



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:44 PM UTC

PDB ID : 6B5H / pdb_00006b5h
Title : ALDH1A2 liganded with NAD and 1-(4-cyanophenyl)-N-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1H-pyrazole-4-carboxamide (compound CM121)
Authors : Chen, Y.; Zhu, J.-Y.; Schonbrunn, E.
Deposited on : 2017-09-29
Resolution : 2.30 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

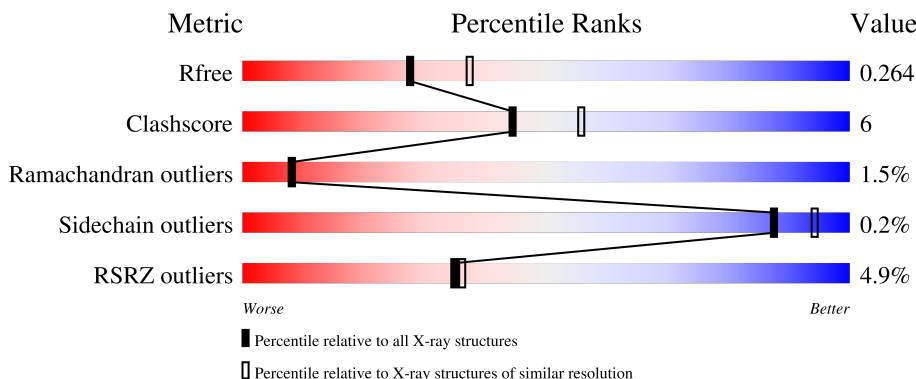
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	493	2% 88% 11%
1	B	493	9% 80% 19%
1	C	493	6% 86% 13%
1	D	493	2% 86% 13%

2 Entry composition ⓘ

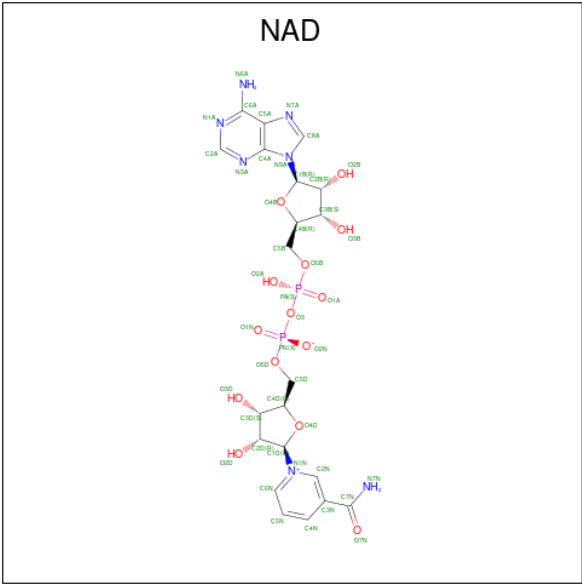
There are 4 unique types of molecules in this entry. The entry contains 15902 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Retinal dehydrogenase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3803	2420	651	714	18			
1	B	492	Total	C	N	O	S	0	0	0
			3803	2420	651	714	18			
1	C	492	Total	C	N	O	S	0	0	0
			3803	2420	651	714	18			
1	D	492	Total	C	N	O	S	0	0	0
			3803	2420	651	714	18			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



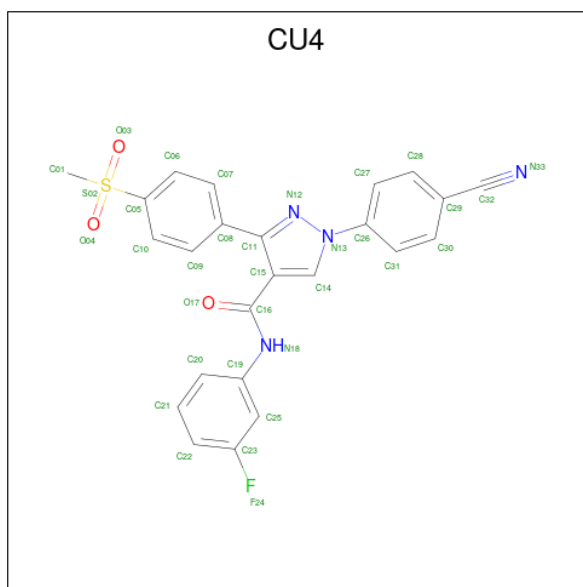
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	B	1	Total	C	N	O	P	0
			44	21	7	14	2	

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

- Molecule 3 is 1-(4-cyanophenyl)-N-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1H-pyrazole-4-carboxamide (CCD ID: CU4) (formula: $C_{24}H_{17}FN_4O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			33	24	1	4	3	1		
3	B	1	Total	C	F	N	O	S	0	0
			33	24	1	4	3	1		
3	C	1	Total	C	F	N	O	S	0	0
			33	24	1	4	3	1		
3	D	1	Total	C	F	N	O	S	0	0
			33	24	1	4	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total	O	0	0
			122	122		
4	B	74	Total	O	0	0
			74	74		

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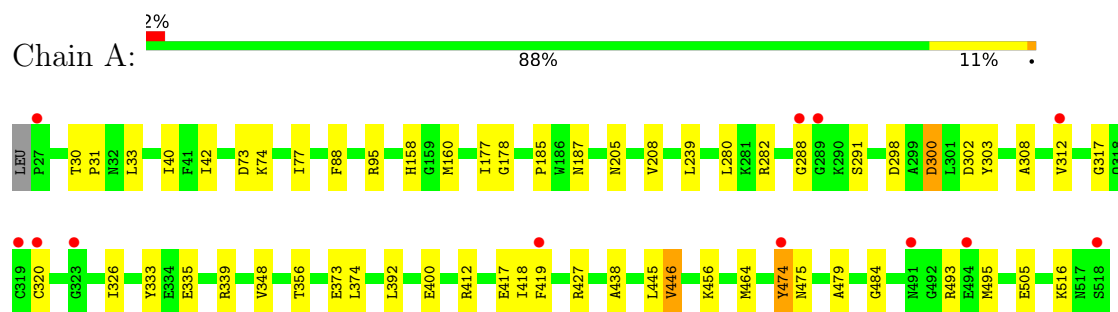
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	64	Total 64	O 64	0	0
4	D	122	Total 122	O 122	0	0

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.

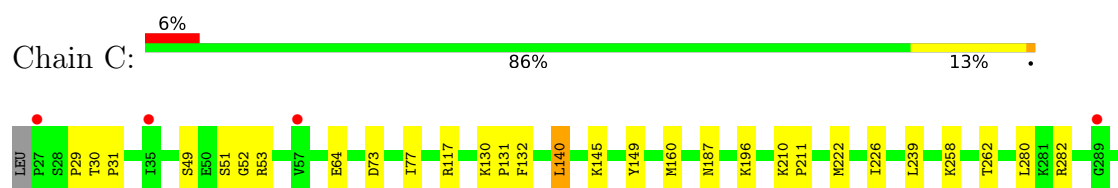
• Molecule 1: Retinal dehydrogenase 2

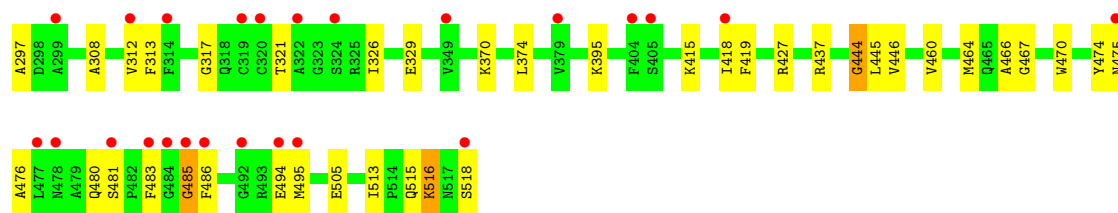


• Molecule 1: Retinal dehydrogenase 2

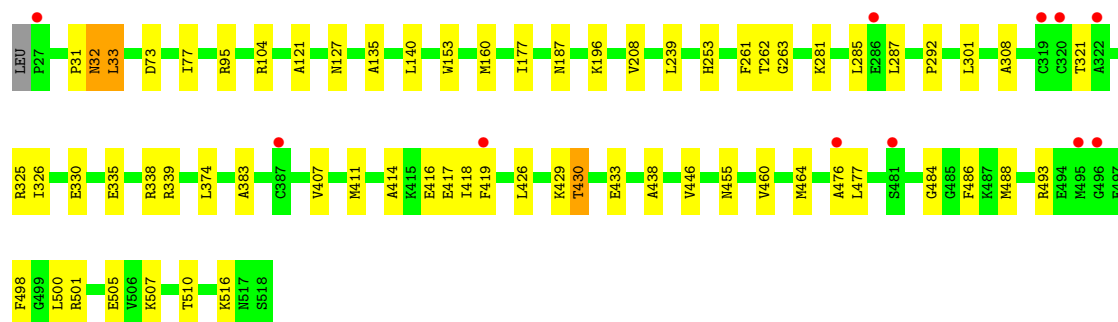
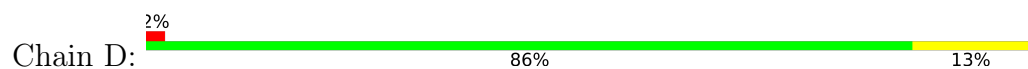


• Molecule 1: Retinal dehydrogenase 2





● Molecule 1: Retinal dehydrogenase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.85Å 141.86Å 164.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.82 – 2.30 72.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (72.82-2.30) 99.8 (72.82-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575_2575	Depositor
R, R_{free}	0.206 , 0.264 0.208 , 0.264	Depositor DCC
R_{free} test set	1776 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15902	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5281e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CU4, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.11	0/3884	0.29	0/5254
1	B	0.14	0/3884	0.36	1/5254 (0.0%)
1	C	0.13	0/3884	0.33	0/5254
1	D	0.10	0/3884	0.31	0/5254
All	All	0.12	0/15536	0.32	1/21016 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	487	LYS	CB-CA-C	-5.90	109.75	116.54

There are no chirality outliers.

There are no planarity outliers.

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	3803	0	3779	42	0
1	B	3803	0	3779	64	0
1	C	3803	0	3777	47	0
1	D	3803	0	3779	41	0
2	A	44	0	24	4	0
2	B	44	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	44	0	23	3	0
2	D	44	0	21	3	0
3	A	33	0	0	0	0
3	B	33	0	0	1	0
3	C	33	0	0	0	0
3	D	33	0	0	0	0
4	A	122	0	0	0	0
4	B	74	0	0	1	0
4	C	64	0	0	2	0
4	D	122	0	0	0	0
All	All	15902	0	15206	184	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 6.

