



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:03 PM UTC

PDB ID : 4M55 / pdb_00004m55
Title : Crystal structure of Human UDP-xylose synthase R236H substitution
Authors : Walsh Jr., R.M.; Polizzi, S.J.; Wood, Z.A.
Deposited on : 2013-08-08
Resolution : 2.86 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

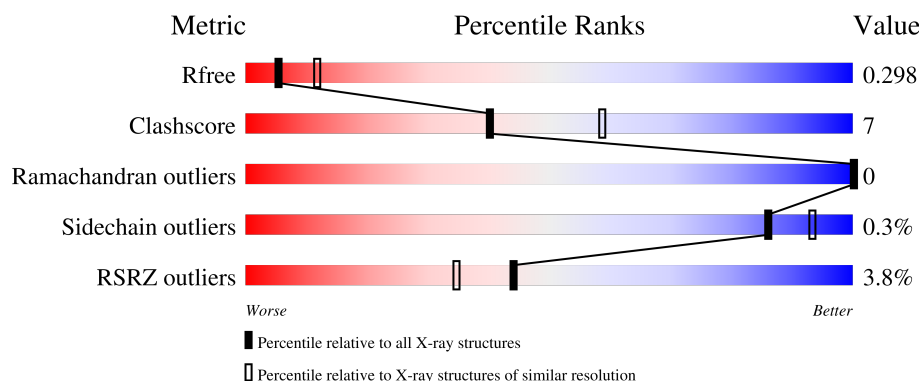
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	336	2% 66% 12% 22%
1	B	336	2% 71% 10% 19%
1	C	336	3% 67% 13% 19%
1	D	336	3% 61% 16% 22%
1	E	336	0% 37% 12% 51%

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Mol	Chain	Length	Quality of chain
1	F	336	4%48%6%46%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11483 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 UDP-glucuronic acid decarboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2086	1332	365	379	10			
1	B	272	Total	C	N	O	S	0	0	0
			2145	1367	374	394	10			
1	C	271	Total	C	N	O	S	0	0	0
			2135	1362	370	393	10			
1	D	261	Total	C	N	O	S	0	0	0
			2070	1323	362	375	10			
1	E	164	Total	C	N	O	S	0	0	0
			1281	816	222	235	8			
1	F	181	Total	C	N	O	S	0	0	0
			1429	917	243	260	9			

There are 6 discrepancies between the modelled and reference sequences:

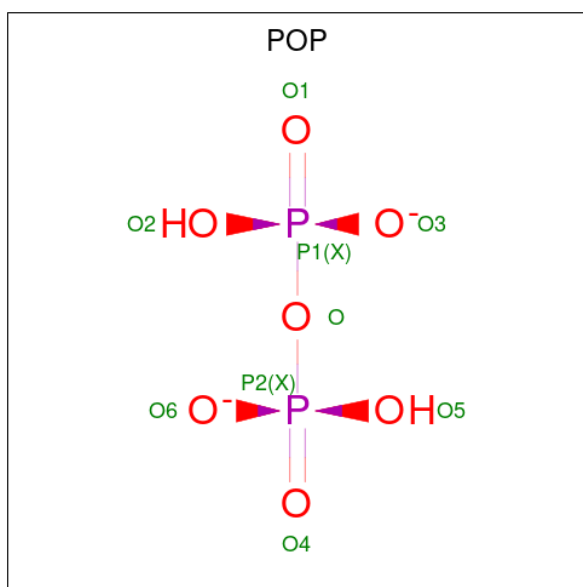
Chain	Residue	Modelled	Actual	Comment	Reference
A	236	HIS	ARG	engineered mutation	UNP Q8NBZ7
B	236	HIS	ARG	engineered mutation	UNP Q8NBZ7
C	236	HIS	ARG	engineered mutation	UNP Q8NBZ7
D	236	HIS	ARG	engineered mutation	UNP Q8NBZ7
E	236	HIS	ARG	engineered mutation	UNP Q8NBZ7
F	236	HIS	ARG	engineered mutation	UNP Q8NBZ7

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 3 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			9	7	2		
3	C	1	Total	O	P	0	0
			9	7	2		

- Molecule 4 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



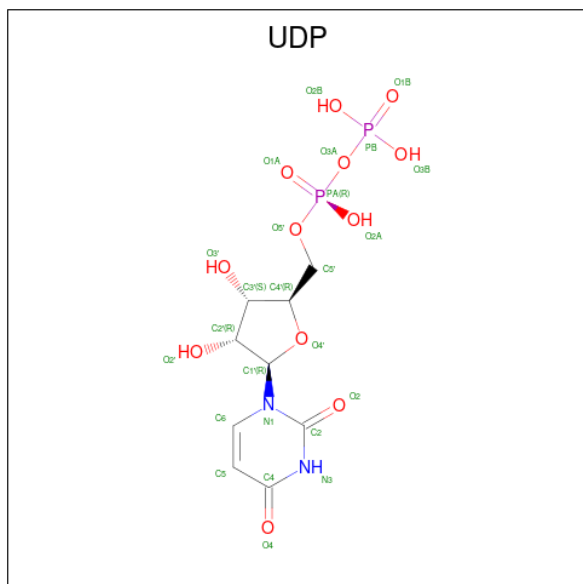
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).

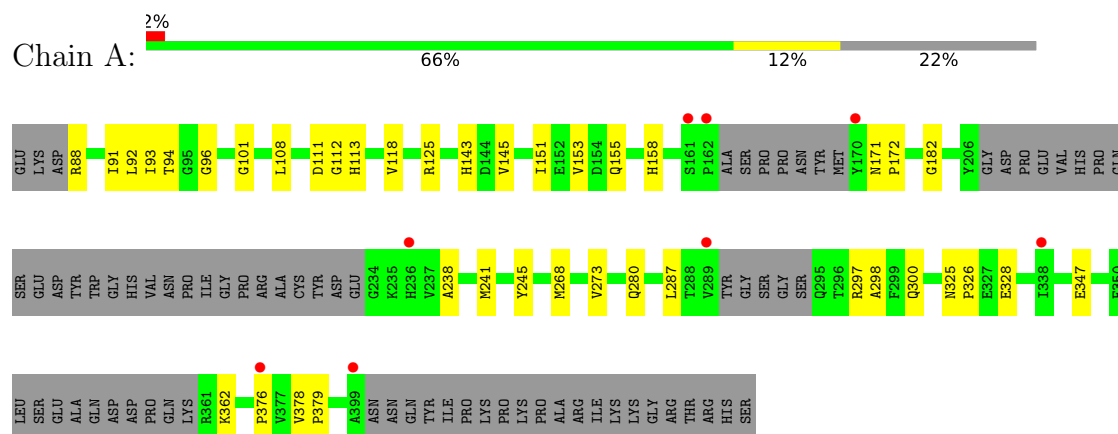


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
5	D	1	Total	C	O	P		0	0
			15	3	10	2			

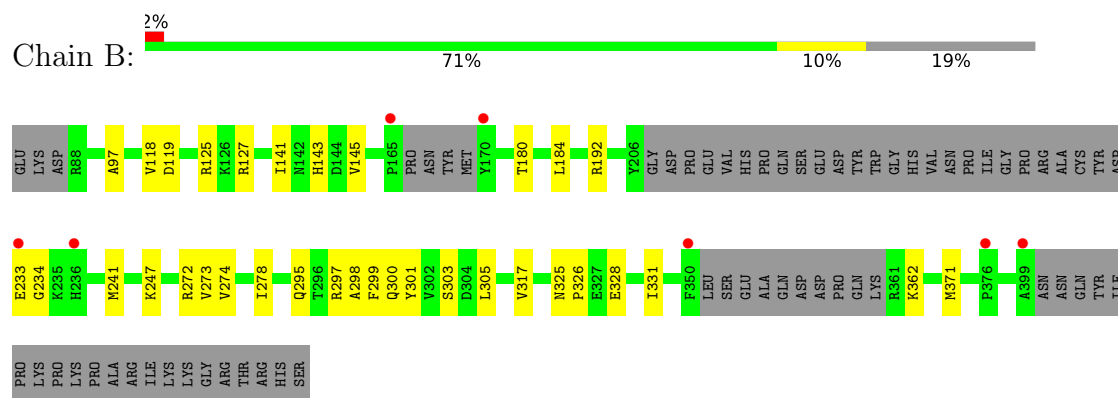
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

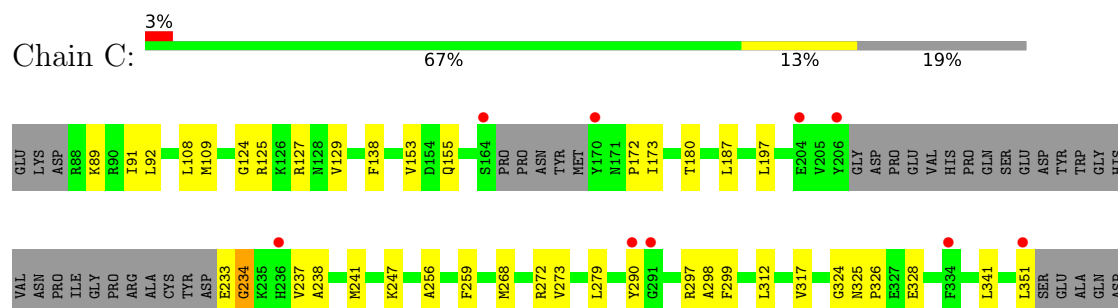
• Molecule 1: UDP-glucuronic acid decarboxylase 1

