



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 04:57 PM JST

PDB ID : 7BSJ
Title : Crystal structure of human ME2 R484W
Authors : Chen, W.L.; Tai, S.C.; Hung, H.C.; Ho, M.C.
Deposited on : 2020-03-30
Resolution : 2.48 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

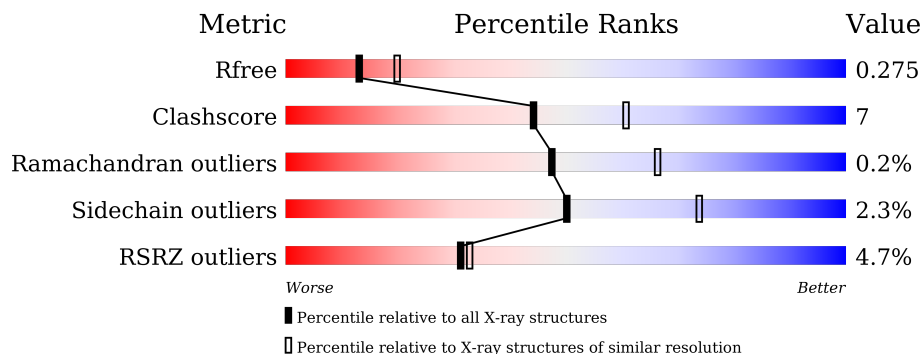
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	566	 3% 83% 14% .
1	B	566	 7% 85% 12% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8961 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.

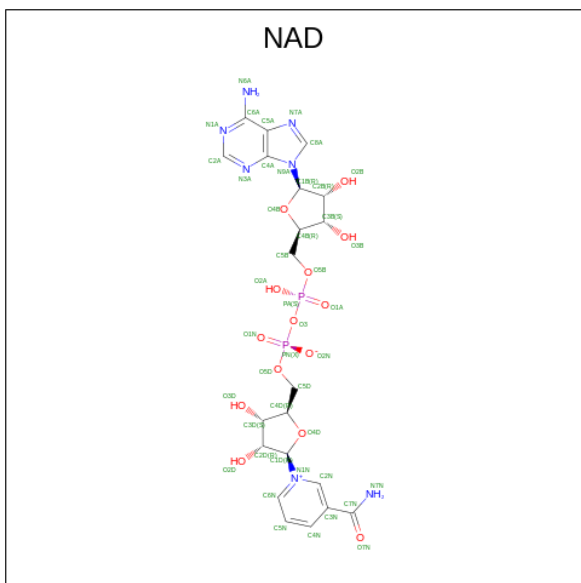
- Molecule 1 is a protein called NAD-dependent malic enzyme, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	553	Total 4373	C 2802	N 744	O 804	S 23	0	0	0
1	B	552	Total 4363	C 2796	N 741	O 803	S 23	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	initiating methionine	UNP P23368
A	484	TRP	ARG	engineered mutation	UNP P23368
B	19	MET	-	initiating methionine	UNP P23368
B	484	TRP	ARG	engineered mutation	UNP P23368

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

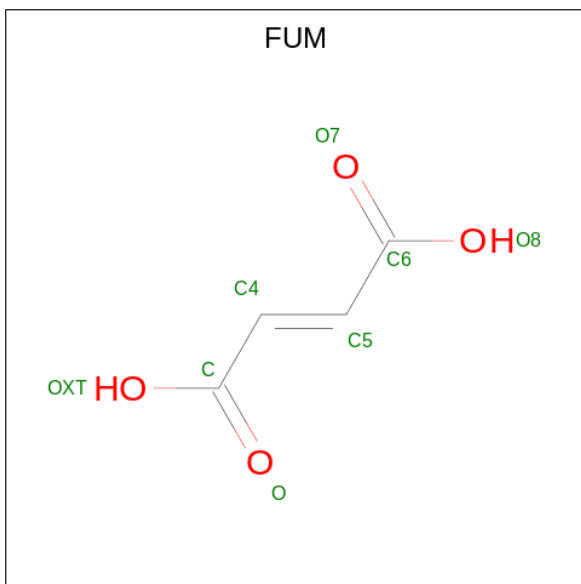


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	44	21	7	14	2	0	0
2	A	1	44	21	7	14	2	0	0
2	B	1	44	21	7	14	2	0	0
2	B	1	44	21	7	14	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
3	B	1	1	1	0	0

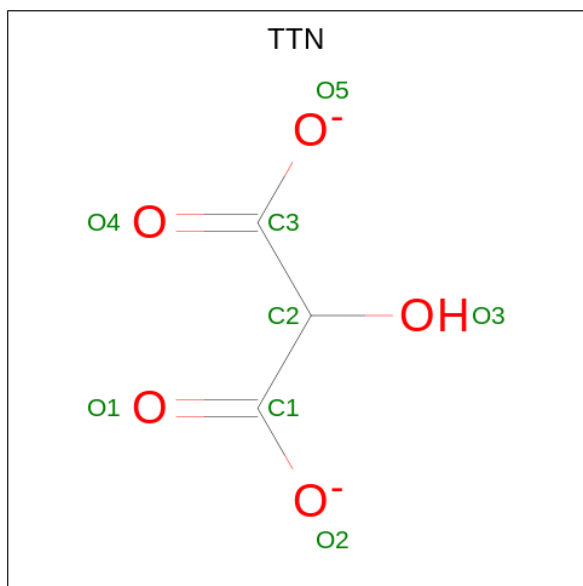
- Molecule 4 is FUMARIC ACID (three-letter code: FUM) (formula: C₄H₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
			Total	C			O
4	A	1	8	4	4	0	0
4	B	1	8	4	4	0	0

- Molecule 5 is TARTRONATE (three-letter code: TTN) (formula: C₃H₂O₅) (labeled as "Lig-

and of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C O	0	0
			8	3 5		
5	B	1	Total	C O	0	0
			8	3 5		

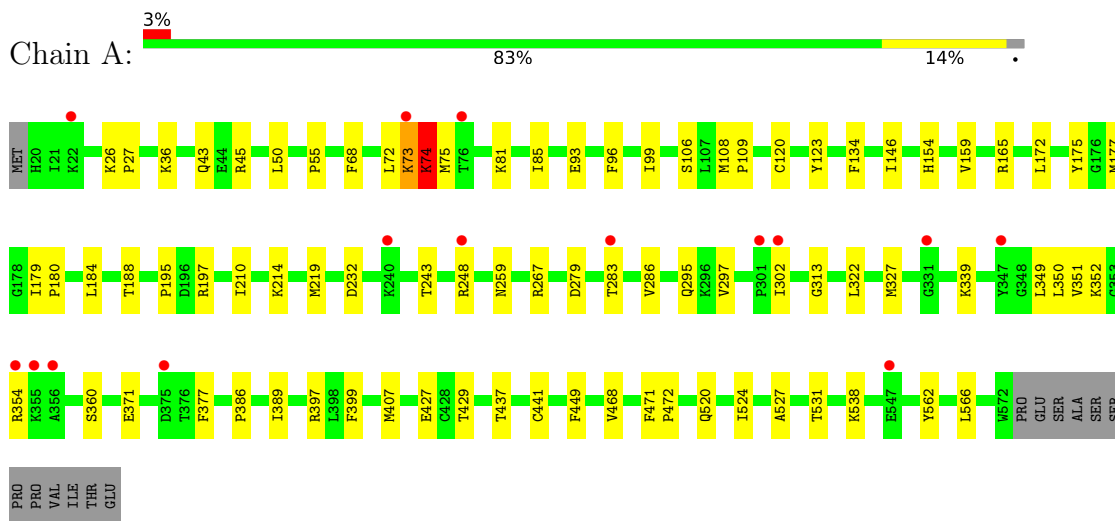
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total	O	0	0
			10	10		
6	B	5	Total	O	0	0
			5	5		

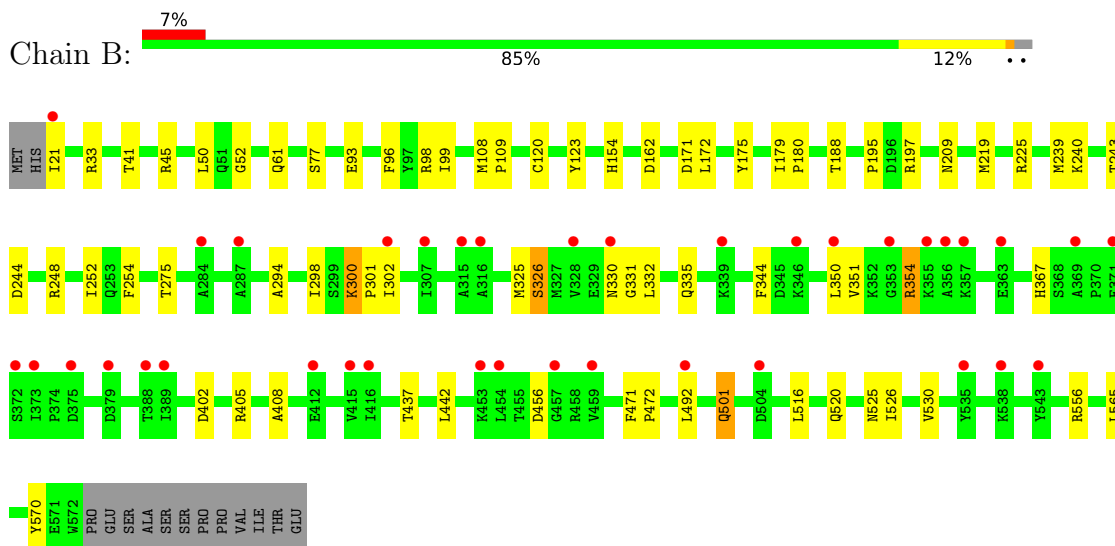
3 Residue-property plots i

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: NAD-dependent malic enzyme, mitochondrial



- Molecule 1: NAD-dependent malic enzyme, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.51Å 58.44Å 141.82Å 90.00° 129.64° 90.00°	Depositor
Resolution (Å)	29.40 – 2.48 29.38 – 2.46	Depositor EDS
% Data completeness (in resolution range)	85.9 (29.40-2.48) 85.9 (29.38-2.46)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.45Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.239 , 0.277 0.237 , 0.275	Depositor DCC
R_{free} test set	1988 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtrriage
Anisotropy	0.170	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 24.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8961	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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, FUM, TTN, MG

