



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:24 AM UTC

PDB ID : 6TGW / pdb_00006tgw
Title : Crystal structure of human Aldehyde dehydrogenase 1A3 in complex with a selective inhibitor
Authors : Garavaglia, S.; Rizzi, M.
Deposited on : 2019-11-18
Resolution : 2.80 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

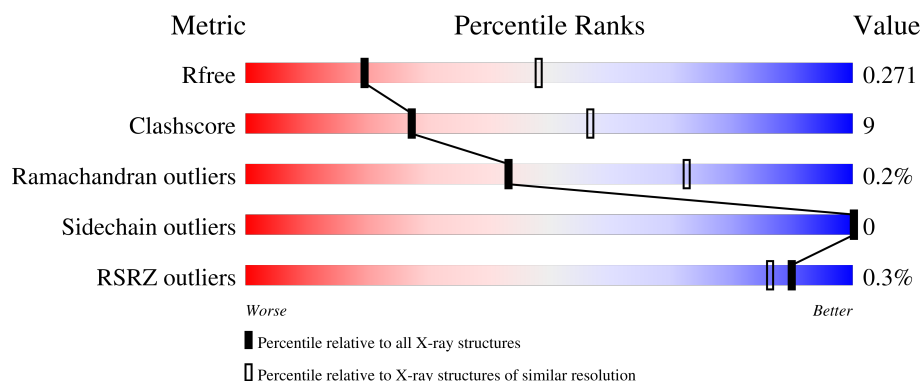
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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.

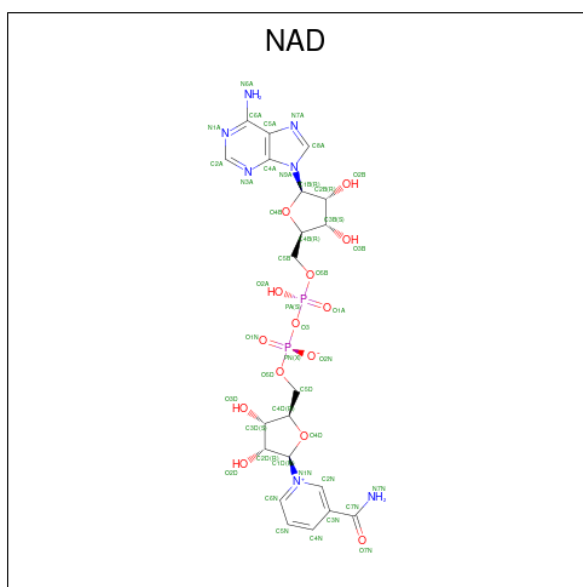
Mol	Chain	Length	Quality of chain
1	A	512	
1	B	512	
1	C	512	
1	D	512	

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 Aldehyde dehydrogenase family 1 member A3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total 3689	C 2354	N 627	O 688	S 20	0	0	0
1	B	478	Total 3689	C 2354	N 627	O 688	S 20	0	0	0
1	C	479	Total 3698	C 2358	N 629	O 691	S 20	0	0	0
1	D	478	Total 3689	C 2352	N 627	O 690	S 20	0	0	0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



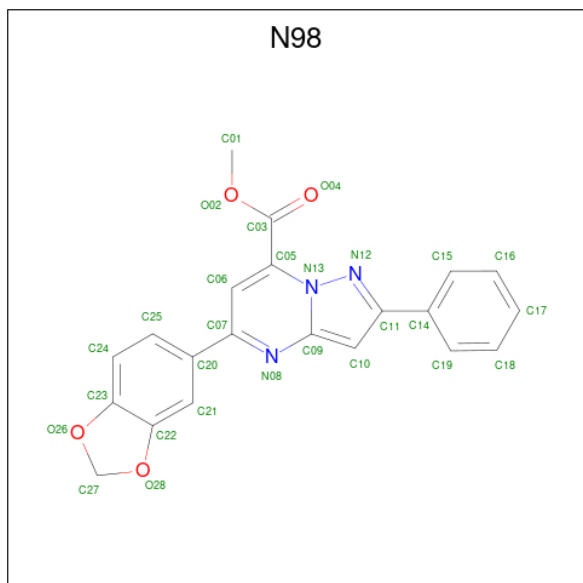
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 methyl 5-(1,3-benzodioxol-5-yl)-2-phenyl-pyrazolo[1,5-a]pyrimidine-7-carboxylate (CCD ID: N98) (formula: C₂₁H₁₅N₃O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	21	3	4		
3	B	1	Total	C	N	O	0	0
			28	21	3	4		
3	C	1	Total	C	N	O	0	0
			28	21	3	4		
3	D	1	Total	C	N	O	0	0
			28	21	3	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	B	52	Total	O	0	0
			52	52		
4	C	73	Total	O	0	0
			73	73		

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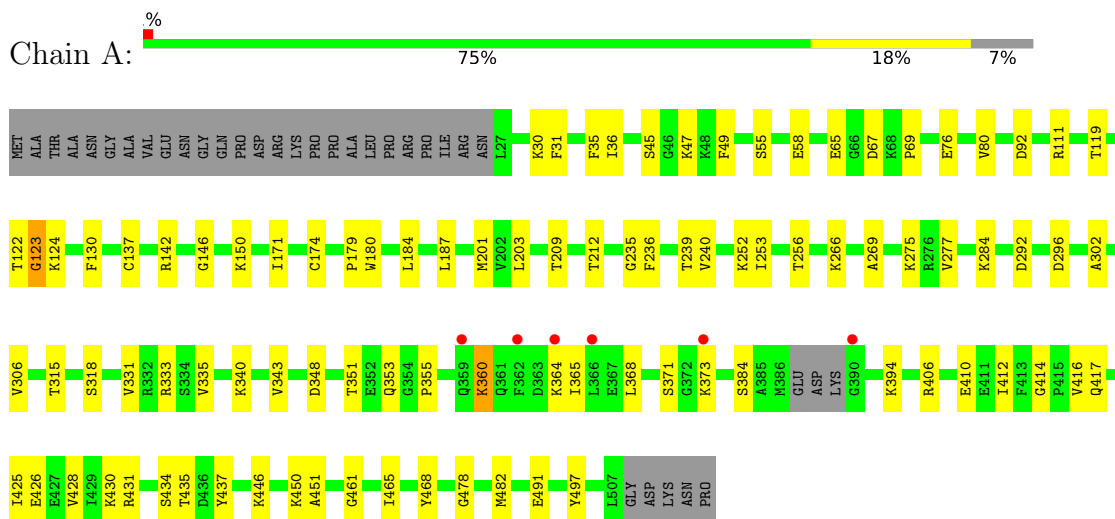
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	70	Total	O	0	0
			70	70		

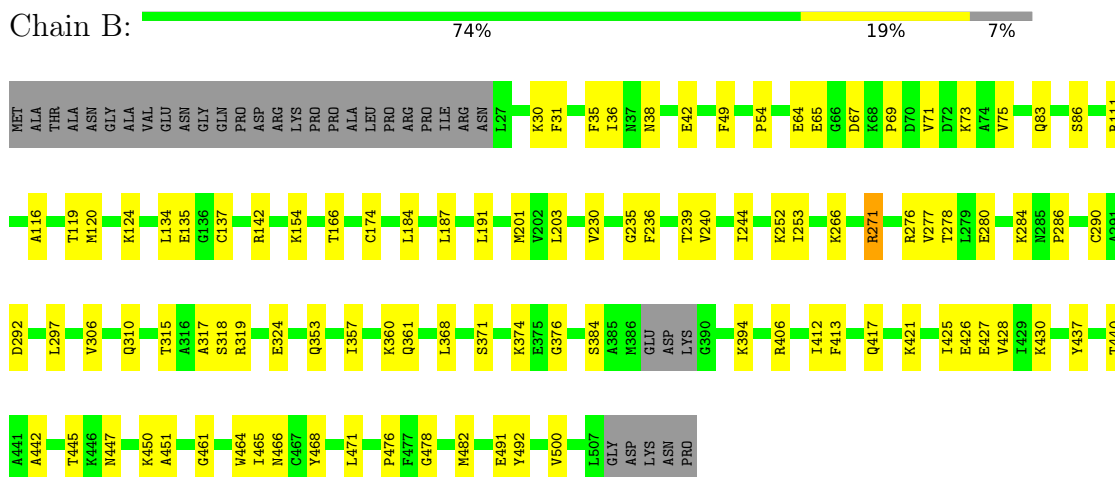
3 Residue-property plots

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: Aldehyde dehydrogenase family 1 member A3

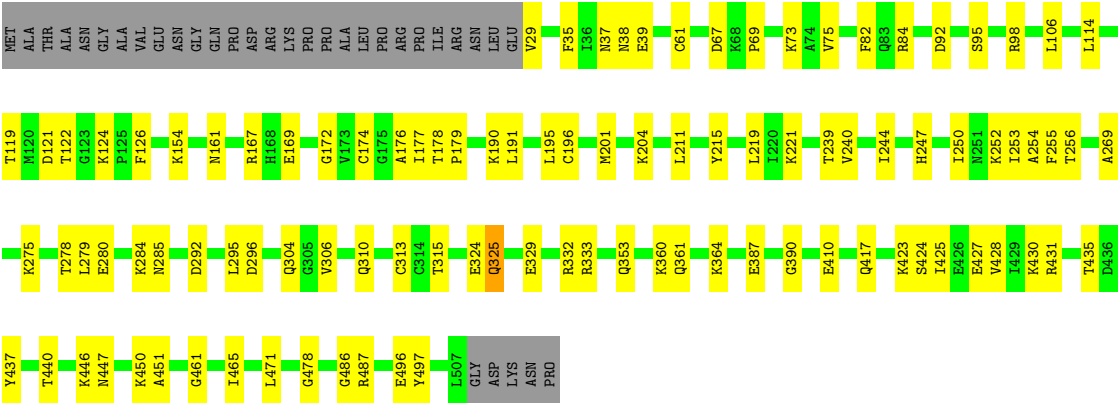


- Molecule 1: Aldehyde dehydrogenase family 1 member A3

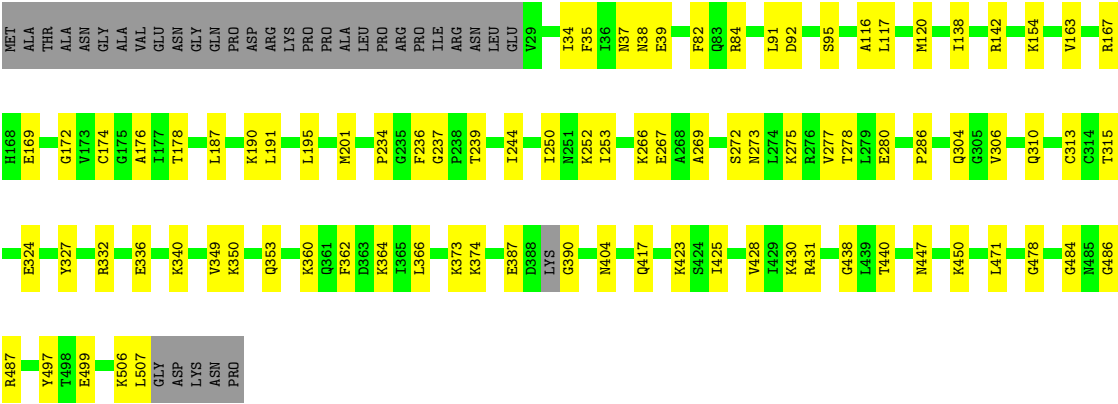


- Molecule 1: Aldehyde dehydrogenase family 1 member A3





- Molecule 1: Aldehyde dehydrogenase family 1 member A3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.03Å 158.47Å 168.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.02 – 2.80 47.02 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.02-2.80) 97.4 (47.02-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.201 , 0.274 0.197 , 0.271	Depositor DCC
R_{free} test set	2634 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15310	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 55.78 % 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 3.0090e-05. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, N98

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	0.47	3/3764 (0.1%)	0.63	5/5092 (0.1%)
1	B	0.46	1/3764 (0.0%)	0.66	1/5092 (0.0%)
1	C	0.39	0/3774	0.58	1/5106 (0.0%)
1	D	0.42	1/3764 (0.0%)	0.58	0/5092
All	All	0.44	5/15066 (0.0%)	0.62	7/20382 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	271	ARG	CB-CG	-9.50	1.24	1.52
1	A	360	LYS	CE-NZ	-8.36	1.24	1.49
1	A	360	LYS	CD-CE	-7.34	1.30	1.52
1	D	236	PHE	CB-CG	6.63	1.65	1.50
1	A	58	GLU	CB-CG	-5.96	1.34	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	ARG	CG-CD-NE	-15.07	78.84	112.00
1	A	58	GLU	CA-CB-CG	-11.70	90.70	114.10
1	A	123	GLY	CA-C-N	7.05	130.51	120.49
1	A	123	GLY	C-N-CA	7.05	130.51	120.49
1	C	325	GLN	CA-CB-CG	-6.99	100.13	114.10
1	A	360	LYS	CG-CD-CE	-6.10	97.27	111.30
1	A	360	LYS	CA-CB-CG	-5.26	103.58	114.10

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	3689	0	3716	65	0
1	B	3689	0	3716	87	1
1	C	3698	0	3723	69	1
1	D	3689	0	3706	68	0
2	A	44	0	25	3	0
2	B	44	0	25	1	0
2	C	44	0	24	1	0
2	D	44	0	23	4	0
3	A	28	0	0	0	0
3	B	28	0	0	1	0
3	C	28	0	0	3	0
3	D	28	0	0	3	0
4	A	62	0	0	2	0
4	B	52	0	0	2	0
4	C	73	0	0	0	0
4	D	70	0	0	1	0
All	All	15310	0	14958	272	1

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 9.

