



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:27 PM UTC

PDB ID : 2BGL / pdb_00002bgl
Title : X-Ray structure of binary-Secoisolariciresinol 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

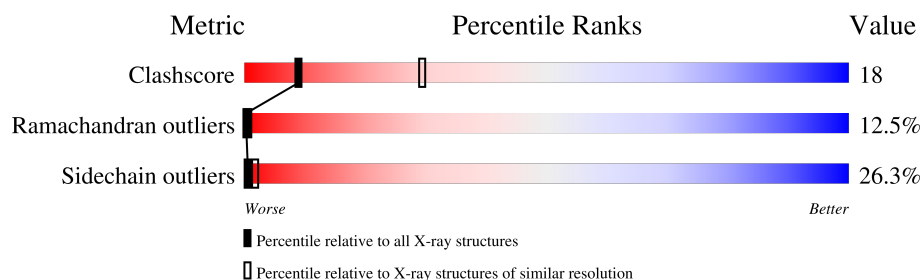
1 Overall quality at a glance

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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 of 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	278	

2 Entry composition [i](#)

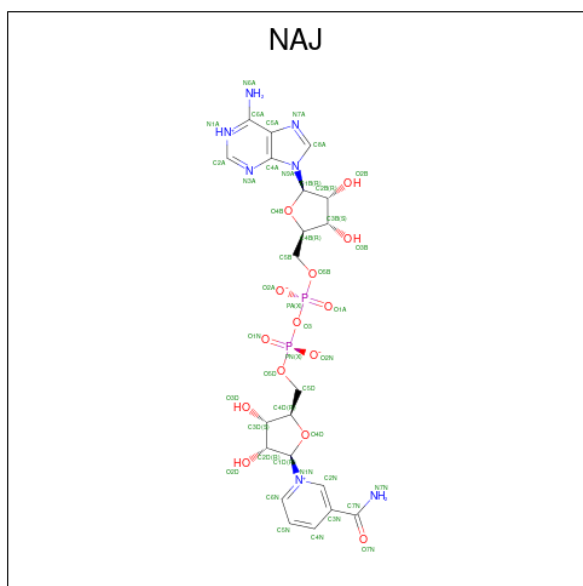
There are 3 unique types of molecules in this entry. The entry contains 2057 atoms, of which 0 are hydrogens and 0 are deuteriums.

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) (CCD ID: NAJ) (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		

- Molecule 3 is water.

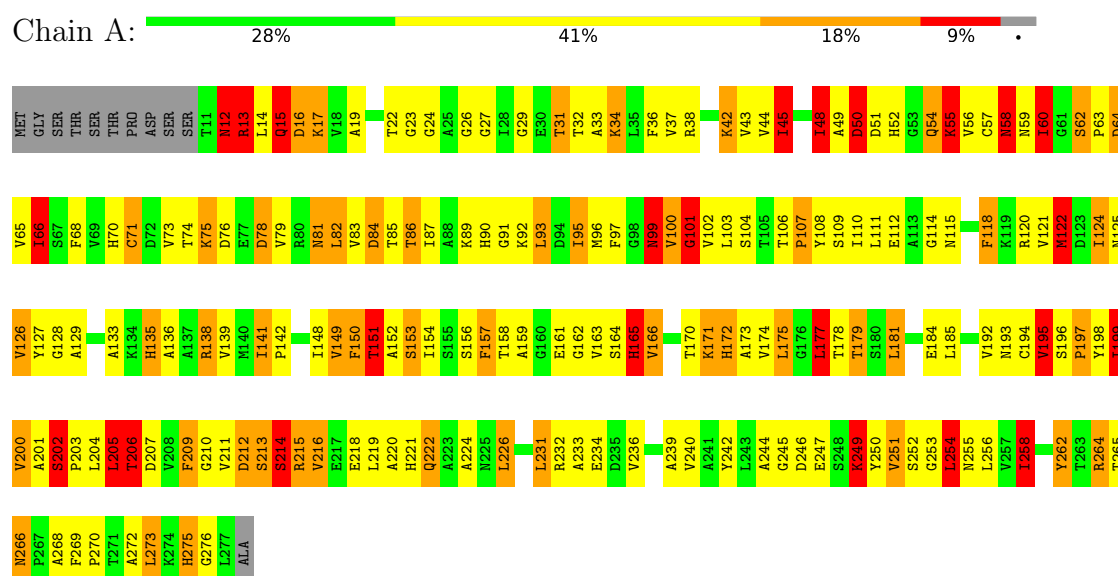
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	28	Total	0	0
			28		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: 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, 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	1.29	15/2017 (0.7%)	2.50	157/2740 (5.7%)