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	0.66	1/4469 (0.0%)	0.86	6/6052 (0.1%)
1	B	0.66	0/4458	0.72	0/6037
All	All	0.66	1/8927 (0.0%)	0.79	6/12089 (0.0%)

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	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	LYS	N-CA	5.17	1.56	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	LYS	C-N-CA	-23.82	62.14	121.70
1	A	73	LYS	CA-C-N	-20.23	72.69	117.20
1	A	74	LYS	O-C-N	-10.20	106.38	122.70
1	A	74	LYS	CA-C-N	7.74	134.23	117.20
1	A	74	LYS	C-N-CA	7.53	140.52	121.70
1	A	73	LYS	O-C-N	5.21	131.03	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	73	LYS	Mainchain
1	A	74	LYS	Peptide
1	B	570	TYR	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4373	0	4404	75	0
1	B	4363	0	4397	44	0
2	A	88	0	52	1	0
2	B	88	0	52	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	1	0	0
4	B	8	0	1	0	0
5	A	8	0	1	0	0
5	B	8	0	1	0	0
6	A	10	0	0	0	0
6	B	5	0	0	0	0
All	All	8961	0	8909	118	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 (118) 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:351:VAL:HG22	1:A:354:ARG:NE	1.10	1.42
1:A:351:VAL:HG13	1:A:354:ARG:NH2	1.39	1.37
1:A:349:LEU:C	1:A:354:ARG:NH1	1.80	1.34
1:A:351:VAL:CG2	1:A:354:ARG:HE	1.41	1.34
1:A:349:LEU:C	1:A:354:ARG:HH12	1.31	1.28
1:A:349:LEU:O	1:A:354:ARG:NH1	1.63	1.27
1:A:351:VAL:CG1	1:A:354:ARG:NH2	1.98	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:VAL:HG22	1:A:354:ARG:CZ	1.80	1.12
1:A:351:VAL:CG2	1:A:354:ARG:NE	2.07	1.05
1:A:72:LEU:C	1:A:74:LYS:H	1.34	1.01
1:A:72:LEU:C	1:A:74:LYS:N	2.10	0.97
1:A:351:VAL:CG1	1:A:354:ARG:HH21	1.79	0.89
1:A:72:LEU:O	1:A:74:LYS:N	2.07	0.83
1:A:74:LYS:O	1:A:74:LYS:HG2	1.77	0.83
1:A:351:VAL:HG13	1:A:354:ARG:HH22	1.41	0.79
1:A:351:VAL:HG13	1:A:354:ARG:CZ	2.15	0.76
1:A:351:VAL:HG11	1:A:354:ARG:NH2	2.02	0.74
1:A:351:VAL:HG11	1:A:354:ARG:HH21	1.54	0.71
1:A:351:VAL:CG2	1:A:354:ARG:CZ	2.60	0.71
1:A:349:LEU:CA	1:A:354:ARG:HH12	2.07	0.68
1:A:351:VAL:CG2	1:A:354:ARG:NH2	2.57	0.67
1:A:350:LEU:N	1:A:354:ARG:NH1	2.42	0.65
1:A:351:VAL:CG2	1:A:354:ARG:HH21	2.10	0.65
1:A:377:PHE:CE2	1:A:389:ILE:HD11	2.33	0.64
1:B:402:ASP:OD1	1:B:405:ARG:NH1	2.30	0.63
1:A:210:ILE:HG22	1:A:214:LYS:HE3	1.83	0.58
1:A:68:PHE:CE2	1:A:99:ILE:HG23	2.38	0.57
1:A:351:VAL:CB	1:A:354:ARG:NH2	2.66	0.57
1:A:302:ILE:HD11	1:A:327:MET:HG2	1.87	0.56
1:A:154:HIS:O	1:A:197:ARG:HG3	2.06	0.56
1:B:21:ILE:HD12	1:B:565:LEU:HD22	1.86	0.55
1:B:123:TYR:HB3	1:B:219:MET:HE1	1.88	0.55
1:A:349:LEU:HD23	1:A:354:ARG:HH22	1.72	0.55
1:B:350:LEU:CD2	1:B:354:ARG:NH1	2.71	0.54
1:B:171:ASP:O	1:B:209:ASN:HB2	2.08	0.54
1:B:123:TYR:HD2	1:B:219:MET:HE3	1.72	0.54
1:B:33:ARG:NH1	1:B:93:GLU:OE1	2.41	0.54
1:A:45:ARG:HA	1:A:50:LEU:HB2	1.91	0.53
1:A:175:TYR:CE1	1:A:219:MET:HE2	2.44	0.53
1:B:240:LYS:HE2	1:B:244:ASP:OD2	2.09	0.53
1:B:252:ILE:HB	1:B:275:THR:HG22	1.89	0.52
1:A:377:PHE:CZ	1:A:389:ILE:HD11	2.44	0.52
1:A:177:MET:O	1:A:180:PRO:HD2	2.10	0.52
1:A:43:GLN:HB3	1:A:566:LEU:HD21	1.91	0.51
1:B:162:ASP:O	1:B:225:ARG:NH2	2.39	0.51
1:B:325:MET:HG2	1:B:492:LEU:HD11	1.93	0.50
1:A:351:VAL:HG22	1:A:354:ARG:NH2	2.18	0.50
1:A:351:VAL:N	1:A:354:ARG:CZ	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:O	1:A:175:TYR:HB2	2.12	0.49
1:B:556:ARG:NE	2:B:1603:NAD:O2A	2.40	0.49
1:A:188:THR:HG21	1:A:195:PRO:HG3	1.95	0.49
1:B:354:ARG:HH21	1:B:354:ARG:CG	2.25	0.49
1:A:349:LEU:CB	1:A:354:ARG:HH12	2.26	0.49
1:A:74:LYS:O	1:A:74:LYS:CG	2.57	0.48
1:A:471:PHE:N	1:A:472:PRO:CD	2.77	0.48
1:B:108:MET:HB3	1:B:109:PRO:HD3	1.95	0.48
1:B:188:THR:HG21	1:B:195:PRO:HG3	1.96	0.48
1:B:61:GLN:HG2	1:B:98:ARG:HG2	1.96	0.47
1:A:350:LEU:N	1:A:354:ARG:HH12	1.98	0.47
1:B:239:MET:HE1	1:B:254:PHE:HZ	1.80	0.47
1:A:283:THR:HB	2:A:601:NAD:H4N	1.97	0.47
1:B:172:LEU:O	1:B:175:TYR:HB2	2.15	0.46
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.97	0.46
1:B:501:GLN:OE1	1:B:525:ASN:HB2	2.16	0.46
1:B:175:TYR:CD1	1:B:219:MET:HE2	2.51	0.46
1:B:298:ILE:HG22	1:B:300:LYS:HB2	1.98	0.46
1:A:108:MET:HB3	1:A:109:PRO:HD3	1.99	0.45
1:A:259:ASN:ND2	1:A:313:GLY:HA2	2.32	0.45
1:B:351:VAL:HA	1:B:367:HIS:O	2.17	0.45
1:B:408:ALA:HB2	1:B:437:THR:HG22	1.98	0.45
1:B:501:GLN:HE21	1:B:501:GLN:HB2	1.52	0.45
1:B:45:ARG:HA	1:B:50:LEU:HB2	1.99	0.45
1:B:471:PHE:CG	1:B:472:PRO:HD3	2.52	0.45
1:B:96:PHE:O	1:B:99:ILE:HG13	2.17	0.44
1:B:108:MET:HG2	1:B:516:LEU:HD21	1.99	0.44
1:A:146:ILE:HG23	1:B:52:GLY:HA3	1.99	0.44
1:A:322:LEU:HD23	1:A:322:LEU:HA	1.90	0.44
1:A:351:VAL:O	1:A:354:ARG:HG3	2.17	0.44
1:B:243:THR:HB	1:B:248:ARG:HA	1.99	0.44
1:B:41:THR:O	1:B:45:ARG:HG3	2.17	0.44
1:A:81:LYS:O	1:A:85:ILE:HG23	2.18	0.44
1:B:179:ILE:HB	1:B:180:PRO:HD3	2.00	0.44
1:A:123:TYR:HB3	1:A:219:MET:HE1	2.00	0.44
1:A:279:ASP:O	1:A:283:THR:HG21	2.19	0.43
1:A:468:VAL:HA	1:A:471:PHE:CE2	2.53	0.43
1:A:45:ARG:NH1	1:A:55:PRO:O	2.45	0.43
1:A:279:ASP:O	1:A:283:THR:CG2	2.65	0.43
1:B:21:ILE:CD1	1:B:565:LEU:HD22	2.49	0.43
1:B:154:HIS:O	1:B:197:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LYS:HE2	1:A:562:TYR:HB3	2.01	0.43
1:A:386:PRO:HG2	1:A:407:MET:CE	2.49	0.43
1:A:159:VAL:HG23	1:A:184:LEU:HD21	2.00	0.42
1:A:397:ARG:HH12	1:A:429:THR:HG23	1.84	0.42
1:A:351:VAL:CB	1:A:354:ARG:CZ	2.97	0.42
1:B:123:TYR:HB3	1:B:219:MET:CE	2.49	0.42
1:B:300:LYS:HG3	1:B:301:PRO:HD2	2.02	0.42
1:B:526:ILE:O	1:B:530:VAL:HG23	2.20	0.42
1:A:429:THR:HA	1:A:449:PHE:CZ	2.55	0.42
2:B:1603:NAD:O1A	2:B:1603:NAD:O2N	2.37	0.42
1:A:259:ASN:HD21	1:A:313:GLY:HA2	1.86	0.41
1:B:471:PHE:N	1:B:472:PRO:CD	2.82	0.41
1:A:93:GLU:O	1:A:96:PHE:HB3	2.20	0.41
1:A:96:PHE:O	1:A:99:ILE:HB	2.20	0.41
1:A:437:THR:HG21	1:A:441:CYS:HB3	2.03	0.41
1:A:26:LYS:N	1:A:27:PRO:CD	2.84	0.41
1:A:134:PHE:O	1:B:52:GLY:HA2	2.20	0.41
1:B:120:CYS:O	1:B:175:TYR:HB3	2.20	0.41
1:B:294:ALA:HA	1:B:442:LEU:HD13	2.02	0.41
1:B:326:SER:O	1:B:330:ASN:HB2	2.20	0.41
1:A:520:GLN:O	1:A:524:ILE:HG12	2.20	0.41
1:A:120:CYS:O	1:A:175:TYR:HB3	2.19	0.41
1:A:399:PHE:CG	1:A:427:GLU:HB3	2.56	0.41
1:A:527:ALA:O	1:A:531:THR:HG23	2.20	0.41
1:B:175:TYR:CD1	1:B:219:MET:CE	3.04	0.41
1:A:283:THR:HA	1:A:286:VAL:HG12	2.03	0.40
1:A:243:THR:HB	1:A:248:ARG:HA	2.03	0.40
1:B:325:MET:CG	1:B:492:LEU:HD11	2.51	0.40
1:A:351:VAL:CB	1:A:354:ARG:HH21	2.31	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	551/566 (97%)	528 (96%)	22 (4%)	1 (0%)	47 66
1	B	550/566 (97%)	524 (95%)	25 (4%)	1 (0%)	47 66
All	All	1101/1132 (97%)	1052 (96%)	47 (4%)	2 (0%)	47 66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	MET
1	B	331	GLY

