



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:14 AM UTC

PDB ID : 2DVM / pdb_00002dvm
Title : NAD complex structure of PH1275 protein from *Pyrococcus horikoshii*
Authors : Lokanath, N.K.; Mizutani, H.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-07-31
Resolution : 1.60 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

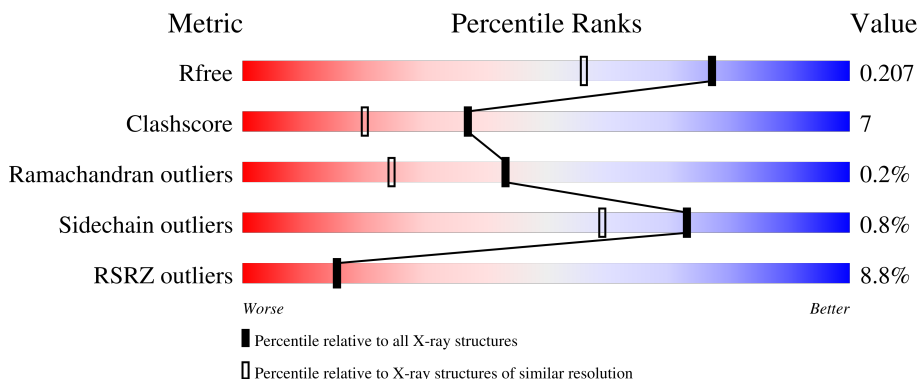
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	439	
1	B	439	
1	C	439	
1	D	439	

2 Entry composition [i](#)

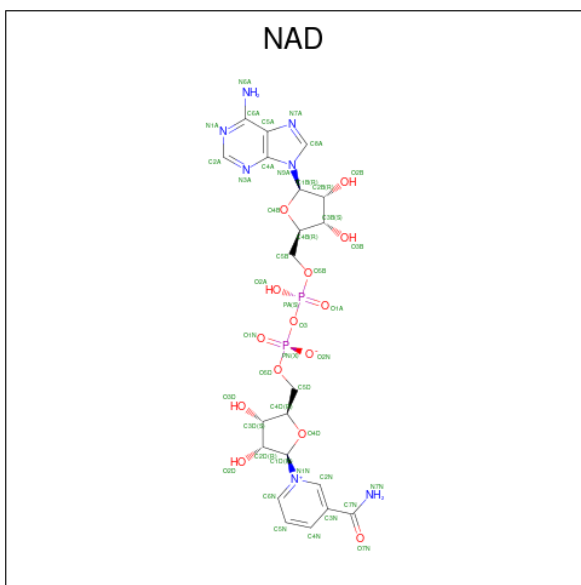
There are 4 unique types of molecules in this entry. The entry contains 15499 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 439aa long hypothetical malate oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	438	Total 3377	C 2166	N 579	O 625	S 7	0	0	0
1	B	434	Total 3345	C 2147	N 572	O 619	S 7	0	0	0
1	C	438	Total 3377	C 2166	N 579	O 625	S 7	0	0	0
1	D	436	Total 3358	C 2156	N 574	O 621	S 7	0	0	0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



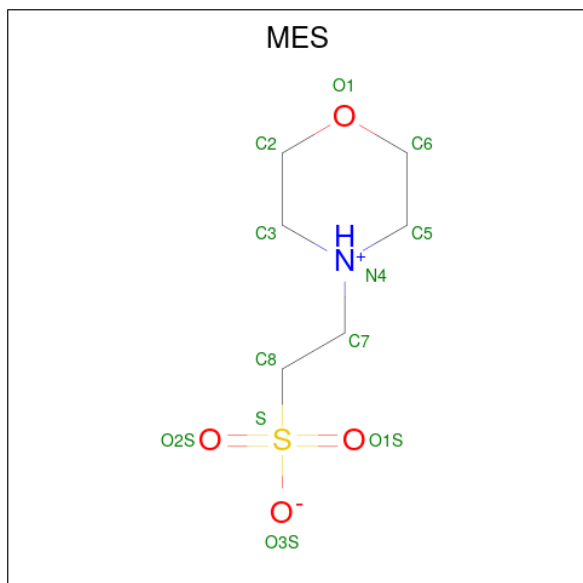
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

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

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			S
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

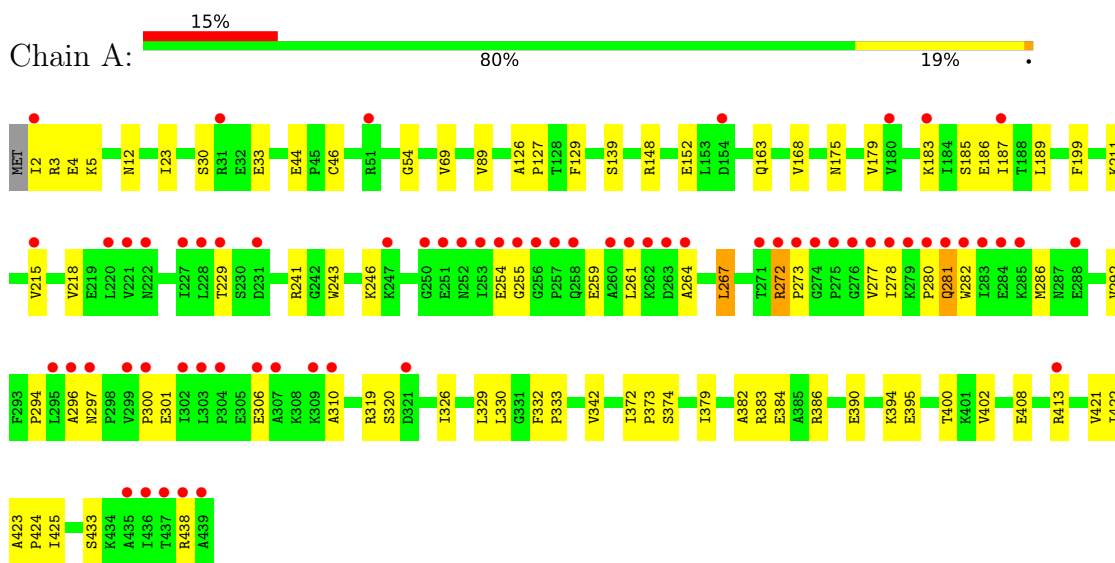
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	383	Total	O	0	0
			383	383		
4	B	454	Total	O	0	0
			454	454		
4	C	483	Total	O	0	0
			483	483		
4	D	510	Total	O	0	0
			510	510		

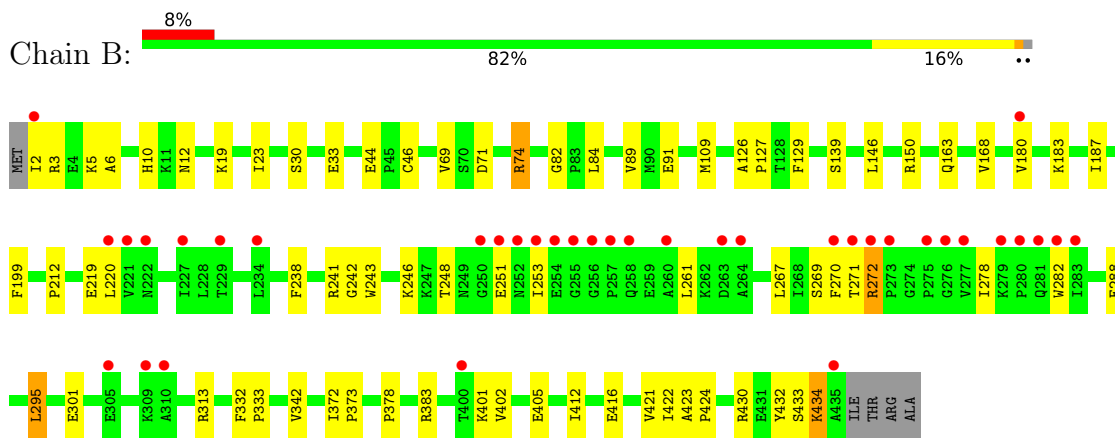
3 Residue-property plots

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 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.

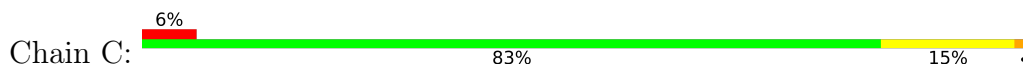
- Molecule 1: 439aa long hypothetical malate oxidoreductase

