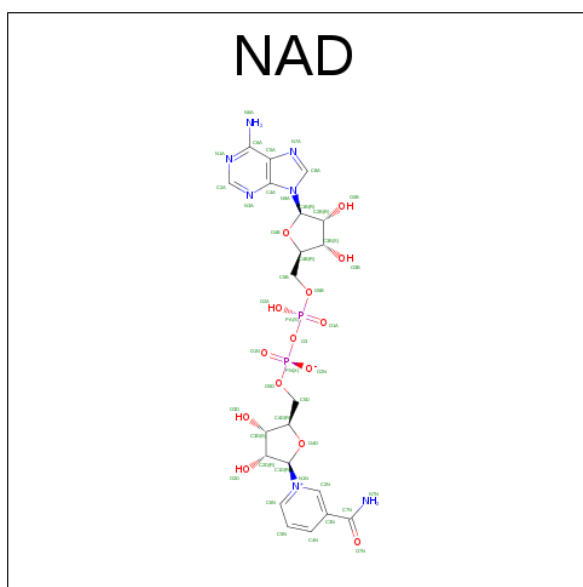
There are 6 unique types of molecules in this entry. The entry contains 8895 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-oxoacyl-[acyl-carrier protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	1	0
			1959	1231	354	367	7			
1	B	258	Total	C	N	O	S	0	2	0
			1970	1237	357	369	7			
1	C	248	Total	C	N	O	S	0	1	0
			1875	1176	344	348	7			
1	D	250	Total	C	N	O	S	0	0	0
			1877	1178	339	353	7			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
2	D	1	Total	C	N	O	P	0	1
			88	42	14	28	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

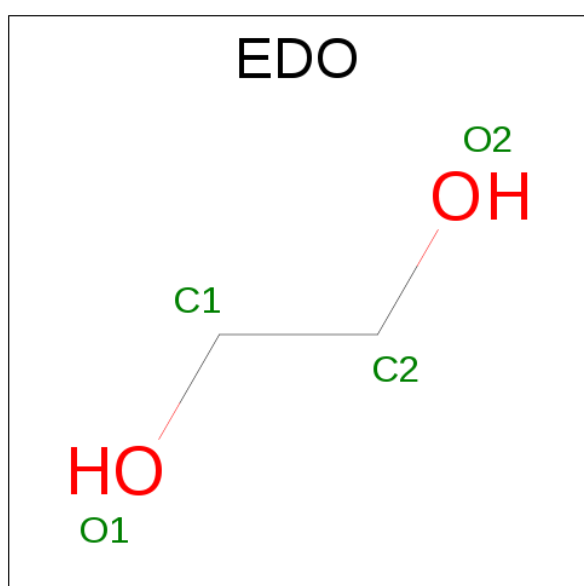


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		

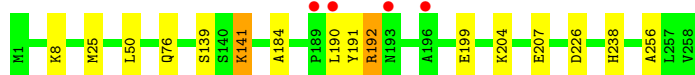
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	236	Total	O	0	2
			238	238		
6	B	259	Total	O	0	0
			259	259		
6	C	169	Total	O	0	0
			169	169		
6	D	202	Total	O	0	1
			203	203		

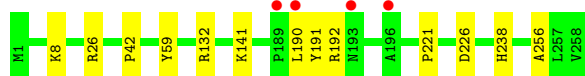
### 3 Residue-property plots [i](#)

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 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.

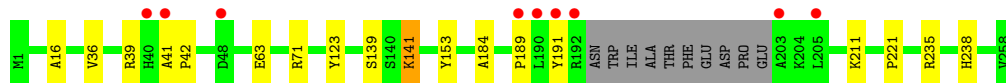
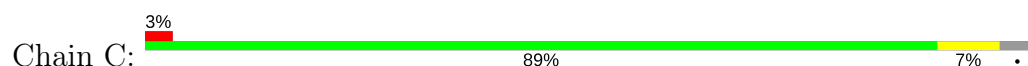
- Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



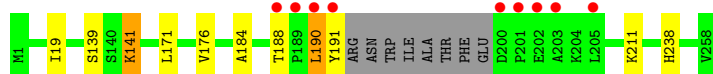
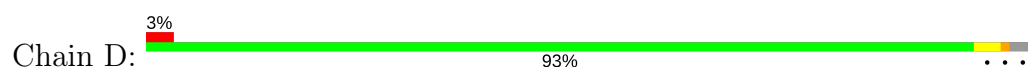
- Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



- Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase



- Molecule 1: 3-oxoacyl-[acyl-carrier protein] reductase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.59Å 99.59Å 206.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.75 – 1.80 28.75 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.75-1.80) 100.0 (28.75-1.80)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 1.80Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, $R_{free}$	0.150 , 0.181 0.149 , 0.179	Depositor DCC
$R_{free}$ test set	5316 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8895	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: CL, EDO, NAD, SO4

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	0.36	0/1997	0.54	0/2718
1	B	0.37	0/2008	0.53	0/2732
1	C	0.33	0/1908	0.51	0/2592
1	D	0.33	0/1911	0.53	0/2599
All	All	0.35	0/7824	0.53	0/10641

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1959	0	1947	12	0
1	B	1970	0	1957	6	0
1	C	1875	0	1880	12	0
1	D	1877	0	1872	7	0
2	A	44	0	26	1	0
2	B	44	0	25	0	0
2	C	88	0	49	4	0
2	D	88	0	52	3	0
3	A	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	1	0
4	C	1	0	0	1	0
4	D	1	0	0	0	0
5	A	8	0	12	0	0
5	B	4	0	6	0	0
5	C	12	0	18	0	0
5	D	8	0	12	1	0
6	A	238	0	0	4	0
6	B	259	0	0	2	1
6	C	169	0	0	0	0
6	D	203	0	0	0	0
All	All	8895	0	7856	35	1

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 2.

All (35) 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:132[A]:ARG:NH1	6:B:618:HOH:O	2.23	0.67
1:A:76[B]:GLN:NE2	6:A:555:HOH:O	2.36	0.58
1:A:199:GLU:N	3:A:304:SO4:O1	2.29	0.57
1:C:39:ARG:NH2	1:C:63:GLU:OE2	2.37	0.56
1:B:8:LYS:NZ	6:B:627:HOH:O	2.42	0.53
1:A:204:LYS:NZ	1:A:207:GLU:OE1	2.46	0.49
1:C:184:ALA:O	2:C:301[A]:NAD:H4N	2.11	0.49
1:B:256:ALA:HA	1:D:211:LYS:HD3	1.96	0.48
1:A:25:MET:HE1	1:A:50:LEU:N	2.28	0.47
1:A:141:LYS:HD2	1:A:184:ALA:HA	1.95	0.47
1:A:226:ASP:OD2	5:D:306:EDO:O1	2.27	0.46
1:D:139:SER:O	2:D:301[A]:NAD:H6N	2.15	0.46
1:B:26:ARG:NE	1:B:226:ASP:OD1	2.23	0.46
1:D:139:SER:O	2:D:301[B]:NAD:H6N	2.15	0.46
1:A:199:GLU:OE1	6:A:469:HOH:O	2.21	0.45
1:C:16:ALA:HB2	1:C:36:VAL:HG11	1.96	0.45
1:C:71:ARG:HB2	1:C:123:TYR:CZ	2.51	0.44
1:A:192:ARG:NH2	6:A:497:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LYS:O	1:A:207:GLU:HG2	2.18	0.44
1:A:8:LYS:NZ	6:A:583:HOH:O	2.19	0.43
1:D:188:THR:OG1	1:D:190:LEU:HB3	2.18	0.43
1:D:19:ILE:HB	2:D:301[A]:NAD:H51N	1.99	0.43
1:A:256:ALA:HA	1:C:211:LYS:HD3	2.00	0.43
1:C:221:PRO:HD2	4:C:304:CL:CL	2.56	0.43
1:B:221:PRO:HD2	4:B:304:CL:CL	2.56	0.43
1:C:139:SER:O	2:C:301[A]:NAD:H6N	2.19	0.42
1:C:184:ALA:O	2:C:301[B]:NAD:H4N	2.18	0.42
1:D:171:LEU:HB3	1:D:176:VAL:HB	2.01	0.42
1:B:42:PRO:HD3	1:B:59:TYR:CZ	2.55	0.42
1:C:141:LYS:HD2	1:C:184:ALA:HA	2.02	0.41
1:A:139:SER:O	2:A:301:NAD:H6N	2.21	0.41
1:C:41:ALA:HA	1:C:42:PRO:HD3	1.92	0.41
1:C:153:TYR:OH	2:C:301[A]:NAD:O2D	2.38	0.41
1:C:235[B]:ARG:HA	1:C:235[B]:ARG:HD3	1.82	0.40
1:D:141:LYS:HD2	1:D:184:ALA:HA	2.03	0.40