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	VAL	CA-CB	8.83	1.63	1.53
1	A	163	VAL	CA-CB	7.94	1.63	1.54
1	A	141	ILE	CA-CB	7.90	1.58	1.54
1	A	90	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	275	HIS	CD2-NE2	-6.64	1.30	1.37
1	A	258	ILE	CA-CB	6.52	1.63	1.54
1	A	52	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	135	HIS	CD2-NE2	-6.45	1.30	1.37
1	A	165	HIS	CD2-NE2	-6.41	1.30	1.37
1	A	221	HIS	CD2-NE2	-5.90	1.31	1.37
1	A	70	HIS	CD2-NE2	-5.76	1.31	1.37
1	A	135	HIS	CG-ND1	-5.58	1.32	1.38
1	A	177	LEU	CA-CB	5.32	1.59	1.52
1	A	150	PHE	N-CA	-5.18	1.43	1.46
1	A	60	ILE	CA-CB	5.09	1.61	1.54

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ASP	CA-CB-CG	14.70	127.30	112.60
1	A	115	ASN	N-CA-C	12.88	128.47	113.01
1	A	201	ALA	N-CA-C	12.10	131.46	107.62
1	A	213	SER	N-CA-C	11.96	127.78	109.96
1	A	56	VAL	N-CA-C	-11.89	102.23	111.62
1	A	58	ASN	CA-CB-CG	10.67	123.27	112.60
1	A	268	ALA	N-CA-C	-10.12	100.21	111.14
1	A	159	ALA	N-CA-C	10.04	121.49	108.34
1	A	118	PHE	N-CA-C	-9.89	100.02	113.18
1	A	66	ILE	CB-CA-C	-9.65	99.41	110.41
1	A	59	ASN	CA-CB-CG	9.23	121.83	112.60
1	A	156	SER	N-CA-C	-8.76	100.71	111.40
1	A	255	ASN	CA-CB-CG	8.72	121.32	112.60
1	A	255	ASN	N-CA-C	-8.69	92.29	110.80
1	A	127	TYR	CA-CB-CG	8.68	129.53	113.90
1	A	101	GLY	O-C-N	8.62	133.91	122.70
1	A	15	GLN	O-C-N	8.27	133.38	122.96
1	A	86	THR	N-CA-C	-8.23	101.36	111.40
1	A	179	THR	N-CA-C	-8.09	102.43	113.18
1	A	272	ALA	N-CA-C	-7.95	102.61	113.18
1	A	54	GLN	CB-CG-CD	7.92	126.06	112.60
1	A	266	ASN	CA-C-N	7.89	129.70	119.84
1	A	266	ASN	C-N-CA	7.89	129.70	119.84
1	A	126	VAL	CB-CA-C	-7.73	101.74	111.94
1	A	246	ASP	CA-CB-CG	7.69	120.29	112.60
1	A	249	LYS	N-CA-C	7.69	127.17	110.80
1	A	254	LEU	N-CA-C	7.66	127.12	110.80
1	A	52	HIS	N-CA-C	-7.62	102.96	112.72
1	A	165	HIS	CA-C-N	7.58	131.65	122.63
1	A	165	HIS	C-N-CA	7.58	131.65	122.63
1	A	150	PHE	N-CA-CB	-7.52	104.60	111.59
1	A	12	ASN	CA-CB-CG	7.32	119.92	112.60
1	A	55	LYS	CA-C-N	7.30	130.90	123.16
1	A	55	LYS	C-N-CA	7.30	130.90	123.16
1	A	214	SER	N-CA-C	-7.30	95.25	110.80
1	A	213	SER	CA-C-O	7.29	129.08	120.70
1	A	75	LYS	N-CA-C	7.17	121.21	109.24
1	A	66	ILE	N-CA-C	7.16	119.57	107.18
1	A	114	GLY	N-CA-C	7.14	124.23	112.66
1	A	276	GLY	N-CA-C	6.96	121.35	110.71
1	A	15	GLN	CA-C-N	6.95	134.81	121.54
1	A	15	GLN	C-N-CA	6.95	134.81	121.54
1	A	54	GLN	OE1-CD-NE2	-6.94	115.66	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	LYS	N-CA-C	6.83	119.87	110.24
