



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 01:27 pm GMT

PDB ID : 5M67
Title : Crystal structure of S-adenosyl-L-homocysteine hydrolase from *Bradyrhizobium elkanii* in complex with adenine and 2'-deoxyadenosine
Authors : Manszewski, T.; Jaskolski, M.
Deposited on : 2016-10-24
Resolution : 1.54 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

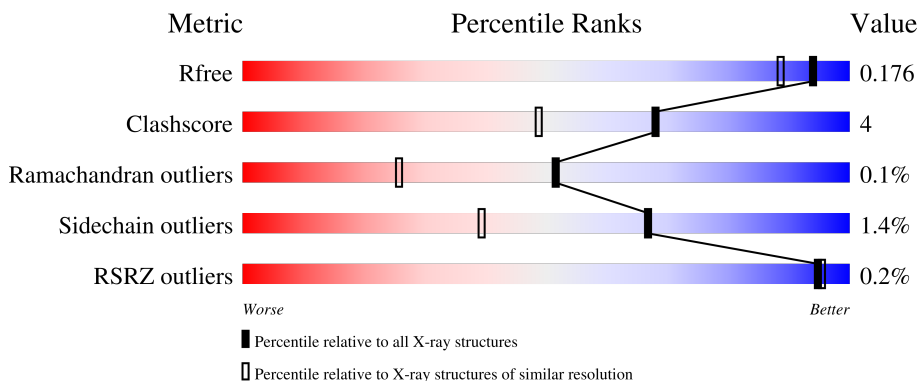
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	479	90% 7% ..
1	B	479	88% 8% ..
1	C	479	91% 6% ..
1	D	479	90% 8% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	A	505	-	-	X	-
5	PEG	D	504	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 17102 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.

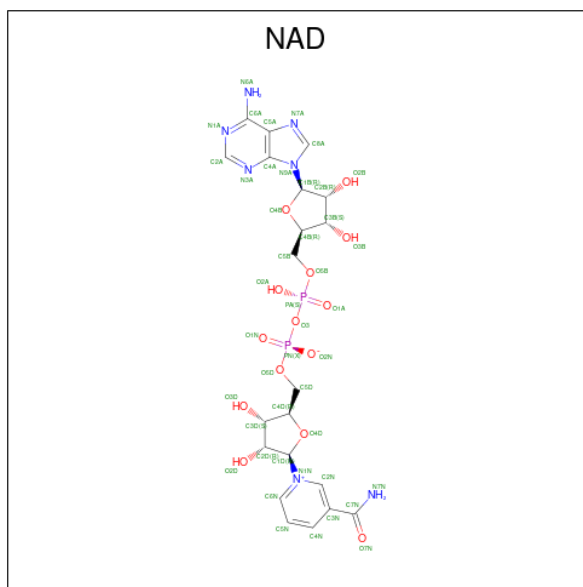
- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	468	3660	2320	630	687	23	0	7	0
1	B	463	3645	2316	621	684	24	0	11	0
1	C	468	3684	2336	633	692	23	0	11	0
1	D	470	3691	2337	636	696	22	0	9	0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

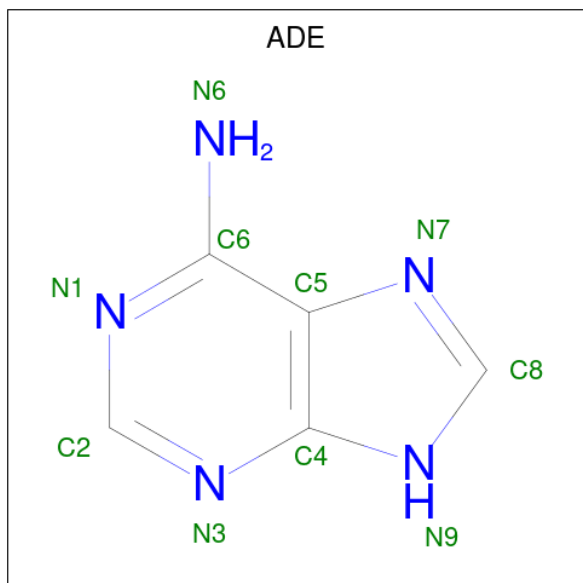
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Na	0	0
			2	2		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



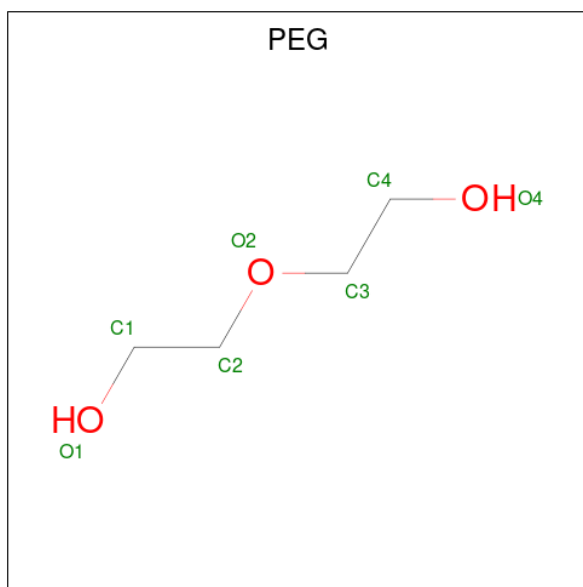
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	N	O			P	
3	A	1	Total	44	21	7	14	2	0	0
3	B	1	Total	44	21	7	14	2	0	0
3	C	1	Total	44	21	7	14	2	0	0
3	D	1	Total	44	21	7	14	2	0	0

- Molecule 4 is ADENINE (three-letter code: ADE) (formula: $C_5H_5N_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			10	5	5		
4	B	1	Total	C	N	0	0
			10	5	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



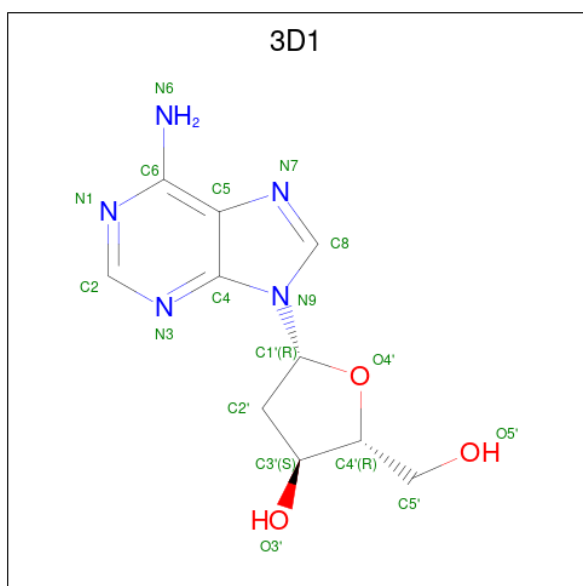
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is (2R,3S,5R)-5-(6-amino-9H-purin-9-yl)-tetrahydro-2-(hydroxymethyl)furan-3-ol (three-letter code: 3D1) (formula: C₁₀H₁₃N₅O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			18	10	5	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	D	1	18	10	5	3	0	0

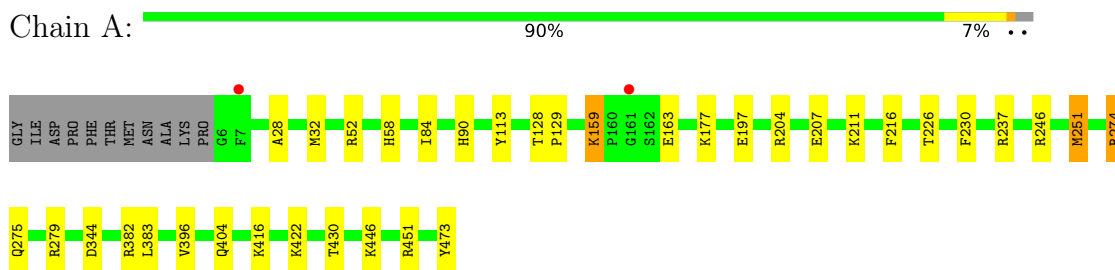
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	561	Total 561	O 561	0	0
8	B	580	Total 580	O 580	0	0
8	C	508	Total 508	O 508	0	0
8	D	507	Total 507	O 507	0	0

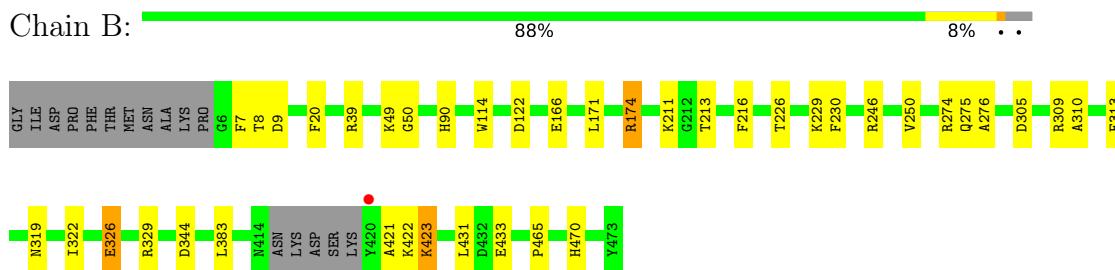
3 Residue-property plots [i](#)

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.