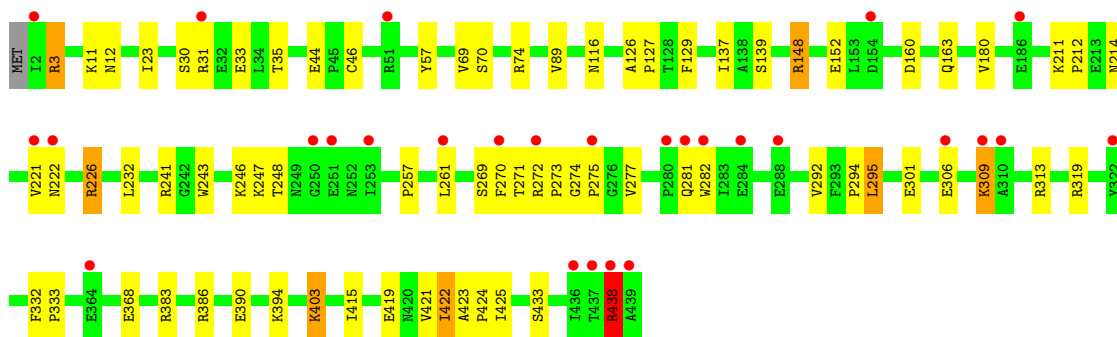


- Molecule 1: 439aa long hypothetical malate oxidoreductase

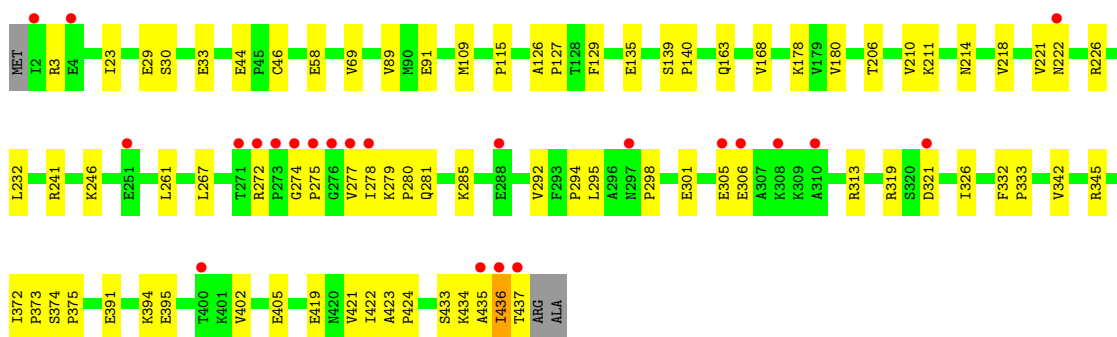
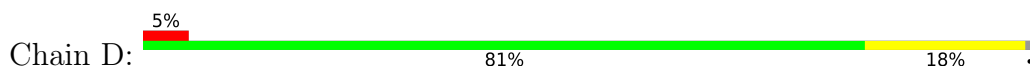


- Molecule 1: 439aa long hypothetical malate oxidoreductase





• Molecule 1: 439aa long hypothetical malate oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.86Å 74.29Å 141.16Å 90.00° 100.37° 90.00°	Depositor
Resolution (Å)	29.84 – 1.60 29.84 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.84-1.60) 99.8 (29.84-1.60)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 1.60Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.191 , 0.207 0.190 , 0.207	Depositor DCC
R_{free} test set	13568 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtrriage
Anisotropy	0.056	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15499	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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, MES

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	0.44	2/3441 (0.1%)	0.93	12/4660 (0.3%)
1	B	0.38	0/3409	0.94	18/4618 (0.4%)
1	C	0.42	1/3441 (0.0%)	0.97	19/4660 (0.4%)
1	D	0.45	0/3422	0.98	12/4636 (0.3%)
All	All	0.42	3/13713 (0.0%)	0.95	61/18574 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	GLU	C-N	7.11	1.43	1.33
1	A	329	LEU	C-N	-6.85	1.24	1.34
1	C	116	ASN	C-N	-5.79	1.26	1.33

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272	ARG	O-C-N	-7.82	115.07	121.80
1	A	374	SER	CA-C-N	7.23	126.93	119.56
1	A	374	SER	C-N-CA	7.23	126.93	119.56
1	A	152	GLU	N-CA-C	7.10	122.20	112.90
1	D	421	VAL	N-CA-C	7.07	117.64	111.56
1	B	421	VAL	N-CA-C	7.03	117.61	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	GLN	N-CA-C	6.79	118.76	111.36
1	C	129	PHE	N-CA-C	6.75	121.03	110.17
1	C	152	GLU	N-CA-C	6.72	121.71	112.90
1	D	129	PHE	N-CA-C	6.70	120.96	110.17
1	D	163	GLN	N-CA-C	6.66	119.55	111.82
1	D	295	LEU	N-CA-C	6.52	120.24	112.93
1	A	129	PHE	N-CA-C	6.51	120.65	110.17
1	B	129	PHE	N-CA-C	6.43	120.53	110.17
1	C	163	GLN	N-CA-C	6.42	119.27	111.82
1	D	298	PRO	CA-C-N	-6.41	117.76	123.33
1	D	298	PRO	C-N-CA	-6.41	117.76	123.33
1	A	163	GLN	N-CA-C	6.14	118.05	111.36
1	B	69	VAL	N-CA-C	6.02	116.60	108.17
1	C	295	LEU	N-CA-C	5.85	120.12	112.92
1	A	69	VAL	N-CA-C	5.85	116.36	108.17
1	A	421	VAL	N-CA-C	5.82	116.22	111.62
1	B	269	SER	CA-C-N	5.80	131.23	122.87
1	B	269	SER	C-N-CA	5.80	131.23	122.87
1	A	139	SER	N-CA-C	-5.79	102.86	110.39
1	D	23	ILE	N-CA-C	5.66	114.12	107.84
1	B	82	GLY	CA-C-N	5.59	125.25	119.05
1	B	82	GLY	C-N-CA	5.59	125.25	119.05
1	B	71	ASP	N-CA-C	-5.59	106.05	112.92
1	C	139	SER	N-CA-C	-5.54	102.65	110.29
1	D	91	GLU	N-CA-C	-5.53	105.33	111.36
1	D	139	SER	N-CA-C	-5.53	102.66	110.29
1	B	295	LEU	N-CA-C	5.53	119.12	112.93
1	D	69	VAL	N-CA-C	5.44	115.79	108.17
1	C	422	ILE	N-CA-C	5.40	116.06	110.82
1	B	23	ILE	N-CA-C	5.39	113.82	107.84
1	C	69	VAL	N-CA-C	5.34	115.99	108.36
1	C	160	ASP	N-CA-C	5.33	117.09	111.28
1	D	422	ILE	N-CA-C	5.32	115.98	110.82
1	B	422	ILE	N-CA-C	5.31	115.97	110.82
1	B	12	ASN	N-CA-C	5.29	118.54	111.24
1	B	91	GLU	N-CA-C	-5.28	105.60	111.36
1	C	12	ASN	N-CA-C	5.28	118.53	111.24
1	C	269	SER	CA-C-N	5.20	130.35	122.87
1	C	269	SER	C-N-CA	5.20	130.35	122.87
1	D	115	PRO	N-CA-C	5.16	121.43	113.75
1	C	319	ARG	CD-NE-CZ	-5.15	117.19	124.40
1	B	272	ARG	CD-NE-CZ	-5.15	117.19	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	ARG	CD-NE-CZ	-5.14	117.21	124.40
1	A	320	SER	CA-C-N	5.12	127.56	120.29
1	A	320	SER	C-N-CA	5.12	127.56	120.29
1	A	23	ILE	N-CA-C	5.11	113.51	107.84
1	C	438	ARG	CD-NE-CZ	-5.09	117.27	124.40
1	C	241	ARG	CD-NE-CZ	-5.09	117.28	124.40
1	C	421	VAL	N-CA-C	5.09	115.64	111.62
1	C	148	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	C	23	ILE	N-CA-C	5.07	113.46	107.84
1	B	74	ARG	CD-NE-CZ	-5.06	117.31	124.40
1	B	378	PRO	N-CD-CG	5.06	110.79	103.20
1	C	226	ARG	CD-NE-CZ	-5.06	117.32	124.40
1	A	12	ASN	N-CA-C	5.04	118.20	111.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	330	LEU	Mainchain

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	3377	0	3490	61	0
1	B	3345	0	3454	45	0
1	C	3377	0	3490	49	0
1	D	3358	0	3467	52	0
2	A	44	0	26	1	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	1	0
3	A	24	0	26	4	0
3	C	12	0	13	3	0
4	A	383	0	0	2	0
4	B	454	0	0	6	0
4	C	483	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	510	0	0	10	0
All	All	15499	0	14044	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 7.

