



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:45 AM GMT

PDB ID : 2BGL
Title : X-RAY STRUCTURE OF BINARY-SECOISOLARICIRE SINOL DEHYDROGENASE
Authors : Youn, B.; Moinuddin, S.G.; Davin, L.B.; Lewis, N.G.; Kang, C.
Deposited on : 2004-12-23
Resolution : 2.80 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
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

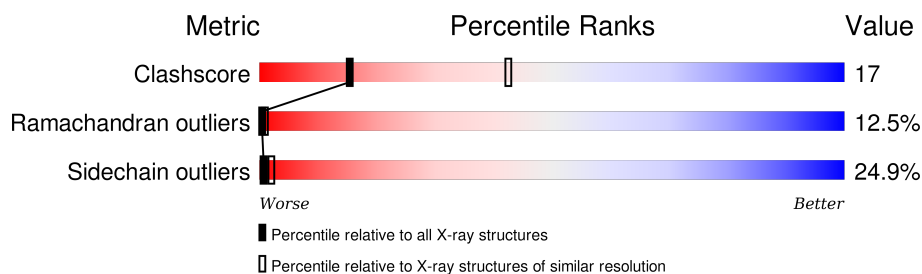
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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 ≥ 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	

2 Entry composition [i](#)

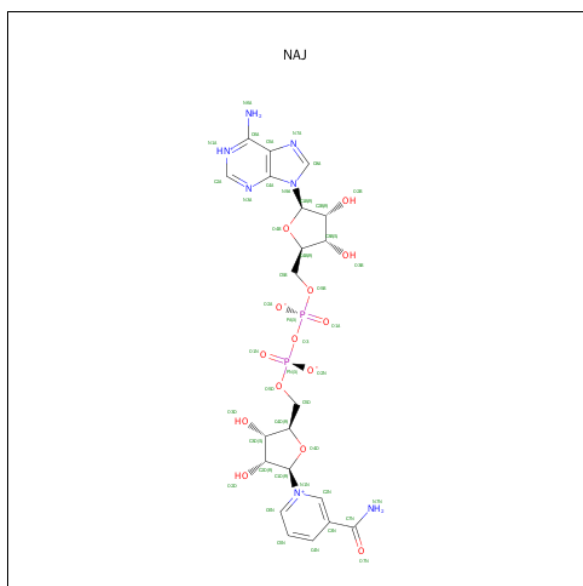
There are 3 unique types of molecules in this entry. The entry contains 2057 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	267	Total	C	N	O	S	0	0	0
			1985	1254	339	385	7			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (ACIDIC FORM) (three-letter code: NAJ) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 3 is water.

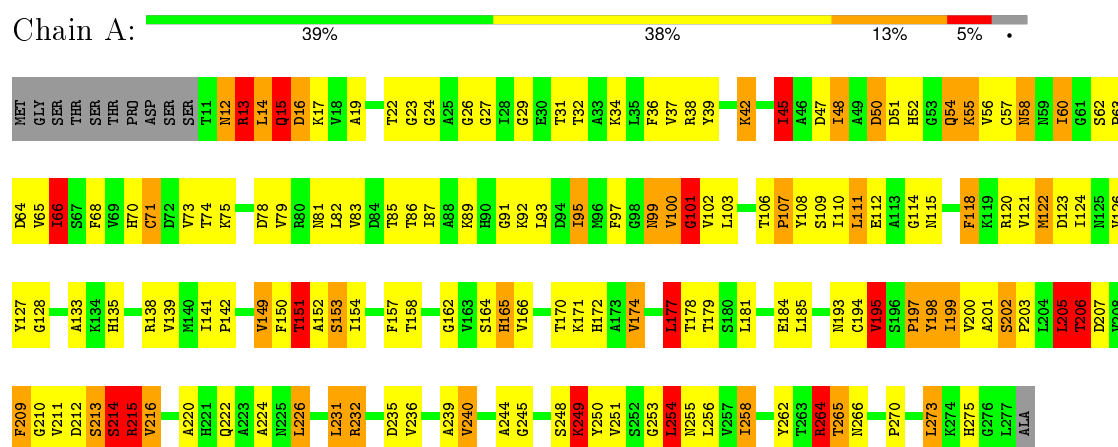
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	28	Total	0	0
			28		

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 ($RSRZ > 2$). 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 will therefore be incomplete.

