WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jul 29, 2024 – 10:09 AM JST

PDB ID	:	8KAO
Title	:	Glutamate dehydrogenase-69O
Authors	:	Sakuraba, H.; Ohshima, T.
Deposited on	:	2023-08-03
Resolution	:	2.55 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

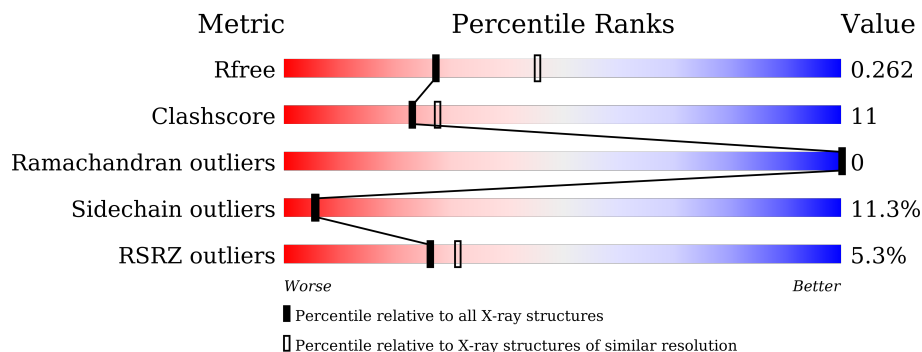|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.55 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	Percentile Ranks	Value
Rfree		0.262
Clashscore		11
Ramachandran outliers		0
Sidechain outliers		11.3%
RSRZ outliers		5.3%

Worse — Better

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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.

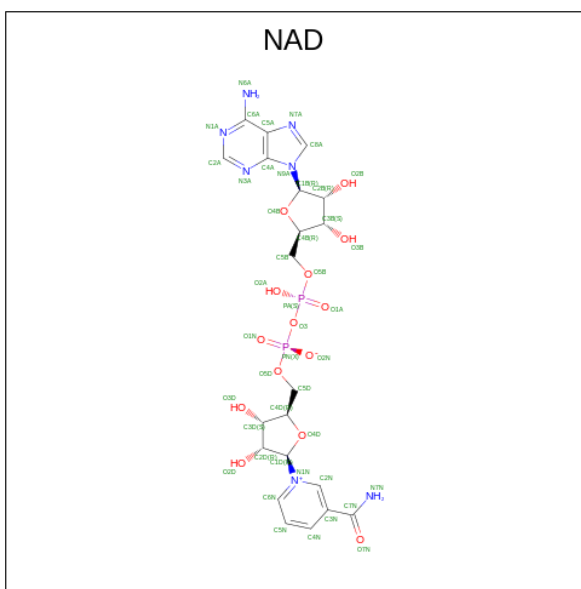| Mol	Chain	Length	Quality of chain
1	A	419	% 71% 23% • •
1	B	419	13% 61% 27% • 10%
1	C	419	% 71% 23% 5% •

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 9341 atoms, of which 0 are hydrogens and 0 are deuteriums.
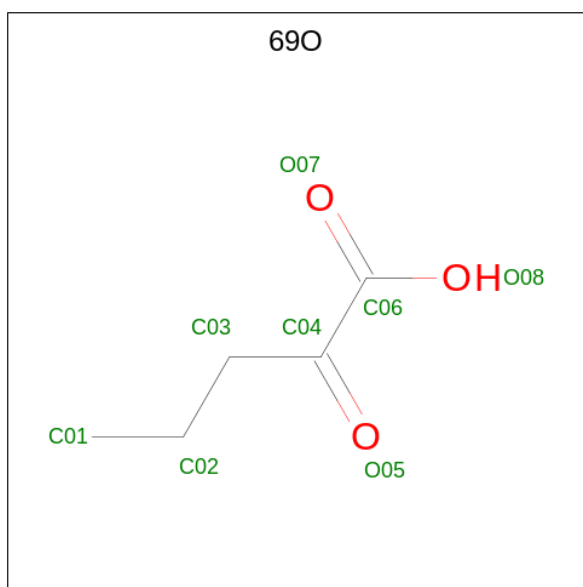
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total 3121	C 1990	N 539	O 582	S 10	0	0	0
1	B	379	Total 2912	C 1859	N 504	O 540	S 9	0	0	0
1	C	412	Total 3147	C 2004	N 544	O 589	S 10	0	0	0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is 2-oxopentanoic acid (three-letter code: 69O) (formula: $C_5H_8O_3$) (labeled as "Ligand of Interest" by depositor).

69O

O07

O

C03   C04   C06   OH   O08

C01

C02   O05

O

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total 39	O 39	0	0
4	B	18	Total 18	O 18	0	0
4	C	52	Total 52	O 52	0	0

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: Glutamate dehydrogenase

• Molecule 1: Glutamate dehydrogenase

• Molecule 1: Glutamate dehydrogenase

Chain C:

%

71%   23%   5% ·
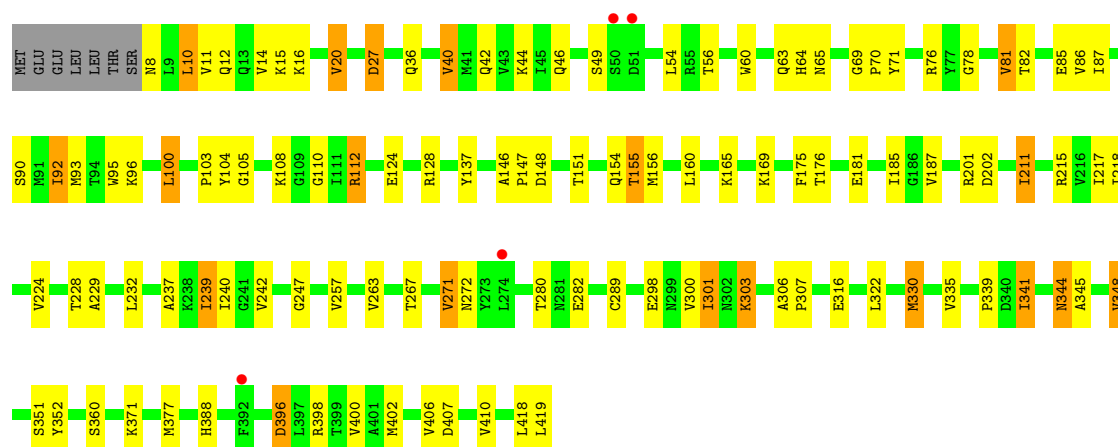
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	99.78Å 153.60Å 110.55Å 90.00° 115.58° 90.00°	Depositor
Resolution (Å)	45.04 – 2.55 45.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.04-2.55) 100.0 (45.00-2.55)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.208 , 0.260 0.212 , 0.262	Depositor DCC
R_{free} test set	2490 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9341	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, 69O

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	0.39	0/3167	0.70	0/4275
1	B	0.41	0/2954	0.66	0/3984
1	C	0.38	0/3194	0.72	0/4313
All	All	0.39	0/9315	0.69	0/12572

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3121	0	3222	70	0
1	B	2912	0	3000	71	0
1	C	3147	0	3246	77	0
2	C	44	0	26	4	0
3	C	8	0	0	3	0
4	A	39	0	0	3	0
4	B	18	0	0	2	0
4	C	52	0	0	5	0
All	All	9341	0	9494	213	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 11.