All (272) 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)
2:B:602:NAD:C1D	2:B:602:NAD:O4D	1.63	1.23
2:D:601:NAD:O4D	2:D:601:NAD:C1D	1.64	1.17
1:B:466:ASN:O	1:D:506:LYS:HE3	1.54	1.07
1:B:142:ARG:HD3	1:C:98:ARG:HH12	1.41	0.85
1:B:271:ARG:NH2	1:D:267:GLU:OE2	2.12	0.82
1:B:142:ARG:HD3	1:C:98:ARG:NH1	1.97	0.79
1:B:466:ASN:O	1:D:506:LYS:CE	2.31	0.77
1:A:266:LYS:HG3	1:A:277:VAL:HG11	1.67	0.76
1:B:324:GLU:HG3	1:B:421:LYS:HE2	1.68	0.75
1:A:426:GLU:OE2	1:C:84:ARG:NH2	2.20	0.75
1:A:360:LYS:HE3	1:A:364:LYS:NZ	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ILE:HG21	1:A:416:VAL:HB	1.74	0.70
1:B:368:LEU:O	1:B:371:SER:HB3	1.92	0.70
1:C:98:ARG:HH11	1:C:98:ARG:HG2	1.56	0.69
1:D:266:LYS:HG3	1:D:277:VAL:HG11	1.75	0.68
1:A:184:LEU:HB2	1:A:212:THR:HG21	1.75	0.68
1:B:284:LYS:NZ	1:B:318:SER:HB2	2.09	0.68
1:C:329:GLU:OE1	1:C:332:ARG:NH1	2.28	0.66
1:B:437:TYR:CD1	1:B:482:MET:HB2	2.31	0.65
1:B:297:LEU:HD21	1:D:506:LYS:HZ1	1.61	0.65
1:A:360:LYS:HE3	1:A:364:LYS:HZ1	1.61	0.64
1:D:425:ILE:O	1:D:428:VAL:HG12	1.98	0.64
1:B:142:ARG:CZ	1:C:98:ARG:HH22	2.11	0.64
1:A:296:ASP:OD1	1:A:333:ARG:NH1	2.31	0.64
1:B:142:ARG:CD	1:C:98:ARG:NH1	2.60	0.64
1:B:266:LYS:HG3	1:B:277:VAL:HG11	1.80	0.63
1:B:361:GLN:NE2	1:B:413:PHE:HD2	1.96	0.63
1:B:284:LYS:HZ3	1:B:318:SER:HB2	1.64	0.63
1:B:297:LEU:CD2	1:D:506:LYS:HZ1	2.12	0.63
1:C:424:SER:HB3	1:C:427:GLU:HB3	1.80	0.62
1:D:304:GLN:HB3	3:D:602:N98:C18	2.29	0.62
1:D:349:VAL:HG13	1:D:350:LYS:HG2	1.81	0.62
1:D:486:GLY:O	1:D:487:ARG:NH1	2.31	0.62
1:B:297:LEU:CD2	1:D:506:LYS:NZ	2.62	0.62
1:A:252:LYS:NZ	4:A:702:HOH:O	2.25	0.62
1:B:252:LYS:NZ	1:B:278:THR:OG1	2.33	0.62
1:B:466:ASN:HB3	1:D:506:LYS:HZ1	1.65	0.61
1:B:437:TYR:HD1	1:B:482:MET:HB2	1.64	0.61
1:B:142:ARG:CZ	1:C:98:ARG:NH2	2.64	0.61
1:C:313:CYS:HG	1:C:315:THR:HG1	1.48	0.61
1:A:142:ARG:NH1	4:A:705:HOH:O	2.34	0.60
1:B:297:LEU:HD21	1:D:506:LYS:NZ	2.17	0.60
1:D:252:LYS:NZ	1:D:278:THR:OG1	2.35	0.60
1:A:180:TRP:NE1	2:A:601:NAD:O5D	2.36	0.59
1:C:167:ARG:NH1	1:C:169:GLU:OE2	2.35	0.59
1:A:302:ALA:O	1:A:306:VAL:HG23	2.03	0.59
1:C:435:THR:HB	1:C:437:TYR:H	1.68	0.58
1:C:176:ALA:HB1	1:C:190:LYS:HD2	1.85	0.58
1:C:361:GLN:HA	1:C:364:LYS:HG3	1.86	0.58
1:A:239:THR:HG23	1:A:240:VAL:HG23	1.86	0.58
1:C:121:ASP:OD2	1:C:211:LEU:HG	2.03	0.58
1:B:286:PRO:HD2	1:B:440:THR:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:GLN:HB3	3:C:602:N98:C17	2.35	0.57
1:A:137:CYS:SG	1:A:184:LEU:HG	2.45	0.56
1:D:324:GLU:HA	1:D:327:TYR:HB2	1.87	0.56
1:C:174:CYS:O	1:C:201:MET:HA	2.05	0.56
1:D:374:LYS:HD2	1:D:374:LYS:O	2.04	0.56
1:D:35:PHE:CZ	1:D:38:ASN:HA	2.41	0.56
1:A:431:ARG:O	1:A:434:SER:HB3	2.06	0.56
1:A:284:LYS:NZ	1:A:318:SER:HB2	2.20	0.56
1:A:368:LEU:O	1:A:371:SER:OG	2.23	0.56
1:A:360:LYS:HG3	1:A:364:LYS:HE3	1.88	0.55
1:C:292:ASP:O	1:C:446:LYS:HG3	2.06	0.55
1:C:471:LEU:HD12	3:C:602:N98:C06	2.36	0.55
1:B:142:ARG:NE	1:C:98:ARG:NH2	2.54	0.55
1:C:284:LYS:HE3	1:C:410:GLU:O	2.05	0.55
1:C:82:PHE:CZ	1:C:172:GLY:HA2	2.42	0.55
1:B:461:GLY:HA3	1:B:478:GLY:O	2.07	0.54
1:B:235:GLY:HA3	1:B:240:VAL:HG21	1.88	0.54
1:A:67:ASP:HB3	1:A:69:PRO:HD2	1.87	0.54
1:D:117:LEU:HD23	1:D:120:MET:HE2	1.89	0.54
1:D:280:GLU:OE1	1:D:478:GLY:HA2	2.08	0.54
1:C:252:LYS:NZ	1:C:278:THR:OG1	2.36	0.54
1:B:427:GLU:O	1:B:430:LYS:HG2	2.08	0.54
1:D:82:PHE:CZ	1:D:172:GLY:HA2	2.43	0.54
1:A:425:ILE:O	1:A:428:VAL:HG12	2.08	0.53
1:C:304:GLN:HB3	3:C:602:N98:C18	2.39	0.53
1:A:435:THR:HB	1:A:437:TYR:H	1.73	0.53
1:B:119:THR:HG23	1:B:124:LYS:O	2.08	0.53
1:B:425:ILE:HD11	1:B:450:LYS:HD3	1.90	0.53
1:D:178:THR:HG22	1:D:190:LYS:HE2	1.91	0.53
1:B:239:THR:HG23	1:B:240:VAL:HG23	1.90	0.52
1:C:177:ILE:HD12	1:C:253:ILE:HD11	1.92	0.52
1:A:384:SER:OG	1:A:394:LYS:HE2	2.09	0.52
1:C:191:LEU:HA	1:C:201:MET:SD	2.50	0.52
1:C:285:ASN:HB3	1:C:440:THR:O	2.10	0.52
1:D:324:GLU:CD	1:D:423:LYS:HZ2	2.18	0.52
1:D:163:VAL:HG23	1:D:507:LEU:HD11	1.92	0.51
1:B:360:LYS:C	1:B:360:LYS:HD3	2.33	0.51
1:A:331:VAL:O	1:A:335:VAL:HG23	2.11	0.51
1:B:290:CYS:HB3	1:B:450:LYS:HZ3	1.76	0.51
1:B:191:LEU:HA	1:B:201:MET:SD	2.51	0.51
1:D:244:ILE:HG23	1:D:250:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:GLN:HG3	1:C:353:GLN:HG3	1.93	0.51
1:D:404:ASN:N	1:D:404:ASN:OD1	2.44	0.51
1:D:387:GLU:O	1:D:390:GLY:HA3	2.10	0.50
1:A:360:LYS:O	1:A:364:LYS:HG2	2.11	0.50
1:D:116:ALA:O	1:D:120:MET:HG3	2.10	0.50
1:D:252:LYS:HE2	1:D:497:TYR:CZ	2.47	0.50
1:A:30:LYS:HD3	1:A:31:PHE:CZ	2.47	0.50
1:A:425:ILE:HD11	1:A:450:LYS:HD3	1.92	0.50
1:C:296:ASP:OD2	1:C:333:ARG:NH1	2.45	0.50
1:B:360:LYS:HD3	1:B:360:LYS:O	2.12	0.50
1:A:340:LYS:O	1:A:340:LYS:HG3	2.11	0.50
1:B:297:LEU:HD22	1:D:506:LYS:NZ	2.26	0.50
1:B:166:THR:CG2	1:B:500:VAL:HG13	2.42	0.50
1:A:269:ALA:HB1	1:A:275:LYS:HG3	1.94	0.49
1:B:154:LYS:NZ	4:B:705:HOH:O	2.45	0.49
1:D:362:PHE:CE2	1:D:366:LEU:HD11	2.47	0.49
1:B:284:LYS:HD3	1:B:318:SER:OG	2.13	0.49
1:B:292:ASP:OD1	1:B:445:THR:OG1	2.25	0.49
1:D:191:LEU:HA	1:D:201:MET:SD	2.52	0.49
1:C:451:ALA:HB1	1:C:465:ILE:HD13	1.95	0.49
1:B:71:VAL:O	1:B:75:VAL:HG23	2.13	0.49
1:A:315:THR:O	1:A:468:TYR:OH	2.28	0.49
1:C:37:ASN:O	1:C:39:GLU:HG3	2.13	0.49
1:A:360:LYS:O	1:A:364:LYS:HE3	2.13	0.49
1:A:235:GLY:HA3	1:A:240:VAL:HG21	1.93	0.49
1:C:98:ARG:NH1	1:C:98:ARG:HG2	2.22	0.49
1:D:387:GLU:O	1:D:387:GLU:HG3	2.12	0.49
1:D:447:ASN:HB3	1:D:450:LYS:HB2	1.95	0.48
1:A:292:ASP:O	1:A:446:LYS:HG3	2.12	0.48
1:B:306:VAL:HG11	1:B:417:GLN:HB2	1.95	0.48
1:D:269:ALA:HB1	1:D:275:LYS:HG3	1.95	0.48
1:A:55:SER:HA	1:A:355:PRO:HG3	1.95	0.48
1:B:280:GLU:HG3	4:B:737:HOH:O	2.14	0.48
1:A:45:SER:OG	1:A:47:LYS:HG3	2.13	0.48
1:B:166:THR:HG21	1:B:500:VAL:HG13	1.95	0.48
1:A:123:GLY:O	1:A:355:PRO:HD2	2.15	0.47
1:A:491:GLU:OE1	1:C:154:LYS:HE2	2.14	0.47
1:B:49:PHE:HD1	1:B:65:GLU:HB2	1.79	0.47
1:A:119:THR:HG23	1:A:124:LYS:O	2.15	0.47
1:A:348:ASP:HB3	1:A:351:THR:OG1	2.14	0.47
1:B:111:ARG:NH2	1:B:135:GLU:OE2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:GLU:HA	1:B:64:GLU:HG3	1.96	0.47
1:A:49:PHE:HD1	1:A:65:GLU:HB2	1.79	0.47
1:A:406:ARG:HD2	1:A:410:GLU:OE2	2.15	0.47
1:B:317:ALA:HB2	1:B:468:TYR:CZ	2.50	0.47
1:C:324:GLU:C	1:C:325:GLN:HG3	2.33	0.47
1:C:92:ASP:OD1	1:C:95:SER:OG	2.13	0.47
1:D:34:ILE:HG12	1:D:234:PRO:HD2	1.97	0.46
1:C:387:GLU:HB2	1:C:390:GLY:H	1.80	0.46
1:A:239:THR:HG23	1:A:240:VAL:N	2.30	0.46
1:A:284:LYS:HZ2	1:A:318:SER:HB2	1.79	0.46
2:A:601:NAD:H2N	2:A:601:NAD:H2D	1.60	0.46
2:A:601:NAD:H8A	2:A:601:NAD:H2B	1.83	0.46
1:B:54:PRO:HB3	1:B:357:ILE:O	2.16	0.46
1:C:486:GLY:O	1:C:487:ARG:NH1	2.44	0.46
1:D:252:LYS:HE2	1:D:497:TYR:CE1	2.51	0.46
1:B:271:ARG:CZ	1:D:267:GLU:OE2	2.64	0.46
1:C:204:LYS:O	1:C:204:LYS:HG3	2.15	0.46
1:C:239:THR:HG22	1:C:240:VAL:N	2.30	0.46
1:B:35:PHE:C	1:B:36:ILE:HG13	2.40	0.46
1:B:361:GLN:HE21	1:B:413:PHE:HD2	1.63	0.46
1:B:471:LEU:HD12	3:B:601:N98:C06	2.45	0.46
1:B:203:LEU:HD13	1:B:230:VAL:HG13	1.98	0.46
1:C:67:ASP:HB3	1:C:69:PRO:HD2	1.98	0.46
1:A:171:ILE:HG13	1:A:497:TYR:C	2.41	0.46
1:A:174:CYS:O	1:A:201:MET:HA	2.15	0.46
1:C:178:THR:HG22	1:C:190:LYS:HE2	1.99	0.45
1:C:195:LEU:HD23	1:C:195:LEU:HA	1.58	0.45
1:C:430:LYS:HG3	1:C:431:ARG:N	2.30	0.45
1:D:304:GLN:HA	1:D:304:GLN:HE21	1.81	0.45
1:A:252:LYS:HG2	1:A:253:ILE:N	2.32	0.45
1:C:35:PHE:CZ	1:C:38:ASN:HA	2.52	0.45
1:A:306:VAL:HG11	1:A:417:GLN:HB2	1.98	0.45
1:B:236:PHE:HB2	1:B:239:THR:HG22	1.99	0.45
1:B:284:LYS:HD2	1:B:319:ARG:HG3	1.98	0.45
1:A:187:LEU:HD11	1:A:203:LEU:HD13	1.98	0.45
1:A:461:GLY:HA3	1:A:478:GLY:O	2.17	0.45
1:B:35:PHE:O	1:B:36:ILE:HG13	2.15	0.45
1:B:116:ALA:O	1:B:120:MET:HG3	2.17	0.45
1:B:447:ASN:HB3	1:B:450:LYS:HB2	1.98	0.45
1:D:138:ILE:O	1:D:142:ARG:HG3	2.17	0.45
1:C:73:LYS:HB3	1:C:73:LYS:HE2	1.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:SER:OG	1:D:273:ASN:N	2.45	0.45
1:B:425:ILE:O	1:B:428:VAL:HG12	2.17	0.45
1:B:187:LEU:HG	1:B:203:LEU:HD23	1.98	0.45
1:B:371:SER:OG	1:B:406:ARG:HB2	2.17	0.45
1:C:122:THR:OG1	1:C:124:LYS:HB2	2.17	0.45
1:B:466:ASN:HB3	1:D:506:LYS:NZ	2.31	0.45
1:B:244:ILE:HG22	1:B:253:ILE:HD12	1.99	0.44
1:C:425:ILE:O	1:C:428:VAL:HG12	2.16	0.44
1:C:306:VAL:HG11	1:C:417:GLN:HB2	2.00	0.44
1:B:368:LEU:HD13	1:B:412:ILE:HG12	1.99	0.44
1:C:252:LYS:HE2	1:C:496:GLU:O	2.17	0.44
1:B:451:ALA:HB1	1:B:465:ILE:HD13	2.00	0.44
1:C:360:LYS:HD3	2:C:601:NAD:O2D	2.17	0.44
1:A:343:VAL:HG22	1:A:353:GLN:HB3	1.99	0.44
1:D:92:ASP:HB2	1:D:95:SER:OG	2.16	0.44
1:A:373:LYS:HB3	1:A:373:LYS:HE3	1.71	0.44
1:B:425:ILE:HD13	1:B:425:ILE:HA	1.84	0.44
1:A:482:MET:HE2	1:A:482:MET:HB3	1.79	0.44
1:B:67:ASP:HB3	1:B:69:PRO:HD2	1.99	0.44
1:C:29:VAL:HG11	1:C:61:CYS:SG	2.58	0.44
1:C:295:LEU:HD12	1:C:295:LEU:HA	1.65	0.44
1:D:167:ARG:NH1	1:D:169:GLU:OE2	2.51	0.44
1:B:361:GLN:HE22	1:B:413:PHE:HB3	1.83	0.43
1:C:269:ALA:HB1	1:C:275:LYS:HG3	2.00	0.43
1:C:461:GLY:HA3	1:C:478:GLY:O	2.18	0.43
1:D:310:GLN:HG3	1:D:353:GLN:HG3	2.00	0.43
1:C:324:GLU:OE1	1:C:423:LYS:HD3	2.18	0.43
1:D:313:CYS:SG	1:D:315:THR:OG1	2.77	0.43
1:B:426:GLU:CD	1:D:84:ARG:HH22	2.26	0.43
1:A:146:GLY:O	1:A:150:LYS:HD2	2.18	0.43
1:B:134:LEU:HD13	1:B:134:LEU:HA	1.81	0.43
1:B:137:CYS:SG	1:B:184:LEU:HG	2.59	0.43
1:C:244:ILE:HG23	1:C:250:ILE:HD13	1.98	0.43
1:A:122:THR:HG22	1:A:209:THR:HG21	2.01	0.43
1:A:184:LEU:HD22	1:A:212:THR:HG21	2.00	0.43
1:B:73:LYS:HE3	1:B:73:LYS:HB3	1.82	0.43
1:A:76:GLU:O	1:A:80:VAL:HG23	2.19	0.43
1:B:35:PHE:CE1	1:B:38:ASN:HA	2.53	0.43
1:B:442:ALA:HA	1:B:464:TRP:O	2.19	0.43
1:D:332:ARG:HE	1:D:332:ARG:HB2	1.62	0.43
1:B:30:LYS:HB3	1:B:31:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ASN:HB3	1:C:221:LYS:HG3	2.00	0.43
1:D:237:GLY:C	1:D:239:THR:H	2.27	0.43
1:D:499:GLU:HA	4:D:742:HOH:O	2.18	0.43
1:A:430:LYS:HG3	1:A:431:ARG:N	2.34	0.43
1:B:276:ARG:NH1	1:D:484:GLY:O	2.51	0.42
1:D:195:LEU:HA	1:D:195:LEU:HD23	1.74	0.42
1:B:482:MET:HE2	1:B:482:MET:HB3	1.74	0.42
1:C:119:THR:OG1	1:C:126:PHE:HA	2.18	0.42
1:C:190:LYS:HD3	1:C:254:ALA:HB3	2.00	0.42
1:D:187:LEU:HD12	1:D:187:LEU:HA	1.80	0.42
1:B:239:THR:HG23	1:B:240:VAL:N	2.33	0.42
1:B:491:GLU:OE2	1:D:154:LYS:HE2	2.19	0.42
1:B:384:SER:OG	1:B:394:LYS:HD2	2.19	0.42
1:A:92:ASP:N	1:A:92:ASP:OD1	2.49	0.42
1:A:111:ARG:HG2	1:A:130:PHE:CE2	2.55	0.42
1:A:451:ALA:HB1	1:A:465:ILE:HD13	2.00	0.42
1:D:286:PRO:HD2	1:D:440:THR:O	2.19	0.42
1:D:471:LEU:HD12	3:D:602:N98:C06	2.49	0.42
1:C:252:LYS:HE3	1:C:497:TYR:CE1	2.55	0.42
2:D:601:NAD:H8A	2:D:601:NAD:H2B	1.86	0.42
1:B:476:PRO:HG3	1:B:492:TYR:CD1	2.55	0.42
1:D:37:ASN:O	1:D:39:GLU:HG3	2.20	0.42
1:D:306:VAL:HG11	1:D:417:GLN:HB2	2.02	0.42
1:B:83:GLN:O	1:B:86:SER:HB3	2.19	0.41
1:C:280:GLU:OE2	1:C:478:GLY:HA2	2.20	0.41
1:C:447:ASN:HB3	1:C:450:LYS:HB2	2.02	0.41
1:D:174:CYS:O	1:D:201:MET:HA	2.19	0.41
1:A:35:PHE:C	1:A:36:ILE:HG13	2.45	0.41
1:C:161:ASN:OD1	1:C:161:ASN:N	2.53	0.41
1:B:174:CYS:O	1:B:201:MET:HA	2.20	0.41
1:B:315:THR:O	1:B:468:TYR:OH	2.33	0.41
1:B:384:SER:O	1:B:394:LYS:HG2	2.21	0.41
1:C:179:PRO:HD3	1:C:256:THR:HB	2.03	0.41
1:D:252:LYS:HG2	1:D:253:ILE:N	2.36	0.41
1:A:179:PRO:HG3	1:A:256:THR:HG22	2.01	0.41
1:A:365:ILE:CD1	1:A:414:GLY:HA3	2.50	0.41
1:D:91:LEU:HD23	1:D:91:LEU:HA	1.93	0.41
1:D:176:ALA:HB1	1:D:190:LYS:HD2	2.02	0.41
1:D:373:LYS:HB2	1:D:373:LYS:HE2	1.76	0.41
1:C:255:PHE:HB3	1:C:279:LEU:HD23	2.03	0.41
1:D:304:GLN:HB3	3:D:602:N98:C17	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:THR:HG23	1:A:240:VAL:H	1.85	0.41
1:D:304:GLN:HA	1:D:304:GLN:NE2	2.36	0.41
1:D:336:GLU:HG2	1:D:340:LYS:HD3	2.03	0.41
1:D:360:LYS:HE3	2:D:601:NAD:O2D	2.20	0.41
1:A:184:LEU:HD13	1:A:212:THR:HG22	2.02	0.41
1:A:239:THR:CG2	1:A:240:VAL:H	2.34	0.41
1:C:75:VAL:HG11	1:C:247:HIS:CE1	2.56	0.41
1:B:310:GLN:HG3	1:B:353:GLN:HG3	2.03	0.40
1:C:106:LEU:HB3	1:C:219:LEU:HD22	2.04	0.40
1:A:236:PHE:HB2	1:A:239:THR:HG22	2.03	0.40
1:B:290:CYS:HB3	1:B:450:LYS:NZ	2.36	0.40
1:C:114:LEU:HD21	1:C:215:TYR:CD1	2.57	0.40
1:C:239:THR:HG22	1:C:240:VAL:HG23	2.04	0.40
1:D:364:LYS:HZ1	2:D:601:NAD:H2N	1.86	0.40
1:D:430:LYS:HG3	1:D:431:ARG:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:GLY:O	1:C:325:GLN:NE2[2_454]	1.68	0.52