1	A	205	LEU	CA-C-N	6.83	134.59	121.54
1	A	205	LEU	C-N-CA	6.83	134.59	121.54
1	A	115	ASN	CB-CG-ND2	-6.79	106.21	116.40
1	A	125	ASN	CA-C-O	-6.78	113.77	120.89
1	A	114	GLY	CA-C-N	6.77	134.59	121.18
1	A	114	GLY	C-N-CA	6.77	134.59	121.18
1	A	254	LEU	CA-C-N	6.73	134.40	121.54
1	A	254	LEU	C-N-CA	6.73	134.40	121.54
1	A	269	PHE	CA-CB-CG	-6.70	107.10	113.80
1	A	48	ILE	CB-CA-C	-6.69	103.28	112.24
1	A	151	THR	N-CA-CB	6.61	121.66	110.49
1	A	212	ASP	CA-CB-CG	6.57	119.17	112.60
1	A	200	VAL	N-CA-C	6.56	122.98	109.34
1	A	49	ALA	CA-C-N	6.55	134.05	121.54
1	A	49	ALA	C-N-CA	6.55	134.05	121.54
1	A	112	GLU	O-C-N	6.51	134.29	122.44
1	A	90	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	A	202	SER	N-CA-C	6.48	124.13	109.81
1	A	76	ASP	N-CA-C	6.46	120.37	112.23
1	A	107	PRO	N-CA-C	6.45	125.76	112.47
1	A	158	THR	N-CA-C	6.44	124.52	110.80
1	A	81	ASN	CA-C-O	6.43	127.78	120.84
1	A	157	PHE	CA-CB-CG	6.41	120.21	113.80
1	A	126	VAL	N-CA-CB	6.33	118.23	110.64
1	A	62	SER	CA-C-N	6.32	127.75	119.84
1	A	62	SER	C-N-CA	6.32	127.75	119.84
1	A	99	ASN	CB-CG-ND2	-6.32	106.93	116.40
1	A	31	THR	N-CA-C	-6.26	104.70	112.90
1	A	112	GLU	CB-CG-CD	6.26	123.24	112.60
1	A	212	ASP	N-CA-C	-6.23	97.54	110.80
1	A	234	GLU	CB-CG-CD	6.20	123.14	112.60
1	A	70	HIS	CA-C-O	6.16	127.79	120.70
1	A	206	THR	CA-CB-OG1	-6.16	100.37	109.60
1	A	258	ILE	CA-C-O	6.15	128.47	120.78
1	A	63	PRO	N-CA-C	6.13	125.11	112.47
1	A	175	LEU	N-CA-C	-6.12	104.44	113.61
1	A	52	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	A	122	MET	N-CA-C	-6.08	97.84	110.80
1	A	210	GLY	N-CA-C	-6.05	98.85	113.18
1	A	251	VAL	N-CA-C	6.02	116.02	106.32
1	A	177	LEU	CB-CA-C	6.00	119.24	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	THR	CA-CB-CG2	5.99	120.69	110.50
1	A	43	VAL	O-C-N	5.96	129.18	122.98
1	A	114	GLY	O-C-N	5.95	130.21	122.71
1	A	115	ASN	OD1-CG-ND2	5.95	128.54	122.60
1	A	165	HIS	CB-CG-CD2	-5.95	123.47	131.20
1	A	275	HIS	CB-CG-CD2	-5.93	123.48	131.20
1	A	266	ASN	OD1-CG-ND2	-5.92	116.69	122.60
1	A	93	LEU	CD1-CG-CD2	-5.91	97.79	110.80
1	A	127	TYR	N-CA-C	5.91	120.76	112.72
1	A	120	ARG	NE-CZ-NH2	5.81	124.42	119.20
1	A	13	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	A	195	VAL	O-C-N	-5.78	115.34	122.57
1	A	55	LYS	N-CA-C	-5.76	106.47	112.93
1	A	266	ASN	CA-CB-CG	5.76	118.36	112.60
1	A	148	ILE	N-CA-C	-5.71	98.92	107.37
