Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 03:20 PM EDT

PDB ID	:	3DHY
Title	:	Crystal Structures of Mycobacterium tuberculosis S-Adenosyl-L-Homocysteine Hydrolase in Ternary Complex with Substrate and Inhibitors
Authors	:	Shetty, N.D.; Ioerger, T.R.; Gokulan, K.; Reddy, M.C.M.; Owen, J.L.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on	:	2008-06-19
Resolution	:	2.00 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:

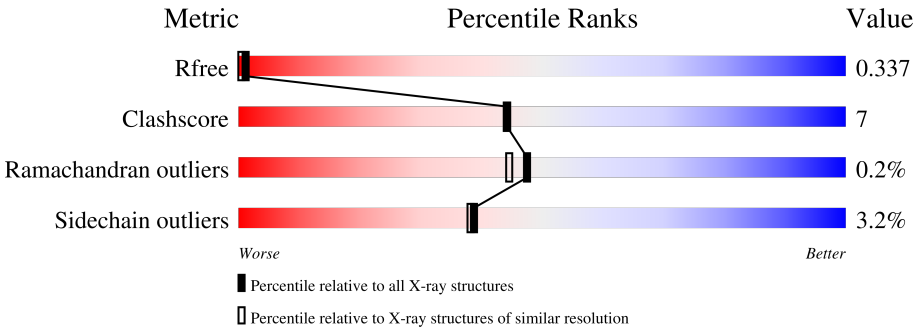
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	495	80% 18% ·
1	B	495	86% 12% ·
1	C	495	81% 15% ··
1	D	495	80% 17% ··

2 Entry composition (i)

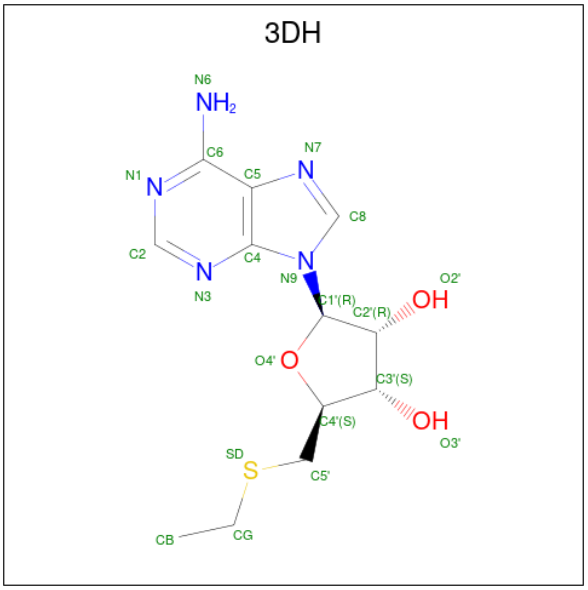
There are 4 unique types of molecules in this entry. The entry contains 15608 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	486	Total	C	N	O	S	0	0	0
			3754	2367	644	726	17			
1	B	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			
1	C	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			
1	D	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			

- Molecule 2 is 5'-S-ethyl-5'-thioadenosine (three-letter code: 3DH) (formula: $C_{12}H_{17}N_5O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			21	12	5	3	1		
2	B	1	Total	C	N	O	S	0	0
			21	12	5	3	1		

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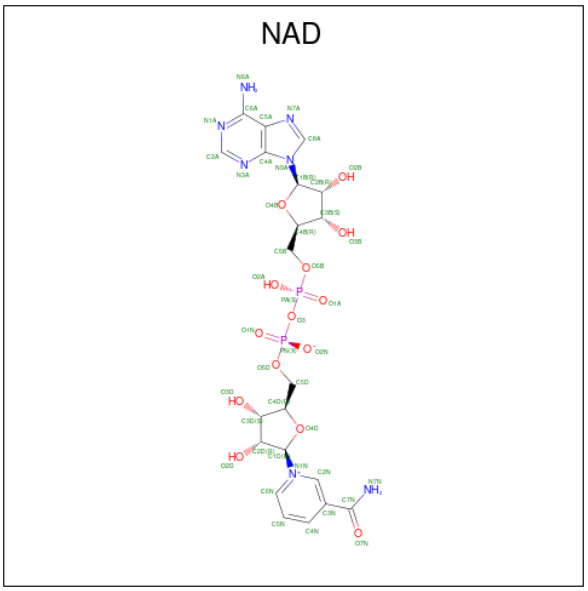
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			21	12	5	3	1		
2	D	1	Total	C	N	O	S	0	0
			21	12	5	3	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total	O	0	0
			72	72		
4	B	90	Total	O	0	0
			90	90		
4	C	91	Total	O	0	0
			91	91		

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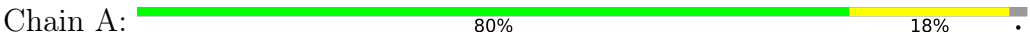
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	97	Total O 97 97	0	0

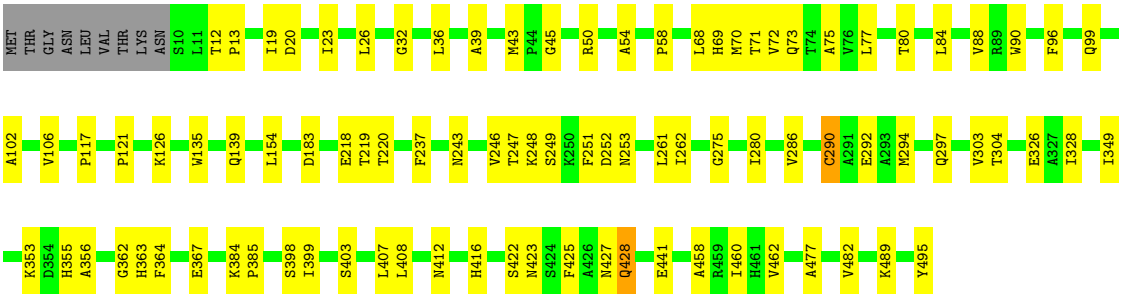
3 Residue-property plots (i)

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. 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. 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

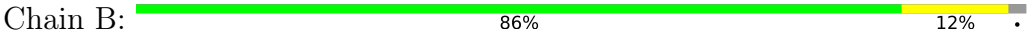
Chain A:





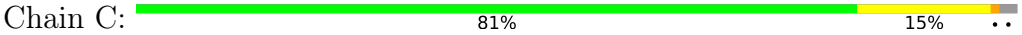
• Molecule 1: Adenosylhomocysteinase

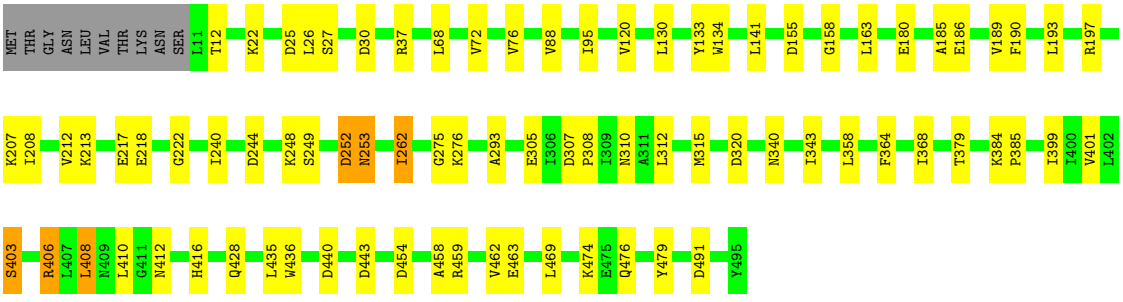
Chain B:



• Molecule 1: Adenosylhomocysteinase

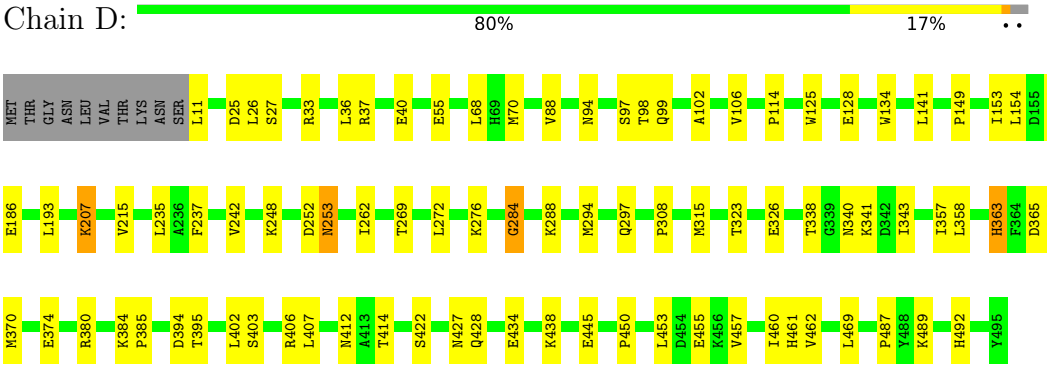
Chain C:





• Molecule 1: Adenosylhomocysteinase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.20Å 111.69Å 100.13Å 90.00° 96.01° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 47.97 – 1.19	Depositor EDS
% Data completeness (in resolution range)	82.5 (30.00-2.00) 58.8 (47.97-1.19)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 1.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.260 , 0.340 0.260 , 0.337	Depositor DCC
R_{free} test set	19267 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	6.6	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 63.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	15608	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3DH, 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	0.64	1/3830 (0.0%)	0.70	0/5194
1	B	0.67	2/3824 (0.1%)	0.75	0/5186
1	C	0.67	1/3824 (0.0%)	0.77	1/5186 (0.0%)
1	D	0.68	0/3824	0.76	1/5186 (0.0%)
All	All	0.67	4/15302 (0.0%)	0.75	2/20752 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	207	LYS	CD-CE	9.13	1.74	1.51
1	B	305	GLU	CG-CD	-6.25	1.42	1.51
1	A	290	CYS	CB-SG	-6.04	1.72	1.82
1	B	290	CYS	CB-SG	-5.15	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	284	GLY	N-CA-C	-5.71	98.83	113.10
1	C	26	LEU	CA-CB-CG	5.01	126.83	115.30

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	3754	0	3698	59	0
1	B	3748	0	3693	35	0
1	C	3748	0	3693	54	0
1	D	3748	0	3693	63	0
2	A	21	0	17	2	0
2	B	21	0	17	1	0
2	C	21	0	17	2	0
2	D	21	0	17	2	0
3	A	44	0	26	6	0
3	B	44	0	26	1	0
3	C	44	0	26	3	0
3	D	44	0	26	1	0
4	A	72	0	0	0	0
4	B	90	0	0	0	0
4	C	91	0	0	1	0
4	D	97	0	0	0	0
All	All	15608	0	14949	200	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 7.