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	469/481 (98%)	458 (98%)	11 (2%)	50 74
1	B	468/481 (97%)	457 (98%)	11 (2%)	49 72
All	All	937/962 (97%)	915 (98%)	22 (2%)	50 74

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	SER
1	A	165	ARG
1	A	232	ASP
1	A	267	ARG
1	A	295	GLN
1	A	297	VAL
1	A	339	LYS
1	A	352	LYS
1	A	360	SER
1	A	371	GLU
1	A	538	LYS
1	B	77	SER
1	B	300	LYS
1	B	302	ILE

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Mol	Chain	Res	Type
1	B	326	SER
1	B	332	LEU
1	B	335	GLN
1	B	344	PHE
1	B	354	ARG
1	B	456	ASP
1	B	501	GLN
1	B	520	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	338	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	B	1601	-	42,48,48	0.81	1 (2%)	50,73,73	1.20	5 (10%)
5	TTN	A	605	3	5,7,7	1.23	0	2,9,9	0.95	0
5	TTN	B	1605	3	5,7,7	1.31	0	2,9,9	0.83	0
4	FUM	B	1604	-	7,7,7	1.06	0	8,8,8	0.80	0
2	NAD	A	601	-	42,48,48	0.90	3 (7%)	50,73,73	1.24	6 (12%)
2	NAD	B	1603	-	42,48,48	0.84	1 (2%)	50,73,73	1.34	5 (10%)
2	NAD	A	603	-	42,48,48	0.90	2 (4%)	50,73,73	1.36	8 (16%)
4	FUM	A	604	-	7,7,7	1.10	0	8,8,8	0.85	0

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	B	1601	-	-	7/26/62/62	0/5/5/5
5	TTN	A	605	3	-	2/8/8/8	-
5	TTN	B	1605	3	-	0/8/8/8	-
4	FUM	B	1604	-	-	0/5/5/5	-
2	NAD	A	601	-	-	7/26/62/62	0/5/5/5
2	NAD	B	1603	-	-	12/26/62/62	0/5/5/5
2	NAD	A	603	-	-	5/26/62/62	0/5/5/5
4	FUM	A	604	-	-	0/5/5/5	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1603	NAD	C5A-C4A	2.39	1.47	1.40
2	B	1601	NAD	C5A-C4A	2.36	1.47	1.40
2	A	601	NAD	C5A-C4A	2.35	1.47	1.40
2	A	603	NAD	C5A-C4A	2.34	1.47	1.40
2	A	603	NAD	O4D-C1D	2.31	1.44	1.41
2	A	601	NAD	O4D-C1D	2.27	1.44	1.41
2	A	601	NAD	C2A-N3A	2.20	1.35	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1603	NAD	PN-O3-PA	-4.68	116.78	132.83
2	A	601	NAD	N3A-C2A-N1A	-4.14	122.20	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	NAD	N3A-C2A-N1A	-4.05	122.35	128.68
2	B	1603	NAD	N3A-C2A-N1A	-3.99	122.44	128.68
2	B	1601	NAD	N3A-C2A-N1A	-3.94	122.52	128.68
2	A	603	NAD	C3D-C2D-C1D	3.74	106.61	100.98
2	B	1601	NAD	PN-O3-PA	-3.50	120.81	132.83
2	A	603	NAD	C4A-C5A-N7A	-3.25	106.02	109.40
2	A	601	NAD	PN-O3-PA	-3.08	122.26	132.83
2	B	1603	NAD	C4A-C5A-N7A	-2.80	106.48	109.40
2	A	603	NAD	C3N-C7N-N7N	2.72	121.02	117.75
2	A	601	NAD	C4A-C5A-N7A	-2.65	106.64	109.40
2	B	1601	NAD	C4A-C5A-N7A	-2.60	106.69	109.40
2	B	1603	NAD	C1B-N9A-C4A	-2.56	122.14	126.64
2	A	603	NAD	PN-O3-PA	-2.54	124.12	132.83
2	A	601	NAD	C3N-C7N-N7N	2.32	120.54	117.75
2	B	1601	NAD	C3N-C7N-N7N	2.23	120.43	117.75
2	B	1603	NAD	C2A-N1A-C6A	2.21	122.54	118.75
2	A	601	NAD	C1B-N9A-C4A	-2.19	122.80	126.64
2	A	603	NAD	C2A-N1A-C6A	2.11	122.37	118.75
2	A	603	NAD	C6N-N1N-C2N	-2.10	120.06	121.97
2	A	603	NAD	O7N-C7N-N7N	-2.08	119.62	122.58
2	B	1601	NAD	C2A-N1A-C6A	2.05	122.26	118.75
2	A	601	NAD	O7N-C7N-N7N	-2.00	119.73	122.58

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAD	C5B-O5B-PA-O1A
2	A	601	NAD	O4D-C1D-N1N-C6N
2	A	603	NAD	C5D-O5D-PN-O1N
2	A	603	NAD	C5D-O5D-PN-O2N
2	A	603	NAD	O4D-C4D-C5D-O5D
2	A	603	NAD	C3D-C4D-C5D-O5D
2	B	1601	NAD	O4B-C4B-C5B-O5B
2	B	1601	NAD	O4D-C1D-N1N-C6N
2	B	1603	NAD	C5D-O5D-PN-O1N
2	B	1603	NAD	C4D-C5D-O5D-PN
2	B	1603	NAD	C3D-C4D-C5D-O5D
2	B	1603	NAD	O4D-C1D-N1N-C6N
2	B	1601	NAD	C3B-C4B-C5B-O5B
2	B	1603	NAD	O4D-C4D-C5D-O5D
2	B	1603	NAD	C4N-C3N-C7N-O7N

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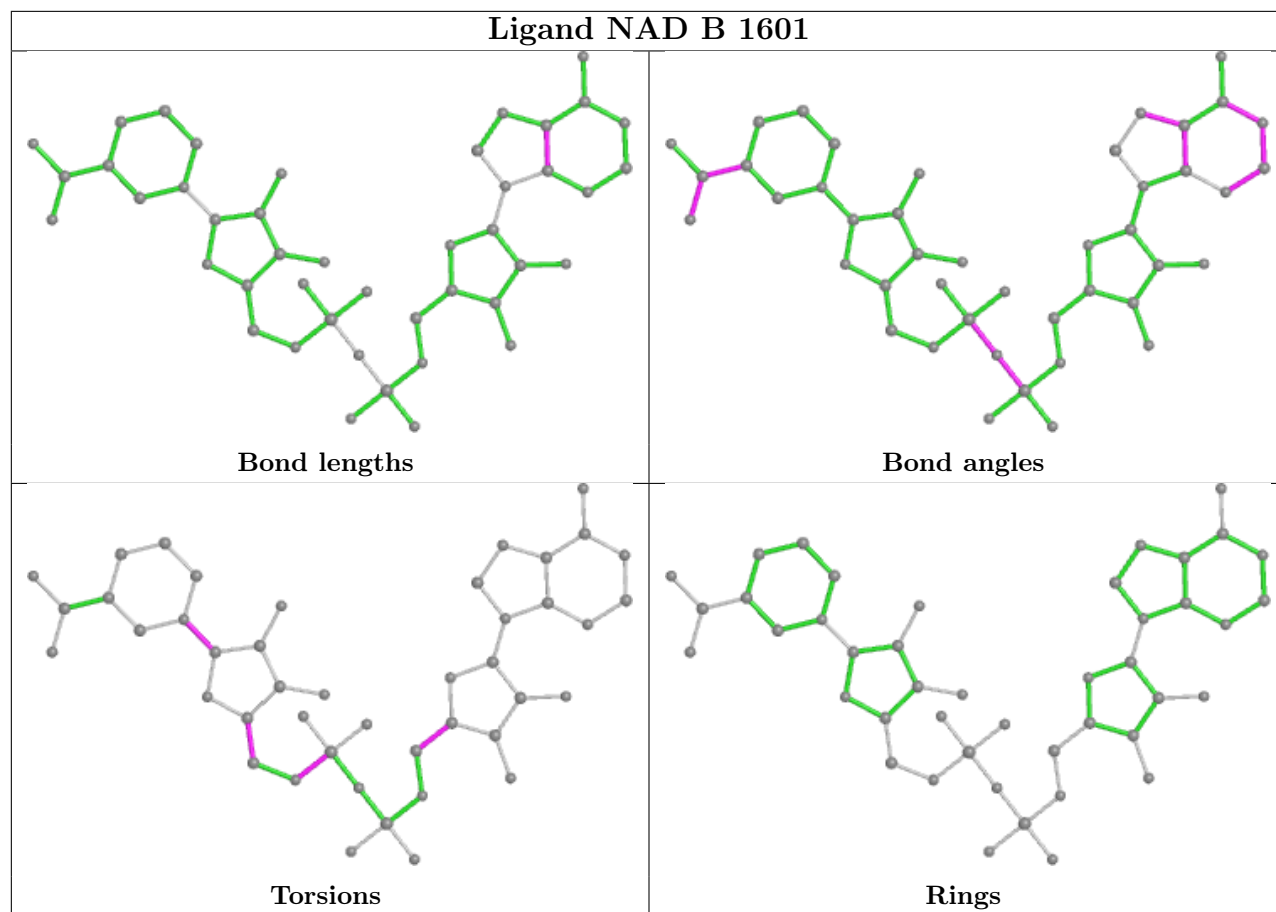
Mol	Chain	Res	Type	Atoms
2	B	1603	NAD	C2N-C3N-C7N-O7N
5	A	605	TTN	O1-C1-C2-O3
5	A	605	TTN	O2-C1-C2-O3
2	B	1601	NAD	O4D-C4D-C5D-O5D
2	B	1603	NAD	C4N-C3N-C7N-N7N
2	A	601	NAD	C5B-O5B-PA-O3
2	A	603	NAD	C5D-O5D-PN-O3
2	B	1601	NAD	C5D-O5D-PN-O3
2	B	1603	NAD	C5B-O5B-PA-O3
2	B	1603	NAD	C2N-C3N-C7N-N7N
2	B	1603	NAD	C5B-O5B-PA-O2A
2	A	601	NAD	PN-O3-PA-O1A
2	B	1601	NAD	C3D-C4D-C5D-O5D
2	A	601	NAD	O4B-C4B-C5B-O5B
2	A	601	NAD	C5D-O5D-PN-O3
2	B	1603	NAD	C5D-O5D-PN-O3
2	A	601	NAD	PN-O3-PA-O2A
2	B	1601	NAD	C5D-O5D-PN-O1N

