



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:05 AM UTC

PDB ID : 2BGM / pdb_00002bgm
Title : X-Ray structure of ternary-Secoisolariciresinol Dehydrogenase
Authors : Youn, B.; Moinuddin, S.G.; Davin, L.B.; Lewis, N.G.; Kang, C.
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

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

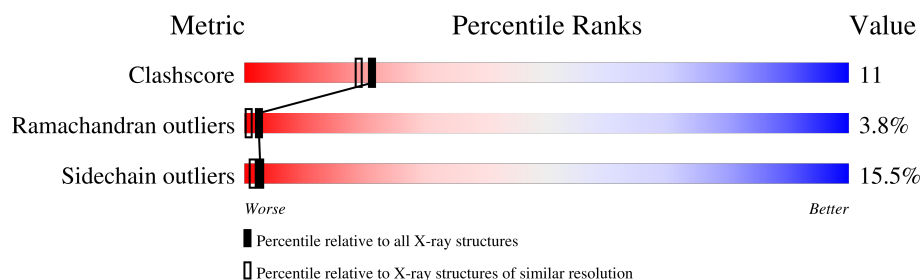
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 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	51% 27% 14% . .

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](#)

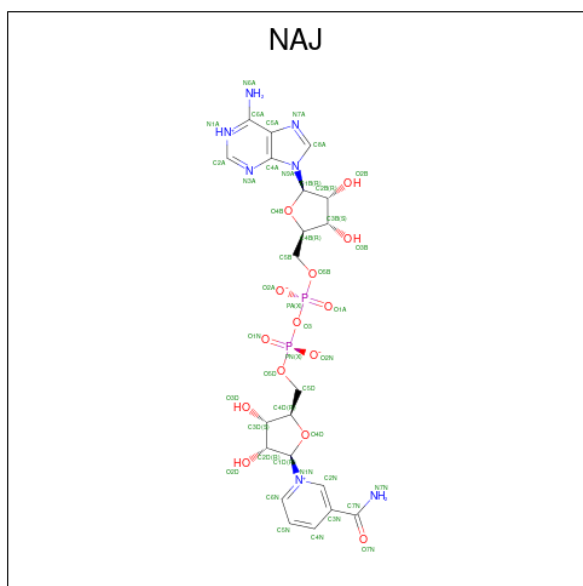
There are 4 unique types of molecules in this entry. The entry contains 2182 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

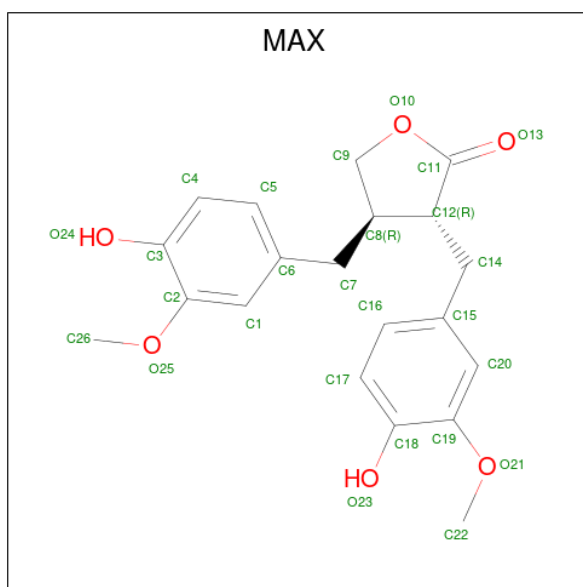
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	1985	1254	339	385	7	0	0	0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (ACIDIC FORM) (CCD ID: 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 (CCD ID: 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.