All (200) 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:248:LYS:HZ3	1:D:253:ASN:HD21	1.23	0.86
1:D:248:LYS:NZ	1:D:253:ASN:HD21	1.73	0.86
1:C:218:GLU:HB2	1:C:428:GLN:HE21	1.42	0.85
1:C:248:LYS:NZ	1:C:253:ASN:HD21	1.74	0.84
1:C:248:LYS:HZ2	1:C:253:ASN:HD21	1.22	0.83
1:B:338:THR:HG21	1:B:343:ILE:HD12	1.62	0.82
1:C:479:TYR:OH	1:D:363:HIS:HE1	1.60	0.82
1:D:253:ASN:HD22	1:D:253:ASN:H	1.25	0.82
1:B:135:TRP:O	1:B:139:GLN:HG2	1.89	0.72
1:A:403:SER:OG	1:A:412:ASN:ND2	2.23	0.72
1:A:423:ASN:O	1:A:427:ASN:ND2	2.24	0.70
1:C:403:SER:OG	1:C:412:ASN:ND2	2.25	0.70
2:A:500:3DH:H3'	3:A:550:NAD:C4N	2.21	0.69
1:C:134:TRP:HE1	1:C:186:GLU:HG2	1.59	0.68
1:D:253:ASN:HD22	1:D:253:ASN:N	1.92	0.67
2:C:500:3DH:H3'	3:C:550:NAD:C4N	2.25	0.67
1:C:252:ASP:C	1:C:252:ASP:OD1	2.34	0.66
1:D:248:LYS:HZ3	1:D:253:ASN:ND2	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ASP:O	1:A:121:PRO:HB3	1.96	0.65
2:B:500:3DH:H3'	3:B:550:NAD:C4N	2.27	0.65
1:C:406:ARG:HH21	1:C:406:ARG:HG3	1.62	0.64
1:A:58:PRO:HD2	1:A:84:LEU:HB3	1.79	0.64
1:A:135:TRP:O	1:A:139:GLN:HG2	1.98	0.64
1:C:248:LYS:NZ	1:C:253:ASN:ND2	2.46	0.64
1:B:489:LYS:HD2	1:B:493:TYR:CD2	2.32	0.63
1:D:323:THR:OG1	1:D:326:GLU:HG2	1.98	0.63
1:A:19:ILE:HD12	1:A:117:PRO:HB2	1.81	0.62
1:D:134:TRP:HB3	1:D:193:LEU:HD13	1.80	0.62
1:A:70:MET:HE1	1:A:90:TRP:CD1	2.36	0.61
1:C:305:GLU:OE2	3:C:550:NAD:O2B	2.11	0.61
1:C:384:LYS:HB2	1:C:385:PRO:HD2	1.82	0.61
1:B:300:ARG:HD2	1:C:320:ASP:OD1	2.00	0.60
1:D:422:SER:HB3	1:D:461:HIS:NE2	2.16	0.60
1:A:262:ILE:HD13	1:A:294:MET:CE	2.31	0.60
1:A:77:LEU:HD13	1:A:425:PHE:HB3	1.83	0.60
1:B:249:SER:O	1:B:253:ASN:HB2	2.01	0.60
1:B:275:GLY:HA2	1:C:315:MET:O	2.02	0.59
1:B:440:ASP:OD2	1:B:441:GLU:HG3	2.01	0.59
1:A:247:THR:HA	1:A:251:PHE:HD2	1.68	0.59
1:B:197:ARG:HD2	1:B:204:LYS:HD2	1.83	0.58
1:C:310:ASN:HD21	1:D:489:LYS:HE2	1.68	0.58
1:B:363:HIS:CD2	1:B:364:PHE:CD2	2.92	0.58
1:A:349:ILE:HG23	1:A:399:ILE:HD13	1.84	0.58
1:C:406:ARG:HH21	1:C:406:ARG:CG	2.16	0.58
1:D:94:ASN:HB3	1:D:97:SER:OG	2.04	0.58
1:C:459:ARG:O	1:C:463:GLU:HG2	2.04	0.58
1:C:479:TYR:OH	1:D:363:HIS:CE1	2.49	0.58
1:D:402:LEU:HB3	1:D:412:ASN:ND2	2.19	0.58
1:A:23:ILE:HD11	1:A:26:LEU:HD13	1.86	0.57
1:A:353:LYS:HG3	1:A:356:ALA:HB2	1.85	0.57
1:A:218:GLU:O	1:A:248:LYS:HE3	2.04	0.57
1:C:253:ASN:H	1:C:253:ASN:HD22	1.52	0.57
1:D:235:LEU:HD23	1:D:445:GLU:HA	1.85	0.57
1:C:244:ASP:OD2	1:D:492:HIS:HE1	1.87	0.57
1:D:36:LEU:O	1:D:40:GLU:HG3	2.05	0.57
1:C:340:ASN:HB3	1:C:343:ILE:HD11	1.87	0.57
1:D:363:HIS:O	1:D:363:HIS:CD2	2.58	0.57
1:D:102:ALA:O	1:D:106:VAL:HG23	2.05	0.56
1:D:363:HIS:NE2	1:D:366:ASN:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LEU:C	1:B:193:LEU:HD23	2.26	0.56
1:D:33:ARG:O	1:D:37:ARG:HG3	2.06	0.56
1:B:56:VAL:HG12	1:B:58:PRO:HD3	1.88	0.56
1:A:326:GLU:OE2	1:B:468:HIS:ND1	2.35	0.55
1:B:477:ALA:HB1	1:B:482:VAL:O	2.07	0.55
1:A:304:THR:OG1	3:A:550:NAD:H2A	2.07	0.55
1:D:68:LEU:HD12	1:D:154:LEU:CD2	2.36	0.55
1:D:262:ILE:CD1	1:D:294:MET:HE2	2.37	0.55
1:A:102:ALA:O	1:A:106:VAL:HG23	2.07	0.55
1:A:262:ILE:CD1	1:A:294:MET:HE2	2.37	0.55
1:A:477:ALA:HB1	1:A:482:VAL:O	2.07	0.55
1:C:217:GLU:CD	1:C:222:GLY:HA3	2.28	0.54
1:A:363:HIS:CD2	1:A:364:PHE:HD2	2.25	0.54
1:C:185:ALA:O	1:C:189:VAL:HG23	2.07	0.54
1:C:240:ILE:HG13	1:C:435:LEU:HD11	1.89	0.54
1:B:315:MET:O	1:C:275:GLY:HA2	2.08	0.54
1:C:130:LEU:HD22	1:C:186:GLU:HG3	1.89	0.54
1:C:155:ASP:OD2	1:C:158:GLY:HA2	2.07	0.54
1:A:262:ILE:HD13	1:A:294:MET:HE2	1.90	0.54
1:B:262:ILE:HD12	1:D:297:GLN:NE2	2.22	0.54
1:B:214:GLY:HA3	1:B:435:LEU:HD13	1.88	0.54
2:C:500:3DH:H3'	3:C:550:NAD:C3N	2.37	0.54
1:C:249:SER:O	1:C:253:ASN:HB2	2.08	0.53
1:A:243:ASN:HA	1:A:248:LYS:HG2	1.91	0.53
1:B:489:LYS:HD2	1:B:493:TYR:CE2	2.43	0.53
1:A:407:LEU:HD22	3:A:550:NAD:N7N	2.23	0.53
1:A:407:LEU:CD2	3:A:550:NAD:N7N	2.72	0.53
1:C:218:GLU:O	1:C:248:LYS:HE3	2.10	0.52
1:D:272:LEU:O	1:D:276:LYS:HG3	2.10	0.52
1:D:402:LEU:HB3	1:D:412:ASN:HD21	1.74	0.52
1:C:276:LYS:NZ	4:C:610:HOH:O	2.42	0.52
1:A:275:GLY:HA2	1:D:315:MET:O	2.10	0.52
1:A:384:LYS:HB2	1:A:385:PRO:HD2	1.92	0.51
1:D:134:TRP:HE1	1:D:186:GLU:HG2	1.75	0.51
1:C:308:PRO:HB3	1:D:469:LEU:HD11	1.92	0.51
1:D:262:ILE:HD13	1:D:294:MET:CE	2.41	0.51
1:C:358:LEU:HG	1:C:368:ILE:HD13	1.93	0.51
1:A:384:LYS:HB2	1:A:385:PRO:CD	2.41	0.50
1:B:20:ASP:O	1:B:121:PRO:HB3	2.11	0.50
1:D:26:LEU:HB3	1:D:114:PRO:HB3	1.93	0.50
1:A:458:ALA:O	1:A:462:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLY:O	1:A:36:LEU:HD13	2.12	0.50
1:C:399:ILE:HD12	1:C:401:VAL:HG23	1.94	0.50
1:D:338:THR:HG21	1:D:343:ILE:HD12	1.93	0.50
1:D:99:GLN:NE2	1:D:414:THR:HB	2.27	0.49
1:A:246:VAL:HG21	1:A:495:TYR:CE1	2.46	0.49
1:D:68:LEU:HG	1:D:156:ASP:HB2	1.95	0.49
2:D:500:3DH:H3'	3:D:550:NAD:C4N	2.42	0.49
1:B:338:THR:HG21	1:B:343:ILE:CD1	2.38	0.49
1:B:39:ALA:O	1:B:43:MET:HG3	2.13	0.49
1:C:25:ASP:OD1	1:C:27:SER:OG	2.29	0.49
1:C:458:ALA:O	1:C:462:VAL:HG23	2.12	0.49
1:C:262:ILE:HG13	1:C:293:ALA:HB1	1.94	0.49
1:C:252:ASP:OD1	1:C:416:HIS:CE1	2.67	0.48
1:B:340:ASN:O	1:B:367:GLU:HG2	2.15	0.47
1:C:248:LYS:HZ3	1:C:253:ASN:ND2	2.12	0.47
1:B:133:TYR:OH	1:B:159:ASP:OD2	2.20	0.47
1:B:163:LEU:HD12	1:B:194:LEU:HD21	1.97	0.47
1:D:253:ASN:N	1:D:253:ASN:ND2	2.61	0.47
1:C:72:VAL:O	1:C:76:VAL:HG23	2.15	0.46
1:D:450:PRO:HG2	1:D:453:LEU:HD12	1.97	0.46
1:D:284:GLY:O	1:D:288:LYS:HG3	2.15	0.46
1:B:363:HIS:HD2	1:B:364:PHE:CD2	2.34	0.46
1:C:406:ARG:CG	1:C:406:ARG:NH2	2.78	0.46
1:C:134:TRP:HB3	1:C:193:LEU:HD13	1.98	0.46
1:B:145:ASP:OD2	1:B:148:LYS:HE3	2.16	0.46
1:A:71:THR:HG22	1:A:99:GLN:NE2	2.31	0.46
1:C:218:GLU:HB2	1:C:428:GLN:NE2	2.20	0.46
1:D:253:ASN:H	1:D:253:ASN:ND2	2.03	0.45
1:A:303:VAL:HG12	1:A:304:THR:N	2.32	0.45
1:C:208:ILE:O	1:C:212:VAL:HG23	2.16	0.45
1:D:125:TRP:O	1:D:128:GLU:HG3	2.17	0.45
1:D:153:ILE:HB	1:D:215:VAL:HG23	1.98	0.45
1:D:358:LEU:HG	1:D:368:ILE:HD13	1.99	0.45
1:A:68:LEU:HD12	1:A:154:LEU:HD22	1.97	0.45
1:B:363:HIS:CD2	1:B:364:PHE:HD2	2.34	0.45
1:D:406:ARG:O	1:D:407:LEU:C	2.55	0.45
1:A:45:GLY:H	1:A:422:SER:HG	1.64	0.45
1:A:407:LEU:HD11	2:A:500:3DH:SD	2.56	0.45
1:D:156:ASP:OD1	2:D:500:3DH:H4'	2.17	0.45
1:C:408:LEU:C	1:C:408:LEU:HD12	2.37	0.45
1:A:73:GLN:H	1:A:73:GLN:CD	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:HIS:N	1:A:398:SER:O	2.46	0.44
1:A:262:ILE:HD12	1:A:297:GLN:HG3	1.99	0.44
1:A:428:GLN:HE21	1:A:428:GLN:HA	1.82	0.44
1:A:407:LEU:HD22	3:A:550:NAD:H72N	1.82	0.44
1:D:149:PRO:HG2	1:D:207:LYS:HD2	1.99	0.44
1:D:242:VAL:HG13	1:D:427:ASN:HB3	1.99	0.44
1:A:247:THR:HA	1:A:251:PHE:CD2	2.50	0.44
1:A:280:ILE:HD12	1:A:290:CYS:HB3	2.00	0.44
1:A:68:LEU:HD12	1:A:154:LEU:CD2	2.48	0.44
1:D:384:LYS:HB2	1:D:385:PRO:HD2	1.99	0.44
1:C:163:LEU:HD12	1:C:190:PHE:CE1	2.53	0.43
1:D:70:MET:HB3	1:D:98:THR:HG23	1.99	0.43
1:D:363:HIS:CD2	1:D:363:HIS:C	2.91	0.43
1:D:365:ASP:HB3	1:D:406:ARG:HG2	2.01	0.43
1:C:312:LEU:HB2	1:D:462:VAL:HG23	2.01	0.43
1:C:384:LYS:HB2	1:C:385:PRO:CD	2.46	0.43
1:A:96:PHE:O	1:A:126:LYS:NZ	2.51	0.43
1:D:370:MET:O	1:D:374:GLU:HG3	2.19	0.43
1:A:428:GLN:HE21	1:A:428:GLN:CA	2.32	0.43
1:C:358:LEU:HG	1:C:368:ILE:CD1	2.49	0.43
1:B:430:ILE:CG2	1:B:453:LEU:HD13	2.49	0.43
1:C:95:ILE:HG22	1:C:133:TYR:HB2	2.01	0.43
1:C:141:LEU:HD12	1:C:163:LEU:HD23	2.00	0.43
1:A:72:VAL:O	1:A:75:ALA:HB3	2.19	0.42
1:D:141:LEU:HD12	1:D:163:LEU:HD23	2.01	0.42
1:C:213:LYS:HD3	1:C:436:TRP:CZ3	2.54	0.42
1:D:457:VAL:HA	1:D:460:ILE:HD12	2.01	0.42
1:D:207:LYS:O	1:D:207:LYS:HD3	2.20	0.42
1:A:362:GLY:HA3	1:A:367:GLU:OE2	2.20	0.42
1:C:476:GLN:HG2	1:D:340:ASN:HD21	1.83	0.42
1:A:45:GLY:HA2	1:A:460:ILE:HG21	2.01	0.42
1:C:307:ASP:OD1	1:C:308:PRO:HD2	2.19	0.42
1:A:246:VAL:HG11	1:B:309:ILE:HG21	2.02	0.41
1:A:286:VAL:HG21	3:A:550:NAD:C6N	2.49	0.41
1:A:39:ALA:O	1:A:43:MET:HG3	2.20	0.41
1:A:70:MET:CE	1:A:90:TRP:CD1	3.01	0.41
1:A:252:ASP:OD1	1:A:416:HIS:CE1	2.73	0.41
1:B:243:ASN:O	1:B:249:SER:HB3	2.21	0.41
1:C:305:GLU:HG3	1:C:307:ASP:H	1.85	0.41
1:D:269:THR:HG21	1:D:357:ILE:HD11	2.01	0.41
1:D:455:GLU:OE1	1:D:487:PRO:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:THR:OG1	1:B:343:ILE:HD11	2.20	0.41
1:D:25:ASP:OD1	1:D:27:SER:OG	2.27	0.41
1:A:80:THR:O	1:A:84:LEU:HG	2.21	0.41
1:B:134:TRP:HE1	1:B:186:GLU:CG	2.34	0.41
1:D:434:GLU:OE1	1:D:438:LYS:HD2	2.20	0.41
1:D:394:ASP:OD1	1:D:395:THR:N	2.53	0.41
1:A:489:LYS:HE2	1:B:310:ASN:HD21	1.86	0.41
1:C:469:LEU:HD21	1:D:308:PRO:HA	2.03	0.41
1:A:50:ARG:O	1:A:54:ALA:HB2	2.20	0.41
1:A:261:LEU:HD12	1:A:408:LEU:HD11	2.02	0.41
1:B:252:ASP:C	1:B:252:ASP:OD1	2.60	0.41
1:D:163:LEU:HD11	1:D:193:LEU:HD22	2.02	0.41
1:B:402:LEU:HB3	1:B:412:ASN:ND2	2.36	0.41
1:D:450:PRO:CG	1:D:453:LEU:HD12	2.51	0.40
1:D:403:SER:OG	1:D:412:ASN:ND2	2.54	0.40
1:A:249:SER:O	1:A:253:ASN:HB2	2.22	0.40
1:B:406:ARG:O	1:B:407:LEU:C	2.60	0.40
1:A:12:THR:HA	1:A:13:PRO:HD3	1.95	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	484/495 (98%)	462 (96%)	21 (4%)	1 (0%)	47	44
1	B	483/495 (98%)	463 (96%)	20 (4%)	0	100	100
1	C	483/495 (98%)	463 (96%)	18 (4%)	2 (0%)	34	30
1	D	483/495 (98%)	460 (95%)	22 (5%)	1 (0%)	47	44
All	All	1933/1980 (98%)	1848 (96%)	81 (4%)	4 (0%)	47	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	D	252	ASP
1	C	364	PHE
1	C	403	SER