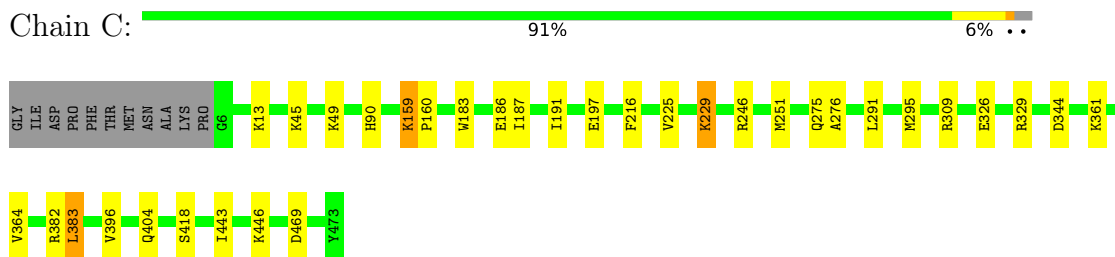
- Molecule 1: Adenosylhomocysteinase



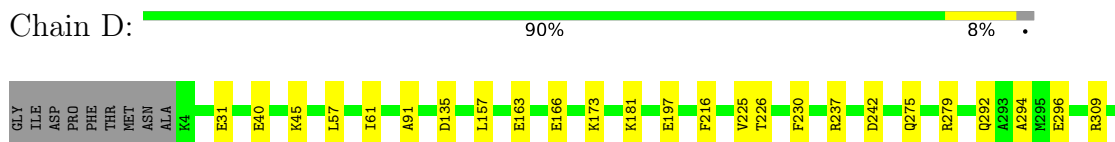
- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase



- Molecule 1: Adenosylhomocysteinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.48Å 174.53Å 96.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.63 – 1.54 84.53 – 1.54	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.63-1.54) 99.6 (84.53-1.54)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.53Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.145 , 0.176 0.144 , 0.176	Depositor DCC
R_{free} test set	1010 reflections (0.38%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtrriage
Anisotropy	0.356	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17102	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PEG, ADE, 3D1, NAD, ACT

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	0.75	0/3748	0.89	12/5056 (0.2%)
1	B	0.75	1/3747 (0.0%)	0.90	8/5055 (0.2%)
1	C	0.74	0/3781	0.83	5/5100 (0.1%)
1	D	0.74	0/3784	0.83	4/5106 (0.1%)
All	All	0.74	1/15060 (0.0%)	0.86	29/20317 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	326	GLU	CG-CD	5.34	1.59	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	A	52	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	D	309	ARG	NE-CZ-NH1	-8.06	116.27	120.30
1	B	246	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	274	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	B	39	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	B	246	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	451	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	204	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	451	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	174	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	309	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	C	383	LEU	CB-CG-CD2	-5.91	100.95	111.00
1	D	382[A]	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	D	382[B]	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	246	ARG	NE-CZ-NH2	-5.76	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	229[A]	LYS	CD-CE-NZ	5.71	124.83	111.70
1	C	229[B]	LYS	CD-CE-NZ	5.71	124.83	111.70
1	A	274	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	251[A]	MET	CG-SD-CE	-5.65	91.15	100.20
1	A	251[B]	MET	CG-SD-CE	-5.65	91.15	100.20
1	C	309	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	C	246	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	204	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	250	VAL	CG1-CB-CG2	5.26	119.31	110.90
1	A	383	LEU	CB-CG-CD1	-5.18	102.20	111.00
1	B	344	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	52	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	D	242	ASP	CB-CG-OD2	-5.01	113.79	118.30

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	3660	0	3695	25	0
1	B	3645	0	3688	26	0
1	C	3684	0	3725	25	0
1	D	3691	0	3715	33	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	44	0	26	1	0
3	B	44	0	26	1	0
3	C	44	0	26	2	0
3	D	44	0	26	2	0
4	A	10	0	4	1	0
4	B	10	0	4	0	0
5	A	7	0	9	10	0
5	B	7	0	9	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	7	0	9	9	0
6	B	4	0	3	0	0
6	C	4	0	3	0	0
7	C	18	0	13	3	0
7	D	18	0	13	4	0
8	A	561	0	0	10	0
8	B	580	0	0	8	0
8	C	508	0	0	7	0
8	D	507	0	0	15	0
All	All	17102	0	14994	114	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 4.