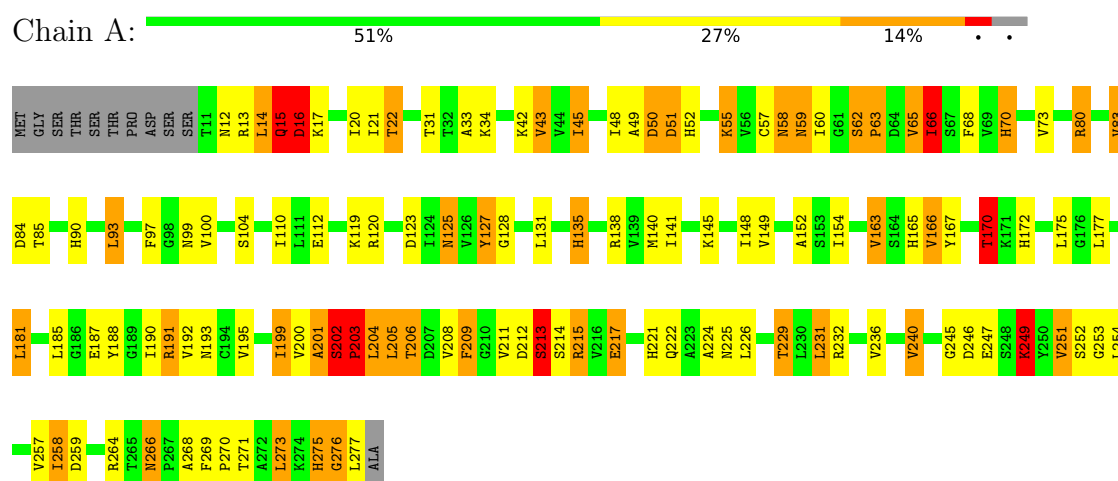
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total	O	0	0
			127	127		

3 Residue-property plots

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	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 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: MAX, 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	1.40	22/2017 (1.1%)	2.47	138/2740 (5.0%)

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 (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	VAL	CA-CB	11.59	1.68	1.54
1	A	141	ILE	CA-CB	11.37	1.60	1.54
1	A	240	VAL	CA-CB	8.69	1.66	1.54
1	A	251	VAL	CA-CB	8.64	1.64	1.54
1	A	172	HIS	CD2-NE2	-7.12	1.30	1.37
1	A	221	HIS	CD2-NE2	-6.90	1.30	1.37
1	A	135	HIS	CD2-NE2	-6.64	1.30	1.37
1	A	70	HIS	CD2-NE2	-6.64	1.30	1.37
1	A	90	HIS	CD2-NE2	-6.38	1.30	1.37
1	A	52	HIS	CD2-NE2	-6.05	1.31	1.37
1	A	166	VAL	CA-CB	5.99	1.62	1.54
1	A	225	ASN	C-O	5.92	1.31	1.24
1	A	275	HIS	CD2-NE2	-5.89	1.31	1.37
1	A	70	HIS	CG-ND1	-5.82	1.31	1.38
1	A	165	HIS	CD2-NE2	-5.76	1.31	1.37
1	A	213	SER	CA-CB	-5.75	1.45	1.53
1	A	253	GLY	CA-C	5.58	1.58	1.52
1	A	152	ALA	CA-C	-5.50	1.50	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	ILE	CA-CB	5.45	1.61	1.54
1	A	211	VAL	CA-CB	5.16	1.59	1.53
1	A	90	HIS	CG-ND1	-5.13	1.32	1.38
1	A	83	VAL	CA-CB	5.05	1.60	1.54