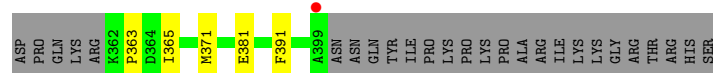


• Molecule 1: UDP-glucuronic acid decarboxylase 1

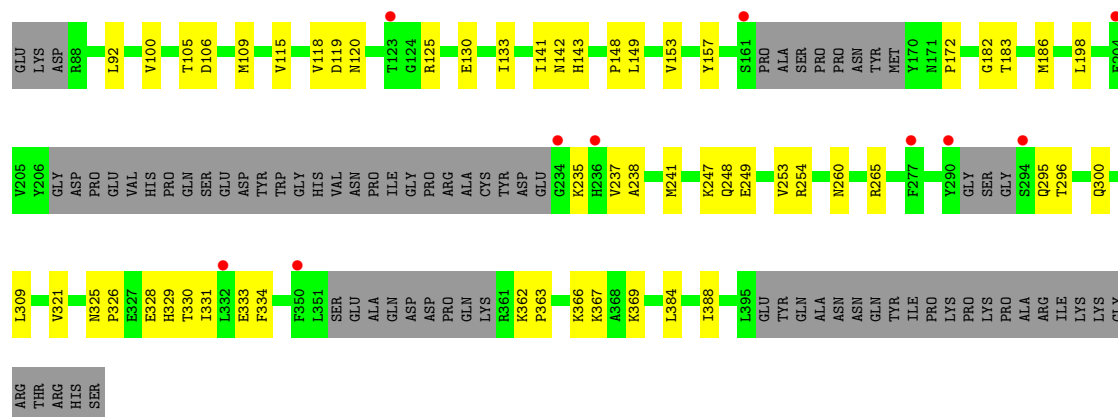


• Molecule 1: UDP-glucuronic acid decarboxylase 1

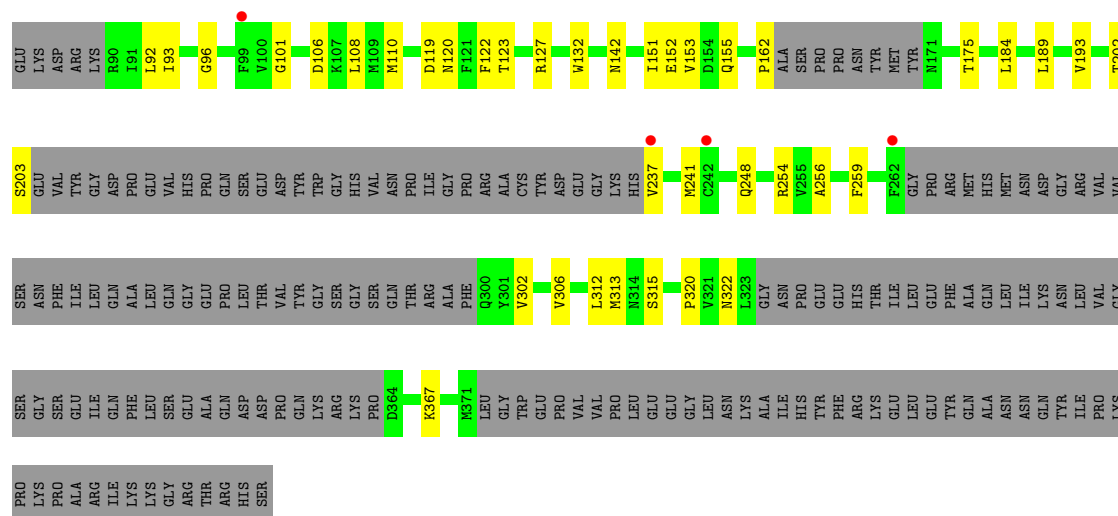
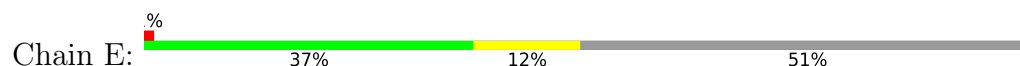




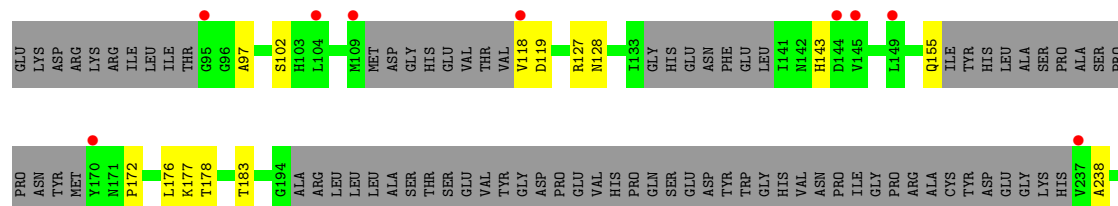
• Molecule 1: UDP-glucuronic acid decarboxylase 1

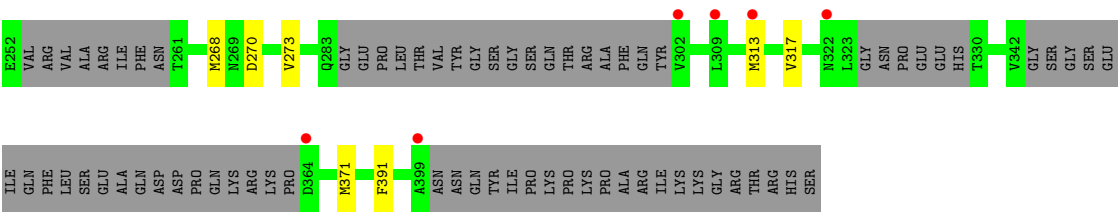


• Molecule 1: UDP-glucuronic acid decarboxylase 1



• Molecule 1: UDP-glucuronic acid decarboxylase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.17Å 85.14Å 292.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.31 – 2.86 42.31 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.31-2.86) 99.9 (42.31-2.86)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.228 , 0.285 0.245 , 0.298	Depositor DCC
R_{free} test set	2451 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	78.4	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 94.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.156 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11483	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: SO4, POP, UDP, 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	0.48	0/2125	0.77	2/2868 (0.1%)
1	B	0.65	0/2187	0.84	0/2954
1	C	0.65	0/2176	0.89	2/2939 (0.1%)
1	D	0.56	0/2108	0.85	0/2844
1	E	0.47	0/1299	0.79	0/1752
1	F	0.43	0/1448	0.73	0/1946
All	All	0.56	0/11343	0.82	4/15303 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ASN	CA-C-N	5.85	125.54	119.05
1	A	171	ASN	C-N-CA	5.85	125.54	119.05
1	C	234	GLY	N-CA-C	-5.69	107.17	114.85
1	C	129	VAL	CB-CA-C	-5.19	105.56	110.70