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	396/404 (98%)	387 (98%)	9 (2%)	50	53
1	B	395/404 (98%)	384 (97%)	11 (3%)	43	44
1	C	395/404 (98%)	374 (95%)	21 (5%)	22	18
1	D	395/404 (98%)	385 (98%)	10 (2%)	47	49
All	All	1581/1616 (98%)	1530 (97%)	51 (3%)	39	38

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	VAL
1	A	183	ASP
1	A	219	THR
1	A	220	THR
1	A	237	PHE
1	A	292	GLU
1	A	328	ILE
1	A	428	GLN
1	A	441	GLU
1	B	11	LEU
1	B	16	ARG
1	B	88	VAL
1	B	182	ASP
1	B	188	LYS
1	B	237	PHE
1	B	252	ASP
1	B	374	GLU
1	B	379	THR

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Mol	Chain	Res	Type
1	B	407	LEU
1	B	428	GLN
1	C	12	THR
1	C	22	LYS
1	C	30	ASP
1	C	37	ARG
1	C	68	LEU
1	C	88	VAL
1	C	120	VAL
1	C	180	GLU
1	C	197	ARG
1	C	252	ASP
1	C	253	ASN
1	C	262	ILE
1	C	379	THR
1	C	406	ARG
1	C	408	LEU
1	C	410	LEU
1	C	440	ASP
1	C	443	ASP
1	C	454	ASP
1	C	474	LYS
1	C	491	ASP
1	D	11	LEU
1	D	55	GLU
1	D	88	VAL
1	D	207	LYS
1	D	237	PHE
1	D	253	ASN
1	D	341	LYS
1	D	363	HIS
1	D	380	ARG
1	D	428	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	99	GLN
1	A	310	ASN
1	A	412	ASN
1	A	416	HIS

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Mol	Chain	Res	Type
1	A	439	ASN
1	B	57	GLN
1	B	310	ASN
1	B	382	ASN
1	B	386	GLN
1	B	412	ASN
1	B	416	HIS
1	B	427	ASN
1	B	428	GLN
1	C	57	GLN
1	C	253	ASN
1	C	259	HIS
1	C	310	ASN
1	C	382	ASN
1	C	412	ASN
1	C	416	HIS
1	C	427	ASN
1	C	428	GLN
1	C	439	ASN
1	D	94	ASN
1	D	253	ASN
1	D	259	HIS
1	D	310	ASN
1	D	340	ASN
1	D	363	HIS
1	D	382	ASN
1	D	412	ASN
1	D	416	HIS
1	D	428	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	NAD	D	550	-	42,48,48	1.53	7 (16%)	50,73,73	1.59	10 (20%)
3	NAD	A	550	-	42,48,48	1.35	4 (9%)	50,73,73	1.59	8 (16%)
3	NAD	C	550	-	42,48,48	1.61	6 (14%)	50,73,73	1.74	8 (16%)
2	3DH	D	500	-	20,23,23	0.80	1 (5%)	20,33,33	1.43	3 (15%)
2	3DH	C	500	-	20,23,23	1.43	1 (5%)	20,33,33	1.86	5 (25%)
2	3DH	A	500	-	20,23,23	1.96	2 (10%)	20,33,33	1.55	2 (10%)
2	3DH	B	500	-	20,23,23	0.79	1 (5%)	20,33,33	1.44	3 (15%)
3	NAD	B	550	-	42,48,48	1.27	4 (9%)	50,73,73	1.43	9 (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	NAD	D	550	-	-	10/26/62/62	0/5/5/5
3	NAD	A	550	-	-	6/26/62/62	0/5/5/5
3	NAD	C	550	-	-	8/26/62/62	0/5/5/5
2	3DH	D	500	-	-	0/4/24/24	0/3/3/3
2	3DH	C	500	-	-	2/4/24/24	0/3/3/3
2	3DH	A	500	-	-	1/4/24/24	0/3/3/3
2	3DH	B	500	-	-	2/4/24/24	0/3/3/3
3	NAD	B	550	-	-	6/26/62/62	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	3DH	O4'-C1'	7.50	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	550	NAD	O7N-C7N	5.84	1.35	1.24
3	D	550	NAD	O7N-C7N	4.92	1.33	1.24
3	A	550	NAD	O7N-C7N	4.87	1.33	1.24
2	C	500	3DH	O4'-C1'	4.77	1.47	1.41
3	B	550	NAD	O7N-C7N	4.59	1.32	1.24
3	C	550	NAD	C7N-N7N	-4.19	1.25	1.33
3	A	550	NAD	C7N-N7N	-3.76	1.25	1.33
3	D	550	NAD	C2D-C1D	-3.31	1.48	1.53
3	C	550	NAD	C2D-C1D	-3.30	1.48	1.53
3	D	550	NAD	C7N-N7N	-3.29	1.26	1.33
3	C	550	NAD	C2B-C1B	-3.28	1.48	1.53
3	D	550	NAD	C2B-C1B	-2.85	1.49	1.53
3	B	550	NAD	C5A-C4A	2.74	1.48	1.40
3	A	550	NAD	C5A-C4A	2.68	1.48	1.40
3	B	550	NAD	C7N-N7N	-2.67	1.27	1.33
3	D	550	NAD	C2A-N3A	2.55	1.36	1.32
3	C	550	NAD	O4B-C4B	-2.38	1.39	1.45
3	D	550	NAD	O4D-C1D	2.37	1.44	1.41
3	B	550	NAD	O4D-C1D	2.30	1.44	1.41
3	C	550	NAD	C5A-C4A	2.17	1.46	1.40
3	D	550	NAD	C2N-N1N	-2.10	1.32	1.35
2	D	500	3DH	O4'-C1'	2.09	1.44	1.41
2	A	500	3DH	C5-N7	-2.08	1.32	1.39
2	B	500	3DH	O4'-C1'	2.05	1.43	1.41
3	A	550	NAD	PN-O1N	-2.01	1.43	1.50