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:C:57:TYR:HE2	3:C:2758:MES:H21	1.28	0.96
1:C:226:ARG:NH1	1:C:232:LEU:HD11	1.85	0.92
1:A:273:PRO:HG3	1:A:297:ASN:O	1.72	0.90
1:B:243:TRP:HA	1:B:246:LYS:HE3	1.57	0.85
1:D:372:ILE:HG13	1:D:373:PRO:HD2	1.63	0.80
1:A:2:ILE:HG12	1:A:5:LYS:HD3	1.66	0.78
1:A:267:LEU:HD12	1:A:292:VAL:HG13	1.65	0.77
1:C:31:ARG:HD3	4:C:2891:HOH:O	1.84	0.77
1:D:394:LYS:HE3	4:D:2667:HOH:O	1.85	0.77
1:C:57:TYR:CE2	3:C:2758:MES:H21	2.17	0.75
3:C:2758:MES:H52	4:C:3090:HOH:O	1.88	0.72
1:D:436:ILE:O	1:D:436:ILE:HG22	1.91	0.70
1:C:180:VAL:HG12	1:C:313:ARG:HD3	1.72	0.70
3:A:2759:MES:O2S	1:B:84:LEU:HD21	1.94	0.68
1:B:372:ILE:HG13	1:B:373:PRO:HD2	1.75	0.68
1:C:292:VAL:HG12	1:C:294:PRO:HD3	1.77	0.67
1:B:261:LEU:HD12	1:B:282:TRP:HB3	1.77	0.65
1:D:274:GLY:HA2	1:D:277:VAL:HG23	1.79	0.64
1:A:127:PRO:HA	3:A:2759:MES:O2S	1.99	0.62
1:C:368:GLU:HG2	4:C:3204:HOH:O	2.00	0.60
1:C:419:GLU:HG2	4:D:2760:HOH:O	1.99	0.60
1:B:219:GLU:HG2	1:B:238:PHE:CE1	2.36	0.60
1:B:261:LEU:HD21	1:B:267:LEU:HD13	1.83	0.60
1:B:6:ALA:O	1:B:10:HIS:HD2	1.85	0.60
1:B:342:VAL:HG12	1:B:402:VAL:HG22	1.81	0.60
1:C:403:LYS:HE2	1:C:403:LYS:HA	1.84	0.59
1:D:292:VAL:HG12	1:D:294:PRO:HD3	1.85	0.59
1:C:46:CYS:SG	1:D:89:VAL:HG23	2.42	0.58
1:C:261:LEU:HD12	1:C:282:TRP:HB3	1.86	0.58
1:D:342:VAL:HG12	1:D:402:VAL:HG22	1.84	0.58
1:C:415:ILE:HD11	4:C:3211:HOH:O	2.04	0.57
1:D:405:GLU:HG3	4:D:2631:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ARG:HA	1:D:44:GLU:HG3	1.85	0.57
1:A:46:CYS:SG	1:B:89:VAL:HG23	2.45	0.57
3:A:2759:MES:H82	1:B:84:LEU:HD11	1.87	0.57
1:D:211:LYS:HB2	1:D:214:ASN:ND2	2.20	0.57
1:B:30:SER:OG	1:B:33:GLU:HG3	2.04	0.57
1:D:30:SER:OG	1:D:33:GLU:HG3	2.06	0.56
1:C:30:SER:OG	1:C:33:GLU:HG3	2.06	0.56
1:C:44:GLU:HG3	1:D:3:ARG:HA	1.87	0.55
1:A:44:GLU:HG3	1:B:3:ARG:HA	1.88	0.55
1:A:30:SER:OG	1:A:33:GLU:HG3	2.07	0.54
1:B:270:PHE:CZ	1:B:295:LEU:HD12	2.43	0.54
1:C:394:LYS:HE3	4:C:3201:HOH:O	2.07	0.54
1:C:74:ARG:HD3	4:C:3232:HOH:O	2.08	0.54
1:C:423:ALA:HB3	1:C:424:PRO:HD3	1.90	0.54
1:A:168:VAL:HG12	1:A:326:ILE:HG23	1.90	0.54
1:B:288:GLU:HG3	4:B:2646:HOH:O	2.08	0.53
1:A:372:ILE:HD12	1:A:373:PRO:HD2	1.89	0.53
1:B:423:ALA:HB3	1:B:424:PRO:HD3	1.90	0.53
1:D:261:LEU:HD21	1:D:267:LEU:HD22	1.90	0.53
1:C:226:ARG:HH12	1:C:232:LEU:HD11	1.68	0.53
1:A:394:LYS:HE3	1:A:395:GLU:OE2	2.09	0.52
1:A:423:ALA:HB3	1:A:424:PRO:HD3	1.90	0.52
1:A:272:ARG:N	1:A:272:ARG:HD3	2.25	0.52
1:D:436:ILE:O	1:D:436:ILE:CG2	2.56	0.52
1:C:211:LYS:HB2	1:C:214:ASN:ND2	2.25	0.52
1:D:435:ALA:C	1:D:437:THR:H	2.18	0.52
1:A:4:GLU:H	1:A:4:GLU:CD	2.19	0.51
1:B:251:GLU:HG3	4:B:2753:HOH:O	2.10	0.51
1:D:345:ARG:O	1:D:345:ARG:HG2	2.10	0.51
1:A:394:LYS:NZ	4:A:2886:HOH:O	2.44	0.51
1:B:242:GLY:O	1:B:246:LYS:HG2	2.10	0.51
1:A:127:PRO:HB2	1:B:109:MET:HB2	1.92	0.51
1:C:422:ILE:O	1:C:425:ILE:HG13	2.10	0.51
1:A:126:ALA:N	1:A:127:PRO:CD	2.74	0.51
1:A:280:PRO:HG3	1:A:306:GLU:HB3	1.93	0.51
1:C:127:PRO:HB2	1:D:109:MET:HB2	1.93	0.51
1:D:180:VAL:HG12	1:D:313:ARG:HD3	1.92	0.51
1:A:272:ARG:HE	1:A:277:VAL:HG13	1.74	0.51
1:A:300:PRO:HD3	1:A:319:ARG:HD2	1.93	0.51
1:C:243:TRP:HA	1:C:246:LYS:HE2	1.92	0.51
1:B:126:ALA:N	1:B:127:PRO:CD	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LEU:O	1:B:150:ARG:HG3	2.10	0.50
1:D:267:LEU:HD21	1:D:278:ILE:HD13	1.92	0.50
1:A:89:VAL:HG23	1:B:46:CYS:SG	2.51	0.50
1:B:405:GLU:HG3	4:B:2587:HOH:O	2.11	0.50
1:D:211:LYS:HB2	1:D:214:ASN:HD22	1.75	0.50
1:C:270:PHE:CZ	1:C:295:LEU:HD12	2.47	0.50
1:B:219:GLU:HG2	1:B:238:PHE:CZ	2.46	0.50
1:C:221:VAL:O	1:C:222:ASN:HB2	2.11	0.50
1:D:178:LYS:HE2	4:D:2803:HOH:O	2.12	0.50
1:D:135:GLU:OE2	4:D:2943:HOH:O	2.19	0.50
1:B:10:HIS:HE1	1:B:19:LYS:NZ	2.10	0.49
1:A:278:ILE:HA	1:A:282:TRP:HZ3	1.76	0.49
1:C:70:SER:HA	1:C:137:ILE:HD11	1.95	0.49
1:A:261:LEU:HD21	1:A:267:LEU:HD23	1.94	0.49
1:A:272:ARG:HD3	1:A:272:ARG:H	1.77	0.49
1:B:2:ILE:HG23	1:B:5:LYS:H	1.78	0.49
1:A:272:ARG:HG3	1:A:272:ARG:HH11	1.78	0.48
1:B:74:ARG:CZ	1:B:139:SER:H	2.26	0.48
1:A:259:GLU:CD	1:A:259:GLU:H	2.21	0.48
1:A:3:ARG:HA	1:B:44:GLU:HG3	1.94	0.48
1:B:401:LYS:HD3	4:B:2762:HOH:O	2.13	0.48
1:A:281:GLN:N	1:A:281:GLN:OE1	2.46	0.48
1:C:247:LYS:HE3	4:C:2989:HOH:O	2.13	0.48
1:A:379:ILE:HG22	1:A:383:ARG:HG3	1.96	0.48
1:D:226:ARG:NH1	1:D:232:LEU:HD11	2.29	0.48
1:D:58:GLU:CG	4:D:2665:HOH:O	2.61	0.47
1:A:438:ARG:HH11	1:A:438:ARG:HG2	1.78	0.47
1:C:212:PRO:O	1:C:248:THR:HA	2.13	0.47
1:D:423:ALA:HB3	1:D:424:PRO:HD3	1.96	0.47
1:C:257:PRO:HD2	4:C:3234:HOH:O	2.14	0.47
1:A:218:VAL:O	2:A:2503:NAD:H2A	2.15	0.47
1:D:434:LYS:HA	1:D:434:LYS:HD3	1.72	0.47
1:D:285:LYS:HB2	4:D:2794:HOH:O	2.15	0.47
1:C:271:THR:OG1	1:C:272:ARG:N	2.48	0.46
1:A:332:PHE:CG	1:A:333:PRO:HD3	2.50	0.46
1:C:309:LYS:HB2	1:C:309:LYS:NZ	2.31	0.46
1:D:126:ALA:N	1:D:127:PRO:CD	2.78	0.46
1:A:292:VAL:HG12	1:A:294:PRO:HD3	1.98	0.46
1:D:261:LEU:HD21	1:D:267:LEU:HD13	1.97	0.46
1:B:2:ILE:N	4:B:2872:HOH:O	2.48	0.46
1:D:285:LYS:HD3	1:D:285:LYS:HA	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:GLY:HA2	1:C:277:VAL:HG23	1.98	0.46
1:A:280:PRO:HB3	1:A:310:ALA:HB2	1.97	0.45
1:C:383:ARG:HH11	1:C:383:ARG:HG3	1.81	0.45
1:A:261:LEU:HD12	1:A:282:TRP:HB3	1.98	0.45
1:A:54:GLY:HA2	3:A:2759:MES:H22	1.98	0.45
1:B:412:ILE:O	1:B:416:GLU:HG3	2.16	0.45
1:A:294:PRO:HB2	1:A:300:PRO:HB3	1.99	0.45
1:C:89:VAL:HG23	1:D:46:CYS:SG	2.57	0.45
1:D:281:GLN:H	1:D:281:GLN:CD	2.23	0.45
1:B:271:THR:OG1	1:B:272:ARG:N	2.49	0.45
1:A:267:LEU:HD12	1:A:292:VAL:CG1	2.41	0.45
1:C:332:PHE:CG	1:C:333:PRO:HD3	2.51	0.45
1:A:278:ILE:HA	1:A:282:TRP:CZ3	2.51	0.44
1:C:126:ALA:N	1:C:127:PRO:CD	2.80	0.44
1:C:148:ARG:HH11	1:C:148:ARG:HD3	1.60	0.44
1:A:413:ARG:HH21	1:B:432:TYR:HA	1.81	0.44
1:B:332:PHE:CG	1:B:333:PRO:HD3	2.53	0.44
1:A:229:THR:HG21	1:A:254:GLU:OE1	2.18	0.44
1:A:386:ARG:O	1:A:390:GLU:HG3	2.17	0.44
1:A:199:PHE:CG	1:A:241:ARG:HG2	2.53	0.44
1:A:2:ILE:HG12	1:A:5:LYS:CD	2.41	0.44
1:B:212:PRO:O	1:B:248:THR:HA	2.17	0.44
1:C:403:LYS:HA	1:C:403:LYS:CE	2.48	0.44
1:D:168:VAL:HG12	1:D:326:ILE:HG23	2.00	0.44
1:A:292:VAL:C	1:A:294:PRO:HD3	2.42	0.43
1:D:278:ILE:HG13	1:D:301:GLU:HB3	1.98	0.43
1:C:211:LYS:HB2	1:C:214:ASN:HD22	1.83	0.43
1:A:296:ALA:HB2	1:A:301:GLU:CD	2.44	0.43
1:C:277:VAL:HB	1:C:301:GLU:HB3	2.00	0.43
1:D:218:VAL:O	2:D:2504:NAD:H2A	2.18	0.43
1:D:274:GLY:HA3	1:D:275:PRO:HA	1.74	0.43
1:B:219:GLU:HG3	1:B:220:LEU:N	2.34	0.43
1:C:11:LYS:NZ	1:D:58:GLU:OE2	2.35	0.43
4:C:3220:HOH:O	1:D:29:GLU:HG2	2.17	0.43
1:D:267:LEU:HD23	1:D:292:VAL:HG13	2.01	0.43
1:D:332:PHE:CG	1:D:333:PRO:HD3	2.54	0.43
1:B:74:ARG:HH12	1:B:139:SER:HB3	1.83	0.43
1:C:31:ARG:O	1:C:35:THR:HG23	2.19	0.43
1:D:140:PRO:HB3	1:D:241:ARG:NH2	2.33	0.43
1:B:278:ILE:HG13	1:B:301:GLU:HB3	2.01	0.42
1:C:438:ARG:HH11	1:C:438:ARG:HD2	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:GLU:CG	4:D:2763:HOH:O	2.65	0.42
1:D:435:ALA:C	1:D:437:THR:N	2.77	0.42
1:A:264:ALA:O	1:A:286:MET:HB3	2.19	0.42
1:A:422:ILE:O	1:A:425:ILE:HG13	2.18	0.42
1:B:383:ARG:HD3	4:B:2754:HOH:O	2.19	0.42
1:A:199:PHE:CD2	1:A:241:ARG:HG2	2.54	0.42
1:B:251:GLU:HB2	1:B:253:ILE:HG13	2.01	0.42
1:A:372:ILE:CD1	1:A:373:PRO:HD2	2.49	0.42
1:C:275:PRO:HB3	4:C:3194:HOH:O	2.18	0.42
1:B:168:VAL:HG13	1:B:372:ILE:HD11	2.00	0.42
1:A:259:GLU:CD	1:A:259:GLU:N	2.78	0.42
1:D:246:LYS:HE2	4:D:2900:HOH:O	2.18	0.42
1:A:4:GLU:CD	1:A:4:GLU:N	2.77	0.42
1:A:183:LYS:HD2	1:A:186:GLU:CD	2.45	0.42
1:C:306:GLU:OE1	4:C:3194:HOH:O	2.22	0.42
1:C:386:ARG:O	1:C:390:GLU:HG3	2.20	0.42
1:A:189:LEU:HB3	1:A:215:VAL:HG22	2.01	0.42
1:C:281:GLN:H	1:C:281:GLN:CD	2.27	0.41
1:D:206:THR:HA	1:D:210:VAL:O	2.20	0.41
1:D:221:VAL:O	1:D:222:ASN:HB2	2.19	0.41
1:D:272:ARG:HD2	4:D:2903:HOH:O	2.20	0.41
1:D:305:GLU:HG2	1:D:306:GLU:N	2.35	0.41
1:A:342:VAL:HG12	1:A:402:VAL:HG22	2.02	0.41
4:A:3082:HOH:O	1:B:430:ARG:HD2	2.20	0.41
1:B:199:PHE:CG	1:B:241:ARG:HG2	2.55	0.41
1:A:255:GLY:HA3	1:A:259:GLU:HG2	2.01	0.41
1:D:279:LYS:HA	1:D:280:PRO:HD3	1.95	0.41
1:B:180:VAL:HG12	1:B:313:ARG:HD3	2.02	0.41
1:B:183:LYS:O	1:B:187:ILE:HG23	2.21	0.41
1:D:319:ARG:HB3	1:D:321:ASP:OD1	2.21	0.41
1:D:391:GLU:OE1	1:D:394:LYS:HE2	2.21	0.41
1:A:185:SER:O	1:A:211:LYS:HE2	2.21	0.40
1:A:342:VAL:C	1:A:400:THR:HG22	2.46	0.40
1:B:434:LYS:HE3	1:B:434:LYS:HA	2.02	0.40
1:C:272:ARG:HB2	1:C:273:PRO:HD2	2.03	0.40
1:A:175:ASN:O	1:A:179:VAL:HG23	2.22	0.40
1:A:243:TRP:HA	1:A:246:LYS:HE2	2.04	0.40
1:A:277:VAL:HB	1:A:301:GLU:HB3	2.02	0.40
1:C:415:ILE:CD1	4:C:3211:HOH:O	2.68	0.40
1:D:374:SER:HA	1:D:375:PRO:HD3	1.94	0.40
1:A:382:ALA:HB1	1:A:408:GLU:HG3	2.04	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	436/439 (99%)	420 (96%)	15 (3%)	1 (0%)	43 24
1	B	432/439 (98%)	419 (97%)	12 (3%)	1 (0%)	43 24
1	C	436/439 (99%)	424 (97%)	11 (2%)	1 (0%)	43 24
1	D	434/439 (99%)	422 (97%)	11 (2%)	1 (0%)	43 24
All	All	1738/1756 (99%)	1685 (97%)	49 (3%)	4 (0%)	43 24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	SER
1	B	433	SER
1	C	433	SER
1	D	433	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	357/358 (100%)	352 (99%)	5 (1%)	59 38
1	B	354/358 (99%)	353 (100%)	1 (0%)	86 78
1	C	357/358 (100%)	354 (99%)	3 (1%)	73 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	355/358 (99%)	353 (99%)	2 (1%)	78	66
All	All	1423/1432 (99%)	1412 (99%)	11 (1%)	73	59