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	2086	0	2100	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2145	0	2149	27	0
1	C	2135	0	2140	31	0
1	D	2070	0	2090	37	0
1	E	1281	0	1301	27	0
1	F	1429	0	1445	13	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	0	0
2	D	44	0	26	1	0
2	E	44	0	26	2	0
2	F	44	0	26	1	0
3	A	9	0	0	1	0
3	C	9	0	0	0	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	B	25	0	11	1	0
5	D	15	0	3	1	0
All	All	11483	0	11395	150	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 (150) 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:118:VAL:HG13	1:D:143:HIS:HB3	1.58	0.83
1:A:92:LEU:HD22	1:A:151:ILE:HD11	1.69	0.74
1:D:321:VAL:HG22	1:D:367:LYS:HE2	1.71	0.73
1:C:187:LEU:HD23	1:C:197:LEU:HD13	1.70	0.72
1:C:247:LYS:HE3	1:D:172:PRO:HG3	1.74	0.70
1:F:178:THR:OG1	2:F:800:NAD:N6A	2.23	0.69
1:B:317:VAL:HG22	1:B:371:MET:HE3	1.77	0.67
1:D:238:ALA:HA	1:D:241:MET:HE2	1.76	0.66
1:A:172:PRO:HG3	1:B:247:LYS:HE3	1.79	0.64
1:C:233:GLU:HG2	1:C:234:GLY:H	1.62	0.63
1:C:238:ALA:HA	1:C:241:MET:HE2	1.80	0.63
1:B:272:ARG:HD3	1:B:299:PHE:HE1	1.63	0.63
1:A:326:PRO:O	1:A:362:LYS:NZ	2.31	0.63
1:C:172:PRO:HG3	1:D:247:LYS:HE3	1.82	0.61
1:D:119:ASP:O	1:D:142:ASN:HA	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:GLU:HG2	1:B:234:GLY:H	1.66	0.60
1:A:238:ALA:HA	1:A:241:MET:HE2	1.82	0.60
2:A:501:NAD:O2N	2:A:501:NAD:N7N	2.33	0.60
1:C:272:ARG:HD3	1:C:299:PHE:HE1	1.67	0.59
1:A:268:MET:N	4:A:503:SO4:O2	2.36	0.59
1:B:326:PRO:O	1:B:362:LYS:NZ	2.36	0.58
1:D:253:VAL:O	1:D:254:ARG:NH1	2.35	0.58
1:A:93:ILE:HD11	1:A:108:LEU:HD12	1.87	0.57
1:C:297:ARG:HB3	1:C:299:PHE:HE2	1.68	0.57
1:D:125:ARG:HH21	1:E:127:ARG:HE	1.51	0.57
1:D:295:GLN:O	1:D:331:ILE:HG12	2.04	0.57
1:A:118:VAL:HG13	1:A:143:HIS:HB3	1.85	0.57
1:D:92:LEU:HB2	1:D:153:VAL:HG11	1.86	0.57
1:D:118:VAL:HG21	1:D:149:LEU:HD21	1.86	0.57
1:E:92:LEU:HB2	1:E:153:VAL:HG11	1.85	0.56
1:D:120:ASN:O	1:E:142:ASN:ND2	2.39	0.56
1:C:298:ALA:HB2	1:C:328:GLU:HG2	1.88	0.56
1:D:329:HIS:ND1	1:D:333:GLU:OE1	2.32	0.55
1:B:192:ARG:NE	5:B:502:UDP:O4	2.36	0.55
1:E:248:GLN:OE1	1:F:172:PRO:HD2	2.07	0.54
1:C:297:ARG:HB3	1:C:299:PHE:CE2	2.42	0.54
1:A:325:ASN:HD22	1:A:376:PRO:HG2	1.71	0.54
1:C:92:LEU:HB2	1:C:153:VAL:HG11	1.90	0.54
1:C:233:GLU:HG2	1:C:234:GLY:N	2.22	0.54
1:D:157:TYR:HD2	1:D:198:LEU:HD22	1.73	0.53
1:D:105:THR:HG23	1:D:115:VAL:HG11	1.91	0.53
1:B:127:ARG:HE	1:C:127:ARG:HH21	1.57	0.52
1:D:198:LEU:HD21	1:D:309:LEU:HD22	1.92	0.52
1:E:106:ASP:OD1	1:E:132:TRP:NE1	2.39	0.52
1:B:127:ARG:HH21	1:C:127:ARG:HE	1.57	0.52
1:E:259:PHE:HE1	1:E:322:ASN:HB3	1.75	0.52
1:A:298:ALA:HB1	1:A:325:ASN:O	2.09	0.52
1:D:300:GLN:HB3	1:D:325:ASN:HB2	1.92	0.51
1:C:326:PRO:HA	1:C:363:PRO:HG2	1.92	0.51
1:E:259:PHE:CE1	1:E:322:ASN:HB3	2.45	0.51
1:D:366:LYS:HA	1:D:369:LYS:HD2	1.93	0.51
1:A:92:LEU:HB2	1:A:153:VAL:HG11	1.93	0.50
1:E:96:GLY:HA2	1:E:101:GLY:HA3	1.93	0.50
1:B:297:ARG:HB3	1:B:299:PHE:CE2	2.47	0.50
1:A:287:LEU:N	1:A:347:GLU:O	2.44	0.50
1:E:119:ASP:OD2	2:E:800:NAD:O3B	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ALA:HB1	1:B:325:ASN:O	2.12	0.50
1:D:326:PRO:HA	1:D:363:PRO:HG2	1.93	0.50
1:D:248:GLN:HG2	1:D:249:GLU:HG2	1.93	0.49
1:A:125:ARG:HH22	1:F:127:ARG:H	1.60	0.49
1:C:268:MET:HE3	1:C:391:PHE:CD2	2.48	0.49
1:E:119:ASP:OD1	1:E:120:ASN:N	2.44	0.49
1:F:268:MET:HE3	1:F:391:PHE:CD2	2.48	0.49
1:E:162:PRO:HG2	1:E:175:THR:HG23	1.95	0.48
1:A:238:ALA:HA	1:A:241:MET:CE	2.44	0.48
1:C:89:LYS:HE3	1:C:155:GLN:NE2	2.29	0.48
1:B:273:VAL:HG11	1:B:297:ARG:HG3	1.95	0.48
1:B:297:ARG:HB3	1:B:299:PHE:HE2	1.78	0.48
1:C:180:THR:HA	1:C:241:MET:HE1	1.95	0.48
1:A:96:GLY:HA2	1:A:101:GLY:HA3	1.96	0.47
1:B:298:ALA:HB2	1:B:328:GLU:HG2	1.96	0.47
1:E:189:LEU:O	1:E:193:VAL:HG22	2.14	0.47
1:A:245:TYR:OH	3:A:502:POP:O5	2.27	0.47
1:A:94:THR:OG1	1:A:158:HIS:HA	2.14	0.47
1:A:145:VAL:O	1:A:182:GLY:HA2	2.15	0.47
1:B:145:VAL:HG22	2:B:501:NAD:N1A	2.29	0.47
1:B:273:VAL:HG21	1:B:331:ILE:HD12	1.97	0.47
1:F:183:THR:HG21	1:F:238:ALA:HB1	1.97	0.47
1:E:151:ILE:HG12	1:E:152:GLU:H	1.79	0.46
1:E:320:PRO:O	1:E:367:LYS:NZ	2.48	0.46
1:B:274:VAL:O	1:B:278:ILE:HG13	2.14	0.46
1:C:341:LEU:HD21	1:C:381:GLU:HG3	1.96	0.46
1:D:329:HIS:HB2	1:D:334:PHE:CE2	2.51	0.46
1:C:109:MET:HE2	1:C:138:PHE:HB2	1.98	0.45
1:C:124:GLY:O	1:C:125:ARG:HD3	2.16	0.45
1:E:302:VAL:O	1:E:306:VAL:HG23	2.16	0.45
1:D:157:TYR:CD2	1:D:198:LEU:HD22	2.51	0.45
1:A:273:VAL:HG11	1:A:297:ARG:HG3	1.99	0.45
1:F:270:ASP:OD1	1:F:270:ASP:N	2.48	0.45
1:D:141:ILE:HG22	1:D:143:HIS:HB2	2.00	0.44
1:F:155:GLN:HB3	1:F:313:MET:HE3	1.99	0.44
1:E:155:GLN:HB3	1:E:313:MET:HE3	1.99	0.44
1:F:317:VAL:HG21	1:F:371:MET:HB3	2.00	0.44
1:A:280:GLN:OE1	1:A:287:LEU:HA	2.17	0.44
1:A:298:ALA:HB2	1:A:328:GLU:HG2	2.00	0.44
1:E:241:MET:HG2	1:F:176:LEU:HD13	2.00	0.44
1:C:290:TYR:CE1	1:C:351:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:VAL:HG21	1:B:371:MET:HB3	1.99	0.44
1:A:111:ASP:HB2	1:A:113:HIS:CD2	2.53	0.44
1:D:100:VAL:HB	2:D:501:NAD:H51N	2.00	0.44
1:A:300:GLN:HB3	1:A:325:ASN:HB2	1.99	0.44
1:B:233:GLU:HG2	1:B:234:GLY:N	2.32	0.44
1:E:254:ARG:NH2	1:E:315:SER:O	2.51	0.43
1:D:118:VAL:HG21	1:D:149:LEU:CD2	2.48	0.43
1:B:118:VAL:HG13	1:B:143:HIS:HB3	2.00	0.43
1:C:298:ALA:HB1	1:C:325:ASN:O	2.18	0.43
1:B:295:GLN:O	1:B:331:ILE:HG12	2.19	0.43
1:C:324:GLY:O	1:C:365:ILE:HG21	2.18	0.43
1:E:93:ILE:HD11	1:E:108:LEU:HD12	1.99	0.43
1:B:180:THR:HA	1:B:241:MET:HE1	2.00	0.43
1:C:91:ILE:HD13	1:C:108:LEU:HD13	2.00	0.43
1:C:256:ALA:HB2	1:C:312:LEU:HD23	2.00	0.42
1:D:148:PRO:HG3	5:D:502:UDP:O2'	2.19	0.42
1:D:296:THR:HA	1:D:330:THR:HA	2.00	0.42
1:E:106:ASP:O	1:E:110:MET:HG2	2.19	0.42
1:F:97:ALA:HB3	1:F:119:ASP:CG	2.44	0.42
1:C:317:VAL:HG22	1:C:371:MET:HE3	2.01	0.42
1:D:130:GLU:HA	1:D:133:ILE:HG13	2.01	0.42
1:D:328:GLU:HG3	1:D:362:LYS:HG3	2.02	0.42
1:B:125:ARG:NH1	1:B:127:ARG:HH22	2.17	0.42
1:B:301:TYR:HD2	1:B:303:SER:HG	1.64	0.42
1:E:184:LEU:HG	1:E:241:MET:SD	2.59	0.42
1:B:300:GLN:OE1	1:B:305:LEU:HB2	2.20	0.42
1:C:273:VAL:HG11	1:C:297:ARG:HG3	2.02	0.42
1:F:177:LYS:HB3	1:F:177:LYS:HE2	1.80	0.42
1:D:106:ASP:OD2	1:D:265:ARG:NH1	2.52	0.42
1:D:183:THR:HB	1:D:241:MET:HE1	2.01	0.42
1:D:182:GLY:O	1:D:186:MET:HG2	2.20	0.42
1:B:184:LEU:HG	1:B:241:MET:SD	2.60	0.42
1:F:102:SER:HB3	1:F:128:ASN:HB3	2.01	0.42
1:C:290:TYR:HD1	1:C:351:LEU:HB2	1.85	0.41
1:F:118:VAL:HG13	1:F:143:HIS:HB3	2.00	0.41
1:B:118:VAL:HG22	1:B:141:ILE:HB	2.01	0.41
1:E:119:ASP:OD1	2:E:800:NAD:O2B	2.37	0.41
1:E:122:PHE:HD2	1:E:123:THR:HG23	1.85	0.41
1:E:256:ALA:HB2	1:E:312:LEU:HD23	2.02	0.41
1:C:259:PHE:CD2	1:C:363:PRO:HB3	2.55	0.41
1:D:235:LYS:HE3	1:D:235:LYS:HB3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ALA:HB3	1:B:119:ASP:OD2	2.21	0.41
1:A:88:ARG:HD2	1:A:112:GLY:O	2.20	0.41
1:C:173:ILE:HG13	1:D:248:GLN:OE1	2.21	0.41
1:C:268:MET:HE2	1:C:279:LEU:HD21	2.03	0.41
1:A:91:ILE:HG12	1:A:155:GLN:HB2	2.03	0.41
1:E:122:PHE:CD2	1:E:123:THR:HG23	2.56	0.41
1:E:151:ILE:HG12	1:E:152:GLU:N	2.35	0.41
1:E:202:THR:OG1	1:E:203:SER:N	2.54	0.41
1:D:109:MET:HE3	1:D:109:MET:HB3	1.85	0.40
1:D:384:LEU:O	1:D:388:ILE:HG13	2.20	0.40
1:A:378:VAL:HA	1:A:379:PRO:HD2	1.97	0.40
1:D:260:ASN:OD1	1:D:260:ASN:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	253/336 (75%)	244 (96%)	9 (4%)	0	100	100
1	B	264/336 (79%)	258 (98%)	6 (2%)	0	100	100
1	C	263/336 (78%)	255 (97%)	8 (3%)	0	100	100
1	D	251/336 (75%)	238 (95%)	13 (5%)	0	100	100
1	E	154/336 (46%)	146 (95%)	8 (5%)	0	100	100
1	F	163/336 (48%)	158 (97%)	5 (3%)	0	100	100
All	All	1348/2016 (67%)	1299 (96%)	49 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	227/290 (78%)	227 (100%)	0	100	100
1	B	233/290 (80%)	233 (100%)	0	100	100
1	C	232/290 (80%)	231 (100%)	1 (0%)	84	92
1	D	226/290 (78%)	225 (100%)	1 (0%)	84	92
1	E	142/290 (49%)	141 (99%)	1 (1%)	76	87
1	F	157/290 (54%)	156 (99%)	1 (1%)	78	89
All	All	1217/1740 (70%)	1213 (100%)	4 (0%)	86	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	237	VAL
1	D	237	VAL
1	E	237	VAL
1	F	273	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	GLN
1	A	267	HIS
1	A	314	ASN
1	A	329	HIS
1	B	155	GLN
1	D	103	HIS
1	D	155	GLN
1	D	314	ASN
1	D	325	ASN
1	D	336	GLN
1	D	340	ASN
1	E	155	GLN
1	E	314	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

13 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	POP	A	502	-	6,8,8	0.66	0	12,13,13	1.08	1 (8%)
5	UDP	D	502	-	12,13,26	1.11	1 (8%)	16,19,40	0.76	0
2	NAD	A	501	-	46,48,48	1.22	6 (13%)	64,73,73	1.63	11 (17%)
2	NAD	F	800	-	46,48,48	1.26	6 (13%)	64,73,73	1.64	10 (15%)
4	SO4	A	503	-	4,4,4	0.23	0	6,6,6	0.10	0
5	UDP	B	502	-	25,26,26	1.05	2 (8%)	38,40,40	1.59	4 (10%)
4	SO4	C	503	-	4,4,4	0.21	0	6,6,6	0.17	0
2	NAD	D	501	-	46,48,48	1.19	6 (13%)	64,73,73	1.54	11 (17%)
2	NAD	C	501	-	46,48,48	1.15	4 (8%)	64,73,73	1.58	12 (18%)
4	SO4	B	503	-	4,4,4	0.25	0	6,6,6	0.19	0
2	NAD	B	501	-	46,48,48	1.28	4 (8%)	64,73,73	1.79	13 (20%)
2	NAD	E	800	-	46,48,48	1.20	5 (10%)	64,73,73	1.59	11 (17%)
3	POP	C	502	-	6,8,8	0.73	0	12,13,13	1.01	1 (8%)

