



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:08 PM UTC

PDB ID : 1F8G / pdb_00001f8g
Title : THE X-RAY STRUCTURE OF NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE FROM RHODOSPIRILLUM RUBRUM COMPLEXED WITH NAD⁺
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Deposited on : 2000-06-30
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

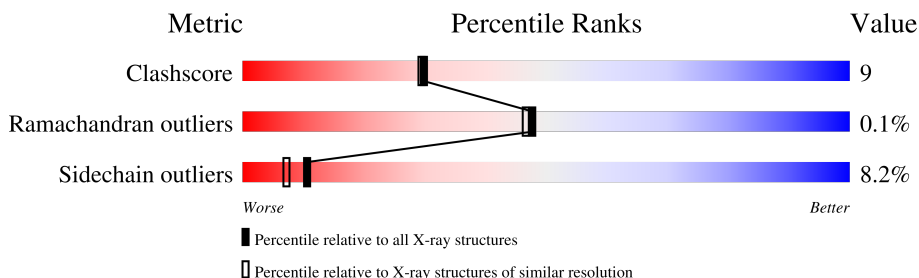
1 Overall quality at a glance

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	384	 81% 16% ...
1	B	384	 80% 16% ..
1	C	384	 79% 16% ...
1	D	384	 70% 24% ...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12733 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 NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	Se	0	0	0
			2795	1763	480	535	3	14			
1	B	381	Total	C	N	O	S	Se	0	0	0
			2792	1761	482	531	3	15			
1	C	375	Total	C	N	O	S	Se	0	0	0
			2759	1742	476	523	3	15			
1	D	377	Total	C	N	O	S	Se	0	0	0
			2770	1749	477	526	3	15			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q60164
A	78	MSE	MET	modified residue	UNP Q60164
A	97	MSE	MET	modified residue	UNP Q60164
A	122	MSE	MET	modified residue	UNP Q60164
A	125	MSE	MET	modified residue	UNP Q60164
A	134	MSE	MET	modified residue	UNP Q60164
A	162	MSE	MET	modified residue	UNP Q60164
A	163	MSE	MET	modified residue	UNP Q60164
A	164	MSE	MET	modified residue	UNP Q60164
A	199	MSE	MET	modified residue	UNP Q60164
A	226	MSE	MET	modified residue	UNP Q60164
A	239	MSE	MET	modified residue	UNP Q60164
A	280	MSE	MET	modified residue	UNP Q60164
A	284	MSE	MET	modified residue	UNP Q60164
A	356	MSE	MET	modified residue	UNP Q60164
B	1	MSE	MET	modified residue	UNP Q60164
B	78	MSE	MET	modified residue	UNP Q60164
B	97	MSE	MET	modified residue	UNP Q60164
B	122	MSE	MET	modified residue	UNP Q60164
B	125	MSE	MET	modified residue	UNP Q60164
B	134	MSE	MET	modified residue	UNP Q60164

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Chain	Residue	Modelled	Actual	Comment	Reference
B	162	MSE	MET	modified residue	UNP Q60164
B	163	MSE	MET	modified residue	UNP Q60164
B	164	MSE	MET	modified residue	UNP Q60164
B	199	MSE	MET	modified residue	UNP Q60164
B	226	MSE	MET	modified residue	UNP Q60164
B	239	MSE	MET	modified residue	UNP Q60164
B	280	MSE	MET	modified residue	UNP Q60164
B	284	MSE	MET	modified residue	UNP Q60164
B	356	MSE	MET	modified residue	UNP Q60164
C	1	MSE	MET	modified residue	UNP Q60164
C	78	MSE	MET	modified residue	UNP Q60164
C	97	MSE	MET	modified residue	UNP Q60164
C	122	MSE	MET	modified residue	UNP Q60164
C	125	MSE	MET	modified residue	UNP Q60164
C	134	MSE	MET	modified residue	UNP Q60164
C	162	MSE	MET	modified residue	UNP Q60164
C	163	MSE	MET	modified residue	UNP Q60164
C	164	MSE	MET	modified residue	UNP Q60164
C	199	MSE	MET	modified residue	UNP Q60164
C	226	MSE	MET	modified residue	UNP Q60164
C	239	MSE	MET	modified residue	UNP Q60164
C	280	MSE	MET	modified residue	UNP Q60164
C	284	MSE	MET	modified residue	UNP Q60164
C	356	MSE	MET	modified residue	UNP Q60164
D	1	MSE	MET	modified residue	UNP Q60164
D	78	MSE	MET	modified residue	UNP Q60164
D	97	MSE	MET	modified residue	UNP Q60164
D	122	MSE	MET	modified residue	UNP Q60164
D	125	MSE	MET	modified residue	UNP Q60164
D	134	MSE	MET	modified residue	UNP Q60164
D	162	MSE	MET	modified residue	UNP Q60164
D	163	MSE	MET	modified residue	UNP Q60164
D	164	MSE	MET	modified residue	UNP Q60164
D	199	MSE	MET	modified residue	UNP Q60164
D	226	MSE	MET	modified residue	UNP Q60164
D	239	MSE	MET	modified residue	UNP Q60164
D	280	MSE	MET	modified residue	UNP Q60164
D	284	MSE	MET	modified residue	UNP Q60164
D	356	MSE	MET	modified residue	UNP Q60164

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: 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
			35	15	5	13	2		
2	C	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	D	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	406	Total	O	0	0
			406	406		
3	B	398	Total	O	0	0
			398	398		
3	C	389	Total	O	0	0
			389	389		
3	D	266	Total	O	0	0
			266	266		

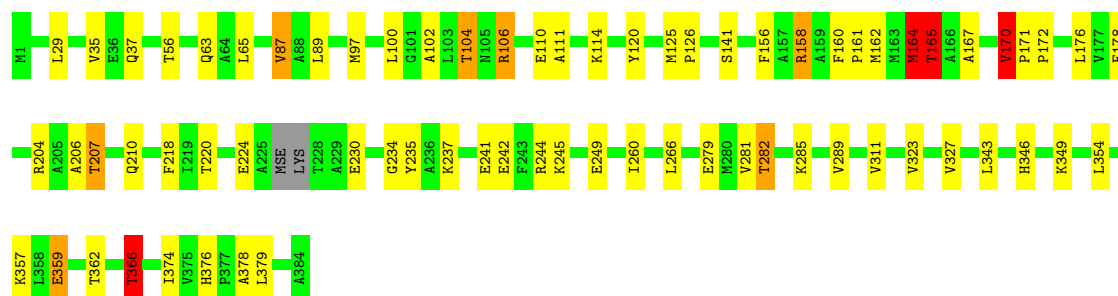
3 Residue-property plots

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.