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ASP	CA-CB-CG	17.75	130.35	112.60
1	A	254	LEU	N-CA-C	15.65	133.42	110.10
1	A	213	SER	N-CA-C	13.97	131.57	111.87
1	A	245	GLY	O-C-N	12.69	139.20	122.70
1	A	205	LEU	N-CA-C	12.54	137.51	110.80
1	A	206	THR	N-CA-C	12.21	128.15	109.96
1	A	212	ASP	CA-CB-CG	12.16	124.76	112.60
1	A	225	ASN	N-CA-C	-11.48	90.53	109.24
1	A	225	ASN	O-C-N	10.89	135.57	123.27
1	A	58	ASN	CA-CB-CG	10.68	123.28	112.60
1	A	204	LEU	CA-C-N	10.17	140.97	121.54
1	A	204	LEU	C-N-CA	10.17	140.97	121.54
1	A	60	ILE	N-CA-C	9.39	119.36	110.53
1	A	249	LYS	N-CA-C	9.29	124.20	113.15
1	A	215	ARG	NE-CZ-NH2	9.13	127.42	119.20
1	A	232	ARG	NE-CZ-NH2	8.73	127.05	119.20
1	A	17	LYS	N-CA-C	8.69	122.84	110.23
1	A	225	ASN	CA-C-O	8.23	129.40	120.43
1	A	222	GLN	CB-CG-CD	7.89	126.01	112.60
1	A	200	VAL	CA-C-O	7.88	129.88	120.74
1	A	201	ALA	N-CA-C	7.86	127.55	110.80
1	A	275	HIS	CB-CG-CD2	-7.84	121.01	131.20
1	A	206	THR	CA-C-O	7.33	129.13	120.70
1	A	21	ILE	CB-CA-C	-7.27	102.08	111.53
1	A	215	ARG	CA-CB-CG	-7.18	99.74	114.10
1	A	163	VAL	N-CA-C	-7.13	98.16	108.36
1	A	172	HIS	CB-CG-CD2	-6.94	122.18	131.20
1	A	203	PRO	N-CA-C	6.82	129.84	112.10
1	A	204	LEU	O-C-N	6.81	131.64	123.33
1	A	225	ASN	CA-C-N	6.81	134.54	121.54
1	A	225	ASN	C-N-CA	6.81	134.54	121.54
1	A	222	GLN	CA-CB-CG	6.76	127.63	114.10
1	A	50	ASP	CA-CB-CG	6.74	119.34	112.60
1	A	217	GLU	CB-CG-CD	6.65	123.91	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	PHE	CA-CB-CG	6.61	120.41	113.80
1	A	13	ARG	CB-CA-C	-6.60	98.34	109.03
1	A	65	VAL	CB-CA-C	-6.58	104.99	111.30
1	A	224	ALA	N-CA-C	6.49	119.89	110.28
1	A	187	GLU	CB-CG-CD	6.45	123.56	112.60
1	A	208	VAL	N-CA-C	6.45	117.10	111.56
1	A	221	HIS	CB-CG-CD2	-6.44	122.83	131.20
1	A	275	HIS	CB-CG-ND1	6.44	132.36	122.70
1	A	131	LEU	CA-C-N	6.42	128.65	120.56
1	A	131	LEU	C-N-CA	6.42	128.65	120.56
1	A	245	GLY	CA-C-O	6.40	131.71	120.57
1	A	59	ASN	CA-C-N	6.36	128.70	120.56
1	A	59	ASN	C-N-CA	6.36	128.70	120.56
1	A	225	ASN	OD1-CG-ND2	-6.35	116.25	122.60
1	A	13	ARG	N-CA-CB	6.34	119.03	110.59
1	A	214	SER	N-CA-C	-6.29	104.66	112.90
1	A	215	ARG	CG-CD-NE	-6.21	98.33	112.00
1	A	208	VAL	CA-C-N	6.17	133.33	121.54
1	A	208	VAL	C-N-CA	6.17	133.33	121.54
1	A	66	ILE	CB-CG1-CD1	-6.10	100.99	113.80
1	A	125	ASN	N-CA-C	6.09	118.88	111.82
1	A	231	LEU	CB-CA-C	-6.07	101.15	110.26
1	A	275	HIS	CA-CB-CG	6.06	119.86	113.80
1	A	43	VAL	N-CA-C	6.00	117.12	108.48
1	A	269	PHE	CA-CB-CG	-5.97	107.83	113.80
1	A	84	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	31	THR	N-CA-C	-5.97	104.86	111.36
1	A	236	VAL	CA-C-N	5.96	128.55	120.38
1	A	236	VAL	C-N-CA	5.96	128.55	120.38
1	A	80	ARG	CG-CD-NE	5.94	125.07	112.00
1	A	62	SER	CA-C-N	5.93	127.26	119.84
1	A	62	SER	C-N-CA	5.93	127.26	119.84
1	A	246	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	112	GLU	CB-CG-CD	5.92	122.67	112.60
1	A	199	ILE	O-C-N	5.92	129.47	122.66