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	POP	A	502	-	-	1/6/6/6	-
5	UDP	D	502	-	-	4/14/14/32	-
2	NAD	A	501	-	-	9/30/62/62	0/5/5/5
2	NAD	F	800	-	-	4/30/62/62	0/5/5/5
5	UDP	B	502	-	-	2/16/32/32	0/2/2/2
2	NAD	D	501	-	-	8/30/62/62	0/5/5/5
2	NAD	C	501	-	-	9/30/62/62	0/5/5/5
2	NAD	B	501	-	-	2/30/62/62	0/5/5/5
2	NAD	E	800	-	-	8/30/62/62	0/5/5/5
3	POP	C	502	-	-	2/6/6/6	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	C5A-C4A	5.65	1.49	1.39
2	E	800	NAD	C5A-C4A	4.82	1.47	1.39
2	D	501	NAD	C5A-C4A	4.74	1.47	1.39
2	A	501	NAD	C5A-C4A	4.70	1.47	1.39
2	F	800	NAD	C5A-C4A	4.48	1.47	1.39
2	C	501	NAD	C5A-C4A	4.40	1.46	1.39
2	C	501	NAD	C8A-N7A	3.26	1.37	1.31
2	B	501	NAD	C8A-N7A	3.00	1.37	1.31
2	F	800	NAD	PA-O3	2.93	1.62	1.59
2	A	501	NAD	C5A-C6A	2.85	1.48	1.41
2	F	800	NAD	PN-O3	2.77	1.62	1.59
2	F	800	NAD	C5A-C6A	2.77	1.48	1.41
2	D	501	NAD	C8A-N7A	2.73	1.36	1.31
2	E	800	NAD	O4D-C1D	2.55	1.44	1.40
2	E	800	NAD	C8A-N7A	2.45	1.36	1.31
2	B	501	NAD	C5A-C6A	2.40	1.47	1.41
2	F	800	NAD	C8A-N7A	2.29	1.36	1.31
2	A	501	NAD	C5A-N7A	-2.29	1.34	1.39
2	D	501	NAD	O4D-C1D	2.28	1.43	1.40
2	E	800	NAD	C5A-C6A	2.26	1.47	1.41
2	F	800	NAD	C4A-N9A	-2.26	1.33	1.37
5	B	502	UDP	C5-C4	-2.24	1.38	1.43
2	B	501	NAD	C5A-N7A	-2.24	1.35	1.39
2	D	501	NAD	C5A-C6A	2.22	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	UDP	PA-O3A	2.21	1.61	1.59
2	C	501	NAD	C5A-C6A	2.20	1.47	1.41
2	E	800	NAD	C5A-N7A	-2.20	1.35	1.39
2	C	501	NAD	C4A-N9A	-2.19	1.33	1.37
2	D	501	NAD	PN-O3	2.10	1.61	1.59
2	A	501	NAD	PN-O3	2.09	1.61	1.59
2	A	501	NAD	C8A-N7A	2.09	1.35	1.31
2	A	501	NAD	O4D-C1D	2.05	1.43	1.40
2	D	501	NAD	C4A-N9A	-2.03	1.33	1.37
5	D	502	UDP	PA-O3A	2.02	1.61	1.59

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAD	C5A-C4A-N3A	-7.16	116.86	126.72
2	B	501	NAD	N3A-C4A-N9A	5.62	136.73	127.17
5	B	502	UDP	C4-N3-C2	-5.58	119.68	126.61
2	A	501	NAD	C5A-C4A-N3A	-5.43	119.23	126.72
2	F	800	NAD	C5A-C4A-N3A	-4.96	119.89	126.72
2	E	800	NAD	C5A-C4A-N3A	-4.76	120.16	126.72
2	A	501	NAD	N3A-C4A-N9A	4.67	135.11	127.17
2	C	501	NAD	C5A-C4A-N3A	-4.63	120.35	126.72
2	D	501	NAD	C5A-C4A-N3A	-4.60	120.38	126.72
2	E	800	NAD	N3A-C4A-N9A	4.41	134.66	127.17
2	F	800	NAD	N3A-C4A-N9A	4.31	134.49	127.17
2	E	800	NAD	C4A-N9A-C8A	4.11	110.05	105.74
2	D	501	NAD	N3A-C2A-N1A	-4.10	122.38	128.58
2	D	501	NAD	N3A-C4A-N9A	4.06	134.08	127.17
2	F	800	NAD	C4A-N9A-C8A	4.03	109.97	105.74
5	B	502	UDP	C5-C4-N3	3.96	120.35	114.80
2	F	800	NAD	N3A-C2A-N1A	-3.71	122.97	128.58
2	C	501	NAD	C4A-C5A-N7A	-3.66	106.40	110.58
2	F	800	NAD	C2A-N3A-C4A	3.63	120.69	111.83
2	A	501	NAD	C2A-N3A-C4A	3.61	120.65	111.83
2	B	501	NAD	C2A-N3A-C4A	3.57	120.54	111.83
5	B	502	UDP	N3-C2-N1	3.48	119.42	114.89
2	A	501	NAD	N3A-C2A-N1A	-3.48	123.31	128.58
2	A	501	NAD	C4A-C5A-N7A	-3.47	106.62	110.58
2	D	501	NAD	C4A-N9A-C8A	3.47	109.38	105.74
2	D	501	NAD	C2A-N3A-C4A	3.44	120.24	111.83
2	A	501	NAD	C4A-N9A-C8A	3.39	109.30	105.74
2	F	800	NAD	C4A-C5A-N7A	-3.35	106.75	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAD	C2A-N3A-C4A	3.31	119.91	111.83
2	C	501	NAD	N3A-C2A-N1A	-3.20	123.74	128.58
2	C	501	NAD	N3A-C4A-N9A	3.16	132.54	127.17
2	E	800	NAD	N3A-C2A-N1A	-3.11	123.88	128.58
2	E	800	NAD	C4A-C5A-N7A	-3.10	107.03	110.58
2	B	501	NAD	C4A-C5A-N7A	-2.99	107.17	110.58
2	B	501	NAD	C5D-C4D-C3D	-2.98	104.48	115.21
2	C	501	NAD	C6A-C5A-N7A	2.97	137.82	132.09
2	C	501	NAD	C4A-N9A-C8A	2.95	108.83	105.74
2	A	501	NAD	C5A-N7A-C8A	2.94	108.07	103.45
2	E	800	NAD	C2A-N3A-C4A	2.92	118.95	111.83
2	E	800	NAD	N9A-C8A-N7A	-2.83	109.92	113.94
5	B	502	UDP	O4-C4-C5	-2.80	120.33	125.16
2	E	800	NAD	C5A-N7A-C8A	2.77	107.81	103.45
2	D	501	NAD	C2A-N1A-C6A	2.77	123.28	118.73
2	B	501	NAD	O2N-PN-O1N	2.76	125.27	112.44
2	F	800	NAD	N9A-C8A-N7A	-2.69	110.12	113.94
2	B	501	NAD	C5N-C4N-C3N	-2.60	117.81	120.36
2	F	800	NAD	C5A-N7A-C8A	2.60	107.54	103.45
2	B	501	NAD	C2N-C3N-C4N	2.56	121.23	118.26
2	C	501	NAD	N9A-C8A-N7A	-2.55	110.32	113.94
2	F	800	NAD	C6A-C5A-N7A	2.54	136.99	132.09
2	A	501	NAD	N9A-C8A-N7A	-2.52	110.36	113.94
2	D	501	NAD	C4A-C5A-N7A	-2.49	107.73	110.58
2	C	501	NAD	C5A-N7A-C8A	2.48	107.34	103.45
2	B	501	NAD	C5A-N7A-C8A	2.45	107.30	103.45
2	C	501	NAD	C4A-N9A-C1B	-2.37	121.10	126.63
2	D	501	NAD	C6A-C5A-N7A	2.31	136.55	132.09
2	F	800	NAD	C2A-N1A-C6A	2.29	122.50	118.73
2	B	501	NAD	O4B-C4B-C5B	2.29	116.66	109.33
2	E	800	NAD	C2D-C3D-C4D	2.24	106.93	102.61
2	C	501	NAD	C3N-C7N-N7N	2.24	120.49	117.74
2	A	501	NAD	C2A-N1A-C6A	2.20	122.35	118.73
2	A	501	NAD	O2N-PN-O1N	2.18	122.61	112.44
2	E	800	NAD	O2N-PN-O1N	2.18	122.59	112.44
2	A	501	NAD	C6A-C5A-N7A	2.16	136.25	132.09
3	A	502	POP	O6-P2-O	2.16	111.86	104.64
2	B	501	NAD	C5A-C6A-N6A	-2.15	117.96	123.29
2	E	800	NAD	O2A-PA-O1A	2.13	122.34	112.44
2	B	501	NAD	O4B-C1B-C2B	-2.12	102.07	106.62
2	D	501	NAD	C5D-C4D-C3D	-2.12	107.60	115.21
3	C	502	POP	O6-P2-O	2.07	111.57	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAD	C5B-C4B-C3B	-2.04	107.85	115.21
2	D	501	NAD	C2D-C3D-C4D	2.04	106.54	102.61
2	D	501	NAD	N9A-C8A-N7A	-2.03	111.05	113.94
2	C	501	NAD	C2D-C3D-C4D	2.02	106.50	102.61

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	C5B-O5B-PA-O2A
2	A	501	NAD	C5B-O5B-PA-O3
2	A	501	NAD	C5D-O5D-PN-O3
2	A	501	NAD	C5D-O5D-PN-O1N
2	A	501	NAD	C5D-O5D-PN-O2N
2	B	501	NAD	C5D-O5D-PN-O1N
2	C	501	NAD	C5B-O5B-PA-O2A
2	C	501	NAD	C5B-O5B-PA-O3
2	C	501	NAD	C5D-O5D-PN-O3
2	C	501	NAD	C5D-O5D-PN-O1N
2	C	501	NAD	C5D-O5D-PN-O2N
2	D	501	NAD	C5B-O5B-PA-O2A
2	D	501	NAD	C5D-O5D-PN-O3
2	D	501	NAD	C5D-O5D-PN-O1N
2	E	800	NAD	C5D-O5D-PN-O3
2	E	800	NAD	C5D-O5D-PN-O1N
2	E	800	NAD	C2N-C3N-C7N-O7N
2	E	800	NAD	C2N-C3N-C7N-N7N
2	F	800	NAD	C5D-O5D-PN-O3
2	F	800	NAD	C5D-O5D-PN-O1N
2	F	800	NAD	C5D-O5D-PN-O2N
3	C	502	POP	P1-O-P2-O5
3	C	502	POP	P1-O-P2-O6
5	D	502	UDP	O3'-C3'-C4'-C5'
2	E	800	NAD	C4N-C3N-C7N-O7N
2	E	800	NAD	C4N-C3N-C7N-N7N
5	D	502	UDP	O3'-C3'-C4'-O4'
2	A	501	NAD	O4B-C4B-C5B-O5B
2	A	501	NAD	C3B-C4B-C5B-O5B
2	C	501	NAD	PA-O3-PN-O1N
5	B	502	UDP	PB-O3A-PA-O2A
2	A	501	NAD	C5B-O5B-PA-O1A
2	B	501	NAD	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
2	C	501	NAD	C5B-O5B-PA-O1A
2	D	501	NAD	C5B-O5B-PA-O1A
2	D	501	NAD	C5B-O5B-PA-O3
2	D	501	NAD	C5D-O5D-PN-O2N
2	E	800	NAD	C5D-O5D-PN-O2N
5	D	502	UDP	PB-O3A-PA-O2A
2	D	501	NAD	O4B-C4B-C5B-O5B
3	A	502	POP	P2-O-P1-O2
2	C	501	NAD	O4B-C4B-C5B-O5B
2	A	501	NAD	PA-O3-PN-O1N
2	C	501	NAD	PA-O3-PN-O2N
5	B	502	UDP	PB-O3A-PA-O1A
5	D	502	UDP	PB-O3A-PA-O1A
2	E	800	NAD	O4B-C4B-C5B-O5B
2	D	501	NAD	C3B-C4B-C5B-O5B
2	F	800	NAD	O4D-C4D-C5D-O5D

