



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 11:02 PM UTC

PDB ID : 9M39 / pdb_00009m39
Title : The crystal structure of DgpA2 protein from P581a bound to Isoschaftosid
Authors : Ma, W.
Deposited on : 2025-03-01
Resolution : 1.92 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) : 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

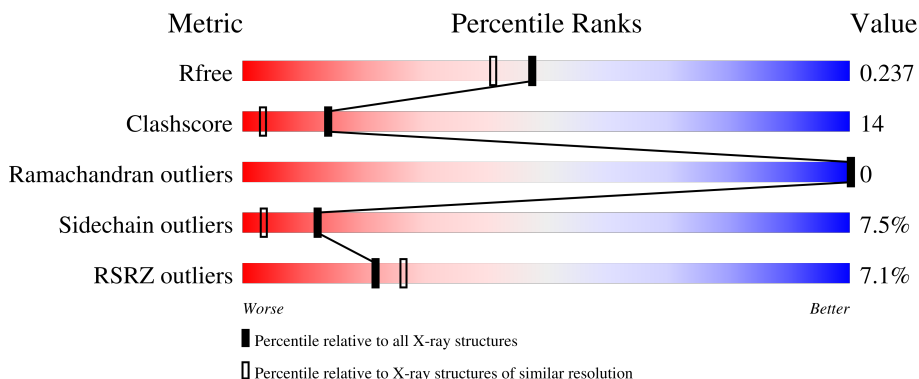
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	361	
1	B	361	

2 Entry composition [i](#)

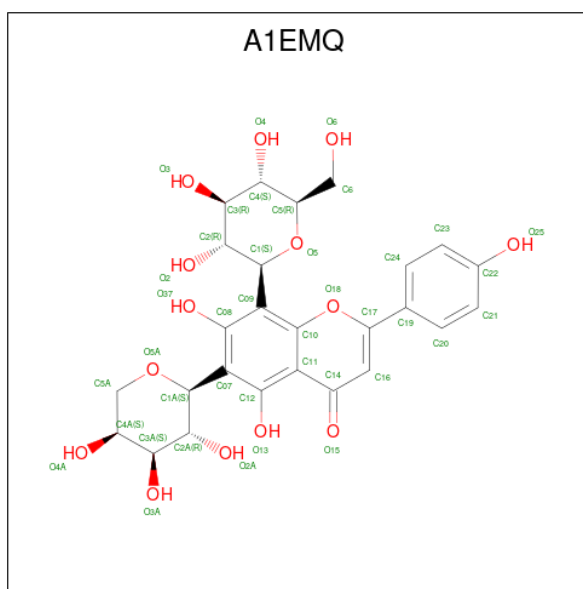
There are 4 unique types of molecules in this entry. The entry contains 5621 atoms, of which 28 are hydrogens and 0 are deuteriums.

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 Gfo/Idh/MocA family protein.

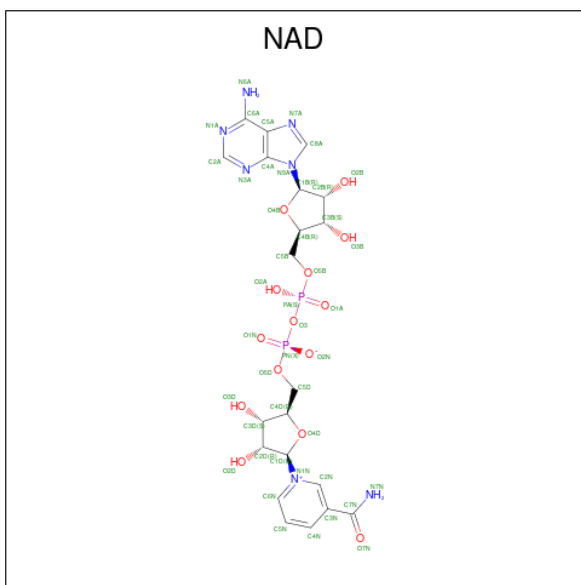
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2591	1664	434	478	15			
1	B	330	Total	C	N	O	S	0	0	0
			2609	1668	442	485	14			

- Molecule 2 is 8-[(2 {S},3 {R},4 {R},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]-2-(4-hydroxyphenyl)-5,7-bis(oxidanyl)-6-[(2 {S},3 {R},4 {S},5 {S})-3,4,5-tris(oxidanyl)oxan-2-yl]chromen-4-one (CCD ID: A1EMQ) (formula: C₂₆H₂₈O₁₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			68	26	28	14		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	176	Total O 176 176	0	0
4	B	89	Total O 89 89	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.83Å 45.91Å 104.73Å 90.00° 103.16° 90.00°	Depositor
Resolution (Å)	21.57 – 1.92 21.57 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.7 (21.57-1.92) 99.6 (21.57-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 1.92Å)	Xtriage
Refinement program	PHENIX 4.7	Depositor
R, R_{free}	0.214 , 0.238 0.215 , 0.237	Depositor DCC
R_{free} test set	2000 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5621	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.88% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, A1EMQ

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	0.24	0/2652	0.43	0/3596
1	B	0.23	0/2668	0.44	2/3617 (0.1%)
All	All	0.24	0/5320	0.43	2/7213 (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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	280	PRO	N-CA-CB	6.83	110.52	103.00
1	B	228	LEU	N-CA-CB	-5.11	102.68	110.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	ARG	Sidechain

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	2591	0	2507	61	0
1	B	2609	0	2517	94	0
2	A	40	28	0	2	0
3	A	44	0	26	5	0
3	B	44	0	25	2	0
4	A	176	0	0	3	0
4	B	89	0	0	7	0
All	All	5593	28	5075	149	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 14.