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	58.51Å 118.91Å 132.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	99.7 (10.00-2.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR NULL	Depositor
R, R_{free}	0.201 , 0.221	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2057	wwPDB-VP
Average B, all atoms (Å ²)	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

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	0.90	0/2017	1.95	61/2740 (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	3

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	101	GLY	CA-C-N	-12.35	90.04	117.20
1	A	127	TYR	CA-CB-CG	8.49	129.53	113.40
1	A	273	LEU	CA-CB-CG	8.48	134.81	115.30
1	A	177	LEU	CA-CB-CG	8.27	134.31	115.30
1	A	120	ARG	NE-CZ-NH2	8.25	124.42	120.30
1	A	13	ARG	NE-CZ-NH2	8.24	124.42	120.30
1	A	138	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	A	213	SER	CA-C-N	-8.05	99.49	117.20
1	A	198	TYR	CB-CG-CD2	-7.76	116.34	121.00
1	A	201	ALA	N-CA-C	7.58	131.46	111.00
1	A	38	ARG	NE-CZ-NH2	7.55	124.08	120.30
1	A	215	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	A	112	GLU	O-C-N	7.25	134.29	122.70
1	A	195	VAL	CG1-CB-CG2	-7.12	99.51	110.90
1	A	198	TYR	CB-CG-CD1	7.05	125.23	121.00
1	A	120	ARG	NE-CZ-NH1	-7.03	116.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	GLY	O-C-N	7.00	133.91	122.70
1	A	255	ASN	N-CA-C	-6.93	92.29	111.00
1	A	114	GLY	CA-C-N	-6.93	101.96	117.20
1	A	15	GLN	O-C-N	6.68	133.38	122.70
1	A	240	VAL	CG1-CB-CG2	-6.56	100.40	110.90
1	A	112	GLU	CA-C-N	-6.47	102.96	117.20
1	A	115	ASN	N-CA-C	6.47	128.47	111.00
1	A	15	GLN	CA-C-N	-6.42	103.07	117.20
1	A	16	ASP	CA-CB-CG	6.32	127.30	113.40
1	A	213	SER	N-CA-C	6.22	127.78	111.00
1	A	66	ILE	CB-CA-C	-6.09	99.41	111.60
1	A	249	LYS	N-CA-C	5.99	127.17	111.00
1	A	151	THR	N-CA-CB	5.98	121.66	110.30
1	A	254	LEU	N-CA-C	5.97	127.12	111.00
1	A	206	THR	CA-CB-CG2	5.92	120.69	112.40
1	A	214	SER	N-CA-C	-5.83	95.25	111.00
1	A	226	LEU	CA-C-N	-5.77	104.50	117.20
1	A	14	LEU	CA-CB-CG	5.72	128.46	115.30
1	A	210	GLY	N-CA-C	-5.70	98.85	113.10
1	A	39	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	A	54	GLN	CB-CG-CD	5.56	126.06	111.60
1	A	232	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	A	215	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	A	13	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	107	PRO	N-CA-C	5.25	125.76	112.10
1	A	45	ILE	CA-CB-CG1	-5.24	101.04	111.00
1	A	15	GLN	C-N-CA	5.24	134.81	121.70
1	A	38	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	A	70	HIS	CA-C-N	-5.20	105.77	117.20
1	A	264	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	248	SER	CB-CA-C	-5.16	100.29	110.10
1	A	114	GLY	C-N-CA	5.16	134.59	121.70
1	A	205	LEU	C-N-CA	5.16	134.59	121.70
1	A	149	VAL	CA-CB-CG1	-5.14	103.18	110.90
1	A	265	THR	CA-CB-CG2	-5.13	105.21	112.40
1	A	258	ILE	CA-C-N	-5.11	105.97	117.20
1	A	174	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	A	56	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	A	126	VAL	CB-CA-C	-5.08	101.74	111.40
1	A	254	LEU	C-N-CA	5.08	134.40	121.70
1	A	209	PHE	CA-C-N	-5.02	106.15	116.20
1	A	235	ASP	CB-CG-OD2	5.02	122.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	A	158	THR	N-CA-C	5.01	124.52	111.00
1	A	63	PRO	N-CA-C	5.00	125.11	112.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	GLY	Mainchain
1	A	202	SER	Peptide
1	A	62	SER	Peptide

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	1985	0	1997	70	0
2	A	44	0	27	3	0
3	A	28	0	0	1	0
All	All	2057	0	2024	70	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 17.