1	A	213	SER	N-CA-CB	-5.88	102.22	111.39
1	A	152	ALA	N-CA-C	-5.86	103.98	108.78
1	A	253	GLY	CA-C-O	5.85	126.53	120.80
1	A	135	HIS	CB-CG-CD2	-5.83	123.62	131.20
1	A	170	THR	N-CA-CB	-5.82	101.54	110.16
1	A	275	HIS	CA-C-N	5.82	132.82	121.41
1	A	275	HIS	C-N-CA	5.82	132.82	121.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	A	249	LYS	CA-CB-CG	-5.82	102.47	114.10
1	A	90	HIS	O-C-N	-5.81	116.40	123.19
1	A	229	THR	N-CA-CB	5.81	121.94	111.37
1	A	264	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	A	127	TYR	CB-CG-CD2	5.79	129.49	120.80
1	A	141	ILE	CA-C-O	-5.79	114.81	118.69
1	A	52	HIS	CA-C-N	5.78	126.39	119.98
1	A	52	HIS	C-N-CA	5.78	126.39	119.98
1	A	185	LEU	N-CA-C	5.74	120.35	113.23
1	A	90	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	A	204	LEU	N-CA-C	5.73	117.62	110.91
1	A	252	SER	N-CA-C	-5.73	107.53	114.75
1	A	212	ASP	CA-C-N	-5.71	113.47	122.79
1	A	212	ASP	C-N-CA	-5.71	113.47	122.79
1	A	127	TYR	CB-CG-CD1	-5.70	112.26	120.80
1	A	206	THR	CA-CB-OG1	-5.64	101.14	109.60
1	A	145	LYS	CA-CB-CG	5.62	125.34	114.10
1	A	195	VAL	CG1-CB-CG2	-5.56	98.56	110.80
1	A	15	GLN	CG-CD-NE2	5.56	124.74	116.40
1	A	85	THR	CA-CB-OG1	-5.55	101.27	109.60
1	A	99	ASN	O-C-N	-5.55	115.44	122.26
1	A	45	ILE	N-CA-CB	-5.50	103.54	110.31
1	A	97	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	221	HIS	CA-C-N	5.46	128.38	120.79
1	A	221	HIS	C-N-CA	5.46	128.38	120.79
1	A	49	ALA	CA-C-N	5.45	131.95	121.54
1	A	49	ALA	C-N-CA	5.45	131.95	121.54
1	A	49	ALA	CA-C-O	5.45	128.64	122.37
1	A	33	ALA	CA-C-N	5.45	127.52	120.44
1	A	33	ALA	C-N-CA	5.45	127.52	120.44
1	A	175	LEU	CA-C-N	5.45	126.14	119.99
1	A	175	LEU	C-N-CA	5.45	126.14	119.99
1	A	204	LEU	CA-C-O	5.41	129.58	122.44
1	A	12	ASN	CA-C-N	5.40	131.64	122.36
1	A	12	ASN	C-N-CA	5.40	131.64	122.36
1	A	50	ASP	N-CA-CB	-5.39	101.38	110.49
1	A	231	LEU	N-CA-CB	5.39	118.01	109.71
1	A	21	ILE	N-CA-CB	5.37	118.43	111.83
1	A	259	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	205	LEU	N-CA-CB	-5.36	101.44	110.49
1	A	34	LYS	CA-CB-CG	5.34	124.78	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ILE	CA-C-N	5.32	128.40	120.31
1	A	110	ILE	C-N-CA	5.32	128.40	120.31
1	A	12	ASN	O-C-N	5.28	128.35	123.50
1	A	199	ILE	CB-CG1-CD1	-5.28	102.72	113.80
1	A	247	GLU	N-CA-C	5.25	120.86	113.56
1	A	154	ILE	N-CA-C	-5.25	106.18	113.00
1	A	42	LYS	N-CA-C	-5.23	100.72	109.24
1	A	276	GLY	N-CA-C	5.19	125.48	113.18
1	A	131	LEU	N-CA-C	5.17	116.91	111.28
1	A	249	LYS	N-CA-CB	-5.11	102.59	110.46
1	A	212	ASP	O-C-N	-5.11	117.66	123.48
1	A	229	THR	CB-CA-C	-5.11	98.70	109.38
1	A	50	ASP	N-CA-C	5.11	121.68	110.80
1	A	22	THR	N-CA-CB	-5.10	102.54	110.04
1	A	22	THR	O-C-N	-5.09	116.55	122.81
1	A	80	ARG	CA-CB-CG	5.07	124.25	114.10
1	A	191	ARG	O-C-N	-5.05	117.30	123.16
1	A	214	SER	CA-C-O	5.04	125.50	119.60
1	A	163	VAL	CA-CB-CG2	5.03	118.95	110.40
1	A	51	ASP	CA-CB-CG	5.01	117.61	112.60