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	3DH	N3-C2-N1	-4.82	121.14	128.68
3	C	550	NAD	N3A-C2A-N1A	-4.65	121.42	128.68
3	D	550	NAD	C1B-N9A-C4A	-4.60	118.56	126.64
3	C	550	NAD	O7N-C7N-C3N	4.48	124.99	119.63
2	B	500	3DH	N3-C2-N1	-4.43	121.75	128.68
2	D	500	3DH	N3-C2-N1	-4.42	121.77	128.68
3	B	550	NAD	N3A-C2A-N1A	-4.17	122.16	128.68
2	C	500	3DH	N3-C2-N1	-4.15	122.19	128.68
3	A	550	NAD	O7N-C7N-N7N	-3.97	116.94	122.58
2	C	500	3DH	O4'-C1'-C2'	-3.86	101.28	106.93
2	C	500	3DH	C4-C5-N7	-3.86	105.38	109.40
3	C	550	NAD	C1B-N9A-C4A	-3.64	120.25	126.64
3	A	550	NAD	N3A-C2A-N1A	-3.61	123.03	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	550	NAD	C3N-C2N-N1N	3.57	123.92	120.43
3	A	550	NAD	O7N-C7N-C3N	3.54	123.87	119.63
3	C	550	NAD	O7N-C7N-N7N	-3.53	117.57	122.58
3	D	550	NAD	N3A-C2A-N1A	-3.38	123.40	128.68
3	C	550	NAD	C2A-N1A-C6A	3.35	124.48	118.75
3	D	550	NAD	C3N-C7N-N7N	3.28	121.69	117.75
3	D	550	NAD	C4A-C5A-N7A	-3.14	106.13	109.40
3	C	550	NAD	O4D-C1D-C2D	-3.07	102.43	106.93
3	C	550	NAD	C2B-C3B-C4B	2.92	108.31	102.64
3	B	550	NAD	C4A-C5A-N7A	-2.75	106.53	109.40
3	C	550	NAD	C4A-C5A-N7A	-2.74	106.54	109.40
3	A	550	NAD	O2N-PN-O1N	2.73	125.72	112.24
3	B	550	NAD	C5N-C4N-C3N	-2.71	117.14	120.34
3	A	550	NAD	C4A-C5A-N7A	-2.69	106.59	109.40
3	D	550	NAD	O3D-C3D-C4D	-2.62	103.48	111.05
2	A	500	3DH	O4'-C1'-C2'	-2.56	103.18	106.93
3	B	550	NAD	C6N-N1N-C2N	-2.46	119.73	121.97
3	B	550	NAD	C1B-N9A-C4A	-2.41	122.41	126.64
3	D	550	NAD	O2N-PN-O1N	2.33	123.77	112.24
3	D	550	NAD	O4D-C1D-C2D	-2.33	103.52	106.93
3	A	550	NAD	C5N-C4N-C3N	-2.32	117.60	120.34
3	B	550	NAD	C3N-C2N-N1N	2.28	122.66	120.43
2	C	500	3DH	O4'-C4'-C3'	-2.27	100.63	105.11
2	C	500	3DH	C3'-C2'-C1'	2.26	104.38	100.98
2	B	500	3DH	C5'-C4'-C3'	-2.23	109.49	115.06
3	B	550	NAD	O4B-C1B-C2B	-2.21	103.70	106.93
2	D	500	3DH	C5'-C4'-C3'	-2.20	109.55	115.06
3	B	550	NAD	O4D-C1D-C2D	-2.20	103.71	106.93
3	B	550	NAD	C2A-N1A-C6A	2.18	122.49	118.75
3	D	550	NAD	O3B-C3B-C4B	-2.13	104.88	111.05
3	A	550	NAD	O4D-C1D-C2D	-2.08	103.88	106.93
3	D	550	NAD	C2B-C3B-C4B	2.08	106.69	102.64
2	B	500	3DH	O4'-C1'-C2'	-2.01	103.99	106.93
2	D	500	3DH	O4'-C1'-C2'	-2.01	103.99	106.93
3	D	550	NAD	O7N-C7N-N7N	-2.00	119.73	122.58

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	3DH	O4'-C4'-C5'-SD
2	B	500	3DH	C3'-C4'-C5'-SD

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Mol	Chain	Res	Type	Atoms
2	C	500	3DH	O4'-C4'-C5'-SD
2	C	500	3DH	C3'-C4'-C5'-SD
3	A	550	NAD	O4B-C4B-C5B-O5B
3	A	550	NAD	O4D-C1D-N1N-C2N
3	A	550	NAD	O4D-C1D-N1N-C6N
3	A	550	NAD	C2D-C1D-N1N-C2N
3	A	550	NAD	C2D-C1D-N1N-C6N
3	B	550	NAD	O4D-C1D-N1N-C2N
3	B	550	NAD	O4D-C1D-N1N-C6N
3	B	550	NAD	C2D-C1D-N1N-C2N
3	B	550	NAD	C2D-C1D-N1N-C6N
3	C	550	NAD	O4D-C1D-N1N-C2N
3	C	550	NAD	O4D-C1D-N1N-C6N
3	C	550	NAD	C2D-C1D-N1N-C2N
3	C	550	NAD	C2D-C1D-N1N-C6N
3	D	550	NAD	O4D-C1D-N1N-C2N
3	D	550	NAD	O4D-C1D-N1N-C6N
3	D	550	NAD	C2D-C1D-N1N-C2N
3	D	550	NAD	C2D-C1D-N1N-C6N
3	A	550	NAD	C3B-C4B-C5B-O5B
2	A	500	3DH	CB-CG-SD-C5'
3	D	550	NAD	C5D-O5D-PN-O3
3	C	550	NAD	PN-O3-PA-O2A
3	D	550	NAD	PN-O3-PA-O2A
3	C	550	NAD	PN-O3-PA-O1A
3	B	550	NAD	O4B-C4B-C5B-O5B
3	D	550	NAD	PN-O3-PA-O1A
3	D	550	NAD	O4B-C4B-C5B-O5B
3	B	550	NAD	C3B-C4B-C5B-O5B
3	C	550	NAD	C5B-O5B-PA-O1A
3	D	550	NAD	C5B-O5B-PA-O1A
3	D	550	NAD	C5D-O5D-PN-O1N
3	C	550	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	550	NAD	1	0
3	A	550	NAD	6	0
3	C	550	NAD	3	0
2	D	500	3DH	2	0

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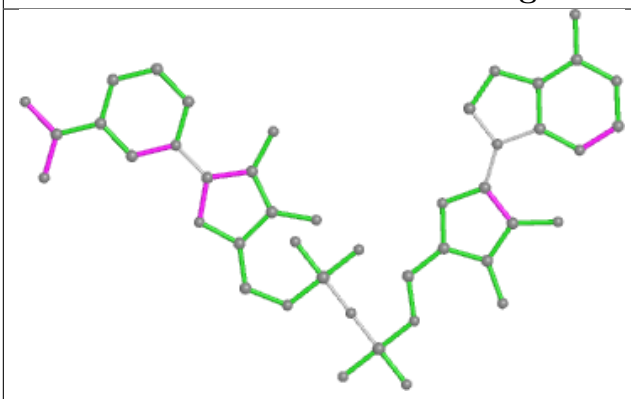
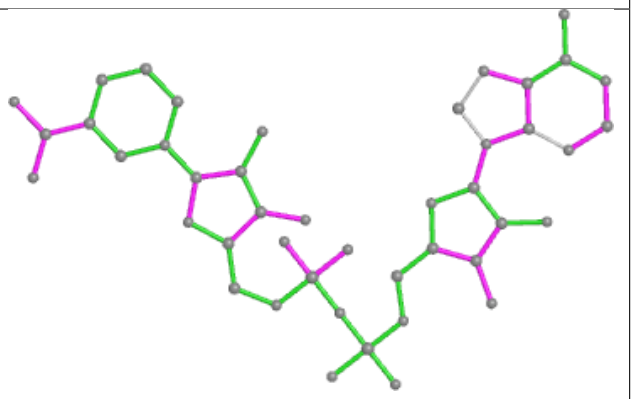
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	3DH	2	0
2	A	500	3DH	2	0
2	B	500	3DH	1	0
3	B	550	NAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