All (149) 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:99:PHE:HE2	1:A:103:MET:HE3	1.22	1.04
1:A:43:PRO:HG2	1:A:46:VAL:HG21	1.45	0.99
1:A:218:THR:HG23	1:B:196:ARG:HH21	1.30	0.97
1:A:263:THR:HG21	1:A:290:GLY:O	1.71	0.89
1:A:245:GLN:HA	1:A:245:GLN:OE1	1.71	0.89
1:B:236:GLU:HG2	1:B:253:PHE:H	1.40	0.86
1:A:191:VAL:HG21	1:A:338:ILE:CD1	2.05	0.85
1:B:73:LEU:HD22	1:B:98:GLU:HG3	1.58	0.84
1:A:99:PHE:CE2	1:A:103:MET:HE3	2.11	0.83
1:A:294:SER:HB2	1:B:230:GLU:OE2	1.78	0.82
1:A:191:VAL:HG21	1:A:338:ILE:HD11	1.63	0.81
1:B:313:ARG:HG3	4:B:501:HOH:O	1.80	0.81
1:A:218:THR:HG23	1:B:196:ARG:NH2	1.96	0.79
1:A:10:GLY:HA3	3:A:402:NAD:O1A	1.85	0.77
1:A:168:LEU:HD23	1:A:339:ARG:HH11	1.50	0.76
1:A:90:LYS:HD2	1:A:90:LYS:C	2.12	0.75
1:A:154:MET:HE3	1:A:167:MET:HE2	1.68	0.75
1:A:294:SER:HB2	1:B:230:GLU:CD	2.11	0.74
1:B:119:ARG:HB2	4:B:513:HOH:O	1.88	0.73
1:B:55:LEU:O	1:B:58:THR:HG22	1.86	0.73
1:B:227:MET:C	1:B:228:LEU:HD13	2.15	0.72
1:A:143:ILE:HG21	1:A:182:MET:HE1	1.72	0.71
1:B:16:HIS:O	1:B:20:ILE:HD12	1.90	0.71
1:B:90:LYS:HE2	1:B:174:HIS:NE2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PHE:CG	1:A:312:LEU:HD22	2.28	0.68
1:A:43:PRO:HG2	1:A:46:VAL:CG2	2.22	0.67
1:B:195:ILE:HD11	1:B:338:ILE:HG22	1.76	0.67
1:A:232:GLU:HG3	1:A:233:ASN:OD1	1.95	0.66
1:B:178:GLN:HE22	1:B:237:ARG:HH22	1.43	0.66
1:B:96:ALA:HB1	1:B:329:TYR:CE1	2.30	0.66
1:B:339:ARG:HH11	1:B:339:ARG:HG3	1.62	0.65
1:B:93:ALA:HB1	1:B:98:GLU:HB3	1.77	0.65
1:B:137:LEU:HB2	1:B:140:ILE:HD11	1.77	0.65
1:A:313:ARG:HB3	1:A:319:GLU:HB2	1.79	0.64
1:B:232:GLU:HG2	1:B:233:ASN:HD22	1.63	0.63
1:B:232:GLU:HG2	1:B:233:ASN:ND2	2.15	0.62
1:A:134:SER:OG	1:A:136:THR:HG23	1.99	0.62
1:B:280:PRO:N	4:B:504:HOH:O	2.33	0.60
1:A:291:ARG:HH11	1:A:291:ARG:CG	2.14	0.60
1:B:154:MET:HE3	1:B:158:HIS:HB3	1.83	0.60
1:B:324:LYS:HE2	1:B:327:GLN:NE2	2.17	0.60
1:A:310:ASN:HD22	1:A:319:GLU:HG2	1.68	0.59
1:B:73:LEU:HD22	1:B:98:GLU:CG	2.31	0.58
1:B:146:SER:OG	1:B:238:HIS:HB2	2.03	0.58
2:A:401:A1EMQ:C6	4:A:591:HOH:O	2.52	0.58
1:B:10:GLY:HA3	3:B:401:NAD:O5B	2.04	0.57
1:A:103:MET:CE	1:A:329:TYR:HB2	2.34	0.57
1:B:229:SER:HB3	1:B:234:TRP:CD2	2.40	0.57
1:B:178:GLN:HE22	1:B:237:ARG:NH2	2.02	0.57
1:B:27:GLU:HG3	1:B:28:LEU:N	2.21	0.56
1:B:58:THR:HG23	1:B:60:ILE:HG23	1.86	0.56
1:B:126:ARG:HG2	1:B:302:VAL:HG11	1.87	0.56
1:B:92:ALA:HB2	1:B:115:ILE:HD12	1.87	0.55
1:A:291:ARG:CG	1:A:291:ARG:NH1	2.68	0.55
1:B:237:ARG:HG3	1:B:238:HIS:N	2.21	0.55
1:B:266:LEU:HD23	1:B:267:GLN:N	2.22	0.55
1:B:73:LEU:HB2	1:B:98:GLU:HG2	1.87	0.55
1:B:96:ALA:HB1	1:B:329:TYR:HE1	1.71	0.55
1:B:236:GLU:HG2	1:B:253:PHE:N	2.16	0.54
1:A:47:GLN:HB3	1:A:49:PHE:CE2	2.43	0.53
1:A:291:ARG:HH12	1:B:150:PHE:HD1	1.55	0.53
1:B:74:GLU:HB3	4:B:557:HOH:O	2.09	0.53
1:A:291:ARG:HH11	1:A:291:ARG:HG3	1.73	0.52
1:A:53:GLU:H	1:A:53:GLU:CD	2.16	0.52
1:A:103:MET:HE1	1:A:326:ASN:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:LEU:C	1:B:223:LEU:HD23	2.34	0.52
1:A:218:THR:CG2	1:B:196:ARG:HH21	2.15	0.51
1:A:223:LEU:C	1:A:223:LEU:HD23	2.36	0.51
1:B:332:MET:HG3	4:B:526:HOH:O	2.10	0.51
1:A:195:ILE:HD11	1:A:338:ILE:HG22	1.92	0.51
1:B:187:ARG:HH11	1:B:187:ARG:HG3	1.75	0.51
1:B:75:MET:O	1:B:79:VAL:HG23	2.11	0.51
1:B:134:SER:OG	1:B:136:THR:HG23	2.11	0.51
1:B:223:LEU:HD23	1:B:224:GLY:N	2.26	0.50
1:B:236:GLU:HB3	1:B:252:GLY:HA2	1.93	0.50
1:B:236:GLU:HG3	1:B:253:PHE:CD2	2.47	0.50
3:A:402:NAD:O1A	3:A:402:NAD:H4B	2.12	0.50
1:A:239:TRP:HB2	1:A:250:ILE:HB	1.94	0.50
1:B:3:LYS:HB2	1:B:60:ILE:HA	1.93	0.50
1:B:339:ARG:HH11	1:B:339:ARG:CG	2.23	0.50
1:B:5:GLY:HA2	1:B:30:ALA:O	2.12	0.49
1:B:150:PHE:HB3	1:B:235:PHE:CE1	2.47	0.49
1:A:90:LYS:HE2	1:A:174:HIS:NE2	2.27	0.49
1:B:311:TYR:C	1:B:313:ARG:H	2.20	0.48
1:B:74:GLU:HG3	1:B:75:MET:N	2.27	0.48
1:B:59:ASP:CG	1:B:59:ASP:O	2.56	0.48
1:A:89:GLU:OE1	3:A:402:NAD:H2N	2.13	0.48
1:B:77:LYS:HZ1	1:B:101:GLU:CD	2.21	0.48
1:B:266:LEU:HD23	1:B:266:LEU:C	2.39	0.48
1:B:195:ILE:HD11	1:B:338:ILE:CG2	2.44	0.47
1:B:55:LEU:C	1:B:55:LEU:HD23	2.39	0.47
1:B:94:MET:HE1	1:B:164:GLY:N	2.28	0.47
1:A:90:LYS:HD2	1:A:91:PRO:N	2.29	0.47
1:A:110:ASN:HA	4:A:565:HOH:O	2.14	0.47
4:A:572:HOH:O	1:B:347:VAL:HG12	2.14	0.47
1:B:324:LYS:HB2	1:B:324:LYS:HE3	1.58	0.47
1:A:291:ARG:NH1	1:B:150:PHE:CD1	2.83	0.46
1:A:146:SER:OG	1:A:238:HIS:HB2	2.15	0.46
1:B:119:ARG:HG2	1:B:174:HIS:HB3	1.96	0.46
1:B:305:GLU:H	1:B:305:GLU:HG2	1.36	0.46
1:A:25:PHE:CD1	1:A:312:LEU:HD22	2.51	0.46
1:B:119:ARG:HD3	1:B:174:HIS:CE1	2.50	0.46
1:B:127:ILE:O	1:B:131:VAL:HG23	2.16	0.46
1:B:121:TRP:CD1	1:B:306:MET:HB2	2.51	0.46
1:B:14:GLN:O	1:B:17:ALA:HB3	2.16	0.45
1:B:189:GLU:OE2	1:B:214:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:MET:HE3	1:A:167:MET:CE	2.43	0.45
1:A:103:MET:HE3	1:A:329:TYR:HB2	1.98	0.45
1:A:192:TYR:HB2	1:A:347:VAL:HG22	1.98	0.45
1:B:333:GLN:NE2	4:B:511:HOH:O	2.50	0.45
1:B:90:LYS:HD3	1:B:174:HIS:CE1	2.51	0.45
1:B:339:ARG:CG	1:B:339:ARG:NH1	2.78	0.45
1:A:32:CYS:HA	1:A:49:PHE:O	2.16	0.45
1:B:73:LEU:HA	1:B:102:MET:HE2	1.99	0.45
2:A:401:A1EMQ:C2	2:A:401:A1EMQ:O18	2.64	0.45
1:B:236:GLU:HG3	1:B:253:PHE:HD2	1.81	0.45
1:B:79:VAL:HG11	1:B:86:ILE:HG12	1.99	0.45
1:A:338:ILE:N	1:A:338:ILE:HD13	2.33	0.44
1:B:229:SER:HB3	1:B:234:TRP:CG	2.52	0.44
1:A:263:THR:O	1:A:264:ALA:C	2.59	0.44
1:A:223:LEU:HD23	1:A:224:GLY:N	2.32	0.44
1:B:137:LEU:HD12	1:B:140:ILE:HD11	2.00	0.44
1:B:228:LEU:HD13	1:B:228:LEU:N	2.30	0.44
1:A:5:GLY:HA2	1:A:30:ALA:O	2.18	0.44
1:B:102:MET:O	1:B:106:THR:HG23	2.17	0.44
1:A:12:MET:HB2	3:A:402:NAD:C6N	2.49	0.43
1:A:212:TYR:CE2	1:A:218:THR:HG22	2.54	0.43
1:B:352:GLU:H	1:B:352:GLU:HG3	1.65	0.43
1:A:345:HIS:O	1:B:347:VAL:HG11	2.18	0.43
1:A:212:TYR:CZ	1:A:218:THR:CG2	3.03	0.42
1:B:187:ARG:HG3	1:B:187:ARG:NH1	2.34	0.42
1:A:140:ILE:HA	1:A:243:GLY:HA2	2.00	0.42
1:B:236:GLU:CB	1:B:252:GLY:HA2	2.50	0.42
1:A:115:ILE:N	1:A:115:ILE:HD12	2.33	0.42
1:B:19:THR:HG23	1:B:305:GLU:OE1	2.19	0.41
1:A:328:ILE:O	1:A:332:MET:HG2	2.19	0.41
1:A:12:MET:SD	3:A:402:NAD:C4N	3.09	0.41
1:A:260:THR:OG1	1:B:230:GLU:OE2	2.34	0.41
1:B:89:GLU:OE1	3:B:401:NAD:H2N	2.21	0.41
1:A:103:MET:HE1	1:A:329:TYR:HB2	2.03	0.41
1:A:229:SER:HB3	1:A:234:TRP:CD2	2.55	0.41
1:A:162:GLU:CD	1:A:162:GLU:H	2.28	0.41
1:B:312:LEU:O	1:B:312:LEU:HD23	2.21	0.41
1:B:37:LEU:H	1:B:37:LEU:HD12	1.86	0.40
1:B:280:PRO:CB	1:B:282:ARG:HH12	2.34	0.40
1:B:154:MET:HB2	1:B:159:VAL:HG12	2.04	0.40
1:B:237:ARG:NH1	1:B:239:TRP:HE1	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ASN:OD1	1:B:153:ASN:O	2.39	0.40
1:B:313:ARG:CG	4:B:501:HOH:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/361 (90%)	316 (98%)	8 (2%)	0	100	100
1	B	322/361 (89%)	306 (95%)	16 (5%)	0	100	100
All	All	646/722 (90%)	622 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	271/303 (89%)	255 (94%)	16 (6%)	18	5
1	B	274/303 (90%)	249 (91%)	25 (9%)	9	1
All	All	545/606 (90%)	504 (92%)	41 (8%)	12	3