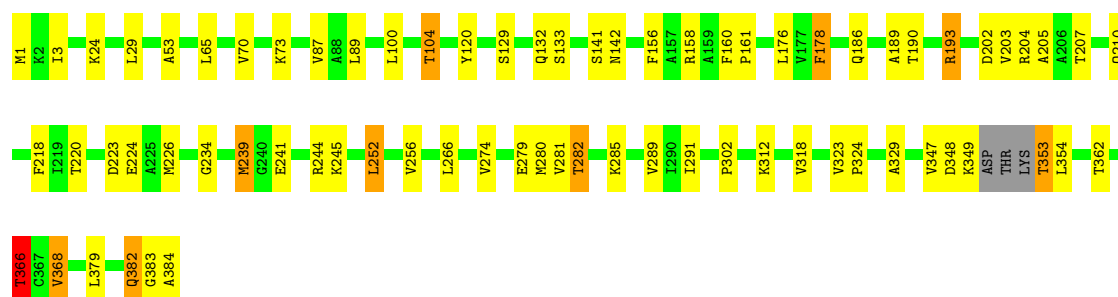
• Molecule 1: NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE

Chain A: 



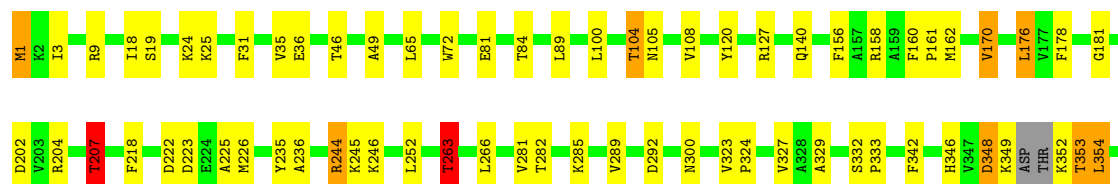
• Molecule 1: NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE

Chain B: 



• Molecule 1: NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE

Chain C: 



D360	E361	T362	T366	H376	P377	ALA	LEU	THR	GLY	GLN	GLY	ALA
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● Molecule 1: NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE



H376	T263	T264	A265	L266	T277	E278	E279	M280	V281	T282	V289	D292	L293	N300	K308	K312	H313	V327	A328	A329	S332	P333	L339	L340	N341	F342	L343	T344	P345	D348	LYS	ASP	THR	K352	T353	L354	L358	E359	D360	E361	T362	T366	C367	V368	T369	R370	V375																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
	R158	A159	F160	M161	M162	M163	M164	T165	A166	A167	G168	T169	V170	P171	P172	L176	V177	F178	Q186	V198	D202	V203	R204	A205	A206	T207	Q210	F218	V221	E224	A225	M226	K227	T228	A229	E230	K237	E238	E242	Q247	V251	L252	K257	T258	D259	I260																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
	M1	K2	I5	R9	S19	V23	F31	I34	Q37	I57	A58	S59	T60	Q63	A64	L65	W72	P77	M78	T84	D85	E86	V87	A88	L89	M97	T104	N105	R106	P107	V108	V109	E110	Y120	A121	M122	M125	S133	N142	F156	A157																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.90Å 116.60Å 102.00Å 90.00° 104.22° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12733	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

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: NAD

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	0.55	0/2818	1.39	23/3798 (0.6%)
1	B	0.55	0/2814	1.33	8/3789 (0.2%)
1	C	0.56	1/2781 (0.0%)	1.38	15/3743 (0.4%)
1	D	0.50	0/2792	1.33	15/3760 (0.4%)
All	All	0.54	1/11205 (0.0%)	1.36	61/15090 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	377	PRO	N-CD	5.41	1.55	1.47

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	LYS	CA-C-O	13.23	134.77	121.14
1	C	170	VAL	N-CA-CB	-12.69	98.92	112.37
1	C	170	VAL	CB-CA-C	11.78	121.55	110.13
1	A	237	LYS	N-CA-C	10.71	121.94	108.45
1	C	348	ASP	CA-CB-CG	10.42	123.02	112.60
1	A	170	VAL	CB-CA-C	9.95	121.02	110.37
1	B	366	THR	N-CA-CB	-9.72	96.23	110.53
1	A	366	THR	N-CA-CB	-9.37	97.65	110.67
1	D	366	THR	N-CA-CB	-9.37	98.13	110.59
1	D	170	VAL	CB-CA-C	9.30	121.55	110.85
1	C	263	THR	N-CA-CB	-8.87	96.63	110.55
1	C	376	HIS	CA-C-O	8.62	127.49	119.99
1	D	263	THR	N-CA-CB	-8.55	97.12	110.55
1	A	237	LYS	CA-C-N	8.39	137.08	122.32
1	A	237	LYS	C-N-CA	8.39	137.08	122.32
1	C	366	THR	N-CA-CB	-8.31	98.33	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	THR	N-CA-CB	-8.23	98.44	110.70
1	A	104	THR	N-CA-CB	-8.14	97.77	111.27
1	A	170	VAL	N-CA-CB	-7.79	103.28	111.61
1	C	207	THR	N-CA-CB	-7.70	98.34	110.28
1	B	382	GLN	OE1-CD-NE2	7.17	129.76	122.60
1	C	353	THR	N-CA-C	7.00	120.82	110.46
1	D	170	VAL	N-CA-CB	-6.67	102.98	111.39
1	A	141	SER	CB-CA-C	-6.57	99.89	110.79
1	A	178	PHE	CA-CB-CG	6.38	120.19	113.80
1	C	346	HIS	CA-CB-CG	-6.38	107.42	113.80
1	C	181	GLY	N-CA-C	-6.38	103.36	112.55
1	D	368	VAL	CB-CA-C	6.34	117.80	110.88
1	D	368	VAL	N-CA-CB	-6.31	103.64	112.35
1	A	346	HIS	CA-CB-CG	-5.97	107.83	113.80
1	B	104	THR	N-CA-CB	-5.96	101.92	110.80
1	B	193	ARG	CB-CA-C	-5.92	101.33	110.81
1	B	178	PHE	CA-CB-CG	5.85	119.65	113.80
1	A	171	PRO	O-C-N	5.82	123.89	121.15
1	D	104	THR	N-CA-CB	-5.79	102.89	110.88
1	D	198	VAL	N-CA-C	5.76	116.23	108.17
1	A	104	THR	CB-CA-C	5.74	120.08	110.44
1	A	164	MSE	CA-C-O	5.54	126.31	120.54
1	A	235	TYR	N-CA-C	5.51	119.05	110.17
1	D	260	ILE	CB-CA-C	-5.47	103.04	110.42
1	C	140	GLN	CA-C-N	5.45	127.58	120.28
1	C	140	GLN	C-N-CA	5.45	127.58	120.28
1	D	263	THR	CB-CA-C	5.39	119.04	110.19
1	C	162	MSE	N-CA-C	-5.35	101.93	109.96
1	D	9	ARG	CD-NE-CZ	5.34	131.87	124.40
1	D	328	ALA	N-CA-C	5.33	118.58	111.75
1	D	224	GLU	N-CA-C	5.33	119.84	113.23
1	A	206	ALA	CA-C-N	5.32	127.41	120.28
1	A	206	ALA	C-N-CA	5.32	127.41	120.28
1	D	366	THR	N-CA-C	5.32	120.42	113.88
1	C	263	THR	CB-CA-C	5.31	118.90	110.19
1	A	102	ALA	N-CA-C	5.30	117.48	111.11
1	A	323	VAL	N-CA-CB	5.29	113.83	110.50
1	A	158	ARG	CD-NE-CZ	5.22	131.71	124.40
1	C	360	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	368	VAL	N-CA-CB	-5.14	102.74	111.23
1	A	260	ILE	CB-CA-C	-5.09	103.55	110.42
1	B	223	ASP	N-CA-C	5.06	117.45	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	239	MSE	N-CA-C	5.06	118.60	112.23
1	A	249	GLU	N-CA-C	5.04	117.16	111.02
1	D	106	ARG	CD-NE-CZ	5.04	131.45	124.40