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	474/512 (93%)	447 (94%)	27 (6%)	0	100	100
1	B	474/512 (93%)	451 (95%)	22 (5%)	1 (0%)	43	72
1	C	477/512 (93%)	456 (96%)	20 (4%)	1 (0%)	43	72
1	D	474/512 (93%)	446 (94%)	27 (6%)	1 (0%)	43	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1899/2048 (93%)	1800 (95%)	96 (5%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	196	CYS
1	B	374	LYS
1	D	438	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	395/422 (94%)	395 (100%)	0	100	100
1	B	395/422 (94%)	395 (100%)	0	100	100
1	C	396/422 (94%)	396 (100%)	0	100	100
1	D	395/422 (94%)	395 (100%)	0	100	100
All	All	1581/1688 (94%)	1581 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	128	HIS
1	A	361	GLN
1	B	152	GLN
1	B	361	GLN
1	B	485	ASN
1	C	152	GLN
1	C	361	GLN
1	C	417	GLN
1	D	304	GLN

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Mol	Chain	Res	Type
1	D	485	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 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$
3	N98	A	602	-	32,32,32	2.87	15 (46%)	41,46,46	3.24	18 (43%)
2	NAD	C	601	-	46,48,48	4.06	20 (43%)	64,73,73	1.76	12 (18%)
3	N98	C	602	-	32,32,32	3.10	16 (50%)	41,46,46	2.97	18 (43%)
2	NAD	A	601	-	46,48,48	4.08	20 (43%)	64,73,73	1.91	14 (21%)
2	NAD	B	602	-	46,48,48	4.19	21 (45%)	64,73,73	1.82	13 (20%)
3	N98	D	602	-	32,32,32	3.17	17 (53%)	41,46,46	3.05	17 (41%)
3	N98	B	601	-	32,32,32	3.26	17 (53%)	41,46,46	3.79	18 (43%)
2	NAD	D	601	-	46,48,48	4.29	17 (36%)	64,73,73	1.84	12 (18%)

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
3	N98	A	602	-	-	0/14/20/20	0/5/5/5
2	NAD	C	601	-	-	7/30/62/62	0/5/5/5
3	N98	C	602	-	-	4/14/20/20	0/5/5/5
2	NAD	A	601	-	-	10/30/62/62	0/5/5/5
2	NAD	B	602	-	-	10/30/62/62	0/5/5/5
3	N98	D	602	-	-	4/14/20/20	0/5/5/5
3	N98	B	601	-	-	1/14/20/20	0/5/5/5
2	NAD	D	601	-	-	17/30/62/62	0/5/5/5