1	A	166	VAL	N-CA-C	-5.68	106.27	111.67
1	A	54	GLN	N-CA-C	-5.66	106.25	114.12
1	A	78	ASP	CA-CB-CG	-5.65	106.95	112.60
1	A	205	LEU	N-CA-C	5.65	122.83	110.80
1	A	64	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	242	TYR	O-C-N	5.62	128.11	122.03
1	A	50	ASP	N-CA-C	5.61	122.74	110.80
1	A	171	LYS	CA-C-N	5.60	132.23	121.54
1	A	171	LYS	C-N-CA	5.60	132.23	121.54
1	A	196	SER	CA-C-N	5.58	126.82	119.84
1	A	196	SER	C-N-CA	5.58	126.82	119.84
1	A	112	GLU	CA-C-N	5.51	132.07	121.54
1	A	112	GLU	C-N-CA	5.51	132.07	121.54
1	A	45	ILE	CA-CB-CG1	-5.51	101.04	110.40
1	A	252	SER	N-CA-C	-5.50	106.16	112.92
1	A	84	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	161	GLU	CA-C-O	5.48	128.67	122.37
1	A	99	ASN	CA-C-N	5.47	131.82	121.97
1	A	99	ASN	C-N-CA	5.47	131.82	121.97
1	A	181	LEU	N-CA-C	-5.46	105.43	111.71
1	A	43	VAL	CA-C-N	5.44	128.13	122.96
1	A	43	VAL	C-N-CA	5.44	128.13	122.96
1	A	199	ILE	O-C-N	5.43	129.36	122.57
1	A	38	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	A	166	VAL	CA-C-O	-5.41	115.01	120.69
1	A	124	ILE	CA-C-O	-5.40	115.33	120.95
1	A	161	GLU	CB-CG-CD	5.36	121.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	GLN	N-CA-C	-5.35	106.72	113.20
1	A	99	ASN	OD1-CG-ND2	5.33	127.93	122.60
1	A	172	HIS	CB-CG-CD2	-5.32	124.28	131.20
1	A	60	ILE	N-CA-C	-5.30	98.31	109.34
1	A	171	LYS	N-CA-C	-5.29	101.68	109.62
1	A	273	LEU	CA-CB-CG	5.29	134.81	116.30
1	A	233	ALA	N-CA-C	-5.23	106.05	112.90
1	A	192	VAL	CA-C-O	5.20	125.97	120.51
1	A	226	LEU	O-C-N	5.20	129.50	122.59
1	A	269	PHE	O-C-N	-5.19	115.36	121.32
1	A	157	PHE	N-CA-C	5.18	116.74	111.14
1	A	209	PHE	CA-C-N	5.18	131.56	121.41
1	A	209	PHE	C-N-CA	5.18	131.56	121.41
1	A	204	LEU	CA-C-N	5.16	131.40	121.54
1	A	204	LEU	C-N-CA	5.16	131.40	121.54
1	A	177	LEU	CA-CB-CG	5.15	134.31	116.30
1	A	33	ALA	CA-C-N	5.14	127.69	120.28
1	A	33	ALA	C-N-CA	5.14	127.69	120.28
1	A	195	VAL	CG1-CB-CG2	-5.13	99.51	110.80
1	A	262	TYR	N-CA-C	5.12	121.69	110.80
1	A	104	SER	CA-CB-OG	5.10	121.31	111.10
1	A	129	ALA	N-CA-C	-5.08	105.44	111.69
1	A	221	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	A	202	SER	CA-C-N	5.05	126.15	119.84
1	A	202	SER	C-N-CA	5.05	126.15	119.84
1	A	86	THR	CA-CB-OG1	-5.04	102.03	109.60
1	A	247	GLU	CB-CG-CD	5.04	121.17	112.60
1	A	218	GLU	N-CA-C	-5.03	105.98	111.82
1	A	70	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	A	104	SER	N-CA-C	5.02	117.32	110.24