All (1) 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)
6:B:651:HOH:O	6:B:659:HOH:O[6_545]	2.16	0.04

## 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	257/258 (100%)	247 (96%)	10 (4%)	0	100	100
1	B	258/258 (100%)	248 (96%)	10 (4%)	0	100	100
1	C	245/258 (95%)	233 (95%)	11 (4%)	1 (0%)	38	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	246/258 (95%)	235 (96%)	10 (4%)	1 (0%)	38	23
All	All	1006/1032 (98%)	963 (96%)	41 (4%)	2 (0%)	51	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	189	PRO
1	D	190	LEU

### 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	198/197 (100%)	193 (98%)	5 (2%)	53	38
1	B	199/197 (101%)	194 (98%)	5 (2%)	53	38
1	C	189/197 (96%)	186 (98%)	3 (2%)	68	58
1	D	190/197 (96%)	187 (98%)	3 (2%)	68	58
All	All	776/788 (98%)	760 (98%)	16 (2%)	59	46

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	LYS
1	A	190	LEU
1	A	191	TYR
1	A	192	ARG
1	A	238	HIS
1	B	141	LYS
1	B	190	LEU
1	B	191	TYR
1	B	192	ARG
1	B	238	HIS
1	C	141	LYS
1	C	191	TYR

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Mol	Chain	Res	Type
1	C	238	HIS
1	D	141	LYS
1	D	191	TYR
1	D	238	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 27 ligands modelled in this entry, 4 are monoatomic - leaving 23 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	NAD	A	301	-	41,48,48	1.51	9 (21%)	43,73,73	1.42	8 (18%)
3	SO4	A	302	-	4,4,4	0.12	0	6,6,6	0.19	0
3	SO4	A	303	-	4,4,4	0.11	0	6,6,6	0.09	0
3	SO4	A	304	-	4,4,4	0.13	0	6,6,6	0.14	0
5	EDO	A	306	-	3,3,3	0.45	0	2,2,2	0.35	0
5	EDO	A	307	-	3,3,3	0.52	0	2,2,2	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	B	301	-	41,48,48	1.50	8 (19%)	43,73,73	1.38	5 (11%)
3	SO4	B	302	-	4,4,4	0.13	0	6,6,6	0.17	0
3	SO4	B	303	-	4,4,4	0.14	0	6,6,6	0.08	0
5	EDO	B	305	-	3,3,3	0.47	0	2,2,2	0.25	0
2	NAD	C	301[A]	-	41,48,48	1.85	10 (24%)	43,73,73	2.37	10 (23%)
2	NAD	C	301[B]	-	41,48,48	1.54	7 (17%)	43,73,73	1.66	10 (23%)
3	SO4	C	302	-	4,4,4	0.11	0	6,6,6	0.23	0
3	SO4	C	303	-	4,4,4	0.14	0	6,6,6	0.06	0
5	EDO	C	305	-	3,3,3	0.43	0	2,2,2	0.30	0
5	EDO	C	306	-	3,3,3	0.46	0	2,2,2	0.31	0
5	EDO	C	307	-	3,3,3	0.43	0	2,2,2	0.35	0
2	NAD	D	301[A]	-	41,48,48	1.43	5 (12%)	43,73,73	1.53	8 (18%)
2	NAD	D	301[B]	-	41,48,48	1.44	5 (12%)	43,73,73	1.56	7 (16%)
3	SO4	D	302	-	4,4,4	0.11	0	6,6,6	0.19	0
3	SO4	D	303	-	4,4,4	0.14	0	6,6,6	0.06	0
5	EDO	D	305	-	3,3,3	0.46	0	2,2,2	0.27	0
5	EDO	D	306	-	3,3,3	0.46	0	2,2,2	0.45	0