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	NAD	O4D-C1D	17.73	1.64	1.40
2	B	602	NAD	O4D-C1D	17.46	1.63	1.40
2	C	601	NAD	O4D-C1D	16.83	1.63	1.40
2	A	601	NAD	O4D-C1D	16.79	1.62	1.40
2	D	601	NAD	O4B-C1B	8.55	1.61	1.42
2	B	602	NAD	O4B-C1B	8.51	1.61	1.42
2	A	601	NAD	O4B-C1B	8.35	1.61	1.42
2	C	601	NAD	O4B-C1B	8.33	1.61	1.42
2	B	602	NAD	C7N-N7N	8.09	1.47	1.33
2	A	601	NAD	C7N-N7N	7.90	1.47	1.33
2	D	601	NAD	C2B-C1B	-7.84	1.28	1.53
2	C	601	NAD	C7N-N7N	7.74	1.47	1.33
2	C	601	NAD	C2B-C1B	-7.73	1.29	1.53
2	A	601	NAD	C2B-C1B	-7.69	1.29	1.53
2	B	602	NAD	C2B-C1B	-7.68	1.29	1.53
2	D	601	NAD	PA-O3	7.52	1.67	1.59
2	D	601	NAD	C7N-N7N	7.49	1.46	1.33
3	D	602	N98	C20-C07	7.32	1.58	1.47
3	D	602	N98	C05-N13	7.04	1.48	1.38
3	D	602	N98	C10-C09	7.03	1.45	1.38
2	D	601	NAD	PN-O3	6.96	1.67	1.59
3	B	601	N98	C14-C11	6.94	1.58	1.47
3	C	602	N98	C10-C09	6.93	1.44	1.38
3	B	601	N98	C20-C07	6.88	1.57	1.47
3	C	602	N98	C20-C07	6.77	1.57	1.47
3	B	601	N98	C05-N13	6.77	1.47	1.38
3	B	601	N98	C11-N12	6.48	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAD	O4B-C4B	-6.35	1.30	1.45
2	B	602	NAD	O4B-C4B	-6.33	1.30	1.45
2	D	601	NAD	O4D-C4D	-6.27	1.31	1.45
2	A	601	NAD	O4D-C4D	-6.23	1.31	1.45
2	B	602	NAD	O4D-C4D	-6.20	1.31	1.45
2	D	601	NAD	O4B-C4B	-6.17	1.31	1.45
2	A	601	NAD	PA-O3	6.11	1.66	1.59
3	C	602	N98	C05-N13	6.10	1.46	1.38
2	C	601	NAD	PA-O3	6.09	1.66	1.59
2	A	601	NAD	C6A-N6A	6.02	1.49	1.34
3	A	602	N98	C20-C07	6.00	1.56	1.47
3	A	602	N98	C14-C11	5.94	1.56	1.47
3	A	602	N98	C11-N12	5.92	1.42	1.34
2	B	602	NAD	PA-O3	5.89	1.65	1.59
3	D	602	N98	C11-N12	5.87	1.42	1.34
3	B	601	N98	C10-C09	5.87	1.43	1.38
2	C	601	NAD	O4D-C4D	-5.85	1.32	1.45
2	C	601	NAD	O4B-C4B	-5.84	1.32	1.45
2	C	601	NAD	C6A-N6A	5.75	1.48	1.34
3	C	602	N98	C14-C11	5.74	1.56	1.47
3	C	602	N98	C11-N12	5.73	1.41	1.34
3	A	602	N98	C05-N13	5.67	1.46	1.38
2	D	601	NAD	C6A-N6A	5.64	1.48	1.34
3	A	602	N98	C10-C09	5.52	1.43	1.38
2	B	602	NAD	C6A-N6A	5.44	1.48	1.34
3	D	602	N98	C14-C11	5.37	1.55	1.47
2	B	602	NAD	PN-O3	4.87	1.64	1.59
2	A	601	NAD	O3D-C3D	-4.51	1.31	1.43
3	B	601	N98	C09-N13	4.38	1.45	1.39
3	C	602	N98	C09-N13	4.31	1.45	1.39
2	B	602	NAD	O3D-C3D	-4.29	1.32	1.43
2	D	601	NAD	O3D-C3D	-4.22	1.32	1.43
2	C	601	NAD	PN-O3	4.19	1.64	1.59
2	A	601	NAD	PN-O3	4.18	1.64	1.59
3	D	602	N98	C09-N13	4.13	1.45	1.39
3	C	602	N98	O02-C03	4.11	1.42	1.33
3	A	602	N98	C09-N13	4.11	1.45	1.39
2	D	601	NAD	O2B-C2B	4.08	1.53	1.43
2	C	601	NAD	O3D-C3D	-4.03	1.33	1.43
2	B	602	NAD	O2B-C2B	4.00	1.52	1.43
2	C	601	NAD	O2B-C2B	3.95	1.52	1.43
2	A	601	NAD	O2D-C2D	3.82	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	N98	O02-C03	3.70	1.41	1.33
2	B	602	NAD	O2D-C2D	3.65	1.52	1.43
3	B	601	N98	C09-N08	3.65	1.43	1.36
3	B	601	N98	O02-C03	3.64	1.41	1.33
2	A	601	NAD	O2B-C2B	3.63	1.51	1.43
2	D	601	NAD	O2D-C2D	3.58	1.51	1.43
2	C	601	NAD	C5D-C4D	3.58	1.62	1.51
3	B	601	N98	N13-N12	3.38	1.44	1.38
3	A	602	N98	C09-N08	3.29	1.42	1.36
3	C	602	N98	C09-N08	3.29	1.42	1.36
2	C	601	NAD	C2N-N1N	3.26	1.38	1.35
2	D	601	NAD	C2N-N1N	3.26	1.38	1.35
3	A	602	N98	O02-C03	3.26	1.40	1.33
2	B	602	NAD	C5D-C4D	3.19	1.61	1.51
2	B	602	NAD	C2N-N1N	3.14	1.38	1.35
2	C	601	NAD	O2D-C2D	3.10	1.50	1.43
3	D	602	N98	N13-N12	3.00	1.43	1.38
2	B	602	NAD	C5A-N7A	-2.97	1.33	1.39
2	A	601	NAD	C5D-C4D	2.96	1.60	1.51
3	D	602	N98	C09-N08	2.92	1.41	1.36
3	D	602	N98	C25-C24	2.91	1.43	1.38
2	B	602	NAD	C3N-C7N	2.89	1.54	1.50
3	C	602	N98	C25-C24	2.88	1.43	1.38
3	A	602	N98	N13-N12	2.88	1.43	1.38
2	C	601	NAD	O3B-C3B	-2.84	1.35	1.43
2	D	601	NAD	C5D-C4D	2.83	1.60	1.51
3	C	602	N98	C06-C07	2.82	1.48	1.43
2	A	601	NAD	C2N-N1N	2.76	1.38	1.35
3	B	601	N98	C15-C14	2.70	1.43	1.39
2	C	601	NAD	C5A-N7A	-2.66	1.34	1.39
3	B	601	N98	C19-C14	2.65	1.43	1.39
3	B	601	N98	C06-C07	2.63	1.48	1.43
3	B	601	N98	C25-C24	2.58	1.43	1.38
3	C	602	N98	C10-C11	2.58	1.45	1.40
3	B	601	N98	O04-C03	2.57	1.26	1.21
2	A	601	NAD	C5A-N7A	-2.54	1.34	1.39
3	A	602	N98	C10-C11	2.53	1.44	1.40
2	C	601	NAD	PA-O5B	2.51	1.69	1.59
2	D	601	NAD	C5A-N7A	-2.51	1.34	1.39
3	B	601	N98	C21-C20	2.50	1.43	1.39
2	D	601	NAD	O3B-C3B	-2.49	1.36	1.43
3	D	602	N98	C10-C11	2.48	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	N98	N13-N12	2.47	1.42	1.38
2	A	601	NAD	C2A-N3A	2.46	1.38	1.33
2	B	602	NAD	PA-O5B	2.42	1.68	1.59
3	C	602	N98	O04-C03	2.41	1.26	1.21
3	B	601	N98	C10-C11	2.40	1.44	1.40
3	D	602	N98	C06-C07	2.35	1.47	1.43
2	A	601	NAD	O3B-C3B	-2.33	1.37	1.43
3	C	602	N98	C15-C14	2.32	1.42	1.39
3	A	602	N98	C15-C14	2.31	1.42	1.39
3	C	602	N98	C05-C03	2.31	1.55	1.48
3	B	601	N98	C16-C15	2.28	1.42	1.38
3	A	602	N98	C06-C07	2.26	1.47	1.43
2	C	601	NAD	C2A-N3A	2.26	1.37	1.33
3	A	602	N98	C25-C24	2.22	1.42	1.38
3	D	602	N98	C05-C03	2.20	1.55	1.48
2	B	602	NAD	O3B-C3B	-2.20	1.37	1.43
3	C	602	N98	C21-C20	2.18	1.42	1.39
3	A	602	N98	C19-C14	2.15	1.42	1.39
3	D	602	N98	O04-C03	2.15	1.25	1.21
2	A	601	NAD	C4N-C3N	-2.14	1.36	1.39
3	D	602	N98	C15-C14	2.14	1.42	1.39
3	D	602	N98	C16-C15	2.14	1.42	1.38
2	B	602	NAD	C5A-C4A	-2.12	1.35	1.39
2	A	601	NAD	PA-O5B	2.12	1.67	1.59
2	C	601	NAD	C4N-C3N	-2.11	1.36	1.39
2	B	602	NAD	C2A-N3A	2.09	1.37	1.33
3	A	602	N98	C16-C15	2.07	1.42	1.38
2	B	602	NAD	C4A-N9A	-2.04	1.33	1.37
2	A	601	NAD	C4A-N9A	-2.04	1.33	1.37
2	C	601	NAD	C5A-C4A	-2.02	1.35	1.39
2	D	601	NAD	C2A-N3A	2.02	1.37	1.33
3	D	602	N98	C19-C14	2.01	1.42	1.39

