



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:06 PM UTC

PDB ID : 3DHY / pdb_00003dhy
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	:	4-5-2 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

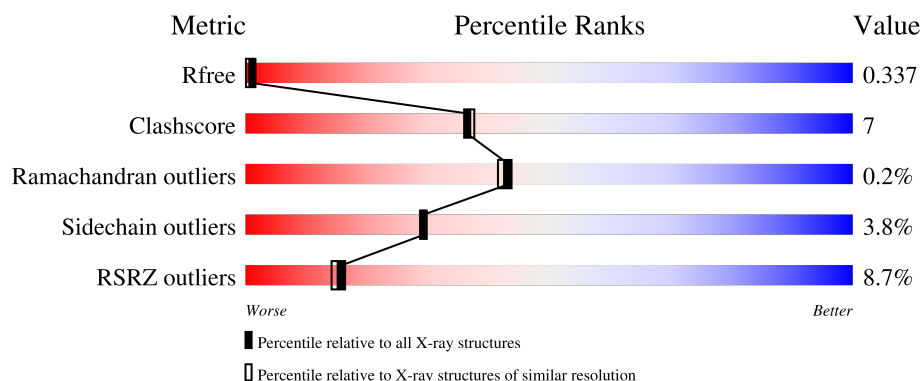
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	495	12% 77% 20% ..
1	B	495	8% 83% 14% ..
1	C	495	8% 79% 17% ..
1	D	495	7% 78% 19% ..

2 Entry composition [i](#)

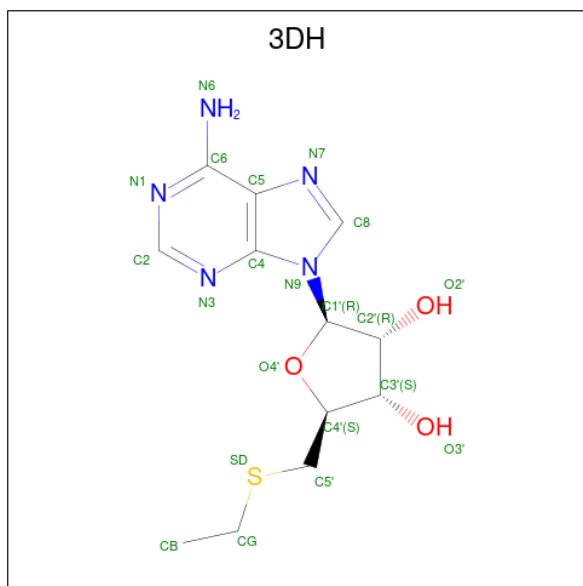
There are 4 unique types of molecules in this entry. The entry contains 15608 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 3DH) (formula: C₁₂H₁₇N₅O₃S).



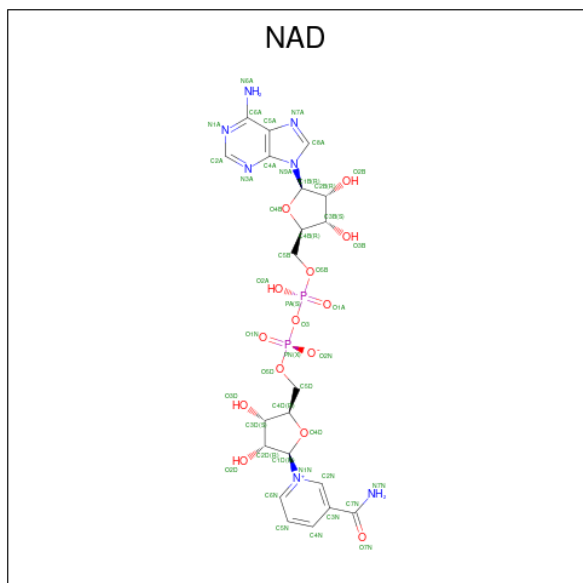
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			21	12	5	3	1		
2	B	1	Total	C	N	O	S	0	0
			21	12	5	3	1		

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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 (CCD ID: 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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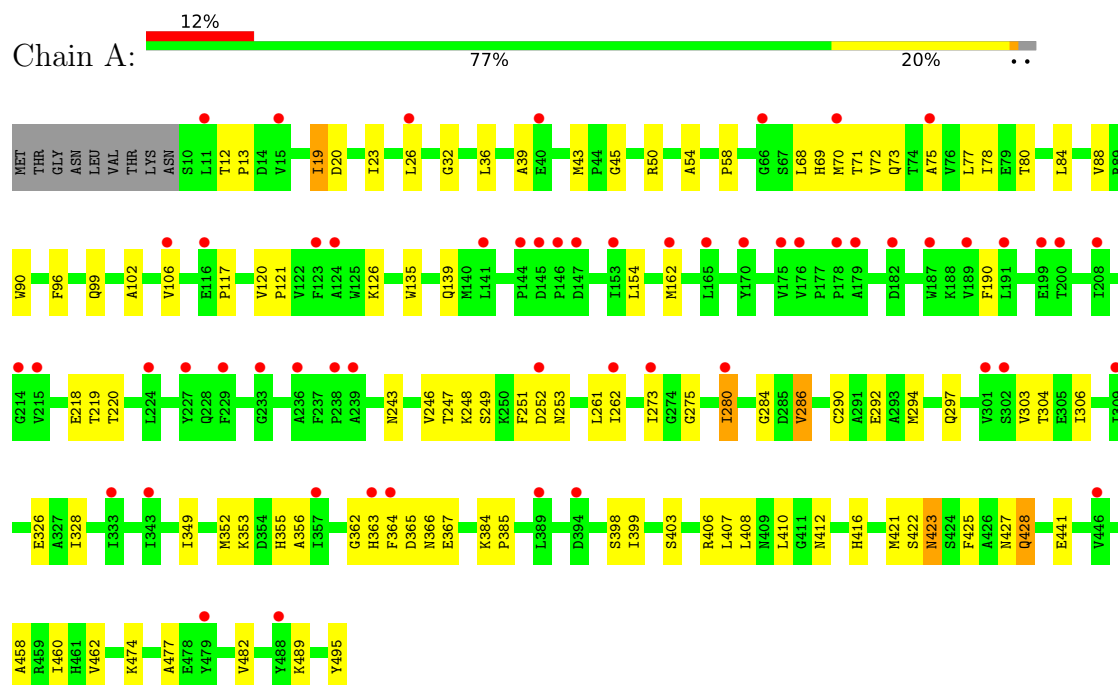
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	97	Total	O	0	0
			97	97		

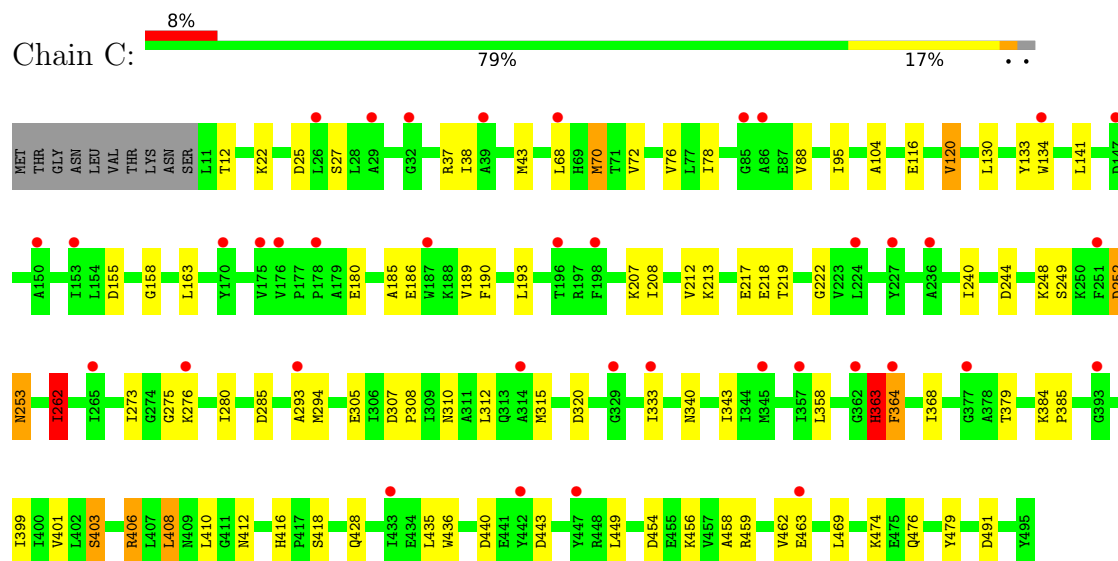
3 Residue-property plots [i](#)

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.