There are no chirality outliers.

There are no planarity outliers.

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	2795	0	2911	38	0
1	B	2792	0	2916	48	0
1	C	2759	0	2887	39	0
1	D	2770	0	2897	75	0
2	A	44	0	26	0	0
2	B	35	0	19	3	0
2	C	35	0	19	1	0
2	D	44	0	26	0	0
3	A	406	0	0	4	0
3	B	398	0	0	3	0
3	C	389	0	0	5	0
3	D	266	0	0	5	0
All	All	12733	0	11701	196	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 9.

All (196) 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:D:263:THR:HG23	1:D:300:ASN:HD22	1.26	0.99
1:C:202:ASP:HB3	1:C:207:THR:HG21	1.48	0.94
1:D:263:THR:HG22	1:D:292:ASP:HA	1.53	0.90
1:A:97:MSE:HE1	1:A:343:LEU:HD13	1.52	0.90
1:A:162:MSE:SE	1:A:164:MSE:HE3	2.23	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:THR:HG23	1:C:49:ALA:H	1.37	0.88
1:D:1:MSE:HE1	1:D:354:LEU:HB2	1.57	0.85
1:C:349:LYS:HA	1:C:352:LYS:HG2	1.65	0.77
1:B:252:LEU:HD21	1:B:280:MSE:HG2	1.66	0.76
1:D:205:ALA:HA	1:D:226:MSE:HE2	1.66	0.75
1:D:263:THR:HG23	1:D:300:ASN:ND2	1.99	0.75
1:D:162:MSE:HG3	1:D:172:PRO:HD3	1.70	0.74
1:D:224:GLU:HA	1:D:227:LYS:HE2	1.71	0.72
1:D:120:TYR:HD2	1:D:366:THR:HG22	1.58	0.69
1:C:1:MSE:HE1	1:C:354:LEU:HD12	1.75	0.68
1:B:349:LYS:H	1:B:349:LYS:HD2	1.57	0.68
1:C:263:THR:HG23	1:C:300:ASN:HB2	1.77	0.67
1:D:202:ASP:HB3	1:D:207:THR:HG21	1.77	0.66
1:D:207:THR:HA	1:D:210:GLN:HE21	1.61	0.66
1:B:142:ASN:HD21	1:B:186:GLN:HE21	1.43	0.66
1:B:207:THR:HG22	1:B:218:PHE:HE1	1.61	0.66
1:C:362:THR:O	1:C:366:THR:HB	1.95	0.65
1:D:9:ARG:HB2	1:D:78:MSE:CE	2.26	0.65
1:D:277:THR:HG22	1:D:278:GLU:H	1.63	0.64
1:B:362:THR:O	1:B:366:THR:HB	1.98	0.64
1:A:207:THR:HA	1:A:210:GLN:HE21	1.64	0.62
1:D:162:MSE:HE3	1:D:164:MSE:HE3	1.80	0.62
1:C:263:THR:CG2	1:C:300:ASN:HB2	2.30	0.62
1:C:263:THR:HG23	1:C:300:ASN:OD1	1.99	0.62
1:A:376:HIS:HD2	1:A:378:ALA:H	1.47	0.61
1:D:165:THR:HG22	1:D:168:GLY:O	2.00	0.61
1:C:263:THR:HG22	1:C:292:ASP:HA	1.80	0.61
1:D:122:MSE:HE2	1:D:339:LEU:HD23	1.82	0.61
1:D:104:THR:HG22	1:D:105:ASN:ND2	2.15	0.61
1:D:263:THR:CG2	1:D:300:ASN:HB2	2.30	0.61
1:B:189:ALA:O	1:B:193:ARG:HG3	2.01	0.60
1:D:165:THR:HG23	1:D:167:ALA:H	1.67	0.60
1:D:375:VAL:O	1:D:376:HIS:HB3	2.02	0.59
1:A:374:ILE:HD13	1:A:379:LEU:O	2.04	0.57
1:B:207:THR:HG22	1:B:218:PHE:CE1	2.39	0.57
1:C:202:ASP:CB	1:C:207:THR:HG21	2.29	0.56
1:C:24:LYS:HZ3	1:C:25:LYS:HG2	1.69	0.56
1:C:24:LYS:NZ	1:C:25:LYS:HG2	2.20	0.56
1:D:9:ARG:HB2	1:D:78:MSE:HE2	1.86	0.56
1:D:342:PHE:CE1	1:D:362:THR:HG23	2.40	0.56
1:D:263:THR:HG23	1:D:300:ASN:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:LEU:HG	3:B:2817:HOH:O	2.04	0.56
1:A:376:HIS:CD2	1:A:378:ALA:H	2.23	0.56
1:A:29:LEU:HD23	1:A:349:LYS:HE2	1.88	0.56
1:B:156:PHE:CE2	1:B:158:ARG:HB2	2.41	0.56
1:D:202:ASP:CB	1:D:207:THR:HG21	2.35	0.56
1:D:125:MSE:HE1	1:D:342:PHE:CD1	2.42	0.55
1:C:120:TYR:HD2	1:C:366:THR:HG22	1.71	0.55
1:B:160:PHE:N	1:B:161:PRO:HD2	2.22	0.54
1:D:19:SER:O	1:D:23:VAL:HG23	2.08	0.54
1:C:120:TYR:HB3	1:C:366:THR:HG23	1.89	0.54
1:D:204:ARG:O	1:D:207:THR:HB	2.08	0.53
1:D:1:MSE:HE3	1:D:31:PHE:CE2	2.44	0.53
1:B:203:VAL:O	1:B:226:MSE:HG3	2.09	0.53
1:B:220:THR:HG23	1:B:226:MSE:HE1	1.91	0.53
1:B:129:SER:O	1:B:132:GLN:HG2	2.10	0.52
1:C:104:THR:HG22	1:C:105:ASN:ND2	2.24	0.52
1:A:120:TYR:HB3	1:A:366:THR:HG23	1.91	0.52
1:D:264:THR:HG22	1:D:293:LEU:HD12	1.90	0.52
1:B:132:GLN:HE21	1:D:166:ALA:HB1	1.74	0.51
1:D:162:MSE:CE	1:D:164:MSE:HE3	2.41	0.51
1:C:332:SER:HB2	1:C:333:PRO:HD3	1.91	0.51
1:D:72:TRP:CD1	1:D:97:MSE:HE3	2.45	0.51
1:A:241:GLU:O	1:A:245:LYS:HD3	2.11	0.51
1:D:165:THR:HG23	1:D:167:ALA:N	2.24	0.51
1:C:349:LYS:HA	1:C:352:LYS:HD3	1.92	0.50
1:A:165:THR:HG23	3:C:2545:HOH:O	2.11	0.50
1:B:120:TYR:HD2	1:B:366:THR:HG22	1.76	0.50
1:A:165:THR:HG22	1:A:167:ALA:H	1.77	0.49
1:B:279:GLU:O	1:B:282:THR:HB	2.11	0.49
1:D:142:ASN:HD21	1:D:186:GLN:HE21	1.60	0.49
1:B:205:ALA:CA	1:B:226:MSE:HG2	2.42	0.49
1:A:376:HIS:HE1	3:A:2675:HOH:O	1.96	0.49
1:A:279:GLU:O	1:A:282:THR:HB	2.13	0.49
1:C:105:ASN:O	1:C:108:VAL:HG12	2.12	0.49
1:B:252:LEU:O	1:B:256:VAL:HG23	2.12	0.49
1:C:3:ILE:HD11	1:C:72:TRP:CE2	2.48	0.48
1:B:204:ARG:NH2	2:B:2501:NAD:H3D	2.28	0.48
1:B:383:GLY:O	1:B:384:ALA:C	2.55	0.48
1:B:132:GLN:HG3	1:B:133:SER:N	2.29	0.48
1:C:24:LYS:HD2	3:C:2804:HOH:O	2.12	0.48
1:D:104:THR:HB	3:D:2599:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:ARG:N	1:D:107:PRO:HD2	2.29	0.48
1:A:158:ARG:HG2	1:C:329:ALA:HB3	1.96	0.48
1:D:360:ASP:OD1	1:D:362:THR:HB	2.14	0.48
1:B:329:ALA:HB3	1:D:158:ARG:HG2	1.96	0.48
1:B:202:ASP:HB3	1:B:207:THR:HG21	1.96	0.48
1:B:207:THR:HA	1:B:210:GLN:HE21	1.78	0.48
1:B:291:ILE:HD13	1:B:318:VAL:HB	1.96	0.47
1:C:222:ASP:HB3	1:C:225:ALA:HB3	1.96	0.47
1:D:162:MSE:CG	1:D:172:PRO:HD3	2.42	0.47