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	NAD	A	301	-	-	0/22/62/62	0/5/5/5
3	SO4	A	302	-	-	0/0/0/0	0/0/0/0
3	SO4	A	303	-	-	0/0/0/0	0/0/0/0
3	SO4	A	304	-	-	0/0/0/0	0/0/0/0
5	EDO	A	306	-	-	0/1/1/1	0/0/0/0
5	EDO	A	307	-	-	0/1/1/1	0/0/0/0
2	NAD	B	301	-	-	0/22/62/62	0/5/5/5
3	SO4	B	302	-	-	0/0/0/0	0/0/0/0
3	SO4	B	303	-	-	0/0/0/0	0/0/0/0
5	EDO	B	305	-	-	0/1/1/1	0/0/0/0
2	NAD	C	301[A]	-	-	0/22/62/62	0/5/5/5
2	NAD	C	301[B]	-	-	0/22/62/62	0/5/5/5
3	SO4	C	302	-	-	0/0/0/0	0/0/0/0
3	SO4	C	303	-	-	0/0/0/0	0/0/0/0
5	EDO	C	305	-	-	0/1/1/1	0/0/0/0
5	EDO	C	306	-	-	0/1/1/1	0/0/0/0
5	EDO	C	307	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	D	301[A]	-	-	0/22/62/62	0/5/5/5
2	NAD	D	301[B]	-	-	0/22/62/62	0/5/5/5
3	SO4	D	302	-	-	0/0/0/0	0/0/0/0
3	SO4	D	303	-	-	0/0/0/0	0/0/0/0
5	EDO	D	305	-	-	0/1/1/1	0/0/0/0
5	EDO	D	306	-	-	0/1/1/1	0/0/0/0