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
1:A:15:GLN:O	1:A:16:ASP:HB2	1.87	0.73
1:A:51:ASP:O	1:A:55:LYS:HE2	1.97	0.64
1:A:202:SER:HB3	1:A:203:PRO:HA	1.79	0.64
1:A:140:MET:HE1	1:A:148:ILE:HD11	1.80	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:191:ARG:HG2	1:A:249:LYS:HZ3	1.72	0.55
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: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:73:VAL:H	2:A:1300:NAJ:H1A	1.66	0.43
1:A:273:LEU:HA	4:A:2117:HOH:O	2.17	0.43
1:A:73:VAL:O	1:A:128:GLY:HA2	2.18	0.43
1:A:104:SER:N	3:A:6001:MAX:H223	2.19	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LYS:HD3	1:A:249:LYS:HA	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%)	2 1

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 ⓘ

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%)	180 (84%)	33 (16%)	2 1

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	15	GLN
1	A	22	THR
1	A	45	ILE
1	A	55	LYS
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	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	257	VAL
1	A	258	ILE
1	A	266	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	271	THR
1	A	273	LEU
1	A	277	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	58	ASN
1	A	99	ASN
1	A	135	HIS
1	A	165	HIS
1	A	193	ASN
1	A	266	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 oligosaccharides 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	-	46,48,48	1.46	6 (13%)	64,73,73	1.78	11 (17%)
3	MAX	A	6001	-	28,28,28	1.61	10 (35%)	38,39,39	2.86	8 (21%)

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	-	-	10/30/62/62	0/5/5/5
3	MAX	A	6001	-	-	6/12/25/25	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1300	NAJ	C2N-N1N	6.21	1.41	1.35
2	A	1300	NAJ	C5A-N7A	-3.08	1.32	1.39
2	A	1300	NAJ	O4D-C1D	2.95	1.44	1.40
3	A	6001	MAX	C4-C3	-2.73	1.34	1.39
3	A	6001	MAX	C18-C19	-2.61	1.35	1.40
2	A	1300	NAJ	C6N-N1N	2.59	1.41	1.35
2	A	1300	NAJ	C3N-C7N	2.54	1.54	1.50
3	A	6001	MAX	C17-C18	-2.54	1.35	1.39
3	A	6001	MAX	C17-C16	-2.52	1.34	1.38
2	A	1300	NAJ	PN-O3	2.50	1.62	1.59
3	A	6001	MAX	C5-C4	-2.48	1.34	1.38
3	A	6001	MAX	C3-C2	-2.44	1.35	1.40
3	A	6001	MAX	C20-C15	-2.36	1.35	1.39
3	A	6001	MAX	C1-C6	-2.34	1.35	1.39
3	A	6001	MAX	C5-C6	-2.04	1.34	1.38
3	A	6001	MAX	C20-C19	-2.01	1.35	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	6001	MAX	C14-C12-C11	13.10	135.19	112.35
3	A	6001	MAX	C7-C8-C9	8.85	124.88	112.66
2	A	1300	NAJ	C5A-C4A-N3A	-5.58	119.05	127.27
2	A	1300	NAJ	C2A-N3A-C4A	5.39	120.42	111.14
2	A	1300	NAJ	C6N-N1N-C2N	-4.57	117.99	121.88
2	A	1300	NAJ	N9A-C4A-N3A	4.52	137.21	126.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1300	NAJ	N1A-C2A-N3A	-4.39	120.59	128.84
2	A	1300	NAJ	C6A-C5A-C4A	3.55	121.21	117.03
3	A	6001	MAX	C26-O25-C2	3.13	122.10	117.51
2	A	1300	NAJ	N6A-C6A-N1A	2.92	122.77	118.72
2	A	1300	NAJ	O4B-C1B-N9A	2.71	114.51	108.36
2	A	1300	NAJ	C2A-N1A-C6A	2.68	122.45	118.55
3	A	6001	MAX	O24-C3-C4	-2.56	112.51	119.36
3	A	6001	MAX	O25-C2-C3	2.44	118.20	114.55
3	A	6001	MAX	O21-C19-C20	-2.43	119.90	124.08
3	A	6001	MAX	C22-O21-C19	2.22	120.77	117.51
3	A	6001	MAX	O21-C19-C18	2.19	117.83	114.55
2	A	1300	NAJ	O3-PA-O1A	-2.14	104.26	110.70
2	A	1300	NAJ	C4B-O4B-C1B	-2.03	104.99	109.47

There are no chirality outliers.