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ARG
1	A	187	ILE
1	A	267	LEU
1	A	272	ARG
1	A	281	GLN
1	B	434	LYS
1	C	309	LYS
1	C	403	LYS
1	C	438	ARG
1	D	395	GLU
1	D	436	ILE

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	214	ASN
1	A	222	ASN
1	A	252	ASN
1	A	297	ASN
1	B	10	HIS
1	B	214	ASN
1	B	252	ASN
1	B	281	GLN
1	B	297	ASN
1	B	370	ASN
1	C	214	ASN
1	C	258	GLN
1	C	297	ASN
1	D	12	ASN
1	D	162	GLN
1	D	214	ASN
1	D	222	ASN
1	D	252	ASN
1	D	258	GLN

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](#)

7 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	A	2503	-	46,48,48	1.75	9 (19%)	64,73,73	1.57	11 (17%)
2	NAD	B	2502	-	46,48,48	1.72	9 (19%)	64,73,73	1.58	11 (17%)
2	NAD	C	2501	-	46,48,48	1.72	9 (19%)	64,73,73	1.54	9 (14%)
3	MES	A	2759	-	12,12,12	2.57	6 (50%)	15,16,16	3.53	7 (46%)
3	MES	A	2760	-	12,12,12	2.54	6 (50%)	15,16,16	3.53	7 (46%)
3	MES	C	2758	-	12,12,12	2.59	6 (50%)	15,16,16	3.38	8 (53%)
2	NAD	D	2504	-	46,48,48	1.71	8 (17%)	64,73,73	1.56	9 (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	NAD	A	2503	-	-	3/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	B	2502	-	-	3/30/62/62	0/5/5/5
2	NAD	C	2501	-	-	3/30/62/62	0/5/5/5
3	MES	A	2759	-	-	2/6/14/14	0/1/1/1
3	MES	A	2760	-	-	3/6/14/14	0/1/1/1
3	MES	C	2758	-	-	1/6/14/14	0/1/1/1
2	NAD	D	2504	-	-	3/30/62/62	0/5/5/5

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2503	NAD	O7N-C7N	7.39	1.37	1.24
2	C	2501	NAD	O7N-C7N	7.25	1.37	1.24
2	D	2504	NAD	O7N-C7N	7.25	1.37	1.24
2	B	2502	NAD	O7N-C7N	7.25	1.37	1.24
3	A	2759	MES	C8-S	5.14	1.84	1.77
3	A	2760	MES	C8-S	4.68	1.84	1.77
3	A	2760	MES	O2S-S	4.65	1.58	1.45
3	C	2758	MES	O2S-S	4.48	1.57	1.45
3	C	2758	MES	C8-S	4.43	1.83	1.77
3	A	2759	MES	O2S-S	4.25	1.57	1.45
2	A	2503	NAD	C2N-N1N	3.58	1.38	1.35
2	B	2502	NAD	C2A-N1A	3.55	1.40	1.33
3	C	2758	MES	C7-N4	3.51	1.55	1.47
2	C	2501	NAD	C2A-N1A	3.50	1.40	1.33
2	D	2504	NAD	C2A-N1A	3.45	1.40	1.33
2	D	2504	NAD	C2N-N1N	3.44	1.38	1.35
2	A	2503	NAD	C2A-N1A	3.42	1.40	1.33
2	B	2502	NAD	C2N-N1N	3.32	1.38	1.35
2	C	2501	NAD	C2N-N1N	3.04	1.38	1.35
3	C	2758	MES	C3-N4	2.89	1.54	1.46
2	C	2501	NAD	C2A-N3A	2.88	1.39	1.33
2	B	2502	NAD	C2A-N3A	2.87	1.39	1.33
3	A	2759	MES	C3-N4	2.82	1.54	1.46
3	A	2759	MES	C7-N4	2.78	1.53	1.47
2	D	2504	NAD	C2A-N3A	2.77	1.38	1.33
3	A	2760	MES	C7-N4	2.76	1.53	1.47
2	A	2503	NAD	C2A-N3A	2.75	1.38	1.33
3	A	2760	MES	C3-N4	2.74	1.54	1.46
2	C	2501	NAD	PA-O3	2.65	1.62	1.59
3	A	2759	MES	O3S-S	-2.62	1.37	1.47
3	A	2760	MES	O3S-S	-2.61	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2758	MES	O3S-S	-2.54	1.37	1.47
2	A	2503	NAD	PA-O3	2.50	1.62	1.59
2	B	2502	NAD	PA-O3	2.28	1.62	1.59
2	A	2503	NAD	PN-O3	2.25	1.61	1.59
3	C	2758	MES	C5-N4	2.24	1.52	1.46
2	C	2501	NAD	PN-O3	2.23	1.61	1.59
2	D	2504	NAD	PA-O3	2.20	1.61	1.59
2	B	2502	NAD	PN-O3	2.19	1.61	1.59
2	D	2504	NAD	C8A-N7A	2.19	1.35	1.31
2	B	2502	NAD	C4N-C3N	2.17	1.42	1.39
3	A	2759	MES	C5-N4	2.15	1.52	1.46
2	B	2502	NAD	C8A-N7A	2.14	1.35	1.31
2	D	2504	NAD	C4N-C3N	2.14	1.42	1.39
3	A	2760	MES	C5-N4	2.10	1.52	1.46
2	A	2503	NAD	C8A-N7A	2.09	1.35	1.31
2	B	2502	NAD	C6N-N1N	2.07	1.40	1.35
2	A	2503	NAD	C6N-N1N	2.06	1.40	1.35
2	A	2503	NAD	C4N-C3N	2.05	1.42	1.39
2	C	2501	NAD	C4N-C3N	2.05	1.42	1.39
2	D	2504	NAD	C6N-N1N	2.05	1.40	1.35
2	C	2501	NAD	C6N-N1N	2.04	1.40	1.35
2	C	2501	NAD	C5A-N7A	-2.01	1.35	1.39