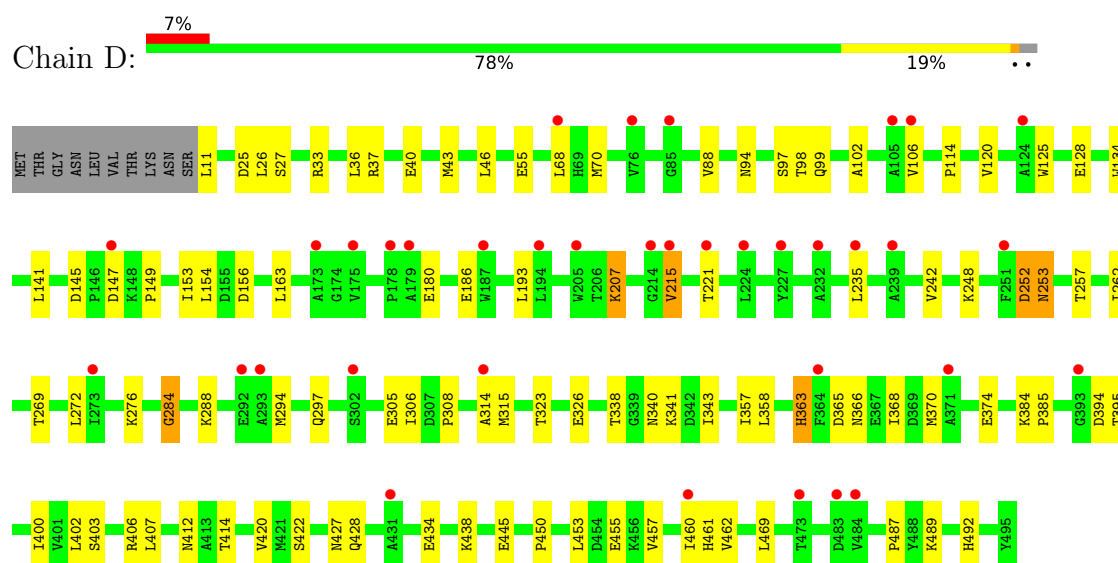
• Molecule 1: Adenosylhomocysteinase



● Molecule 1: Adenosylhomocysteinase



● Molecule 1: Adenosylhomocysteinase



4 Data and refinement statistics

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 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	82.5 (30.00-2.00) 82.5 (30.00-2.00)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (2.95%)	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)	0.35 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

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: 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	0.86	2/3830 (0.1%)	1.03	4/5194 (0.1%)
1	B	0.91	3/3824 (0.1%)	1.06	7/5186 (0.1%)
1	C	0.90	6/3824 (0.2%)	1.10	10/5186 (0.2%)
1	D	0.92	1/3824 (0.0%)	1.08	5/5186 (0.1%)
All	All	0.90	12/15302 (0.1%)	1.07	26/20752 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	280	ILE	CA-CB	9.72	1.65	1.54
1	C	207	LYS	CD-CE	7.21	1.74	1.52
1	C	280	ILE	CA-CB	6.26	1.61	1.53
1	D	215	VAL	CA-CB	6.25	1.63	1.54
1	B	460	ILE	CA-CB	5.76	1.60	1.54
1	C	38	ILE	CA-CB	5.67	1.60	1.54
1	C	104	ALA	CA-CB	-5.52	1.44	1.53
1	B	357	ILE	CA-CB	5.48	1.60	1.54
1	A	280	ILE	CA-CB	5.43	1.60	1.54
1	C	120	VAL	C-O	-5.42	1.20	1.24
1	C	70	MET	SD-CE	-5.34	1.66	1.79
1	A	286	VAL	CA-CB	5.31	1.60	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	449	LEU	CA-C-N	8.32	128.39	119.90
1	C	449	LEU	C-N-CA	8.32	128.39	119.90
1	D	284	GLY	N-CA-C	-8.01	98.83	112.77
1	C	285	ASP	N-CA-C	7.50	119.09	111.07
1	A	284	GLY	N-CA-C	-6.49	103.32	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	MET	CA-C-N	6.39	126.15	119.05
1	C	43	MET	C-N-CA	6.39	126.15	119.05
1	B	265	ILE	N-CA-C	6.30	117.05	110.62
1	D	420	VAL	CB-CA-C	-6.19	103.95	111.88
1	B	256	GLY	N-CA-C	-5.77	105.38	112.77
1	C	418	SER	N-CA-C	5.67	117.91	111.11
1	D	257	THR	N-CA-C	5.66	118.18	111.33
1	A	423	ASN	N-CA-C	5.64	117.51	111.36
1	B	219	THR	N-CA-C	5.56	118.14	109.52
1	D	420	VAL	N-CA-C	5.37	116.00	110.36
1	C	363	HIS	N-CA-C	5.34	117.31	109.24
1	D	314	ALA	N-CA-C	5.30	117.47	111.11
1	B	412	ASN	N-CA-C	5.28	119.57	113.18
1	A	365	ASP	N-CA-C	-5.18	106.06	114.09
1	C	262	ILE	N-CA-C	5.18	115.90	110.62
1	B	159	ASP	N-CA-C	5.16	116.99	111.36
1	B	89	ARG	N-CA-C	-5.15	101.37	109.50
1	B	136	ALA	N-CA-C	-5.11	105.63	111.14
1	C	116	GLU	CA-C-N	5.10	125.02	119.76
1	C	116	GLU	C-N-CA	5.10	125.02	119.76
1	A	366	ASN	N-CA-C	5.01	119.54	113.38

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	64	0
1	B	3748	0	3693	39	0
1	C	3748	0	3693	59	0
1	D	3748	0	3693	66	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	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	217	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 (217) 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: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:HZ2	1:C:253:ASN:HD21	1.21	0.85
1:C:248:LYS:NZ	1:C:253:ASN:HD21	1.74	0.84
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:D:248:LYS:HZ2	1:D:253:ASN:HD21	1.28	0.80
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:252:ASP:OD1	1:C:252:ASP:C	2.34	0.70
1:C:403:SER:OG	1:C:412:ASN:ND2	2.25	0.70
1:C:273:ILE:HD13	1:C:294:MET:HE1	1.74	0.69
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:C:305:GLU:OE2	3:C:550:NAD:O2B	2.11	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: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:HG3	1:C:406:ARG:HH21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:78:ILE:HD11	1.81	0.61
1:C:384:LYS:HB2	1:C:385:PRO:HD2	1.82	0.61
1:B:193:LEU:C	1:B:193:LEU:HD23	2.26	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:C:217:GLU:CD	1:C:222:GLY:HA3	2.28	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:A:70:MET:HE2	1:A:90:TRP:CD1	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:102:ALA:O	1:A:106:VAL:HG23	2.07	0.55
1:A:477:ALA:HB1	1:A:482:VAL:O	2.07	0.55
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: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:D:262:ILE:CD1	1:D:294:MET:HE2	2.38	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:C:70:MET:HE1	1:C:78:ILE:CD1	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
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:406:ARG:O	1:D:407:LEU:C	2.55	0.49
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:C:408:LEU:HD12	1:C:408:LEU:C	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:LEU:HG	1:D:156:ASP:HB2	1.95	0.49
1:A:73:GLN:CD	1:A:73:GLN:H	2.20	0.49
1:D:43:MET:HE2	1:D:46:LEU:HD12	1.94	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:A:262:ILE:CD1	1:A:294:MET:HE2	2.43	0.48
1:A:273:ILE:HD13	1:A:294:MET:HE1	1.95	0.48
1:D:363:HIS:CD2	1:D:363:HIS:C	2.91	0.48
1:C:252:ASP:OD1	1:C:416:HIS:CE1	2.67	0.48
1:A:70:MET:HE1	1:A:78:ILE:CD1	2.44	0.47
1:B:340:ASN:O	1:B:367:GLU:HG2	2.15	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:B:273:ILE:HD13	1:B:294:MET:HE1	1.96	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:C:248:LYS:HZ3	1:C:253:ASN:ND2	2.14	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: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:B:406:ARG:O	1:B:407:LEU:C	2.60	0.45
1:D:305:GLU:OE2	3:D:550:NAD:O2B	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ASP:C	1:B:252:ASP:OD1	2.60	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:A:352:MET:HE2	1:A:352:MET:HB3	1.73	0.43
1:A:70:MET:CE	1:A:90:TRP:CD1	3.01	0.43
1:B:408:LEU:C	1:B:408:LEU:HD12	2.42	0.43
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:B:138:GLU:CD	1:B:197:ARG:HH21	2.26	0.43
1:D:145:ASP:C	1:D:147:ASP:H	2.27	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:A:406:ARG:O	1:A:407:LEU:C	2.61	0.43
1:A:421:MET:O	1:A:422:SER:C	2.62	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:248:LYS:HD3	1:D:248:LYS:C	2.44	0.42
1:C:307:ASP:CG	1:C:310:ASN:HD22	2.27	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:253:ASN:N	1:D:253:ASN:ND2	2.61	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:D:252:ASP:OD2	1:D:252:ASP:C	2.62	0.42
1:A:162:MET:HE3	1:A:190:PHE:CE1	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:363:HIS:O	1:C:364:PHE:C	2.63	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
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: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:C:70:MET:HE1	1:C:78:ILE:HD11	2.02	0.40
1:D:450:PRO:CG	1:D:453:LEU:HD12	2.51	0.40
1:B:162:MET:HE3	1:B:190:PHE:CE1	2.56	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: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%)	43	42
1	B	483/495 (98%)	463 (96%)	20 (4%)	0	100	100
1	C	483/495 (98%)	463 (96%)	18 (4%)	2 (0%)	30	27
1	D	483/495 (98%)	460 (95%)	22 (5%)	1 (0%)	43	42
All	All	1933/1980 (98%)	1848 (96%)	81 (4%)	4 (0%)	43	42

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 ⓘ

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%)	384 (97%)	12 (3%)	36	38
1	B	395/404 (98%)	383 (97%)	12 (3%)	36	38
1	C	395/404 (98%)	372 (94%)	23 (6%)	18	15
1	D	395/404 (98%)	382 (97%)	13 (3%)	33	34
All	All	1581/1616 (98%)	1521 (96%)	60 (4%)	29	29

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	88	VAL
1	A	120	VAL
1	A	219	THR
1	A	220	THR
1	A	292	GLU
1	A	306	ILE