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 ⓘ

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	75	0
2	A	44	0	27	3	0
3	A	28	0	0	1	0
All	All	2057	0	2024	75	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 18.

All (75) 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:122:MET:HE3	1:A:170:THR:HG22	1.65	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
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:12:ASN:H	1:A:12:ASN:HD22	1.51	0.57
1:A:149:VAL:HA	1:A:193:ASN:O	2.05	0.57
1:A:42:LYS:HG3	1:A:65:VAL:HG12	1.85	0.57
1:A:214:SER:C	1:A:216:VAL:H	2.13	0.56
1:A:133:ALA:HB1	1:A:181:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:HB3	1:A:264:ARG:NH1	2.21	0.55
1:A:13:ARG:HH21	1:A:13:ARG:HG3	1.71	0.55
1:A:205:LEU:HB2	1:A:213:SER:H	1.72	0.55
1:A:211:VAL:HG11	3:A:2021:HOH:O	2.06	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: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:65:VAL:C	1:A:66:ILE:HD13	2.38	0.49
1:A:96:MET:HE2	1:A:136:ALA:HB2	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:48:ILE:HG23	1:A:71:CYS:O	2.14	0.47
1:A:205:LEU:HB3	1:A:206:THR:H	1.52	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
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:73:VAL:C	1:A:75:LYS:H	2.25	0.44
1:A:173:ALA:C	1:A:175:LEU:H	2.25	0.44
1:A:34:LYS:CE	1:A:60:ILE:HG12	2.48	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:22:THR:HG22	1:A:22:THR:O	2.21	0.41
1:A:153:SER:HB3	2:A:1300:NAJ:H6N	2.02	0.41
1:A:250:TYR:CD2	1:A:250:TYR:O	2.74	0.41
1:A:32:THR:HG21	1:A:97:PHE:CE2	2.56	0.40
1:A:84:ASP:CG	1:A:138:ARG:HH22	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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 0

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

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Mol	Chain	Res	Type
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%)	157 (74%)	56 (26%)	0 2

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	13	ARG
1	A	14	LEU
1	A	15	GLN

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Mol	Chain	Res	Type
1	A	31	THR
1	A	34	LYS
1	A	42	LYS
1	A	45	ILE
1	A	48	ILE
1	A	50	ASP
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	82	LEU
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	122	MET
1	A	126	VAL
1	A	138	ARG
1	A	142	PRO
1	A	149	VAL
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
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

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Mol	Chain	Res	Type
1	A	219	LEU
1	A	222	GLN
1	A	226	LEU
1	A	231	LEU
1	A	249	LYS
1	A	258	ILE
1	A	264	ARG
1	A	265	THR
1	A	270	PRO
1	A	273	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	15	GLN
1	A	58	ASN
1	A	81	ASN
1	A	99	ASN
1	A	135	HIS
1	A	255	ASN
1	A	266	ASN
1	A	275	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	46,48,48	1.39	4 (8%)	64,73,73	1.95	13 (20%)

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	-	-	6/30/62/62	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1300	NAJ	C2N-N1N	6.00	1.41	1.35
2	A	1300	NAJ	O4D-C1D	3.23	1.45	1.40
2	A	1300	NAJ	C6N-N1N	3.02	1.42	1.35
2	A	1300	NAJ	C5A-N7A	-2.79	1.33	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1300	NAJ	C5A-C4A-N3A	-6.38	117.88	127.27
2	A	1300	NAJ	C6N-N1N-C2N	-5.36	117.32	121.88
2	A	1300	NAJ	C2A-N3A-C4A	5.34	120.33	111.14
2	A	1300	NAJ	N9A-C4A-N3A	4.78	137.79	126.90
2	A	1300	NAJ	C6A-C5A-C4A	4.25	122.03	117.03
2	A	1300	NAJ	N1A-C2A-N3A	-3.88	121.55	128.84
2	A	1300	NAJ	C4B-O4B-C1B	-2.65	103.62	109.47
2	A	1300	NAJ	O3-PA-O1A	-2.47	103.28	110.70
2	A	1300	NAJ	O4B-C1B-N9A	2.35	113.69	108.36
2	A	1300	NAJ	O4B-C1B-C2B	-2.29	101.72	106.62
2	A	1300	NAJ	C2B-C1B-N9A	2.17	119.29	113.25
2	A	1300	NAJ	N6A-C6A-N1A	2.17	121.73	118.72
2	A	1300	NAJ	C2A-N1A-C6A	2.13	121.65	118.55

There are no chirality outliers.