All (114) 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:D:344[A]:ASP:O	8:D:601:HOH:O	1.64	1.15
1:D:344[B]:ASP:O	8:D:602:HOH:O	1.74	1.03
1:C:344[A]:ASP:O	8:C:602:HOH:O	1.82	0.97
1:C:382[B]:ARG:NH2	8:C:603:HOH:O	1.99	0.94
5:A:505:PEG:H41	8:A:970:HOH:O	1.69	0.93
1:B:305[B]:ASP:OD2	8:B:601:HOH:O	1.91	0.88
5:D:504:PEG:H12	8:D:990:HOH:O	1.75	0.86
1:C:159:LYS:HD3	1:C:160:PRO:HD2	1.56	0.85
5:A:505:PEG:H31	1:C:275:GLN:O	1.77	0.83
1:C:326:GLU:OE1	1:C:329:ARG:NH1	2.12	0.81
1:A:237:ARG:HG2	5:A:505:PEG:H11	1.64	0.79
1:A:237:ARG:CZ	5:A:505:PEG:H42	2.13	0.77
1:D:237:ARG:HG2	5:D:504:PEG:H42	1.66	0.76
7:D:503:3D1:H2'2	8:D:609:HOH:O	1.83	0.76
1:B:122[A]:ASP:OD1	8:B:602:HOH:O	2.05	0.74
1:B:275:GLN:O	5:D:504:PEG:H22	1.87	0.73
7:C:503:3D1:H2'2	8:C:609:HOH:O	1.88	0.73
1:D:449[B]:GLU:OE1	8:D:604:HOH:O	2.06	0.72
1:C:469[B]:ASP:OD2	8:C:604:HOH:O	2.10	0.69
1:D:31:GLU:OE2	1:D:442:LYS:NZ	2.24	0.69
1:B:166[A]:GLU:OE1	8:B:603:HOH:O	2.13	0.66
4:A:504:ADE:N9	8:A:604:HOH:O	2.29	0.65
1:A:446:LYS:HD2	8:A:936:HOH:O	1.97	0.64
1:B:470:HIS:HD2	8:B:852:HOH:O	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:505:PEG:H22	1:C:276:ALA:HA	1.81	0.61
1:B:211:LYS:HG3	1:B:213:THR:HG23	1.82	0.61
1:B:274[B]:ARG:HD2	8:B:854:HOH:O	2.01	0.61
5:A:505:PEG:H12	8:A:812:HOH:O	2.02	0.60
1:B:383[B]:LEU:HD22	3:B:502:NAD:N7N	2.16	0.60
1:D:446:LYS:HG2	8:D:711:HOH:O	2.02	0.59
1:A:237:ARG:NE	5:A:505:PEG:H42	2.17	0.59
1:C:229[A]:LYS:HE3	1:D:472:ARG:HB2	1.85	0.58
1:C:469[B]:ASP:CG	8:C:604:HOH:O	2.42	0.58
1:B:275:GLN:O	5:D:504:PEG:H31	2.05	0.57
1:D:237:ARG:HG2	5:D:504:PEG:C4	2.34	0.57
1:D:163:GLU:O	1:D:166:GLU:HG3	2.04	0.56
1:C:159:LYS:HD3	1:C:160:PRO:CD	2.34	0.55
1:D:342:HIS:HA	1:D:383:LEU:HD21	1.87	0.55
1:A:275:GLN:CB	5:A:505:PEG:H21	2.36	0.55
1:B:326:GLU:HG3	8:B:618:HOH:O	2.07	0.55
1:B:20:PHE:HB2	5:B:504:PEG:H11	1.89	0.54
1:C:344[A]:ASP:HB3	1:C:382[A]:ARG:HG2	1.89	0.53
1:D:279[B]:ARG:HD2	8:D:603:HOH:O	2.06	0.53
1:B:20:PHE:CG	5:B:504:PEG:H32	2.44	0.53
1:D:237:ARG:CZ	5:D:504:PEG:H11	2.38	0.53
1:A:275:GLN:HB2	5:A:505:PEG:H21	1.91	0.52
1:C:13:LYS:HE2	8:C:1006:HOH:O	2.09	0.52
1:B:174:ARG:NE	8:B:606:HOH:O	2.23	0.51
1:A:446:LYS:HB3	8:A:997:HOH:O	2.12	0.50
5:B:504:PEG:H31	1:D:361:LYS:HA	1.93	0.50
1:B:49:LYS:HD3	1:B:50:GLY:N	2.26	0.50
1:B:7:PHE:CE1	1:B:9:ASP:HB3	2.46	0.49
1:B:423:LYS:HA	1:B:423:LYS:HE3	1.94	0.49
1:D:449[A]:GLU:HG2	8:D:618:HOH:O	2.13	0.49
7:D:503:3D1:H1'	8:D:621:HOH:O	2.13	0.49
3:D:502:NAD:C4N	7:D:503:3D1:H3'	2.43	0.48
5:A:505:PEG:H22	1:C:275:GLN:O	2.13	0.48
1:A:473:TYR:O	1:B:229:LYS:HE2	2.14	0.48
3:C:502:NAD:C4N	7:C:503:3D1:H3'	2.44	0.48
1:D:279[B]:ARG:NH1	8:D:603:HOH:O	1.96	0.48
1:D:275:GLN:HG3	5:D:504:PEG:H32	1.96	0.47
1:A:251[A]:MET:HE1	1:C:396:VAL:HB	1.95	0.47
1:D:57:LEU:HD21	8:D:621:HOH:O	2.14	0.47
1:C:197:GLU:HB2	1:C:404:GLN:HE21	1.80	0.47
1:A:430:THR:HG23	8:A:963:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:503:3D1:C2'	8:C:609:HOH:O	2.54	0.47
1:C:361:LYS:HE2	1:C:364:VAL:HG21	1.97	0.46
1:C:443:ILE:HD12	1:D:294:ALA:HB1	1.97	0.46
1:D:135:ASP:OD2	1:D:197:GLU:HG2	2.15	0.46
1:A:344:ASP:HB3	1:A:382[A]:ARG:HG2	1.98	0.46
1:B:319:ASN:HB3	1:B:322:ILE:HD11	1.97	0.46
1:C:225:VAL:HG22	1:D:472:ARG:CZ	2.45	0.46
1:D:423:LYS:HB2	8:D:907:HOH:O	2.16	0.46
7:D:503:3D1:C2'	8:D:609:HOH:O	2.54	0.46
1:A:84:ILE:HG22	1:A:113:TYR:HB2	1.97	0.46
1:A:251[A]:MET:CE	1:C:396:VAL:HB	2.46	0.45
1:D:371:ASP:OD1	1:D:373:HIS:HB3	2.15	0.45
1:D:442:LYS:HE3	8:D:1028:HOH:O	2.18	0.44
1:A:128:THR:HB	1:A:129:PRO:HD2	1.99	0.44
1:A:382[A]:ARG:NH2	8:A:624:HOH:O	2.50	0.44
1:B:433:GLU:OE1	1:B:465:PRO:HA	2.18	0.44
1:B:226:THR:HA	1:B:230:PHE:CD1	2.53	0.43
1:B:329:ARG:HD2	8:B:618:HOH:O	2.17	0.43
1:B:114:TRP:HB3	1:B:171:LEU:HD22	2.00	0.43
1:D:446:LYS:HD3	8:D:705:HOH:O	2.17	0.43
1:D:292:GLN:O	1:D:296:GLU:HG2	2.19	0.43
1:A:226:THR:HA	1:A:230:PHE:CD1	2.53	0.43
1:A:177:LYS:HB2	1:A:177:LYS:NZ	2.34	0.42
1:A:128:THR:HB	1:A:129:PRO:CD	2.49	0.42
1:D:225:VAL:HG21	1:D:473:TYR:CE1	2.54	0.42
1:A:396:VAL:HB	1:C:251[A]:MET:CE	2.49	0.42
1:C:291:LEU:O	1:C:295[A]:MET:HG2	2.20	0.41
1:A:159:LYS:HA	1:A:159:LYS:NZ	2.35	0.41
1:C:383:LEU:HD22	3:C:502:NAD:N7N	2.35	0.41
3:A:503:NAD:H8A	8:A:829:HOH:O	2.19	0.41
1:B:276:ALA:HA	5:D:504:PEG:H31	2.01	0.41
1:A:197:GLU:HB2	1:A:404:GLN:HE21	1.86	0.41
1:D:157:LEU:HB3	1:D:173:LYS:HE3	2.03	0.41
1:D:275:GLN:CB	5:D:504:PEG:H32	2.51	0.41
1:D:383:LEU:HD22	3:D:502:NAD:N7N	2.35	0.41
1:A:207:GLU:O	1:A:211:LYS:HG3	2.21	0.41
1:A:274:ARG:HD2	8:A:821:HOH:O	2.20	0.41
1:A:279[A]:ARG:NH1	8:A:615:HOH:O	2.43	0.41
1:B:310:ALA:HB3	1:B:313:PHE:CZ	2.56	0.41
1:D:325:ILE:HA	1:D:325:ILE:HD12	1.84	0.41
1:D:61:ILE:HD13	1:D:91:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:LYS:HE2	1:D:423:LYS:HB3	1.90	0.40
1:A:28:ALA:O	1:A:32:MET:HG3	2.21	0.40
1:C:49:LYS:HB2	1:C:49:LYS:HE3	1.86	0.40
1:C:187:ILE:O	1:C:191:ILE:HG12	2.21	0.40
1:C:183:TRP:O	1:C:186:GLU:HB3	2.21	0.40
1:B:431:LEU:HD23	1:B:431:LEU:HA	1.90	0.40
1:D:226:THR:HA	1:D:230:PHE:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	473/479 (99%)	461 (98%)	11 (2%)	1 (0%)	47 24
1	B	471/479 (98%)	458 (97%)	12 (2%)	1 (0%)	47 24
1	C	477/479 (100%)	463 (97%)	14 (3%)	0	100 100
1	D	477/479 (100%)	467 (98%)	10 (2%)	0	100 100
All	All	1898/1916 (99%)	1849 (97%)	47 (2%)	2 (0%)	51 26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	421	ALA
1	A	58	HIS

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	385/387 (100%)	379 (98%)	6 (2%)	62	33
1	B	385/387 (100%)	381 (99%)	4 (1%)	76	55
1	C	389/387 (100%)	383 (98%)	6 (2%)	65	36
1	D	389/387 (100%)	383 (98%)	6 (2%)	65	36
All	All	1548/1548 (100%)	1526 (99%)	22 (1%)	67	39

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

Mol	Chain	Res	Type
1	A	90	HIS
1	A	159	LYS
1	A	163	GLU
1	A	216	PHE
1	A	416	LYS
1	A	422	LYS
1	B	90	HIS
1	B	216	PHE
1	B	422	LYS
1	B	423	LYS
1	C	45	LYS
1	C	90	HIS
1	C	159	LYS
1	C	216	PHE
1	C	418	SER
1	C	446	LYS
1	D	40	GLU
1	D	45	LYS
1	D	181	LYS
1	D	216	PHE
1	D	469[A]	ASP
1	D	469[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 5 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	C	502	-	42,48,48	1.82	10 (23%)	50,73,73	1.57	9 (18%)
3	NAD	D	502	-	42,48,48	1.97	12 (28%)	50,73,73	1.64	8 (16%)
6	ACT	C	504	-	3,3,3	0.86	0	3,3,3	1.68	2 (66%)
3	NAD	B	502	-	42,48,48	1.78	14 (33%)	50,73,73	1.85	11 (22%)
4	ADE	A	504	-	9,11,11	0.70	0	7,15,15	1.12	1 (14%)
3	NAD	A	503	-	42,48,48	1.96	12 (28%)	50,73,73	1.34	8 (16%)
5	PEG	B	504	-	6,6,6	0.66	0	5,5,5	0.72	0
5	PEG	D	504	-	6,6,6	0.73	0	5,5,5	1.47	1 (20%)
7	3D1	C	503	-	18,20,20	1.63	5 (27%)	17,29,29	1.83	5 (29%)
5	PEG	A	505	-	6,6,6	0.82	0	5,5,5	1.00	0
4	ADE	B	503	-	9,11,11	1.26	2 (22%)	7,15,15	1.16	1 (14%)
6	ACT	B	505	-	3,3,3	1.02	0	3,3,3	1.13	0
7	3D1	D	503	-	18,20,20	1.38	2 (11%)	17,29,29	2.21	6 (35%)