All (16) torsion outliers are listed below:

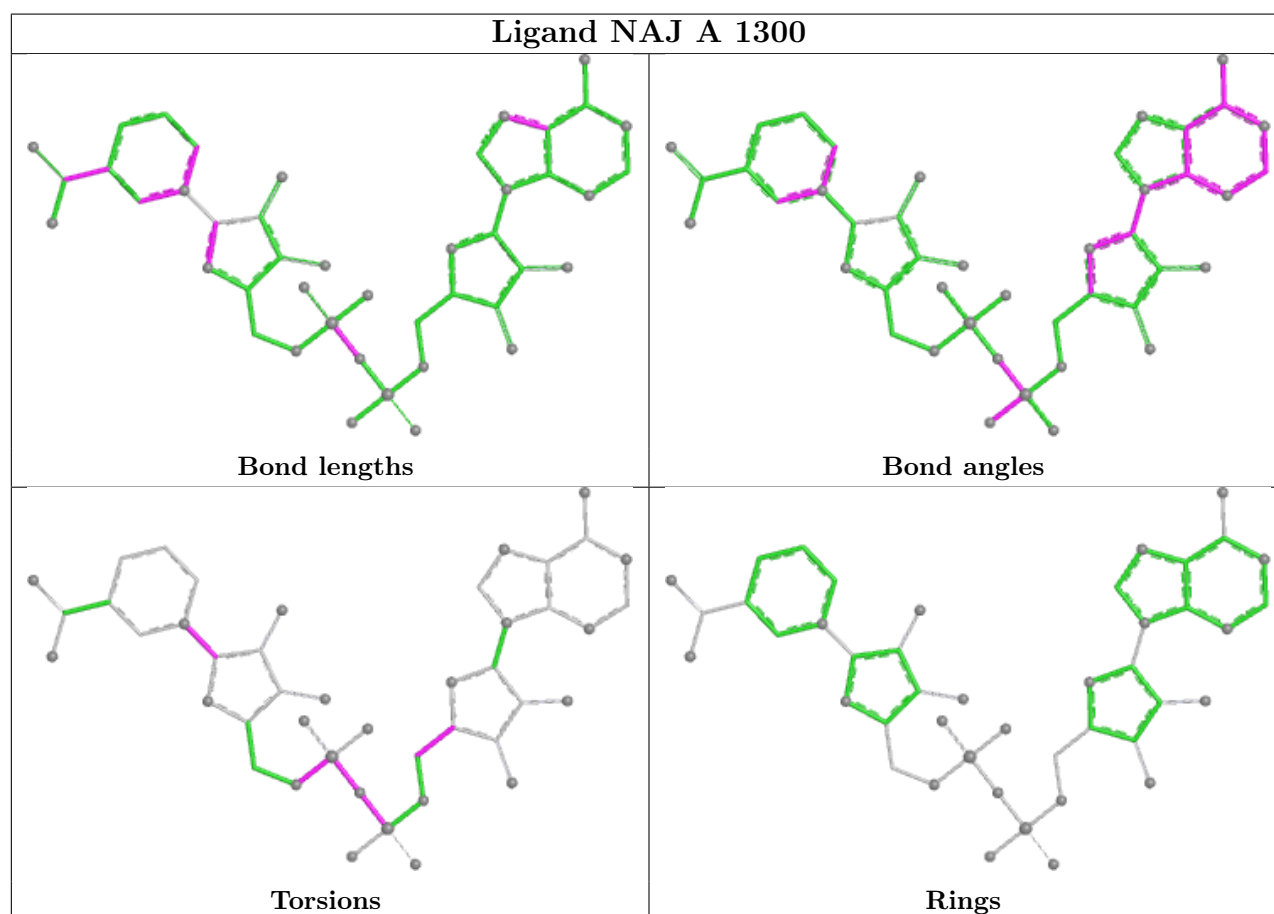
Mol	Chain	Res	Type	Atoms
2	A	1300	NAJ	PN-O3-PA-O5B
2	A	1300	NAJ	C5D-O5D-PN-O3
2	A	1300	NAJ	C5D-O5D-PN-O1N
2	A	1300	NAJ	C5D-O5D-PN-O2N
2	A	1300	NAJ	O4D-C1D-N1N-C2N
2	A	1300	NAJ	O4D-C1D-N1N-C6N
3	A	6001	MAX	C8-C12-C14-C15
3	A	6001	MAX	C11-C12-C14-C15
3	A	6001	MAX	C18-C19-O21-C22
3	A	6001	MAX	C3-C2-O25-C26
3	A	6001	MAX	C1-C2-O25-C26
3	A	6001	MAX	C20-C19-O21-C22
2	A	1300	NAJ	PA-O3-PN-O2N
2	A	1300	NAJ	C2D-C1D-N1N-C6N
2	A	1300	NAJ	PA-O3-PN-O1N
2	A	1300	NAJ	O4B-C4B-C5B-O5B