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	47	GLN
1	A	53	GLU
1	A	74	GLU
1	A	90	LYS
1	A	162	GLU
1	A	189	GLU
1	A	201	LYS
1	A	212	TYR
1	A	245	GLN
1	A	291	ARG
1	A	321	LEU
1	A	326	ASN
1	A	338	ILE
1	A	339	ARG
1	A	345	HIS
1	B	3	LYS
1	B	27	GLU
1	B	59	ASP
1	B	74	GLU
1	B	90	LYS
1	B	95	ASN
1	B	119	ARG
1	B	126	ARG
1	B	144	LYS
1	B	151	ASN
1	B	155	HIS
1	B	162	GLU
1	B	197	ASN
1	B	214	GLU
1	B	228	LEU
1	B	236	GLU
1	B	256	LYS
1	B	267	GLN
1	B	281	THR
1	B	292	ILE
1	B	302	VAL
1	B	305	GLU
1	B	339	ARG
1	B	349	THR
1	B	352	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	202	ASN
1	A	249	ASN
1	A	310	ASN
1	B	16	HIS
1	B	151	ASN
1	B	153	ASN
1	B	178	GLN
1	B	233	ASN
1	B	303	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	A1EMQ	A	401	-	44,44,44	2.99	15 (34%)	63,67,67	2.32	21 (33%)
3	NAD	B	401	-	46,48,48	4.02	21 (45%)	64,73,73	2.19	13 (20%)
3	NAD	A	402	-	46,48,48	0.64	1 (2%)	64,73,73	0.52	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	A1EMQ	A	401	-	-	8/14/51/51	0/5/5/5
3	NAD	B	401	-	-	10/30/62/62	0/5/5/5
3	NAD	A	402	-	-	3/30/62/62	0/5/5/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	NAD	O4D-C1D	-10.28	1.27	1.40
3	B	401	NAD	PN-O3	9.73	1.70	1.59
2	A	401	A1EMQ	O18-C17	9.09	1.49	1.36
3	B	401	NAD	C3B-C4B	-8.94	1.30	1.53
3	B	401	NAD	C7N-N7N	8.86	1.49	1.33
3	B	401	NAD	C3D-C4D	-8.28	1.32	1.53
2	A	401	A1EMQ	O18-C10	8.21	1.50	1.38
2	A	401	A1EMQ	O5A-C1A	7.97	1.51	1.43
3	B	401	NAD	O4D-C4D	7.62	1.61	1.45
3	B	401	NAD	O4B-C4B	7.41	1.61	1.45
3	B	401	NAD	C6A-N6A	5.95	1.49	1.34
2	A	401	A1EMQ	O5-C1	5.74	1.50	1.43
2	A	401	A1EMQ	C16-C17	5.20	1.51	1.37
3	B	401	NAD	PA-O3	4.76	1.64	1.59
3	B	401	NAD	C3N-C7N	4.57	1.57	1.50
3	B	401	NAD	O4B-C1B	-4.50	1.31	1.42
3	B	401	NAD	O3D-C3D	4.30	1.53	1.43
2	A	401	A1EMQ	O15-C14	-4.14	1.15	1.24
2	A	401	A1EMQ	C19-C17	3.96	1.56	1.48
2	A	401	A1EMQ	C24-C19	3.67	1.45	1.39
2	A	401	A1EMQ	O5A-C5A	3.15	1.49	1.43
3	B	401	NAD	O3B-C3B	3.12	1.50	1.43
3	B	401	NAD	C5A-C4A	-2.75	1.34	1.39
2	A	401	A1EMQ	O25-C22	2.69	1.43	1.37
3	B	401	NAD	C2A-N1A	2.68	1.38	1.33
2	A	401	A1EMQ	C21-C22	2.60	1.43	1.39
3	B	401	NAD	O2B-C2B	-2.59	1.36	1.43
3	B	401	NAD	C8A-N9A	-2.58	1.33	1.37
2	A	401	A1EMQ	O5-C5	2.54	1.50	1.44
3	B	401	NAD	O7N-C7N	-2.53	1.19	1.24
3	B	401	NAD	C2N-N1N	2.52	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	NAD	C2N-N1N	2.51	1.37	1.35
3	B	401	NAD	C8A-N7A	2.27	1.36	1.31
2	A	401	A1EMQ	C08-C09	2.27	1.43	1.40
2	A	401	A1EMQ	C2A-C1A	-2.25	1.48	1.53
3	B	401	NAD	PA-O5B	2.11	1.67	1.59
2	A	401	A1EMQ	O3-C3	2.02	1.48	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	NAD	C4A-N9A-C1B	-6.87	110.58	126.63
3	B	401	NAD	N3A-C2A-N1A	-5.61	120.09	128.58
2	A	401	A1EMQ	C6-C5-C4	-5.53	99.44	113.02
2	A	401	A1EMQ	O5-C5-C6	5.53	120.14	106.44
3	B	401	NAD	N9A-C8A-N7A	-5.40	106.27	113.94
3	B	401	NAD	C1B-N9A-C8A	5.39	139.06	127.09
2	A	401	A1EMQ	C12-C07-C08	5.08	120.80	116.58
2	A	401	A1EMQ	C4A-C3A-C2A	5.01	119.67	110.86
3	B	401	NAD	N6A-C6A-N1A	-4.85	107.58	118.38
2	A	401	A1EMQ	O2A-C2A-C1A	-4.70	99.38	109.28
3	B	401	NAD	C5A-C4A-N3A	-4.52	120.50	126.72
2	A	401	A1EMQ	O4-C4-C5	4.47	120.33	109.32
2	A	401	A1EMQ	C10-O18-C17	-4.42	115.11	120.04
3	B	401	NAD	C4A-N9A-C8A	4.41	110.37	105.74
2	A	401	A1EMQ	O3A-C3A-C4A	-4.05	101.79	110.05
3	B	401	NAD	C5A-C6A-N6A	3.67	132.36	123.29
2	A	401	A1EMQ	C17-C16-C14	-3.61	118.43	122.14
2	A	401	A1EMQ	O3-C3-C2	-3.59	101.91	110.38
2	A	401	A1EMQ	O3-C3-C4	3.48	118.58	110.38
3	B	401	NAD	C4D-O4D-C1D	-3.44	106.77	109.92
3	B	401	NAD	N3A-C4A-N9A	3.43	133.00	127.17
2	A	401	A1EMQ	O2-C2-C1	-3.25	102.42	109.28
3	B	401	NAD	C5A-N7A-C8A	3.25	108.55	103.45
3	B	401	NAD	C2A-N3A-C4A	3.18	119.60	111.83
2	A	401	A1EMQ	C20-C19-C17	-3.00	116.00	120.77
2	A	401	A1EMQ	O5-C1-C09	2.78	113.44	107.70
2	A	401	A1EMQ	C4-C3-C2	-2.76	105.98	110.83
2	A	401	A1EMQ	C08-C07-C1A	-2.58	115.33	121.19
2	A	401	A1EMQ	O2A-C2A-C3A	-2.40	104.73	110.38
2	A	401	A1EMQ	O18-C10-C09	-2.26	113.89	116.10
2	A	401	A1EMQ	C11-C14-C16	2.22	120.47	116.31
2	A	401	A1EMQ	C5A-O5A-C1A	2.17	116.12	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	NAD	C2B-C3B-C4B	2.10	106.66	102.61
2	A	401	A1EMQ	O4-C4-C3	-2.05	105.54	110.38