1:A:160:PHE:N	1:A:161:PRO:HD2	2.29	0.47
1:D:106:ARG:NH2	1:D:110:GLU:OE2	2.47	0.47
1:D:207:THR:HG22	1:D:218:PHE:CE1	2.49	0.47
1:C:24:LYS:HG3	1:C:25:LYS:N	2.30	0.47
1:D:133:SER:HB2	1:D:341:ASN:ND2	2.30	0.47
1:B:29:LEU:HB3	1:B:347:VAL:HG11	1.97	0.47
1:B:203:VAL:HG11	1:B:239:MSE:HG3	1.96	0.47
1:D:308:LYS:HD2	3:D:2709:HOH:O	2.13	0.47
1:D:120:TYR:HB3	1:D:366:THR:CG2	2.45	0.47
1:D:312:LYS:HD2	1:D:313:HIS:CD2	2.50	0.47
1:D:9:ARG:HB2	1:D:78:MSE:HE1	1.96	0.46
1:B:204:ARG:O	1:B:207:THR:HB	2.15	0.46
1:C:349:LYS:HA	1:C:352:LYS:CG	2.39	0.46
1:A:207:THR:HG22	1:A:218:PHE:CE1	2.51	0.46
1:B:158:ARG:HG2	1:D:329:ALA:HB3	1.97	0.46
1:C:218:PHE:HE2	1:C:226:MSE:HE1	1.80	0.46
1:D:277:THR:HG22	1:D:278:GLU:N	2.28	0.46
1:A:165:THR:CG2	1:A:167:ALA:H	2.29	0.45
1:C:204:ARG:O	1:C:207:THR:HB	2.16	0.45
1:B:241:GLU:HG3	1:B:245:LYS:HE3	1.98	0.45
1:C:246:LYS:HA	3:C:2736:HOH:O	2.15	0.45
1:C:342:PHE:CZ	1:C:366:THR:HG21	2.52	0.45
1:D:332:SER:HB2	1:D:333:PRO:HD3	1.99	0.45
1:A:63:GLN:HB2	3:A:2728:HOH:O	2.17	0.45
1:A:362:THR:O	1:A:366:THR:HB	2.17	0.45
1:C:160:PHE:N	1:C:161:PRO:HD2	2.32	0.45
1:D:358:LEU:HD21	1:D:370:ARG:NH1	2.32	0.45
1:A:204:ARG:O	1:A:207:THR:HB	2.17	0.45
1:A:125:MSE:SE	1:A:126:PRO:HD2	2.66	0.44
1:C:9:ARG:NH2	1:C:36:GLU:OE2	2.50	0.44
1:D:37:GLN:HG2	3:D:2642:HOH:O	2.17	0.44
1:B:176:LEU:HG	1:B:178:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ARG:HH22	2:B:2501:NAD:H3D	1.81	0.44
1:C:156:PHE:CE2	1:C:158:ARG:HB2	2.52	0.44
1:D:58:ALA:HB3	1:D:64:ALA:HB2	1.98	0.44
1:C:236:ALA:HB2	2:C:2502:NAD:O2B	2.17	0.44
1:A:110:GLU:OE1	1:A:114:LYS:NZ	2.50	0.44
1:A:359:GLU:CD	1:A:359:GLU:H	2.24	0.44
1:B:202:ASP:CB	1:B:207:THR:HG21	2.48	0.44
1:B:348:ASP:O	1:B:349:LYS:C	2.60	0.44
1:C:1:MSE:HE2	1:C:31:PHE:HE2	1.83	0.44
1:A:87:VAL:HG21	1:A:111:ALA:HB1	2.00	0.44
1:A:242:GLU:H	1:A:242:GLU:CD	2.26	0.44
1:D:156:PHE:CZ	1:D:259:ASP:HB3	2.53	0.44
1:C:176:LEU:HG	1:C:178:PHE:CE2	2.53	0.44
1:D:228:THR:O	1:D:237:LYS:HE3	2.18	0.44
1:D:160:PHE:N	1:D:161:PRO:HD2	2.34	0.43
1:B:132:GLN:HG3	1:B:133:SER:H	1.84	0.43
1:D:120:TYR:CD2	1:D:366:THR:HG22	2.46	0.43
1:D:344:THR:HB	1:D:345:PRO:HD3	2.00	0.43
1:D:263:THR:CG2	1:D:292:ASP:HA	2.37	0.43
1:B:205:ALA:HA	1:B:226:MSE:HG2	2.01	0.43
1:D:362:THR:HG21	3:D:2527:HOH:O	2.19	0.43
1:A:241:GLU:OE2	1:A:244:ARG:HD3	2.19	0.42
1:B:234:GLY:O	2:B:2501:NAD:H4D	2.19	0.42
1:D:230:GLU:HB3	3:D:2690:HOH:O	2.19	0.42
1:C:18:ILE:HG13	1:C:19:SER:N	2.35	0.42
1:C:244:ARG:HG2	1:C:244:ARG:HH21	1.83	0.42
1:D:37:GLN:HB2	1:D:57:ILE:CG2	2.50	0.42
1:A:311:VAL:HB	3:A:2848:HOH:O	2.20	0.42
1:B:190:THR:O	1:B:193:ARG:HB2	2.19	0.42
1:D:60:THR:OG1	1:D:63:GLN:HG3	2.20	0.42
1:A:162:MSE:HB2	1:A:172:PRO:HD3	2.01	0.42
1:A:170:VAL:HG13	3:C:2559:HOH:O	2.18	0.42
1:B:226:MSE:HE2	3:B:2734:HOH:O	2.19	0.42
1:B:274:VAL:HG13	1:B:302:PRO:HD3	2.01	0.42
1:D:2:LYS:HD3	1:D:34:ILE:HD11	2.00	0.42
1:D:156:PHE:CE2	1:D:158:ARG:HB2	2.55	0.42
1:D:5:ILE:HG13	1:D:72:TRP:HB2	2.02	0.42
1:A:343:LEU:HD11	1:A:354:LEU:HD11	2.02	0.41
1:C:3:ILE:HD11	1:C:72:TRP:CD2	2.55	0.41
1:D:77:PRO:HB2	1:D:87:VAL:HG12	2.01	0.41
1:D:162:MSE:HG3	1:D:171:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:THR:HG22	1:D:218:PHE:HE1	1.85	0.41
1:D:312:LYS:HD2	1:D:313:HIS:NE2	2.35	0.41
1:A:207:THR:HG22	1:A:218:PHE:HE1	1.84	0.41
1:C:127:ARG:HD2	1:C:235:TYR:CE1	2.55	0.41
1:C:323:VAL:N	1:C:324:PRO:CD	2.83	0.41
1:A:230:GLU:OE1	1:A:234:GLY:HA2	2.20	0.41
1:D:221:VAL:HG13	1:D:247:GLN:HA	2.01	0.41
1:A:244:ARG:HH12	1:A:245:LYS:HG3	1.86	0.41
1:B:120:TYR:HB3	1:B:366:THR:HG23	2.01	0.41
1:D:105:ASN:O	1:D:108:VAL:HG12	2.20	0.41
1:A:106:ARG:HA	1:A:106:ARG:HD2	1.75	0.41
1:D:176:LEU:HG	1:D:178:PHE:CE1	2.56	0.41
1:B:241:GLU:OE1	1:B:244:ARG:HD3	2.21	0.41
1:B:1:MSE:SE	1:B:353:THR:HA	2.71	0.41
1:A:156:PHE:CE2	1:A:158:ARG:HB2	2.56	0.40
1:B:323:VAL:N	1:B:324:PRO:CD	2.84	0.40
1:B:24:LYS:HG3	1:B:53:ALA:HB1	2.04	0.40
1:B:120:TYR:CD2	1:B:366:THR:HG22	2.56	0.40
1:B:193:ARG:HD2	3:B:2602:HOH:O	2.21	0.40
1:D:85:ASP:OD2	1:D:88:ALA:HB2	2.21	0.40
1:D:203:VAL:O	1:D:226:MSE:HG2	2.21	0.40
1:D:221:VAL:HG21	1:D:247:GLN:HG3	2.02	0.40
1:A:165:THR:HG22	1:A:167:ALA:N	2.36	0.40
1:A:170:VAL:HG22	3:C:2645:HOH:O	2.21	0.40
1:B:3:ILE:HA	1:B:70:VAL:O	2.20	0.40
1:D:279:GLU:O	1:D:282:THR:HB	2.22	0.40
1:A:114:LYS:HE3	3:A:2777:HOH:O	2.22	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	378/384 (98%)	370 (98%)	8 (2%)	0	100	100
1	B	377/384 (98%)	367 (97%)	10 (3%)	0	100	100
1	C	371/384 (97%)	357 (96%)	13 (4%)	1 (0%)	36	35
1	D	373/384 (97%)	360 (96%)	12 (3%)	1 (0%)	36	35
All	All	1499/1536 (98%)	1454 (97%)	43 (3%)	2 (0%)	48	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	223	ASP
1	D	376	HIS