All (184) 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:B:453:ASP:HB3	1:B:456:LYS:HD2	1.50	0.93
1:A:417:GLU:CD	1:A:419:PHE:HE1	1.81	0.87
1:C:370:LYS:HZ1	1:C:419:PHE:H	1.22	0.86
1:A:320:CYS:HG	1:A:419:PHE:HZ	0.88	0.84
1:A:417:GLU:OE2	1:A:419:PHE:HE1	1.60	0.84
1:A:320:CYS:SG	2:A:601:NAD:H2D	2.17	0.84
1:A:479:ALA:HA	1:A:495:MET:HE3	1.63	0.80
1:D:383:ALA:HB2	1:D:411:MET:HE1	1.60	0.80
1:A:417:GLU:CD	1:A:419:PHE:CE1	2.59	0.79
1:C:370:LYS:NZ	1:C:419:PHE:H	1.83	0.76
1:C:187:ASN:HD21	2:C:601:NAD:H5N	1.52	0.74
1:C:494:GLU:HG3	1:C:495:MET:HG2	1.70	0.74
1:B:388:GLY:HA3	1:B:402:THR:HA	1.69	0.73
1:B:187:ASN:HD21	2:B:601:NAD:H5N	1.54	0.72
1:B:383:ALA:HB2	1:B:411:MET:HE1	1.72	0.72
1:B:74:LYS:NZ	4:B:701:HOH:O	2.22	0.72
1:B:77:ILE:HD13	1:B:239:LEU:HD22	1.72	0.71
1:D:77:ILE:HD13	1:D:239:LEU:HD22	1.72	0.71
1:B:320:CYS:SG	2:B:601:NAD:H2D	2.30	0.71
1:C:474:TYR:O	1:C:476:ALA:N	2.21	0.71
1:A:77:ILE:HD13	1:A:239:LEU:HD22	1.73	0.69
1:A:374:LEU:HD13	1:A:418:ILE:HG12	1.74	0.68
1:C:427:ARG:O	1:C:437:ARG:NH2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:CYS:SG	1:A:419:PHE:HZ	2.08	0.67
1:C:77:ILE:HD13	1:C:239:LEU:HD22	1.78	0.66
1:A:187:ASN:HD21	2:A:601:NAD:H5N	1.61	0.65
1:B:518:SER:HA	1:D:95:ARG:HH11	1.61	0.65
1:D:177:ILE:HG12	1:D:505:GLU:HG2	1.77	0.65
1:D:374:LEU:HD13	1:D:418:ILE:HG12	1.80	0.64
1:D:135:ALA:O	1:D:140:LEU:HD12	1.99	0.63
1:A:158:HIS:CG	1:C:160:MET:HE2	2.34	0.62
1:D:31:PRO:O	1:D:33:LEU:N	2.32	0.61
1:B:321:THR:O	1:B:474:TYR:OH	2.17	0.61
1:A:288:GLY:HA2	1:A:445:LEU:HD22	1.82	0.59
1:B:489:SER:O	1:B:489:SER:OG	2.14	0.59
1:C:64:GLU:N	1:C:64:GLU:OE2	2.32	0.59
1:B:111:ASP:OD1	1:B:148:ARG:NH2	2.33	0.59
1:C:445:LEU:HD12	1:C:485:GLY:HA2	1.85	0.59
1:D:460:VAL:HG13	1:D:464:MET:HE3	1.86	0.58
1:B:337:VAL:O	1:B:341:VAL:HG12	2.03	0.58
1:B:386:GLU:OE2	1:B:405:SER:OG	2.18	0.58
1:C:467:GLY:HA3	1:C:485:GLY:H	1.67	0.58
1:A:298:ASP:OD2	1:A:456:LYS:NZ	2.36	0.57
1:A:438:ALA:HB3	1:A:464:MET:HE1	1.86	0.57
1:A:348:VAL:HG11	1:A:356:THR:HG22	1.86	0.57
1:A:392:LEU:HD13	1:A:400:GLU:HG3	1.85	0.57
1:B:285:LEU:HB3	1:B:287:LEU:HD21	1.86	0.57
1:C:444:GLY:O	1:C:486:PHE:HB2	2.05	0.56
1:A:187:ASN:ND2	2:A:601:NAD:H5N	2.21	0.56
1:B:160:MET:HA	1:D:160:MET:HA	1.87	0.56
1:C:145:LYS:NZ	4:C:702:HOH:O	2.38	0.55
1:B:288:GLY:HA2	1:B:445:LEU:HD22	1.87	0.55
1:B:372:LEU:HD21	1:B:390:LYS:HB3	1.89	0.55
1:D:498:PHE:HA	1:D:501:ARG:HG3	1.89	0.55
1:B:266:GLU:H	1:B:266:GLU:CD	2.14	0.55
1:C:513:ILE:HD11	1:C:516:LYS:HB2	1.87	0.54
1:D:430:THR:HG22	1:D:433:GLU:H	1.72	0.54
1:B:287:LEU:HB2	1:B:489:SER:HA	1.89	0.54
1:C:258:LYS:HD3	1:C:282:ARG:HB2	1.87	0.54
1:B:389:GLY:O	1:B:390:LYS:HB3	2.06	0.54
1:D:484:GLY:HA3	1:D:493:ARG:HD3	1.90	0.54
1:B:295:ILE:HD12	1:B:304:ALA:HB1	1.89	0.53
1:B:452:ASN:ND2	1:D:455:ASN:OD1	2.42	0.53
1:A:335:GLU:HG2	1:A:339:ARG:HE	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:ASN:HD21	2:D:601:NAD:H5N	1.73	0.53
1:B:443:PHE:HD1	1:B:489:SER:HB2	1.73	0.53
1:A:417:GLU:HG2	1:A:419:PHE:HD1	1.75	0.52
1:A:291:SER:HB3	1:A:446:VAL:HG12	1.90	0.52
1:B:173:ARG:NH1	1:B:175:GLU:OE2	2.43	0.52
1:B:430:THR:HG22	1:B:432:ASP:H	1.75	0.52
1:B:388:GLY:HA2	1:B:400:GLU:OE1	2.10	0.51
1:C:130:LYS:HD2	1:C:131:PRO:HD2	1.92	0.51
1:A:302:ASP:OD1	1:A:339:ARG:NH1	2.43	0.51
1:B:475:ASN:HB3	3:B:602:CU4:N12	2.26	0.51
1:A:160:MET:HA	1:C:160:MET:HA	1.93	0.51
1:D:330:GLU:HB2	1:D:429:LYS:HG2	1.92	0.51
1:B:308:ALA:HB1	1:B:326:ILE:HD13	1.92	0.50
1:D:321:THR:HG22	1:D:446:VAL:HG21	1.93	0.50
1:C:460:VAL:HG13	1:C:464:MET:HE3	1.93	0.50
1:D:253:HIS:O	1:D:281:LYS:NZ	2.45	0.50
1:C:464:MET:O	1:D:507:LYS:NZ	2.44	0.50
1:D:335:GLU:OE2	1:D:339:ARG:NH2	2.37	0.50
1:B:447:ALA:HB1	1:B:464:MET:HE3	1.93	0.49
1:B:427:ARG:O	1:B:437:ARG:NH1	2.39	0.49
1:B:321:THR:HG22	1:B:446:VAL:HG11	1.95	0.49
1:D:419:PHE:CZ	2:D:601:NAD:H2D	2.48	0.49
1:A:73:ASP:OD1	1:A:74:LYS:N	2.46	0.49
1:C:196:LYS:NZ	1:C:262:THR:OG1	2.44	0.49
1:B:390:LYS:HZ1	1:B:392:LEU:H	1.61	0.48
1:D:121:ALA:HB2	1:D:140:LEU:HD13	1.94	0.48
1:C:321:THR:HG22	1:C:446:VAL:HG21	1.95	0.48
1:A:484:GLY:HA3	1:A:493:ARG:HD3	1.95	0.48
1:B:393:GLY:O	1:B:395:LYS:N	2.46	0.48
1:D:335:GLU:OE1	1:D:338:ARG:NH2	2.42	0.48
1:A:417:GLU:HG2	1:A:419:PHE:CD1	2.49	0.48
1:C:149:TYR:CE1	1:C:480:GLN:HG3	2.49	0.48
1:B:390:LYS:HB2	1:B:399:ILE:HG23	1.96	0.47
1:B:208:VAL:HG13	1:B:239:LEU:HD13	1.96	0.47
1:A:308:ALA:HB1	1:A:326:ILE:HD13	1.97	0.47
1:B:112:LEU:HB3	1:B:225:LEU:HD22	1.95	0.47
1:C:312:VAL:O	1:C:317:GLY:HA2	2.15	0.47
1:D:153:TRP:CG	1:D:500:LEU:HD11	2.49	0.47
1:B:460:VAL:O	1:B:464:MET:HG2	2.15	0.47
1:B:393:GLY:C	1:B:395:LYS:H	2.22	0.47
1:C:470:TRP:HD1	1:D:510:THR:HB	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:THR:HB	1:A:33:LEU:HD13	1.97	0.46
1:B:324:SER:OG	1:B:325:ARG:N	2.47	0.46
1:B:374:LEU:HA	1:B:377:SER:HB3	1.97	0.46
1:B:143:VAL:HG21	1:B:190:LEU:HG	1.97	0.46
1:B:289:GLY:HA3	1:B:443:PHE:HB3	1.98	0.46
1:C:187:ASN:ND2	2:C:601:NAD:H5N	2.27	0.46
1:C:419:PHE:CZ	2:C:601:NAD:H2D	2.51	0.46
1:A:373:GLU:CD	1:A:412:ARG:HH22	2.24	0.45
1:D:196:LYS:NZ	1:D:262:THR:OG1	2.47	0.45
1:D:263:GLY:C	2:D:601:NAD:H1D	2.41	0.45
1:B:439:ASN:O	1:B:441:SER:N	2.49	0.45
1:C:505:GLU:HG2	1:D:486:PHE:CE1	2.52	0.45
1:A:282:ARG:NH2	1:A:505:GLU:OE1	2.50	0.45
1:B:323:GLY:O	1:B:325:ARG:N	2.50	0.45
1:C:480:GLN:H	1:C:480:GLN:CD	2.25	0.44
2:A:601:NAD:H8A	2:A:601:NAD:H2B	1.88	0.44
1:C:73:ASP:O	1:C:77:ILE:HG12	2.18	0.44
1:B:493:ARG:HD3	1:B:493:ARG:HA	1.89	0.44
1:B:41:PHE:CZ	1:B:44:ASN:HA	2.52	0.44
1:B:372:LEU:HD21	1:B:390:LYS:CB	2.48	0.44
1:A:300:ASP:HB3	1:A:303:TYR:HB3	2.00	0.44
1:B:61:ALA:HA	1:B:361:PRO:HG3	2.00	0.44
1:C:297:ALA:N	1:C:329:GLU:OE1	2.39	0.44
1:C:312:VAL:HG23	1:C:313:PHE:CD2	2.53	0.44
1:B:487:LYS:HB3	1:B:488:MET:H	1.52	0.44
1:C:308:ALA:O	1:C:312:VAL:HG22	2.17	0.44
1:B:131:PRO:HB2	1:B:134:GLN:HG2	1.99	0.43
1:B:210:LYS:NZ	1:B:211:PRO:O	2.49	0.43
1:D:308:ALA:HB1	1:D:326:ILE:HD13	1.99	0.43
1:D:73:ASP:O	1:D:77:ILE:HG12	2.17	0.43
1:A:177:ILE:N	1:A:205:ASN:OD1	2.51	0.43
1:B:484:GLY:HA3	1:B:493:ARG:HD3	2.00	0.43
1:D:263:GLY:O	1:D:287:LEU:HA	2.19	0.43
1:A:464:MET:HA	1:A:464:MET:HE2	2.01	0.43
1:C:415:LYS:HE2	1:C:415:LYS:HB3	1.83	0.43
1:B:149:TYR:CE1	1:B:480:GLN:HG3	2.54	0.42
1:B:192:MET:HE2	1:B:192:MET:HB3	1.90	0.42
1:A:417:GLU:OE2	1:A:419:PHE:CE1	2.52	0.42
1:A:312:VAL:O	1:A:317:GLY:HA2	2.19	0.42
1:A:333:TYR:CD1	1:A:427:ARG:HB3	2.55	0.42
1:B:104:ARG:HA	1:B:104:ARG:HD2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:GLU:HG2	1:B:495:MET:H	1.84	0.42
1:C:444:GLY:O	1:C:466:ALA:HA	2.20	0.42
1:B:284:THR:HG21	1:B:502:GLU:HG3	2.00	0.42
1:D:104:ARG:HA	1:D:104:ARG:HD2	1.85	0.42
1:C:395:LYS:HG3	4:C:723:HOH:O	2.20	0.42
1:B:35:ILE:HD13	1:B:217:LEU:HD13	2.02	0.41
1:C:210:LYS:HE3	1:C:211:PRO:O	2.20	0.41
1:A:280:LEU:HB2	1:B:488:MET:HG2	2.02	0.41
1:B:312:VAL:HG23	1:B:324:SER:H	1.84	0.41
1:C:222:MET:O	1:C:226:ILE:HG12	2.20	0.41
1:D:32:ASN:OD1	1:D:33:LEU:N	2.53	0.41
1:D:292:PRO:HG3	1:D:438:ALA:HB1	2.02	0.41
1:A:95:ARG:HH21	1:C:518:SER:HA	1.86	0.41
1:A:474:TYR:HA	1:A:475:ASN:HA	1.69	0.41
1:D:208:VAL:HG13	1:D:239:LEU:HD13	2.03	0.41
1:D:301:LEU:HD12	1:D:301:LEU:HA	1.82	0.41
1:A:88:PHE:CE2	1:A:178:GLY:HA2	2.54	0.41
1:B:287:LEU:O	2:B:601:NAD:O2D	2.37	0.41
1:C:30:THR:HA	1:C:31:PRO:HD3	1.93	0.41
1:A:288:GLY:HA3	1:A:320:CYS:SG	2.60	0.41
1:B:301:LEU:HD23	1:B:301:LEU:HA	1.85	0.41
1:D:127:ASN:O	1:D:127:ASN:ND2	2.53	0.41
1:A:40:ILE:HG22	1:A:42:ILE:HG13	2.02	0.41
1:A:208:VAL:HG13	1:A:239:LEU:HD13	2.02	0.41
1:B:33:LEU:HD11	1:B:119:VAL:HG13	2.03	0.41
1:C:280:LEU:HD12	1:D:488:MET:HE2	2.01	0.41
1:C:515:GLN:O	1:C:516:LYS:HB3	2.21	0.41
1:B:451:THR:OG1	1:B:452:ASN:N	2.52	0.41
1:C:29:PRO:HG3	1:C:132:PHE:CG	2.55	0.41
1:C:49:SER:HB2	1:C:52:GLY:H	1.86	0.41
1:C:308:ALA:HB1	1:C:326:ILE:HD13	2.03	0.41
1:C:374:LEU:HD13	1:C:418:ILE:HG12	2.04	0.40
1:D:325:ARG:HD3	1:D:414:ALA:O	2.21	0.40
1:C:117:ARG:HG3	1:C:140:LEU:HD22	2.03	0.40
1:D:417:GLU:CD	1:D:419:PHE:CE1	2.99	0.40
1:C:51:SER:OG	1:C:53:ARG:HG3	2.20	0.40
1:D:261:PHE:HB3	1:D:285:LEU:HD23	2.03	0.40
1:D:407:VAL:HB	1:D:426:LEU:HG	2.02	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	490/493 (99%)	469 (96%)	16 (3%)	5 (1%)	12	15
1	B	490/493 (99%)	455 (93%)	23 (5%)	12 (2%)	4	4
1	C	490/493 (99%)	455 (93%)	29 (6%)	6 (1%)	10	12
1	D	490/493 (99%)	463 (94%)	20 (4%)	7 (1%)	9	9
All	All	1960/1972 (99%)	1842 (94%)	88 (4%)	30 (2%)	8	8