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	N98	C11-C10-C09	10.20	110.82	105.56
3	B	601	N98	C14-C11-N12	9.73	133.29	120.49
3	D	602	N98	C11-N12-N13	8.41	110.25	104.06
3	A	602	N98	C11-C10-C09	7.97	109.67	105.56
3	A	602	N98	C14-C11-N12	7.96	130.97	120.49
3	B	601	N98	C11-N12-N13	7.91	109.88	104.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	N98	C11-N12-N13	7.62	109.67	104.06
3	C	602	N98	C01-O02-C03	6.94	128.72	115.85
2	B	602	NAD	N3A-C2A-N1A	-6.73	118.39	128.58
3	A	602	N98	C11-N12-N13	6.70	108.99	104.06
3	B	601	N98	C01-O02-C03	6.58	128.06	115.85
3	D	602	N98	C01-O02-C03	6.24	127.42	115.85
3	B	601	N98	C19-C14-C15	-6.01	110.92	118.57
3	D	602	N98	O02-C03-O04	-5.97	112.10	123.50
3	C	602	N98	C11-C10-C09	5.94	108.62	105.56
2	A	601	NAD	N3A-C2A-N1A	-5.90	119.65	128.58
2	C	601	NAD	N3A-C2A-N1A	-5.81	119.78	128.58
2	D	601	NAD	N3A-C2A-N1A	-5.81	119.78	128.58
3	B	601	N98	C14-C11-C10	-5.61	120.82	128.69
3	D	602	N98	C11-C10-C09	5.58	108.44	105.56
3	B	601	N98	C18-C19-C14	5.51	125.78	120.36
3	B	601	N98	N13-C09-N08	5.47	125.46	121.49
3	A	602	N98	C19-C14-C15	-5.41	111.69	118.57
3	C	602	N98	O02-C03-O04	-5.25	113.48	123.50
2	D	601	NAD	C5A-C4A-N3A	-5.19	119.57	126.72
2	C	601	NAD	C5A-C4A-N3A	-5.12	119.66	126.72
3	B	601	N98	C15-C14-C11	5.00	126.48	120.87
3	B	601	N98	C10-C11-N12	-4.94	105.69	111.11
3	C	602	N98	O02-C03-C05	4.91	127.83	111.70
3	A	602	N98	C14-C11-C10	-4.79	121.97	128.69
3	D	602	N98	C19-C14-C15	-4.77	112.50	118.57
3	D	602	N98	O02-C03-C05	4.72	127.19	111.70
3	C	602	N98	C19-C14-C15	-4.71	112.58	118.57
3	A	602	N98	C18-C19-C14	4.69	124.98	120.36
3	B	601	N98	O02-C03-O04	-4.65	114.61	123.50
3	A	602	N98	C01-O02-C03	4.65	124.47	115.85
2	A	601	NAD	N6A-C6A-N1A	-4.64	108.05	118.38
2	B	602	NAD	N6A-C6A-N1A	-4.62	108.08	118.38
3	C	602	N98	C16-C15-C14	4.58	124.87	120.36
2	A	601	NAD	N9A-C8A-N7A	-4.53	107.51	113.94
3	A	602	N98	C16-C15-C14	4.49	124.78	120.36
3	A	602	N98	N13-C09-N08	4.47	124.73	121.49
3	D	602	N98	C14-C11-N12	4.41	126.29	120.49
2	B	602	NAD	N9A-C8A-N7A	-4.35	107.76	113.94
3	A	602	N98	O02-C03-O04	-4.34	115.22	123.50
3	B	601	N98	C16-C15-C14	4.33	124.63	120.36
2	D	601	NAD	N6A-C6A-N1A	-4.25	108.92	118.38
3	D	602	N98	C18-C19-C14	4.12	124.41	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	N98	C15-C14-C11	4.08	125.45	120.87
3	A	602	N98	C15-C14-C11	4.06	125.42	120.87
2	A	601	NAD	C5A-C4A-N3A	-4.05	121.14	126.72
2	D	601	NAD	N9A-C8A-N7A	-4.00	108.25	113.94
2	C	601	NAD	N6A-C6A-N1A	-4.00	109.46	118.38
3	A	602	N98	O02-C03-C05	4.00	124.82	111.70
3	C	602	N98	C18-C19-C14	3.97	124.27	120.36
3	D	602	N98	C16-C15-C14	3.97	124.27	120.36
2	A	601	NAD	C3N-C7N-N7N	3.90	122.54	117.74
3	A	602	N98	C10-C11-N12	-3.90	106.83	111.11
3	C	602	N98	C14-C11-N12	3.89	125.61	120.49
2	C	601	NAD	N9A-C8A-N7A	-3.87	108.44	113.94
2	B	602	NAD	C5A-C4A-N3A	-3.79	121.49	126.72
2	D	601	NAD	N3A-C4A-N9A	3.73	133.51	127.17
3	D	602	N98	C10-C11-N12	-3.73	107.02	111.11
2	D	601	NAD	C2A-N3A-C4A	3.67	120.79	111.83
2	A	601	NAD	C5A-C6A-N6A	3.67	132.36	123.29
2	C	601	NAD	N3A-C4A-N9A	3.57	133.24	127.17
3	C	602	N98	C10-C11-N12	-3.52	107.25	111.11
2	B	602	NAD	C3N-C7N-N7N	3.50	122.05	117.74
2	C	601	NAD	C2A-N3A-C4A	3.48	120.32	111.83
3	D	602	N98	C09-N13-N12	-3.47	107.01	111.96
2	D	601	NAD	C6N-N1N-C2N	-3.47	118.93	121.88
2	B	602	NAD	C5A-C6A-N6A	3.46	131.85	123.29
2	A	601	NAD	C4A-N9A-C8A	3.38	109.28	105.74
3	A	602	N98	C20-C07-N08	3.32	120.48	116.94
3	B	601	N98	O02-C03-C05	3.31	122.56	111.70
2	B	602	NAD	C2A-N3A-C4A	3.24	119.73	111.83
2	B	602	NAD	O7N-C7N-N7N	-3.18	118.02	122.62
3	C	602	N98	N13-C09-N08	3.14	123.77	121.49
2	A	601	NAD	C2A-N3A-C4A	3.04	119.25	111.83
2	B	602	NAD	C4A-N9A-C8A	3.03	108.92	105.74
3	D	602	N98	C20-C07-N08	2.95	120.08	116.94
2	A	601	NAD	N3A-C4A-N9A	2.90	132.10	127.17
2	A	601	NAD	C5A-N7A-C8A	2.90	108.01	103.45
3	C	602	N98	C25-C20-C07	2.84	124.05	120.87
3	D	602	N98	C24-C25-C20	2.83	123.82	120.80
3	B	601	N98	C20-C07-N08	2.82	119.95	116.94
3	B	601	N98	C09-N13-N12	-2.82	107.94	111.96
2	C	601	NAD	C5A-C6A-N6A	2.79	130.18	123.29
2	D	601	NAD	C5A-C6A-N6A	2.78	130.16	123.29
2	B	602	NAD	N3A-C4A-N9A	2.76	131.86	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	N98	C10-C09-N13	2.75	107.29	105.65
2	C	601	NAD	O3-PA-O1A	-2.72	102.52	110.70
3	C	602	N98	C09-N13-N12	-2.71	108.09	111.96
2	B	602	NAD	C5A-N7A-C8A	2.64	107.60	103.45
2	D	601	NAD	C5A-N7A-C8A	2.63	107.58	103.45
3	C	602	N98	C19-C14-C11	2.60	123.78	120.87
3	C	602	N98	C20-C07-N08	2.60	119.71	116.94
2	A	601	NAD	C4D-O4D-C1D	-2.58	107.56	109.92
2	D	601	NAD	C5D-C4D-C3D	-2.45	106.41	115.21
2	D	601	NAD	C4A-N9A-C8A	2.44	108.30	105.74
3	A	602	N98	C20-C07-C06	-2.44	118.23	121.40
2	C	601	NAD	C5A-N7A-C8A	2.42	107.25	103.45
2	C	601	NAD	C3N-C7N-N7N	2.40	120.69	117.74
3	C	602	N98	C15-C14-C11	2.40	123.56	120.87
3	B	601	N98	C10-C09-N08	-2.39	128.89	132.64
3	A	602	N98	C25-C20-C07	2.37	123.52	120.87
3	A	602	N98	C09-N13-N12	-2.36	108.59	111.96
2	D	601	NAD	O7N-C7N-N7N	-2.32	119.26	122.62
3	B	601	N98	C25-C20-C07	2.30	123.45	120.87
3	D	602	N98	C25-C20-C21	-2.30	116.59	119.25
3	D	602	N98	C25-C20-C07	2.30	123.44	120.87
2	C	601	NAD	C4A-N9A-C8A	2.29	108.14	105.74
3	C	602	N98	O04-C03-C05	-2.19	118.68	124.34
2	B	602	NAD	C6N-N1N-C2N	-2.18	120.02	121.88
2	A	601	NAD	O2B-C2B-C3B	-2.18	104.83	111.82
2	A	601	NAD	O2A-PA-O3	-2.18	101.39	107.27
2	C	601	NAD	C6N-N1N-C2N	-2.15	120.05	121.88
2	A	601	NAD	O4B-C1B-N9A	-2.07	104.11	108.09
3	B	601	N98	C05-C06-C07	2.07	125.46	120.05
3	A	602	N98	C10-C09-N08	-2.07	129.40	132.64
3	C	602	N98	C05-C06-C07	2.05	125.40	120.05
2	B	602	NAD	C4D-O4D-C1D	-2.04	108.06	109.92

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAD	C5B-O5B-PA-O1A
2	A	601	NAD	C5B-O5B-PA-O3
2	A	601	NAD	C2D-C1D-N1N-C2N
2	A	601	NAD	C2D-C1D-N1N-C6N
2	B	602	NAD	PN-O3-PA-O5B

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Mol	Chain	Res	Type	Atoms
2	B	602	NAD	C5D-O5D-PN-O3
2	B	602	NAD	C5D-O5D-PN-O1N
2	B	602	NAD	C5D-O5D-PN-O2N
2	D	601	NAD	O4B-C4B-C5B-O5B
2	D	601	NAD	C5D-O5D-PN-O3
2	D	601	NAD	C5D-O5D-PN-O1N
2	D	601	NAD	C5D-O5D-PN-O2N
2	D	601	NAD	C2D-C1D-N1N-C2N
2	D	601	NAD	C2D-C1D-N1N-C6N
3	C	602	N98	C10-C11-C14-C15
3	C	602	N98	N12-C11-C14-C15
3	C	602	N98	N12-C11-C14-C19
3	C	602	N98	C10-C11-C14-C19
2	A	601	NAD	C3D-C4D-C5D-O5D
2	D	601	NAD	C3B-C4B-C5B-O5B
2	A	601	NAD	O4D-C4D-C5D-O5D
2	D	601	NAD	O4D-C4D-C5D-O5D
2	D	601	NAD	C3D-C4D-C5D-O5D
3	D	602	N98	N12-C11-C14-C15
3	D	602	N98	C10-C11-C14-C15
3	D	602	N98	N12-C11-C14-C19
2	B	602	NAD	O4D-C4D-C5D-O5D
2	B	602	NAD	C3D-C4D-C5D-O5D
2	C	601	NAD	C2N-C3N-C7N-O7N
3	D	602	N98	C10-C11-C14-C19
2	C	601	NAD	C2N-C3N-C7N-N7N
2	C	601	NAD	PN-O3-PA-O5B
2	C	601	NAD	C4N-C3N-C7N-O7N
2	C	601	NAD	C4N-C3N-C7N-N7N
2	A	601	NAD	C2B-C1B-N9A-C8A
2	B	602	NAD	C2B-C1B-N9A-C8A
2	C	601	NAD	C2B-C1B-N9A-C8A
2	D	601	NAD	C2B-C1B-N9A-C8A
3	B	601	N98	C10-C11-C14-C19
2	D	601	NAD	C4D-C5D-O5D-PN
2	A	601	NAD	C5B-O5B-PA-O2A
2	A	601	NAD	C5D-O5D-PN-O3
2	A	601	NAD	C4D-C5D-O5D-PN
2	D	601	NAD	C2N-C3N-C7N-N7N
2	D	601	NAD	C2N-C3N-C7N-O7N
2	D	601	NAD	C4N-C3N-C7N-N7N
2	B	602	NAD	O4B-C1B-N9A-C8A

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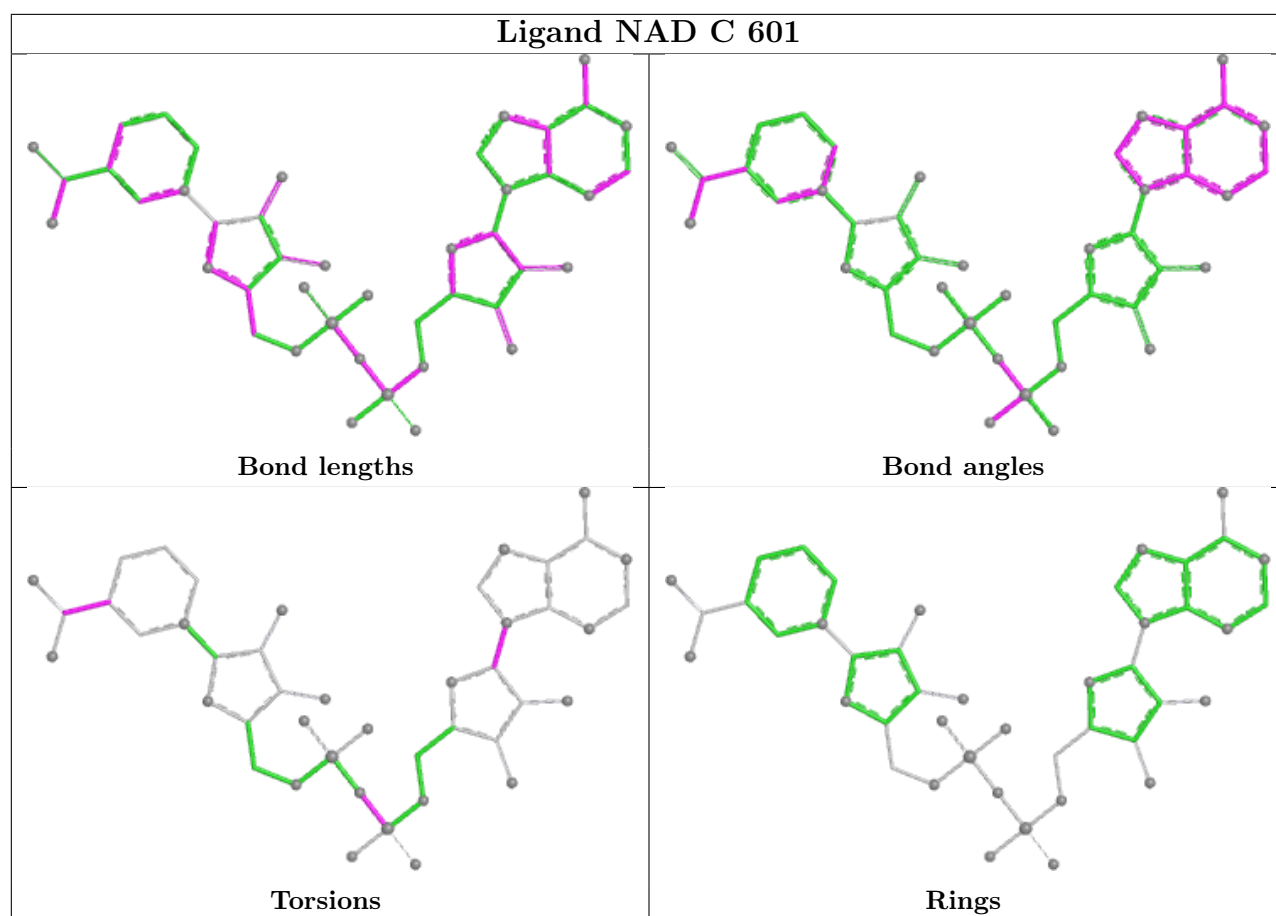
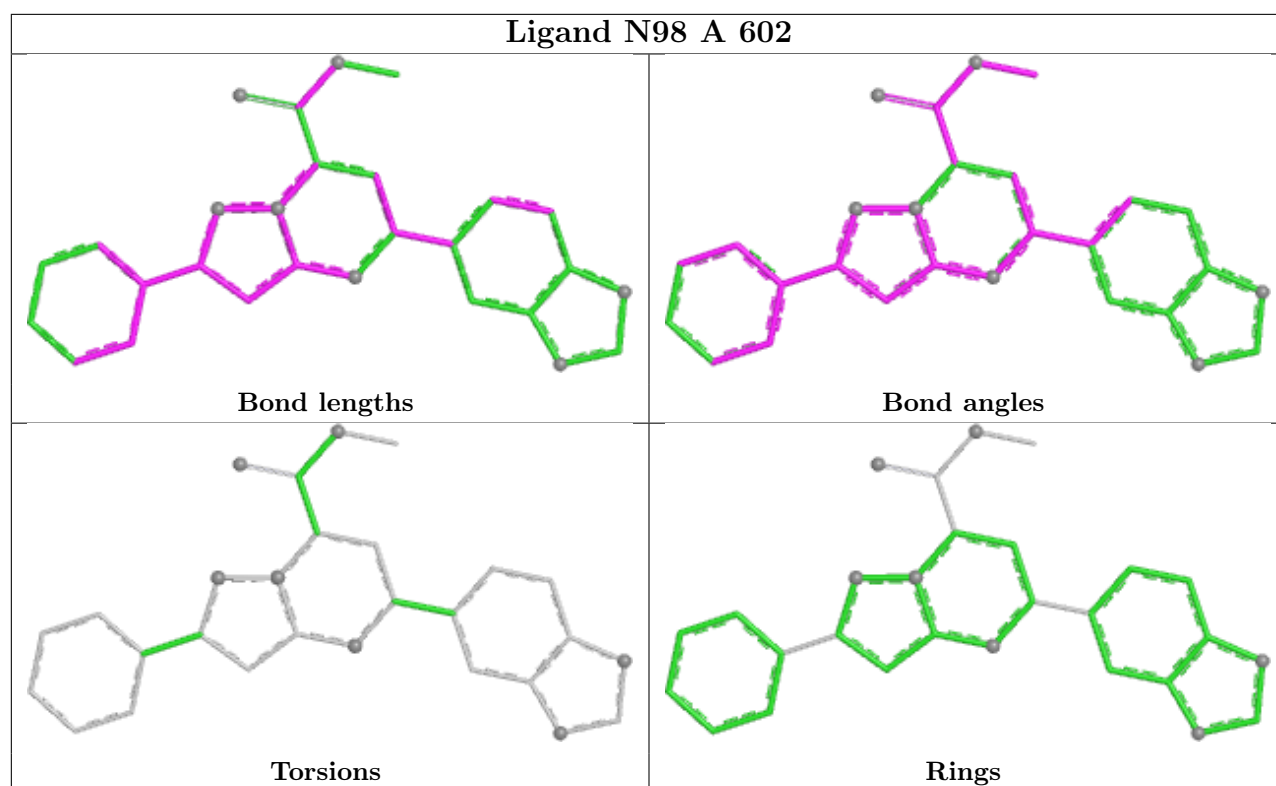
Mol	Chain	Res	Type	Atoms
2	D	601	NAD	C4N-C3N-C7N-O7N
2	B	602	NAD	C2B-C1B-N9A-C4A
2	C	601	NAD	O4B-C1B-N9A-C8A
2	D	601	NAD	O4B-C1B-N9A-C8A
2	B	602	NAD	C4D-C5D-O5D-PN
2	D	601	NAD	PN-O3-PA-O2A