All (70) 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:55:LYS:HA	1:A:58:ASN:HD22	1.44	0.82
1:A:206:THR:HA	1:A:211:VAL:HG23	1.63	0.78
1:A:264:ARG:HH11	1:A:264:ARG:HB3	1.53	0.73
1:A:54:GLN:O	1:A:58:ASN:HB3	1.87	0.73
1:A:200:VAL:HG22	1:A:231:LEU:HD22	1.72	0.72
1:A:45:ILE:HB	1:A:57:CYS:SG	2.33	0.69
1:A:86:THR:HG21	1:A:93:LEU:HD12	1.74	0.68
1:A:178:THR:HG21	1:A:194:CYS:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:HE3	2:A:1300:NAJ:O2D	1.99	0.63
1:A:166:VAL:O	1:A:170:THR:HG23	1.99	0.62
1:A:205:LEU:HB2	1:A:213:SER:HB2	1.83	0.60
1:A:141:ILE:HD11	1:A:185:LEU:HD11	1.83	0.60
1:A:151:THR:HA	1:A:195:VAL:HG13	1.83	0.59
1:A:197:PRO:HA	1:A:258:ILE:HG23	1.84	0.58
1:A:205:LEU:HD12	1:A:213:SER:HB2	1.84	0.58
1:A:87:ILE:HD11	1:A:139:VAL:HG21	1.86	0.58
1:A:34:LYS:HE2	1:A:60:ILE:HG12	1.86	0.57
1:A:154:ILE:HG23	1:A:197:PRO:O	2.05	0.57
1:A:149:VAL:HA	1:A:193:ASN:O	2.05	0.57
1:A:12:ASN:HD22	1:A:12:ASN:H	1.51	0.57
1:A:42:LYS:HG3	1:A:65:VAL:HG12	1.85	0.57
1:A:133:ALA:HB1	1:A:181:LEU:HD21	1.87	0.56
1:A:264:ARG:NH1	1:A:264:ARG:HB3	2.21	0.55
1:A:13:ARG:HG3	1:A:13:ARG:HH21	1.71	0.55
1:A:211:VAL:HG11	3:A:2021:HOH:O	2.06	0.55
1:A:205:LEU:HB2	1:A:213:SER:H	1.72	0.55
1:A:102:VAL:HG21	1:A:124:ILE:HD13	1.89	0.53
1:A:73:VAL:HG21	1:A:100:VAL:HG21	1.91	0.53
1:A:101:GLY:HA3	2:A:1300:NAJ:H3D	1.92	0.52
1:A:198:TYR:O	1:A:200:VAL:HG23	2.10	0.52
1:A:109:SER:HB3	1:A:111:LEU:HD23	1.91	0.52
1:A:214:SER:C	1:A:216:VAL:H	2.13	0.51
1:A:254:LEU:HD23	1:A:256:LEU:HD12	1.92	0.51
1:A:36:PHE:HZ	1:A:240:VAL:HG12	1.77	0.49
1:A:118:PHE:O	1:A:122:MET:HB2	2.11	0.49
1:A:231:LEU:HD23	1:A:232:ARG:H	1.77	0.49
1:A:177:LEU:HD22	1:A:181:LEU:HD22	1.95	0.49
1:A:152:ALA:HA	1:A:171:LYS:HD2	1.95	0.48
1:A:51:ASP:O	1:A:55:LYS:HG2	2.14	0.47
1:A:205:LEU:HB3	1:A:206:THR:H	1.52	0.47
1:A:48:ILE:HG23	1:A:71:CYS:O	2.14	0.47
1:A:83:VAL:O	1:A:86:THR:HG22	2.15	0.47
1:A:239:ALA:HB1	1:A:256:LEU:HD22	1.95	0.47
1:A:95:ILE:HG21	1:A:244:ALA:HB1	1.96	0.47
1:A:36:PHE:CZ	1:A:240:VAL:HG12	2.50	0.46
1:A:24:GLY:HA2	1:A:29:GLY:HA3	1.97	0.46
1:A:170:THR:O	1:A:174:VAL:HG23	2.16	0.46
1:A:32:THR:HG22	1:A:32:THR:O	2.16	0.45
1:A:17:LYS:HE2	1:A:245:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:VAL:HG21	1:A:254:LEU:HD13	1.99	0.45
1:A:12:ASN:OD1	1:A:15:GLN:HG3	2.17	0.44
1:A:34:LYS:CE	1:A:60:ILE:HG12	2.48	0.44
1:A:65:VAL:C	1:A:66:ILE:HD13	2.38	0.43
1:A:110:ILE:HG23	1:A:111:LEU:N	2.32	0.43
1:A:195:VAL:HG21	1:A:236:VAL:HG13	2.00	0.43
1:A:50:ASP:HA	1:A:68:PHE:CZ	2.53	0.43
1:A:199:ILE:CG2	1:A:220:ALA:HB2	2.48	0.43
1:A:83:VAL:HG21	1:A:135:HIS:HB3	2.01	0.43
1:A:50:ASP:HA	1:A:68:PHE:CE2	2.53	0.43
1:A:45:ILE:CG2	1:A:57:CYS:SG	3.06	0.42
1:A:75:LYS:O	1:A:79:VAL:HG23	2.19	0.42
1:A:121:VAL:O	1:A:170:THR:HG21	2.20	0.42
1:A:19:ALA:HB2	1:A:95:ILE:HD12	2.02	0.41
1:A:45:ILE:HG22	1:A:68:PHE:HD1	1.85	0.41
1:A:37:VAL:HG21	1:A:66:ILE:HD12	2.02	0.41
1:A:89:LYS:HE3	1:A:89:LYS:HB2	1.64	0.41
1:A:153:SER:HB3	2:A:1300:NAJ:H6N	2.02	0.41
1:A:250:TYR:O	1:A:250:TYR:CD2	2.74	0.41
1:A:22:THR:O	1:A:22:THR:HG22	2.21	0.41
1:A:32:THR:HG21	1:A:97:PHE:CE2	2.56	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%)	168 (63%)	64 (24%)	33 (12%)	0 1