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Mol	Chain	Res	Type
1	A	328	ILE
1	A	410	LEU
1	A	428	GLN
1	A	441	GLU
1	A	474	LYS
1	B	11	LEU
1	B	16	ARG
1	B	56	VAL
1	B	88	VAL
1	B	182	ASP
1	B	188	LYS
1	B	252	ASP
1	B	374	GLU
1	B	379	THR
1	B	399	ILE
1	B	407	LEU
1	B	428	GLN
1	C	12	THR
1	C	22	LYS
1	C	37	ARG
1	C	68	LEU
1	C	88	VAL
1	C	120	VAL
1	C	180	GLU
1	C	219	THR
1	C	252	ASP
1	C	253	ASN
1	C	262	ILE
1	C	333	ILE
1	C	363	HIS
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	456	LYS
1	C	474	LYS
1	C	491	ASP
1	D	11	LEU
1	D	55	GLU

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Mol	Chain	Res	Type
1	D	88	VAL
1	D	120	VAL
1	D	180	GLU
1	D	207	LYS
1	D	221	THR
1	D	253	ASN
1	D	306	ILE
1	D	341	LYS
1	D	363	HIS
1	D	400	ILE
1	D	428	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	111	HIS
1	A	139	GLN
1	A	297	GLN
1	A	310	ASN
1	A	412	ASN
1	A	416	HIS
1	A	423	ASN
1	A	439	ASN
1	B	17	ASN
1	B	94	ASN
1	B	310	ASN
1	B	382	ASN
1	B	386	GLN
1	B	412	ASN
1	B	416	HIS
1	B	492	HIS
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	444	ASN
1	C	452	HIS

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Mol	Chain	Res	Type
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	412	ASN
1	D	416	HIS
1	D	428	GLN

5.3.3 RNA [i](#)

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 oligosaccharides 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$
2	3DH	C	500	-	23,23,23	1.05	1 (4%)	32,33,33	2.31	11 (34%)
2	3DH	D	500	-	23,23,23	1.03	3 (13%)	32,33,33	2.02	10 (31%)
3	NAD	B	550	-	46,48,48	1.47	7 (15%)	64,73,73	1.73	13 (20%)
3	NAD	C	550	-	46,48,48	1.61	6 (13%)	64,73,73	1.85	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	3DH	A	500	-	23,23,23	1.59	4 (17%)	32,33,33	2.27	10 (31%)
3	NAD	D	550	-	46,48,48	1.52	7 (15%)	64,73,73	1.97	18 (28%)
3	NAD	A	550	-	46,48,48	1.48	5 (10%)	64,73,73	2.01	17 (26%)
2	3DH	B	500	-	23,23,23	1.03	3 (13%)	32,33,33	2.03	10 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3DH	C	500	-	-	2/8/24/24	0/3/3/3
2	3DH	D	500	-	-	0/8/24/24	0/3/3/3
3	NAD	B	550	-	-	6/30/62/62	0/5/5/5
3	NAD	C	550	-	-	7/30/62/62	0/5/5/5
2	3DH	A	500	-	-	1/8/24/24	0/3/3/3
3	NAD	D	550	-	-	10/30/62/62	0/5/5/5
3	NAD	A	550	-	-	6/30/62/62	0/5/5/5
2	3DH	B	500	-	-	2/8/24/24	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	550	NAD	O7N-C7N	6.01	1.35	1.24
3	B	550	NAD	C5A-C4A	5.10	1.48	1.39
3	D	550	NAD	O7N-C7N	5.07	1.33	1.24
3	A	550	NAD	O7N-C7N	5.02	1.33	1.24
3	A	550	NAD	C5A-C4A	5.01	1.48	1.39
3	B	550	NAD	O7N-C7N	4.73	1.32	1.24
3	C	550	NAD	C7N-N7N	-4.32	1.25	1.33
3	C	550	NAD	C5A-C4A	4.26	1.46	1.39
2	A	500	3DH	O4'-C1'	4.13	1.51	1.42
3	D	550	NAD	C5A-C4A	3.92	1.46	1.39
3	A	550	NAD	C7N-N7N	-3.88	1.25	1.33
2	A	500	3DH	C5-N7	-3.78	1.32	1.39
3	D	550	NAD	C7N-N7N	-3.39	1.26	1.33
2	D	500	3DH	C5-N7	-3.14	1.33	1.39
2	B	500	3DH	C5-N7	-3.13	1.33	1.39
3	C	550	NAD	C8A-N7A	2.89	1.37	1.31
3	B	550	NAD	C8A-N7A	2.80	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	550	NAD	C7N-N7N	-2.75	1.27	1.33
3	D	550	NAD	C8A-N7A	2.75	1.37	1.31
3	D	550	NAD	O4D-C1D	2.66	1.44	1.40
3	B	550	NAD	C5A-N7A	-2.62	1.34	1.39
3	B	550	NAD	O4D-C1D	2.59	1.44	1.40
3	B	550	NAD	C4A-N9A	-2.48	1.32	1.37
2	C	500	3DH	O4'-C1'	2.48	1.47	1.42
2	A	500	3DH	C8-N9	-2.48	1.33	1.37
2	A	500	3DH	C1'-N9	2.40	1.53	1.46
3	C	550	NAD	O4B-C4B	-2.39	1.39	1.45
3	D	550	NAD	C2N-N1N	-2.36	1.32	1.35
2	B	500	3DH	C8-N9	-2.22	1.33	1.37
2	D	500	3DH	C8-N9	-2.20	1.33	1.37
3	A	550	NAD	C8A-N7A	2.11	1.35	1.31
2	B	500	3DH	C4-N9	-2.08	1.33	1.37
3	C	550	NAD	C4A-N9A	-2.08	1.33	1.37
2	D	500	3DH	C4-N9	-2.05	1.33	1.37
3	D	550	NAD	C5A-N7A	-2.05	1.35	1.39
3	A	550	NAD	PN-O1N	-2.03	1.43	1.50