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	293/281 (104%)	268 (92%)	25 (8%)	10	7
1	B	293/281 (104%)	273 (93%)	20 (7%)	14	11
1	C	291/281 (104%)	266 (91%)	25 (9%)	10	6
1	D	292/281 (104%)	266 (91%)	26 (9%)	9	6
All	All	1169/1124 (104%)	1073 (92%)	96 (8%)	10	7

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	37	GLN
1	A	56	THR
1	A	65	LEU
1	A	87	VAL
1	A	89	LEU
1	A	100	LEU
1	A	104	THR
1	A	106	ARG

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Mol	Chain	Res	Type
1	A	164	MSE
1	A	165	THR
1	A	170	VAL
1	A	176	LEU
1	A	207	THR
1	A	220	THR
1	A	224	GLU
1	A	266	LEU
1	A	281	VAL
1	A	282	THR
1	A	285	LYS
1	A	289	VAL
1	A	327	VAL
1	A	357	LYS
1	A	359	GLU
1	A	366	THR
1	B	65	LEU
1	B	73	LYS
1	B	87	VAL
1	B	89	LEU
1	B	100	LEU
1	B	104	THR
1	B	141	SER
1	B	224	GLU
1	B	252	LEU
1	B	266	LEU
1	B	281	VAL
1	B	282	THR
1	B	285	LYS
1	B	289	VAL
1	B	312	LYS
1	B	353	THR
1	B	354	LEU
1	B	366	THR
1	B	368	VAL
1	B	382	GLN
1	C	1	MSE
1	C	35	VAL
1	C	65	LEU
1	C	81	GLU
1	C	84	THR
1	C	89	LEU