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	31	PRO
1	B	386	GLU
1	C	475	ASN
1	D	32	ASN
1	A	516	LYS
1	B	324	SER
1	B	394	ARG
1	B	444	GLY
1	B	491	ASN
1	D	416	GLU
1	A	31	PRO
1	B	384	LYS
1	B	440	ASN
1	C	481	SER
1	C	483	PHE
1	D	476	ALA
1	D	477	LEU
1	A	300	ASP
1	A	474	TYR
1	C	444	GLY
1	C	485	GLY
1	C	516	LYS

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Mol	Chain	Res	Type
1	D	33	LEU
1	D	430	THR
1	B	390	LYS
1	B	395	LYS
1	D	516	LYS
1	B	185	PRO
1	B	391	GLY
1	A	185	PRO

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	401/402 (100%)	400 (100%)	1 (0%)	87	94
1	B	401/402 (100%)	400 (100%)	1 (0%)	87	94
1	C	401/402 (100%)	400 (100%)	1 (0%)	87	94
1	D	401/402 (100%)	401 (100%)	0	100	100
All	All	1604/1608 (100%)	1601 (100%)	3 (0%)	87	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	446	VAL
1	B	192	MET
1	C	140	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	182	GLN
1	A	307	GLN
1	A	318	GLN
1	A	367	GLN

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Mol	Chain	Res	Type
1	B	43	ASN
1	B	134	GLN
1	B	187	ASN
1	B	272	GLN
1	B	316	GLN
1	B	452	ASN
1	B	465	GLN
1	C	32	ASN
1	C	47	GLN
1	C	141	GLN
1	C	182	GLN
1	C	272	GLN
1	C	316	GLN
1	C	318	GLN
1	C	359	GLN
1	C	455	ASN
1	D	82	GLN
1	D	478	ASN
1	D	515	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAD	D	601	-	46,48,48	3.61	15 (32%)	64,73,73	1.68	12 (18%)
3	CU4	C	602	-	36,36,36	2.70	10 (27%)	51,52,52	2.07	12 (23%)
3	CU4	A	602	-	36,36,36	2.77	11 (30%)	51,52,52	2.19	13 (25%)
3	CU4	B	602	-	36,36,36	2.71	10 (27%)	51,52,52	2.04	12 (23%)
3	CU4	D	602	-	36,36,36	2.69	10 (27%)	51,52,52	2.08	12 (23%)
2	NAD	C	601	-	46,48,48	3.64	15 (32%)	64,73,73	1.62	10 (15%)
2	NAD	B	601	-	46,48,48	3.69	15 (32%)	64,73,73	1.70	13 (20%)
2	NAD	A	601	-	46,48,48	3.79	15 (32%)	64,73,73	1.75	13 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	D	601	-	-	9/30/62/62	0/5/5/5
3	CU4	C	602	-	-	2/24/24/24	0/4/4/4
3	CU4	A	602	-	-	0/24/24/24	0/4/4/4
3	CU4	B	602	-	-	8/24/24/24	0/4/4/4
3	CU4	D	602	-	-	6/24/24/24	0/4/4/4
2	NAD	C	601	-	-	5/30/62/62	0/5/5/5
2	NAD	B	601	-	-	12/30/62/62	0/5/5/5
2	NAD	A	601	-	-	7/30/62/62	0/5/5/5

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAD	O4D-C1D	16.76	1.62	1.40
2	B	601	NAD	O4D-C1D	16.00	1.61	1.40
2	C	601	NAD	O4D-C1D	15.73	1.61	1.40
2	D	601	NAD	O4D-C1D	15.53	1.61	1.40
2	B	601	NAD	O4B-C1B	8.82	1.62	1.42
2	C	601	NAD	O4B-C1B	8.76	1.62	1.42
2	A	601	NAD	O4B-C1B	8.74	1.62	1.42
2	D	601	NAD	O4B-C1B	8.60	1.61	1.42
2	B	601	NAD	C2B-C1B	-7.84	1.28	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAD	C2B-C1B	-7.84	1.28	1.53
2	C	601	NAD	C2B-C1B	-7.69	1.29	1.53
2	D	601	NAD	C2B-C1B	-7.55	1.29	1.53
3	A	602	CU4	O04-S02	6.98	1.61	1.44
3	B	602	CU4	O03-S02	6.85	1.61	1.44
3	D	602	CU4	O03-S02	6.85	1.61	1.44
3	C	602	CU4	O03-S02	6.83	1.61	1.44
3	C	602	CU4	O04-S02	6.78	1.60	1.44
3	B	602	CU4	O04-S02	6.77	1.60	1.44
3	A	602	CU4	O03-S02	6.76	1.60	1.44
3	D	602	CU4	O04-S02	6.75	1.60	1.44
2	D	601	NAD	O4B-C4B	-6.72	1.30	1.45
3	A	602	CU4	C29-C32	-6.61	1.30	1.44
3	C	602	CU4	C29-C32	-6.59	1.30	1.44
3	B	602	CU4	C29-C32	-6.58	1.30	1.44
2	A	601	NAD	O4D-C4D	-6.58	1.30	1.45
3	D	602	CU4	C29-C32	-6.55	1.30	1.44
2	B	601	NAD	C7N-N7N	6.54	1.45	1.33
2	A	601	NAD	C7N-N7N	6.52	1.45	1.33
2	C	601	NAD	C7N-N7N	6.47	1.44	1.33
2	D	601	NAD	C7N-N7N	6.46	1.44	1.33
2	C	601	NAD	O4B-C4B	-6.41	1.30	1.45
2	A	601	NAD	O4B-C4B	-6.30	1.31	1.45
2	D	601	NAD	O4D-C4D	-6.25	1.31	1.45
2	B	601	NAD	O4B-C4B	-6.21	1.31	1.45
2	B	601	NAD	O4D-C4D	-6.15	1.31	1.45
2	C	601	NAD	O4D-C4D	-6.02	1.31	1.45
3	A	602	CU4	N13-N12	-5.83	1.29	1.36
3	B	602	CU4	N13-N12	-5.70	1.29	1.36
3	C	602	CU4	N13-N12	-5.56	1.29	1.36
3	D	602	CU4	N13-N12	-5.52	1.30	1.36
3	A	602	CU4	C08-C11	-4.66	1.41	1.48
2	A	601	NAD	C2N-N1N	4.46	1.39	1.35
3	C	602	CU4	C08-C11	-4.08	1.42	1.48
3	B	602	CU4	C08-C11	-4.07	1.42	1.48
3	D	602	CU4	C08-C11	-4.07	1.42	1.48
2	B	601	NAD	C2N-N1N	3.93	1.39	1.35
2	A	601	NAD	C3N-C7N	3.76	1.56	1.50
2	D	601	NAD	C6A-N6A	3.74	1.43	1.34
2	B	601	NAD	C6A-N6A	3.72	1.43	1.34
2	A	601	NAD	C6A-N6A	3.70	1.43	1.34
2	B	601	NAD	C3N-C7N	3.67	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAD	C6A-N6A	3.65	1.43	1.34
3	A	602	CU4	C26-N13	-3.57	1.36	1.43
2	C	601	NAD	C3N-C7N	3.55	1.55	1.50
2	C	601	NAD	C2N-N1N	3.39	1.38	1.35
3	D	602	CU4	C26-N13	-3.37	1.36	1.43
2	D	601	NAD	C3N-C7N	3.36	1.55	1.50
3	C	602	CU4	C26-N13	-3.36	1.36	1.43
3	B	602	CU4	C26-N13	-3.36	1.36	1.43
2	C	601	NAD	O3D-C3D	-3.06	1.35	1.43
2	D	601	NAD	O3D-C3D	-3.03	1.35	1.43
2	D	601	NAD	O2B-C2B	3.03	1.50	1.43
2	B	601	NAD	O3D-C3D	-2.96	1.35	1.43
2	B	601	NAD	O3B-C3B	-2.90	1.35	1.43
2	A	601	NAD	O3B-C3B	-2.88	1.35	1.43
2	D	601	NAD	O3B-C3B	-2.81	1.36	1.43
2	A	601	NAD	O3D-C3D	-2.78	1.36	1.43
2	C	601	NAD	O3B-C3B	-2.77	1.36	1.43
2	C	601	NAD	O2B-C2B	2.75	1.49	1.43
2	D	601	NAD	C2N-N1N	2.71	1.38	1.35
2	A	601	NAD	O2B-C2B	2.68	1.49	1.43
2	B	601	NAD	O2B-C2B	2.49	1.49	1.43
3	B	602	CU4	C15-C16	-2.48	1.42	1.49
3	A	602	CU4	C15-C16	-2.48	1.42	1.49
3	C	602	CU4	C15-C16	-2.44	1.42	1.49
3	C	602	CU4	C01-S02	2.43	1.83	1.75
3	B	602	CU4	C01-S02	2.42	1.83	1.75
3	D	602	CU4	C15-C16	-2.35	1.42	1.49
2	B	601	NAD	O2D-C2D	2.31	1.48	1.43
2	D	601	NAD	C8A-N7A	2.30	1.36	1.31
3	A	602	CU4	C01-S02	2.30	1.83	1.75
2	D	601	NAD	O2D-C2D	2.29	1.48	1.43
2	C	601	NAD	O2D-C2D	2.25	1.48	1.43
2	C	601	NAD	C5A-C4A	-2.25	1.35	1.39
3	A	602	CU4	F24-C23	-2.24	1.30	1.36
3	D	602	CU4	C01-S02	2.23	1.83	1.75
3	C	602	CU4	F24-C23	-2.22	1.31	1.36
2	C	601	NAD	C8A-N7A	2.20	1.35	1.31
3	B	602	CU4	F24-C23	-2.20	1.31	1.36
3	D	602	CU4	F24-C23	-2.20	1.31	1.36
3	B	602	CU4	C25-C23	2.19	1.41	1.37
2	B	601	NAD	C8A-N7A	2.19	1.35	1.31
3	A	602	CU4	C06-C05	2.19	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAD	O2D-C2D	2.18	1.48	1.43
2	A	601	NAD	C8A-N7A	2.14	1.35	1.31
2	A	601	NAD	C5A-C4A	-2.14	1.35	1.39
2	B	601	NAD	C5A-C4A	-2.13	1.35	1.39
2	D	601	NAD	C5A-C4A	-2.11	1.35	1.39
3	A	602	CU4	C25-C23	2.09	1.41	1.37
3	C	602	CU4	C25-C23	2.06	1.41	1.37
3	D	602	CU4	C25-C23	2.05	1.41	1.37