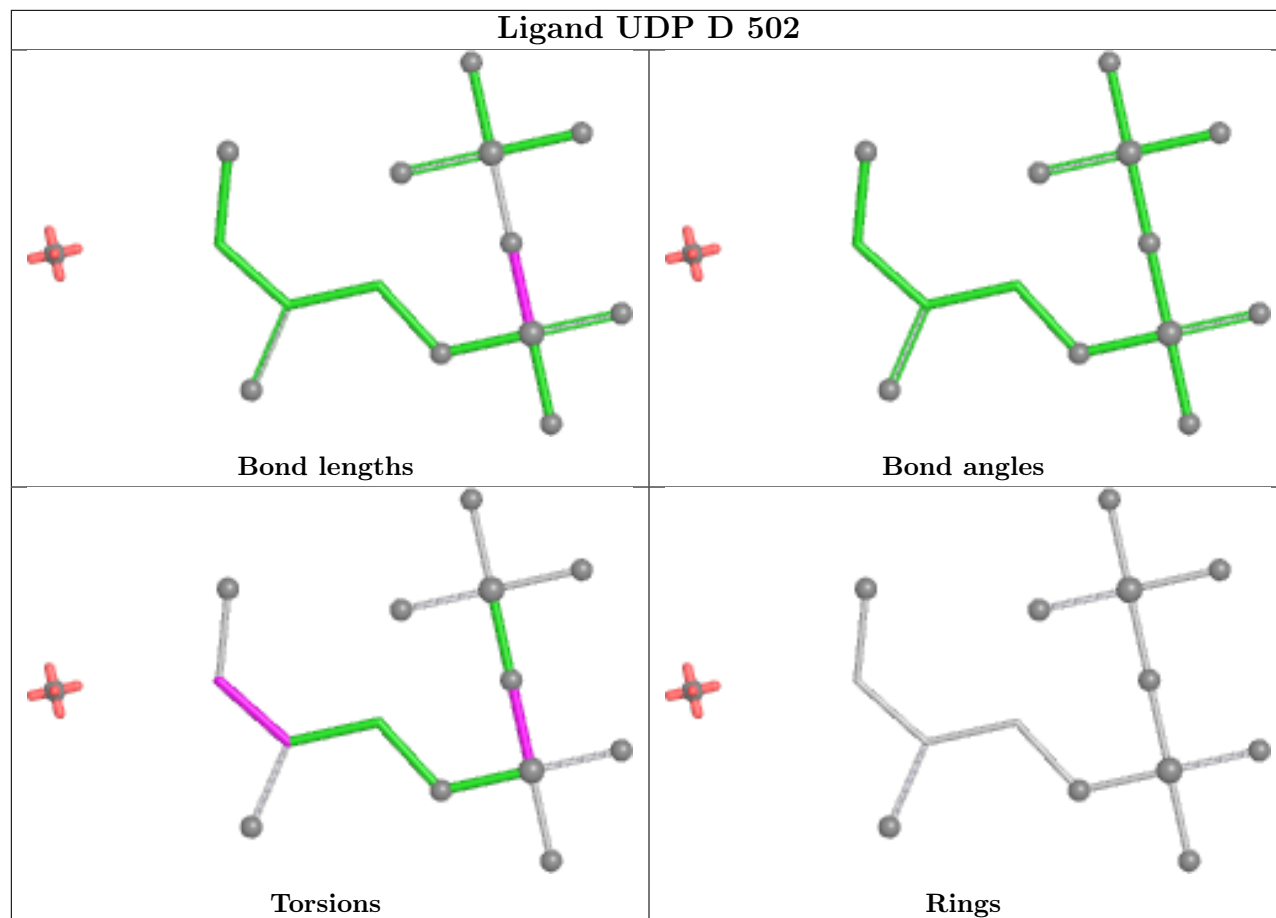
There are no ring outliers.

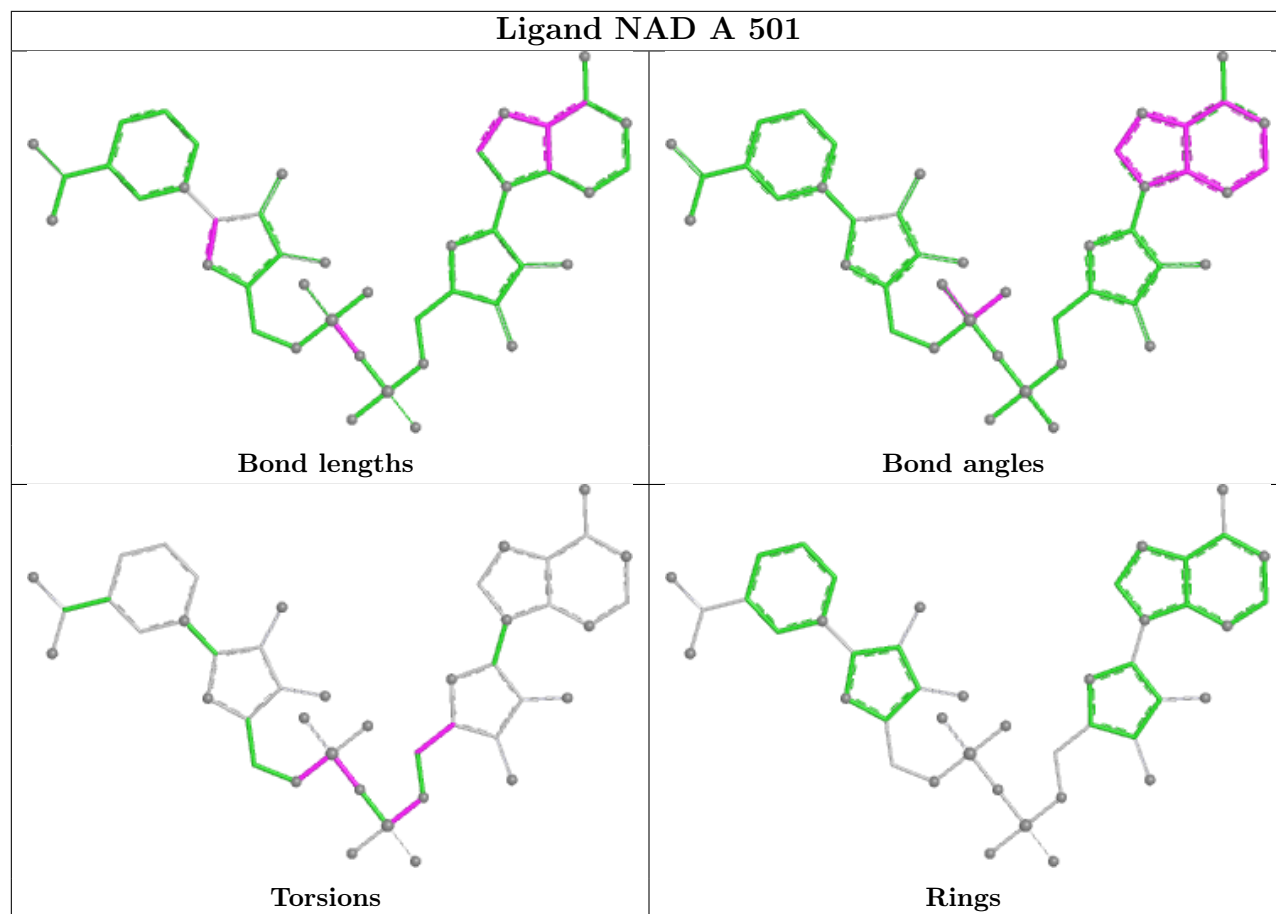
9 monomers are involved in 10 short contacts:

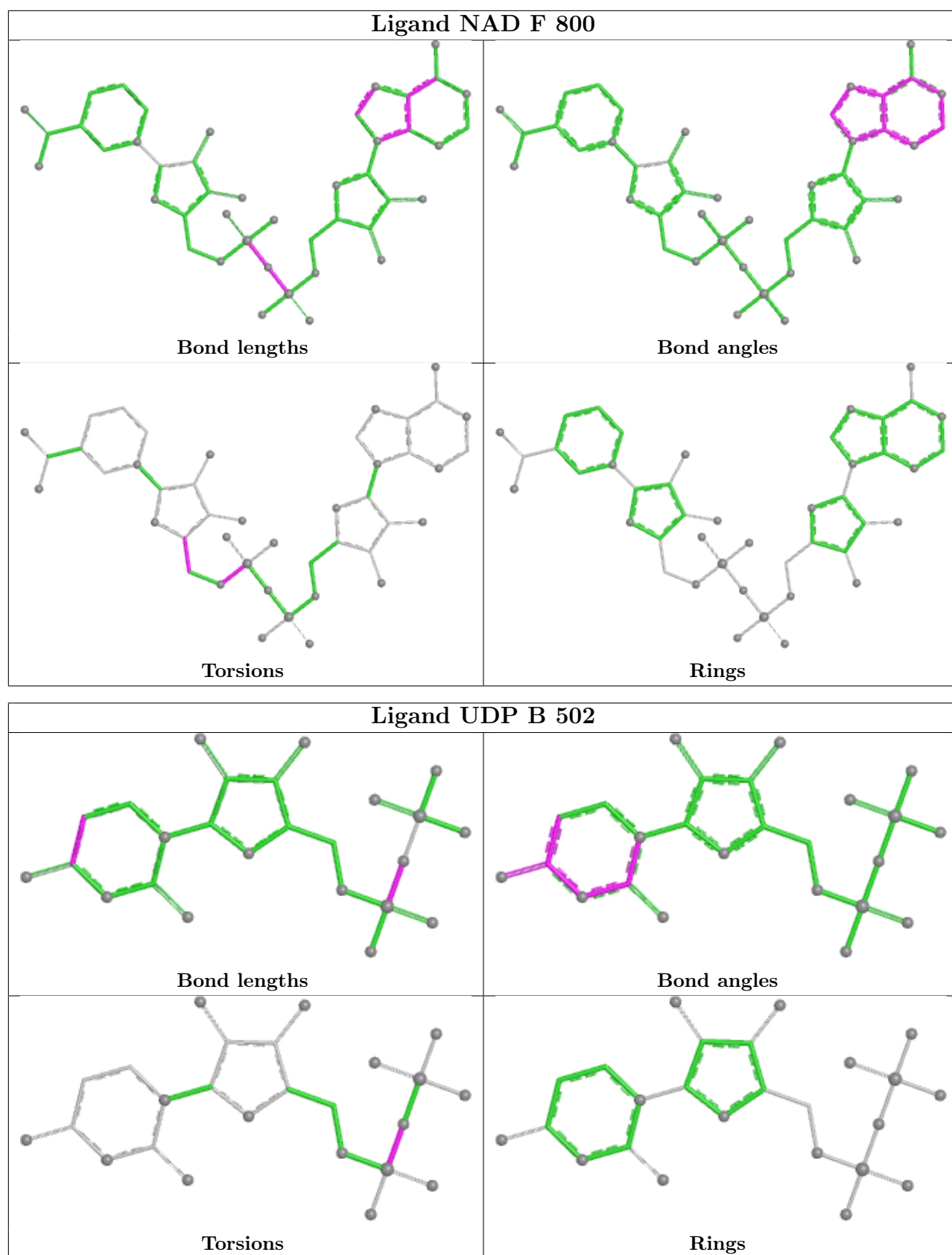
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	POP	1	0
5	D	502	UDP	1	0
2	A	501	NAD	1	0
2	F	800	NAD	1	0
4	A	503	SO4	1	0
5	B	502	UDP	1	0
2	D	501	NAD	1	0
2	B	501	NAD	1	0
2	E	800	NAD	2	0