All (213) 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:64:HIS:HB2	1:C:90:SER:HB3	1.50	0.93
1:B:64:HIS:HB2	1:B:90:SER:HB3	1.56	0.87
1:C:96:LYS:HD2	1:C:348:VAL:HG21	1.55	0.86
1:C:263:VAL:O	1:C:267:THR:HB	1.76	0.85
1:C:176:THR:HB	1:C:351:SER:HB2	1.60	0.84
1:B:307:PRO:HA	1:B:333:ARG:HH11	1.42	0.83
2:C:501:NAD:H5N	3:C:502:69O:C04	2.09	0.83
1:B:176:THR:HG21	1:B:351:SER:HB2	1.60	0.82
1:B:147:PRO:HA	1:B:151:THR:HG22	1.63	0.79
1:C:339:PRO:HG3	1:C:398:ARG:HA	1.66	0.78
1:A:303:LYS:HE2	1:A:323:THR:HG21	1.73	0.71
1:C:239:ILE:HD11	1:C:242:VAL:CG2	2.21	0.70
1:C:410:VAL:HG23	1:C:419:LEU:HD23	1.74	0.70
1:A:239:ILE:O	1:A:255:ILE:HG23	1.92	0.69
1:B:147:PRO:HA	1:B:151:THR:CG2	2.22	0.68
1:C:96:LYS:HZ2	1:C:344:ASN:HD21	1.40	0.68
1:A:100:LEU:HD11	1:A:345:ALA:CB	2.24	0.67
1:C:95:TRP:CD1	1:C:402:MET:HE1	2.31	0.66
1:B:198:THR:HG21	1:B:374:VAL:HG22	1.76	0.66
1:C:11:VAL:O	1:C:15:LYS:HD3	1.95	0.66
1:C:20:VAL:HG21	1:C:402:MET:HB3	1.77	0.66
1:A:146:ALA:CB	1:A:176:THR:HG22	2.27	0.65
1:A:146:ALA:HB2	1:A:176:THR:HG22	1.79	0.65
1:A:49:SER:HB3	1:A:122:GLU:OE2	1.96	0.65
1:B:307:PRO:HA	1:B:333:ARG:NH1	2.12	0.64
2:C:501:NAD:C5N	3:C:502:69O:C06	2.76	0.64
1:A:215:ARG:HB3	1:A:240:ILE:HD13	1.80	0.64
1:B:406:VAL:O	1:B:410:VAL:HG12	1.99	0.62
2:C:501:NAD:H5N	3:C:502:69O:C06	2.30	0.61
1:B:244:ASP:N	1:B:247:GLY:O	2.34	0.61
1:C:87:ILE:O	1:C:90:SER:HB2	2.00	0.60
1:B:44:LYS:HD3	1:C:36:GLN:HB2	1.84	0.60
1:B:320:GLY:N	1:B:321:PRO:HD3	2.17	0.60
1:C:257:VAL:HG23	4:C:626:HOH:O	2.01	0.60
1:B:176:THR:CG2	1:B:351:SER:HB2	2.32	0.59
1:B:282:GLU:O	1:B:286:ILE:HG12	2.02	0.59
1:C:95:TRP:CD1	1:C:402:MET:CE	2.86	0.59
1:B:68:LEU:HD11	1:B:408:ARG:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:HIS:CD2	1:A:400:VAL:HG21	2.38	0.59
1:A:64:HIS:HB2	1:A:90:SER:HB2	1.84	0.58
1:B:100:LEU:HD11	1:B:345:ALA:HB3	1.86	0.58
1:C:215:ARG:HB3	1:C:240:ILE:HD13	1.84	0.58
1:A:100:LEU:CD1	1:A:345:ALA:HB1	2.34	0.58
1:C:60:TRP:HB2	1:C:86:VAL:HG11	1.85	0.58
1:C:176:THR:CB	1:C:351:SER:HB2	2.32	0.58
1:C:92:ILE:HD12	1:C:341:ILE:HG13	1.85	0.58
1:A:283:GLU:O	1:A:287:SER:OG	2.22	0.57
1:A:152:ASN:HB2	1:A:153:PRO:HD2	1.86	0.57
1:B:302:ASN:OD1	1:B:305:ASN:ND2	2.36	0.57
1:A:188:ARG:NH1	4:A:502:HOH:O	2.38	0.57
1:C:267:THR:HG21	1:C:272:ASN:HB2	1.87	0.57
1:A:57:PHE:CE1	1:A:113:VAL:HG23	2.40	0.56
1:B:82:THR:HG23	1:B:85:GLU:HB3	1.87	0.56
1:B:309:VAL:HG23	1:B:311:ALA:H	1.70	0.56
1:C:301:ILE:HB	1:C:322:LEU:HD22	1.87	0.56
1:B:156:MET:HE2	1:B:175:PHE:HB3	1.88	0.55
1:B:18:TYR:OH	1:B:32:ASP:OD1	2.23	0.55
1:B:316:GLU:HB3	1:B:321:PRO:HG2	1.88	0.55
1:C:10:LEU:O	1:C:14:VAL:HG23	2.07	0.55
1:C:76:ARG:HB3	1:C:148:ASP:OD2	2.07	0.55
1:A:244:ASP:HB3	1:A:269:SER:OG	2.07	0.55
1:B:319:ASN:OD1	1:B:344:ASN:ND2	2.40	0.55
1:A:143:ASP:O	1:A:145:PRO:HD3	2.07	0.54
1:A:174:VAL:HG12	1:A:174:VAL:O	2.08	0.53
1:A:10:LEU:HD12	1:A:84:ASP:CB	2.38	0.53
1:B:87:ILE:O	1:B:90:SER:HB2	2.09	0.53
1:C:267:THR:HG21	1:C:272:ASN:CB	2.39	0.53
1:C:388:HIS:HD2	1:C:400:VAL:HG21	1.74	0.53
1:A:146:ALA:HB1	1:A:147:PRO:CD	2.39	0.53
1:B:112:ARG:HB3	4:B:501:HOH:O	2.08	0.52
1:A:10:LEU:HD12	1:A:84:ASP:HB3	1.91	0.52
1:A:83:GLN:O	1:A:87:ILE:HG13	2.09	0.52
1:A:302:ASN:HB2	1:A:303:LYS:HE3	1.92	0.52
1:A:330:MET:HG3	1:A:335:VAL:HG22	1.93	0.51
1:B:64:HIS:HB2	1:B:90:SER:CB	2.34	0.51
1:B:156:MET:CE	1:B:175:PHE:HB3	2.40	0.51
1:C:93:MET:SD	1:C:96:LYS:HE3	2.50	0.51
1:C:229:ALA:HB1	1:C:239:ILE:HD13	1.93	0.51
1:C:70:PRO:HD2	1:C:103:PRO:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLN:HE22	1:A:300:VAL:HG21	1.75	0.51
1:B:40:VAL:HG23	1:C:42:GLN:HB3	1.93	0.51
1:A:10:LEU:HD12	1:A:84:ASP:CG	2.31	0.51
1:A:176:THR:HG21	1:A:351:SER:CB	2.40	0.51
1:B:42:GLN:HB3	1:C:40:VAL:HG23	1.93	0.50
1:B:41:MET:CE	1:B:137:TYR:HB2	2.42	0.50
1:C:218:ILE:HD12	1:C:239:ILE:HD12	1.93	0.50
1:A:364:ILE:HG23	1:A:368:GLU:HB2	1.93	0.50
1:C:388:HIS:CD2	1:C:400:VAL:HG21	2.47	0.50
1:C:398:ARG:O	1:C:402:MET:HB2	2.11	0.50
1:A:64:HIS:HB2	1:A:90:SER:CB	2.41	0.50
1:A:188:ARG:HD3	4:A:508:HOH:O	2.11	0.50
1:B:187:VAL:HG12	1:B:190:TYR:CE2	2.47	0.50
1:A:42:GLN:HB2	1:A:60:TRP:CD1	2.46	0.49
1:A:402:MET:O	1:A:406:VAL:HG23	2.12	0.49
1:C:85:GLU:OE1	1:C:298:GLU:OE2	2.30	0.49
1:B:154:GLN:OE1	1:B:158:TRP:CE2	2.66	0.49
1:B:62:SER:HB3	1:B:90:SER:OG	2.13	0.49
1:B:146:ALA:CB	1:B:176:THR:HG22	2.43	0.49
1:B:242:VAL:O	1:B:248:GLY:HA3	2.13	0.49
1:B:147:PRO:CA	1:B:151:THR:HG22	2.38	0.49
1:C:151:THR:HG22	1:C:155:THR:HG21	1.95	0.49
1:C:104:TYR:OH	1:C:352:TYR:HA	2.13	0.48
1:B:100:LEU:HD11	1:B:345:ALA:CB	2.42	0.48
1:B:76:ARG:O	1:B:110:GLY:HA2	2.14	0.48
1:C:96:LYS:NZ	1:C:344:ASN:OD1	2.44	0.48
1:C:402:MET:O	1:C:406:VAL:HG23	2.14	0.48
1:C:316:GLU:OE1	1:C:398:ARG:NH2	2.45	0.48
1:A:320:GLY:N	1:A:321:PRO:CD	2.77	0.48
1:B:136:LYS:HB2	1:C:137:TYR:CZ	2.48	0.48
1:B:40:VAL:CG2	1:C:42:GLN:HB3	2.44	0.48
1:C:146:ALA:HB1	1:C:147:PRO:CD	2.43	0.48