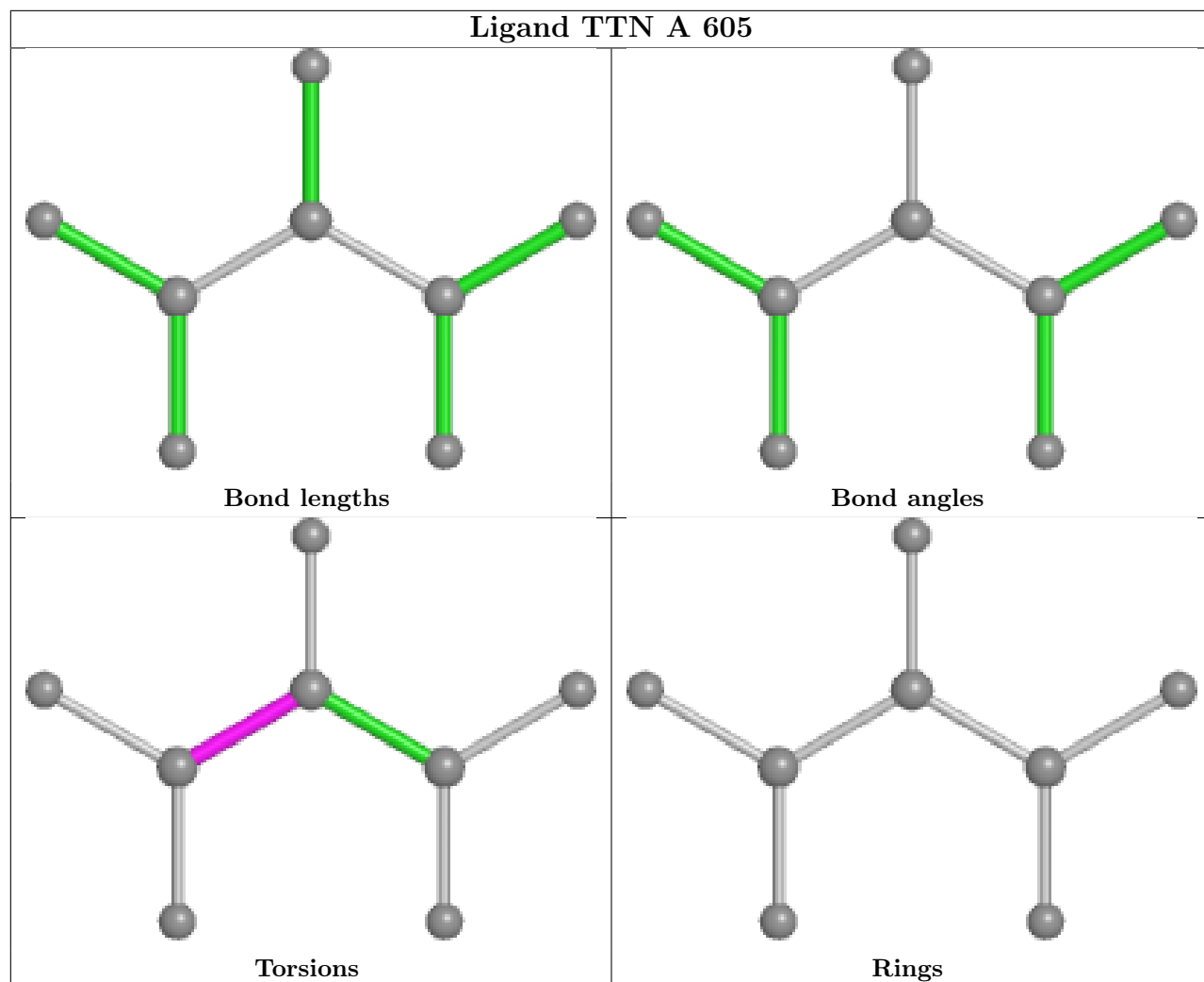
There are no ring outliers.

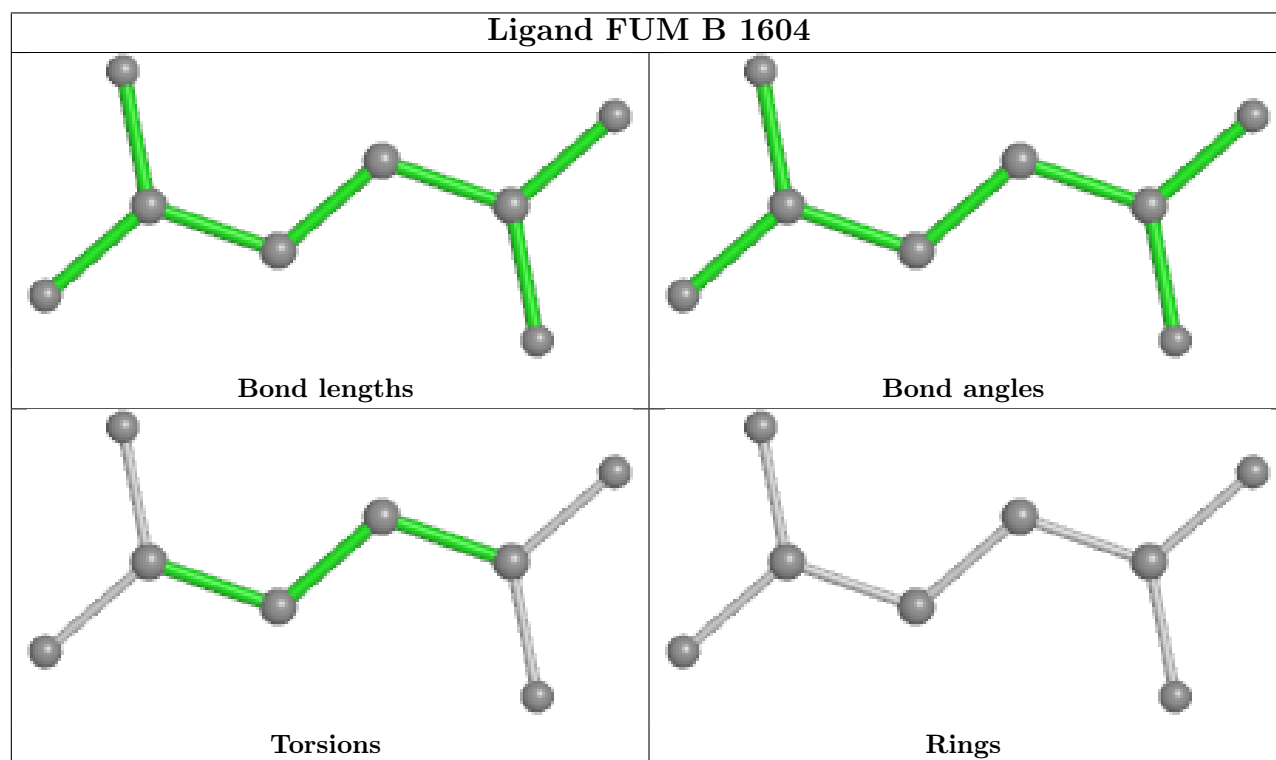
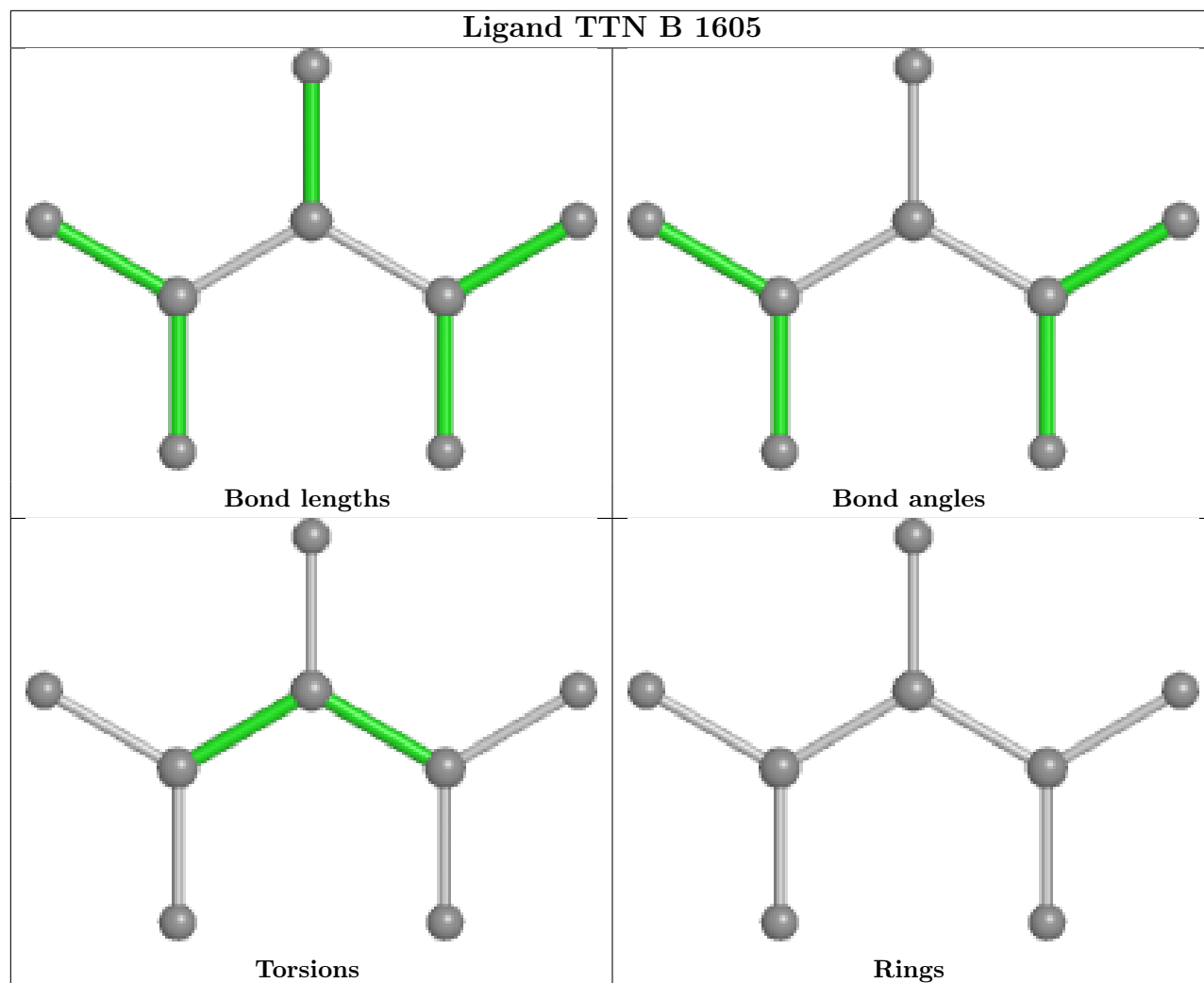
2 monomers are involved in 3 short contacts:

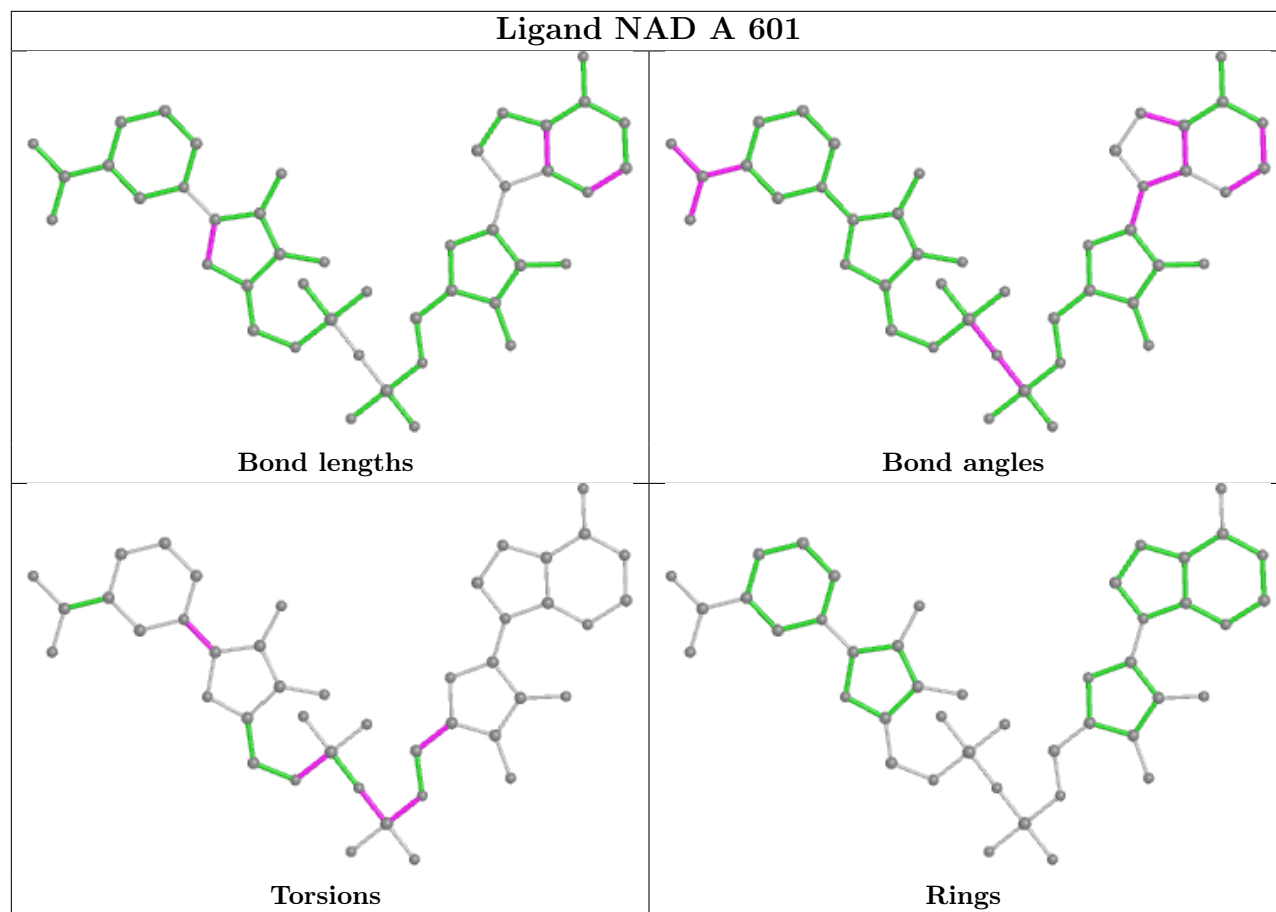
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAD	1	0
2	B	1603	NAD	2	0

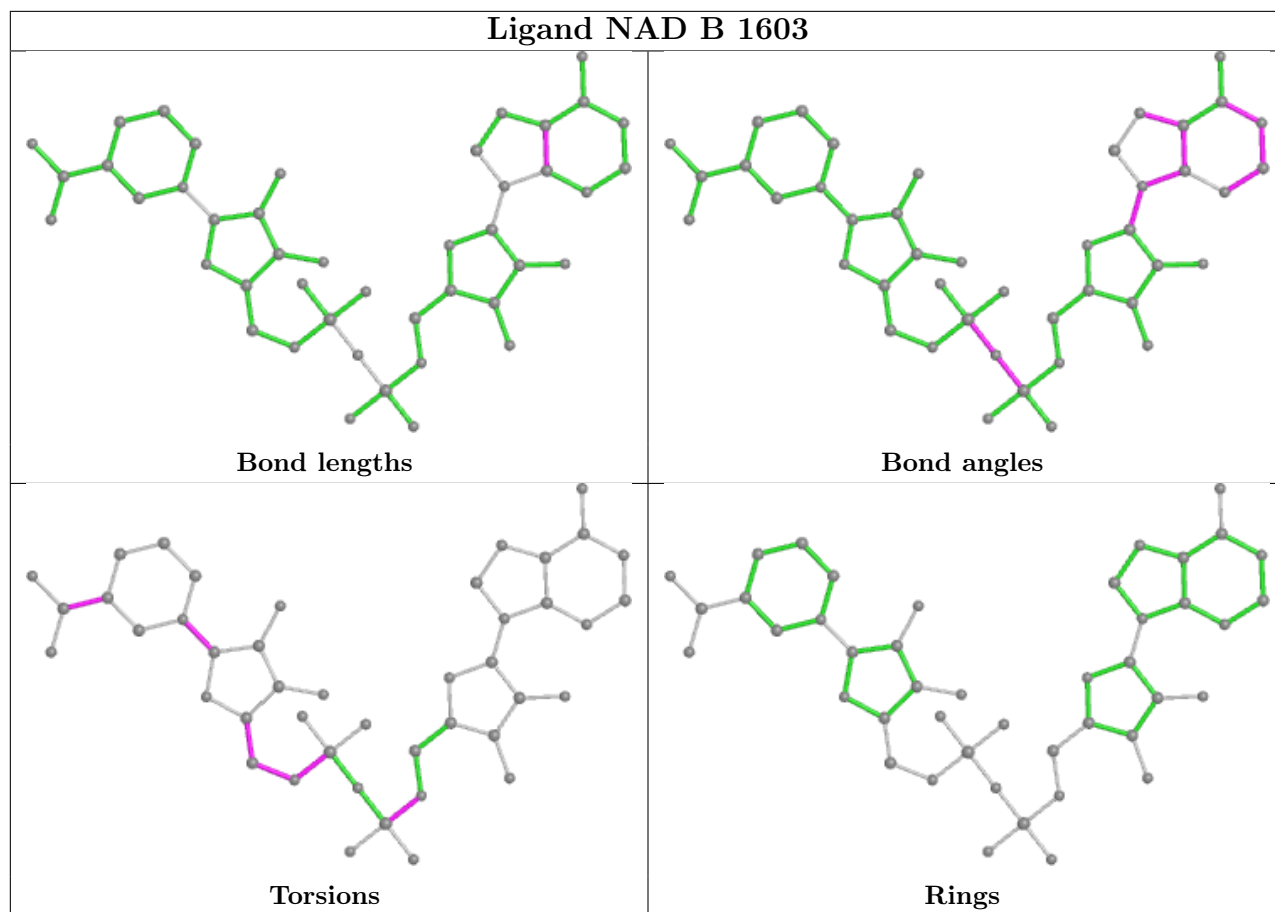
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