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	3DH	C5-C4-N3	-5.86	118.65	126.72
3	A	550	NAD	C5A-C4A-N3A	-5.51	119.12	126.72
2	C	500	3DH	C5-C4-N3	-5.35	119.35	126.72
2	B	500	3DH	C5-C4-N3	-5.31	119.41	126.72
2	D	500	3DH	C5-C4-N3	-5.30	119.42	126.72
3	B	550	NAD	C5A-C4A-N3A	-5.14	119.64	126.72
3	A	550	NAD	N3A-C4A-N9A	5.12	135.87	127.17
2	A	500	3DH	N1-C2-N3	-4.92	121.14	128.58
3	D	550	NAD	C4A-N9A-C8A	4.80	110.78	105.74
3	C	550	NAD	N3A-C2A-N1A	-4.73	121.42	128.58
2	C	500	3DH	C4-C5-N7	-4.55	105.38	110.58
2	B	500	3DH	N1-C2-N3	-4.51	121.75	128.58
2	D	500	3DH	N1-C2-N3	-4.50	121.77	128.58
3	C	550	NAD	O7N-C7N-C3N	4.41	124.99	119.60
2	C	500	3DH	C5-N7-C8	4.38	110.33	103.45
3	A	550	NAD	C4A-N9A-C8A	4.27	110.22	105.74
3	D	550	NAD	C5A-C4A-N3A	-4.25	120.86	126.72
3	B	550	NAD	N3A-C2A-N1A	-4.24	122.16	128.58
2	C	500	3DH	N1-C2-N3	-4.22	122.19	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	3DH	N9-C8-N7	-4.20	107.98	113.94
2	A	500	3DH	N3-C4-N9	4.19	134.29	127.17
3	D	550	NAD	N9A-C8A-N7A	-4.17	108.02	113.94
3	C	550	NAD	C5A-C4A-N3A	-3.96	121.27	126.72
3	A	550	NAD	O7N-C7N-N7N	-3.93	116.94	122.62
3	D	550	NAD	C4A-C5A-N7A	-3.89	106.13	110.58
2	A	500	3DH	C4'-O4'-C1'	-3.80	101.09	109.47
3	A	550	NAD	N3A-C2A-N1A	-3.67	123.03	128.58
3	D	550	NAD	C5A-N7A-C8A	3.65	109.18	103.45
3	D	550	NAD	O3-PN-O1N	-3.65	99.73	110.70
3	D	550	NAD	O2A-PA-O3	3.64	117.11	107.27
2	B	500	3DH	N3-C4-N9	3.63	133.34	127.17
2	D	500	3DH	N3-C4-N9	3.61	133.31	127.17
3	D	550	NAD	N3A-C4A-N9A	3.58	133.26	127.17
3	A	550	NAD	O3-PN-O1N	-3.58	99.94	110.70
3	C	550	NAD	C4A-N9A-C8A	3.57	109.49	105.74
3	B	550	NAD	C4A-C5A-N7A	-3.54	106.53	110.58
3	C	550	NAD	C4A-C5A-N7A	-3.53	106.54	110.58
2	A	500	3DH	C2-N3-C4	3.53	120.45	111.83
2	D	500	3DH	C2-N3-C4	3.51	120.41	111.83
2	B	500	3DH	C2-N3-C4	3.51	120.40	111.83
3	C	550	NAD	C2A-N1A-C6A	3.50	124.48	118.73
3	C	550	NAD	O7N-C7N-N7N	-3.49	117.57	122.62
3	A	550	NAD	O7N-C7N-C3N	3.49	123.87	119.60
3	A	550	NAD	C4A-C5A-N7A	-3.49	106.59	110.58
3	B	550	NAD	N3A-C4A-N9A	3.45	133.04	127.17
3	D	550	NAD	C4A-N9A-C1B	-3.45	118.56	126.63
3	D	550	NAD	N3A-C2A-N1A	-3.42	123.40	128.58
2	C	500	3DH	C2-N3-C4	3.34	119.99	111.83
3	A	550	NAD	C5A-N7A-C8A	3.31	108.65	103.45
3	B	550	NAD	C5N-C4N-C3N	-3.28	117.14	120.36
2	D	500	3DH	N9-C8-N7	-3.26	109.31	113.94
2	B	500	3DH	N9-C8-N7	-3.24	109.34	113.94
3	D	550	NAD	C3N-C7N-N7N	3.20	121.69	117.74
3	C	550	NAD	O2A-PA-O3	3.20	115.93	107.27
2	A	500	3DH	O4'-C1'-N9	3.14	114.12	108.09
3	B	550	NAD	C2A-N3A-C4A	3.11	119.42	111.83
3	A	550	NAD	N9A-C8A-N7A	-3.11	109.53	113.94
3	A	550	NAD	C2A-N3A-C4A	3.08	119.35	111.83
2	A	500	3DH	C5-N7-C8	3.02	108.19	103.45
2	A	500	3DH	N9-C8-N7	-2.98	109.70	113.94
3	C	550	NAD	N3A-C4A-N9A	2.97	132.22	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	550	NAD	C2B-C3B-C4B	2.95	108.31	102.61
3	B	550	NAD	O2N-PN-O3	2.92	115.16	107.27
3	A	550	NAD	O2N-PN-O1N	2.85	125.72	112.44
2	C	500	3DH	N3-C4-N9	2.83	131.98	127.17
3	A	550	NAD	C5N-C4N-C3N	-2.82	117.60	120.36
2	D	500	3DH	C5-N7-C8	2.80	107.86	103.45
2	B	500	3DH	C5-N7-C8	2.80	107.84	103.45
3	C	550	NAD	C4A-N9A-C1B	-2.73	120.25	126.63
3	B	550	NAD	C6N-N1N-C1D	2.68	124.98	119.73
2	B	500	3DH	C4-C5-N7	-2.67	107.53	110.58
3	C	550	NAD	C2A-N3A-C4A	2.66	118.34	111.83
2	D	500	3DH	C4-C5-N7	-2.66	107.54	110.58
3	D	550	NAD	O3D-C3D-C4D	-2.65	103.48	111.08
2	C	500	3DH	C5-C4-N9	2.61	108.66	105.81
3	A	550	NAD	O3-PA-O1A	-2.61	102.85	110.70
3	B	550	NAD	O3-PA-O1A	-2.56	103.00	110.70
3	B	550	NAD	C6N-N1N-C2N	-2.52	119.73	121.88
2	C	500	3DH	O4'-C1'-C2'	-2.49	101.28	106.62
3	C	550	NAD	C6A-C5A-N7A	2.49	136.89	132.09
2	D	500	3DH	C4'-O4'-C1'	-2.45	104.05	109.47
2	B	500	3DH	C4'-O4'-C1'	-2.44	104.09	109.47
3	D	550	NAD	O2N-PN-O1N	2.43	123.77	112.44
3	C	550	NAD	C4D-O4D-C1D	2.43	112.15	109.92
3	C	550	NAD	N9A-C8A-N7A	-2.39	110.55	113.94
3	A	550	NAD	C6N-N1N-C1D	2.35	124.35	119.73
3	B	550	NAD	C4D-O4D-C1D	2.30	112.03	109.92
2	A	500	3DH	C6-C5-C4	2.29	120.31	117.18
3	B	550	NAD	C2A-N1A-C6A	2.29	122.49	118.73
2	C	500	3DH	O4'-C4'-C3'	-2.28	100.63	105.15
2	A	500	3DH	C4-C5-N7	-2.27	107.99	110.58
3	C	550	NAD	C5A-N7A-C8A	2.23	106.95	103.45
2	B	500	3DH	C5'-C4'-C3'	-2.23	109.49	115.06
2	D	500	3DH	C5'-C4'-C3'	-2.20	109.55	115.06
2	B	500	3DH	C4-N9-C8	2.19	108.04	105.74
3	B	550	NAD	C5A-N7A-C8A	2.19	106.89	103.45
3	D	550	NAD	C4B-O4B-C1B	-2.18	104.66	109.47
2	D	500	3DH	C4-N9-C8	2.17	108.02	105.74
3	D	550	NAD	O3B-C3B-C4B	-2.16	104.88	111.08
3	D	550	NAD	C2A-N3A-C4A	2.14	117.06	111.83
3	D	550	NAD	C2B-C3B-C4B	2.11	106.69	102.61
2	C	500	3DH	C4'-O4'-C1'	-2.07	104.90	109.47
3	A	550	NAD	C5B-C4B-C3B	-2.04	107.86	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	550	NAD	C6N-N1N-C2N	-2.02	120.16	121.88
3	D	550	NAD	C2A-N1A-C6A	2.02	122.04	118.73
3	C	550	NAD	C5B-C4B-C3B	-2.00	108.00	115.21

There are no chirality outliers.

All (34) torsion outliers are listed below:

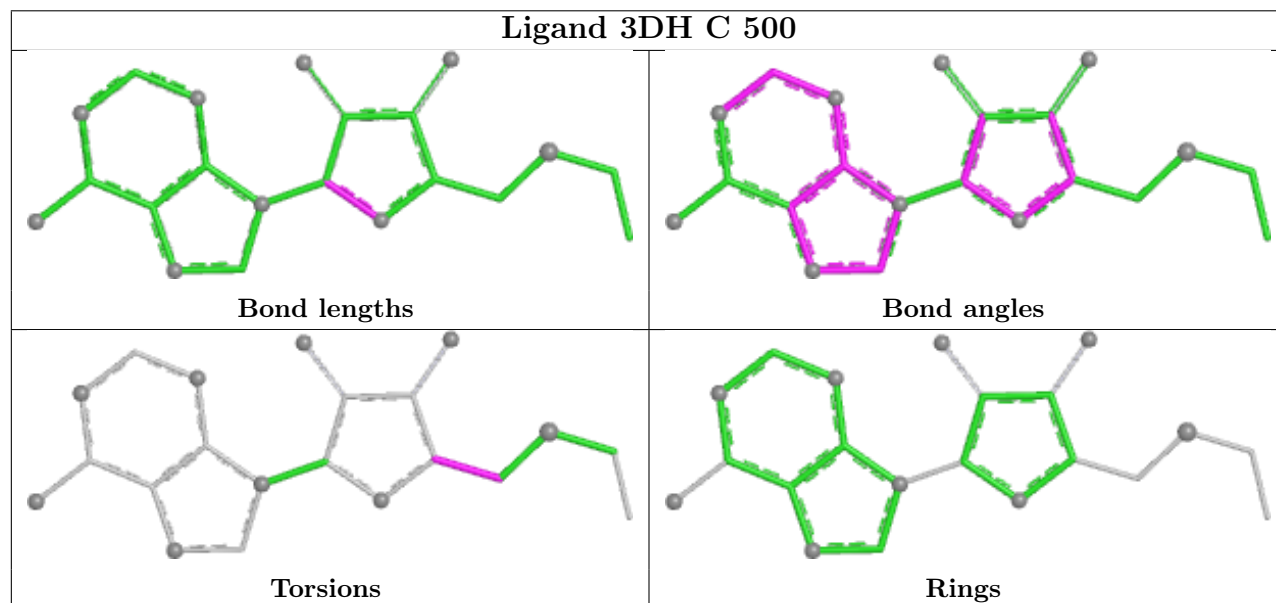
Mol	Chain	Res	Type	Atoms
2	B	500	3DH	O4'-C4'-C5'-SD
2	B	500	3DH	C3'-C4'-C5'-SD
2	C	500	3DH	O4'-C4'-C5'-SD
2	C	500	3DH	C3'-C4'-C5'-SD
3	A	550	NAD	O4D-C1D-N1N-C2N
3	A	550	NAD	O4D-C1D-N1N-C6N
3	A	550	NAD	C2D-C1D-N1N-C2N
3	A	550	NAD	C2D-C1D-N1N-C6N
3	B	550	NAD	O4D-C1D-N1N-C2N
3	B	550	NAD	O4D-C1D-N1N-C6N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