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	CU4	C11-N12-N13	6.43	110.12	104.89
3	C	602	CU4	C01-S02-C05	6.03	111.20	104.55
3	C	602	CU4	O04-S02-O03	-6.00	107.82	117.99
3	D	602	CU4	C11-N12-N13	5.98	109.75	104.89
3	C	602	CU4	C11-N12-N13	5.94	109.71	104.89
3	A	602	CU4	O04-S02-O03	-5.81	108.14	117.99
3	B	602	CU4	O04-S02-O03	-5.79	108.18	117.99
3	D	602	CU4	O04-S02-O03	-5.75	108.24	117.99
2	A	601	NAD	N3A-C2A-N1A	-5.58	120.13	128.58
2	B	601	NAD	N3A-C2A-N1A	-5.57	120.15	128.58
3	A	602	CU4	C01-S02-C05	5.54	110.65	104.55
2	C	601	NAD	N3A-C2A-N1A	-5.47	120.31	128.58
2	D	601	NAD	N3A-C2A-N1A	-5.40	120.41	128.58
3	A	602	CU4	C11-N12-N13	5.34	109.23	104.89
3	B	602	CU4	C01-S02-C05	5.25	110.33	104.55
2	D	601	NAD	C4D-O4D-C1D	-5.12	105.23	109.92
2	B	601	NAD	C5A-C4A-N3A	-5.00	119.83	126.72
2	A	601	NAD	C5A-C4A-N3A	-4.83	120.07	126.72
3	D	602	CU4	C15-C16-N18	4.76	122.32	115.61
3	A	602	CU4	O03-S02-C05	4.74	111.91	108.23
2	C	601	NAD	N9A-C8A-N7A	-4.62	107.38	113.94
2	D	601	NAD	C5A-C4A-N3A	-4.47	120.56	126.72
2	C	601	NAD	C5A-C4A-N3A	-4.36	120.72	126.72
2	D	601	NAD	N9A-C8A-N7A	-4.29	107.84	113.94
3	D	602	CU4	O04-S02-C05	4.29	111.56	108.23
2	A	601	NAD	N9A-C8A-N7A	-4.28	107.86	113.94
2	B	601	NAD	N9A-C8A-N7A	-4.26	107.89	113.94
3	C	602	CU4	C15-C16-N18	4.24	121.59	115.61
3	A	602	CU4	C15-C16-N18	4.22	121.56	115.61
2	A	601	NAD	C6N-N1N-C2N	-4.22	118.29	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	CU4	O04-S02-C05	4.17	111.47	108.23
2	B	601	NAD	C4D-O4D-C1D	-4.11	106.16	109.92
3	C	602	CU4	O03-S02-C05	4.07	111.39	108.23
3	D	602	CU4	O03-S02-C05	3.97	111.31	108.23
3	A	602	CU4	C06-C05-S02	3.94	123.08	119.58
3	D	602	CU4	C01-S02-C05	3.88	108.83	104.55
3	D	602	CU4	C19-C25-C23	3.78	121.72	117.96
3	C	602	CU4	C19-C25-C23	3.59	121.52	117.96
3	B	602	CU4	O03-S02-C05	3.58	111.01	108.23
3	B	602	CU4	C15-C16-N18	3.44	120.46	115.61
2	B	601	NAD	C2A-N3A-C4A	3.39	120.11	111.83
2	A	601	NAD	C2A-N3A-C4A	3.33	119.96	111.83
3	A	602	CU4	C19-C25-C23	3.31	121.24	117.96
2	A	601	NAD	C4D-O4D-C1D	-3.24	106.95	109.92
2	C	601	NAD	C2A-N3A-C4A	3.15	119.54	111.83
3	B	602	CU4	C19-C25-C23	3.13	121.07	117.96
2	D	601	NAD	C2A-N3A-C4A	3.11	119.42	111.83
2	C	601	NAD	C5A-N7A-C8A	3.11	108.33	103.45
2	B	601	NAD	C5A-N7A-C8A	3.01	108.18	103.45
3	B	602	CU4	O04-S02-C05	2.99	110.55	108.23
2	C	601	NAD	C4D-O4D-C1D	-2.97	107.20	109.92
2	C	601	NAD	C3B-C2B-C1B	2.97	107.08	101.46
2	A	601	NAD	C5A-N7A-C8A	2.93	108.06	103.45
2	B	601	NAD	N3A-C4A-N9A	2.93	132.14	127.17
2	A	601	NAD	N3A-C4A-N9A	2.91	132.11	127.17
2	D	601	NAD	C5A-N7A-C8A	2.89	107.99	103.45
2	C	601	NAD	C4A-N9A-C8A	2.78	108.65	105.74
3	B	602	CU4	C14-N13-N12	-2.77	109.46	112.31
3	D	602	CU4	C22-C23-C25	-2.71	119.66	123.23
3	C	602	CU4	C22-C23-C25	-2.67	119.70	123.23
3	A	602	CU4	C22-C23-C25	-2.63	119.76	123.23
3	C	602	CU4	C14-N13-N12	-2.62	109.62	112.31
3	D	602	CU4	C14-N13-N12	-2.56	109.68	112.31
2	D	601	NAD	C3B-C2B-C1B	2.53	106.24	101.46
2	B	601	NAD	C6N-N1N-C2N	-2.51	119.74	121.88
2	C	601	NAD	C4A-C5A-N7A	-2.50	107.72	110.58
3	B	602	CU4	C22-C23-C25	-2.48	119.95	123.23
2	C	601	NAD	N3A-C4A-N9A	2.47	131.37	127.17
3	D	602	CU4	C08-C11-N12	2.46	122.67	118.99
2	D	601	NAD	C4A-C5A-N7A	-2.43	107.80	110.58
2	B	601	NAD	C4A-C5A-N7A	-2.38	107.86	110.58
2	A	601	NAD	C4A-N9A-C8A	2.38	108.23	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	NAD	N3A-C4A-N9A	2.37	131.19	127.17
3	A	602	CU4	C14-C15-C11	-2.33	103.41	104.76
2	A	601	NAD	C3N-C7N-N7N	2.32	120.60	117.74
2	D	601	NAD	C6N-N1N-C2N	-2.32	119.90	121.88
3	A	602	CU4	C14-N13-N12	-2.30	109.94	112.31
2	D	601	NAD	C4A-N9A-C8A	2.27	108.12	105.74
2	B	601	NAD	C5B-C4B-C3B	-2.26	107.08	115.21
3	D	602	CU4	O17-C16-C15	-2.26	117.11	121.04
2	D	601	NAD	C5A-C4A-N9A	2.24	108.25	105.81
2	A	601	NAD	C4A-C5A-N7A	-2.23	108.03	110.58
3	C	602	CU4	C26-N13-N12	2.23	122.64	119.93
2	B	601	NAD	C4A-N9A-C8A	2.20	108.05	105.74
3	D	602	CU4	C26-N13-N12	2.15	122.55	119.93
3	B	602	CU4	C10-C05-S02	2.15	121.48	119.58
3	B	602	CU4	C26-N13-N12	2.14	122.53	119.93
2	A	601	NAD	C2D-C3D-C4D	2.14	106.74	102.61
3	A	602	CU4	C10-C05-S02	-2.11	117.71	119.58
3	C	602	CU4	C15-C14-N13	2.09	108.60	107.13
2	B	601	NAD	C6A-C5A-C4A	2.05	119.98	117.18
3	B	602	CU4	C15-C14-N13	2.05	108.58	107.13
3	A	602	CU4	O17-C16-C15	-2.04	117.48	121.04
2	A	601	NAD	O7N-C7N-N7N	-2.03	119.68	122.62
2	B	601	NAD	C5A-C4A-N9A	2.03	108.03	105.81
3	C	602	CU4	O17-C16-C15	-2.03	117.51	121.04
3	C	602	CU4	C14-C15-C11	-2.01	103.60	104.76

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	NAD	C5B-O5B-PA-O1A
2	B	601	NAD	C5B-O5B-PA-O2A
2	B	601	NAD	C5B-O5B-PA-O3
2	B	601	NAD	PN-O3-PA-O5B
2	B	601	NAD	C5D-O5D-PN-O3
2	B	601	NAD	C5D-O5D-PN-O1N
2	B	601	NAD	C5D-O5D-PN-O2N
2	C	601	NAD	PN-O3-PA-O5B
2	D	601	NAD	C5B-O5B-PA-O1A
3	B	602	CU4	C06-C05-S02-O03
2	A	601	NAD	C3D-C4D-C5D-O5D
2	B	601	NAD	C3D-C4D-C5D-O5D

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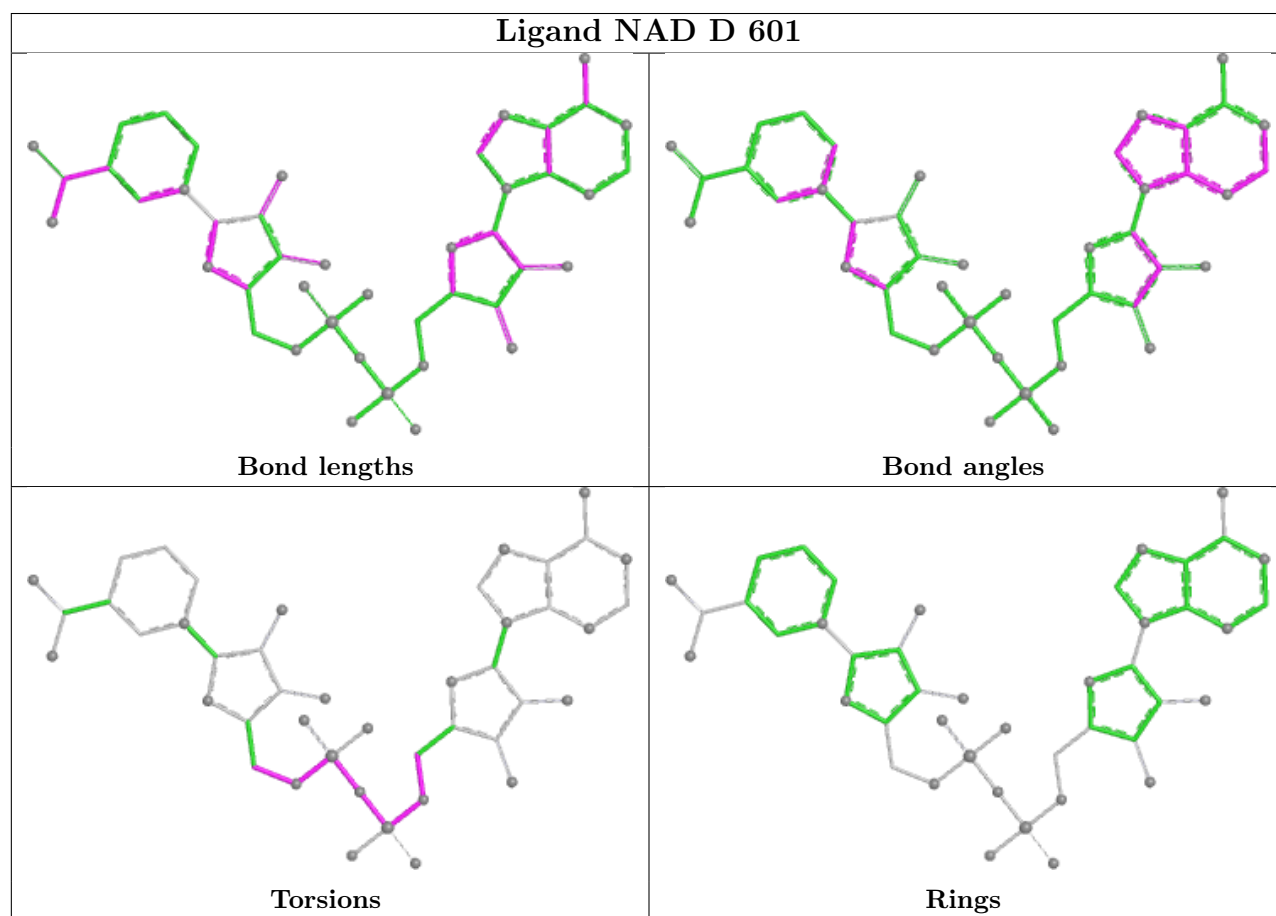
Mol	Chain	Res	Type	Atoms
3	D	602	CU4	C06-C05-S02-O03
3	D	602	CU4	C10-C05-S02-O03
2	A	601	NAD	O4D-C4D-C5D-O5D
2	B	601	NAD	O4D-C4D-C5D-O5D
2	C	601	NAD	O4D-C4D-C5D-O5D
2	C	601	NAD	C3D-C4D-C5D-O5D
3	D	602	CU4	C10-C05-S02-C01
3	B	602	CU4	C10-C05-S02-O03
2	D	601	NAD	C4D-C5D-O5D-PN
3	D	602	CU4	C06-C05-S02-C01
2	B	601	NAD	C3B-C4B-C5B-O5B
2	C	601	NAD	C4D-C5D-O5D-PN
2	A	601	NAD	PN-O3-PA-O5B
2	D	601	NAD	PN-O3-PA-O5B
3	B	602	CU4	C06-C05-S02-C01
2	A	601	NAD	C2B-C1B-N9A-C8A
3	B	602	CU4	C27-C26-N13-N12
2	D	601	NAD	C5B-O5B-PA-O2A
2	D	601	NAD	C5B-O5B-PA-O3
2	D	601	NAD	C5D-O5D-PN-O2N
2	A	601	NAD	C4D-C5D-O5D-PN
2	B	601	NAD	C4D-C5D-O5D-PN
2	D	601	NAD	C4B-C5B-O5B-PA
3	B	602	CU4	C10-C05-S02-C01
3	B	602	CU4	C31-C26-N13-N12
3	B	602	CU4	C27-C26-N13-C14
2	D	601	NAD	PA-O3-PN-O1N
2	D	601	NAD	PA-O3-PN-O2N
2	A	601	NAD	O4B-C1B-N9A-C8A
2	B	601	NAD	O4B-C4B-C5B-O5B
2	A	601	NAD	C2B-C1B-N9A-C4A
3	D	602	CU4	C09-C08-C11-N12
3	D	602	CU4	C07-C08-C11-N12
3	B	602	CU4	C31-C26-N13-C14
3	C	602	CU4	C09-C08-C11-N12
3	C	602	CU4	C07-C08-C11-N12
2	C	601	NAD	C2B-C1B-N9A-C8A