1:C:96:LYS:NZ	1:C:344:ASN:HD21	2.12	0.47
1:C:228:THR:O	1:C:232:LEU:HB2	2.14	0.47
1:C:330:MET:HE2	1:C:335:VAL:HG11	1.95	0.47
1:B:124:GLU:HA	1:B:158:TRP:CE3	2.49	0.47
1:C:78:GLY:O	1:C:81:VAL:HG13	2.14	0.47
1:B:286:ILE:HG23	1:B:308:LYS:HG2	1.95	0.47
1:C:124:GLU:O	1:C:128:ARG:HG3	2.14	0.47
1:B:117:LYS:C	1:B:118:LEU:HD23	2.35	0.47
1:A:387:PHE:CD2	1:A:404:LEU:HD13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ASP:OD1	1:C:27:ASP:N	2.46	0.47
1:B:176:THR:HG23	1:B:177:GLY:N	2.29	0.47
1:A:36:GLN:HG3	1:A:37:PRO:HD2	1.97	0.46
1:A:40:VAL:HG12	1:A:62:SER:HA	1.97	0.46
1:A:100:LEU:HD11	1:A:345:ALA:HB1	1.93	0.46
1:C:211:ILE:HD12	1:C:237:ALA:HB2	1.97	0.46
1:A:341:ILE:HA	4:A:531:HOH:O	2.14	0.46
1:A:289:CYS:SG	1:A:311:ALA:HB2	2.56	0.46
1:A:244:ASP:CB	1:A:269:SER:OG	2.62	0.46
1:B:62:SER:CB	1:B:90:SER:OG	2.64	0.46
1:A:259:ARG:HA	1:A:262:GLU:HG3	1.97	0.46
1:C:377:MET:HE2	1:C:377:MET:HA	1.96	0.46
1:B:103:PRO:HB2	4:B:503:HOH:O	2.15	0.45
1:A:176:THR:HG23	1:A:177:GLY:N	2.31	0.45
1:A:65:ASN:O	1:A:105:GLY:HA3	2.16	0.45
1:A:176:THR:HG21	1:A:351:SER:HB3	1.98	0.45
1:A:73:GLY:HA3	1:A:107:GLY:O	2.16	0.45
1:C:339:PRO:HG3	1:C:398:ARG:CA	2.40	0.45
1:A:223:ASN:O	1:A:227:PHE:HD2	1.99	0.45
1:B:243:SER:HA	1:B:247:GLY:O	2.17	0.45
1:C:8:ASN:N	4:C:603:HOH:O	2.49	0.45
1:A:163:TYR:CE1	1:A:174:VAL:HG21	2.52	0.45
1:B:340:ASP:O	1:B:344:ASN:OD1	2.35	0.45
1:C:82:THR:O	1:C:86:VAL:HG12	2.17	0.45
1:B:89:LEU:HB3	1:B:108:LYS:HD2	1.99	0.44
1:B:136:LYS:HB2	1:C:137:TYR:CE2	2.52	0.44
1:A:49:SER:CB	1:A:122:GLU:OE2	2.64	0.44
1:B:163:TYR:CE2	1:B:174:VAL:HG21	2.52	0.44
1:B:302:ASN:O	1:B:306:ALA:HB2	2.18	0.44
1:B:41:MET:HE2	1:B:137:TYR:HB2	1.99	0.44
1:B:288:ASP:HA	1:B:310:ARG:HB2	1.99	0.44
1:B:289:CYS:SG	1:B:311:ALA:HB2	2.58	0.44
1:A:205:ASN:ND2	1:A:210:GLY:HA2	2.32	0.44
1:C:76:ARG:O	1:C:110:GLY:HA2	2.18	0.44
1:A:203:ALA:HB1	1:A:313:LEU:HD11	2.00	0.44
1:C:282:GLU:OE1	1:C:282:GLU:N	2.41	0.44
1:B:89:LEU:HA	1:B:92:ILE:HG22	2.00	0.43
1:B:115:PRO:HG2	1:B:150:ASN:HB3	1.99	0.43
1:A:330:MET:HE2	1:A:335:VAL:HG21	1.99	0.43
1:B:40:VAL:HG12	1:B:62:SER:HA	1.98	0.43
1:B:176:THR:HG21	1:B:351:SER:CB	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ASN:HB2	4:C:622:HOH:O	2.18	0.43
1:C:247:GLY:C	1:C:271:VAL:HG13	2.38	0.43
1:B:152:ASN:HB2	1:B:153:PRO:HD2	2.00	0.43
1:C:217:ILE:HD12	1:C:289:CYS:HB3	2.01	0.43
1:C:306:ALA:HB3	1:C:307:PRO:HD3	2.01	0.43
1:C:232:LEU:HD12	1:C:232:LEU:HA	1.93	0.43
1:B:364:ILE:N	1:B:364:ILE:HD12	2.33	0.43
1:C:224:VAL:CG2	2:C:501:NAD:H2N	2.48	0.43
1:A:326:ALA:O	1:A:330:MET:HB2	2.19	0.43
1:C:345:ALA:HB3	1:C:377:MET:HE3	2.01	0.43
1:A:60:TRP:HB2	1:A:86:VAL:HG21	2.01	0.43
1:A:17:LEU:HA	1:A:20:VAL:HG12	2.01	0.42
1:B:218:ILE:HD12	1:B:229:ALA:HB2	2.02	0.42
1:A:302:ASN:HA	1:A:323:THR:CG2	2.49	0.42
1:A:297:VAL:HG22	1:A:298:GLU:H	1.85	0.42
1:B:22:GLU:HG2	1:B:23:LEU:N	2.34	0.42
1:B:160:LEU:O	1:B:164:ILE:HG13	2.19	0.42
1:A:23:LEU:HD21	1:A:392:PHE:CD1	2.55	0.42
1:A:70:PRO:HD2	1:A:103:PRO:O	2.19	0.42
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.89	0.42
1:B:11:VAL:O	1:B:15:LYS:HD2	2.20	0.42
1:A:63:GLN:HB3	1:A:71:TYR:CD2	2.55	0.41
1:A:81:VAL:HA	1:A:85:GLU:OE2	2.20	0.41
1:A:63:GLN:HB3	1:A:71:TYR:CE2	2.55	0.41
1:A:174:VAL:O	1:A:174:VAL:CG1	2.68	0.41
1:A:370:LYS:O	1:A:374:VAL:HG23	2.20	0.41
1:B:36:GLN:HB2	1:C:44:LYS:HD3	2.01	0.41
1:B:49:SER:HB3	1:B:51:ASP:OD1	2.20	0.41
1:C:418:LEU:HD13	4:C:637:HOH:O	2.20	0.41
1:B:72:LYS:HD3	1:B:104:TYR:CZ	2.56	0.41
1:C:100:LEU:HD21	1:C:377:MET:CE	2.50	0.41
1:C:303:LYS:CE	1:C:303:LYS:H	2.34	0.41
1:A:170:VAL:HG11	1:C:69:GLY:HA2	2.02	0.41
1:C:96:LYS:HD2	1:C:348:VAL:CG2	2.37	0.41
1:C:112:ARG:HB3	4:C:604:HOH:O	2.20	0.41
1:A:176:THR:HG21	1:A:351:SER:HB2	2.03	0.41
1:A:404:LEU:HD12	1:A:404:LEU:HA	1.88	0.41
1:C:407:ASP:HA	1:C:410:VAL:HG12	2.03	0.41
1:C:63:GLN:HB3	1:C:71:TYR:CE2	2.56	0.41
1:C:156:MET:CE	1:C:175:PHE:HB3	2.51	0.41
1:C:396:ASP:OD1	1:C:398:ARG:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HD13	1:B:349:VAL:HG23	2.02	0.41
1:C:65:ASN:O	1:C:105:GLY:HA3	2.21	0.41
1:A:124:GLU:HA	1:A:158:TRP:CE3	2.56	0.40
1:B:94:THR:OG1	1:B:106:GLY:HA3	2.22	0.40
1:B:217:ILE:HG21	1:B:284:LEU:HG	2.03	0.40
1:A:115:PRO:HG2	1:A:150:ASN:OD1	2.20	0.40
1:A:176:THR:CG2	1:A:351:SER:HB3	2.52	0.40
1:A:192:THR:HG22	1:A:224:VAL:HG13	2.04	0.40
1:C:201:ARG:HA	1:C:211:ILE:CG1	2.52	0.40
1:B:286:ILE:HD11	1:B:305:ASN:HB2	2.04	0.40
1:C:156:MET:HE2	1:C:175:PHE:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	404/419 (96%)	388 (96%)	16 (4%)	0	100	100
1	B	369/419 (88%)	349 (95%)	20 (5%)	0	100	100
1	C	410/419 (98%)	399 (97%)	11 (3%)	0	100	100
All	All	1183/1257 (94%)	1136 (96%)	47 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/344 (97%)	302 (90%)	32 (10%)	8	9
1	B	311/344 (90%)	270 (87%)	41 (13%)	4	3
1	C	337/344 (98%)	299 (89%)	38 (11%)	6	5
All	All	982/1032 (95%)	871 (89%)	111 (11%)	6	5