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	NAD	C	502	-	-	5/26/62/62	0/5/5/5
3	NAD	D	502	-	-	5/26/62/62	0/5/5/5
3	NAD	B	502	-	-	5/26/62/62	0/5/5/5
4	ADE	A	504	-	-	-	0/2/2/2
3	NAD	A	503	-	-	5/26/62/62	0/5/5/5
5	PEG	B	504	-	-	2/4/4/4	-
5	PEG	D	504	-	-	3/4/4/4	-
7	3D1	C	503	-	-	0/2/18/18	0/3/3/3
5	PEG	A	505	-	-	1/4/4/4	-
7	3D1	D	503	-	-	1/2/18/18	0/3/3/3
4	ADE	B	503	-	-	-	0/2/2/2

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	NAD	C7N-N7N	5.28	1.43	1.33
3	A	503	NAD	C7N-N7N	5.23	1.43	1.33
3	D	502	NAD	C4N-C3N	4.62	1.47	1.39
3	C	502	NAD	C2N-N1N	4.59	1.40	1.35
3	A	503	NAD	C2B-C1B	-4.34	1.47	1.53
3	A	503	NAD	C4N-C3N	4.13	1.46	1.39
3	C	502	NAD	C2B-C1B	-4.09	1.47	1.53
3	B	502	NAD	C2N-N1N	4.07	1.39	1.35
3	C	502	NAD	C5N-C4N	4.04	1.47	1.38
3	A	503	NAD	C2B-C3B	-3.94	1.42	1.53
3	B	502	NAD	C5N-C4N	3.91	1.47	1.38
3	D	502	NAD	C2B-C1B	-3.91	1.47	1.53
3	D	502	NAD	C5N-C4N	3.68	1.46	1.38
3	A	503	NAD	C2N-N1N	3.63	1.39	1.35
3	B	502	NAD	C4N-C3N	3.63	1.45	1.39
3	C	502	NAD	C6A-N6A	3.46	1.46	1.34
3	D	502	NAD	C2B-C3B	-3.42	1.44	1.53
3	C	502	NAD	C7N-N7N	3.37	1.39	1.33
3	C	502	NAD	C2B-C3B	-3.27	1.44	1.53
3	B	502	NAD	C2B-C3B	-3.16	1.44	1.53
3	D	502	NAD	C6N-N1N	3.16	1.43	1.35
3	D	502	NAD	C6A-N6A	3.05	1.45	1.34
3	C	502	NAD	C4N-C3N	2.98	1.44	1.39
3	A	503	NAD	C6N-N1N	2.96	1.42	1.35
3	B	502	NAD	O4D-C1D	2.95	1.45	1.41
7	C	503	3D1	C4-N3	2.87	1.39	1.35
3	A	503	NAD	C8A-N7A	2.87	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	NAD	C6A-N6A	2.86	1.44	1.34
3	B	502	NAD	C6A-N6A	2.80	1.44	1.34
3	A	503	NAD	C5N-C4N	2.75	1.44	1.38
3	C	502	NAD	O4B-C4B	-2.72	1.38	1.45
3	B	502	NAD	C2A-N1A	2.71	1.38	1.33
3	C	502	NAD	O2B-C2B	2.68	1.49	1.43
3	D	502	NAD	C2N-N1N	2.63	1.38	1.35
7	C	503	3D1	C1'-N9	-2.60	1.41	1.49
3	D	502	NAD	O4D-C1D	2.57	1.44	1.41
7	D	503	3D1	C1'-N9	-2.54	1.41	1.49
3	B	502	NAD	C6N-N1N	2.51	1.41	1.35
3	D	502	NAD	C2A-N1A	2.48	1.38	1.33
3	B	502	NAD	C7N-N7N	2.45	1.37	1.33
3	A	503	NAD	C2D-C1D	-2.42	1.50	1.53
4	B	503	ADE	C4-N3	-2.39	1.33	1.37
7	C	503	3D1	C6-N6	2.39	1.42	1.34
3	B	502	NAD	C2B-C1B	-2.27	1.50	1.53
3	D	502	NAD	O4B-C4B	-2.27	1.39	1.45
4	B	503	ADE	C2-N3	2.25	1.35	1.32
3	C	502	NAD	C2A-N1A	2.21	1.38	1.33
7	C	503	3D1	O3'-C3'	2.20	1.48	1.43
3	B	502	NAD	C4A-N3A	2.20	1.38	1.35
7	D	503	3D1	C2-N1	2.16	1.37	1.33
3	B	502	NAD	O4B-C4B	-2.16	1.40	1.45
3	B	502	NAD	C6N-C5N	2.15	1.43	1.38
3	A	503	NAD	C2A-N3A	2.10	1.35	1.32
3	D	502	NAD	C8A-N7A	2.06	1.38	1.34
3	A	503	NAD	O4D-C1D	2.06	1.44	1.41
3	B	502	NAD	C2D-C1D	-2.04	1.50	1.53
7	C	503	3D1	C2-N1	2.00	1.37	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	NAD	C5N-C4N-C3N	-5.58	113.75	120.34
7	D	503	3D1	O4'-C1'-C2'	-4.86	97.07	106.25
3	D	502	NAD	N3A-C2A-N1A	-4.73	121.29	128.68
3	C	502	NAD	C4A-C5A-N7A	-4.70	104.50	109.40
3	C	502	NAD	C5N-C4N-C3N	-4.49	115.03	120.34
3	C	502	NAD	N3A-C2A-N1A	-4.44	121.74	128.68
3	B	502	NAD	O4D-C1D-C2D	-4.23	100.74	106.93
3	D	502	NAD	C5N-C4N-C3N	-4.16	115.42	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	503	3D1	N3-C2-N1	-4.14	122.20	128.68
3	A	503	NAD	N3A-C2A-N1A	-4.14	122.21	128.68
7	D	503	3D1	C4-C5-N7	-4.02	105.21	109.40
3	B	502	NAD	C4A-C5A-N7A	-3.89	105.34	109.40
3	B	502	NAD	C3B-C2B-C1B	3.77	106.66	100.98
3	B	502	NAD	N3A-C2A-N1A	-3.70	122.89	128.68
3	B	502	NAD	C2N-C3N-C4N	3.67	122.42	118.26
3	B	502	NAD	O4B-C1B-C2B	-3.64	101.61	106.93
3	D	502	NAD	O4B-C1B-C2B	-3.63	101.61	106.93
3	D	502	NAD	C6N-N1N-C2N	-3.58	118.71	121.97
7	D	503	3D1	O5'-C5'-C4'	-3.35	99.81	111.29
7	C	503	3D1	O4'-C1'-C2'	-3.22	100.17	106.25
3	A	503	NAD	C2N-C3N-C4N	3.21	121.90	118.26
3	C	502	NAD	C2N-C3N-C4N	3.20	121.89	118.26
3	D	502	NAD	C2N-C3N-C4N	3.14	121.81	118.26
7	D	503	3D1	C2'-C1'-N9	-3.12	107.07	114.27
3	C	502	NAD	O4D-C1D-C2D	-2.87	102.73	106.93
3	B	502	NAD	PN-O3-PA	-2.66	123.70	132.83
5	D	504	PEG	C3-O2-C2	2.66	124.80	113.29
3	A	503	NAD	C3N-C2N-N1N	-2.65	117.84	120.43
3	A	503	NAD	O4B-C1B-C2B	-2.56	103.19	106.93
7	D	503	3D1	C5-C6-N6	2.51	124.16	120.35
3	B	502	NAD	C6N-N1N-C2N	-2.49	119.70	121.97
7	C	503	3D1	C2'-C1'-N9	-2.42	108.69	114.27
3	A	503	NAD	C4A-C5A-N7A	-2.41	106.89	109.40
3	D	502	NAD	C3B-C2B-C1B	2.41	104.60	100.98
7	C	503	3D1	O5'-C5'-C4'	-2.40	103.04	111.29
3	D	502	NAD	C5N-C6N-N1N	2.35	123.78	120.40
4	A	504	ADE	C5-C6-N6	2.31	123.86	120.35
3	C	502	NAD	PN-O3-PA	-2.28	125.01	132.83
4	B	503	ADE	C5-C6-N6	2.24	123.76	120.35
3	C	502	NAD	O4B-C1B-C2B	-2.21	103.69	106.93
3	D	502	NAD	O4D-C1D-C2D	-2.21	103.69	106.93
7	D	503	3D1	C5'-C4'-C3'	-2.19	109.28	114.81
3	B	502	NAD	C3N-C7N-N7N	2.14	120.32	117.75
3	B	502	NAD	C5A-C6A-N6A	-2.13	117.11	120.35
3	A	503	NAD	O7N-C7N-N7N	-2.10	119.59	122.58
6	C	504	ACT	OXT-C-CH3	2.08	123.76	115.18
3	C	502	NAD	O4B-C4B-C3B	2.06	109.18	105.11
7	C	503	3D1	C2-N1-C6	2.04	122.25	118.75
3	A	503	NAD	C2N-N1N-C1D	-2.03	114.61	119.14
3	A	503	NAD	PN-O3-PA	-2.03	125.88	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	504	ACT	OXT-C-O	-2.03	114.59	122.05
3	C	502	NAD	C5A-C6A-N6A	-2.01	117.30	120.35