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	A1EMQ	C10-C09-C1-O5
2	A	401	A1EMQ	C08-C09-C1-O5
3	B	401	NAD	O4D-C1D-N1N-C2N
3	B	401	NAD	O4D-C1D-N1N-C6N
2	A	401	A1EMQ	O5-C5-C6-O6
2	A	401	A1EMQ	C4-C5-C6-O6
3	A	402	NAD	C4B-C5B-O5B-PA
3	B	401	NAD	C3B-C4B-C5B-O5B
3	B	401	NAD	O4B-C4B-C5B-O5B
3	B	401	NAD	O4D-C4D-C5D-O5D
3	B	401	NAD	C2B-C1B-N9A-C8A
2	A	401	A1EMQ	C08-C07-C1A-C2A
3	B	401	NAD	C2D-C1D-N1N-C2N
3	B	401	NAD	C2D-C1D-N1N-C6N
3	A	402	NAD	O4D-C1D-N1N-C2N
3	B	401	NAD	PA-O3-PN-O2N
2	A	401	A1EMQ	C10-C09-C1-C2
2	A	401	A1EMQ	C08-C09-C1-C2
2	A	401	A1EMQ	C12-C07-C1A-C2A
3	A	402	NAD	O4B-C4B-C5B-O5B
3	B	401	NAD	O4B-C1B-N9A-C8A