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Mol	Chain	Res	Type
1	C	100	LEU
1	C	104	THR
1	C	170	VAL
1	C	176	LEU
1	C	207	THR
1	C	244	ARG
1	C	245	LYS
1	C	252	LEU
1	C	263	THR
1	C	266	LEU
1	C	281	VAL
1	C	282	THR
1	C	285	LYS
1	C	289	VAL
1	C	327	VAL
1	C	348	ASP
1	C	353	THR
1	C	354	LEU
1	C	366	THR
1	D	65	LEU
1	D	84	THR
1	D	87	VAL
1	D	89	LEU
1	D	104	THR
1	D	106	ARG
1	D	163	MSE
1	D	164	MSE
1	D	170	VAL
1	D	207	THR
1	D	238	GLU
1	D	242	GLU
1	D	251	VAL
1	D	252	LEU
1	D	257	LYS
1	D	263	THR
1	D	266	LEU
1	D	281	VAL
1	D	282	THR
1	D	289	VAL
1	D	312	LYS
1	D	327	VAL
1	D	362	THR

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Mol	Chain	Res	Type
1	D	366	THR
1	D	368	VAL
1	D	376	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	105	ASN
1	A	210	GLN
1	A	320	HIS
1	A	322	ASN
1	A	376	HIS
1	B	132	GLN
1	B	186	GLN
1	B	210	GLN
1	B	313	HIS
1	B	338	ASN
1	C	105	ASN
1	C	322	ASN
1	C	338	ASN
1	D	105	ASN
1	D	132	GLN
1	D	142	ASN
1	D	210	GLN
1	D	300	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 oligosaccharides in this entry.

5.6 Ligand geometry

4 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	NAD	D	2503	-	46,48,48	1.08	3 (6%)	64,73,73	1.79	7 (10%)
2	NAD	A	2500	-	46,48,48	1.09	3 (6%)	64,73,73	1.79	7 (10%)
2	NAD	C	2502	-	38,38,48	0.79	1 (2%)	53,58,73	0.90	2 (3%)
2	NAD	B	2501	-	38,38,48	0.80	0	53,58,73	0.77	2 (3%)

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	D	2503	-	-	1/30/62/62	0/5/5/5
2	NAD	A	2500	-	-	2/30/62/62	0/5/5/5
2	NAD	C	2502	-	-	3/22/51/62	0/4/4/5
2	NAD	B	2501	-	-	4/22/51/62	0/4/4/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2500	NAD	C3N-C7N	3.89	1.56	1.50
2	D	2503	NAD	C3N-C7N	3.89	1.56	1.50
2	A	2500	NAD	C6N-N1N	2.95	1.42	1.35
2	D	2503	NAD	C6N-N1N	2.92	1.42	1.35
2	D	2503	NAD	PA-O3	2.38	1.62	1.59
2	A	2500	NAD	C2A-N1A	2.30	1.38	1.33
2	C	2502	NAD	C2A-N1A	2.11	1.37	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2500	NAD	C5N-C4N-C3N	-7.50	112.99	120.36
2	D	2503	NAD	C5N-C4N-C3N	-7.19	113.29	120.36
2	A	2500	NAD	C6N-C5N-C4N	5.94	128.01	119.45
2	D	2503	NAD	C6N-C5N-C4N	5.81	127.82	119.45
2	D	2503	NAD	C5N-C6N-N1N	-5.13	113.38	120.38
2	A	2500	NAD	C5N-C6N-N1N	-4.95	113.63	120.38
2	D	2503	NAD	C4D-O4D-C1D	-4.71	105.61	109.92
2	A	2500	NAD	C2N-C3N-C4N	4.18	123.12	118.26
2	D	2503	NAD	C2N-C3N-C4N	3.96	122.86	118.26
2	A	2500	NAD	C4N-C3N-C7N	-3.52	111.48	121.06
2	A	2500	NAD	O2A-PA-O3	3.43	116.55	107.27
2	D	2503	NAD	C4N-C3N-C7N	-3.00	112.88	121.06
2	D	2503	NAD	C3N-C7N-N7N	-2.73	114.37	117.74
2	C	2502	NAD	O4D-C1D-C2D	-2.60	101.28	105.76
2	C	2502	NAD	O3D-C3D-C2D	-2.22	106.72	111.97
2	B	2501	NAD	O4B-C1B-C2B	-2.09	102.14	106.62
2	A	2500	NAD	C2N-C3N-C7N	2.06	125.40	119.46
2	B	2501	NAD	O4D-C4D-C3D	-2.05	102.74	104.63

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2501	NAD	C5D-O5D-PN-O3
2	B	2501	NAD	C5D-O5D-PN-O1N
2	B	2501	NAD	O4D-C4D-C5D-O5D
2	B	2501	NAD	C3D-C4D-C5D-O5D
2	C	2502	NAD	O4D-C4D-C5D-O5D
2	C	2502	NAD	C3D-C4D-C5D-O5D
2	A	2500	NAD	O4D-C4D-C5D-O5D
2	A	2500	NAD	C3D-C4D-C5D-O5D
2	D	2503	NAD	C5B-O5B-PA-O1A
2	C	2502	NAD	PN-O3-PA-O2A