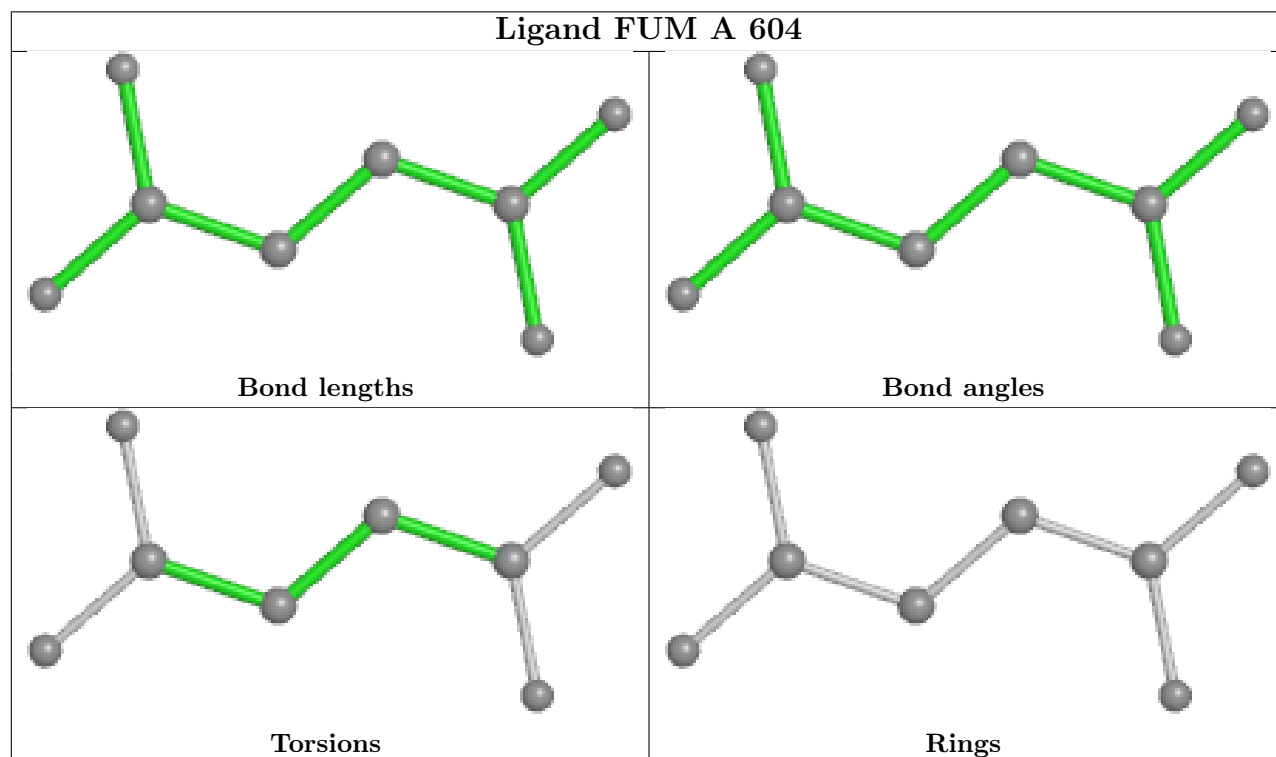
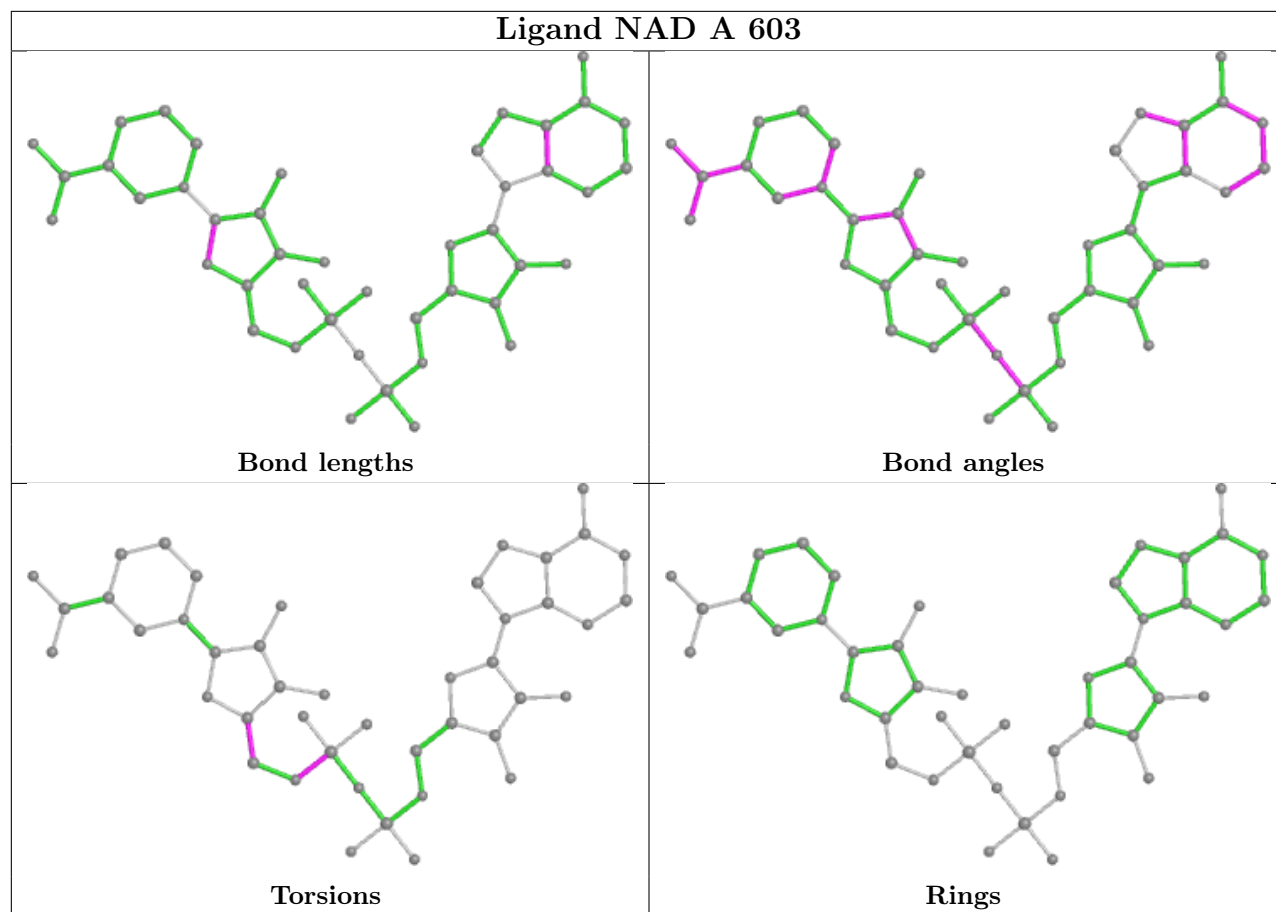












5.7 Other polymers [i](#)

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	553/566 (97%)	0.16	15 (2%) 54 56	19, 37, 60, 79	0
1	B	552/566 (97%)	0.38	37 (6%) 17 17	21, 41, 72, 89	0
All	All	1105/1132 (97%)	0.27	52 (4%) 31 33	19, 39, 69, 89	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354	ARG	5.4
1	B	453	LYS	4.7
1	A	355	LYS	4.3
1	B	373	ILE	4.2
1	B	21	ILE	3.8
1	A	331	GLY	3.7
1	B	372	SER	3.6
1	A	283	THR	3.6
1	B	457	GLY	3.5
1	B	375	ASP	3.0
1	B	543	TYR	2.9
1	B	353	GLY	2.9
1	B	459	VAL	2.8
1	A	248	ARG	2.8
1	A	375	ASP	2.8
1	B	412	GLU	2.8
1	A	302	ILE	2.8
1	B	355	LYS	2.7
1	A	301	PRO	2.7
1	B	330	ASN	2.6
1	B	316	ALA	2.6
1	B	369	ALA	2.5
1	B	538	LYS	2.5
1	B	357	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	22	LYS	2.4
1	B	346	LYS	2.3
1	B	415	VAL	2.3
1	B	302	ILE	2.3
1	B	315	ALA	2.3
1	B	416	ILE	2.3
1	A	240	LYS	2.3
1	A	347	TYR	2.3
1	B	379	ASP	2.3
1	B	535	TYR	2.3
1	B	339	LYS	2.3
1	A	73	LYS	2.3
1	B	307	ILE	2.3
1	B	389	ILE	2.3
1	B	492	LEU	2.2
1	B	371	GLU	2.2
1	A	356	ALA	2.2
1	A	76	THR	2.2
1	B	356	ALA	2.2
1	B	504	ASP	2.2
1	B	454	LEU	2.2
1	B	388	THR	2.1
1	B	328	VAL	2.1
1	A	547	GLU	2.1
1	B	287	ALA	2.1
1	B	363	GLU	2.1
1	B	284	ALA	2.0
1	B	350	LEU	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 monosaccharides in this entry.