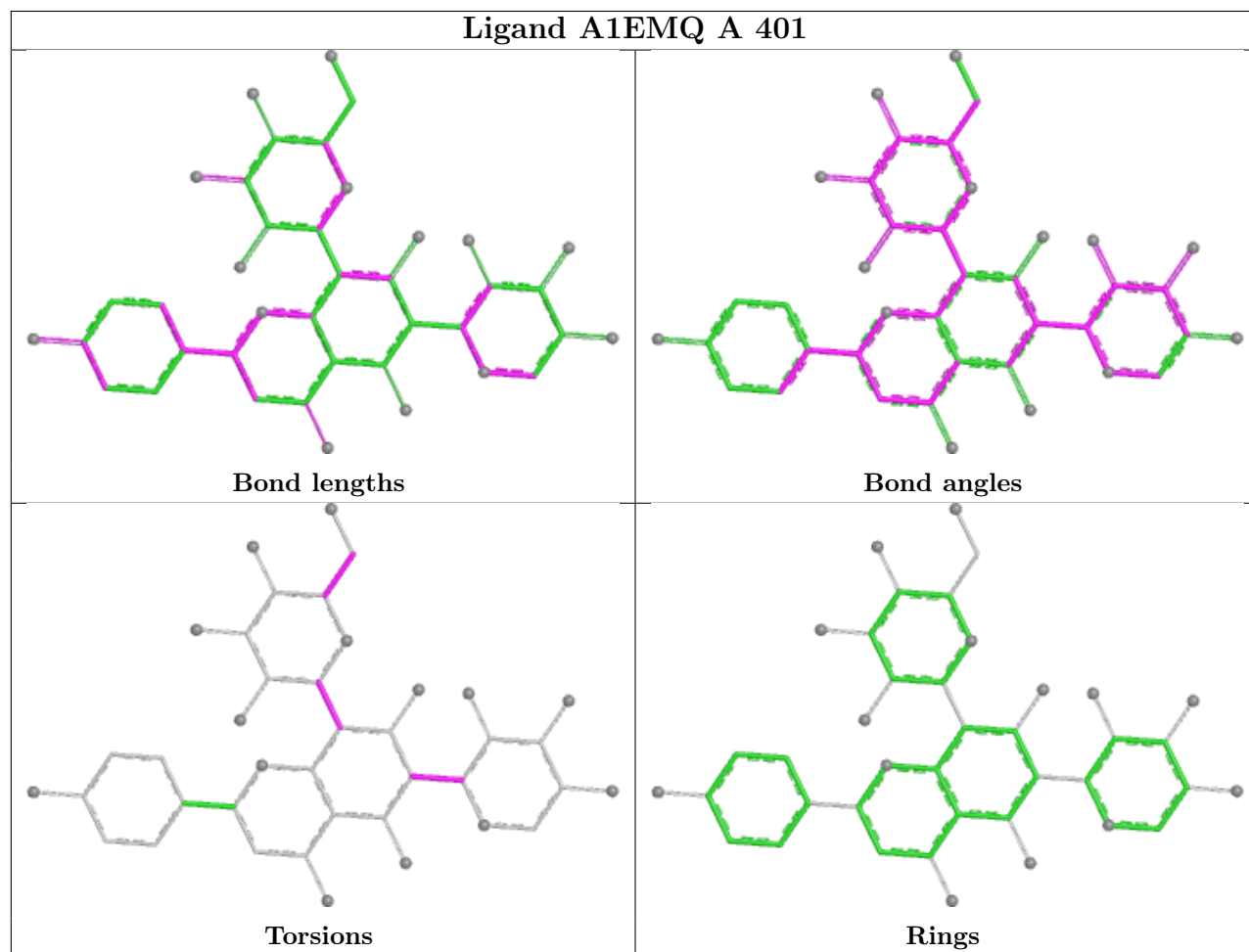
There are no ring outliers.

