



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 10:48 pm GMT

PDB ID : 2BGM  
Title : X-RAY STRUCTURE OF TERNARY-SECOISOLARICIRESINOL DEHYDROGENASE  
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Deposited on : 2004-12-23  
Resolution : 2.00 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) : **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) : recalc28949

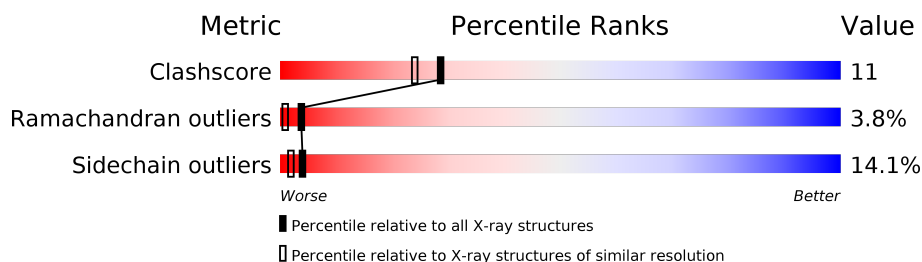
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	278	

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
3	MAX	A	6001	-	-	X	-

## 2 Entry composition [i](#)

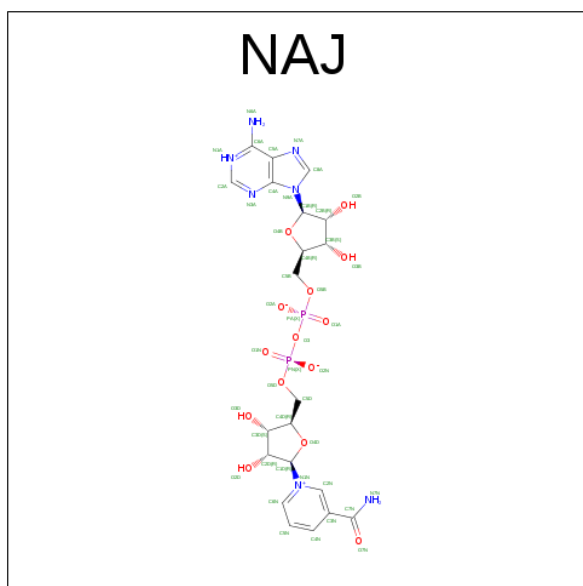
There are 4 unique types of molecules in this entry. The entry contains 2182 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RHIZOME SECOISOLARICIRE SINOL DEHYDROGENASE.

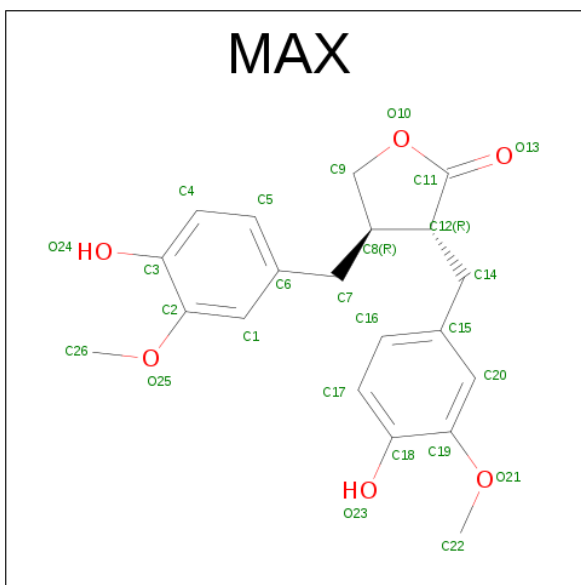
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	1985	1254	339	385	7	0	0	0

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



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

- Molecule 3 is MATAIRESINOL (three-letter code: MAX) (formula:  $C_{20}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			26	20	6		

- Molecule 4 is water.