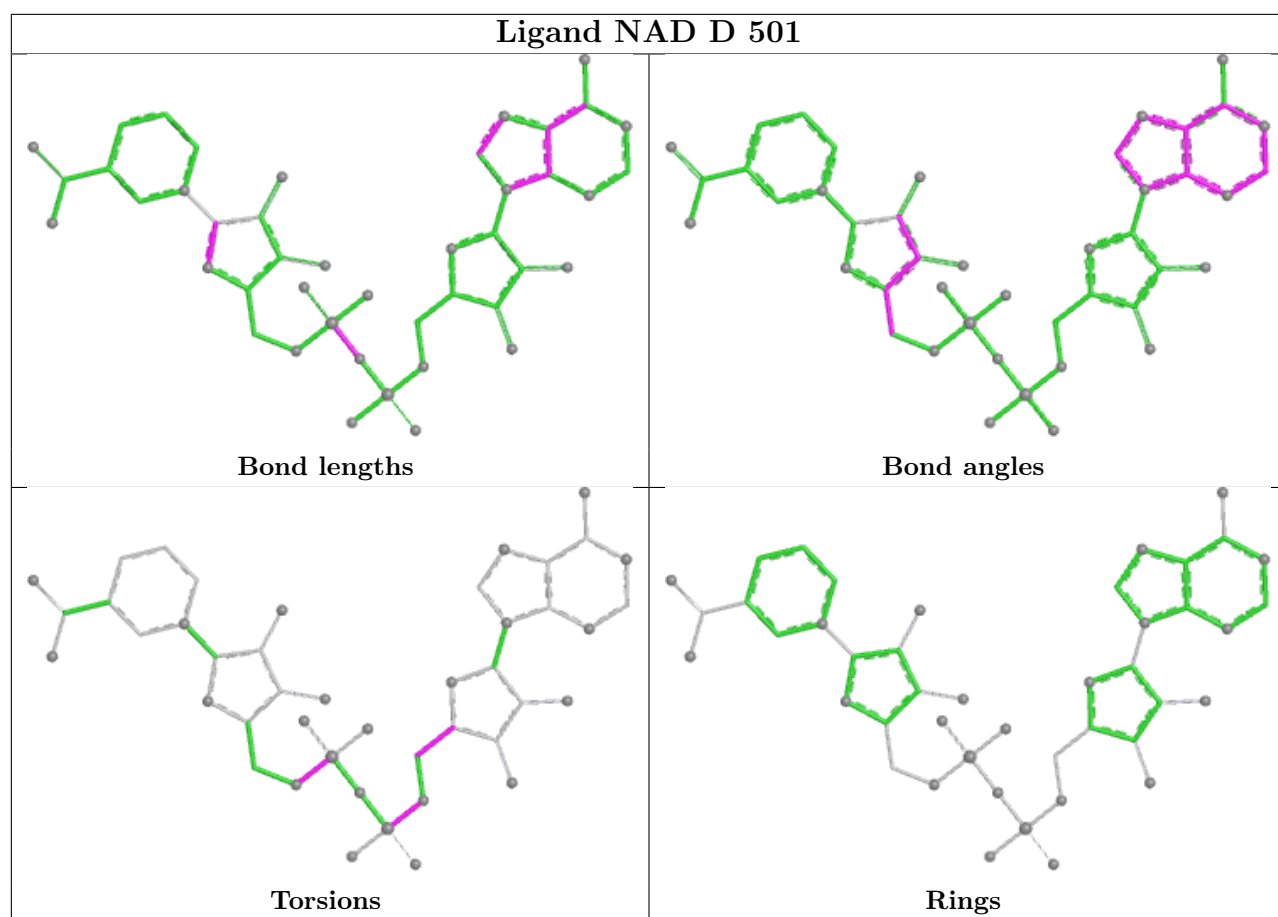
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

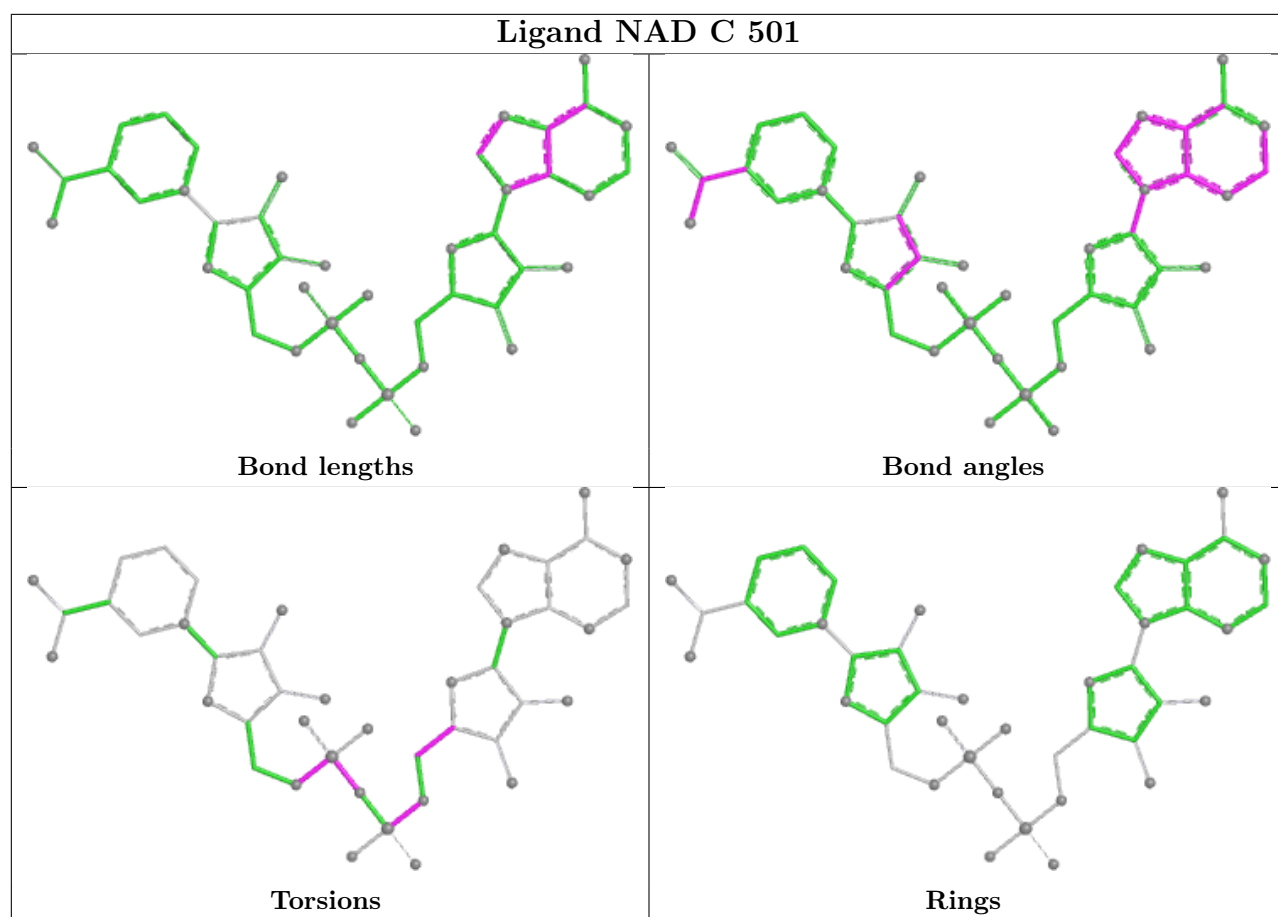
equivalents in the CSD to analyse the geometry.