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	35	SER
1	A	41	MET
1	A	51	ASP
1	A	54	LEU
1	A	56	THR
1	A	82	THR
1	A	90	SER
1	A	108	LYS
1	A	118	LEU
1	A	120	LEU
1	A	129	LYS
1	A	142	VAL
1	A	176	THR
1	A	188	ARG
1	A	238	LYS
1	A	244	ASP
1	A	255	ILE
1	A	259	ARG
1	A	300	VAL
1	A	303	LYS
1	A	310	ARG
1	A	312	LYS
1	A	313	LEU
1	A	323	THR
1	A	330	MET
1	A	332	GLN
1	A	335	VAL
1	A	351	SER
1	A	370	LYS
1	A	372	LEU
1	A	408	ARG

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Mol	Chain	Res	Type
1	B	10	LEU
1	B	12	GLN
1	B	15	LYS
1	B	19	LYS
1	B	22	GLU
1	B	41	MET
1	B	48	ARG
1	B	50	SER
1	B	54	LEU
1	B	56	THR
1	B	82	THR
1	B	85	GLU
1	B	96	LYS
1	B	102	LEU
1	B	112	ARG
1	B	129	LYS
1	B	140	SER
1	B	142	VAL
1	B	151	THR
1	B	154	GLN
1	B	155	THR
1	B	176	THR
1	B	202	ASP
1	B	221	PHE
1	B	226	PHE
1	B	230	LYS
1	B	282	GLU
1	B	283	GLU
1	B	290	ASP
1	B	303	LYS
1	B	305	ASN
1	B	330	MET
1	B	335	VAL
1	B	371	LYS
1	B	373	ILE
1	B	376	ARG
1	B	378	ILE
1	B	389	LYS
1	B	394	ASP
1	B	396	ASP
1	B	399	THR
1	C	10	LEU

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Mol	Chain	Res	Type
1	C	12	GLN
1	C	16	LYS
1	C	20	VAL
1	C	27	ASP
1	C	40	VAL
1	C	46	GLN
1	C	49	SER
1	C	54	LEU
1	C	56	THR
1	C	81	VAL
1	C	92	ILE
1	C	100	LEU
1	C	108	LYS
1	C	112	ARG
1	C	154	GLN
1	C	155	THR
1	C	160	LEU
1	C	165	LYS
1	C	169	LYS
1	C	181	GLU
1	C	185	ILE
1	C	187	VAL
1	C	202	ASP
1	C	211	ILE
1	C	239	ILE
1	C	271	VAL
1	C	280	THR
1	C	300	VAL
1	C	301	ILE
1	C	303	LYS
1	C	330	MET
1	C	341	ILE
1	C	344	ASN
1	C	348	VAL
1	C	360	SER
1	C	371	LYS
1	C	396	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN

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Mol	Chain	Res	Type
1	B	154	GLN
1	B	205	ASN
1	B	344	ASN

5.3.3　RNA　ⓘ

There are no RNA molecules in this entry.