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ILE
1	A	100	VAL
1	A	107	PRO
1	A	205	LEU
1	A	209	PHE
1	A	212	ASP
1	A	214	SER
1	A	254	LEU
1	A	266	ASN
1	A	275	HIS
1	A	16	ASP
1	A	27	GLY
1	A	82	LEU
1	A	99	ASN
1	A	108	TYR
1	A	151	THR
1	A	224	ALA
1	A	262	TYR
1	A	23	GLY
1	A	165	HIS
1	A	203	PRO
1	A	253	GLY
1	A	13	ARG
1	A	206	THR
1	A	207	ASP
1	A	215	ARG
1	A	249	LYS
1	A	202	SER
1	A	26	GLY
1	A	162	GLY
1	A	91	GLY
1	A	128	GLY
1	A	197	PRO

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	213/222 (96%)	160 (75%)	53 (25%)	1 2

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	14	LEU
1	A	15	GLN
1	A	31	THR
1	A	42	LYS
1	A	45	ILE
1	A	47	ASP
1	A	48	ILE
1	A	50	ASP
1	A	52	HIS
1	A	55	LYS
1	A	58	ASN
1	A	64	ASP
1	A	66	ILE
1	A	71	CYS
1	A	74	THR
1	A	78	ASP
1	A	81	ASN
1	A	85	THR
1	A	92	LYS
1	A	95	ILE
1	A	99	ASN
1	A	103	LEU
1	A	106	THR
1	A	111	LEU
1	A	118	PHE
1	A	122	MET
1	A	123	ASP
1	A	142	PRO
1	A	150	PHE
1	A	153	SER
1	A	157	PHE
1	A	164	SER
1	A	165	HIS
1	A	172	HIS
1	A	177	LEU
1	A	179	THR
1	A	184	GLU

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Mol	Chain	Res	Type
1	A	195	VAL
1	A	199	ILE
1	A	205	LEU
1	A	206	THR
1	A	214	SER
1	A	215	ARG
1	A	216	VAL
1	A	222	GLN
1	A	226	LEU
1	A	231	LEU
1	A	249	LYS
1	A	264	ARG
1	A	265	THR
1	A	270	PRO
1	A	273	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	58	ASN
1	A	59	ASN
1	A	81	ASN
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 ⓘ

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

1 ligand is 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	-	38,48,48	1.01	2 (5%)	47,73,73	2.08	7 (14%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1300	NAJ	C6N-N1N	2.52	1.42	1.35
2	A	1300	NAJ	O4D-C1D	3.11	1.45	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1300	NAJ	N3A-C2A-N1A	-9.59	121.55	128.89
2	A	1300	NAJ	C4B-O4B-C1B	-5.55	103.62	109.72
2	A	1300	NAJ	C1B-N9A-C4A	-2.73	122.82	126.94
2	A	1300	NAJ	O4B-C1B-N9A	2.67	113.69	108.10
2	A	1300	NAJ	C4A-C5A-N7A	2.87	112.12	109.48
2	A	1300	NAJ	C2B-C1B-N9A	3.27	119.29	114.29
2	A	1300	NAJ	O4D-C1D-N1N	3.66	112.15	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1300	NAJ	3	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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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