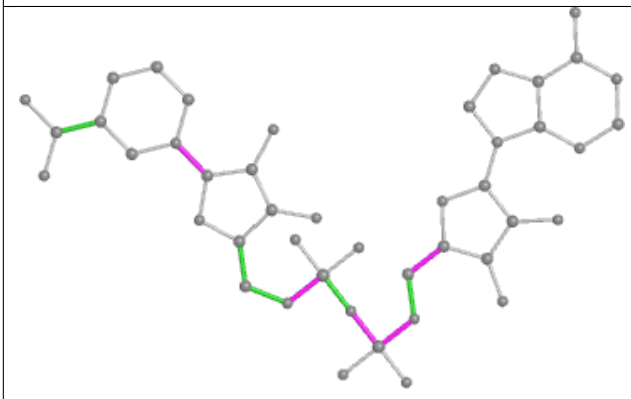
Ligand NAD D 550



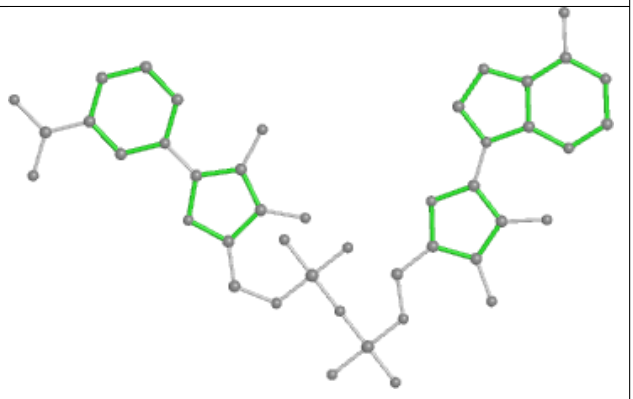
Bond lengths



Bond angles

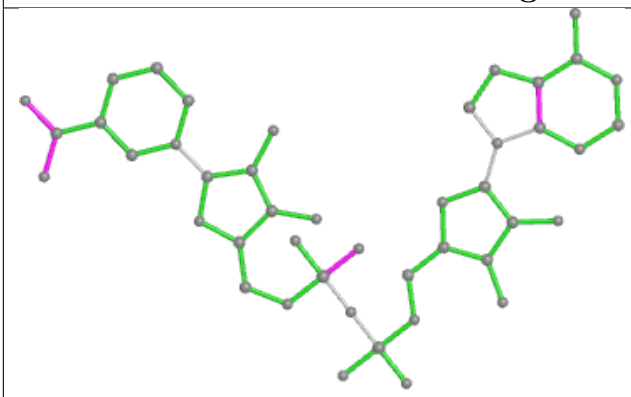


Torsions

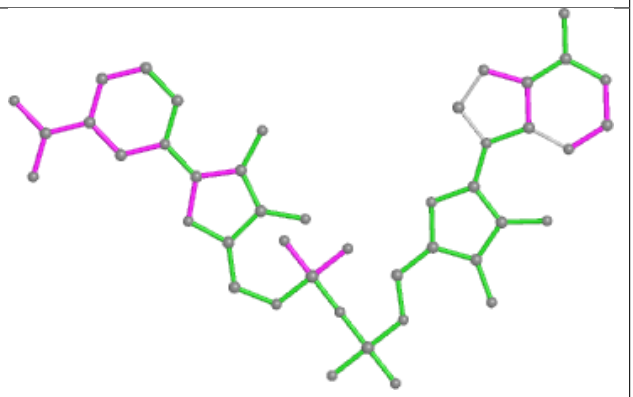


Rings

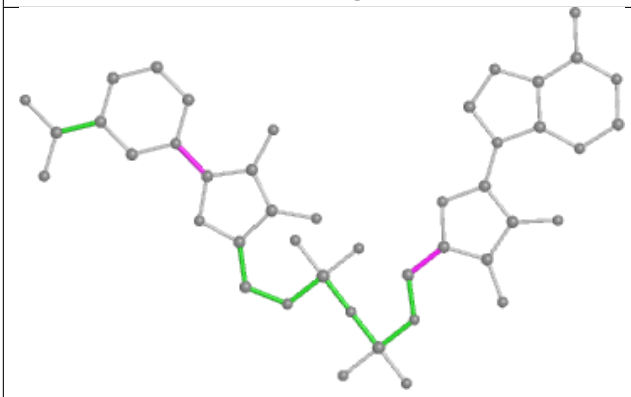
Ligand NAD A 550



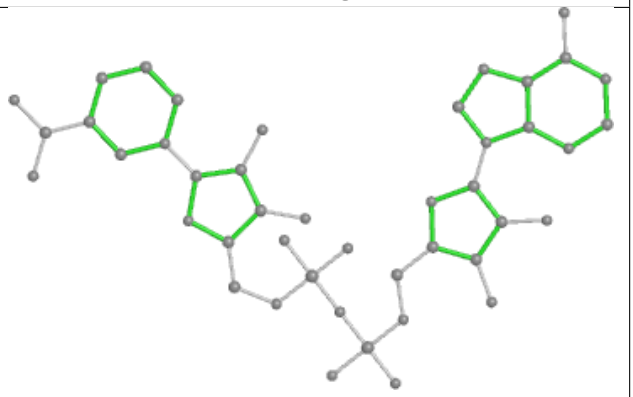
Bond lengths



Bond angles

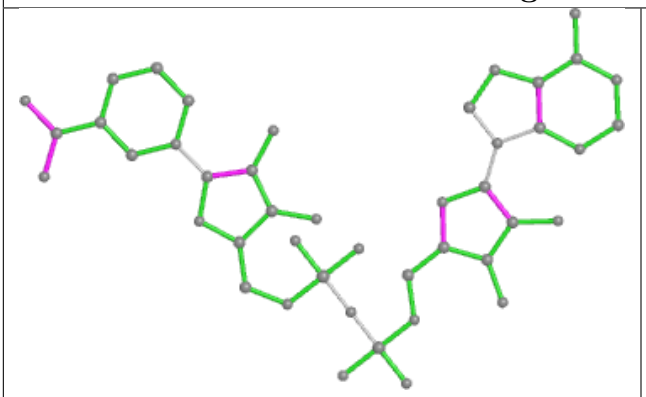


Torsions

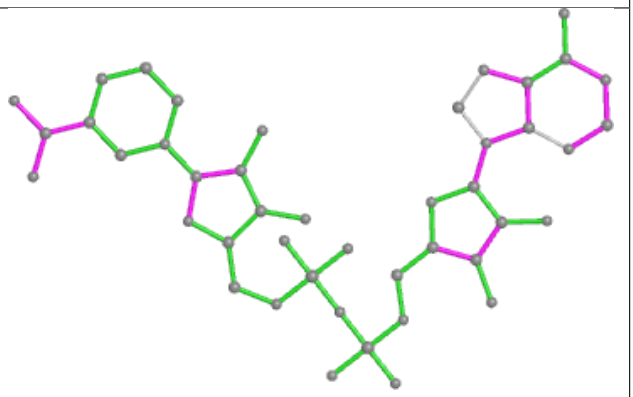


Rings

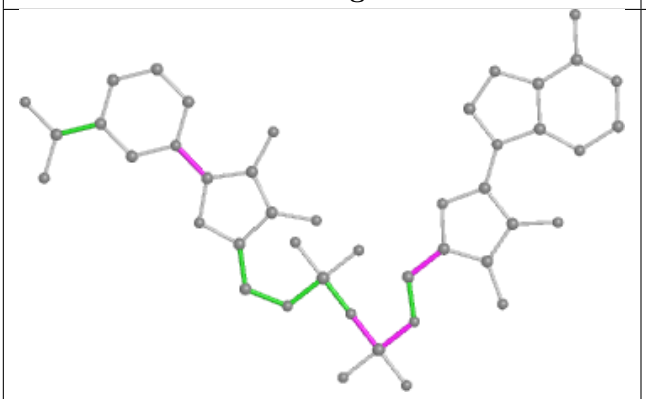
Ligand NAD C 550



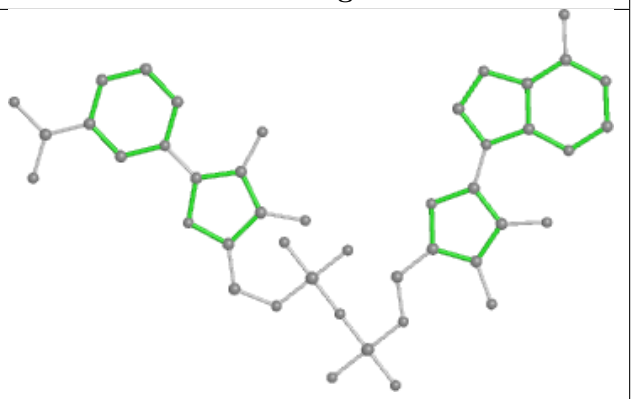
Bond lengths



Bond angles

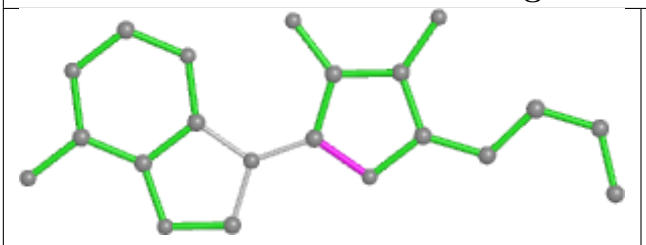


Torsions

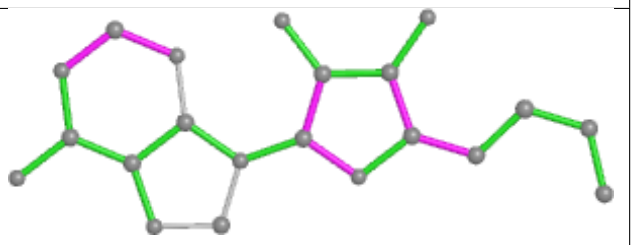


Rings

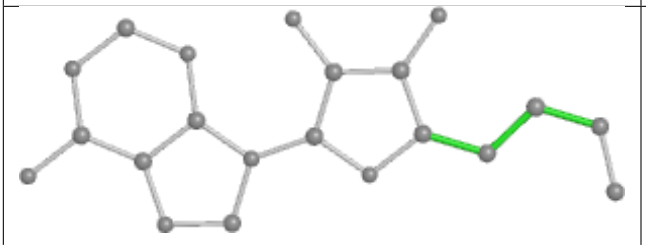
Ligand 3DH D 500



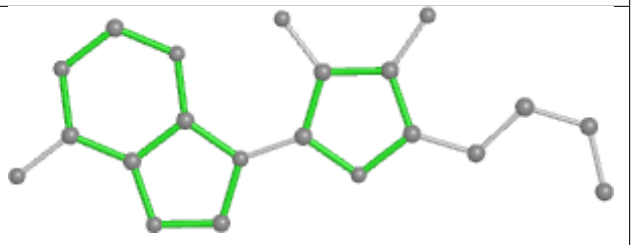
Bond lengths



Bond angles

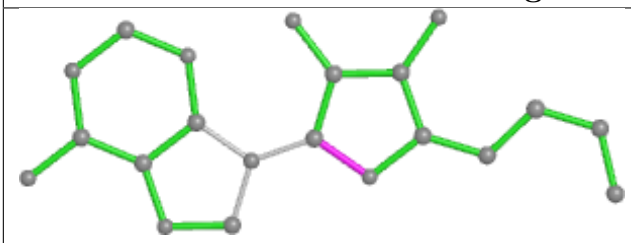


Torsions

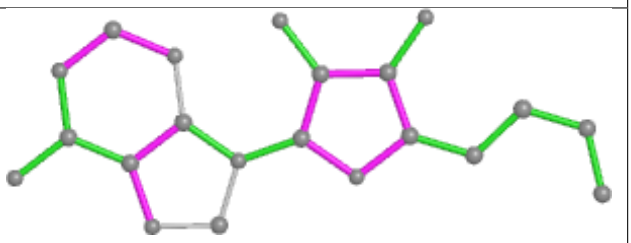


Rings

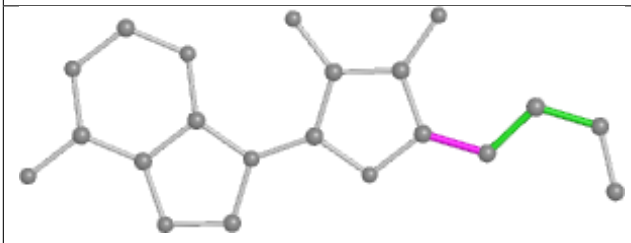