All (6) torsion outliers are listed below:

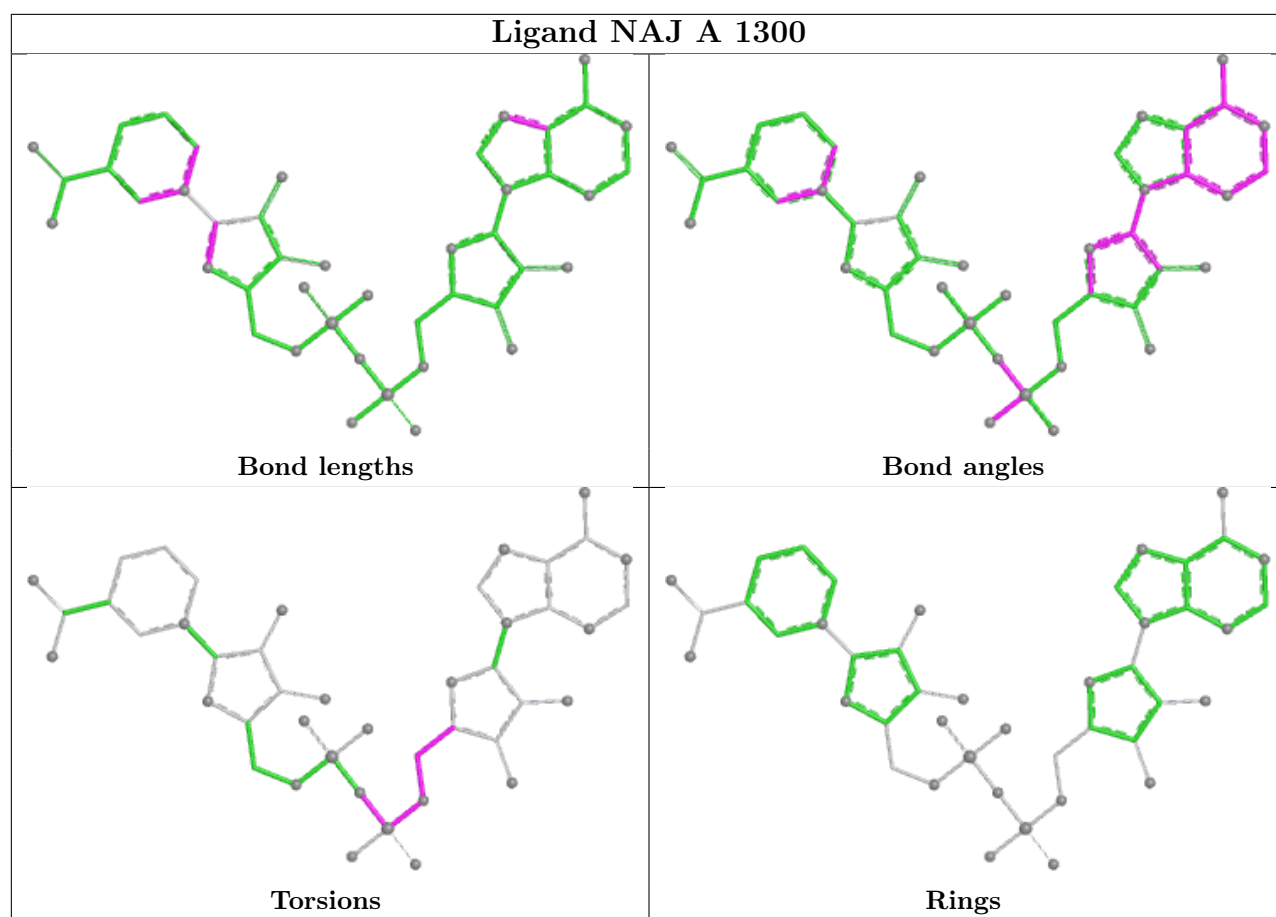
Mol	Chain	Res	Type	Atoms
2	A	1300	NAJ	C5B-O5B-PA-O1A
2	A	1300	NAJ	O4B-C4B-C5B-O5B
2	A	1300	NAJ	PN-O3-PA-O1A
2	A	1300	NAJ	C5B-O5B-PA-O2A
2	A	1300	NAJ	C4B-C5B-O5B-PA
2	A	1300	NAJ	PN-O3-PA-O5B

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.