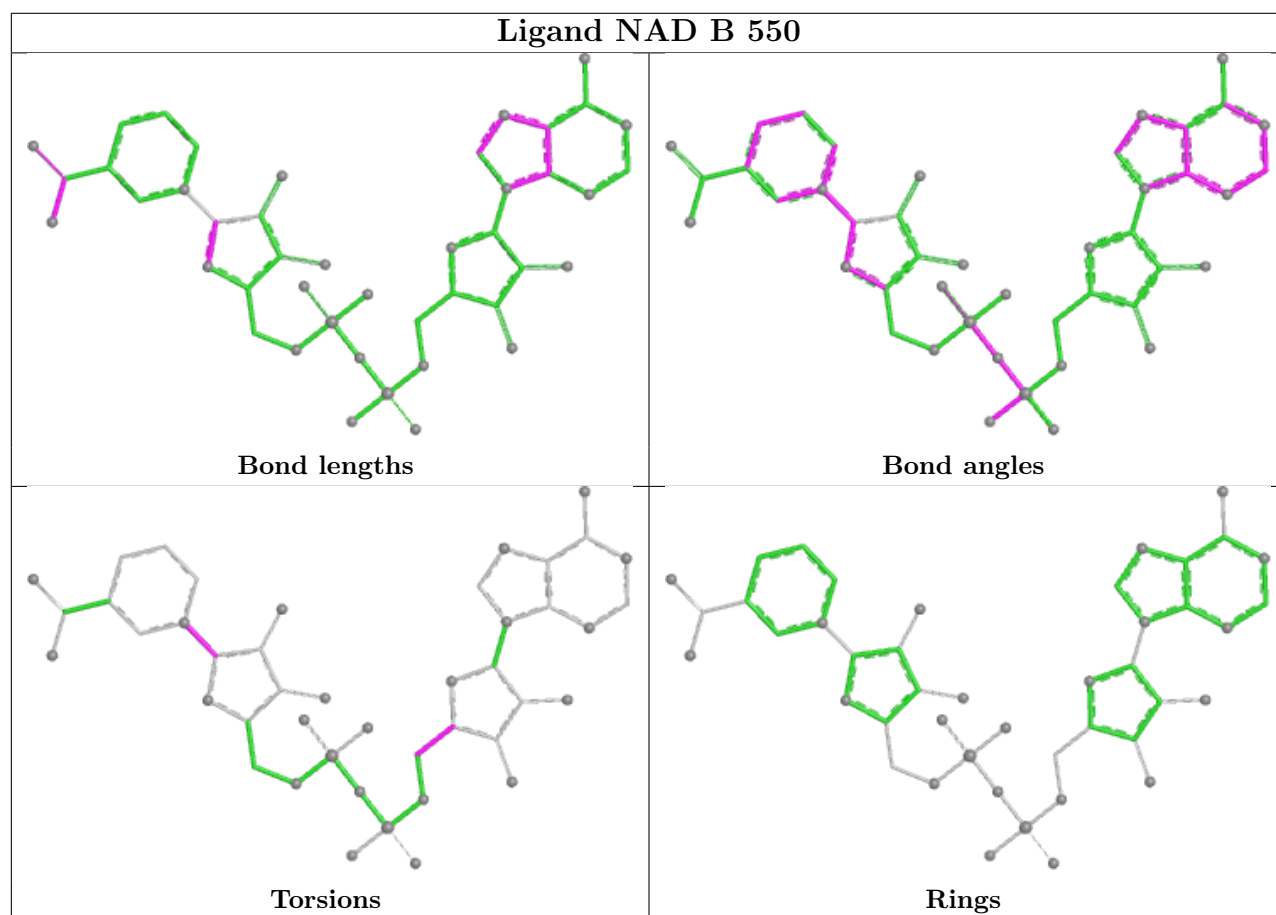
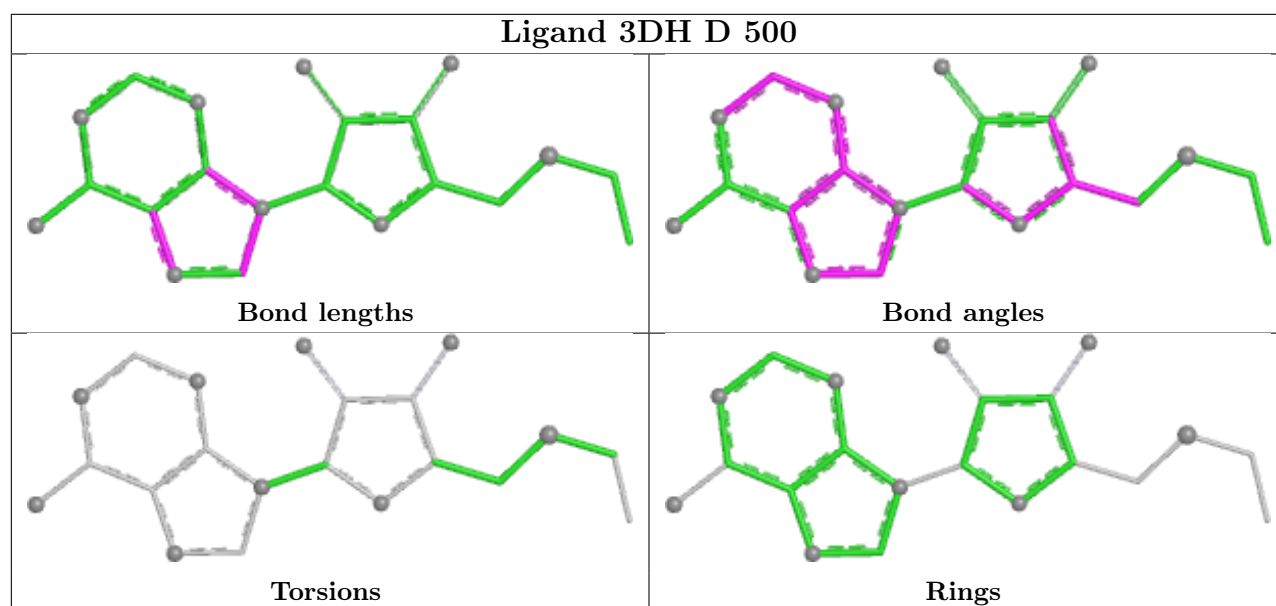
There are no ring outliers.

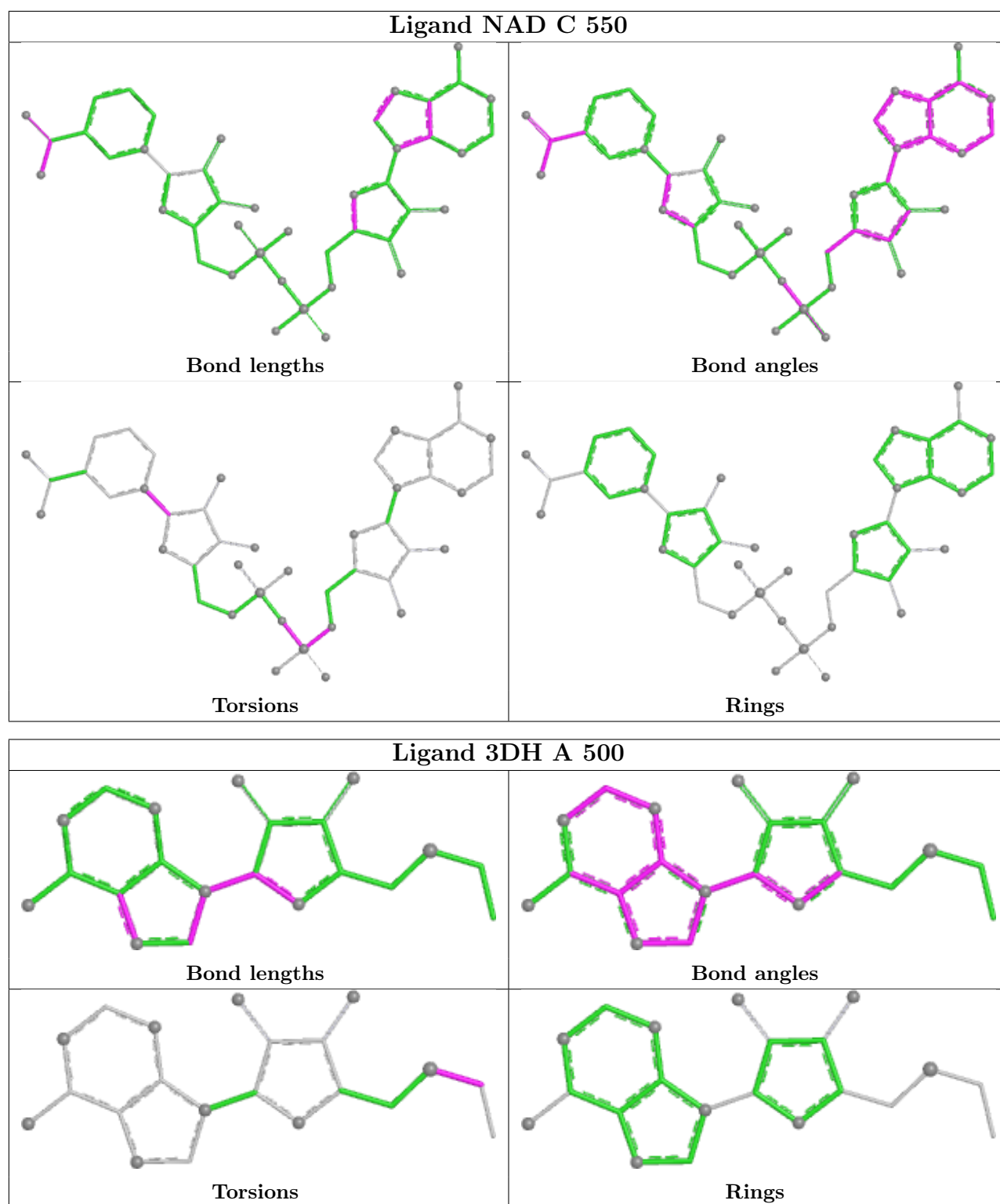
8 monomers are involved in 14 short contacts:

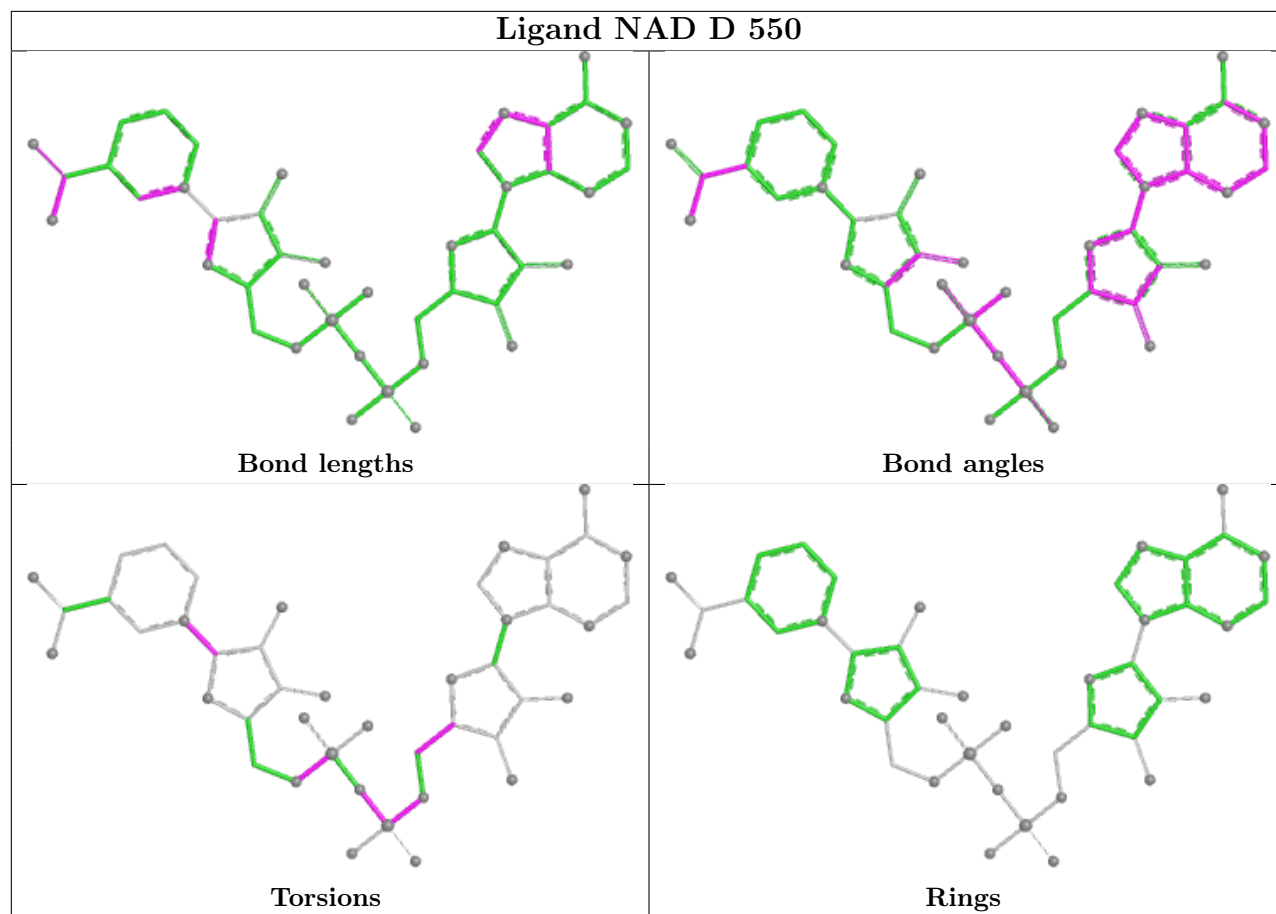
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	3DH	2	0
2	D	500	3DH	2	0
3	B	550	NAD	1	0
3	C	550	NAD	3	0
2	A	500	3DH	2	0
3	D	550	NAD	2	0
3	A	550	NAD	6	0
2	B	500	3DH	1	0

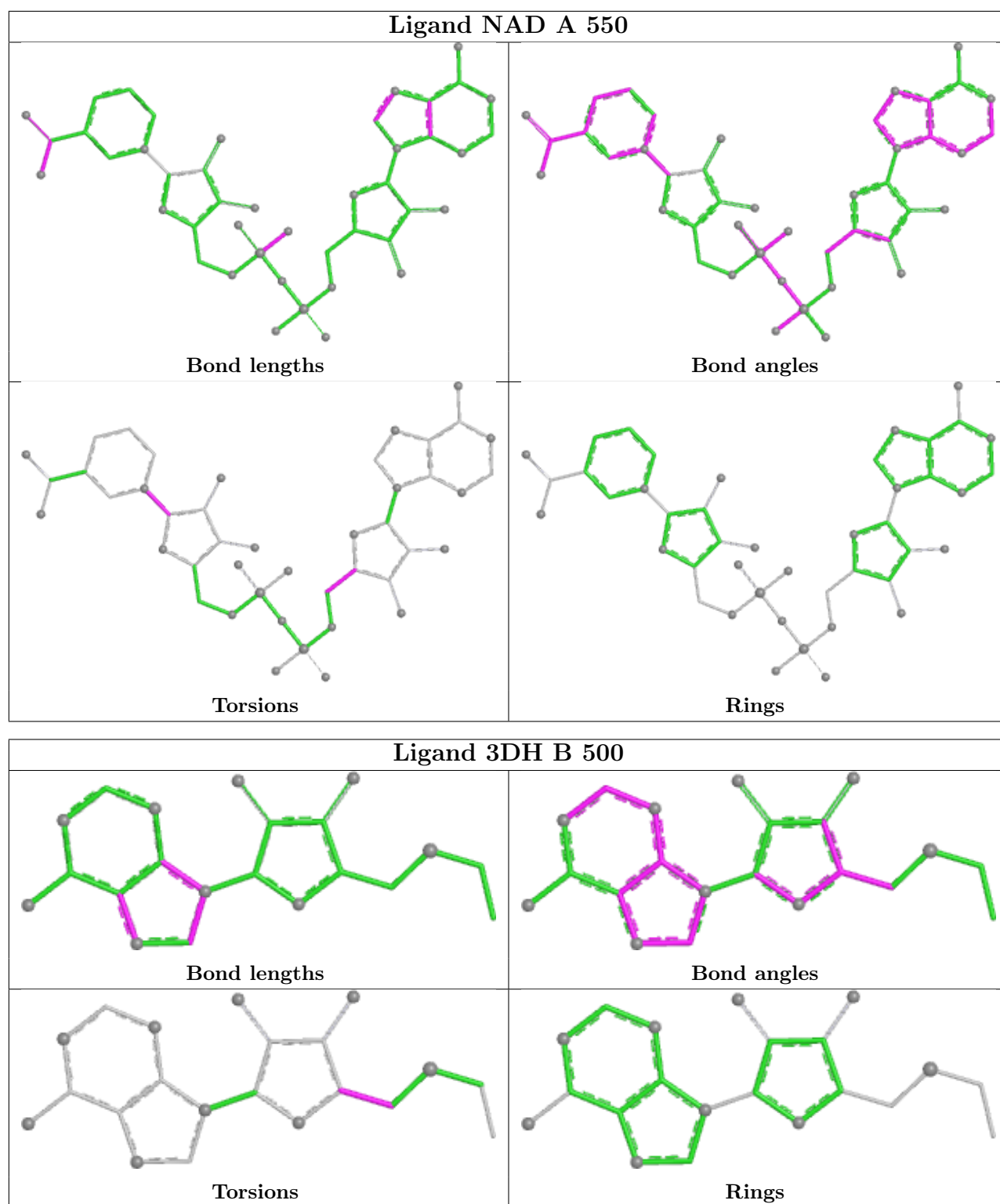
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	486/495 (98%)	0.99	57 (11%) 9 8	19, 36, 57, 88	0
1	B	485/495 (97%)	0.86	38 (7%) 19 18	15, 33, 51, 82	0
1	C	485/495 (97%)	0.85	38 (7%) 19 18	18, 32, 52, 66	0
1	D	485/495 (97%)	0.83	36 (7%) 20 19	16, 32, 49, 67	0
All	All	1941/1980 (98%)	0.88	169 (8%) 16 15	15, 33, 53, 88	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	144	PRO	5.6
1	D	175	VAL	5.5
1	C	150	ALA	5.2
1	C	147	ASP	4.9
1	A	153	ILE	4.5
1	A	239	ALA	4.4
1	C	175	VAL	4.1
1	B	11	LEU	3.8
1	D	484	VAL	3.7
1	C	463	GLU	3.6
1	B	364	PHE	3.5
1	A	66	GLY	3.5
1	A	280	ILE	3.5
1	B	198	PHE	3.4
1	D	371	ALA	3.4
1	A	147	ASP	3.3
1	A	233	GLY	3.3
1	C	227	TYR	3.2
1	B	214	GLY	3.2
1	C	86	ALA	3.2
1	B	147	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	123	PHE	3.2
1	B	106	VAL	3.1
1	D	483	ASP	3.1
1	D	85	GLY	3.1
1	A	178	PRO	3.1
1	A	75	ALA	3.1
1	C	447	TYR	3.0
1	D	364	PHE	3.0
1	A	40	GLU	3.0
1	A	214	GLY	3.0
1	A	364	PHE	2.9
1	D	293	ALA	2.9
1	D	147	ASP	2.9
1	A	302	SER	2.9
1	C	393	GLY	2.9
1	A	273	ILE	2.9
1	C	26	LEU	2.8
1	D	68	LEU	2.8
1	B	75	ALA	2.8
1	D	105	ALA	2.8
1	A	208	ILE	2.8
1	A	479	TYR	2.8
1	B	479	TYR	2.8
1	D	314	ALA	2.8
1	B	177	PRO	2.8
1	A	357	ILE	2.7
1	A	224	LEU	2.7
1	B	229	PHE	2.7
1	A	165	LEU	2.7
1	D	221	THR	2.7
1	B	377	GLY	2.7
1	B	302	SER	2.6
1	A	215	VAL	2.6
1	D	215	VAL	2.6
1	C	29	ALA	2.6
1	B	178	PRO	2.6
1	A	394	ASP	2.6
1	A	189	VAL	2.6
1	A	301	VAL	2.6
1	D	187	TRP	2.6
1	C	377	GLY	2.5
1	A	363	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	11	LEU	2.5
1	A	26	LEU	2.5
1	D	235	LEU	2.5
1	B	228	GLN	2.5
1	C	224	LEU	2.5
1	B	76	VAL	2.4
1	D	460	ILE	2.5
1	C	170	TYR	2.4
1	D	302	SER	2.4
1	A	124	ALA	2.4
1	C	293	ALA	2.4
1	A	191	LEU	2.4
1	B	226	LEU	2.4
1	C	176	VAL	2.4
1	B	227	TYR	2.4
1	B	488	TYR	2.4
1	B	182	ASP	2.4
1	D	251	PHE	2.4
1	A	227	TYR	2.3
1	A	199	GLU	2.3
1	D	239	ALA	2.3
1	D	431	ALA	2.3
1	B	278	VAL	2.3
1	C	39	ALA	2.3
1	D	227	TYR	2.3
1	B	394	ASP	2.3
1	A	229	PHE	2.3
1	C	364	PHE	2.3
1	D	178	PRO	2.3
1	D	232	ALA	2.3
1	A	170	TYR	2.3
1	C	187	TRP	2.3
1	C	251	PHE	2.3
1	A	333	ILE	2.3
1	C	153	ILE	2.3
1	B	303	VAL	2.3
1	D	76	VAL	2.3
1	B	247	THR	2.3
1	D	473	THR	2.3
1	B	66	GLY	2.3
1	A	309	ILE	2.2
1	B	399	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	146	PRO	2.2
1	B	56	VAL	2.2
1	B	215	VAL	2.2
1	A	179	ALA	2.2
1	B	162	MET	2.2
1	D	124	ALA	2.2
1	D	194	LEU	2.2
1	B	189	VAL	2.2
1	A	162	MET	2.2
1	B	330	ASP	2.2
1	D	173	ALA	2.2
1	A	389	LEU	2.2
1	C	68	LEU	2.2
1	D	224	LEU	2.2
1	C	276	LYS	2.2
1	A	238	PRO	2.2
1	B	483	ASP	2.2
1	D	273	ILE	2.2
1	A	175	VAL	2.2
1	D	106	VAL	2.2
1	C	85	GLY	2.2
1	B	402	LEU	2.2
1	C	134	TRP	2.2
1	A	182	ASP	2.2
1	C	196	THR	2.2
1	A	262	ILE	2.1
1	A	106	VAL	2.1
1	B	481	GLY	2.1
1	D	179	ALA	2.1
1	A	488	TYR	2.1
1	B	262	ILE	2.1
1	A	15	VAL	2.1
1	D	214	GLY	2.1
1	D	393	GLY	2.1
1	B	230	ALA	2.1
1	A	187	TRP	2.1
1	A	176	VAL	2.1
1	B	232	ALA	2.1
1	C	314	ALA	2.1
1	A	141	LEU	2.1
1	A	145	ASP	2.1
1	B	183	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	433	ILE	2.1
1	A	446	VAL	2.1
1	B	123	PHE	2.1
1	C	198	PHE	2.1
1	A	70	MET	2.0
1	A	116	GLU	2.0
1	C	236	ALA	2.1
1	A	252	ASP	2.0
1	A	200	THR	2.0
1	C	32	GLY	2.0
1	C	362	GLY	2.0
1	C	442	TYR	2.0
1	A	343	ILE	2.0
1	C	265	ILE	2.0
1	C	333	ILE	2.0
1	C	357	ILE	2.0
1	D	292	GLU	2.0
1	C	345	MET	2.0
1	A	236	ALA	2.0
1	D	205	TRP	2.0
1	C	178	PRO	2.0
1	C	329	GLY	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
2	3DH	D	500	21/21	0.74	0.16	18,26,43,61	0