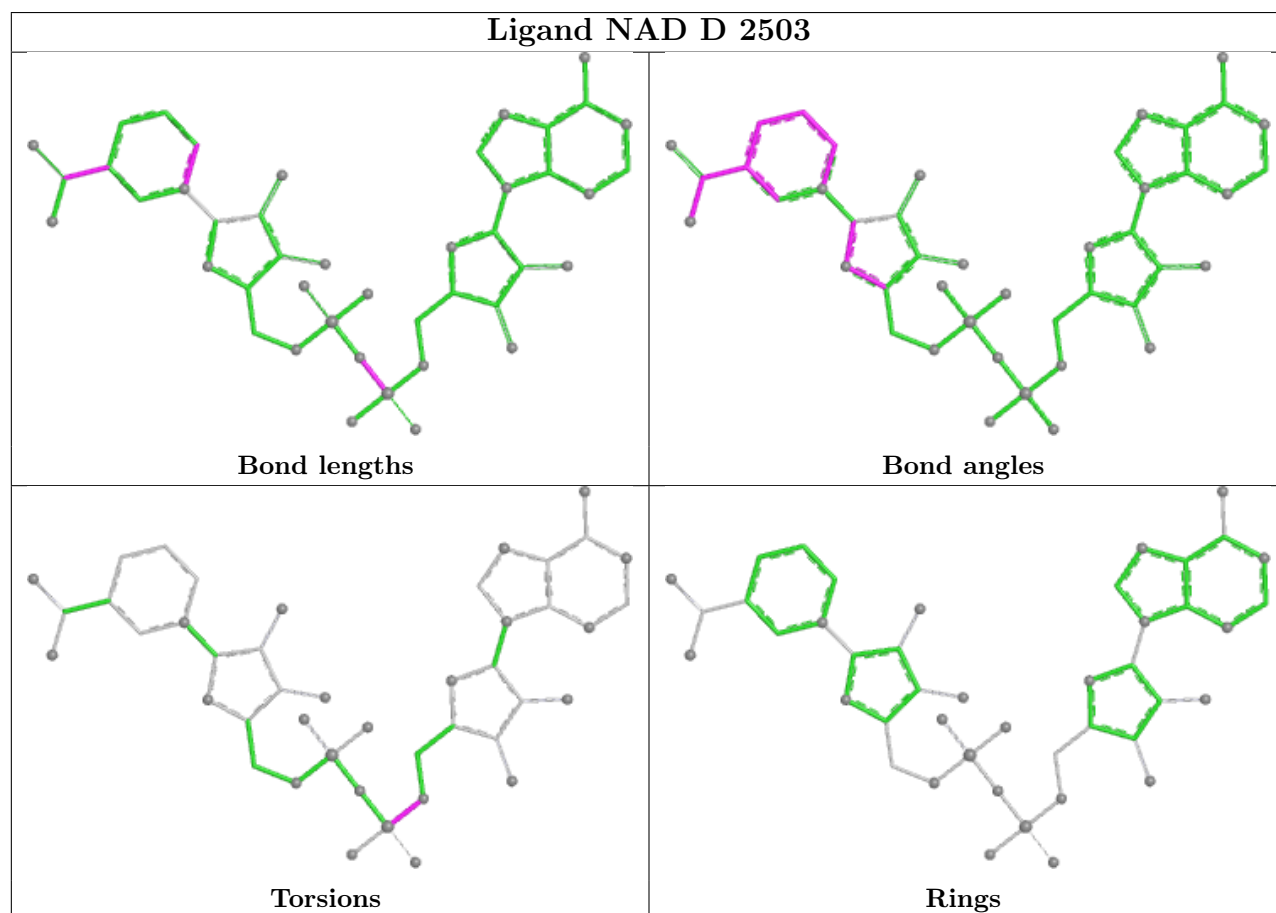
There are no ring outliers.

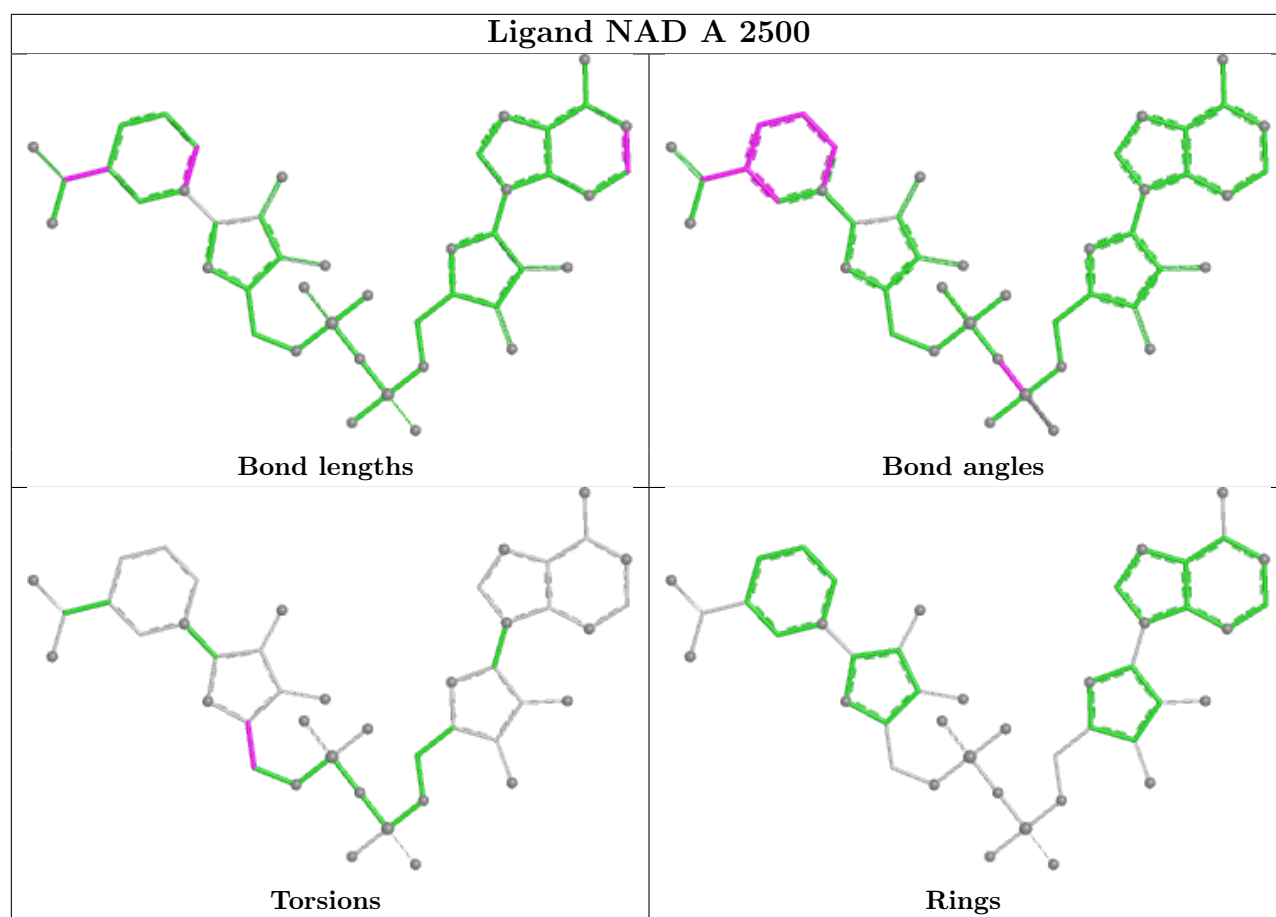
2 monomers are involved in 4 short contacts:

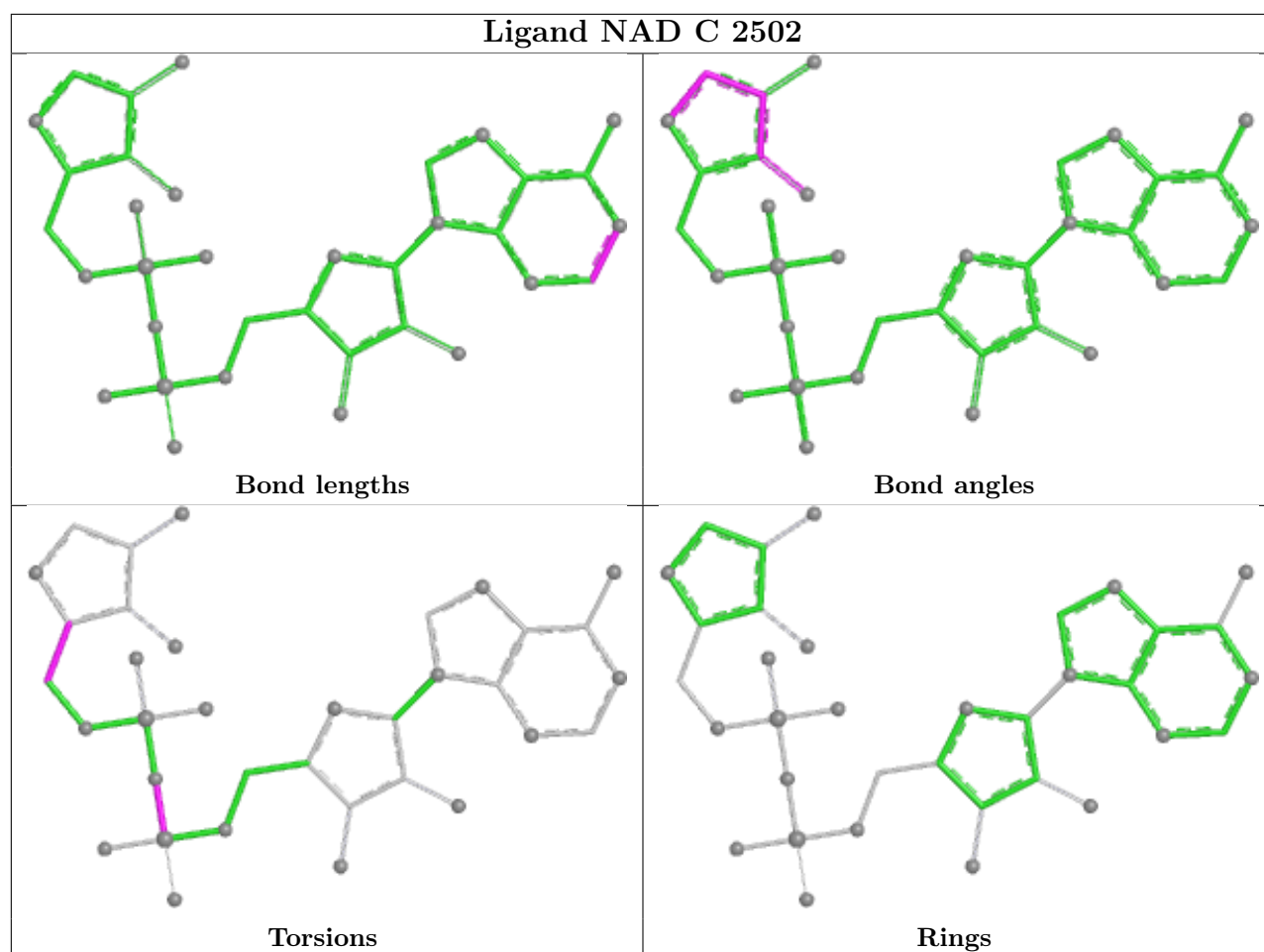
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2502	NAD	1	0
2	B	2501	NAD	3	0

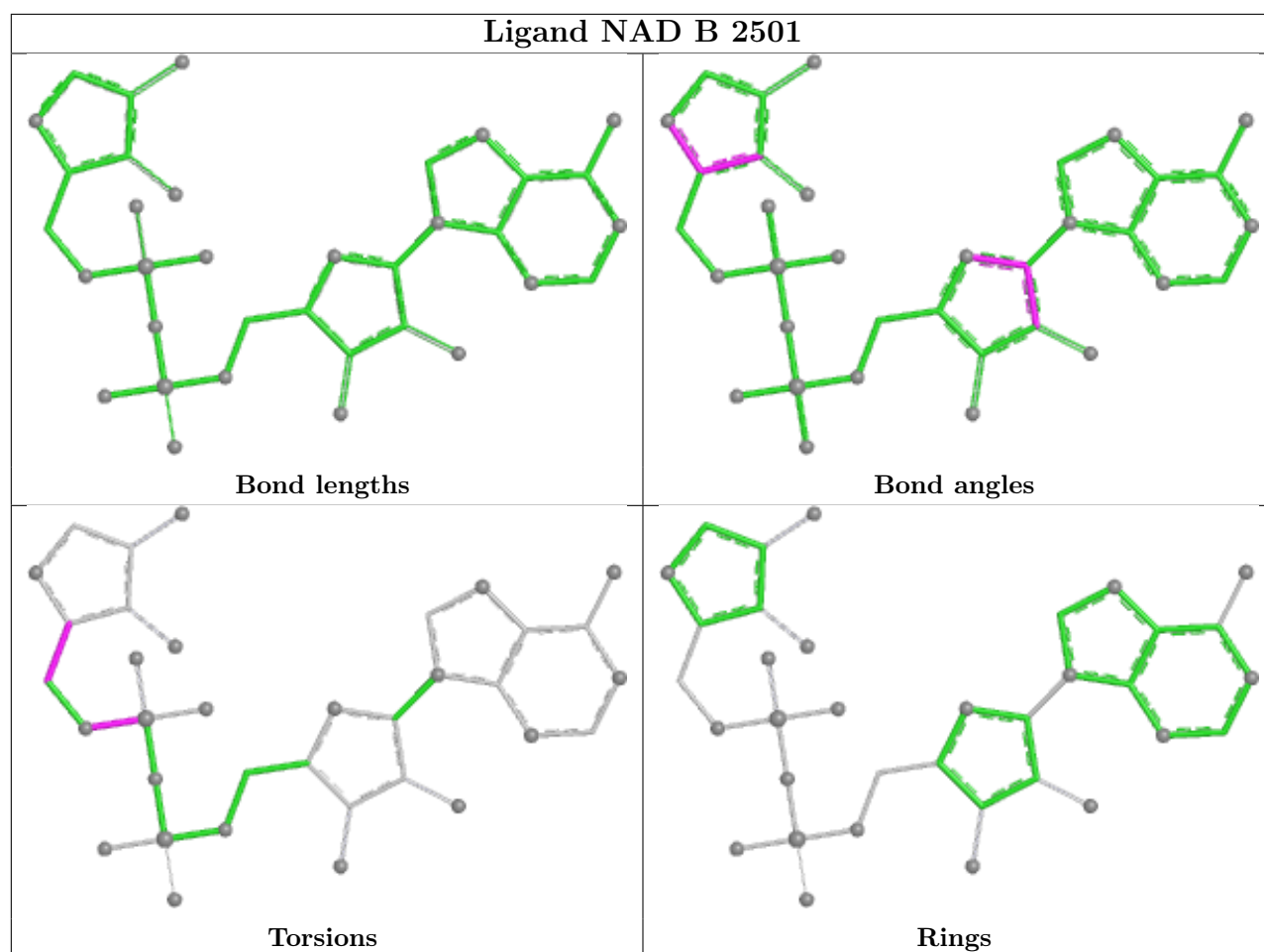
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.