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2759	MES	O3S-S-O1S	8.01	131.44	111.40
3	A	2760	MES	O3S-S-O1S	7.93	131.24	111.40
3	C	2758	MES	O3S-S-O1S	7.78	130.87	111.40
3	A	2759	MES	O1S-S-C8	-7.10	95.99	106.73
3	A	2760	MES	O1S-S-C8	-6.64	96.69	106.73
3	A	2760	MES	O3S-S-C8	-5.76	94.73	106.00
3	C	2758	MES	O1S-S-C8	-5.71	98.11	106.73
3	C	2758	MES	O3S-S-C8	-5.31	95.62	106.00
2	B	2502	NAD	N3A-C2A-N1A	-5.31	120.55	128.58
2	C	2501	NAD	N3A-C2A-N1A	-5.28	120.59	128.58
2	D	2504	NAD	N3A-C2A-N1A	-5.26	120.62	128.58
2	A	2503	NAD	N3A-C2A-N1A	-5.19	120.72	128.58
2	A	2503	NAD	C3N-C7N-N7N	4.66	123.49	117.74
3	A	2759	MES	O3S-S-C8	-4.63	96.95	106.00
2	D	2504	NAD	C3N-C7N-N7N	4.61	123.42	117.74
2	B	2502	NAD	C3N-C7N-N7N	4.57	123.36	117.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2501	NAD	C3N-C7N-N7N	4.33	123.08	117.74
3	C	2758	MES	O2S-S-C8	-4.29	100.24	106.73
3	A	2759	MES	C2-C3-N4	-3.84	104.29	110.12
3	A	2760	MES	C2-C3-N4	-3.73	104.46	110.12
2	B	2502	NAD	N9A-C8A-N7A	-3.71	108.68	113.94
2	A	2503	NAD	N9A-C8A-N7A	-3.69	108.69	113.94
2	C	2501	NAD	N9A-C8A-N7A	-3.65	108.76	113.94
2	D	2504	NAD	N9A-C8A-N7A	-3.64	108.78	113.94
3	A	2759	MES	O2S-S-C8	-3.63	101.24	106.73
2	B	2502	NAD	C5A-N7A-C8A	3.47	108.90	103.45
2	C	2501	NAD	C5A-N7A-C8A	3.47	108.90	103.45
2	A	2503	NAD	C5A-N7A-C8A	3.44	108.86	103.45
2	D	2504	NAD	C5A-N7A-C8A	3.40	108.80	103.45
3	A	2760	MES	O2S-S-C8	-3.19	101.91	106.73
2	C	2501	NAD	C5A-C4A-N3A	-3.16	122.36	126.72
3	C	2758	MES	C2-C3-N4	-3.13	105.36	110.12
2	D	2504	NAD	C5A-C4A-N3A	-3.09	122.46	126.72
2	A	2503	NAD	C5A-C4A-N3A	-3.08	122.47	126.72
2	B	2502	NAD	C5A-C4A-N3A	-3.08	122.48	126.72
2	D	2504	NAD	C2A-N3A-C4A	2.95	119.03	111.83
2	C	2501	NAD	C2A-N3A-C4A	2.95	119.03	111.83
2	B	2502	NAD	C2A-N3A-C4A	2.94	119.00	111.83
2	A	2503	NAD	C2A-N3A-C4A	2.90	118.90	111.83
2	A	2503	NAD	C4A-C5A-N7A	-2.84	107.33	110.58
2	B	2502	NAD	C4A-C5A-N7A	-2.83	107.34	110.58
2	C	2501	NAD	C4A-C5A-N7A	-2.81	107.36	110.58
2	D	2504	NAD	C4A-C5A-N7A	-2.78	107.40	110.58
2	A	2503	NAD	O7N-C7N-N7N	-2.72	118.69	122.62
3	C	2758	MES	C6-C5-N4	2.70	114.23	110.12
2	B	2502	NAD	O7N-C7N-N7N	-2.70	118.72	122.62
3	A	2759	MES	C6-C5-N4	2.69	114.22	110.12
2	D	2504	NAD	O7N-C7N-N7N	-2.67	118.75	122.62
2	C	2501	NAD	O7N-C7N-N7N	-2.63	118.82	122.62
3	A	2760	MES	C6-C5-N4	2.60	114.08	110.12
3	A	2759	MES	O3S-S-O2S	-2.42	105.34	111.40
2	C	2501	NAD	C2B-C1B-N9A	2.39	119.23	113.30
3	A	2760	MES	O3S-S-O2S	-2.36	105.51	111.40
2	D	2504	NAD	C2B-C1B-N9A	2.35	119.15	113.30
2	A	2503	NAD	C2B-C1B-N9A	2.28	118.96	113.30
2	B	2502	NAD	C2B-C1B-N9A	2.24	118.86	113.30
3	C	2758	MES	O3S-S-O2S	-2.17	105.97	111.40
2	B	2502	NAD	C4B-O4B-C1B	-2.13	104.76	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2502	NAD	O4B-C1B-C2B	-2.07	102.18	106.62
2	A	2503	NAD	C4B-O4B-C1B	-2.03	104.98	109.47
3	C	2758	MES	C7-N4-C3	-2.02	105.86	111.24
2	A	2503	NAD	O4B-C1B-C2B	-2.01	102.33	106.62

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2503	NAD	O4D-C1D-N1N-C6N
2	B	2502	NAD	O4D-C1D-N1N-C6N
2	C	2501	NAD	O4D-C1D-N1N-C6N
2	D	2504	NAD	O4D-C1D-N1N-C6N
3	A	2759	MES	C8-C7-N4-C5
3	A	2760	MES	C7-C8-S-O3S
3	A	2759	MES	C8-C7-N4-C3
3	A	2760	MES	C8-C7-N4-C3
3	A	2760	MES	C8-C7-N4-C5
3	C	2758	MES	N4-C7-C8-S
2	A	2503	NAD	O4D-C1D-N1N-C2N
2	B	2502	NAD	O4D-C1D-N1N-C2N
2	C	2501	NAD	O4D-C1D-N1N-C2N
2	D	2504	NAD	O4D-C1D-N1N-C2N
2	A	2503	NAD	O4B-C4B-C5B-O5B
2	C	2501	NAD	O4B-C4B-C5B-O5B
2	D	2504	NAD	O4B-C4B-C5B-O5B
2	B	2502	NAD	O4B-C4B-C5B-O5B