5.4　Non-standard residues in protein, DNA, RNA chains　ⓘ

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

5.5　Carbohydrates　ⓘ

There are no monosaccharides in this entry.

5.6　Ligand geometry　ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	NAD	C	501	-	42,48,48	0.81	1 (2%)	50,73,73	1.25	5 (10%)
3	69O	C	502	-	7,7,7	1.71	2 (28%)	8,8,8	1.38	1 (12%)

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	C	501	-	-	8/26/62/62	0/5/5/5

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PROTEIN DATA BANK

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	69O	C	502	-	-	0/7/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NAD	C2N-N1N	3.64	1.39	1.35
3	C	502	69O	C03-C04	3.36	1.55	1.51
3	C	502	69O	O07-C06	2.61	1.29	1.22

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	NAD	C4N-C3N-C7N	-3.71	111.10	121.04
2	C	501	NAD	C6N-N1N-C2N	-3.28	118.98	121.97
2	C	501	NAD	C2N-C3N-C7N	3.06	128.33	119.46
2	C	501	NAD	C2N-N1N-C1D	2.45	124.59	119.14
3	C	502	69O	C02-C03-C04	-2.21	109.62	113.87
2	C	501	NAD	C2N-C3N-C4N	2.03	120.56	118.26

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	NAD	C5D-O5D-PN-O1N
2	C	501	NAD	C5D-O5D-PN-O2N
2	C	501	NAD	C4N-C3N-C7N-N7N
2	C	501	NAD	C2N-C3N-C7N-N7N
2	C	501	NAD	C4N-C3N-C7N-O7N
2	C	501	NAD	C2N-C3N-C7N-O7N
2	C	501	NAD	O4B-C4B-C5B-O5B
2	C	501	NAD	C5D-O5D-PN-O3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NAD	4	0
3	C	502	69O	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand NAD C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand 69O C 502