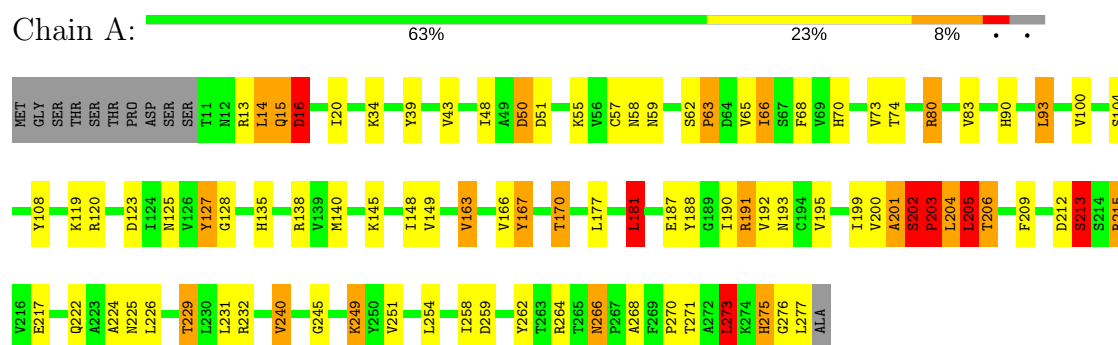
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total	O	0	0
			127	127		

### 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.

Note EDS was not executed.

#### • Molecule 1: RHIZOME SECOISOLARICIRESINOL DEHYDROGENASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.35Å 118.74Å 131.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	79.1 (10.00-2.00)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.200 , 0.229	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2182	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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: NAJ, MAX

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	1.00	3/2017 (0.1%)	1.98	59/2740 (2.2%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	VAL	CA-CB	6.36	1.68	1.54
1	A	240	VAL	CA-CB	5.43	1.66	1.54
1	A	187	GLU	CB-CG	5.38	1.62	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	GLY	CA-C-N	-15.45	83.22	117.20
1	A	127	TYR	CB-CG-CD1	-14.57	112.26	121.00
1	A	215	ARG	NE-CZ-NH2	14.24	127.42	120.30
1	A	127	TYR	CB-CG-CD2	14.15	129.49	121.00
1	A	232	ARG	NE-CZ-NH2	13.51	127.05	120.30
1	A	80	ARG	NE-CZ-NH1	11.18	125.89	120.30
1	A	225	ASN	CA-C-N	-11.00	93.00	117.20
1	A	245	GLY	O-C-N	10.31	139.20	122.70
1	A	205	LEU	N-CA-C	9.82	137.51	111.00
1	A	204	LEU	CA-C-N	-8.42	98.68	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	LEU	N-CA-C	8.30	133.42	111.00
1	A	264	ARG	NE-CZ-NH2	8.25	124.43	120.30
1	A	225	ASN	O-C-N	8.04	135.57	122.70
1	A	108	TYR	CB-CG-CD2	-7.79	116.33	121.00
1	A	195	VAL	CG1-CB-CG2	-7.71	98.56	110.90
1	A	204	LEU	C-N-CA	7.71	140.97	121.70
1	A	16	ASP	CA-CB-CG	7.70	130.35	113.40
1	A	213	SER	N-CA-C	7.62	131.57	111.00
1	A	225	ASN	N-CA-C	-7.58	90.53	111.00
1	A	200	VAL	CA-C-N	-7.44	100.83	117.20
1	A	264	ARG	NE-CZ-NH1	-7.35	116.62	120.30
1	A	203	PRO	N-CA-C	6.82	129.84	112.10
1	A	222	GLN	CA-CB-CG	6.47	127.63	113.40
1	A	215	ARG	CG-CD-NE	-6.41	98.33	111.80
1	A	206	THR	N-CA-C	6.35	128.15	111.00
1	A	167	TYR	CB-CG-CD1	-6.32	117.21	121.00
1	A	80	ARG	CG-CD-NE	6.32	125.07	111.80
1	A	215	ARG	CA-CB-CG	-6.21	99.74	113.40
1	A	80	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	245	GLY	CA-C-O	6.17	131.71	120.60
1	A	191	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	A	201	ALA	N-CA-C	6.13	127.55	111.00
1	A	229	THR	N-CA-CB	6.12	121.94	110.30
1	A	273	LEU	CA-CB-CG	6.10	129.32	115.30
1	A	13	ARG	CB-CA-C	-6.03	98.34	110.40
1	A	90	HIS	CA-C-N	5.89	127.97	116.20
1	A	204	LEU	O-C-N	5.59	131.64	122.70
1	A	222	GLN	CB-CG-CD	5.54	126.01	111.60
1	A	213	SER	N-CA-CB	-5.52	102.22	110.50
1	A	206	THR	CA-C-N	-5.51	105.07	117.20
1	A	74	THR	CA-CB-CG2	-5.50	104.70	112.40
1	A	262	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	A	145	LYS	CA-CB-CG	5.43	125.34	113.40
1	A	213	SER	CA-C-N	-5.42	105.27	117.20
1	A	259	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	215	ARG	NH1-CZ-NH2	-5.38	113.48	119.40
1	A	163	VAL	CA-CB-CG2	5.37	118.95	110.90
1	A	224	ALA	CB-CA-C	-5.33	102.11	110.10
1	A	232	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	A	205	LEU	CA-C-N	5.28	128.81	117.20
1	A	16	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	181	LEU	CA-CB-CG	5.21	127.29	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	LYS	CA-CB-CG	5.17	124.78	113.40
1	A	212	ASP	CA-CB-CG	5.16	124.76	113.40
1	A	39	TYR	CB-CG-CD2	-5.16	117.91	121.00
1	A	277	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	225	ASN	C-N-CA	5.14	134.54	121.70
1	A	50	ASP	N-CA-CB	-5.12	101.38	110.60
1	A	275	HIS	C-N-CA	5.01	132.82	122.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	SER	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	1985	0	1997	42	0
2	A	44	0	27	2	0
3	A	26	0	22	9	0
4	A	127	0	0	5	0
All	All	2182	0	2046	45	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 11.