There are no ring outliers.

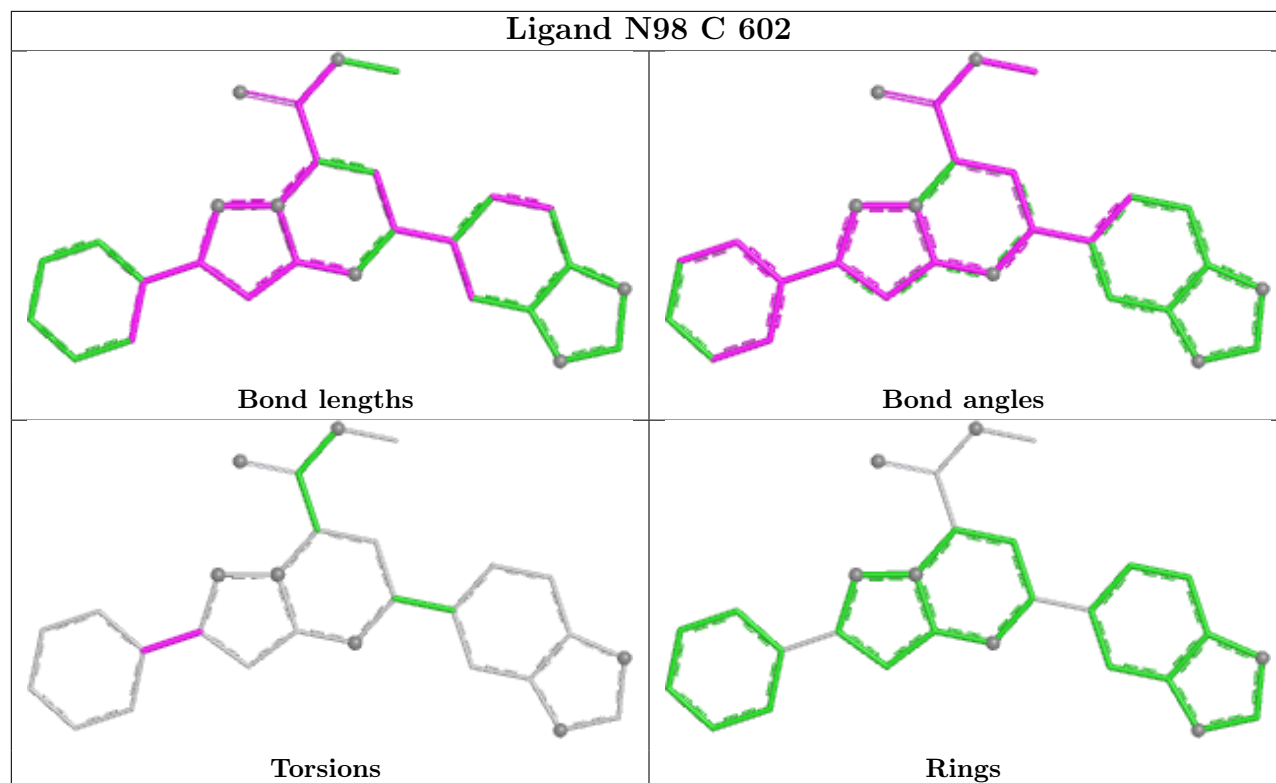
7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	NAD	1	0
3	C	602	N98	3	0
2	A	601	NAD	3	0
2	B	602	NAD	1	0
3	D	602	N98	3	0
3	B	601	N98	1	0
2	D	601	NAD	4	0

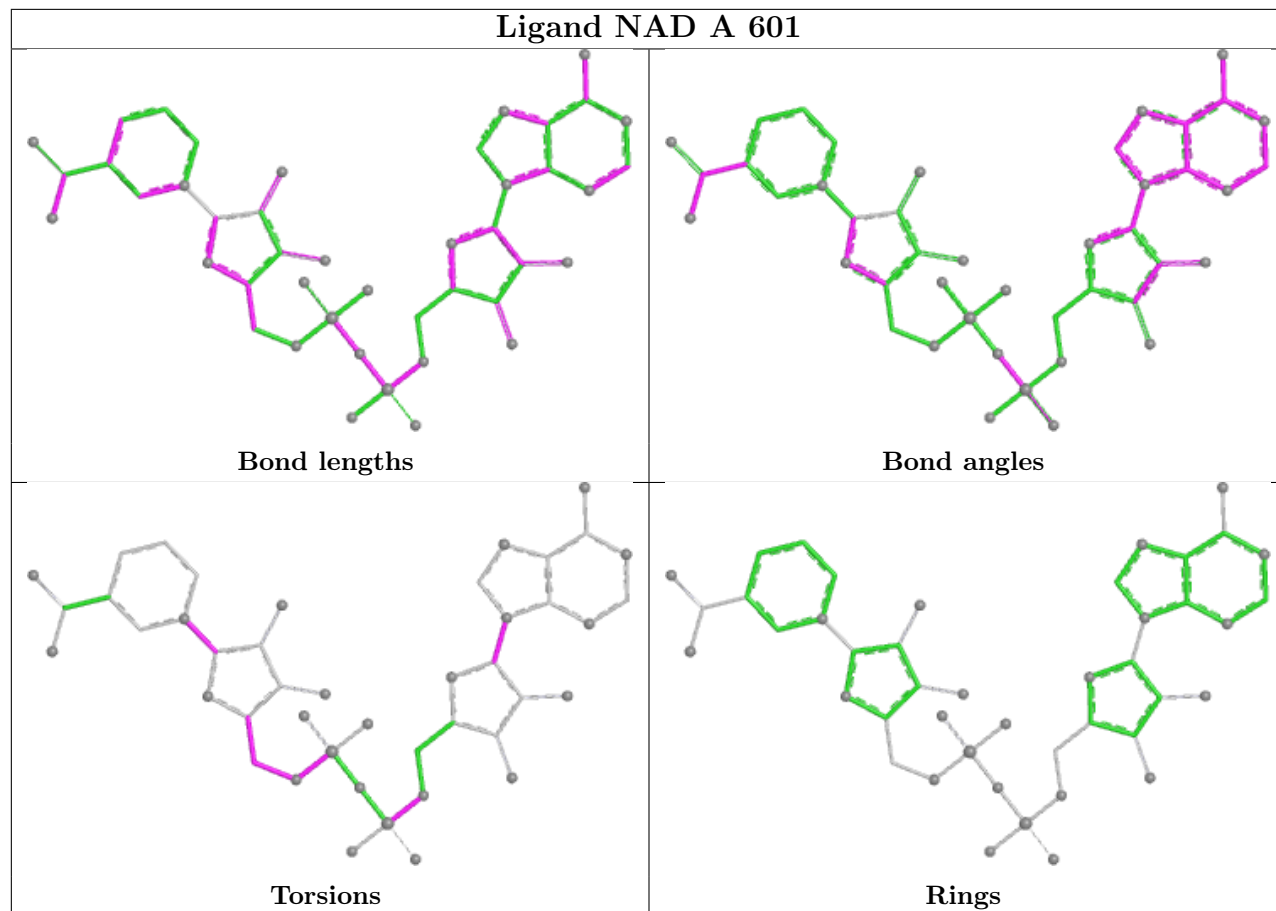
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