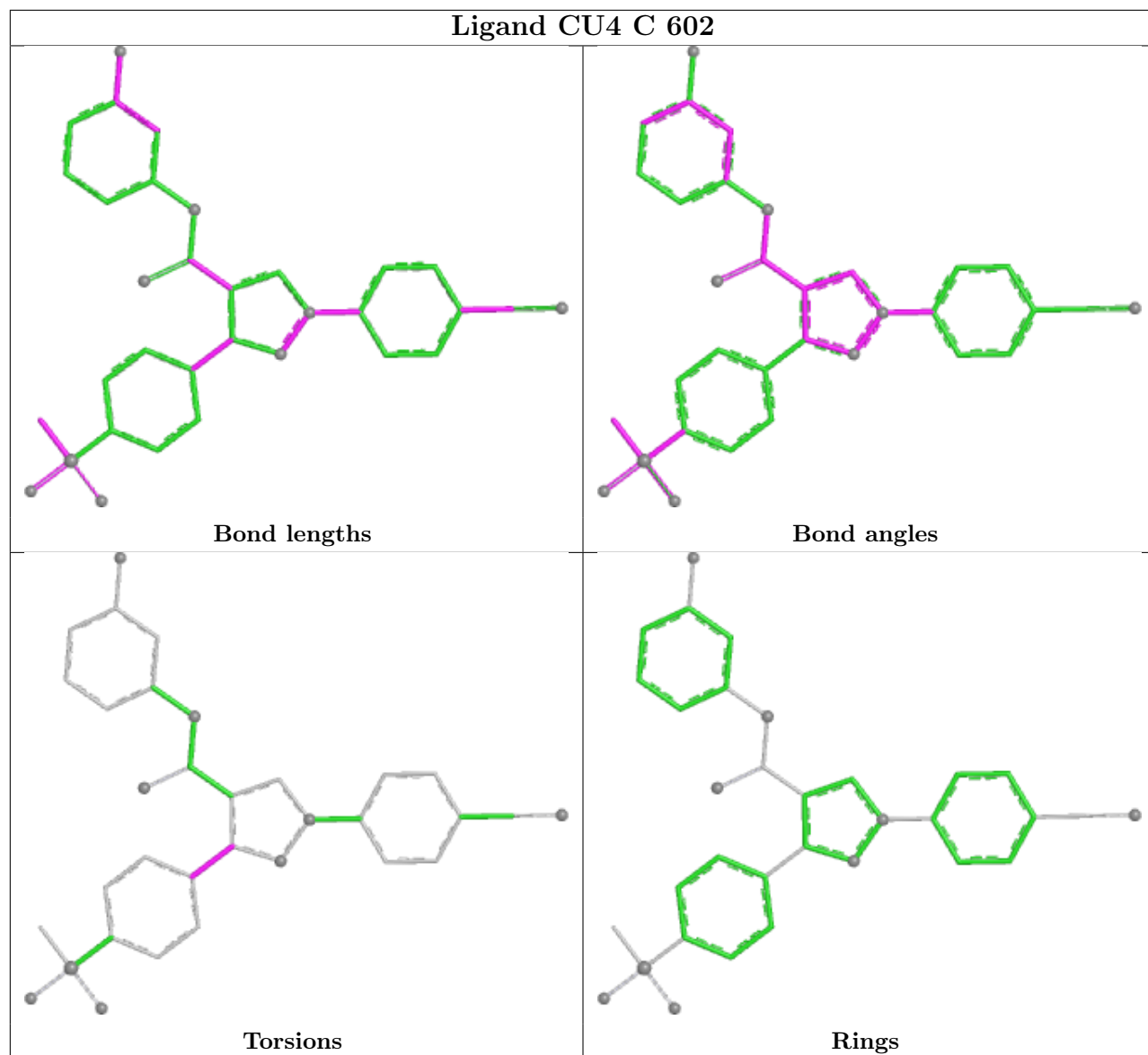
There are no ring outliers.

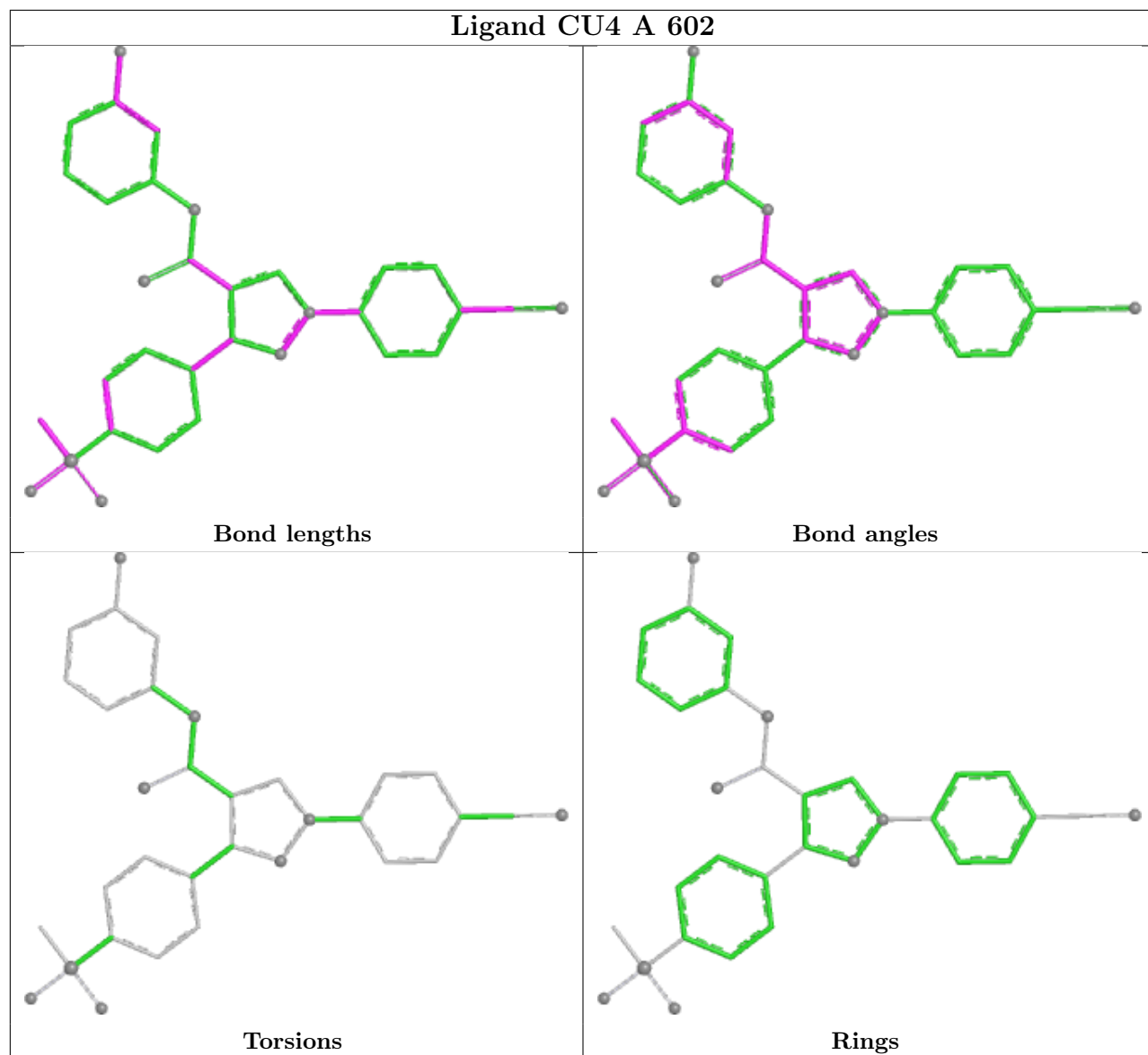
5 monomers are involved in 14 short contacts:

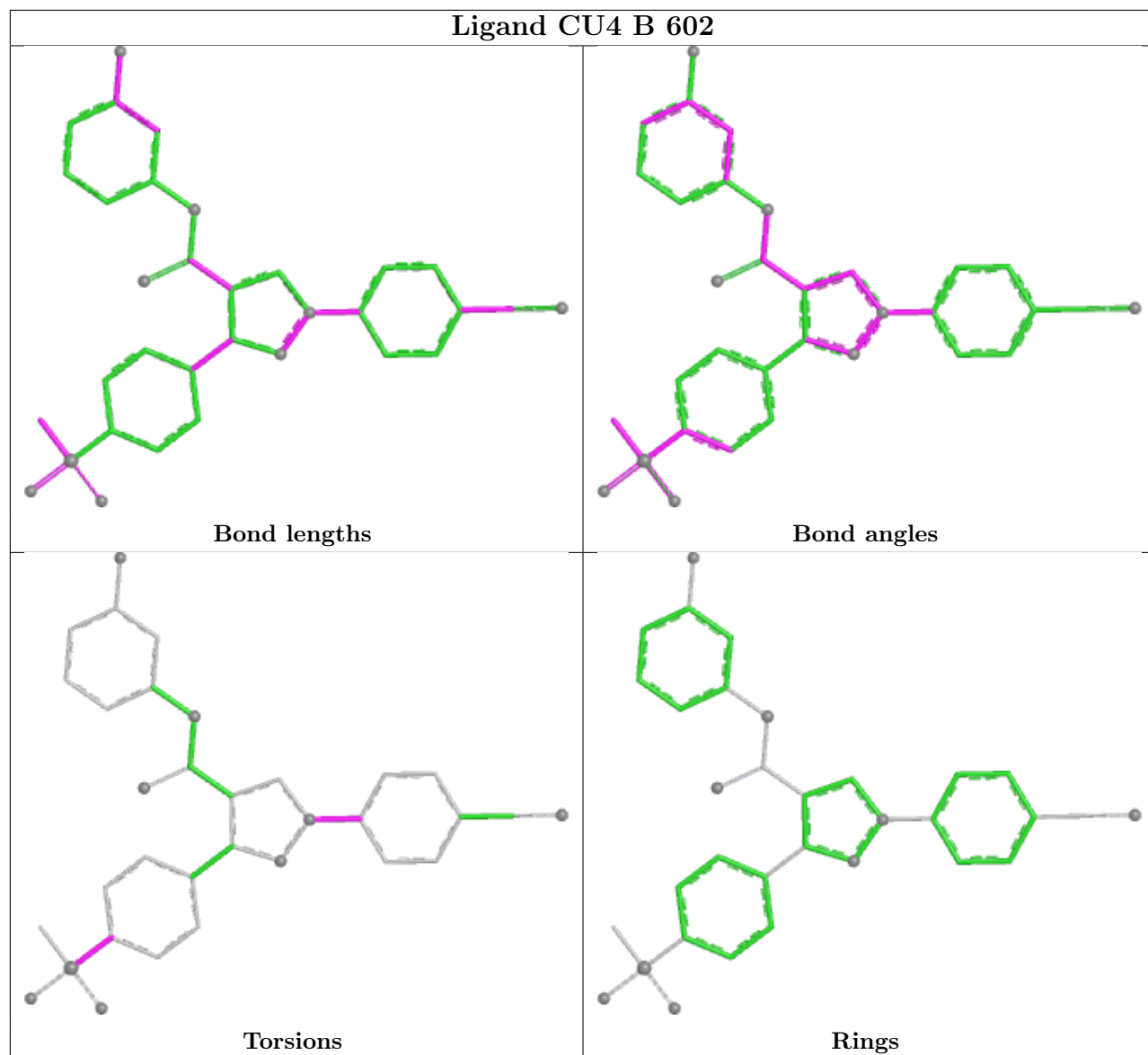
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	NAD	3	0
3	B	602	CU4	1	0
2	C	601	NAD	3	0
2	B	601	NAD	3	0
2	A	601	NAD	4	0

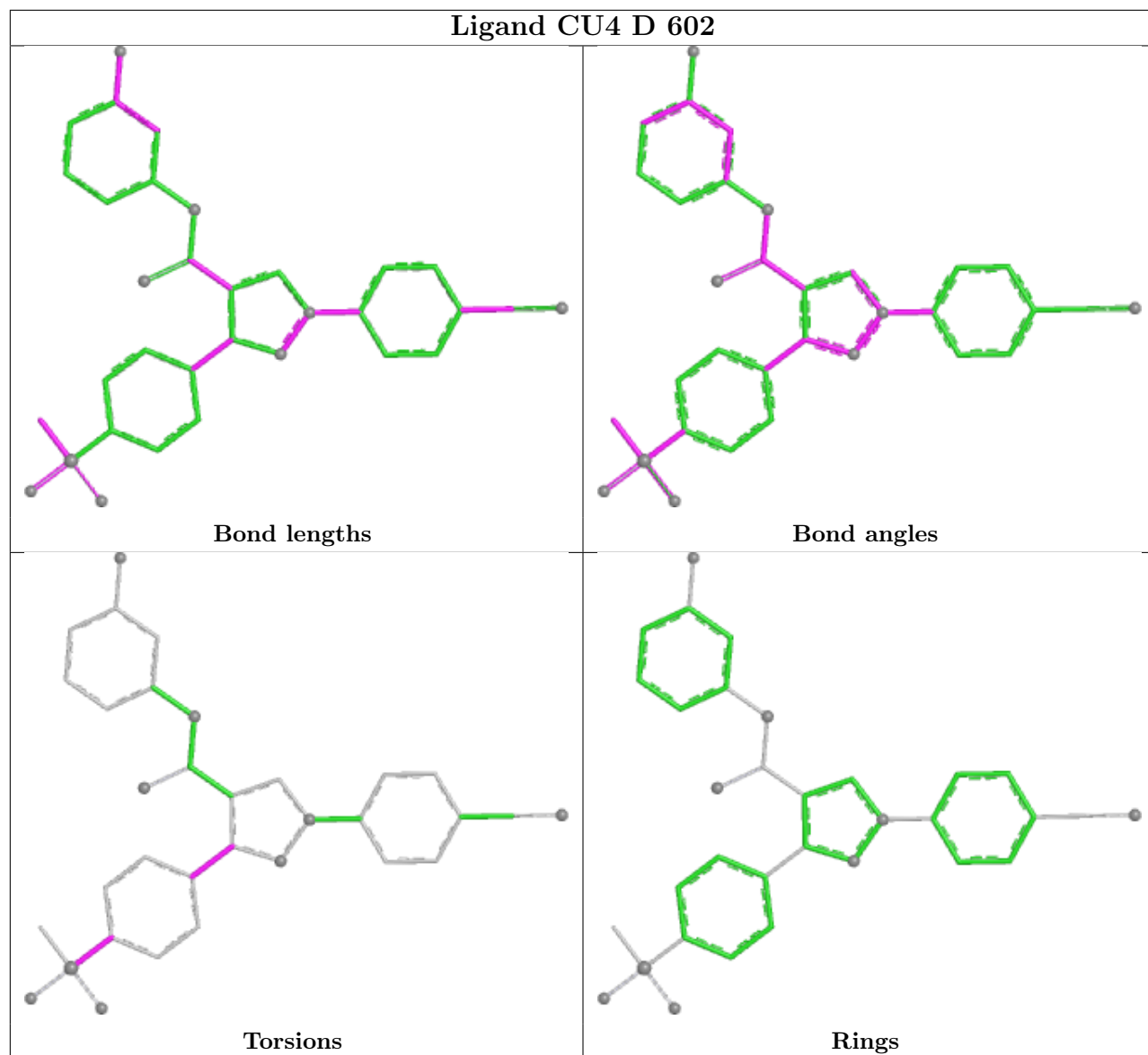
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