Ligand 3DH C 500



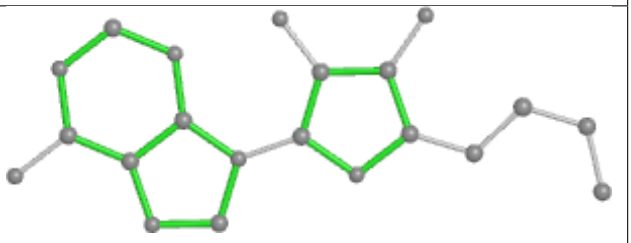
Bond lengths



Bond angles

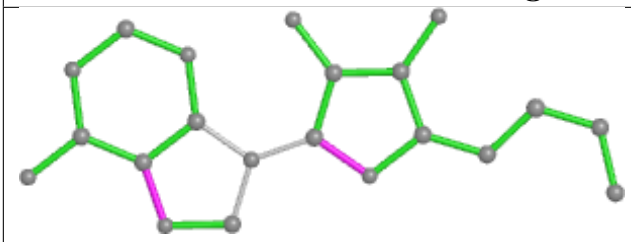


Torsions

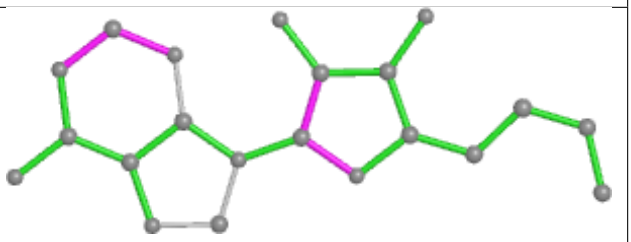


Rings

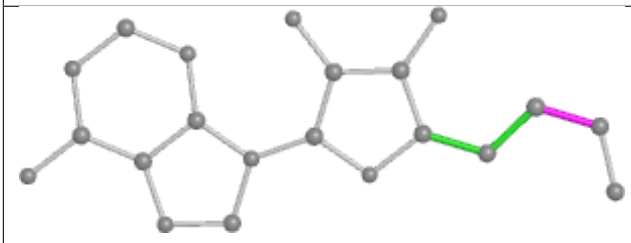
Ligand 3DH A 500



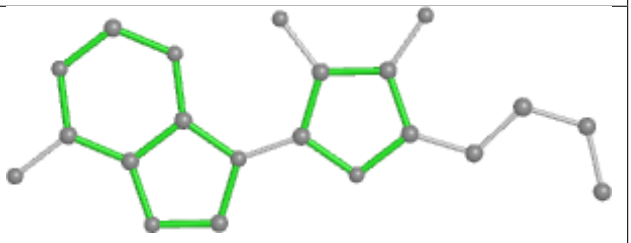
Bond lengths



Bond angles

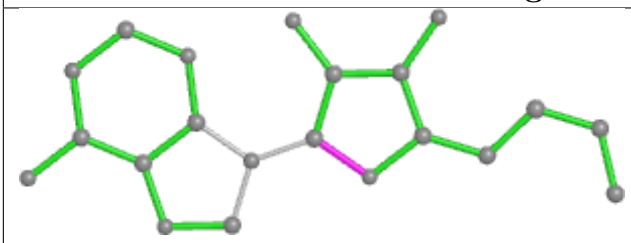


Torsions

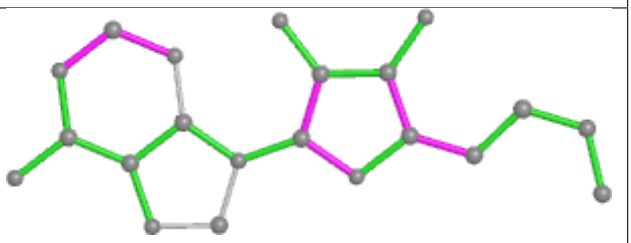


Rings

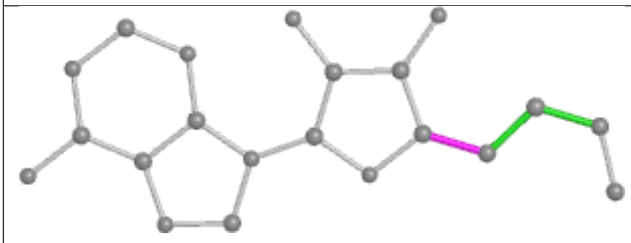
Ligand 3DH B 500



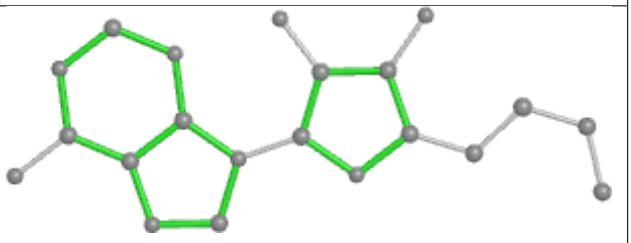
Bond lengths



Bond angles

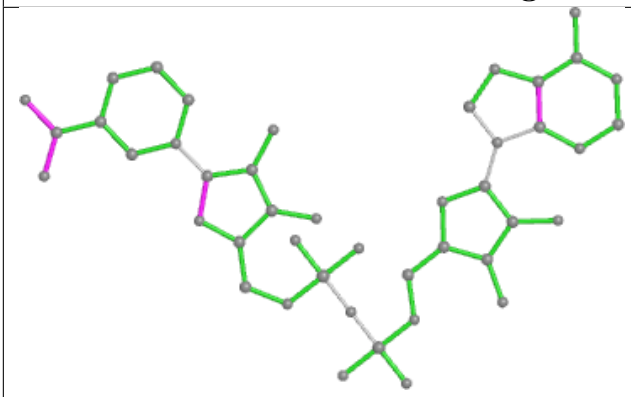


Torsions

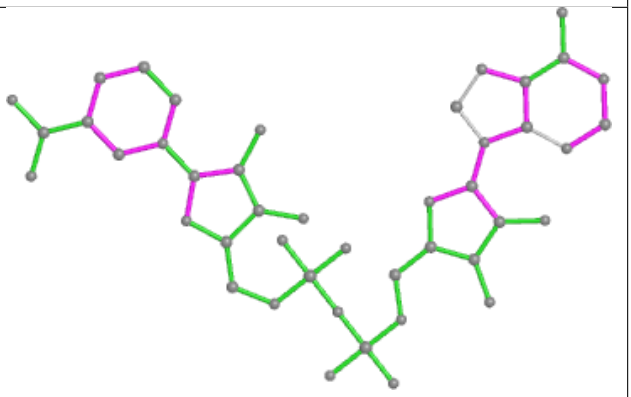


Rings

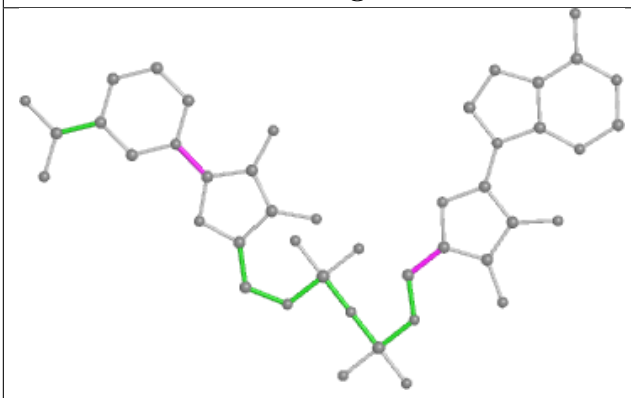
Ligand NAD B 550



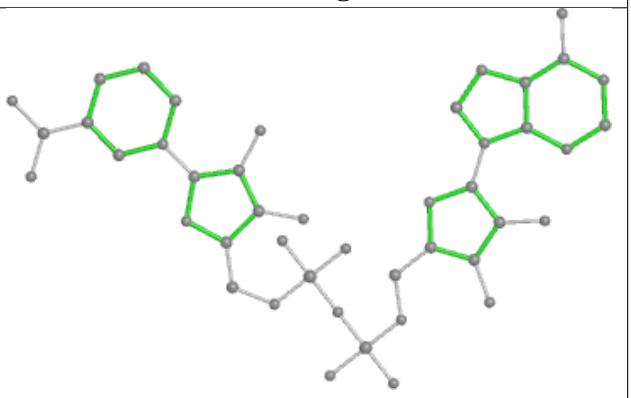
Bond lengths



Bond angles



Torsions



Rings

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

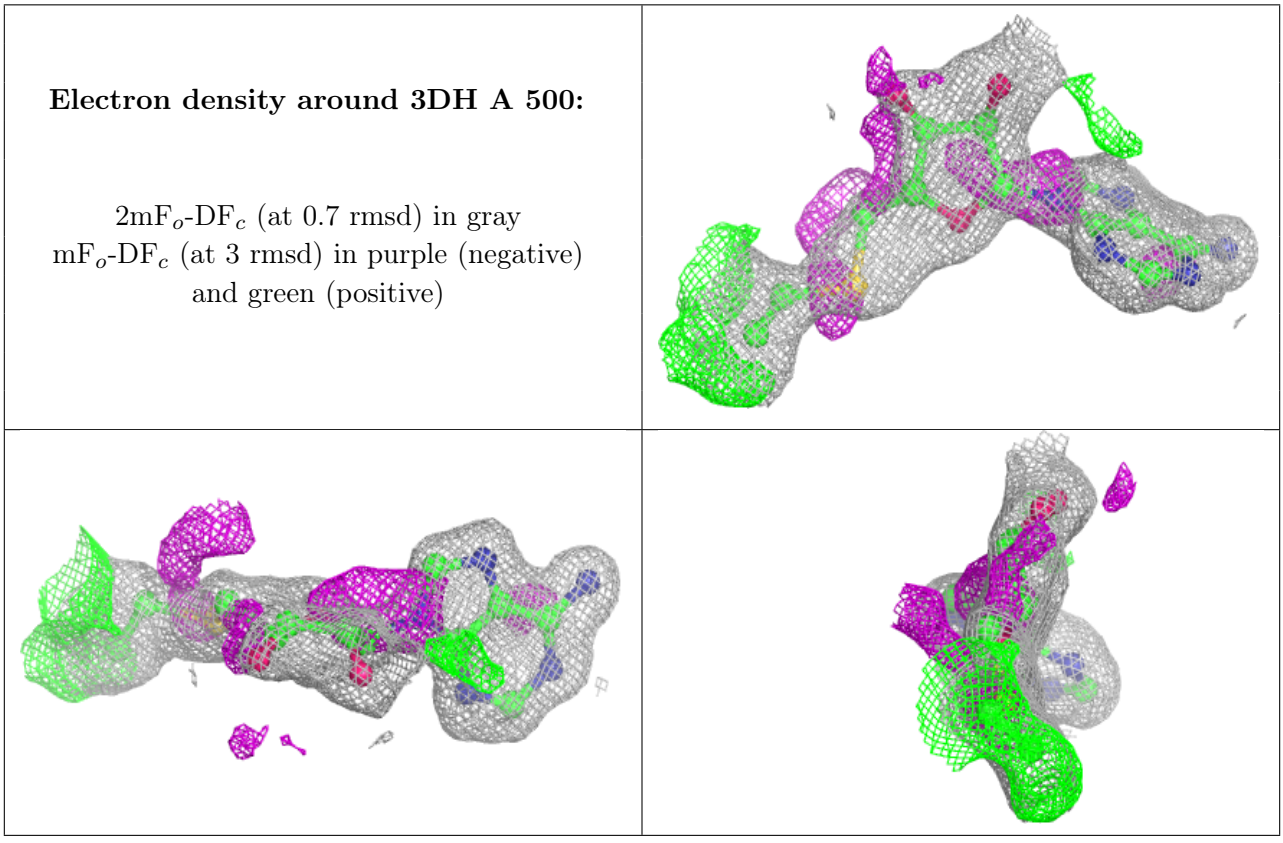
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