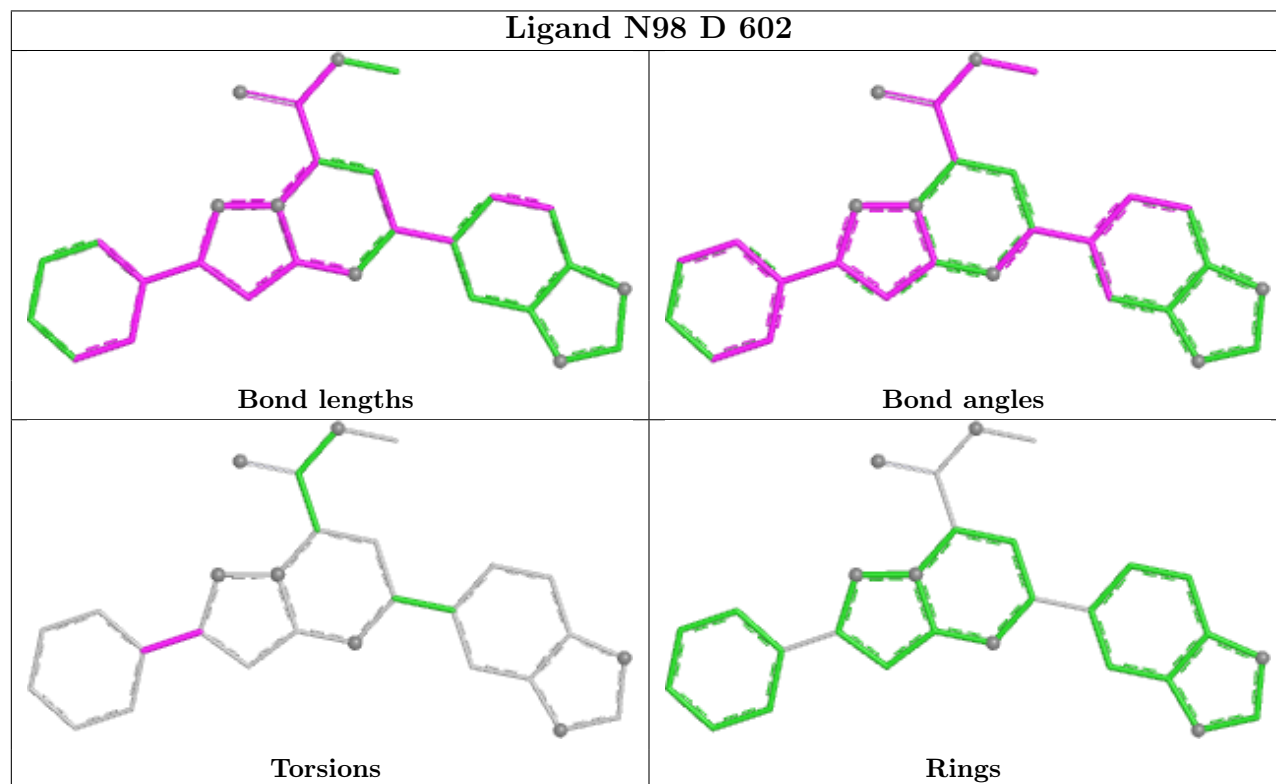
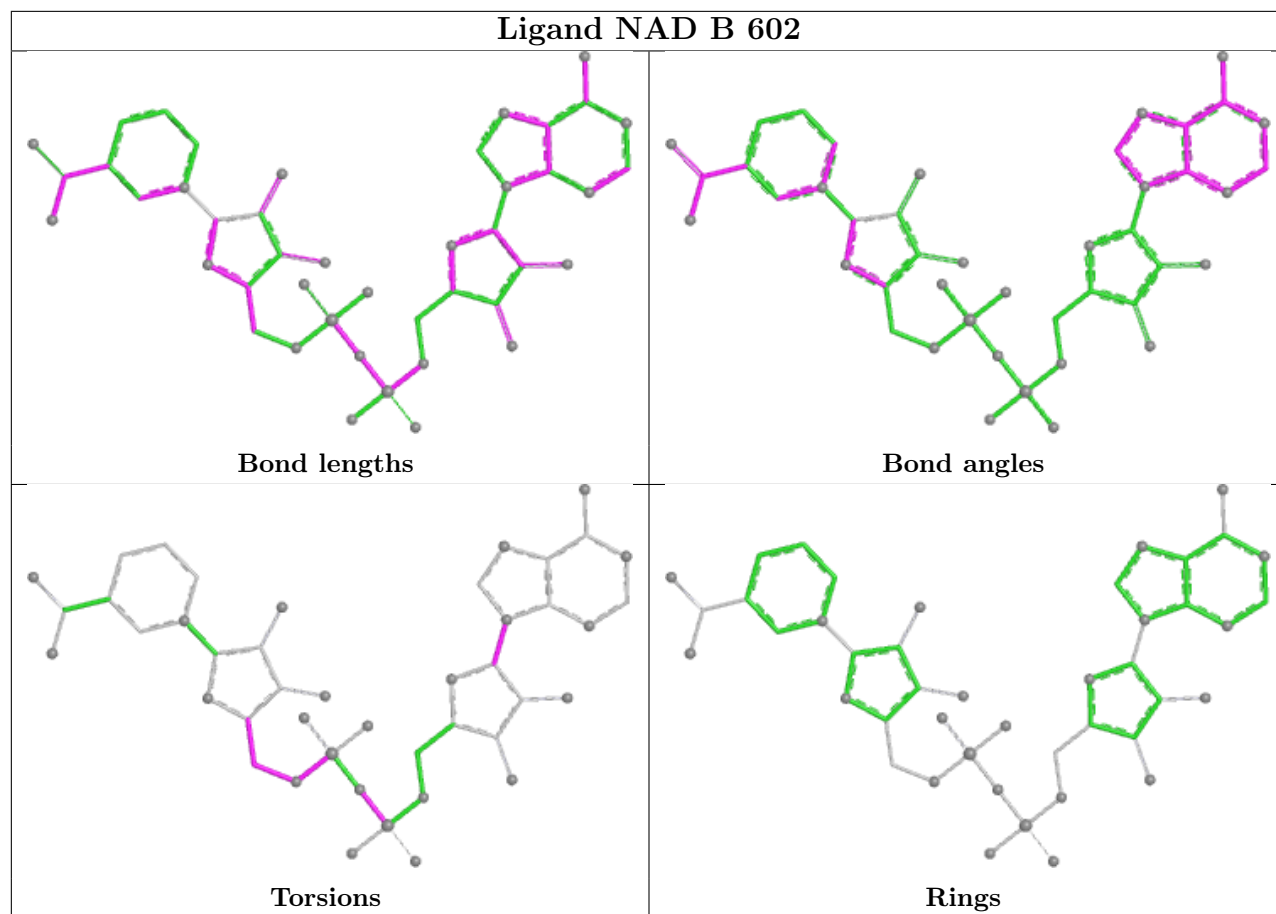


Ligand N98 C 602

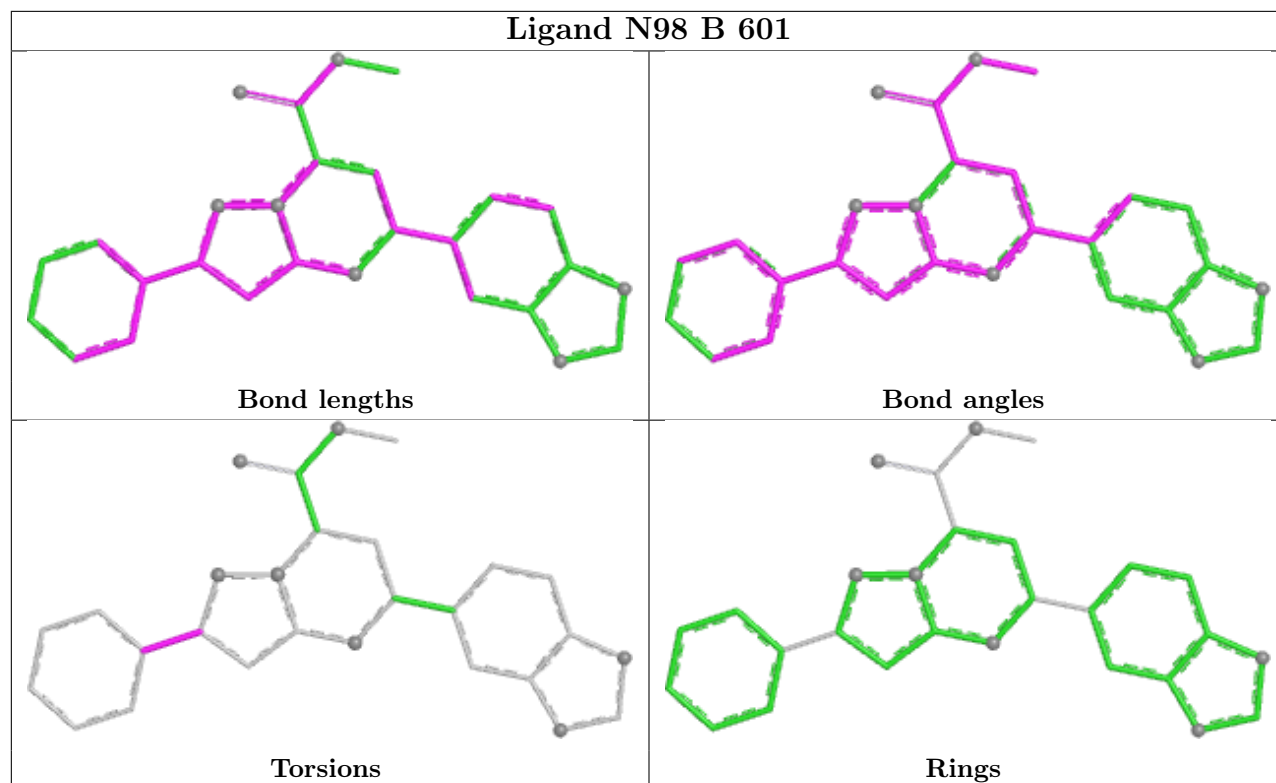


Ligand NAD A 601

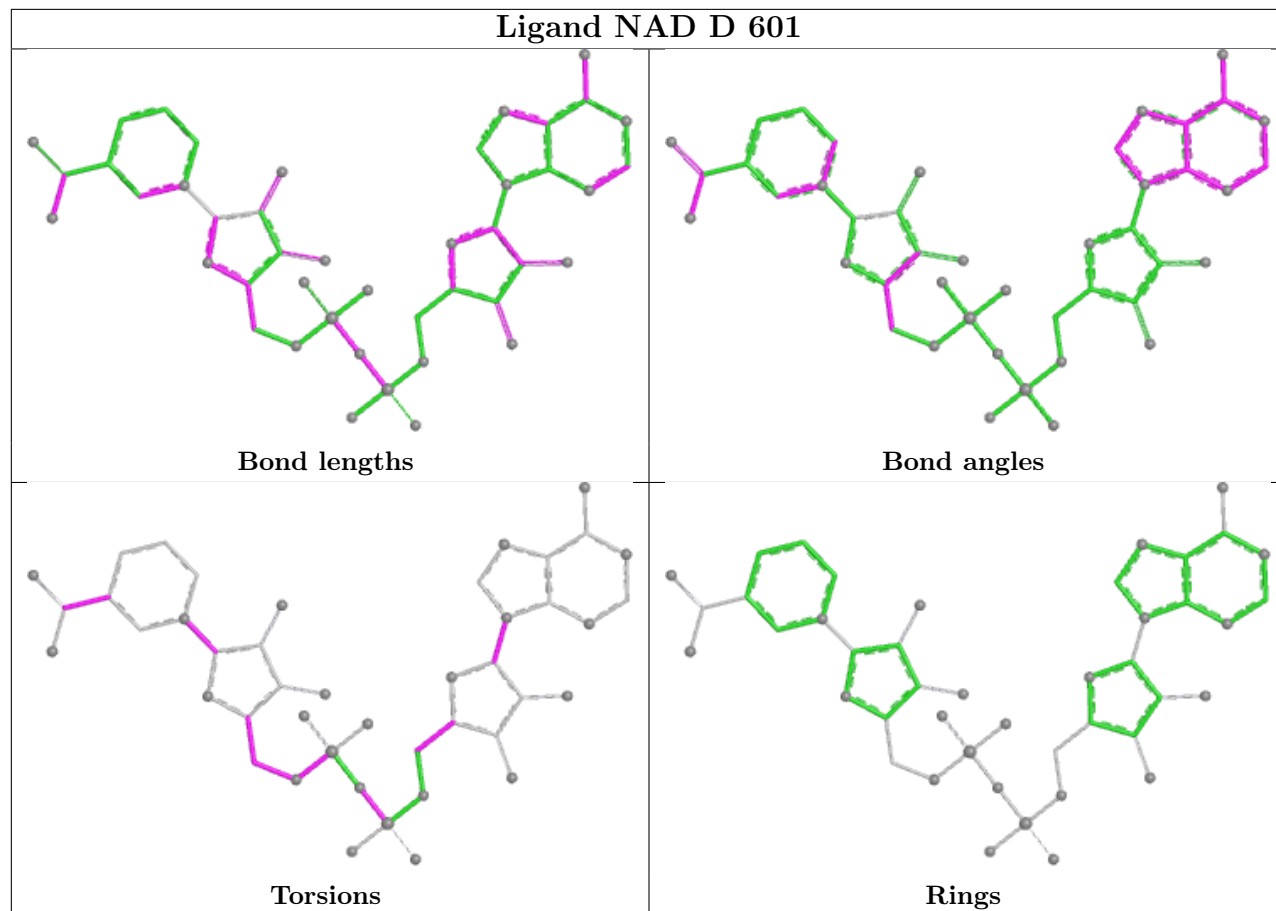




Ligand N98 B 601



Ligand NAD D 601



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	478/512 (93%)	-0.23	6 (1%) 75 66	7, 20, 55, 65	0
1	B	478/512 (93%)	-0.32	0 100 100	7, 19, 44, 56	0
1	C	479/512 (93%)	-0.43	0 100 100	7, 19, 40, 81	0
1	D	478/512 (93%)	-0.41	0 100 100	6, 19, 39, 75	0
All	All	1913/2048 (93%)	-0.34	6 (0%) 90 86	6, 19, 44, 81	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	LEU	4.1
1	A	390	GLY	3.3
1	A	362	PHE	3.0
1	A	364	LYS	2.6
1	A	359	GLN	2.2
1	A	373	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

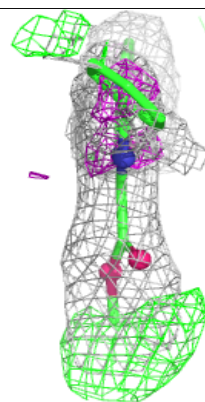
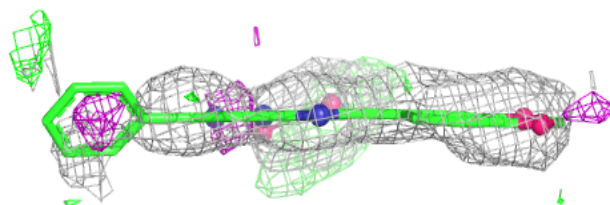
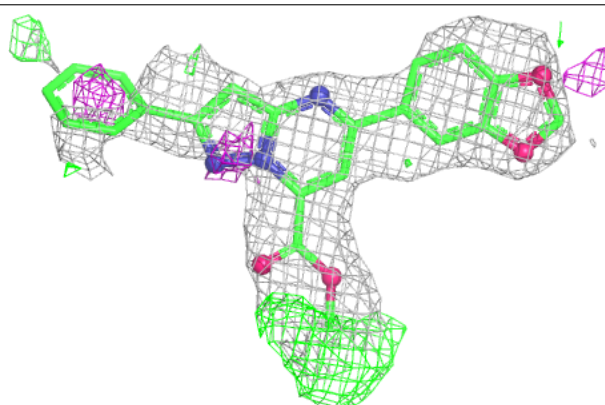
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	N98	D	602	28/28	0.78	0.17	15,34,57,60	0
3	N98	C	602	28/28	0.80	0.15	12,35,50,57	0
3	N98	B	601	28/28	0.82	0.16	17,30,56,58	0
3	N98	A	602	28/28	0.84	0.16	13,30,59,64	0
2	NAD	D	601	44/44	0.93	0.12	8,28,81,87	0
2	NAD	C	601	44/44	0.94	0.12	10,22,82,88	0
2	NAD	A	601	44/44	0.95	0.11	9,19,72,77	0
2	NAD	B	602	44/44	0.95	0.10	7,20,67,72	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.