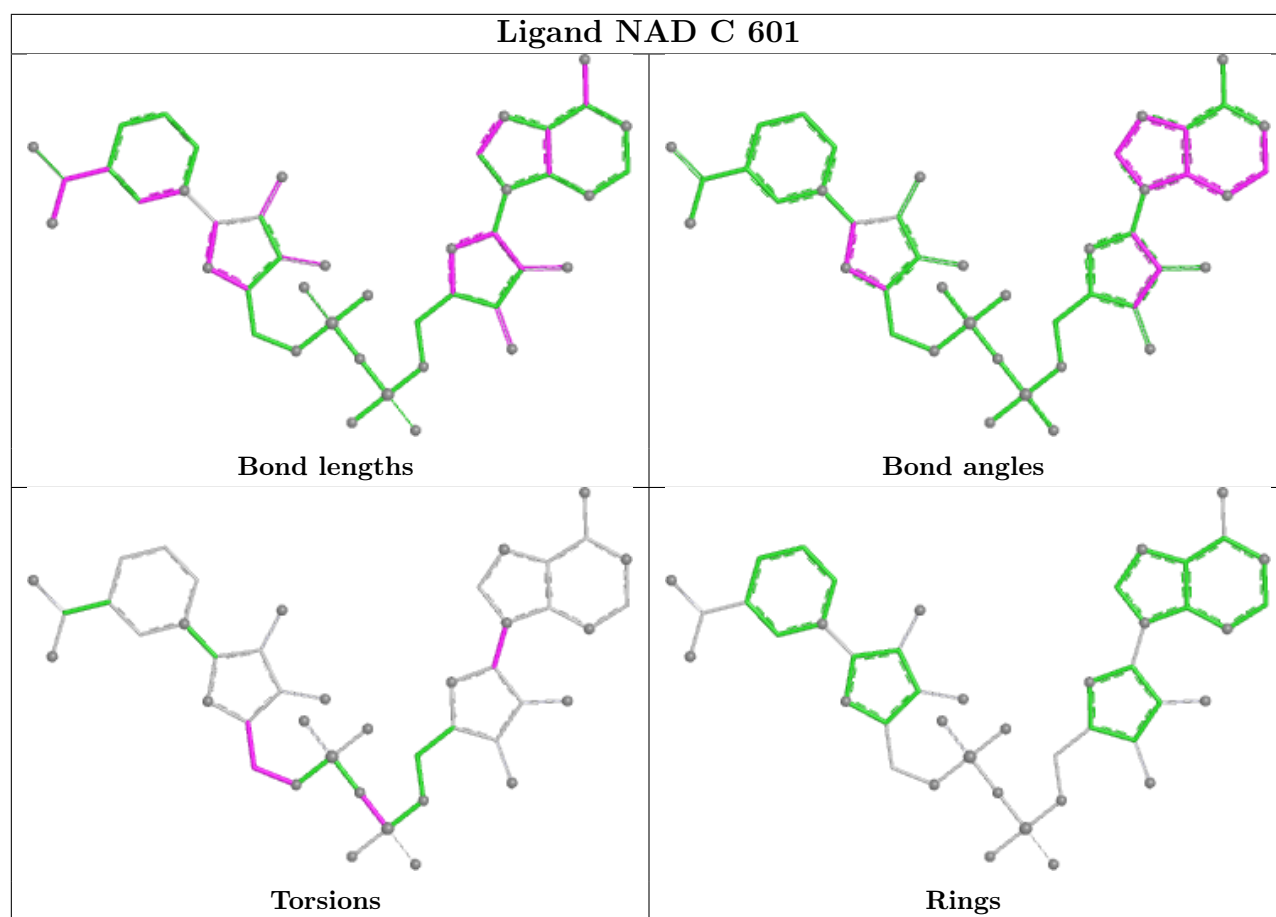


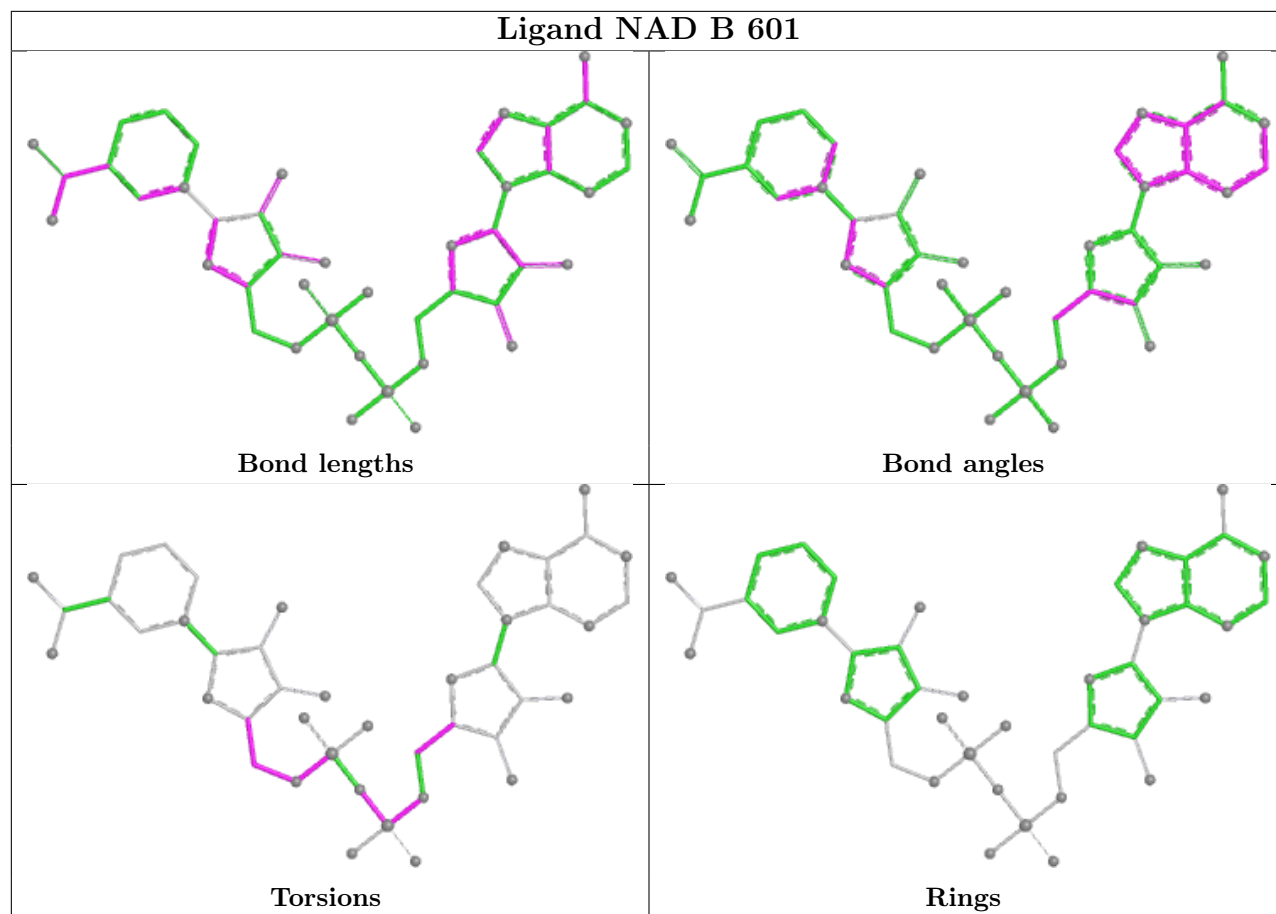


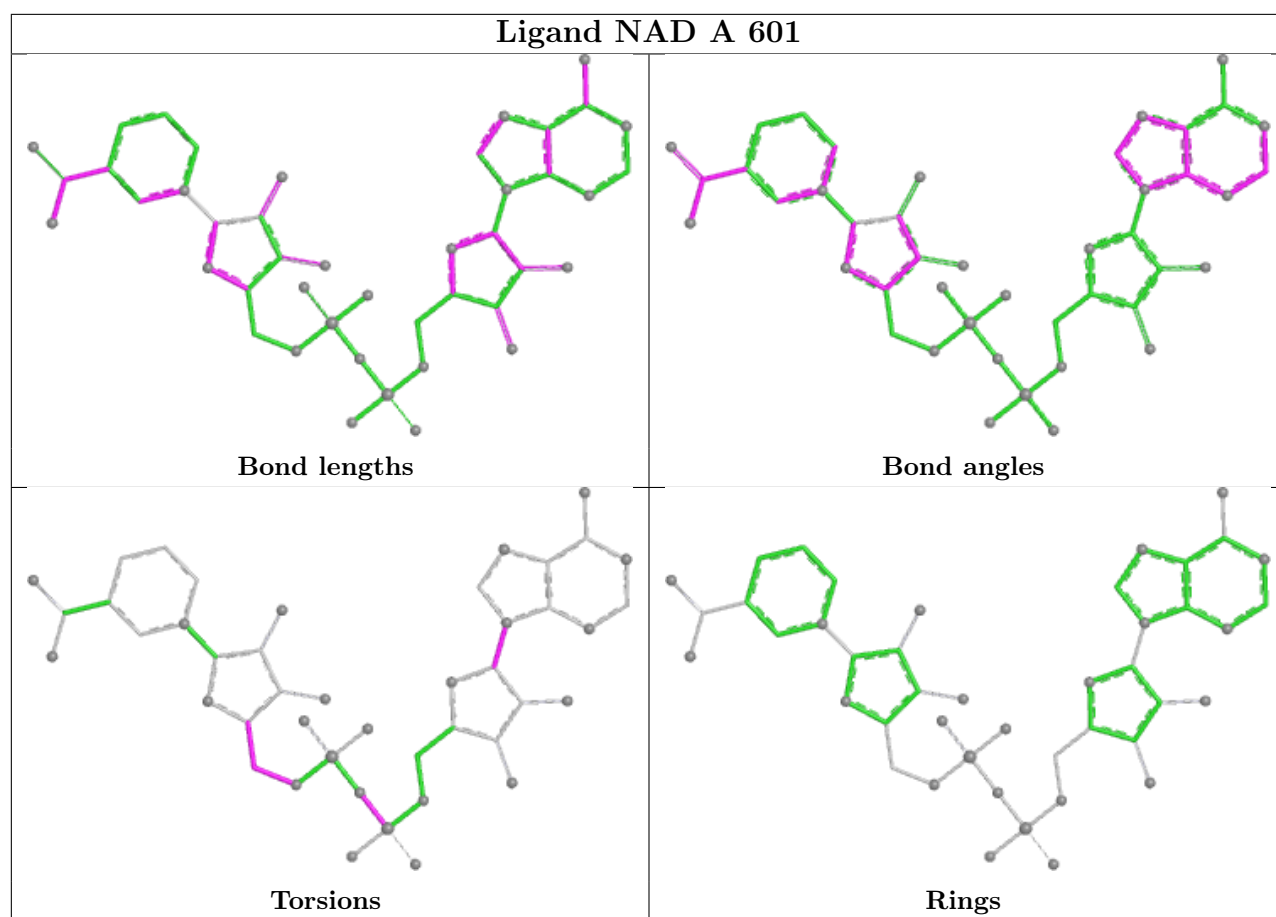












5.7 Other polymers [i](#)

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	492/493 (99%)	0.16	12 (2%) 59 62	22, 35, 49, 65	0
1	B	492/493 (99%)	0.73	45 (9%) 15 16	22, 49, 74, 86	0
1	C	492/493 (99%)	0.58	28 (5%) 29 31	26, 46, 61, 77	0
1	D	492/493 (99%)	0.16	11 (2%) 62 64	20, 34, 49, 64	0
All	All	1968/1972 (99%)	0.41	96 (4%) 35 36	20, 40, 67, 86	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	483	PHE	4.5
1	A	518	SER	4.4
1	B	492	GLY	4.3
1	B	391	GLY	4.1
1	D	419	PHE	3.8
1	A	474	TYR	3.7
1	D	322	ALA	3.6
1	B	483	PHE	3.6
1	B	392	LEU	3.4
1	A	419	PHE	3.4
1	B	419	PHE	3.4
1	B	477	LEU	3.3
1	B	404	PHE	3.3
1	C	518	SER	3.3
1	D	387	CYS	3.2
1	C	484	GLY	3.1
1	B	320	CYS	3.1
1	C	320	CYS	2.9
1	D	319	CYS	2.9
1	A	289	GLY	2.9
1	A	320	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	374	LEU	2.9
1	D	320	CYS	2.9
1	B	476	ALA	2.9
1	C	485	GLY	2.8
1	B	479	ALA	2.8
1	B	491	ASN	2.8
1	B	319	CYS	2.7
1	C	477	LEU	2.7
1	B	326	ILE	2.7
1	D	495	MET	2.7
1	C	289	GLY	2.6
1	C	319	CYS	2.6
1	C	478	ASN	2.6
1	B	403	VAL	2.6
1	B	288	GLY	2.6
1	B	389	GLY	2.6
1	D	496	GLY	2.6
1	B	327	PHE	2.5
1	A	494	GLU	2.5
1	B	311	GLY	2.5
1	B	494	GLU	2.5
1	B	322	ALA	2.5
1	C	324	SER	2.5
1	C	492	GLY	2.5
1	B	518	SER	2.4
1	C	481	SER	2.4
1	B	407	VAL	2.4
1	A	319	CYS	2.4
1	C	405	SER	2.4
1	C	312	VAL	2.4
1	D	27	PRO	2.4
1	A	288	GLY	2.4
1	B	379	VAL	2.4
1	C	35	ILE	2.4
1	B	410	ASP	2.4
1	B	418	ILE	2.4
1	C	314	PHE	2.4
1	D	286	GLU	2.4
1	B	31	PRO	2.3
1	B	481	SER	2.3
1	B	312	VAL	2.3
1	B	486	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	476	ALA	2.3
1	B	502	GLU	2.3
1	C	57	VAL	2.3
1	B	393	GLY	2.3
1	B	356	THR	2.3
1	C	494	GLU	2.3
1	C	404	PHE	2.2
1	C	486	PHE	2.2
1	D	481	SER	2.2
1	C	495	MET	2.2
1	B	408	THR	2.2
1	B	349	VAL	2.2
1	B	336	PHE	2.2
1	C	475	ASN	2.2
1	A	27	PRO	2.2
1	B	420	GLY	2.2
1	B	371	ILE	2.1
1	B	425	ILE	2.1
1	C	322	ALA	2.1
1	C	418	ILE	2.1
1	C	27	PRO	2.1
1	B	387	CYS	2.1
1	B	489	SER	2.1
1	B	495	MET	2.1
1	C	379	VAL	2.1
1	B	428	PHE	2.1
1	B	333	TYR	2.1
1	C	349	VAL	2.1
1	A	323	GLY	2.1
1	C	299	ALA	2.0
1	A	491	ASN	2.0
1	B	332	ILE	2.0
1	A	312	VAL	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 oligosaccharides in this entry.

6.4 Ligands

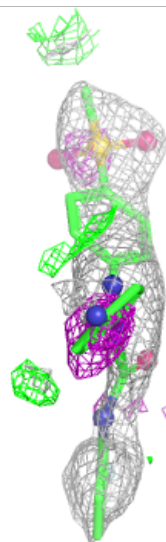
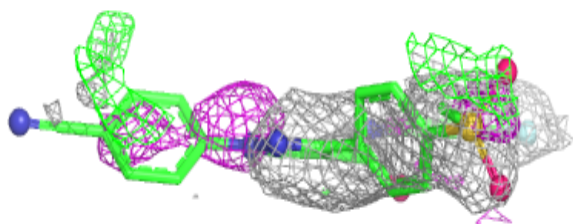
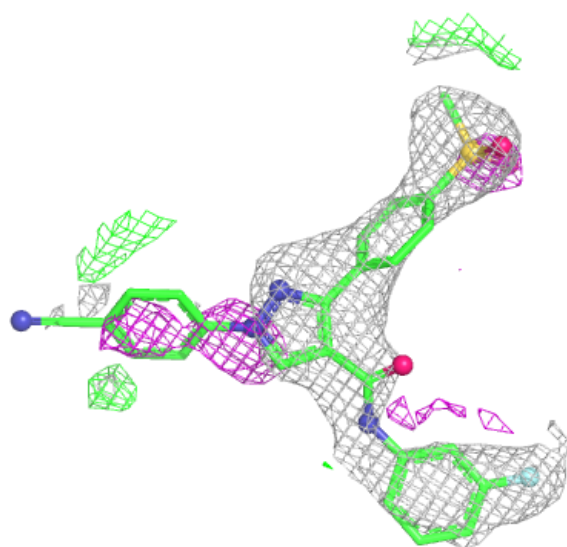
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CU4	B	602	33/33	0.68	0.20	58,73,83,83	0
3	CU4	D	602	33/33	0.82	0.14	40,50,60,70	0
3	CU4	C	602	33/33	0.83	0.14	50,61,68,74	0
2	NAD	D	601	44/44	0.84	0.17	24,48,64,66	0
2	NAD	B	601	44/44	0.87	0.12	39,59,69,71	0
3	CU4	A	602	33/33	0.88	0.13	44,52,58,62	0
2	NAD	C	601	44/44	0.89	0.11	36,50,64,65	0
2	NAD	A	601	44/44	0.91	0.12	25,43,57,61	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.