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	NAD	O4D-C1D-N1N-C2N
3	A	503	NAD	O4D-C1D-N1N-C6N
3	A	503	NAD	C2D-C1D-N1N-C2N
3	A	503	NAD	C2D-C1D-N1N-C6N
3	B	502	NAD	O4D-C1D-N1N-C2N
3	B	502	NAD	O4D-C1D-N1N-C6N
3	B	502	NAD	C2D-C1D-N1N-C2N
3	B	502	NAD	C2D-C1D-N1N-C6N
3	C	502	NAD	O4D-C1D-N1N-C2N
3	C	502	NAD	O4D-C1D-N1N-C6N
3	C	502	NAD	C2D-C1D-N1N-C2N
3	C	502	NAD	C2D-C1D-N1N-C6N
3	D	502	NAD	O4D-C1D-N1N-C2N
3	D	502	NAD	O4D-C1D-N1N-C6N
3	D	502	NAD	C2D-C1D-N1N-C2N
3	D	502	NAD	C2D-C1D-N1N-C6N
5	A	505	PEG	O1-C1-C2-O2
5	D	504	PEG	O2-C3-C4-O4
5	B	504	PEG	O1-C1-C2-O2
5	D	504	PEG	O1-C1-C2-O2
5	B	504	PEG	C1-C2-O2-C3
5	D	504	PEG	C1-C2-O2-C3
3	A	503	NAD	O4B-C4B-C5B-O5B
3	B	502	NAD	O4B-C4B-C5B-O5B
3	C	502	NAD	O4B-C4B-C5B-O5B
3	D	502	NAD	O4B-C4B-C5B-O5B
7	D	503	3D1	O4'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 34 short contacts:

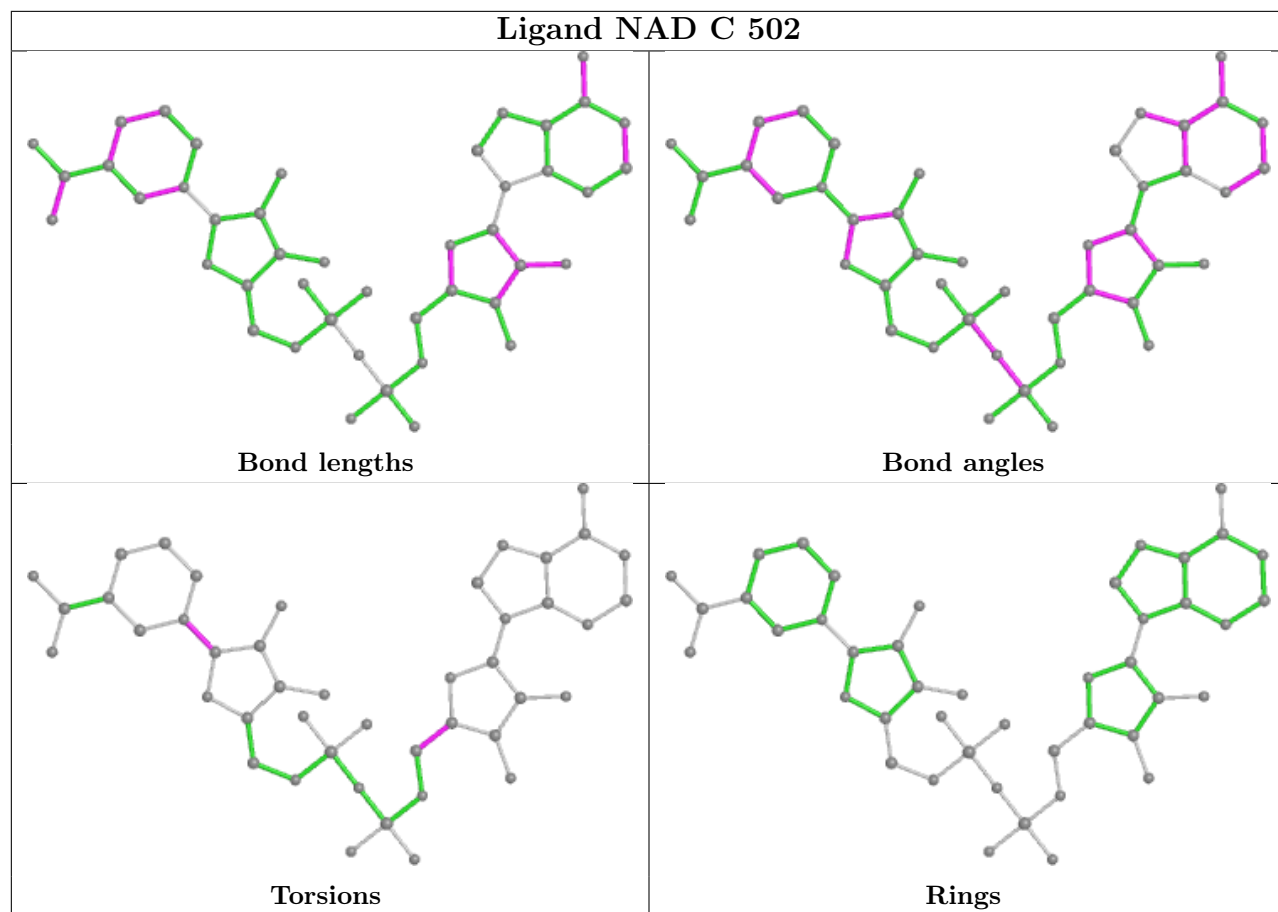
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	NAD	2	0
3	D	502	NAD	2	0