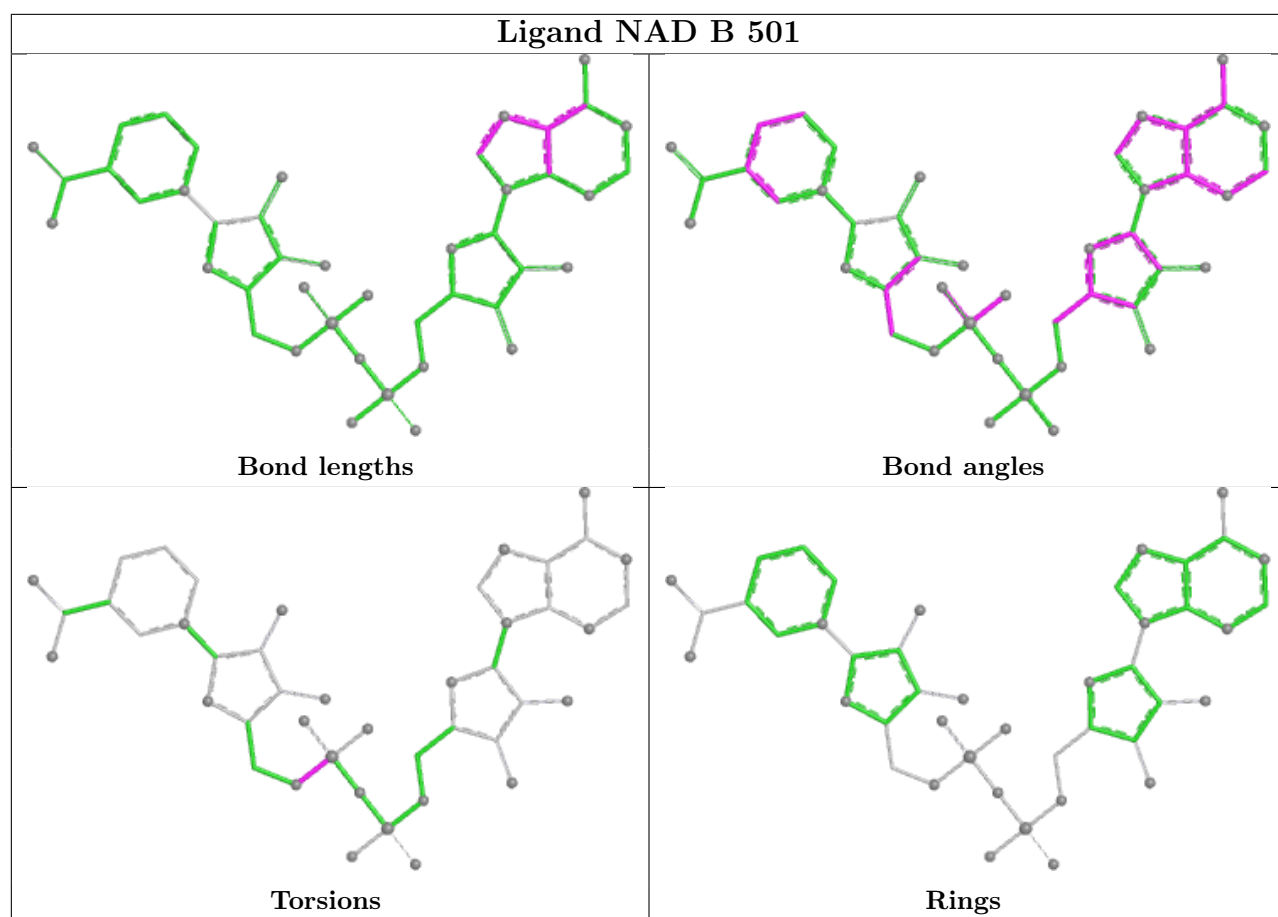


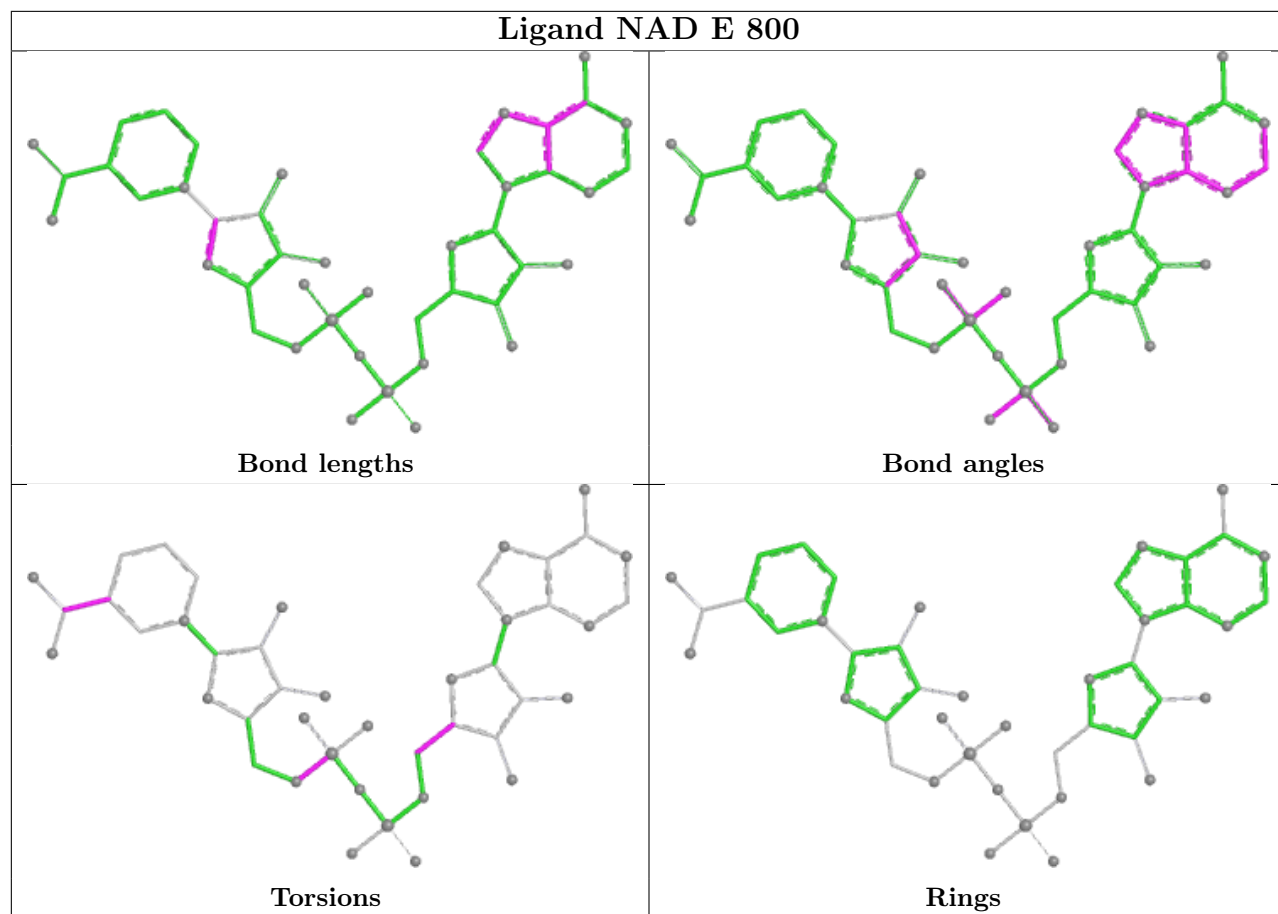












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	263/336 (78%)	0.41	8 (3%)	52	44	52, 131, 173, 208	0
1	B	272/336 (80%)	0.07	7 (2%)	57	48	47, 88, 152, 174	0
1	C	271/336 (80%)	0.12	10 (3%)	45	35	47, 91, 143, 169	0
1	D	261/336 (77%)	0.35	10 (3%)	44	35	47, 110, 182, 212	0
1	E	164/336 (48%)	0.43	4 (2%)	59	51	84, 125, 169, 204	0
1	F	181/336 (53%)	0.61	15 (8%)	17	13	85, 142, 175, 184	0
All	All	1412/2016 (70%)	0.30	54 (3%)	44	35	47, 112, 170, 212	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	HIS	5.8
1	C	399	ALA	5.6
1	D	236	HIS	5.1
1	D	161	SER	5.1
1	A	399	ALA	5.1
1	B	236	HIS	4.8
1	A	162	PRO	4.6
1	C	236	HIS	4.4
1	B	399	ALA	3.7
1	B	170	TYR	3.5
1	F	309	LEU	3.5
1	F	399	ALA	3.5
1	B	376	PRO	3.4
1	D	234	GLY	3.4
1	C	204	GLU	3.4
1	F	104	LEU	3.3
1	E	237	VAL	3.3
1	D	294	SER	3.3
1	C	351	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	237	VAL	3.2
1	D	290	TYR	3.1
1	D	204	GLU	3.1
1	C	290	TYR	3.1
1	D	350	PHE	2.9
1	A	376	PRO	2.8
1	B	165	PRO	2.8
1	E	99	PHE	2.7
1	D	332	LEU	2.7
1	F	302	VAL	2.6
1	C	206	TYR	2.5
1	E	242	CYS	2.5
1	C	164	SER	2.4
1	A	170	TYR	2.4
1	B	233	GLU	2.4
1	C	170	TYR	2.4
1	F	145	VAL	2.3
1	F	109	MET	2.3
1	F	170	TYR	2.3
1	F	364	ASP	2.3
1	A	338	ILE	2.3
1	B	350	PHE	2.3
1	F	149	LEU	2.3
1	F	95	GLY	2.2
1	F	313	MET	2.2
1	F	144	ASP	2.2
1	A	161	SER	2.2
1	F	322	ASN	2.1
1	C	291	GLY	2.1
1	C	334	PHE	2.1
1	E	262	PHE	2.1
1	A	289	VAL	2.1
1	D	277	PHE	2.1
1	D	123	THR	2.0
1	F	118	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

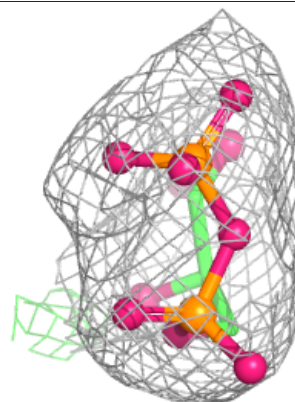
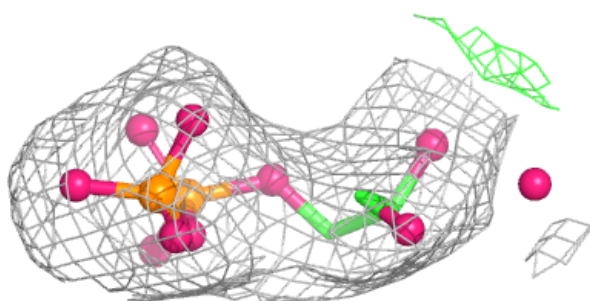
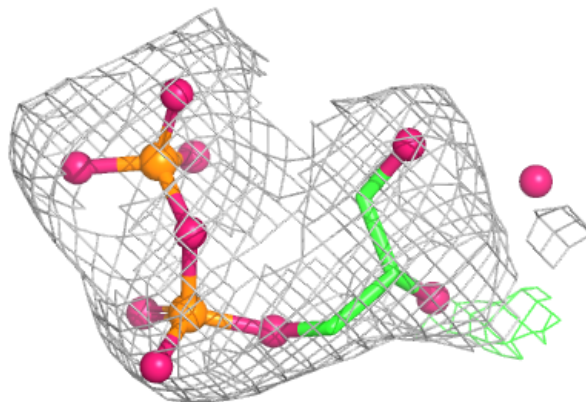
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	POP	A	502	9/9	0.73	0.09	111,120,154,274	1
3	POP	C	502	9/9	0.76	0.08	103,111,174,175	1
4	SO4	A	503	5/5	0.77	0.08	164,165,168,168	0
5	UDP	D	502	15/25	0.79	0.11	100,135,199,289	0
5	UDP	B	502	25/25	0.82	0.09	101,130,171,323	0
4	SO4	B	503	5/5	0.83	0.09	125,131,133,141	0
4	SO4	C	503	5/5	0.84	0.08	131,133,138,146	0
2	NAD	E	800	44/44	0.86	0.12	70,125,168,299	0
2	NAD	F	800	44/44	0.87	0.10	82,123,143,153	0
2	NAD	D	501	44/44	0.90	0.10	63,99,118,122	0
2	NAD	A	501	44/44	0.95	0.09	52,107,118,120	0
2	NAD	B	501	44/44	0.95	0.09	43,72,87,276	0
2	NAD	C	501	44/44	0.96	0.08	49,76,95,183	0