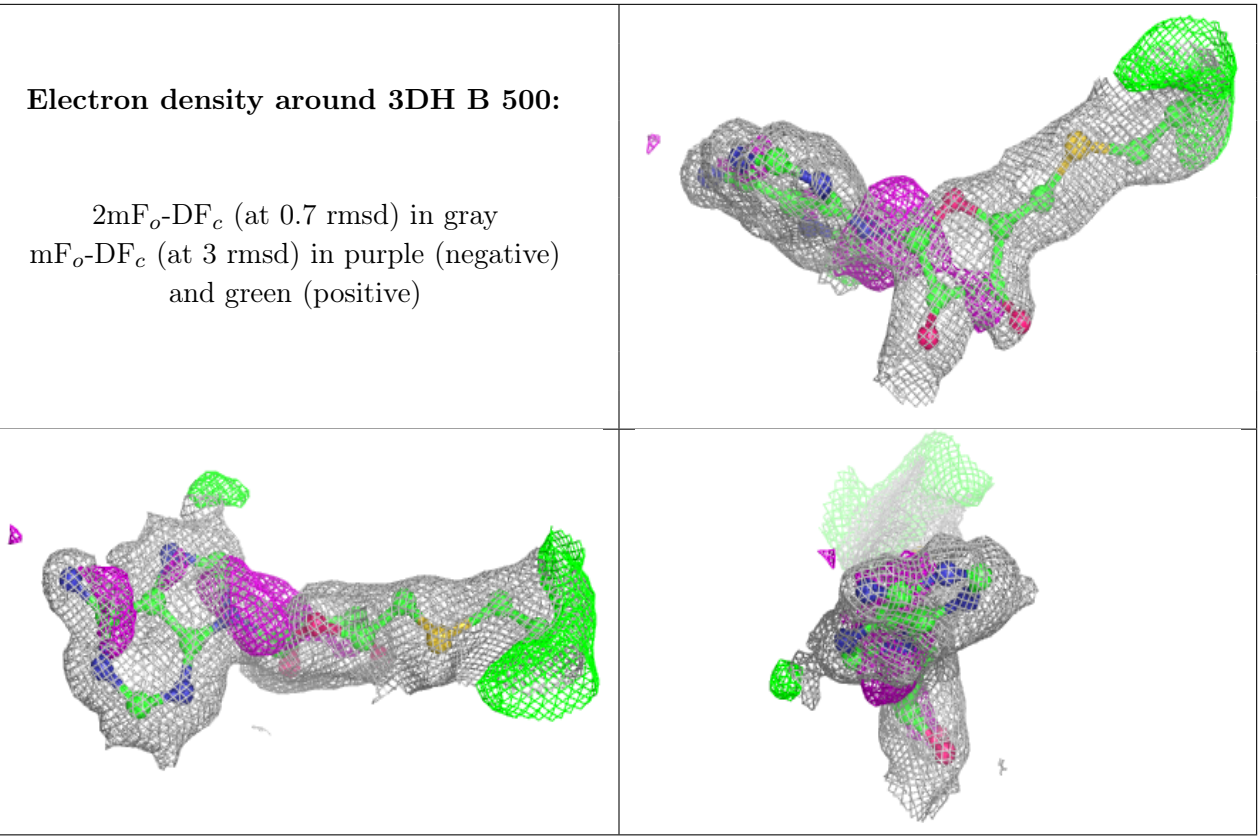
Electron density around 3DH A 500:

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



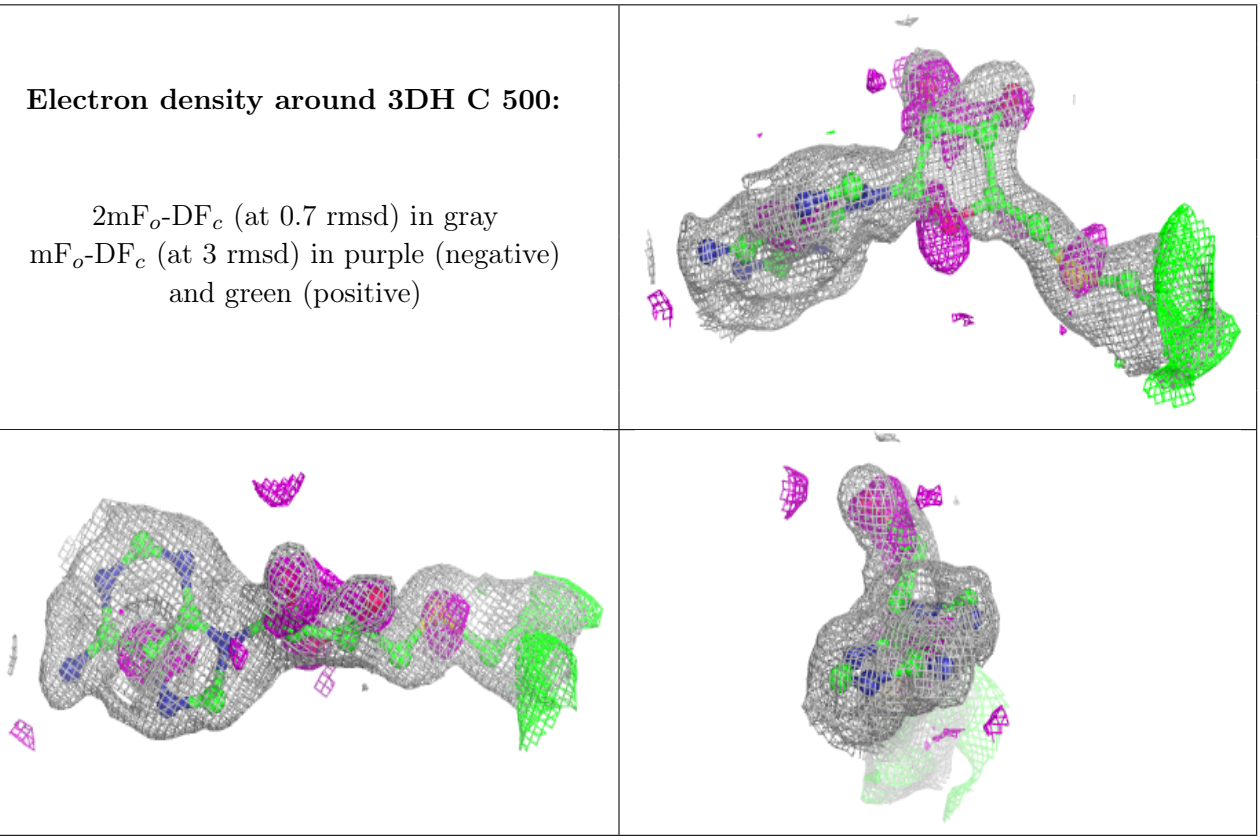
Electron density around 3DH B 500:

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



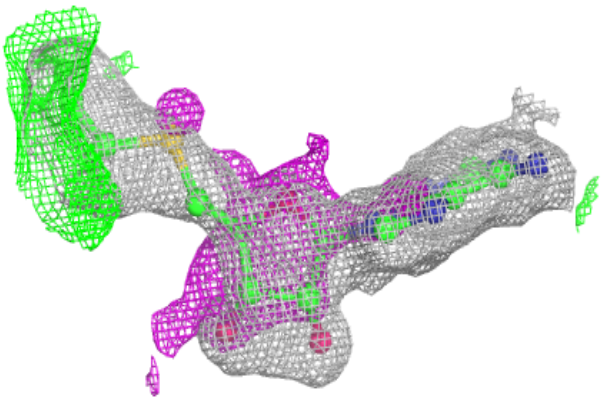
Electron density around 3DH C 500:

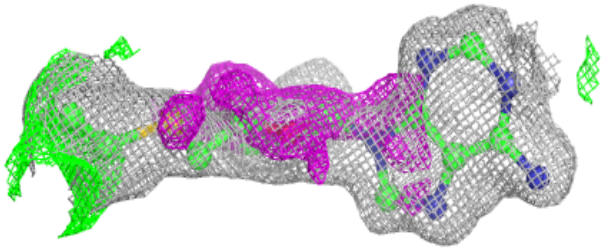
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

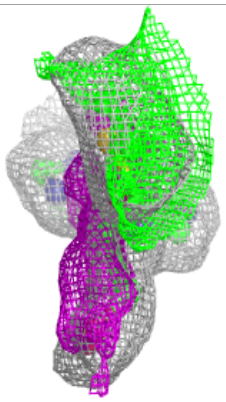


Electron density around 3DH D 500:

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

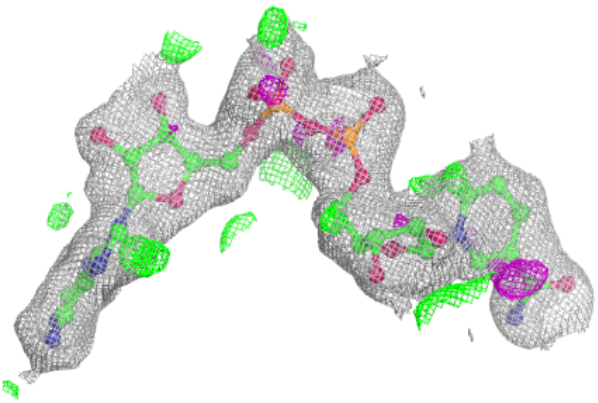


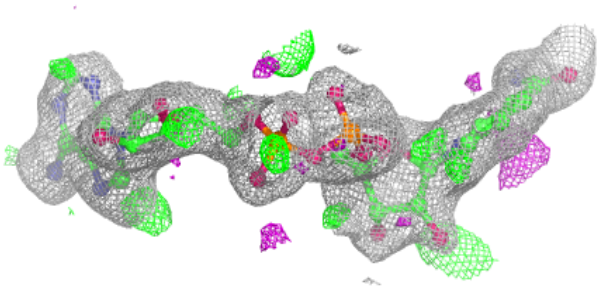


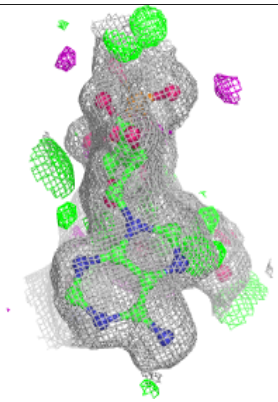


Electron density around NAD A 550:

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

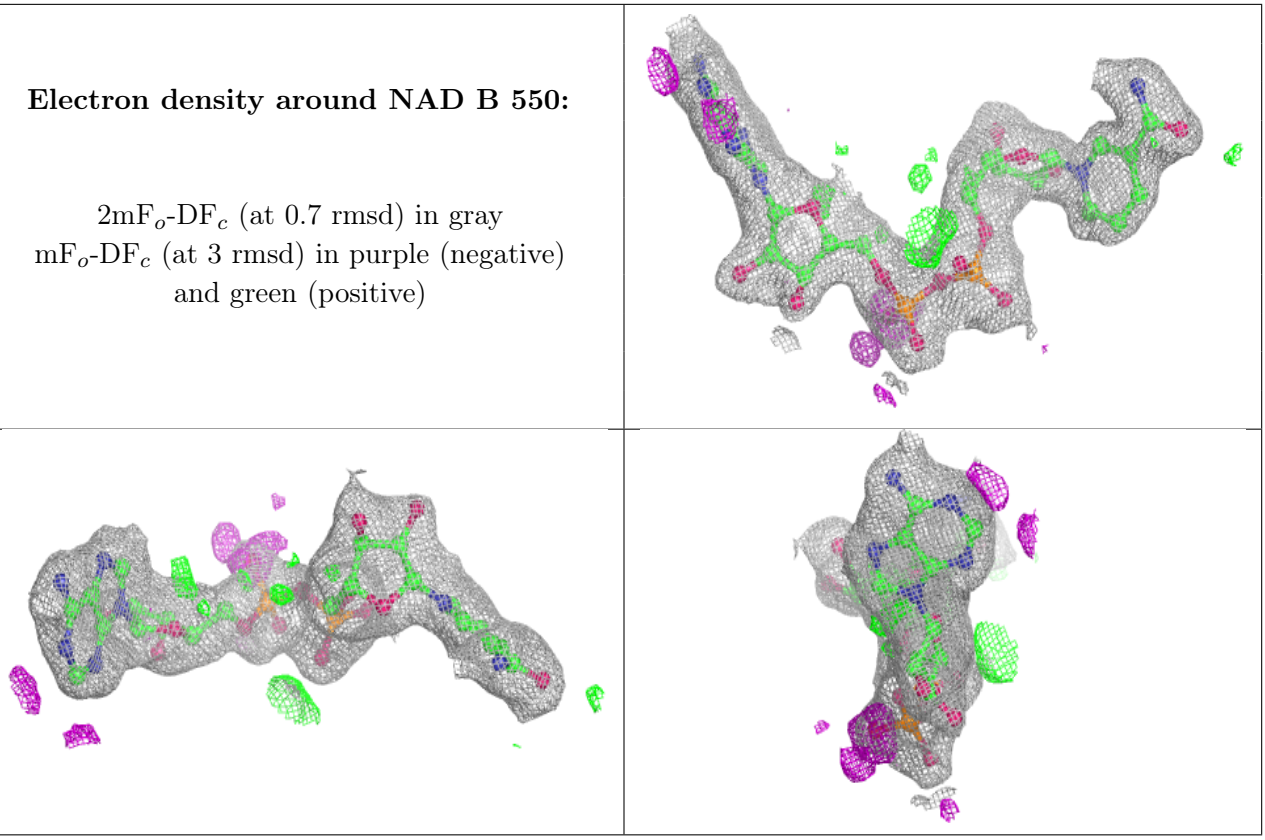






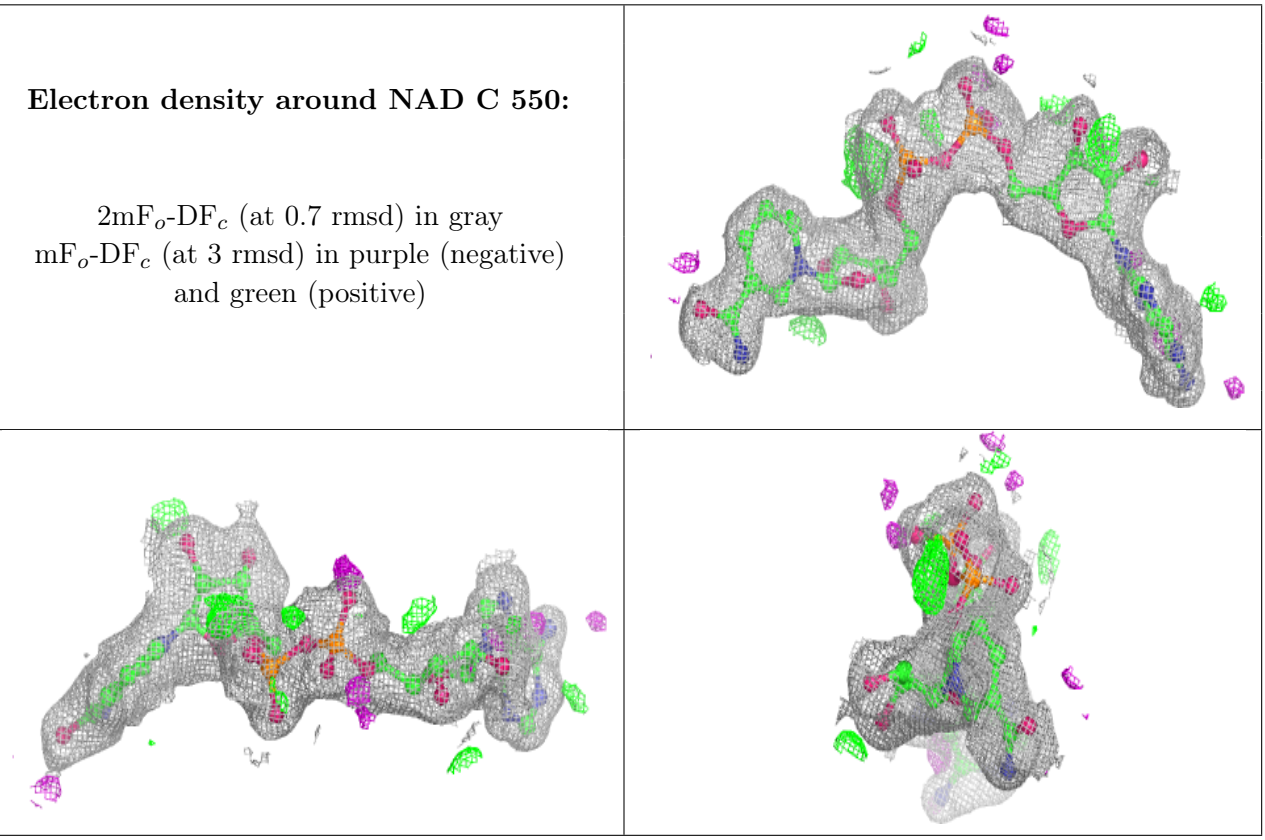
Electron density around NAD B 550:

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



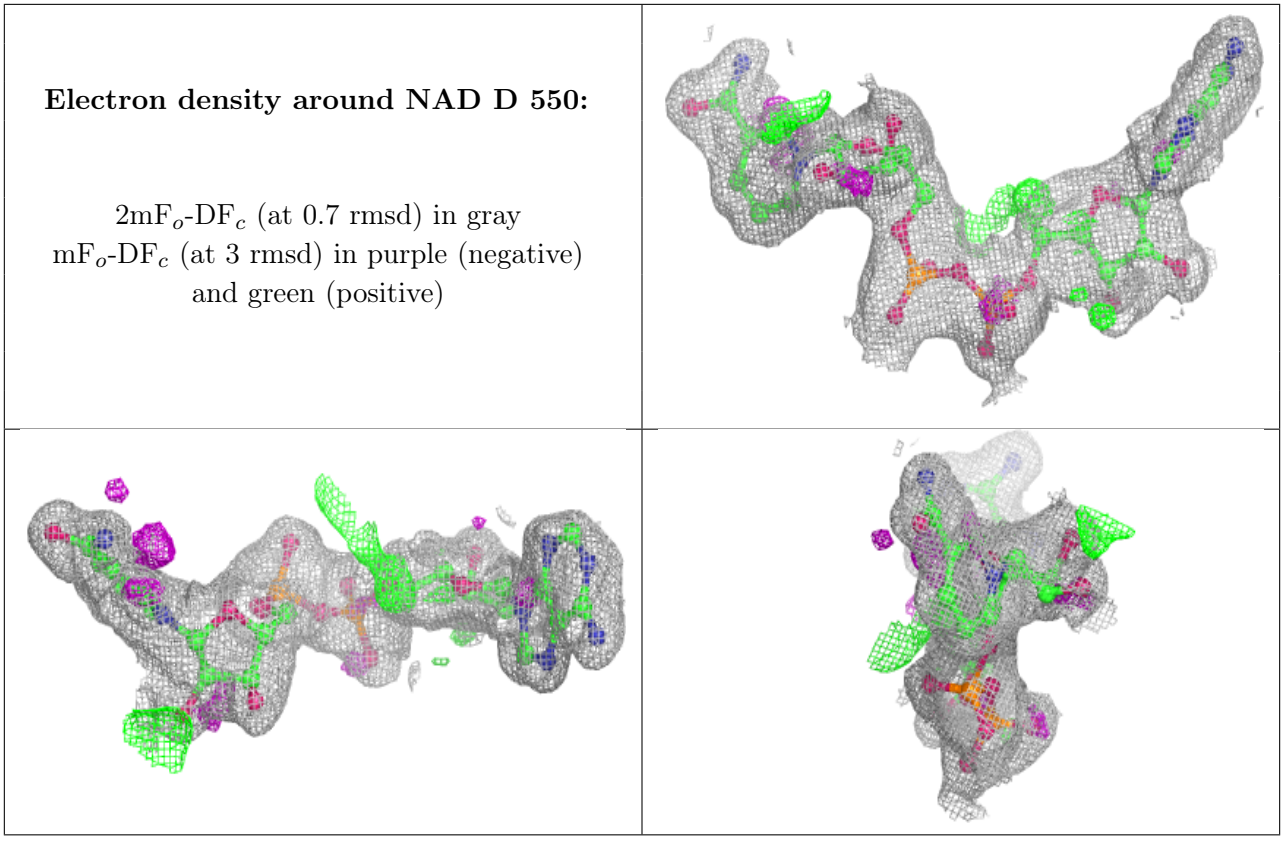
Electron density around NAD C 550:

$2mF_o$-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 550:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.