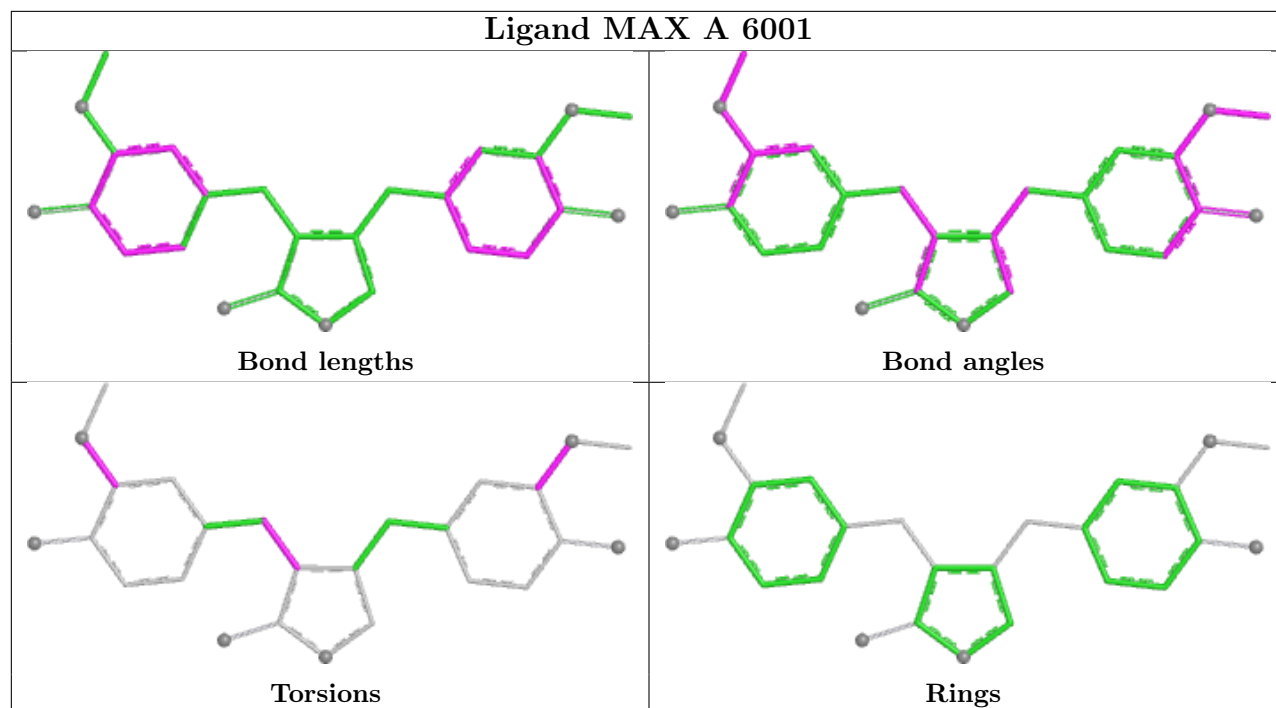
There are no ring outliers.

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

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.