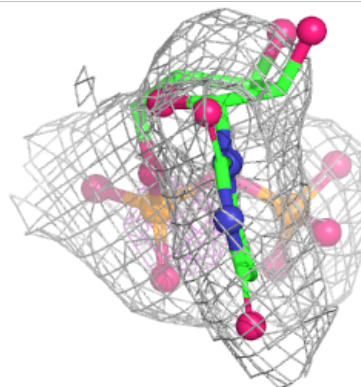
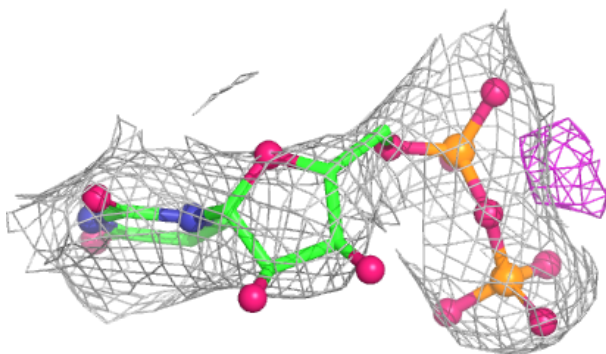
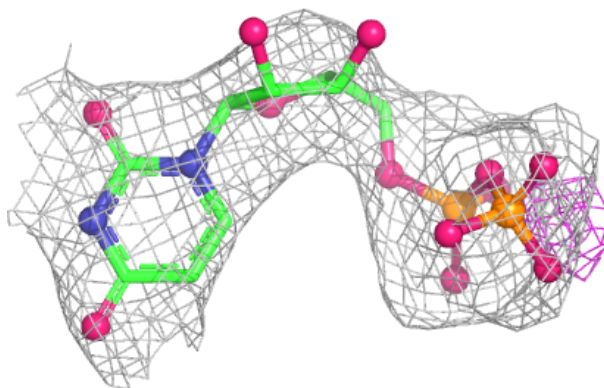
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDP 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)

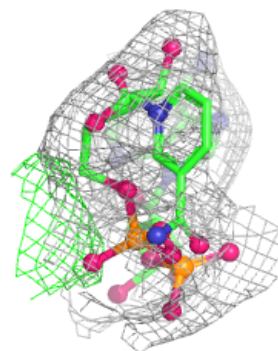
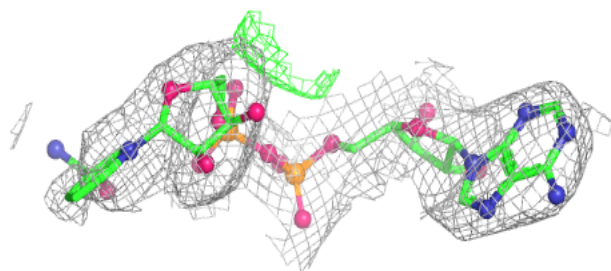
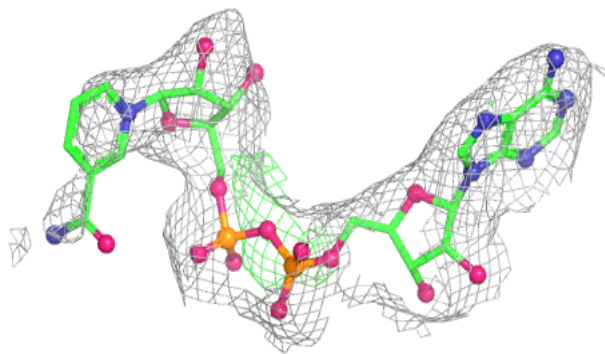
**Electron density around UDP B 502:**

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

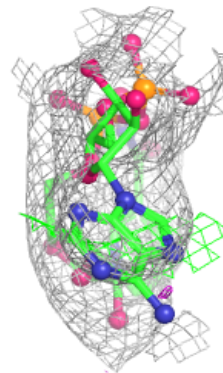
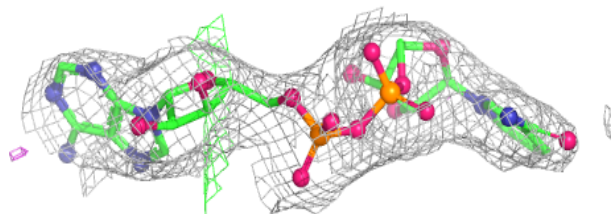
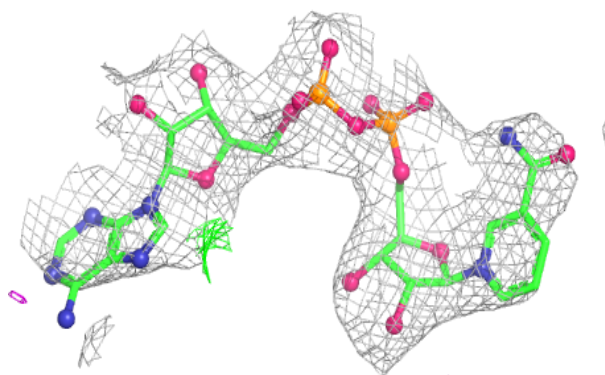


Electron density around NAD E 800:

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

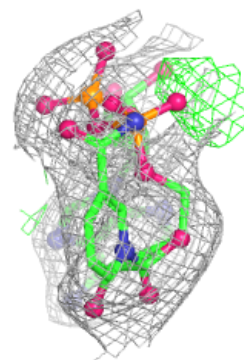
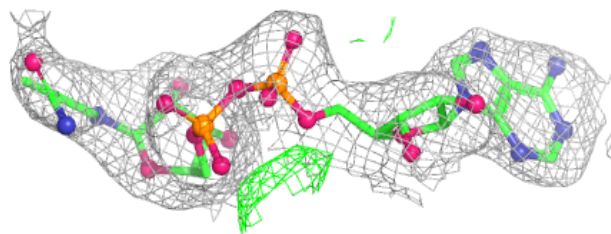
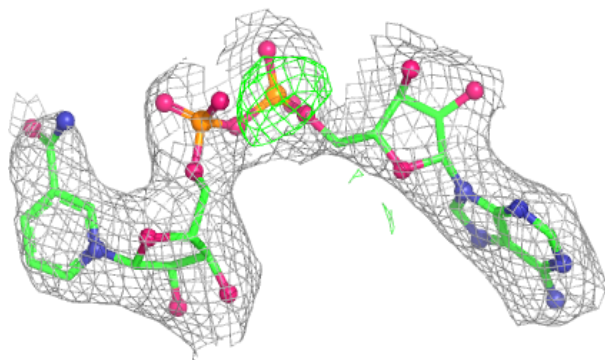
**Electron density around NAD F 800:**

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

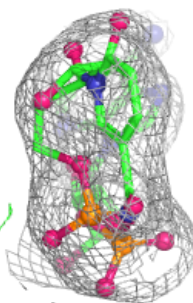
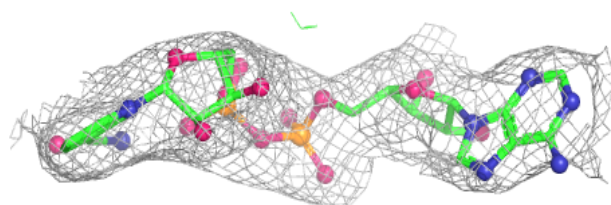
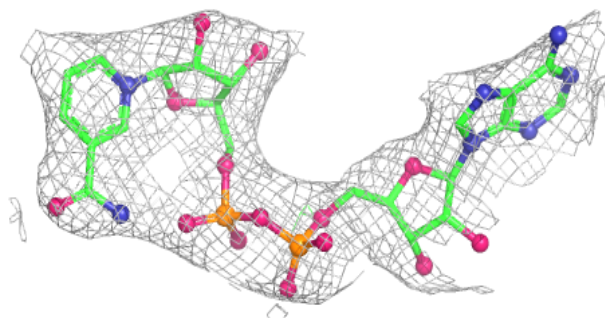


Electron density around NAD D 501:

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

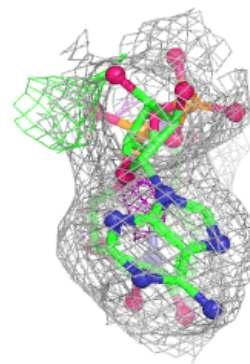
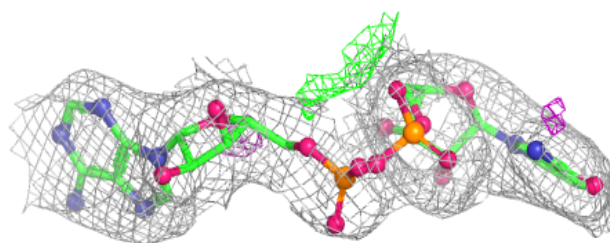
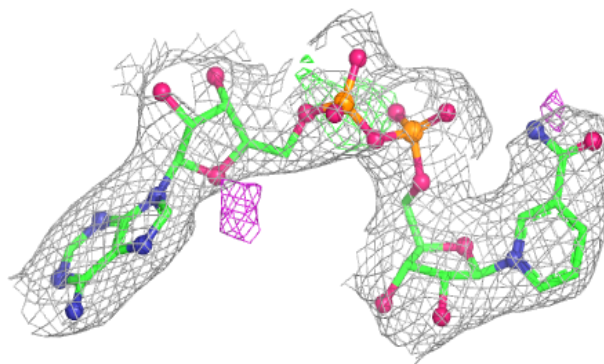
**Electron density around NAD A 501:**

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

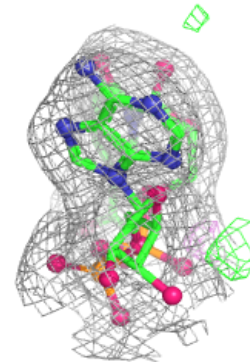
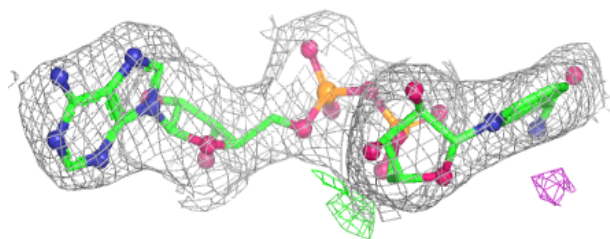
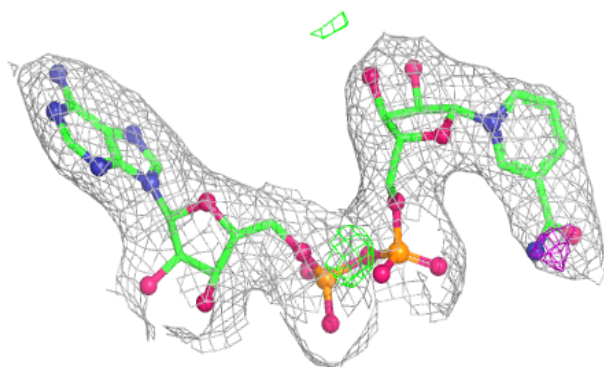


Electron density around NAD B 501:

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

**Electron density around NAD C 501:**

$2mF_o-DF_c$ (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.