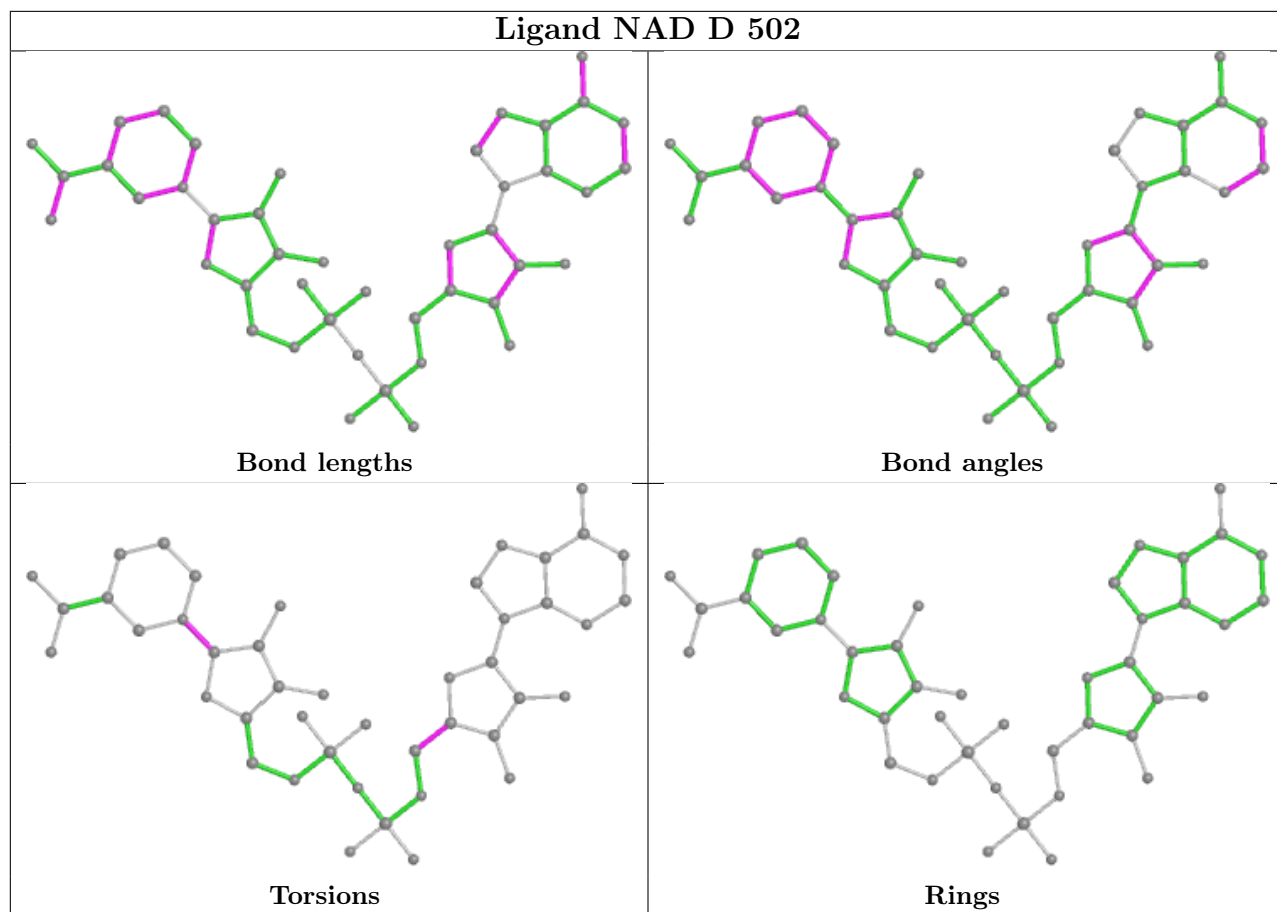
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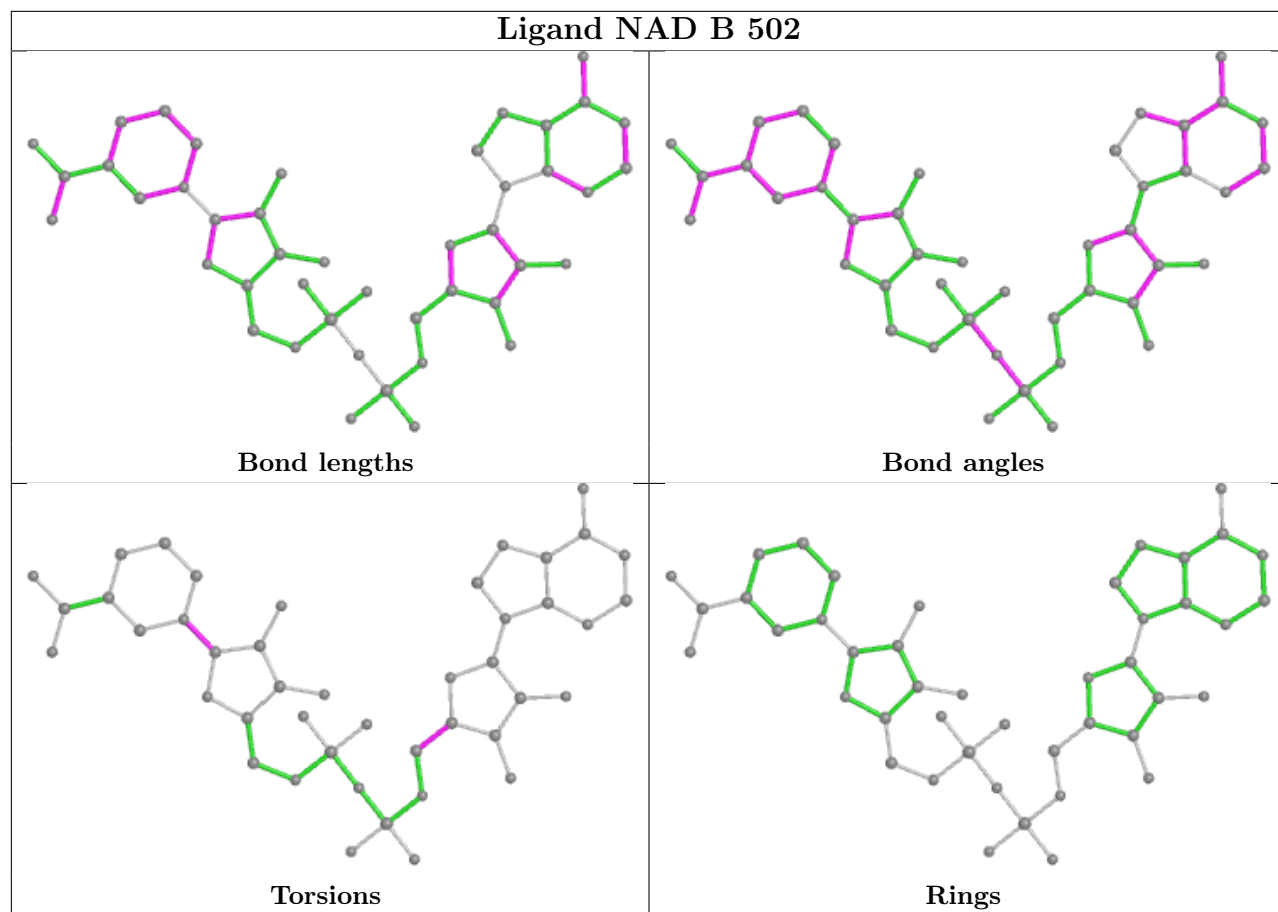
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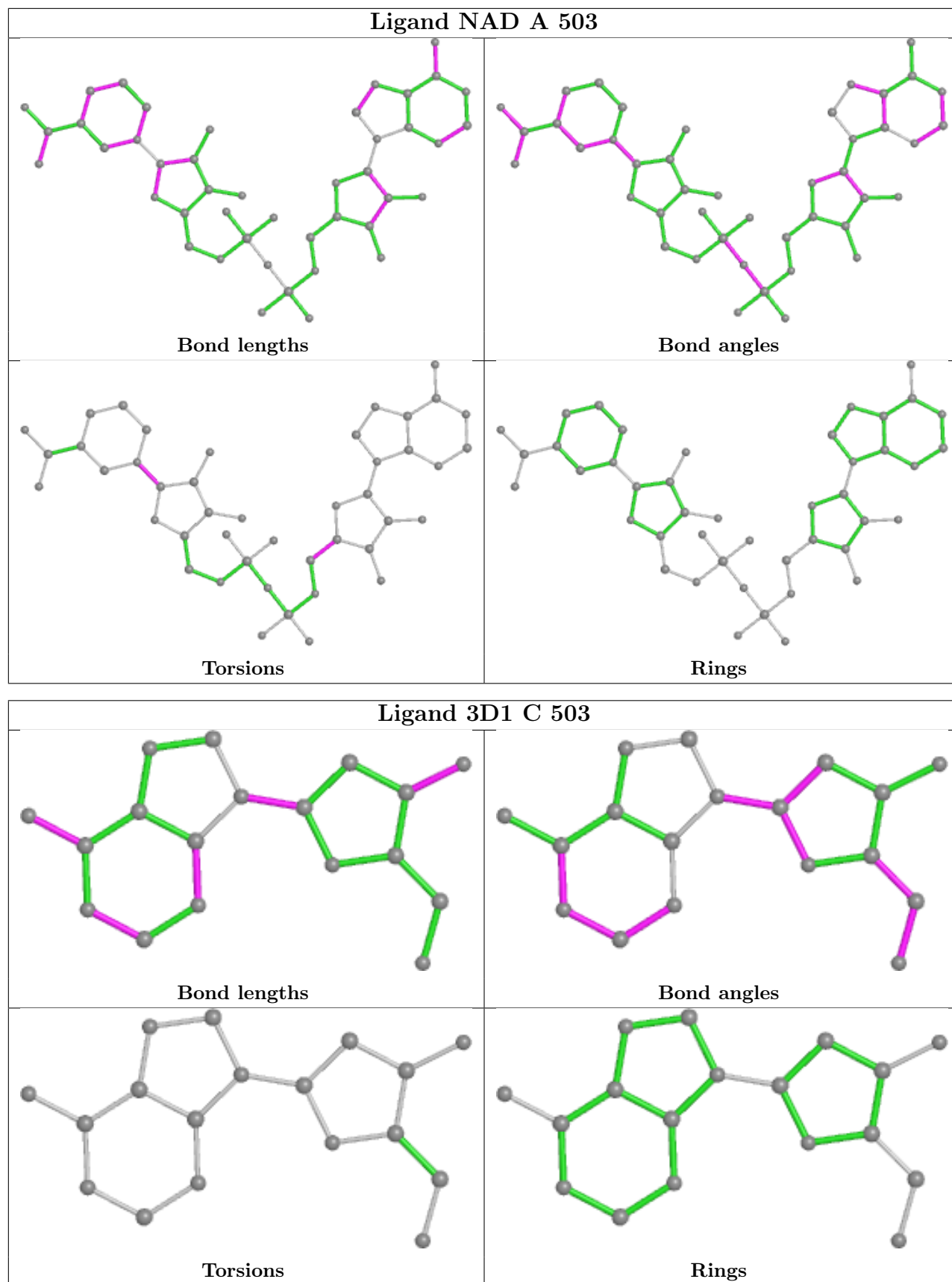
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	NAD	1	0
4	A	504	ADE	1	0
3	A	503	NAD	1	0
5	B	504	PEG	3	0
5	D	504	PEG	9	0
7	C	503	3D1	3	0
5	A	505	PEG	10	0
7	D	503	3D1	4	0