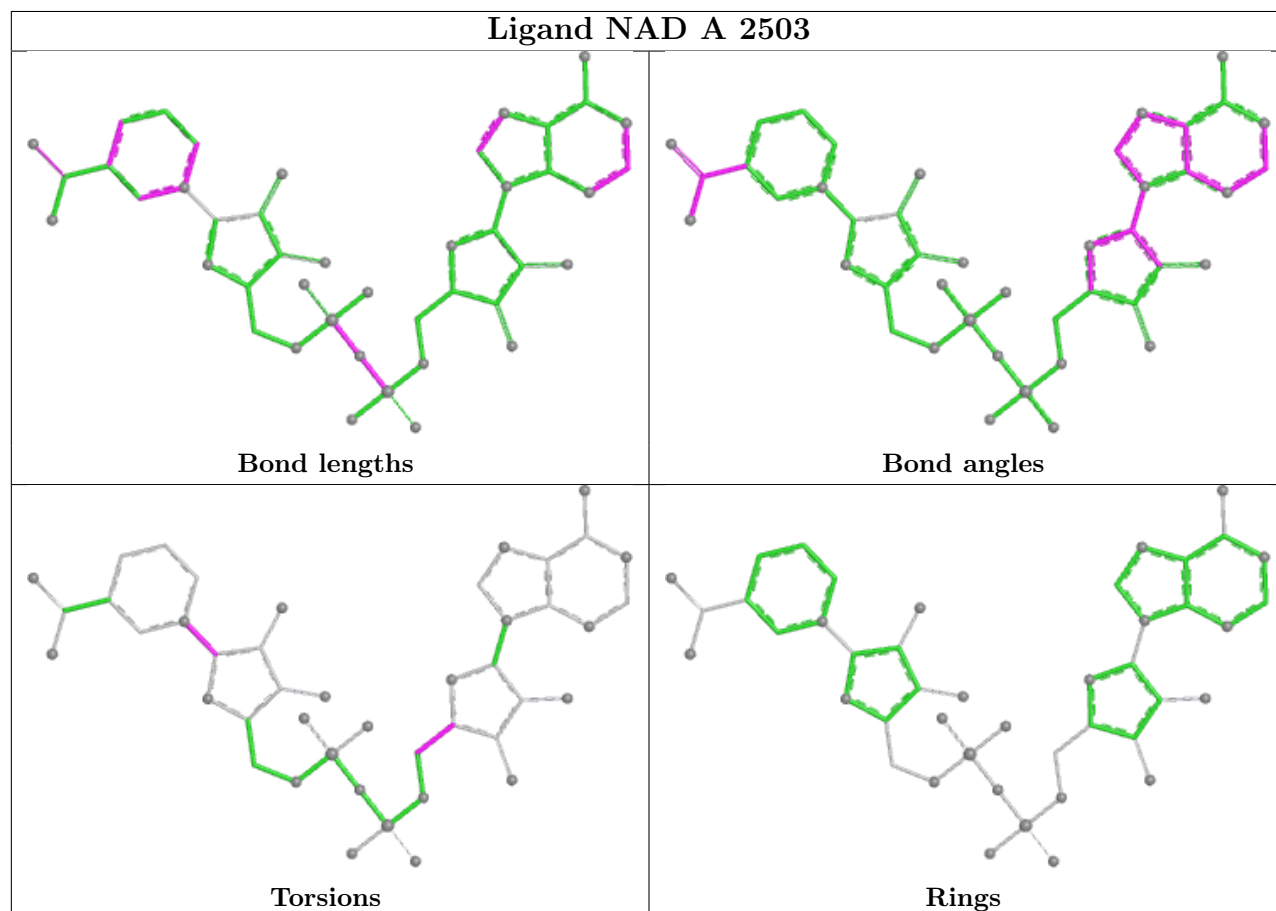
There are no ring outliers.

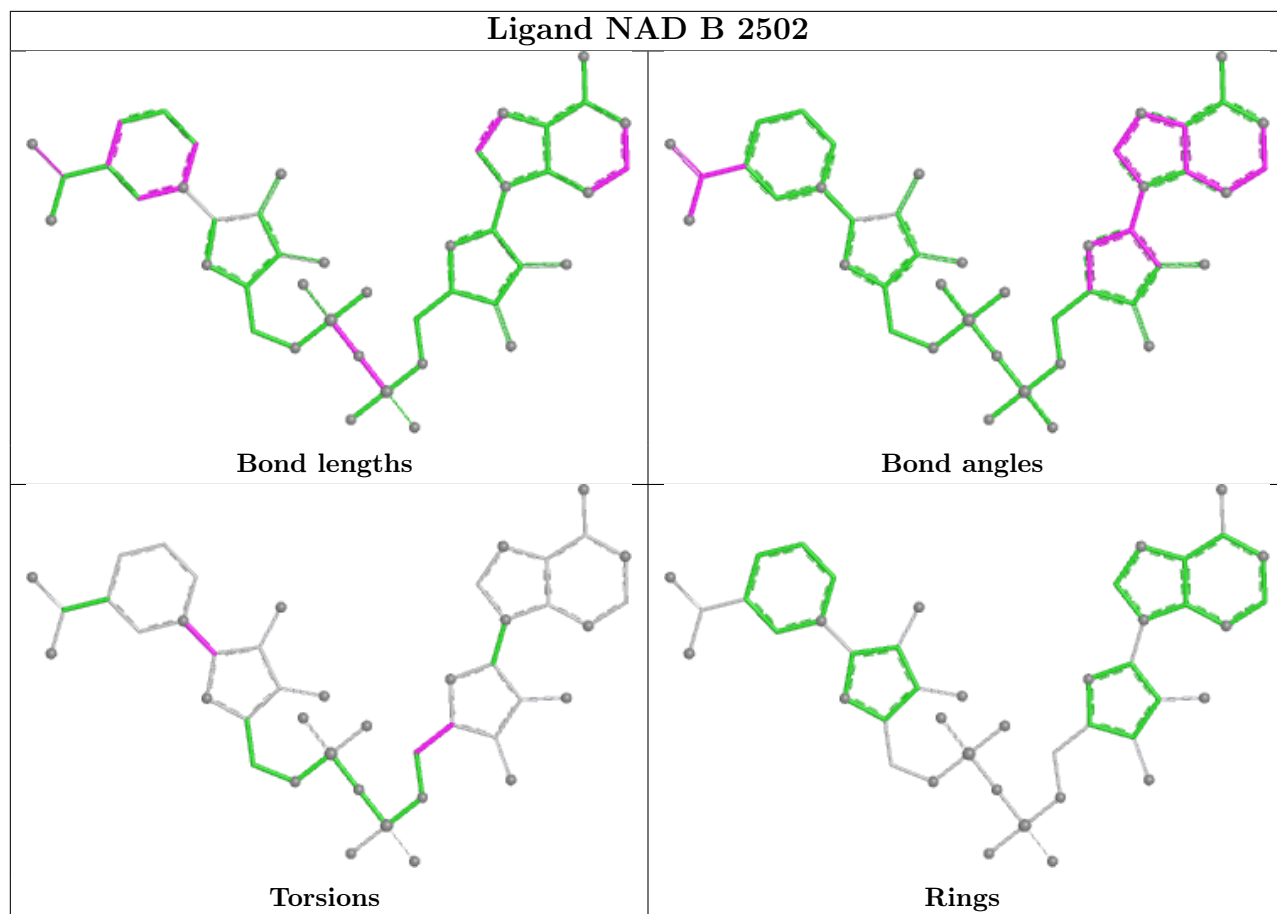
4 monomers are involved in 9 short contacts:

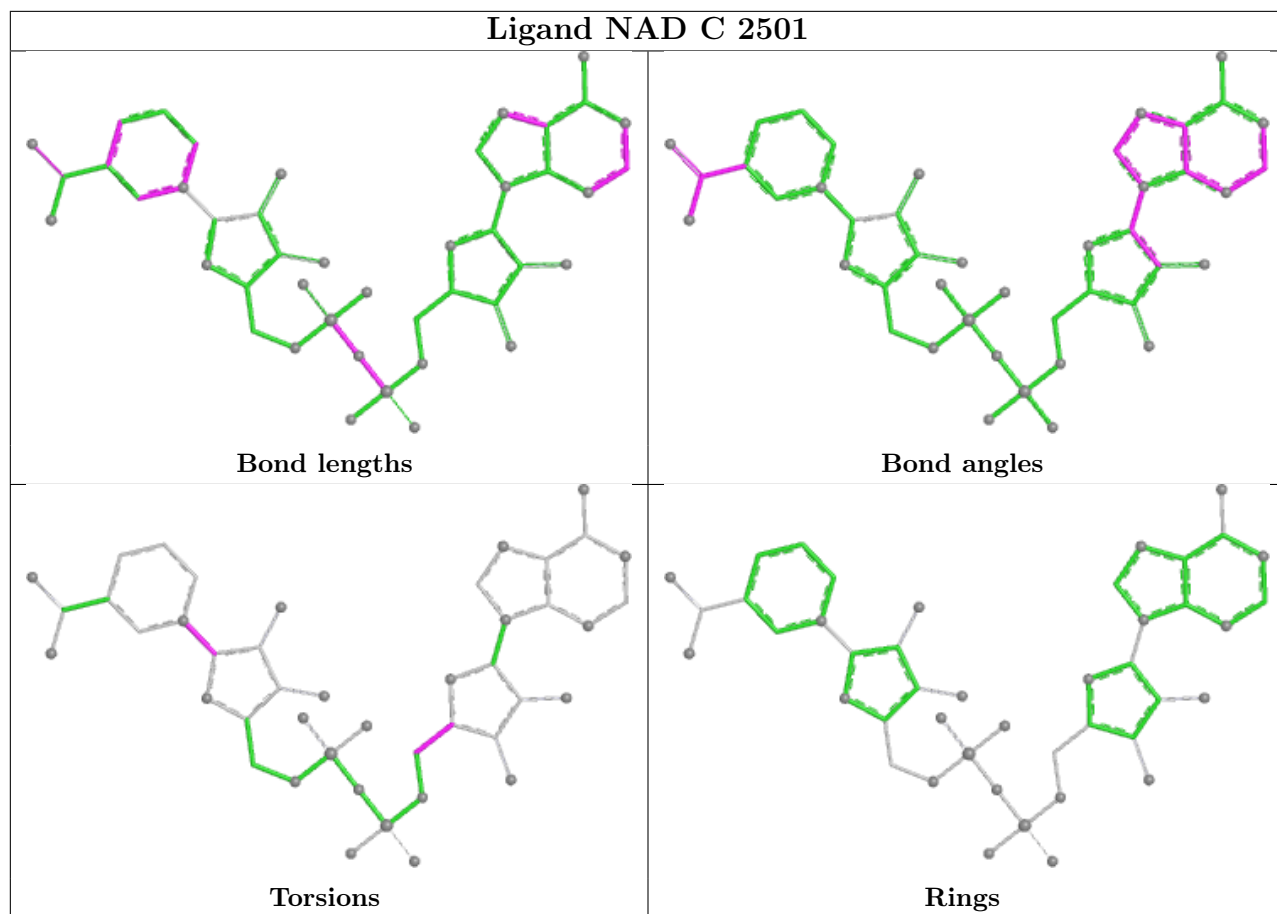
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2503	NAD	1	0
3	A	2759	MES	4	0
3	C	2758	MES	3	0
2	D	2504	NAD	1	0