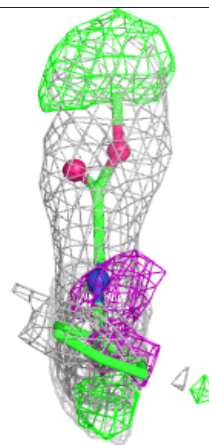
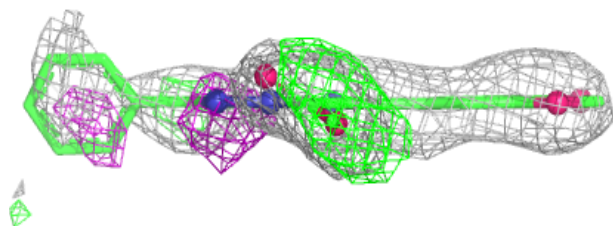
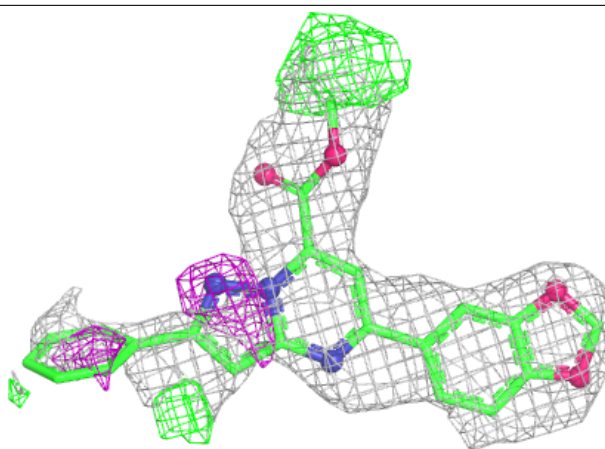
Electron density around N98 D 602:

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

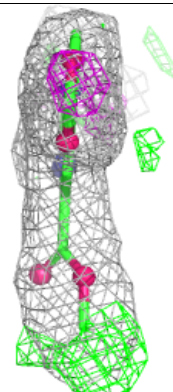
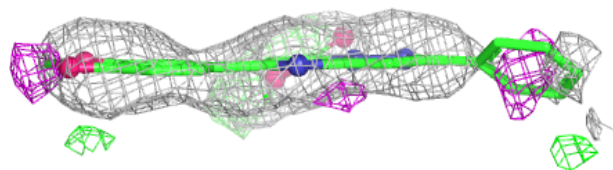
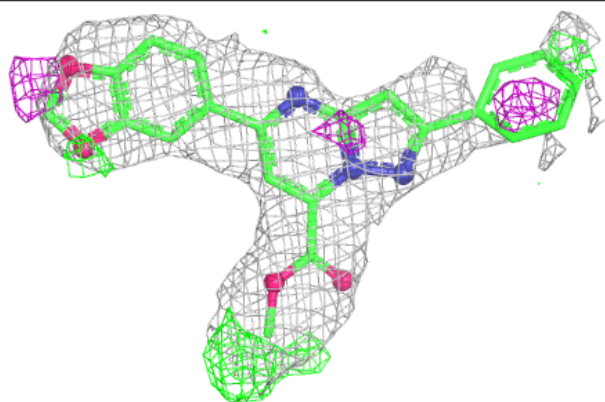


Electron density around N98 C 602:

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

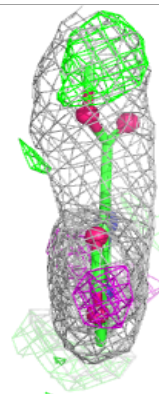
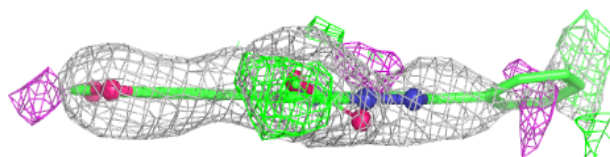
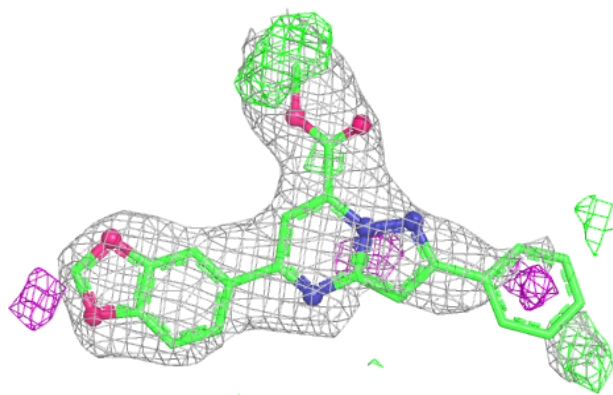
**Electron density around N98 B 601:**

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



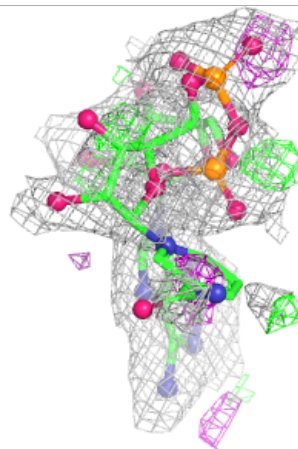
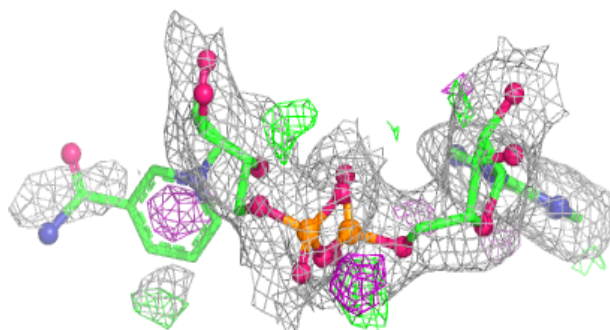
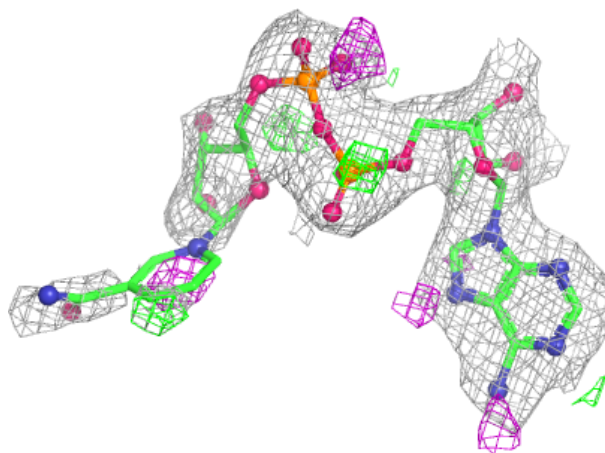
Electron density around N98 A 602:

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



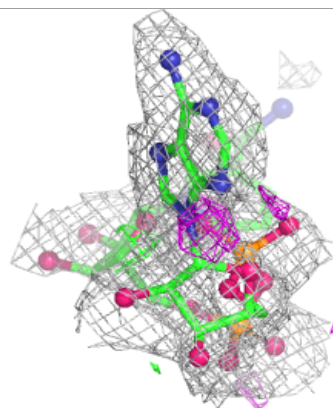
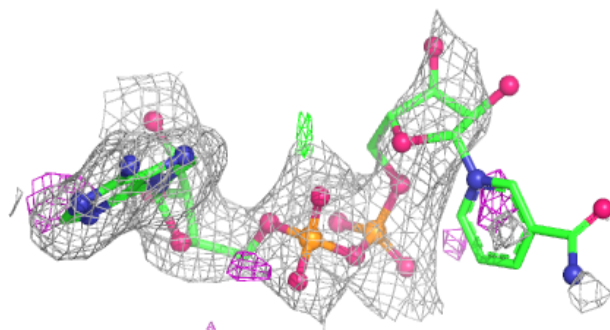
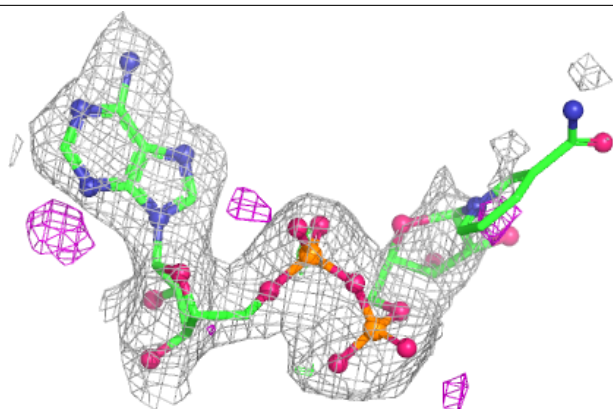
Electron density around NAD D 601:

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

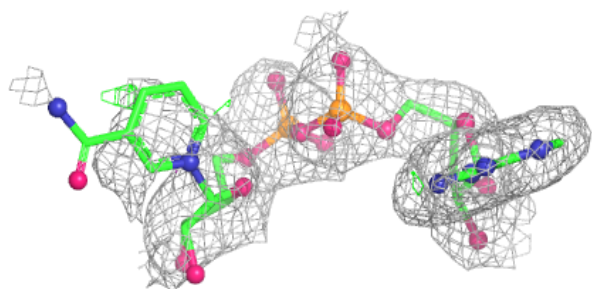
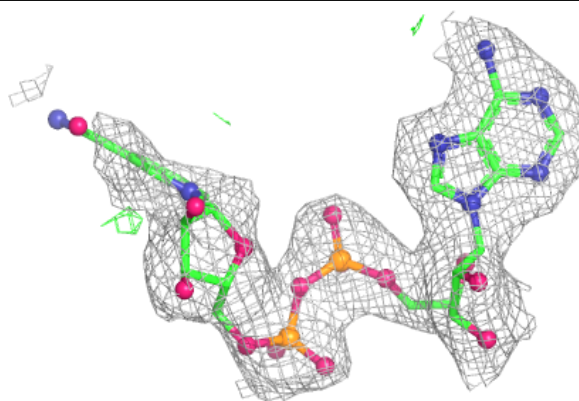


Electron density around NAD C 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

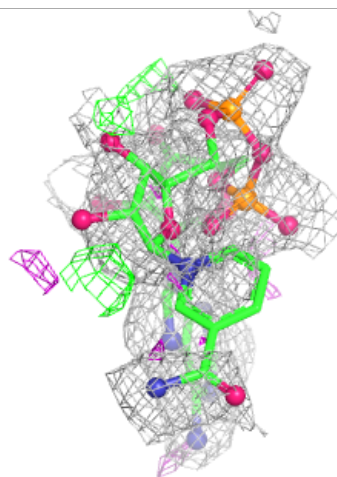
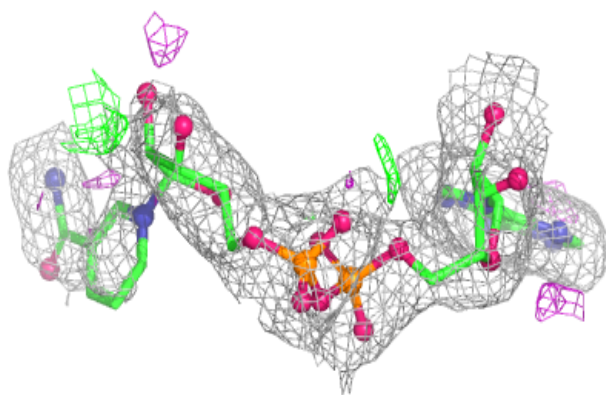
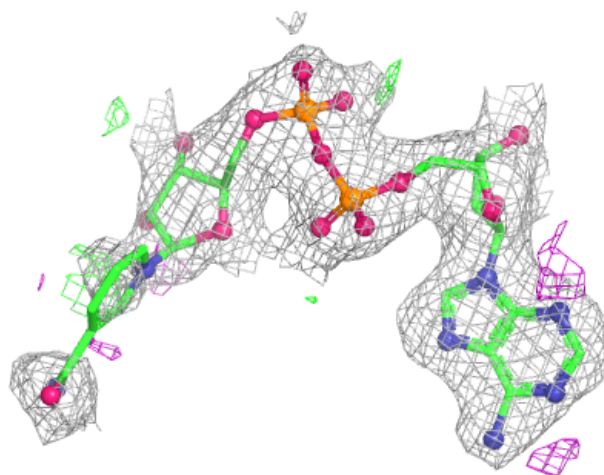
**Electron density around NAD A 601:**

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



Electron density around NAD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.