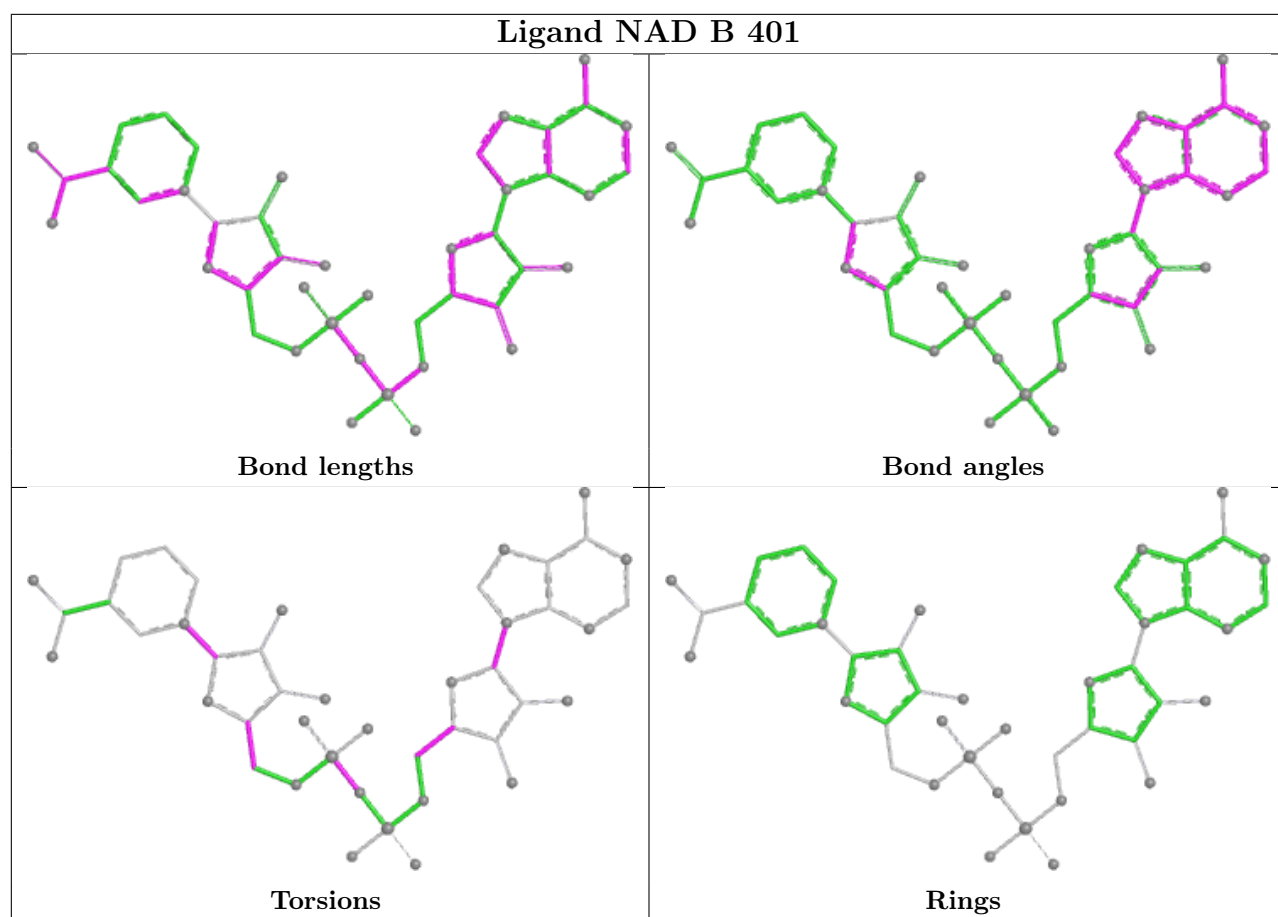
3 monomers are involved in 9 short contacts:

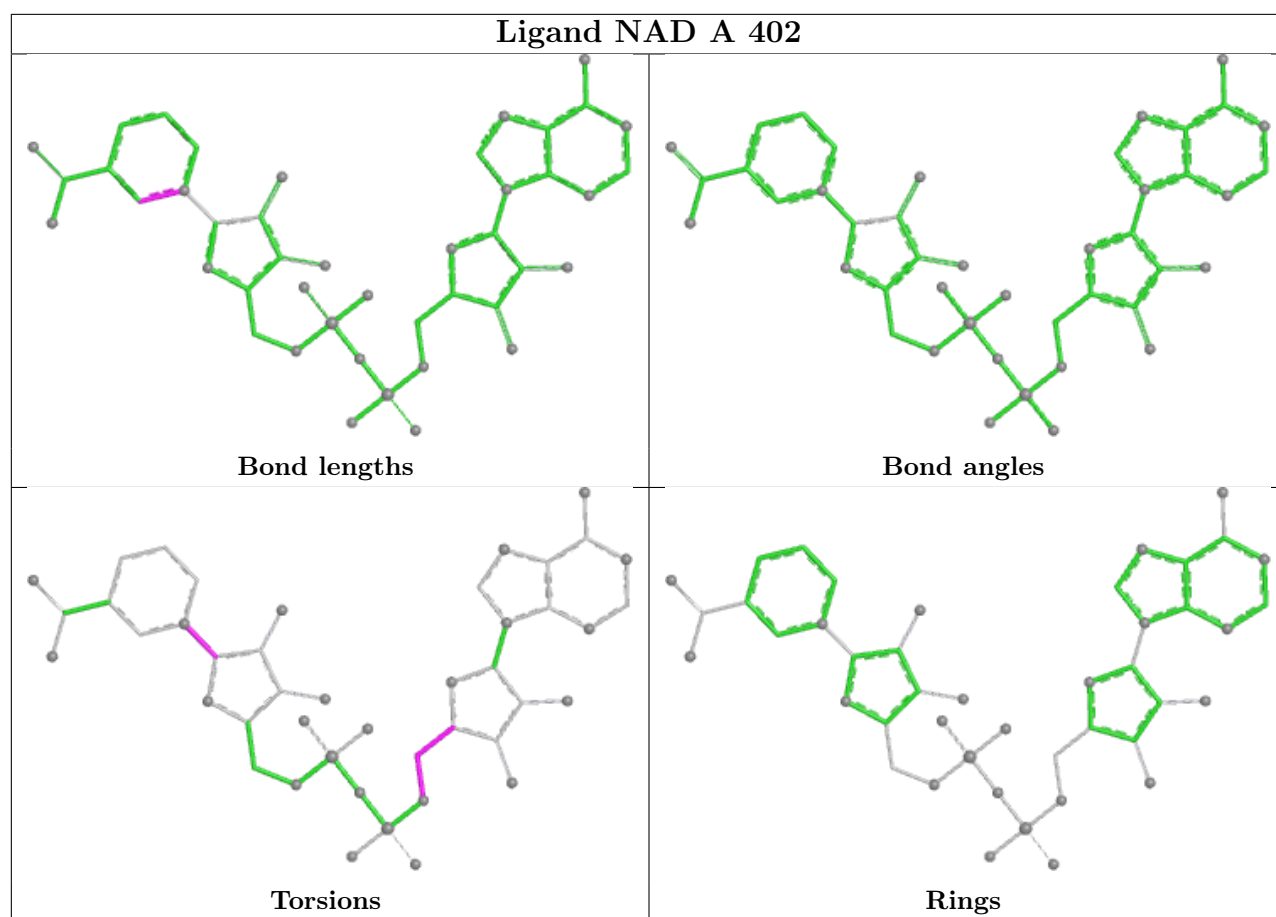
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	A1EMQ	2	0
3	B	401	NAD	2	0
3	A	402	NAD	5	0

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	328/361 (90%)	0.16	11 (3%)	48	53	19, 27, 44, 71	0
1	B	330/361 (91%)	0.84	36 (10%)	10	14	21, 39, 67, 83	0
All	All	658/722 (91%)	0.50	47 (7%)	22	26	19, 32, 65, 83	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	TYR	5.1
1	A	317	GLY	5.0
1	A	287	PRO	4.4
1	A	289	ALA	3.9
1	A	316	GLN	3.7
1	A	264	ALA	3.5
1	B	302	VAL	3.5
1	B	313	ARG	3.4
1	A	245	GLN	3.4
1	B	103	MET	3.4
1	B	10	GLY	3.3
1	B	25	PHE	3.2
1	B	151	ASN	3.1
1	B	301	PHE	3.1
1	B	42	ALA	3.0
1	B	325	PRO	3.0
1	B	108	ALA	3.0
1	B	237	ARG	2.9
1	B	163	PHE	2.9
1	B	97	ALA	2.9
1	B	21	ALA	2.8
1	B	11	PHE	2.7
1	A	263	THR	2.7
1	B	37	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	318	GLU	2.7
1	B	312	LEU	2.7
1	A	291	ARG	2.6
1	B	96	ALA	2.5
1	B	322	VAL	2.5
1	B	280	PRO	2.5
1	B	59	ASP	2.5
1	B	329	TYR	2.4
1	B	39	LEU	2.4
1	B	228	LEU	2.4
1	B	2	LEU	2.4
1	B	332	MET	2.4
1	B	1	MET	2.4
1	B	110	ASN	2.3
1	A	232	GLU	2.3
1	B	48	THR	2.3
1	B	41	HIS	2.2
1	B	300	VAL	2.2
1	B	169	TYR	2.2
1	B	155	HIS	2.1
1	B	111	VAL	2.1
1	B	50	LEU	2.1
1	B	347	VAL	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](#)