All (45) 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:125:ASN:HD22	1:A:170:THR:HG21	1.28	0.97
1:A:104:SER:H	3:A:6001:MAX:H223	1.37	0.89
1:A:204:LEU:HD23	1:A:213:SER:H	1.43	0.83
1:A:140:MET:SD	4:A:2060:HOH:O	2.40	0.79
1:A:73:VAL:HG21	1:A:100:VAL:HG11	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLN:O	1:A:16:ASP:HB2	1.87	0.73
1:A:140:MET:HE1	1:A:148:ILE:HD11	1.75	0.68
1:A:202:SER:HB3	1:A:203:PRO:HA	1.79	0.64
1:A:51:ASP:O	1:A:55:LYS:HE2	1.97	0.64
1:A:167:TYR:HB2	3:A:6001:MAX:H221	1.78	0.64
1:A:199:ILE:HG13	3:A:6001:MAX:C5	2.28	0.64
1:A:191:ARG:HG2	1:A:249:LYS:NZ	2.17	0.60
1:A:188:TYR:HB2	1:A:190:ILE:HD12	1.85	0.57
1:A:125:ASN:HD22	1:A:170:THR:CG2	2.07	0.56
1:A:202:SER:OG	1:A:213:SER:HB3	2.08	0.54
2:A:1300:NAJ:H4N	3:A:6001:MAX:H4	1.90	0.52
1:A:57:CYS:SG	1:A:68:PHE:HB2	2.50	0.52
1:A:119:LYS:HB3	1:A:120:ARG:HH21	1.74	0.51
1:A:166:VAL:O	1:A:170:THR:HB	2.11	0.50
1:A:191:ARG:HG2	1:A:249:LYS:HZ3	1.77	0.49
1:A:202:SER:CB	1:A:203:PRO:HA	2.42	0.49
1:A:55:LYS:O	1:A:59:ASN:HB2	2.13	0.49
1:A:83:VAL:HG21	1:A:135:HIS:HB3	1.95	0.48
1:A:167:TYR:HB2	3:A:6001:MAX:C22	2.44	0.48
1:A:149:VAL:HA	1:A:193:ASN:O	2.15	0.47
3:A:6001:MAX:H17	4:A:2125:HOH:O	2.16	0.45
3:A:6001:MAX:H9C2	4:A:2127:HOH:O	2.15	0.45
1:A:266:ASN:ND2	1:A:268:ALA:H	2.15	0.45
1:A:181:LEU:HB3	1:A:192:VAL:HG21	2.00	0.44
1:A:20:ILE:HG13	1:A:93:LEU:HD21	2.01	0.43
1:A:273:LEU:HA	4:A:2117:HOH:O	2.17	0.43
1:A:73:VAL:H	2:A:1300:NAJ:H1A	1.66	0.43
1:A:104:SER:N	3:A:6001:MAX:H223	2.19	0.43
1:A:73:VAL:O	1:A:128:GLY:HA2	2.18	0.43
1:A:135:HIS:HD2	1:A:138:ARG:HH21	1.68	0.42
1:A:43:VAL:O	1:A:66:ILE:HA	2.20	0.42
1:A:204:LEU:CD2	1:A:213:SER:H	2.22	0.41
1:A:249:LYS:HA	1:A:249:LYS:HD3	1.88	0.41
1:A:270:PRO:O	1:A:273:LEU:HB3	2.20	0.41
1:A:249:LYS:HD2	4:A:2023:HOH:O	2.20	0.41
1:A:199:ILE:HG13	3:A:6001:MAX:C4	2.50	0.41
1:A:177:LEU:O	1:A:181:LEU:HB2	2.21	0.41
1:A:14:LEU:HD12	1:A:14:LEU:HA	1.99	0.40
1:A:270:PRO:HA	1:A:273:LEU:HB3	2.03	0.40
1:A:48:ILE:HA	1:A:70:HIS:CE1	2.55	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	265/278 (95%)	237 (89%)	18 (7%)	10 (4%)	<b>4</b> <b>1</b>