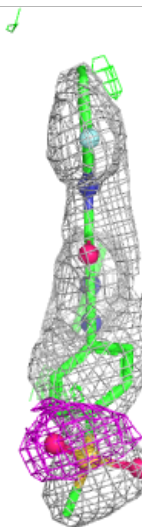
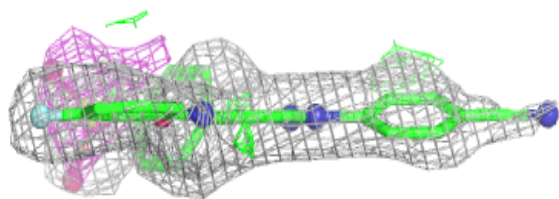
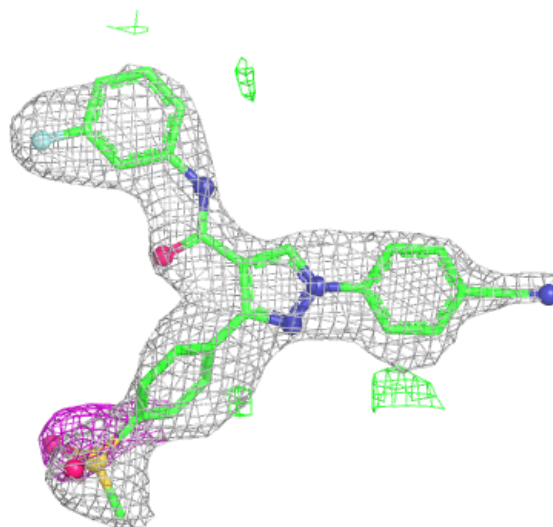
Electron density around CU4 B 602:

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



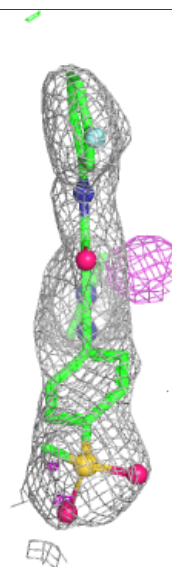
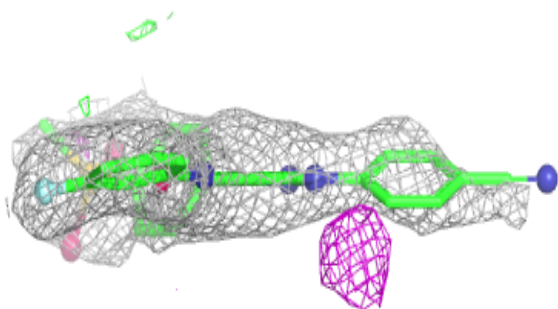
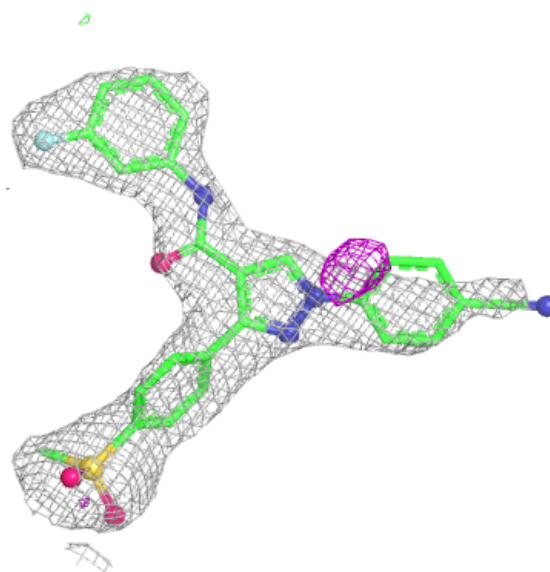
Electron density around CU4 D 602:

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



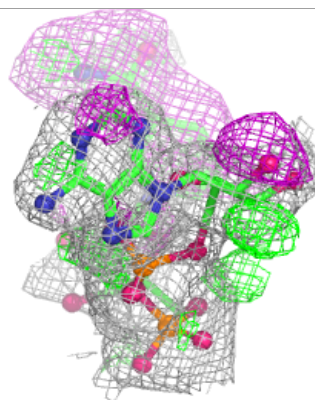
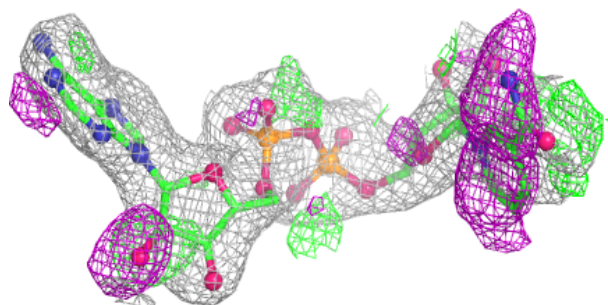
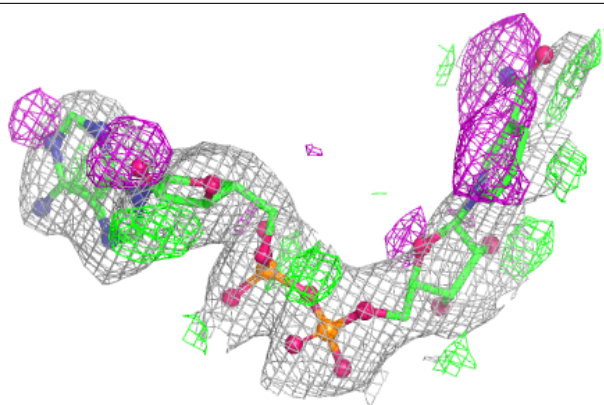
Electron density around CU4 C 602:

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

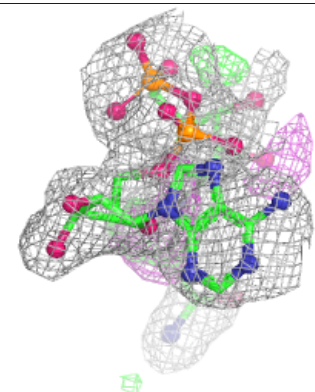
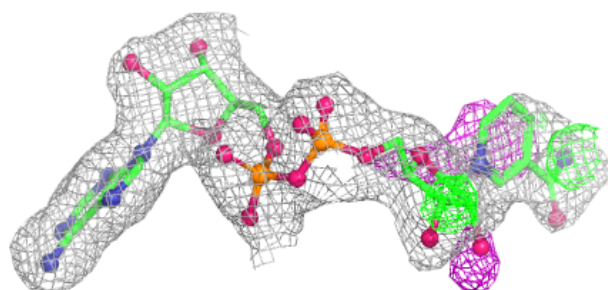
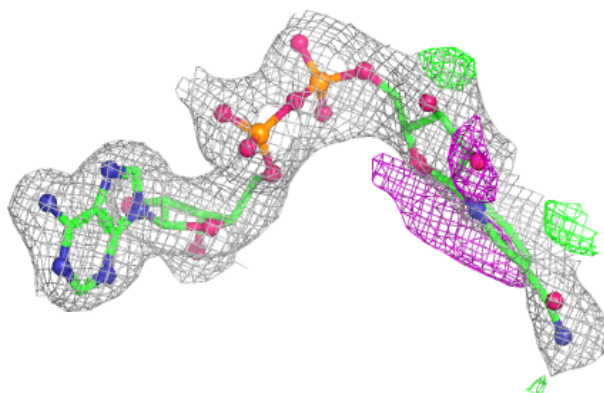


Electron density around NAD D 601:

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

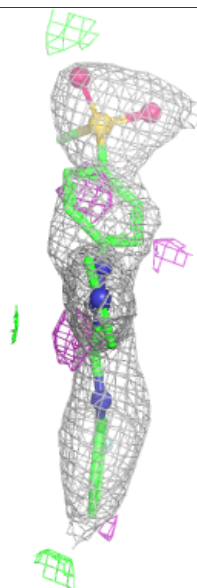
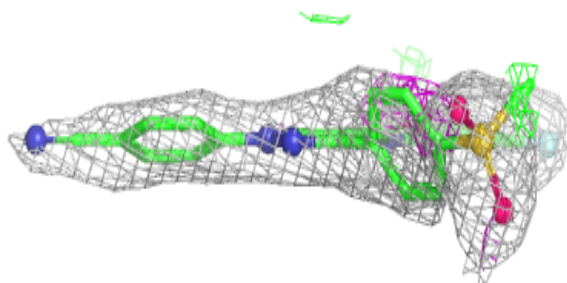
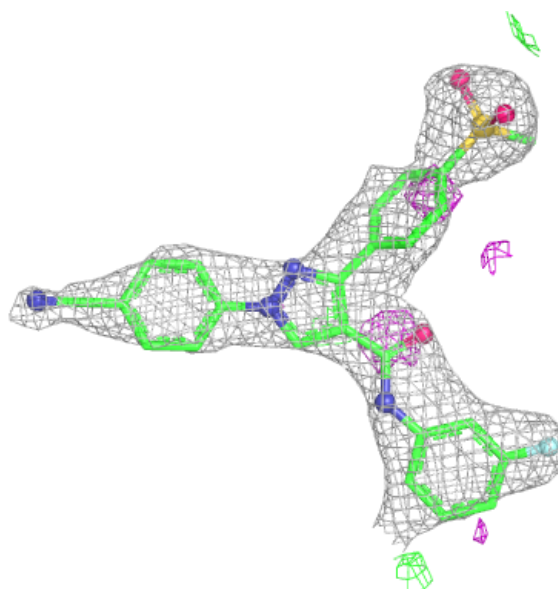
**Electron density around NAD B 601:**

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



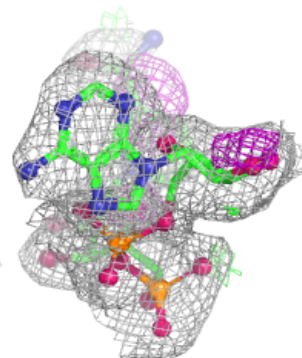
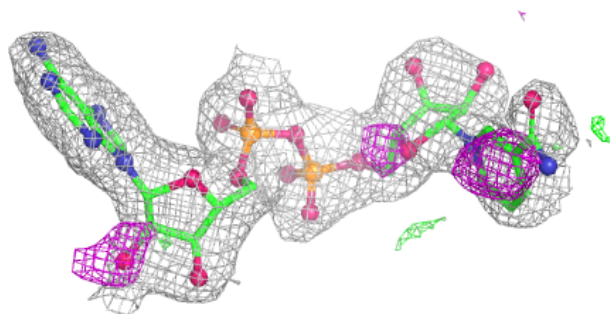
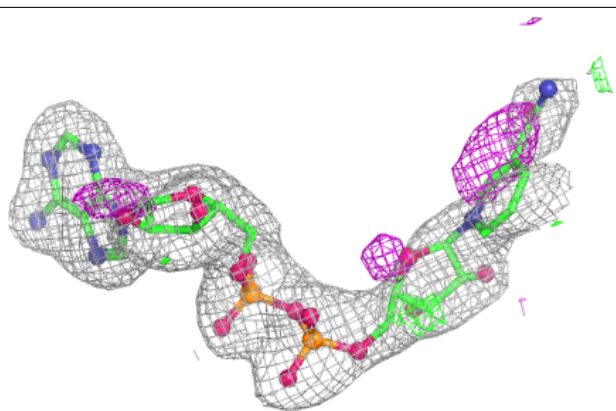
Electron density around CU4 A 602:

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

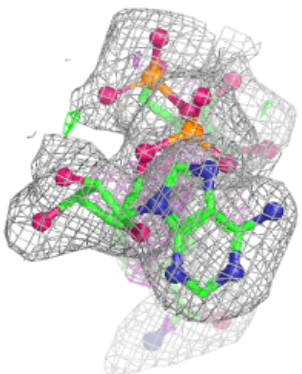
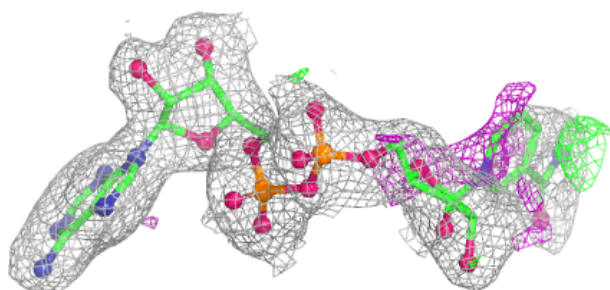
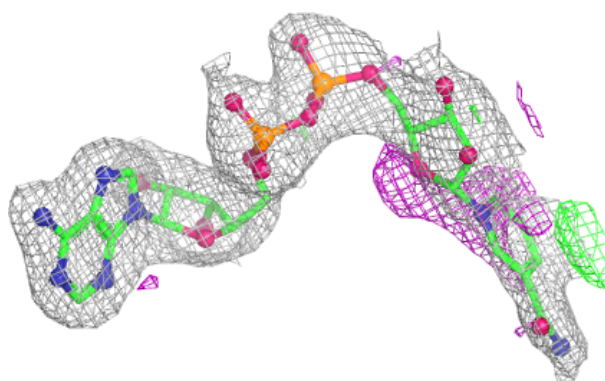


Electron density around NAD C 601:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.