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301[A]	NAD	O3B-C3B	-5.08	1.31	1.43
2	D	301[B]	NAD	PN-O1N	-4.79	1.33	1.50
2	D	301[A]	NAD	PN-O2N	-4.77	1.31	1.55
2	C	301[B]	NAD	PN-O1N	-4.37	1.34	1.50
2	C	301[B]	NAD	O7N-C7N	-3.94	1.16	1.24
2	B	301	NAD	PN-O2N	-3.55	1.37	1.55
2	A	301	NAD	PN-O2N	-3.54	1.37	1.55
2	A	301	NAD	O4D-C4D	-3.09	1.38	1.45
2	C	301[A]	NAD	O2D-C2D	-2.99	1.36	1.43
2	D	301[B]	NAD	O4D-C4D	-2.94	1.38	1.45
2	C	301[A]	NAD	O2B-C2B	-2.92	1.36	1.43
2	D	301[A]	NAD	O4D-C4D	-2.87	1.38	1.45
2	B	301	NAD	O3D-C3D	-2.86	1.36	1.43
2	C	301[A]	NAD	O4B-C4B	-2.82	1.38	1.45
2	C	301[B]	NAD	O4D-C4D	-2.80	1.38	1.45
2	B	301	NAD	O7N-C7N	-2.78	1.18	1.24
2	B	301	NAD	O4D-C4D	-2.78	1.38	1.45
2	C	301[A]	NAD	C2B-C1B	-2.65	1.49	1.53
2	A	301	NAD	C4N-C3N	-2.63	1.35	1.39
2	C	301[B]	NAD	C5A-N7A	-2.46	1.31	1.39
2	B	301	NAD	C5A-N7A	-2.43	1.31	1.39
2	C	301[A]	NAD	O4B-C1B	-2.42	1.37	1.41
2	A	301	NAD	PA-O2A	-2.40	1.43	1.55
2	D	301[B]	NAD	O7N-C7N	-2.36	1.19	1.24
2	D	301[A]	NAD	O7N-C7N	-2.34	1.19	1.24
2	A	301	NAD	C6N-N1N	-2.34	1.29	1.35
2	C	301[A]	NAD	C2B-C3B	-2.34	1.47	1.53
2	A	301	NAD	PN-O1N	-2.32	1.42	1.50
2	D	301[B]	NAD	C4N-C3N	-2.30	1.35	1.39
2	D	301[A]	NAD	C4N-C3N	-2.30	1.35	1.39
2	A	301	NAD	C5N-C4N	-2.23	1.34	1.38
2	B	301	NAD	C6N-N1N	-2.20	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301[B]	NAD	C4N-C3N	-2.07	1.35	1.39
2	B	301	NAD	PA-O1A	-2.05	1.43	1.50
2	A	301	NAD	O3D-C3D	-2.01	1.38	1.43
2	C	301[B]	NAD	C5A-C4A	2.09	1.45	1.40
2	C	301[B]	NAD	O4D-C1D	2.24	1.44	1.41
2	C	301[A]	NAD	C6A-N6A	2.66	1.45	1.34
2	A	301	NAD	C5A-C4A	2.72	1.46	1.40
2	D	301[A]	NAD	C5A-C4A	2.95	1.47	1.40
2	D	301[B]	NAD	C5A-C4A	2.99	1.47	1.40
2	C	301[A]	NAD	C2A-N3A	3.00	1.37	1.32
2	B	301	NAD	C5A-C4A	3.32	1.48	1.40
2	C	301[A]	NAD	C7N-N7N	4.56	1.41	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301[A]	NAD	N3A-C2A-N1A	-10.05	120.10	128.86
2	C	301[A]	NAD	O5B-PA-O1A	-6.81	81.76	109.25
2	C	301[A]	NAD	O2A-PA-O1A	-5.58	83.38	112.28
2	C	301[B]	NAD	N3A-C2A-N1A	-5.30	124.24	128.86
2	D	301[B]	NAD	N3A-C2A-N1A	-4.81	124.67	128.86
2	D	301[A]	NAD	N3A-C2A-N1A	-4.79	124.69	128.86
2	B	301	NAD	N3A-C2A-N1A	-4.68	124.78	128.86
2	D	301[A]	NAD	C4B-O4B-C1B	-3.18	106.39	109.77
2	D	301[B]	NAD	C4B-O4B-C1B	-2.92	106.66	109.77
2	D	301[B]	NAD	C4A-C5A-N7A	-2.68	106.82	109.41
2	D	301[A]	NAD	C4A-C5A-N7A	-2.64	106.86	109.41
2	A	301	NAD	N3A-C2A-N1A	-2.61	126.58	128.86
2	C	301[B]	NAD	O7N-C7N-C3N	-2.57	116.62	119.62
2	C	301[A]	NAD	C4D-O4D-C1D	-2.54	107.06	109.77
2	C	301[A]	NAD	C4B-O4B-C1B	-2.43	107.19	109.77
2	A	301	NAD	C4B-O4B-C1B	-2.27	107.35	109.77
2	B	301	NAD	O5B-PA-O1A	-2.26	100.14	109.25
2	C	301[B]	NAD	O3B-C3B-C4B	-2.24	104.54	111.09
2	C	301[A]	NAD	C4A-C5A-N7A	-2.20	107.28	109.41
2	D	301[A]	NAD	O3B-C3B-C4B	-2.11	104.93	111.09
2	A	301	NAD	C5A-C6A-N6A	-2.05	116.28	120.47
2	C	301[A]	NAD	O7N-C7N-N7N	-2.05	119.67	122.58
2	C	301[B]	NAD	C6N-C5N-C4N	-2.03	116.38	119.44
2	C	301[B]	NAD	C4A-C5A-N7A	-2.02	107.46	109.41
2	A	301	NAD	C4A-C5A-N7A	-2.01	107.47	109.41
2	D	301[B]	NAD	O3B-C3B-C4B	-2.00	105.23	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAD	C4D-O4D-C1D	2.03	111.94	109.77
2	C	301[B]	NAD	C2N-C3N-C7N	2.05	125.29	119.34
2	D	301[B]	NAD	O5D-PN-O1N	2.06	117.56	109.25
2	D	301[A]	NAD	C4D-O4D-C1D	2.10	112.01	109.77
2	A	301	NAD	O5D-C5D-C4D	2.11	116.47	109.00
2	C	301[A]	NAD	O4B-C4B-C3B	2.18	109.50	105.17
2	B	301	NAD	C4D-O4D-C1D	2.19	112.10	109.77
2	C	301[B]	NAD	C4D-O4D-C1D	2.21	112.13	109.77
2	C	301[A]	NAD	O2A-PA-O5B	2.22	118.61	108.14
2	A	301	NAD	O4B-C4B-C3B	2.23	109.61	105.17
2	D	301[B]	NAD	N6A-C6A-N1A	2.24	123.21	118.77
2	D	301[A]	NAD	N6A-C6A-N1A	2.29	123.30	118.77
2	D	301[A]	NAD	O2N-PN-O5D	2.42	119.55	108.14
2	D	301[A]	NAD	O5D-C5D-C4D	2.55	118.03	109.00
2	B	301	NAD	O2N-PN-O1N	2.76	126.57	112.28
2	B	301	NAD	N6A-C6A-N1A	2.78	124.28	118.77
2	C	301[B]	NAD	N6A-C6A-N1A	2.89	124.50	118.77
2	A	301	NAD	N6A-C6A-N1A	3.44	125.59	118.77
2	C	301[B]	NAD	C3N-C7N-N7N	3.62	121.91	117.77
2	C	301[B]	NAD	O5D-C5D-C4D	3.70	122.11	109.00
2	C	301[A]	NAD	C3N-C7N-N7N	3.81	122.13	117.77
2	D	301[B]	NAD	O5D-C5D-C4D	4.32	124.33	109.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAD	1	0
3	A	304	SO4	1	0
2	C	301[A]	NAD	3	0
2	C	301[B]	NAD	1	0
2	D	301[A]	NAD	2	0
2	D	301[B]	NAD	1	0
5	D	306	EDO	1	0