Bond lengths

Bond angles

Torsions

Rings
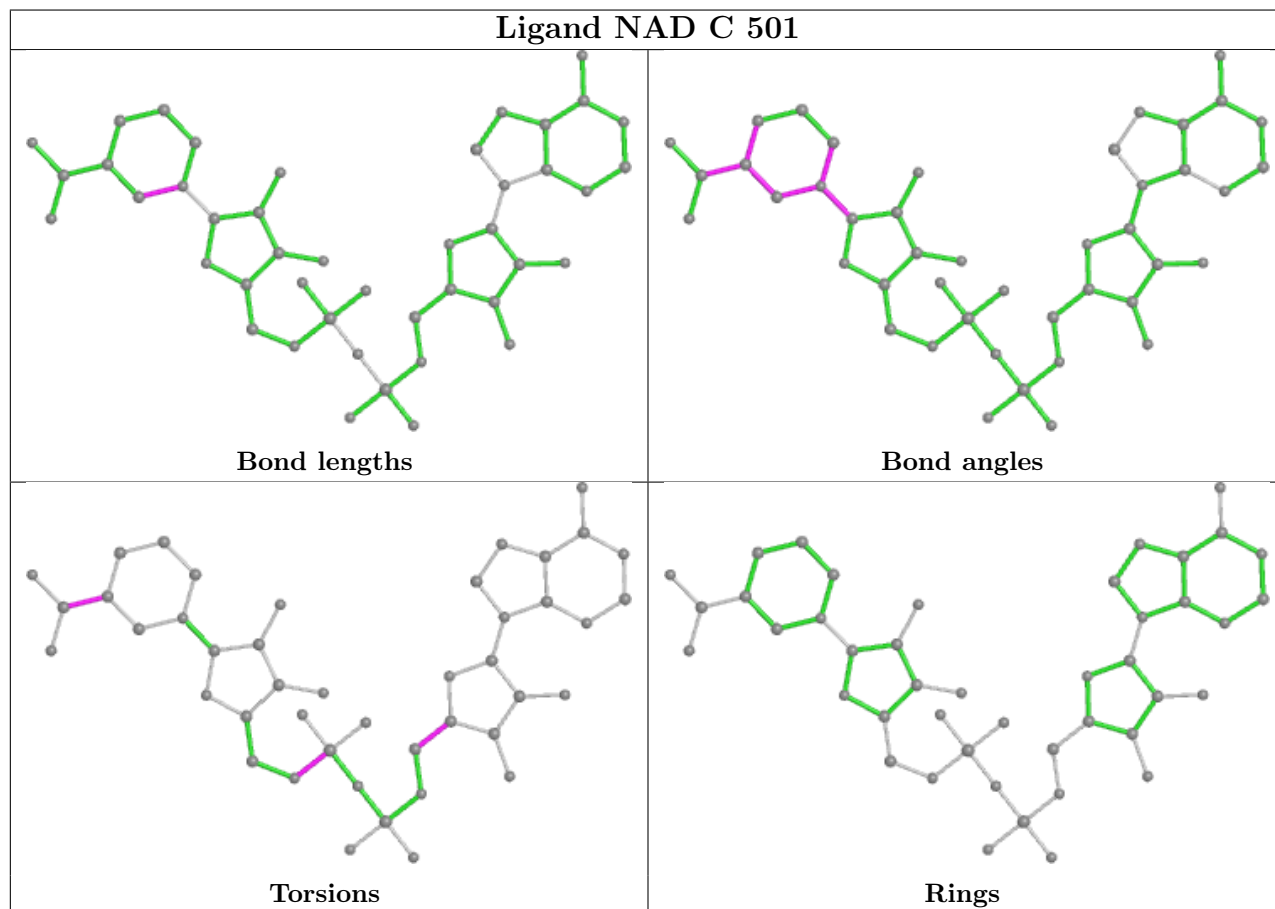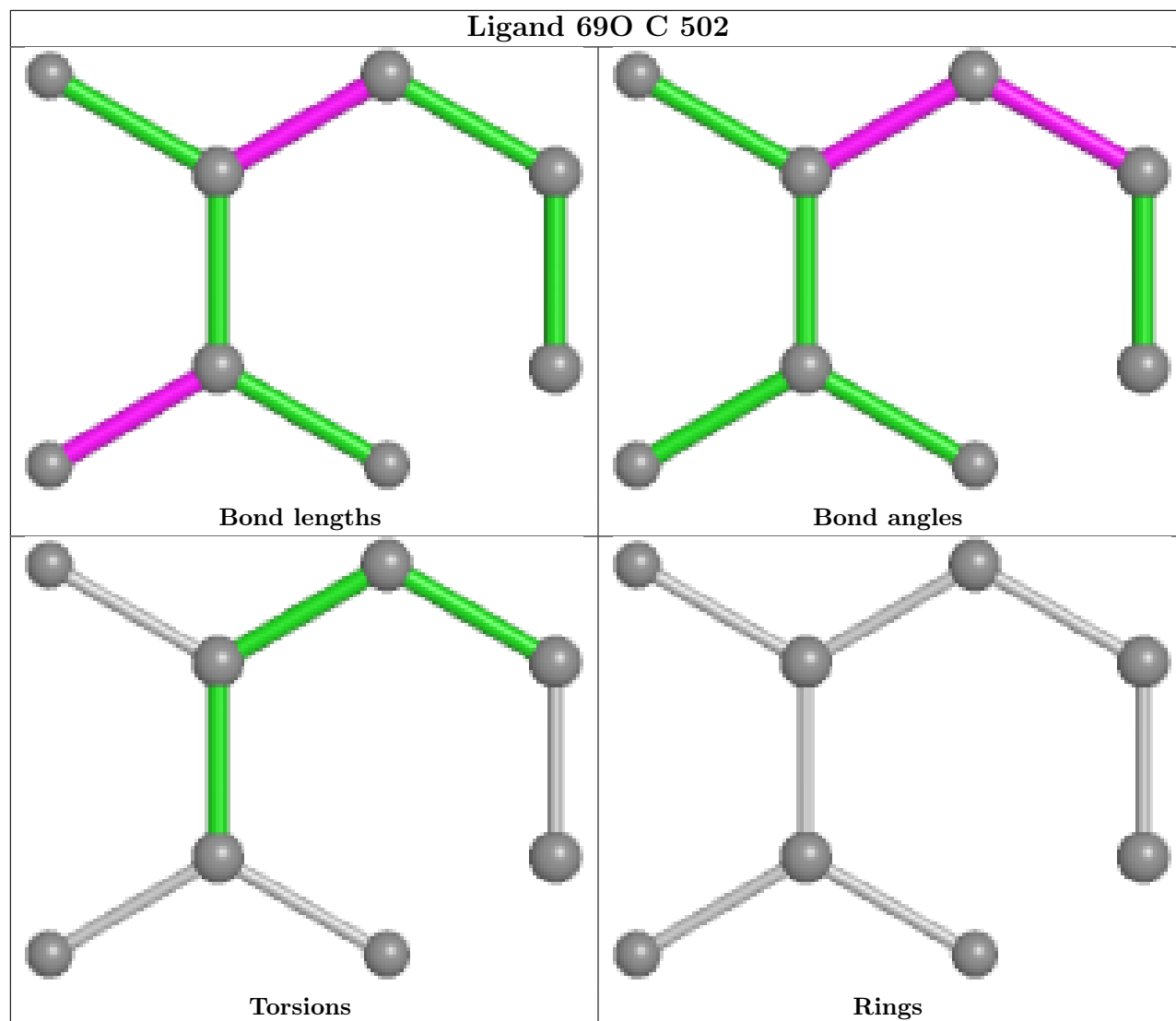
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	408/419 (97%)	-0.07	4 (0%)	82 86	28, 47, 71, 92	0
1	B	379/419 (90%)	0.70	55 (14%)	2 3	28, 57, 117, 141	0
1	C	412/419 (98%)	-0.16	4 (0%)	82 86	25, 39, 62, 80	0
All	All	1199/1257 (95%)	0.14	63 (5%)	26 31	25, 45, 99, 141	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	255	ILE	6.8
1	B	240	ILE	5.9
1	B	291	ILE	5.6
1	B	220	GLY	5.2
1	B	253	ASN	5.0
1	B	289	CYS	5.0
1	B	231	PHE	5.0
1	B	313	LEU	4.9
1	B	261	LEU	4.8
1	B	258	ASN	4.7
1	B	252	GLU	4.7
1	B	246	GLY	4.5
1	B	232	LEU	4.5
1	B	257	VAL	4.5
1	B	250	ILE	4.4
1	B	247	GLY	4.3
1	B	323	THR	4.3
1	B	249	VAL	4.2
1	B	217	ILE	4.1
1	B	254	GLY	4.0
1	B	290	ASP	4.0
1	B	218	ILE	3.9
1	B	244	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	204	ALA	3.8
1	B	293	ILE	3.8
1	B	311	ALA	3.7
1	B	259	ARG	3.4
1	A	275	GLU	3.4
1	B	242	VAL	3.3
1	B	239	ILE	3.3
1	B	314	ILE	3.2
1	A	276	GLY	3.2
1	A	274	LEU	3.2
1	B	263	VAL	3.1
1	B	337	VAL	3.1
1	B	262	GLU	3.0
1	B	256	ASP	3.0
1	B	245	ILE	3.0