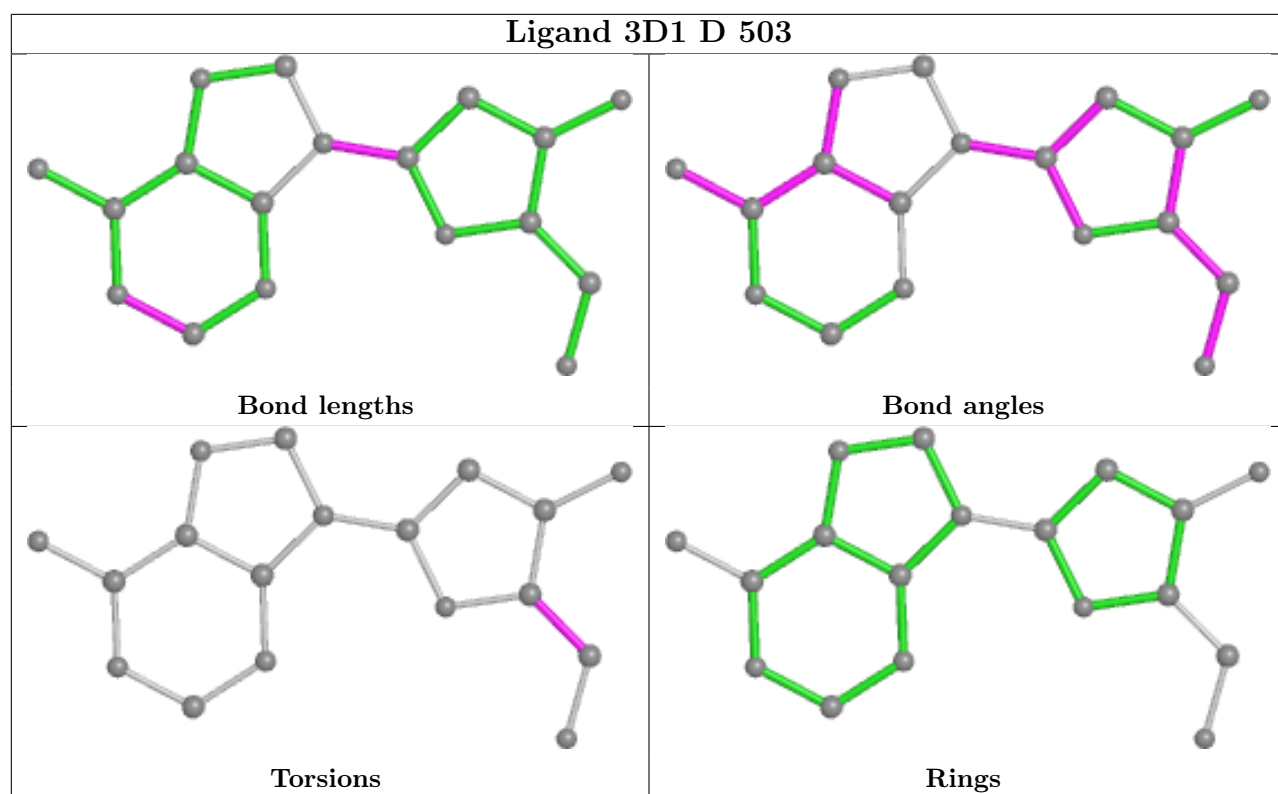
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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	468/479 (97%)	-0.76	2 (0%) 92 94	11, 18, 40, 66	1 (0%)
1	B	463/479 (96%)	-0.76	1 (0%) 95 95	11, 17, 37, 68	1 (0%)
1	C	468/479 (97%)	-0.73	0 100 100	11, 20, 43, 86	0
1	D	470/479 (98%)	-0.66	0 100 100	11, 20, 42, 70	0
All	All	1869/1916 (97%)	-0.73	3 (0%) 95 95	11, 19, 40, 86	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	420	TYR	2.8
1	A	161	GLY	2.7
1	A	7	PHE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

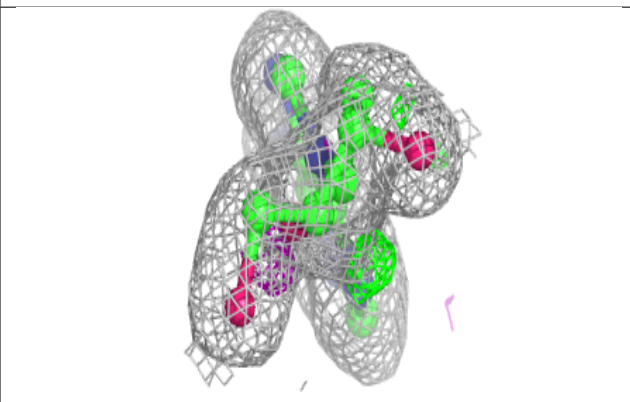
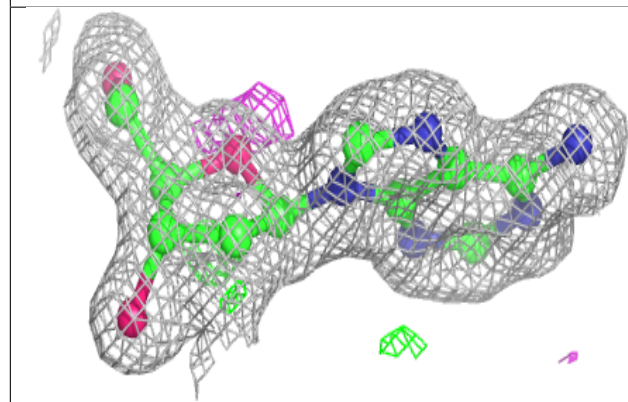
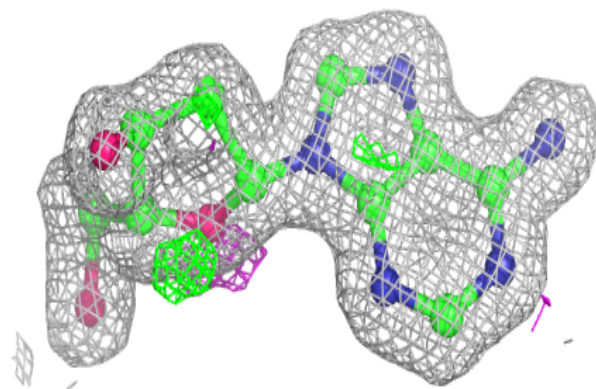
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PEG	B	504	7/7	0.80	0.21	45,50,55,56	0
6	ACT	B	505	4/4	0.89	0.13	31,32,35,37	0
5	PEG	A	505	7/7	0.90	0.20	15,18,24,27	7
5	PEG	D	504	7/7	0.91	0.24	14,18,20,36	7
6	ACT	C	504	4/4	0.94	0.14	27,35,36,37	0
7	3D1	C	503	18/18	0.97	0.06	12,15,27,30	0
7	3D1	D	503	18/18	0.97	0.07	11,14,26,29	0
3	NAD	C	502	44/44	0.98	0.05	10,15,18,20	0
3	NAD	D	502	44/44	0.98	0.06	10,14,19,19	0
4	ADE	B	503	10/10	0.98	0.04	11,11,13,14	0
3	NAD	A	503	44/44	0.98	0.06	12,15,17,19	0
3	NAD	B	502	44/44	0.98	0.05	12,15,18,18	0
2	NA	A	502	1/1	0.99	0.07	24,24,24,24	0
4	ADE	A	504	10/10	0.99	0.05	10,11,12,13	0
2	NA	B	501	1/1	1.00	0.04	13,13,13,13	0
2	NA	C	501	1/1	1.00	0.04	14,14,14,14	0
2	NA	D	501	1/1	1.00	0.03	14,14,14,14	0
2	NA	A	501	1/1	1.00	0.04	13,13,13,13	0