## 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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	258/258 (100%)	-0.51	4 (1%) 72 69	4, 12, 39, 65	0
1	B	258/258 (100%)	-0.63	4 (1%) 72 69	4, 11, 36, 52	0
1	C	248/258 (96%)	-0.40	9 (3%) 43 38	7, 16, 42, 64	0
1	D	250/258 (96%)	-0.46	9 (3%) 43 38	7, 15, 37, 74	0
All	All	1014/1032 (98%)	-0.50	26 (2%) 56 52	4, 13, 39, 74	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	190	LEU	7.9
1	A	189	PRO	6.0
1	D	203	ALA	5.2
1	D	189	PRO	5.1
1	D	190	LEU	4.8
1	C	189	PRO	4.5
1	D	201	PRO	4.3
1	A	193	ASN	4.3
1	A	196	ALA	4.2
1	C	205	LEU	4.1
1	D	200	ASP	3.8
1	B	189	PRO	3.7
1	B	190	LEU	3.6
1	C	203	ALA	3.6
1	D	205	LEU	3.4
1	D	202	GLU	3.4
1	C	192	ARG	3.4
1	C	191	TYR	3.2
1	A	190	LEU	3.1
1	D	191	TYR	2.7
1	B	196	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	41	ALA	2.4
1	C	40	HIS	2.2
1	B	193	ASN	2.2
1	C	48	ASP	2.1
1	D	188	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	B	305	4/4	0.97	0.14	9.36	7,12,16,18	0
5	EDO	C	305	4/4	0.94	0.22	8.14	30,30,30,36	0
5	EDO	D	306	4/4	0.94	0.12	7.84	19,23,31,32	0
5	EDO	C	306	4/4	0.97	0.09	5.68	10,19,19,20	0
5	EDO	A	307	4/4	0.96	0.09	4.52	8,13,14,16	0
3	SO4	D	302	5/5	0.97	0.09	3.90	16,16,16,17	5
5	EDO	C	307	4/4	0.87	0.14	2.69	28,30,32,36	0
5	EDO	A	306	4/4	0.91	0.09	2.64	23,26,29,34	0
5	EDO	D	305	4/4	0.97	0.07	1.31	8,17,17,19	0
3	SO4	B	302	5/5	0.99	0.07	0.81	9,9,12,21	5
3	SO4	A	302	5/5	0.99	0.07	0.76	7,11,12,17	5
3	SO4	A	304	5/5	0.92	0.17	0.71	36,45,46,49	5
2	NAD	D	301[B]	44/44	0.88	0.14	0.65	3,21,33,36	44
2	NAD	D	301[A]	44/44	0.88	0.14	0.65	4,21,32,38	44
3	SO4	C	302	5/5	0.97	0.08	0.63	18,21,22,26	5
2	NAD	C	301[A]	44/44	0.85	0.16	0.47	11,27,41,45	44

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	C	301[B]	44/44	0.85	0.16	0.47	5,28,40,46	44
2	NAD	B	301	44/44	0.93	0.10	0.24	1,16,29,34	44
2	NAD	A	301	44/44	0.94	0.10	0.17	5,15,26,37	44
3	SO4	C	303	5/5	0.94	0.29	-	68,68,69,70	5
3	SO4	A	303	5/5	0.96	0.14	-	46,49,55,56	5
4	CL	B	304	1/1	0.99	0.25	-	35,35,35,35	0
4	CL	A	305	1/1	0.98	0.22	-	31,31,31,31	0
3	SO4	D	303	5/5	0.91	0.20	-	64,64,65,67	5
3	SO4	B	303	5/5	0.95	0.14	-	50,52,54,56	5
4	CL	C	304	1/1	0.99	0.22	-	36,36,36,36	0
4	CL	D	304	1/1	0.99	0.27	-	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.