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	201	ALA
1	A	205	LEU
1	A	209	PHE
1	A	50	ASP
1	A	203	PRO
1	A	276	GLY
1	A	275	HIS
1	A	63	PRO
1	A	226	LEU

### 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	213/222 (96%)	183 (86%)	30 (14%)	<b>4</b> <b>2</b>

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU

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Mol	Chain	Res	Type
1	A	15	GLN
1	A	16	ASP
1	A	58	ASN
1	A	62	SER
1	A	63	PRO
1	A	65	VAL
1	A	66	ILE
1	A	80	ARG
1	A	93	LEU
1	A	123	ASP
1	A	127	TYR
1	A	163	VAL
1	A	170	THR
1	A	181	LEU
1	A	202	SER
1	A	205	LEU
1	A	206	THR
1	A	213	SER
1	A	215	ARG
1	A	217	GLU
1	A	229	THR
1	A	231	LEU
1	A	240	VAL
1	A	249	LYS
1	A	251	VAL
1	A	258	ILE
1	A	266	ASN
1	A	271	THR
1	A	273	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	135	HIS
1	A	266	ASN

### 5.3.3 RNA ⓘ

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](#)

2 ligands are modelled in this entry.

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	NAJ	A	1300	-	41,48,48	1.05	5 (12%)	43,73,73	1.92	6 (13%)
3	MAX	A	6001	-	28,28,28	1.56	8 (28%)	37,39,39	2.48	7 (18%)

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	NAJ	A	1300	-	-	0/22/62/62	0/5/5/5
3	MAX	A	6001	-	-	0/12/25/25	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	6001	MAX	C18-C19	-3.03	1.35	1.40
3	A	6001	MAX	C3-C2	-2.84	1.35	1.40
3	A	6001	MAX	C4-C3	-2.59	1.34	1.39
3	A	6001	MAX	C17-C18	-2.40	1.35	1.39
3	A	6001	MAX	C20-C15	-2.25	1.35	1.39
3	A	6001	MAX	C17-C16	-2.24	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	6001	MAX	C1-C6	-2.23	1.35	1.39
3	A	6001	MAX	C5-C4	-2.20	1.34	1.38
2	A	1300	NAJ	C2B-C1B	-2.10	1.50	1.53
2	A	1300	NAJ	O4B-C1B	2.23	1.44	1.41
2	A	1300	NAJ	C6N-N1N	2.23	1.41	1.35
2	A	1300	NAJ	C3N-C7N	2.48	1.54	1.50
2	A	1300	NAJ	O4D-C1D	2.53	1.44	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1300	NAJ	N3A-C2A-N1A	-9.49	120.59	128.86
2	A	1300	NAJ	C4B-O4B-C1B	-4.49	104.99	109.77
2	A	1300	NAJ	C1B-N9A-C4A	-2.84	121.73	126.64
3	A	6001	MAX	O21-C19-C20	-2.54	119.90	124.17
3	A	6001	MAX	O24-C3-C4	-2.51	112.51	119.35
2	A	1300	NAJ	N6A-C6A-N1A	2.02	122.77	118.77
2	A	1300	NAJ	C2A-N1A-C6A	2.10	122.45	118.77
3	A	6001	MAX	C22-O21-C19	2.24	120.77	117.54
3	A	6001	MAX	O21-C19-C18	2.69	117.83	114.55
3	A	6001	MAX	O25-C2-C3	3.00	118.20	114.55
3	A	6001	MAX	C26-O25-C2	3.17	122.10	117.54
2	A	1300	NAJ	C4A-C5A-N7A	3.70	112.99	109.41
3	A	6001	MAX	C14-C12-C11	12.68	135.19	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1300	NAJ	2	0
3	A	6001	MAX	9	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

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.