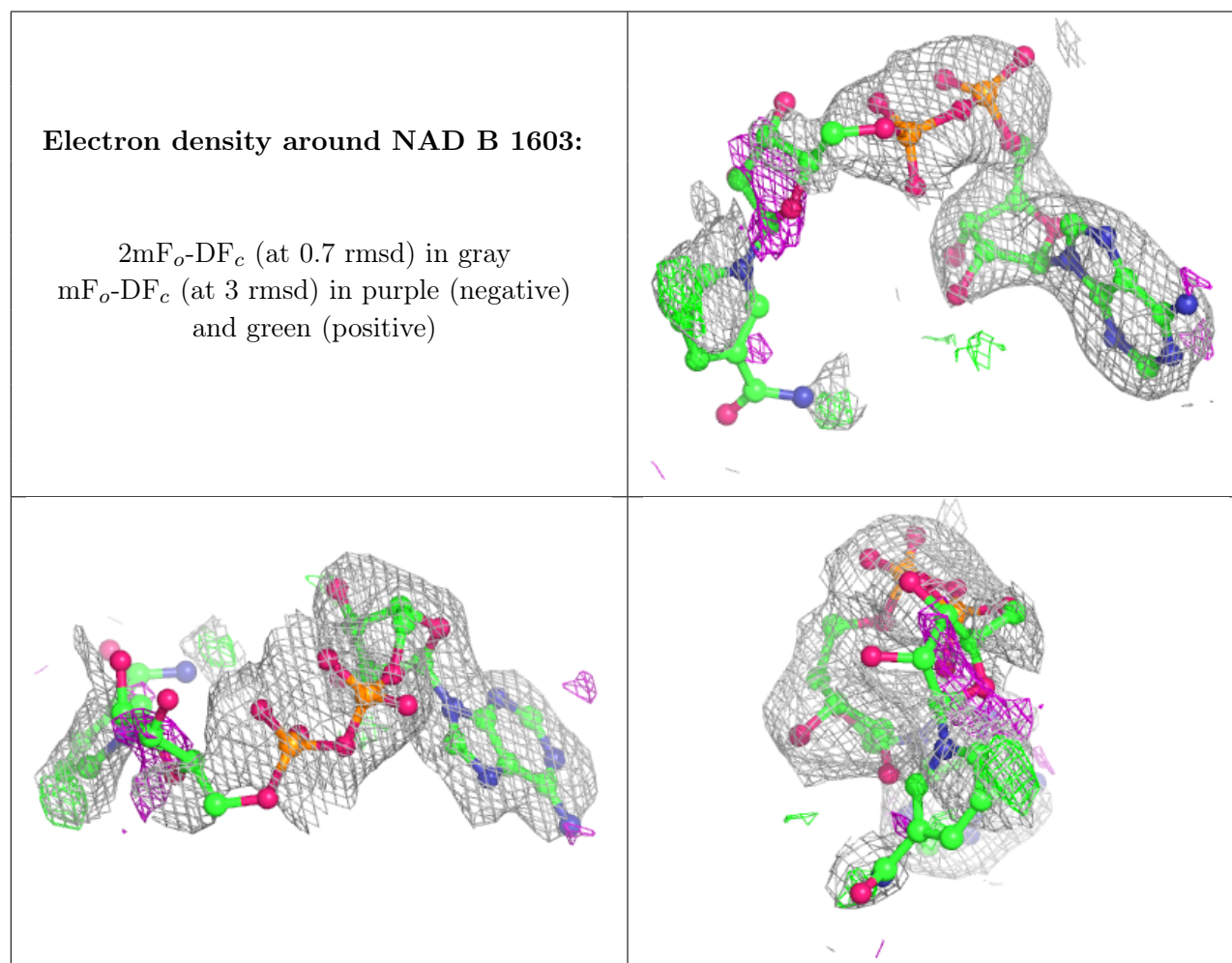
6.4 Ligands [i](#)

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.

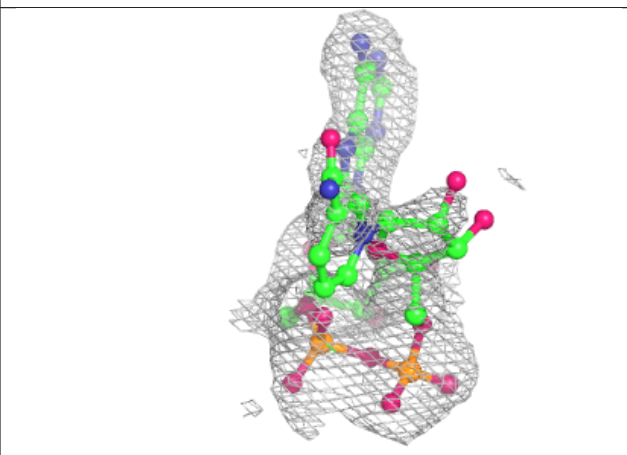
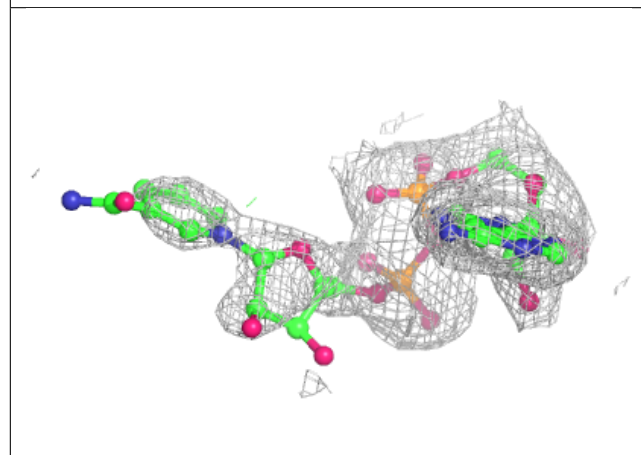
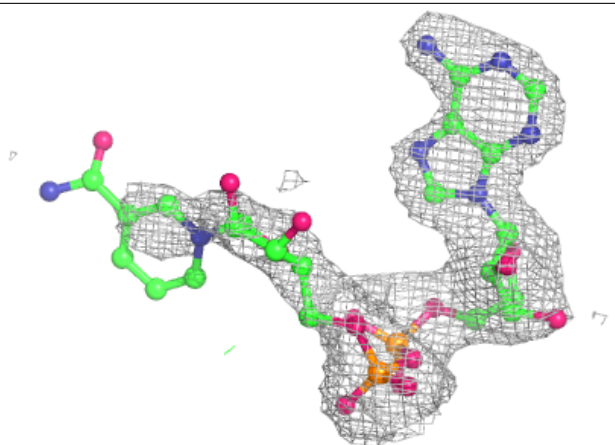
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	B	1602	1/1	0.78	0.18	41,41,41,41	0
2	NAD	B	1603	44/44	0.83	0.30	46,75,117,118	0
3	MG	A	602	1/1	0.84	0.25	37,37,37,37	0
2	NAD	A	603	44/44	0.87	0.23	36,56,102,104	0
5	TTN	A	605	8/8	0.90	0.23	43,45,53,53	0
5	TTN	B	1605	8/8	0.91	0.20	38,40,46,47	0
2	NAD	B	1601	44/44	0.92	0.14	29,42,48,49	0
2	NAD	A	601	44/44	0.93	0.14	27,39,43,45	0
4	FUM	B	1604	8/8	0.93	0.14	30,34,36,38	0
4	FUM	A	604	8/8	0.95	0.12	23,25,26,26	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.



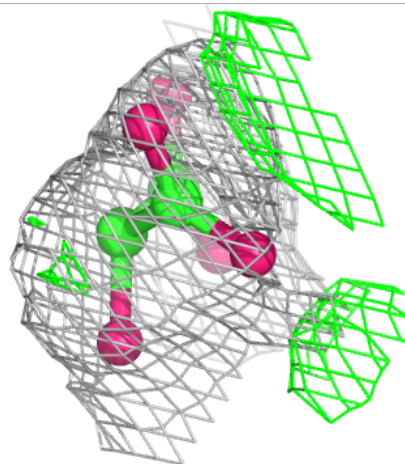
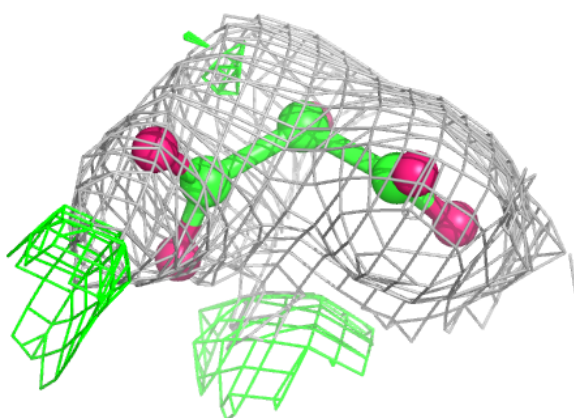
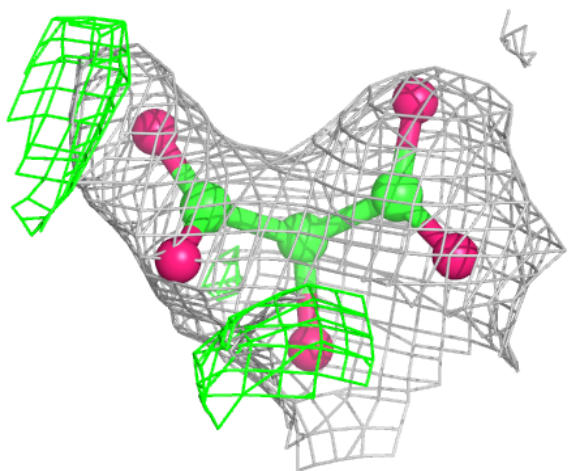
Electron density around NAD A 603:

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



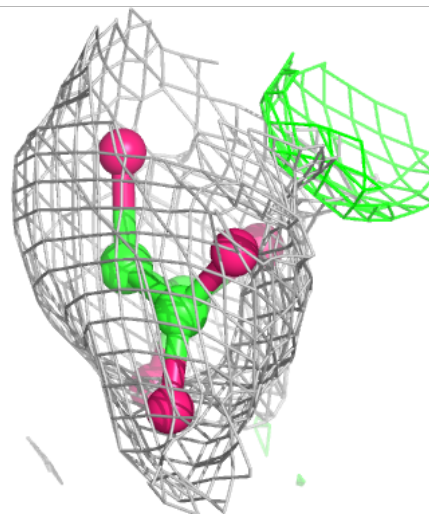
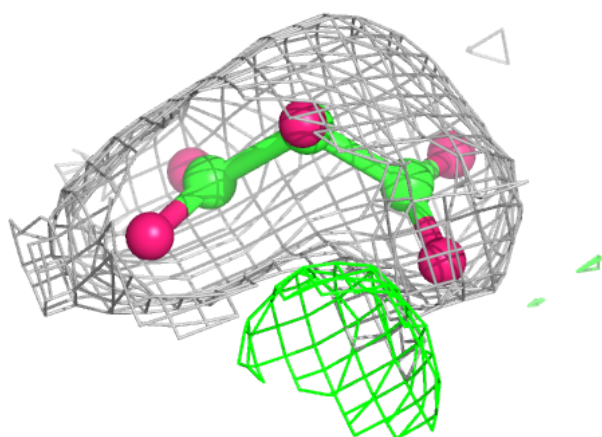
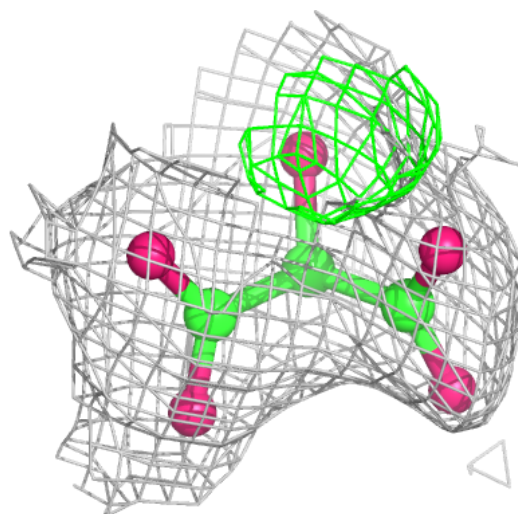
Electron density around TTN A 605:

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



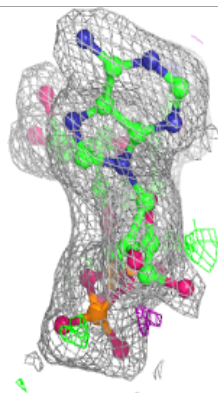
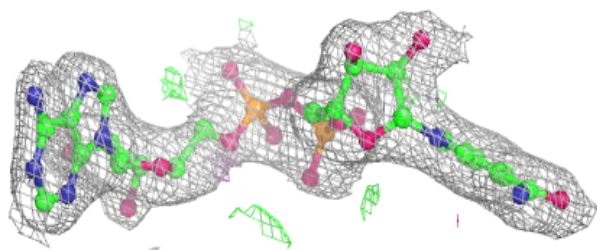
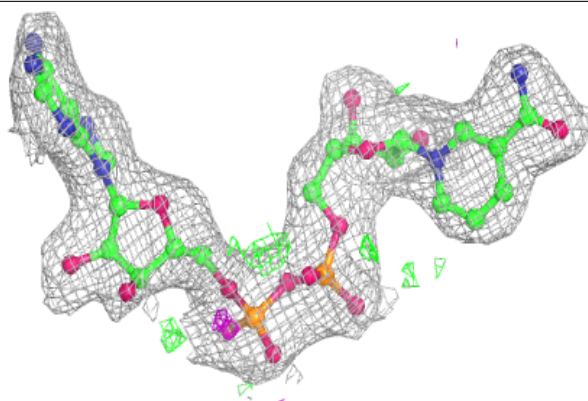
Electron density around TTN B 1605:

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

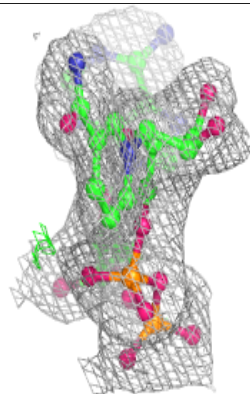
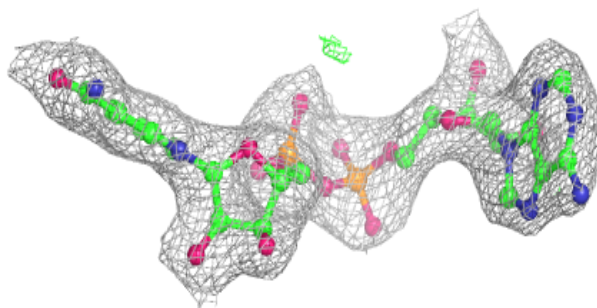
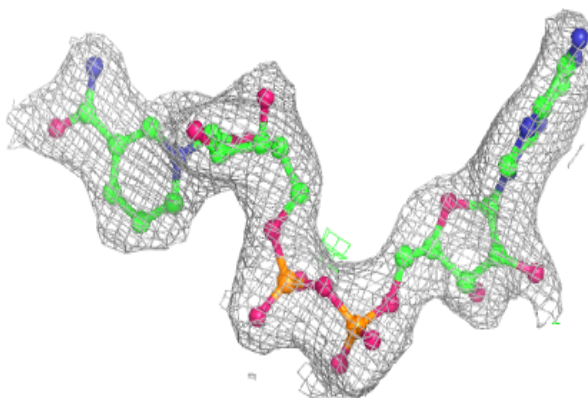


Electron density around NAD B 1601:

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

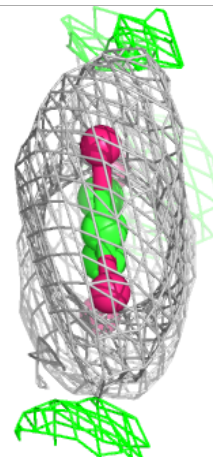
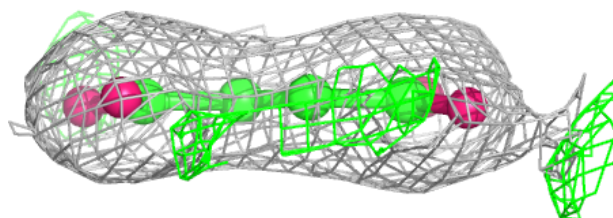
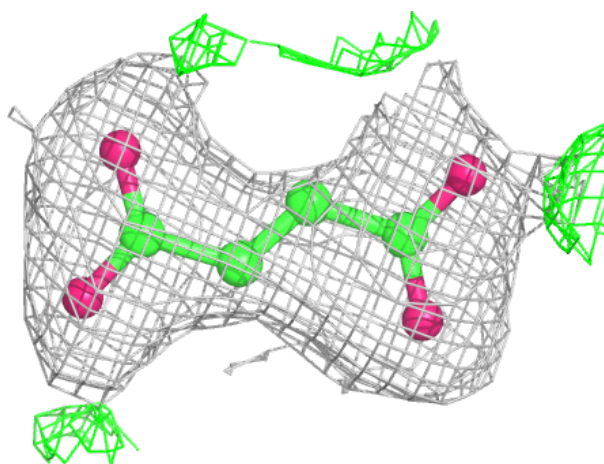
**Electron density around NAD A 601:**

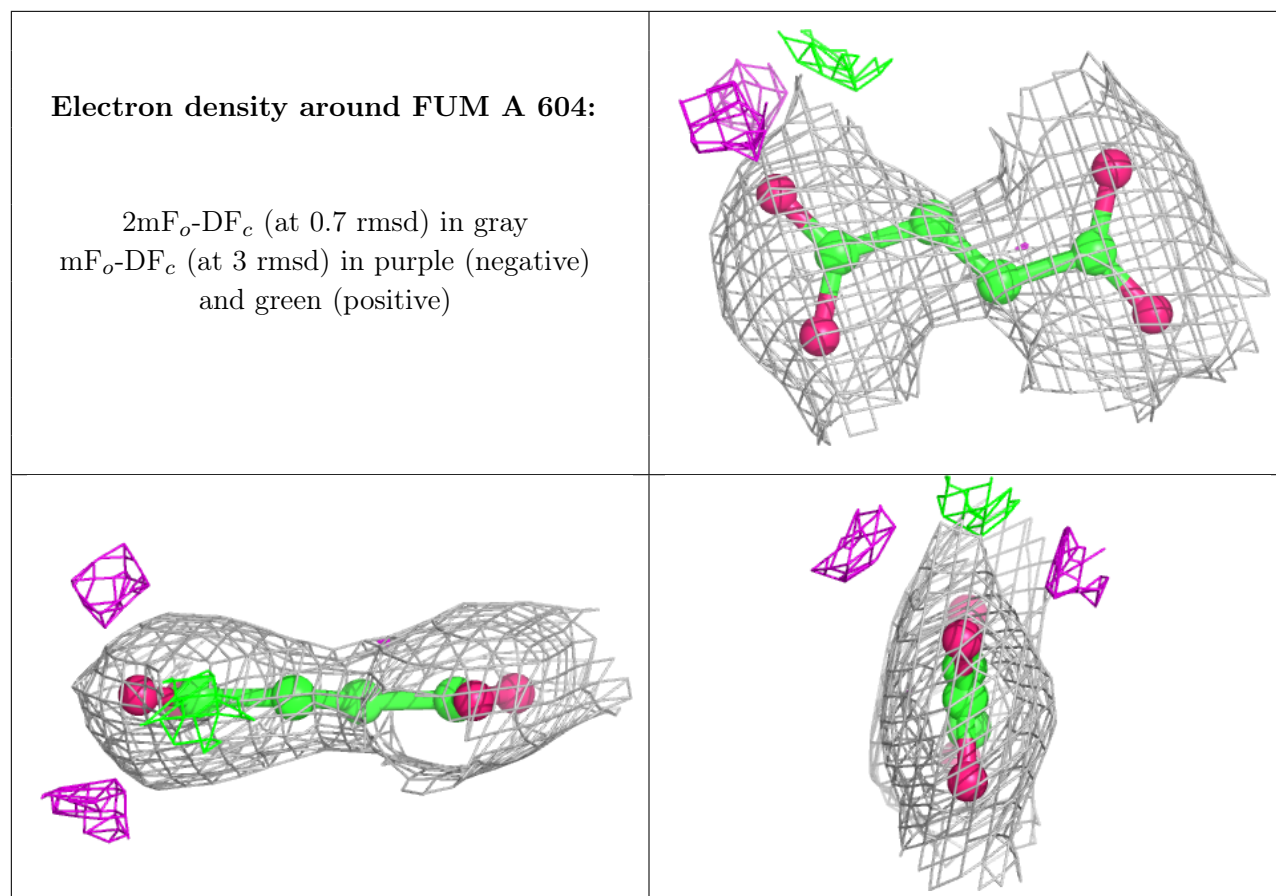
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FUM B 1604:

$2mF_o-DF_c$ (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.