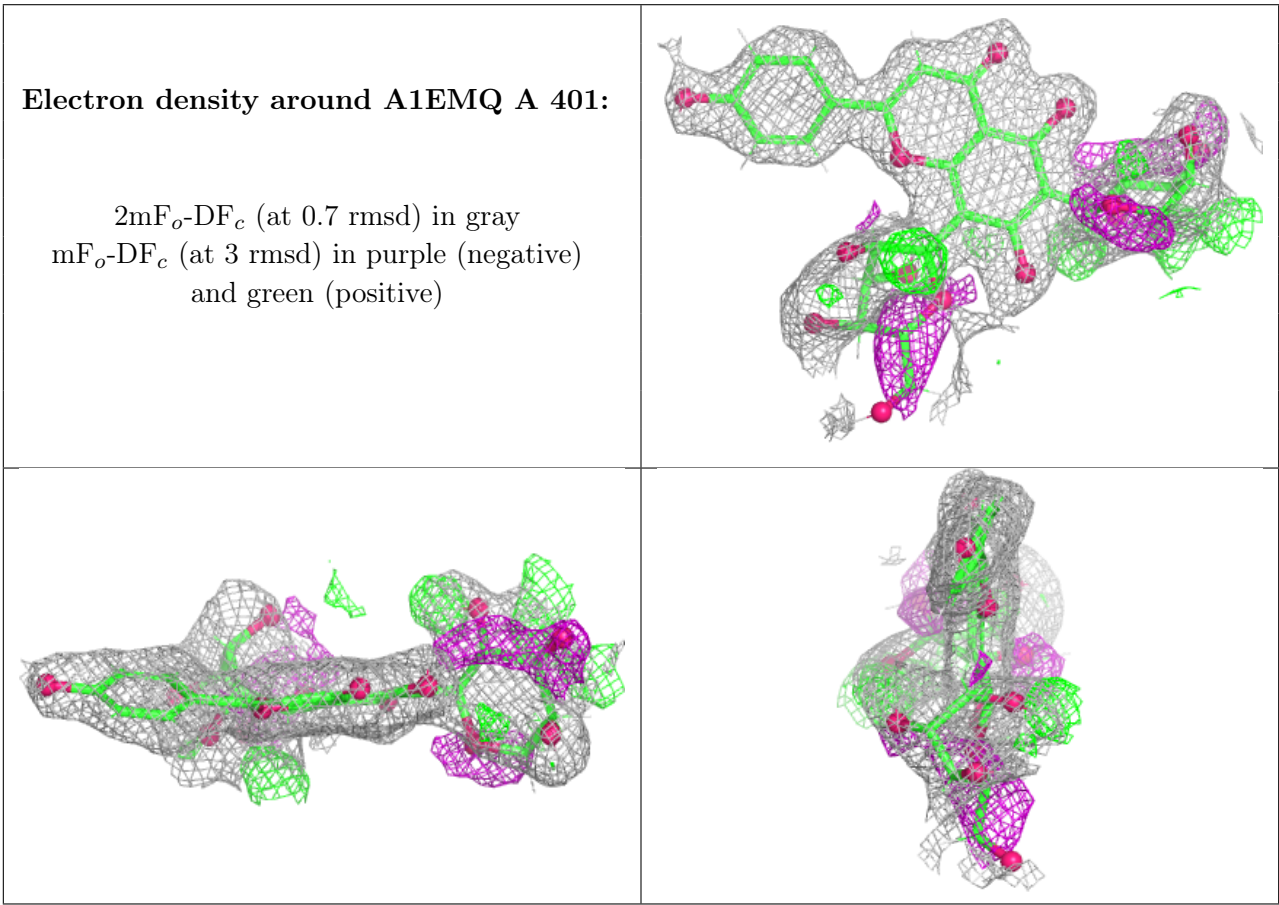
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

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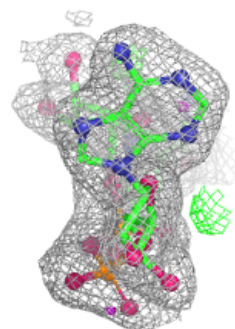
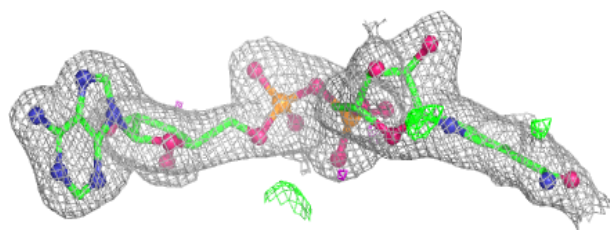
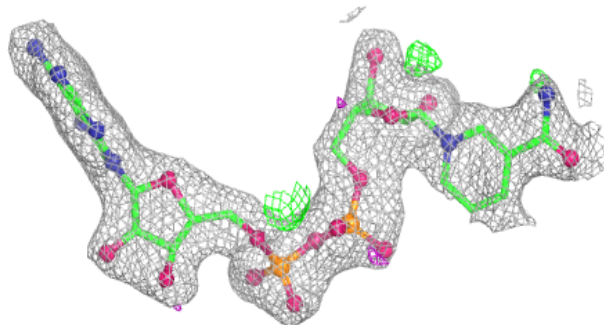
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1EMQ	A	401	40/40	0.77	0.14	29,45,69,76	0
3	NAD	B	401	44/44	0.90	0.09	33,46,53,55	0
3	NAD	A	402	44/44	0.91	0.09	19,25,34,42	0

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.

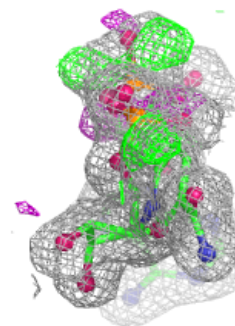
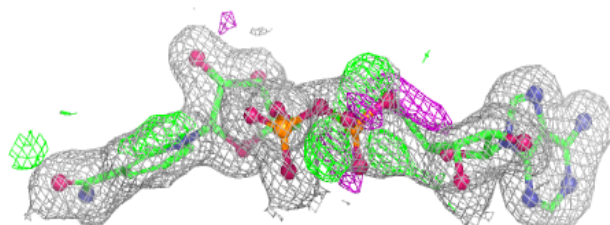
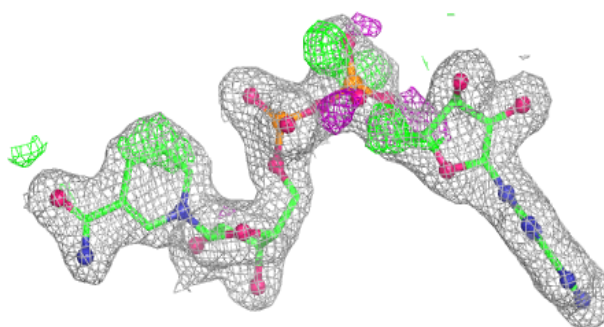


Electron density around NAD B 401:

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

**Electron density around NAD A 402:**

$2mF_o-DF_c$ (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.