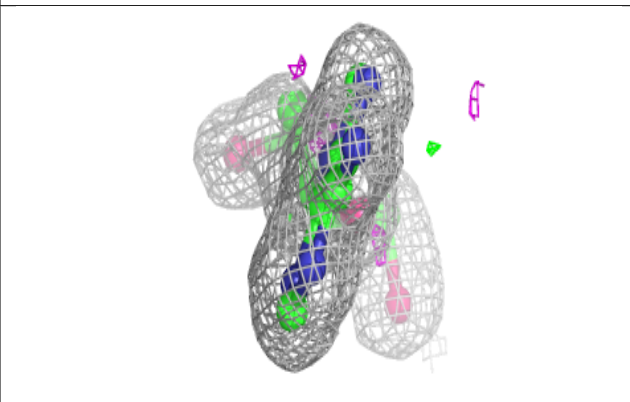
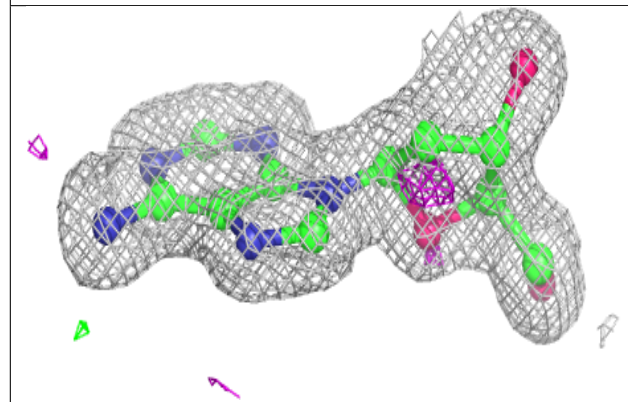
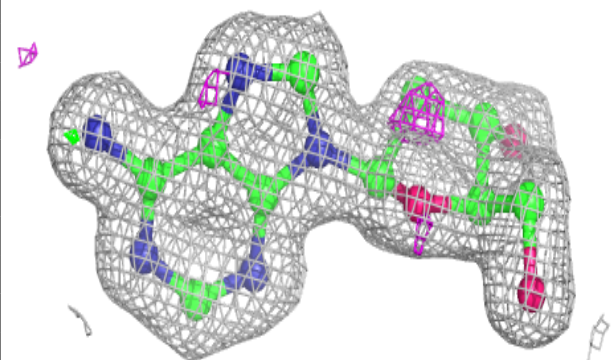
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 3D1 C 503:

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

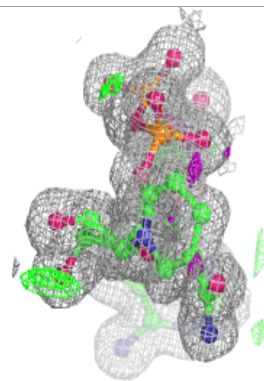
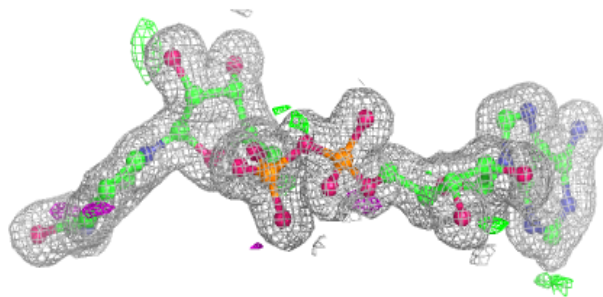
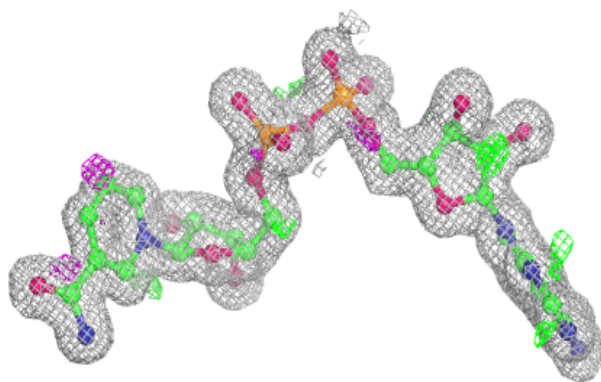
**Electron density around 3D1 D 503:**

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

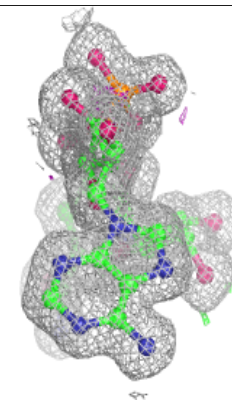
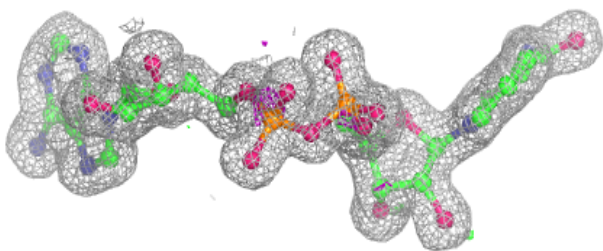
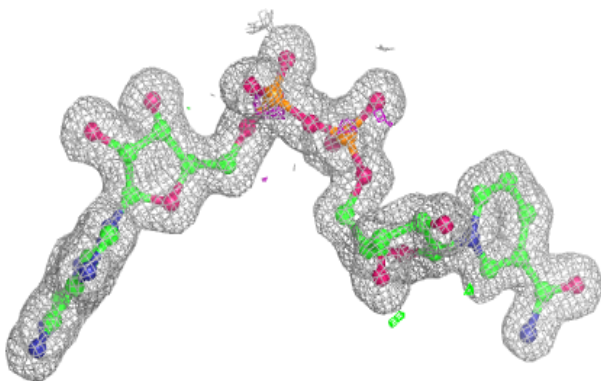


Electron density around NAD C 502:

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

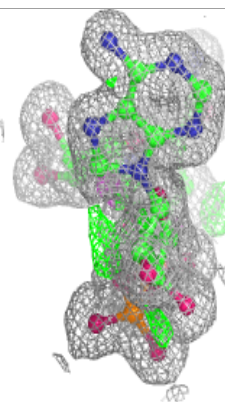
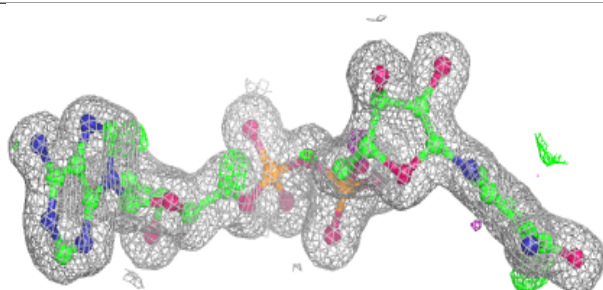
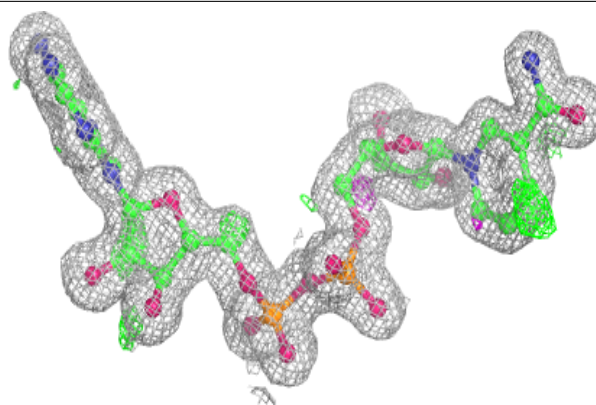
**Electron density around NAD D 502:**

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

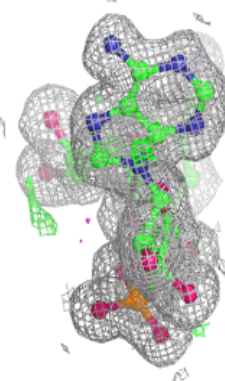
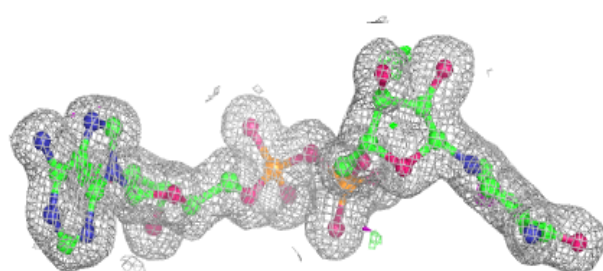
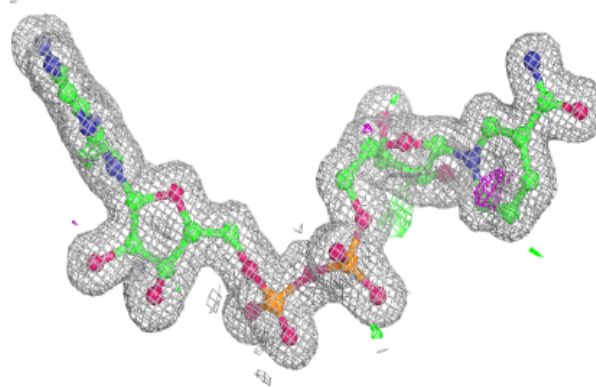


Electron density around NAD A 503:

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

**Electron density around NAD B 502:**

$2mF_o-DF_c$ (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.