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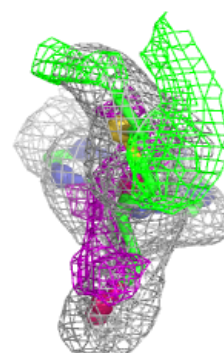
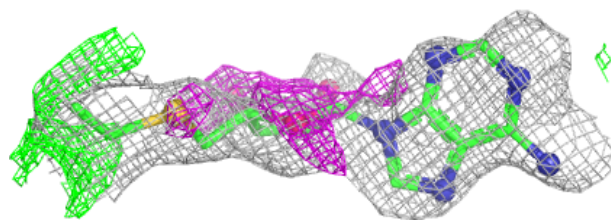
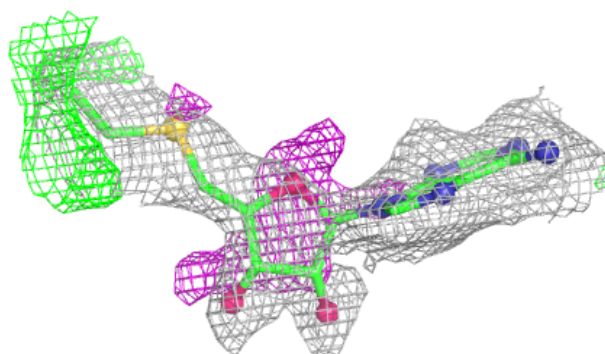
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	3DH	A	500	21/21	0.76	0.13	21,27,38,52	0
2	3DH	B	500	21/21	0.80	0.15	12,28,53,65	0
2	3DH	C	500	21/21	0.84	0.13	7,28,38,46	0
3	NAD	A	550	44/44	0.91	0.10	15,32,41,47	0
3	NAD	B	550	44/44	0.93	0.09	18,30,39,44	0
3	NAD	C	550	44/44	0.93	0.10	16,26,35,38	0
3	NAD	D	550	44/44	0.93	0.09	9,25,33,36	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.

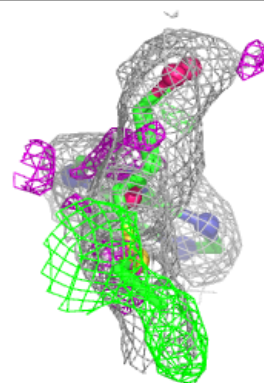
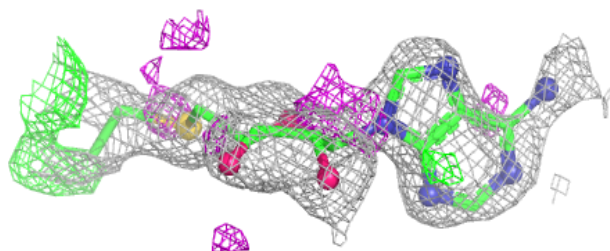
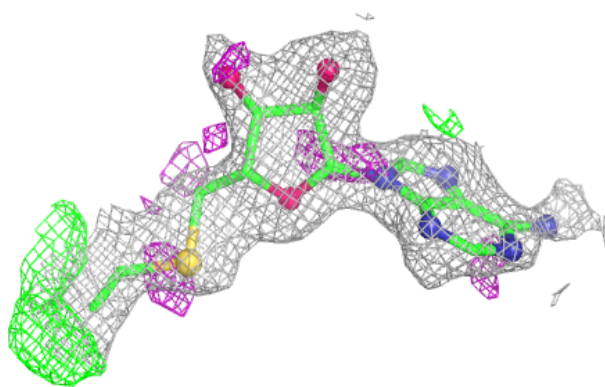
Electron density around 3DH D 500:

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

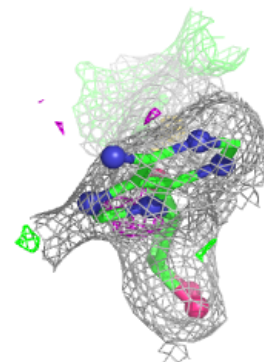
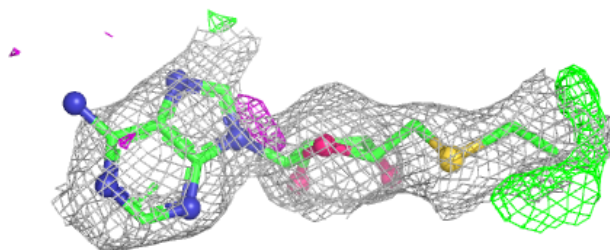
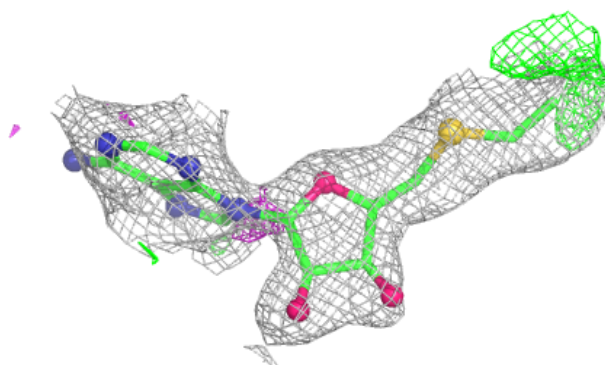


Electron density around 3DH A 500:

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

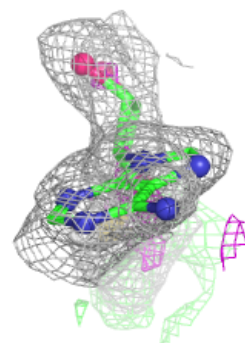
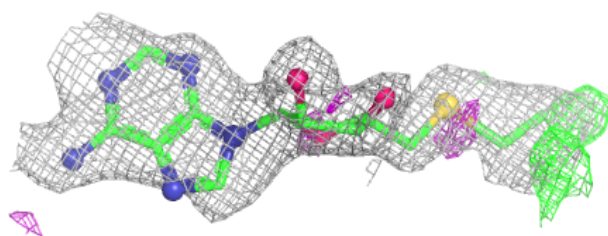
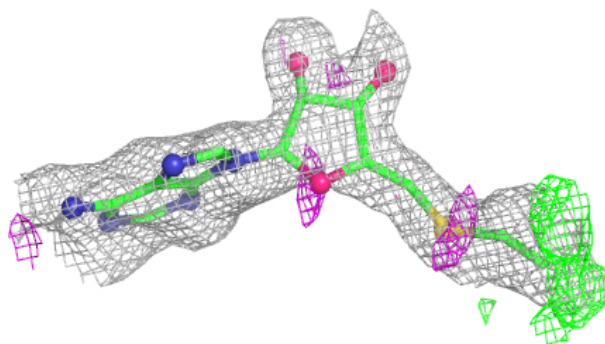
**Electron density around 3DH B 500:**

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

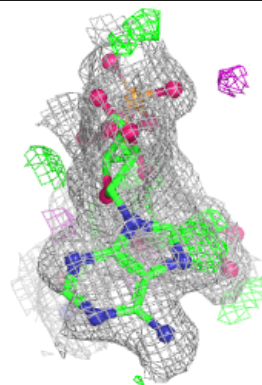
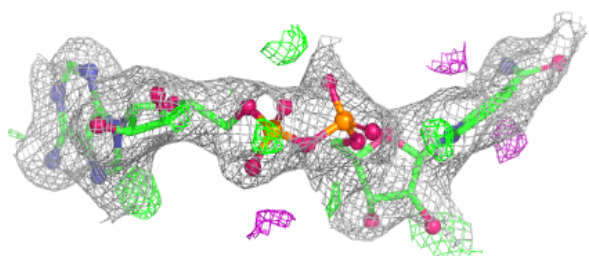
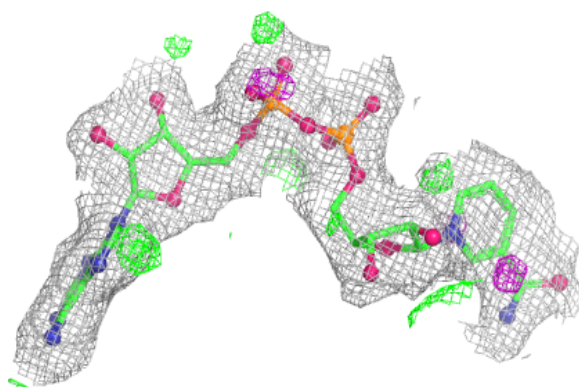


Electron density around 3DH C 500:

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

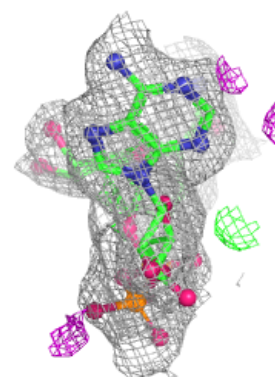
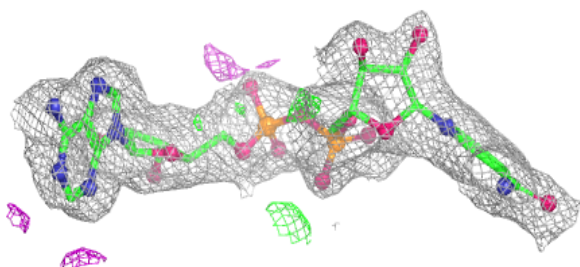
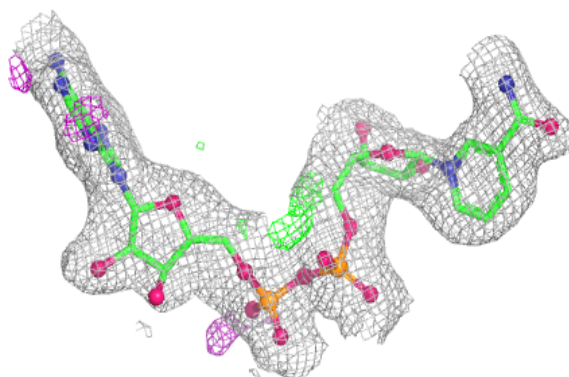
**Electron density around NAD A 550:**

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

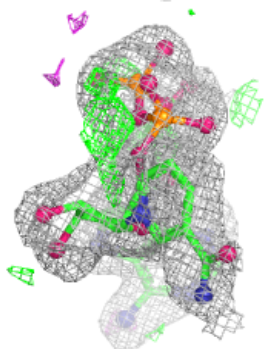
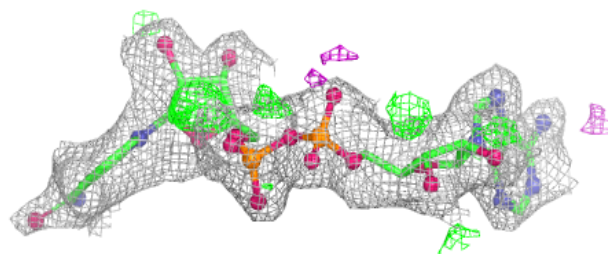
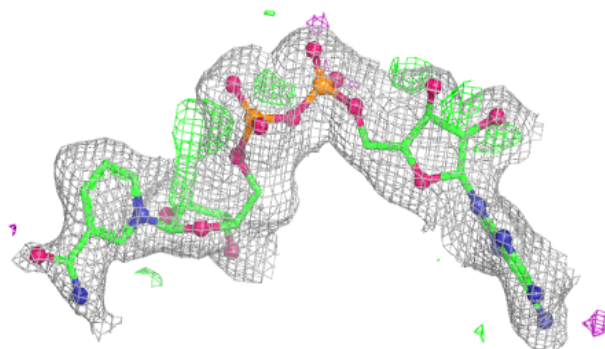


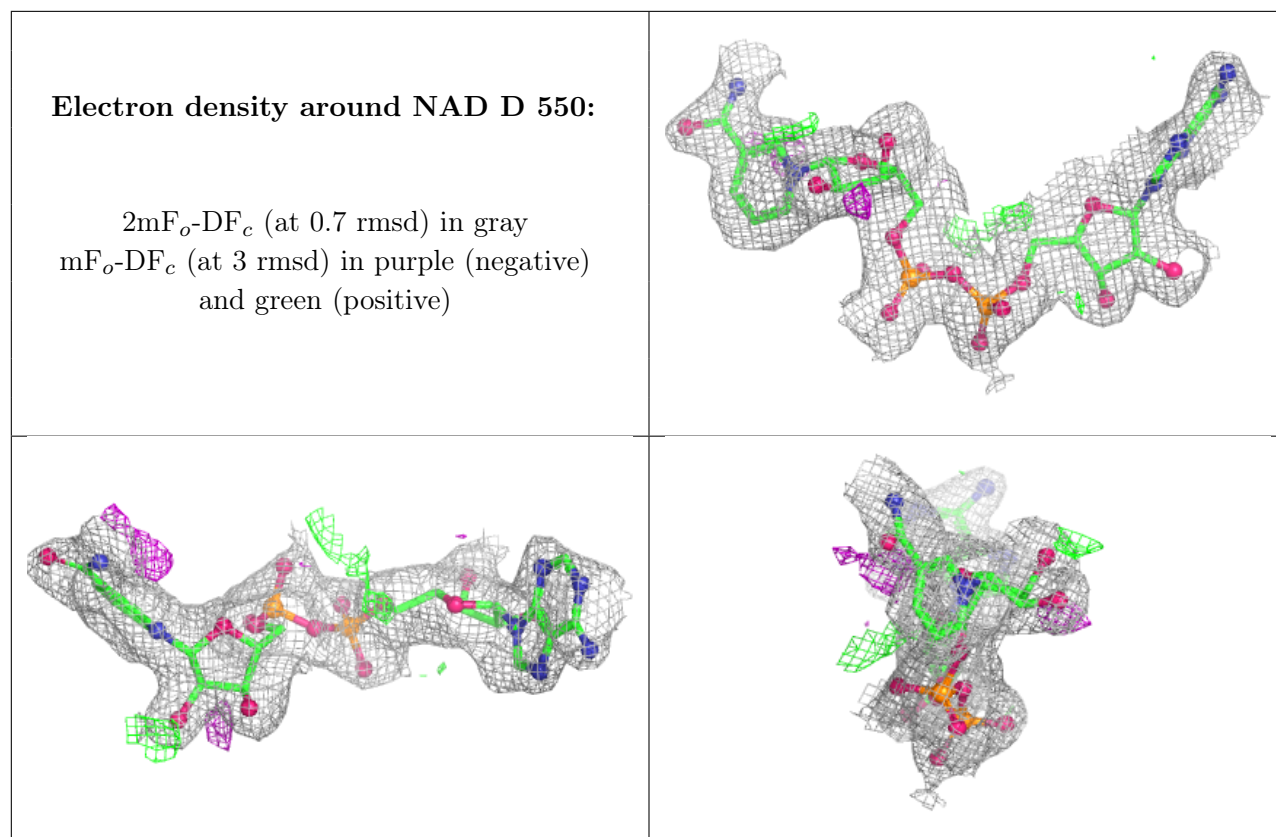
Electron density around NAD B 550:

$2mF_o-DF_c$ (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)





6.5 Other polymers ⓘ

There are no such residues in this entry.