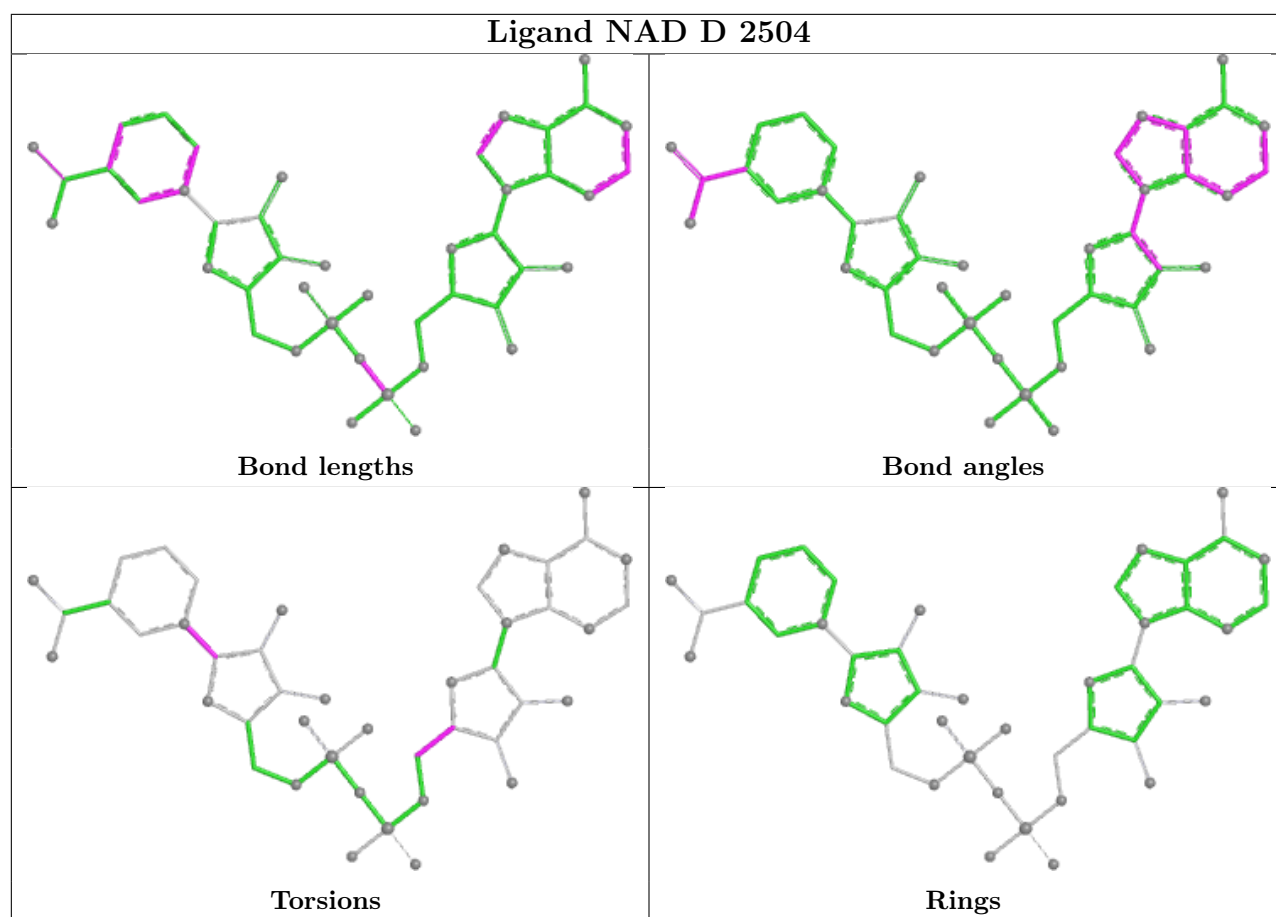
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	438/439 (99%)	0.70	65 (14%) 5 5	14, 24, 54, 59	0
1	B	434/439 (98%)	0.41	37 (8%) 16 16	13, 21, 44, 53	0
1	C	438/439 (99%)	0.31	28 (6%) 25 26	11, 20, 41, 48	0
1	D	436/439 (99%)	0.19	23 (5%) 32 33	10, 19, 38, 54	0
All	All	1746/1756 (99%)	0.40	153 (8%) 15 15	10, 21, 46, 59	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ILE	6.2
1	D	436	ILE	5.8
1	D	437	THR	5.7
1	A	437	THR	5.5
1	B	435	ALA	5.4
1	D	273	PRO	5.2
1	C	439	ALA	5.0
1	A	439	ALA	5.0
1	D	435	ALA	4.9
1	A	277	VAL	4.6
1	B	2	ILE	4.6
1	A	280	PRO	4.6
1	A	282	TRP	4.5
1	B	221	VAL	4.4
1	A	2	ILE	4.3
1	A	436	ILE	4.3
1	B	271	THR	4.1
1	A	275	PRO	4.1
1	B	275	PRO	4.0
1	A	272	ARG	3.9
1	A	271	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	277	VAL	3.8
1	D	276	GLY	3.8
1	A	435	ALA	3.8
1	C	288	GLU	3.7
1	D	2	ILE	3.7
1	A	278	ILE	3.6
1	A	297	ASN	3.6
1	A	221	VAL	3.6
1	D	271	THR	3.5
1	B	253	ILE	3.5
1	D	274	GLY	3.5
1	A	260	ALA	3.4
1	B	276	GLY	3.4
1	D	275	PRO	3.4
1	D	222	ASN	3.4
1	A	253	ILE	3.4
1	B	279	LYS	3.3
1	A	310	ALA	3.3
1	B	277	VAL	3.2
1	C	436	ILE	3.2
1	B	220	LEU	3.2
1	C	310	ALA	3.2
1	A	251	GLU	3.1
1	C	306	GLU	3.1
1	A	321	ASP	3.1
1	A	296	ALA	3.1
1	B	222	ASN	3.1
1	C	437	THR	3.1
1	A	228	LEU	3.0
1	A	283	ILE	3.0
1	A	279	LYS	3.0
1	B	270	PHE	3.0
1	B	251	GLU	3.0
1	A	263	ASP	3.0
1	A	276	GLY	3.0
1	A	303	LEU	2.9
1	A	227	ILE	2.9
1	B	256	GLY	2.9
1	A	281	GLN	2.9
1	C	261	LEU	2.9
1	C	282	TRP	2.9
1	A	252	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	220	LEU	2.8
1	A	261	LEU	2.8
1	B	273	PRO	2.8
1	B	282	TRP	2.8
1	A	285	LYS	2.8
1	A	300	PRO	2.8
1	B	280	PRO	2.8
1	A	302	ILE	2.8
1	A	307	ALA	2.8
1	A	413	ARG	2.8
1	D	272	ARG	2.8
1	A	51	ARG	2.7
1	D	4	GLU	2.7
1	C	275	PRO	2.7
1	B	283	ILE	2.7
1	A	262	LYS	2.7
1	B	257	PRO	2.7
1	A	229	THR	2.7
1	C	154	ASP	2.7
1	C	251	GLU	2.7
1	B	263	ASP	2.7
1	A	273	PRO	2.6
1	A	250	GLY	2.6
1	B	264	ALA	2.6
1	A	222	ASN	2.6
1	C	186	GLU	2.6
1	B	252	ASN	2.6
1	C	250	GLY	2.5
1	D	288	GLU	2.5
1	B	310	ALA	2.5
1	A	180	VAL	2.5
1	A	256	GLY	2.5
1	B	180	VAL	2.5
1	C	253	ILE	2.5
1	B	254	GLU	2.5
1	A	255	GLY	2.4
1	A	438	ARG	2.4
1	B	260	ALA	2.4
1	B	227	ILE	2.4
1	A	254	GLU	2.4
1	C	51	ARG	2.4
1	C	438	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	31	ARG	2.4
1	C	322	TYR	2.4
1	C	309	LYS	2.4
1	D	278	ILE	2.4
1	A	304	PRO	2.3
1	D	321	ASP	2.3
1	D	400	THR	2.3
1	C	272	ARG	2.3
1	A	257	PRO	2.3
1	B	272	ARG	2.3
1	C	281	GLN	2.3
1	D	310	ALA	2.3
1	A	215	VAL	2.3
1	A	299	VAL	2.3
1	A	231	ASP	2.2
1	B	258	GLN	2.2
1	C	284	GLU	2.2
1	B	281	GLN	2.2
1	A	187	ILE	2.2
1	A	258	GLN	2.2
1	A	288	GLU	2.2
1	B	234	LEU	2.2
1	B	305	GLU	2.1
1	A	309	LYS	2.1
1	A	306	GLU	2.1
1	C	222	ASN	2.1
1	A	154	ASP	2.1
1	B	229	THR	2.1
1	B	400	THR	2.1
1	C	280	PRO	2.1
1	A	264	ALA	2.1
1	A	274	GLY	2.1
1	B	250	GLY	2.1
1	B	255	GLY	2.1
1	B	309	LYS	2.1
1	C	221	VAL	2.1
1	D	297	ASN	2.1
1	A	284	GLU	2.1
1	C	364	GLU	2.1
1	D	305	GLU	2.1
1	D	308	LYS	2.1
1	C	270	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	306	GLU	2.0
1	A	295	LEU	2.0
1	A	183	LYS	2.0
1	A	247	LYS	2.0
1	D	251	GLU	2.0
1	A	31	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