1	B	304	PHE	2.9
1	B	295	ALA	2.9
1	B	215	ARG	2.8
1	B	385	TYR	2.8
1	B	221	PHE	2.8
1	B	53	LYS	2.8
1	B	284	LEU	2.7
1	B	335	VAL	2.5
1	B	322	LEU	2.5
1	C	274	LEU	2.5
1	B	285	LEU	2.4
1	B	387	PHE	2.4
1	B	229	ALA	2.4
1	B	292	LEU	2.3
1	C	50	SER	2.3
1	B	233	SER	2.3
1	C	392	PHE	2.2
1	B	54	LEU	2.2
1	C	51	ASP	2.2
1	A	11	VAL	2.1
1	B	341	ILE	2.0
1	B	207	PHE	2.0
1	B	288	ASP	2.0
1	B	331	LYS	2.0
1	B	234	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, $95^{th}$ 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	69O	C	502	8/8	0.82	0.23	28,45,49,52	0
2	NAD	C	501	44/44	0.96	0.14	23,33,79,100	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.
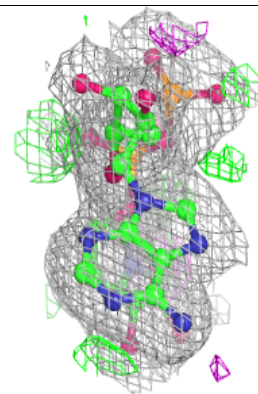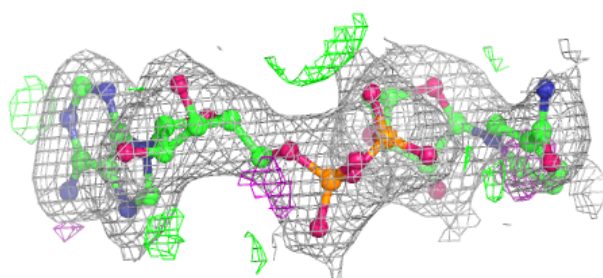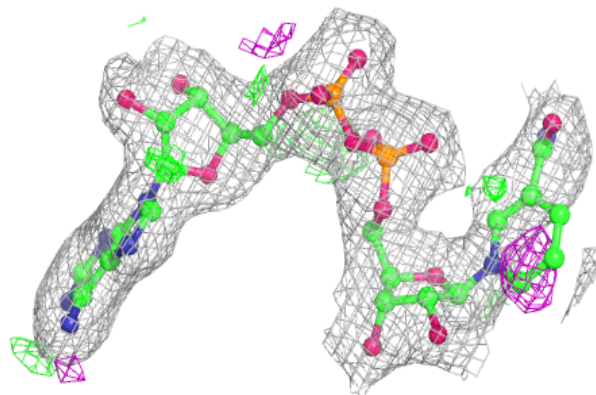
Electron density around 69O C 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
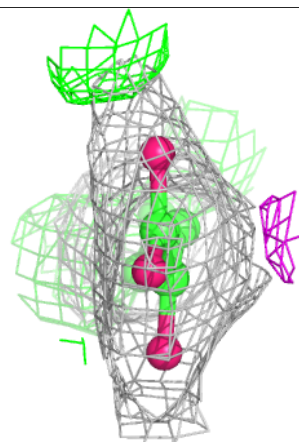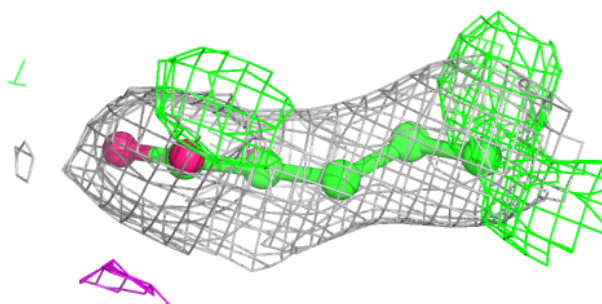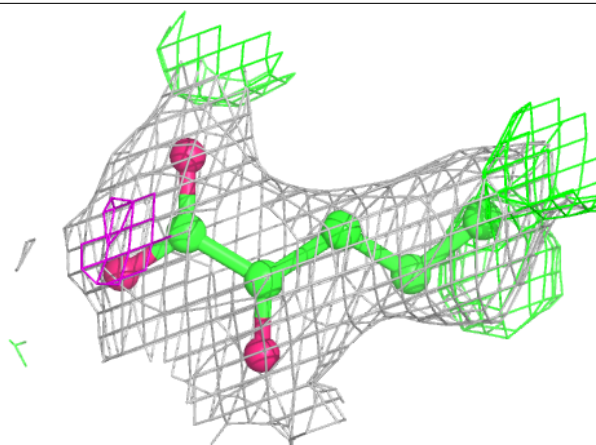
Electron density around NAD C 501:

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 ⓘ

There are no such residues in this entry.