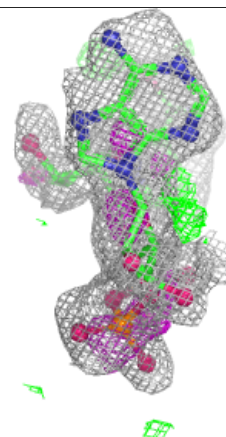
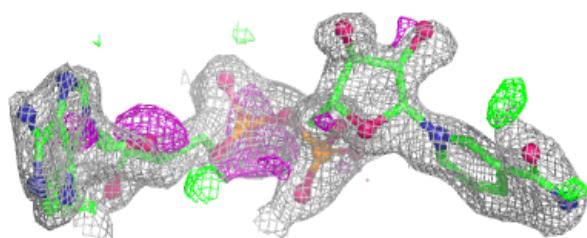
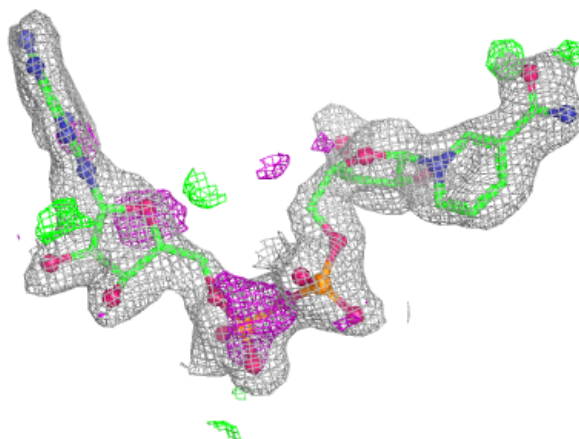
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MES	A	2759	12/12	0.65	0.24	45,46,50,51	0
3	MES	A	2760	12/12	0.77	0.18	48,48,49,49	0
2	NAD	A	2503	44/44	0.84	0.13	41,45,48,49	0
2	NAD	B	2502	44/44	0.84	0.13	34,36,41,43	0
2	NAD	D	2504	44/44	0.85	0.14	32,36,41,43	0
3	MES	C	2758	12/12	0.88	0.17	26,34,36,37	0
2	NAD	C	2501	44/44	0.94	0.09	23,27,35,35	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

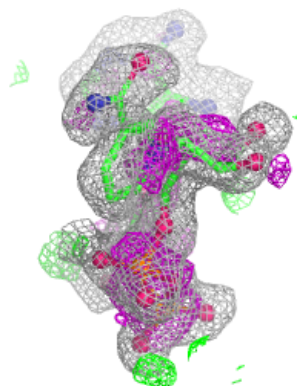
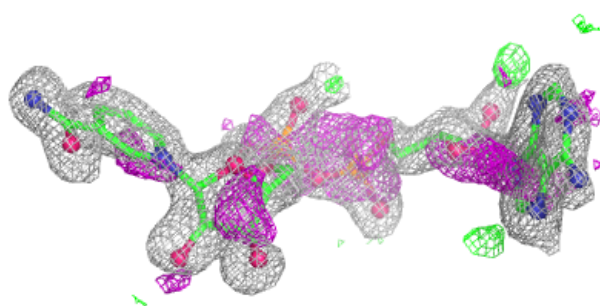
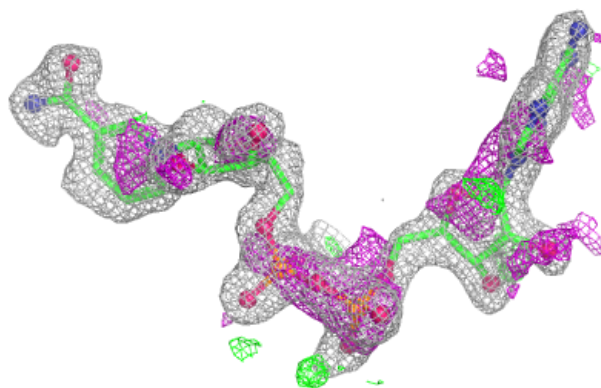
Electron density around NAD A 2503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

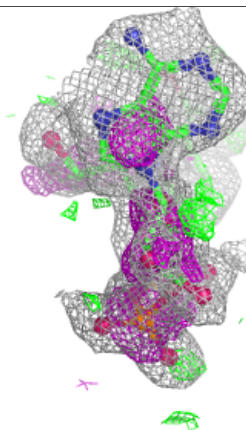
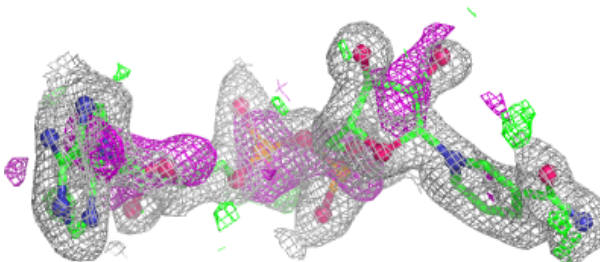
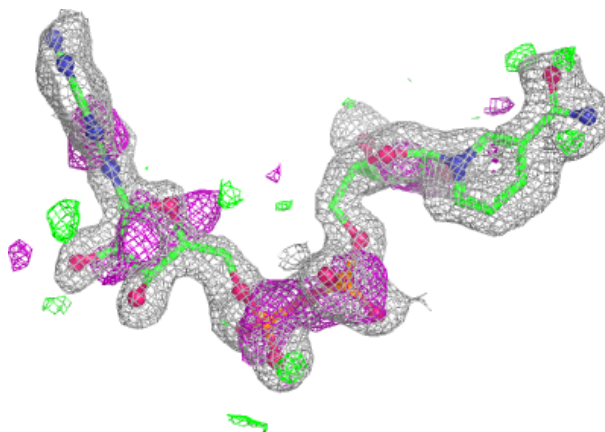


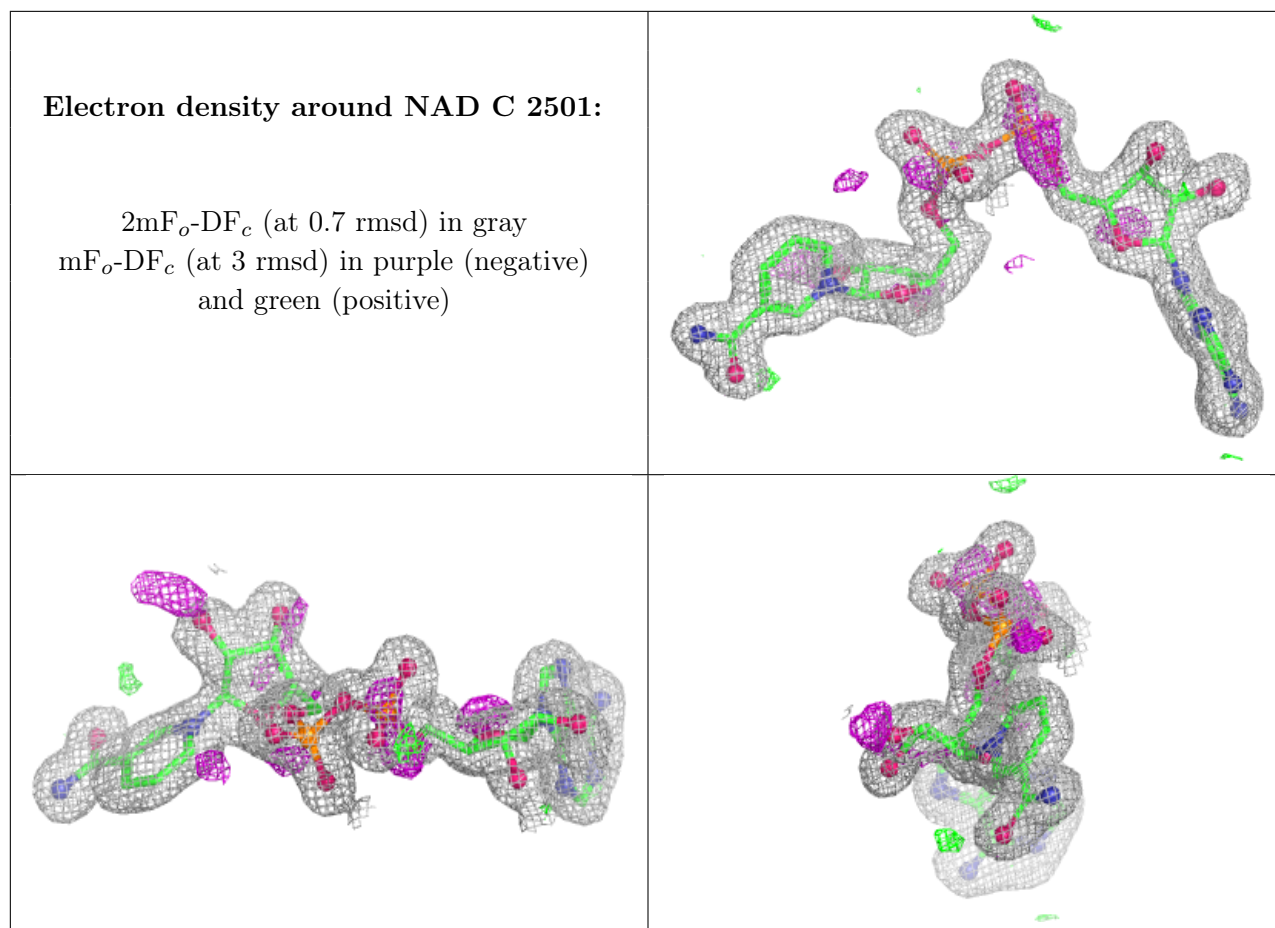
Electron density around NAD B 2502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAD D 2504:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.