



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 08:03 pm BST

PDB ID : 4M55
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 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 : 2.11
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) : 2.11

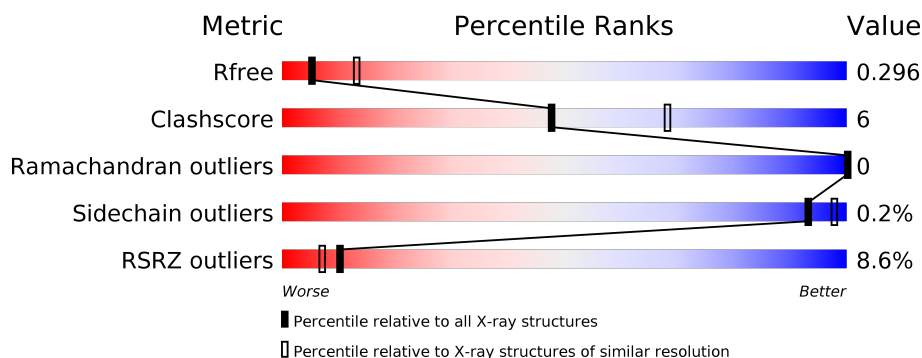
1 Overall quality at a glance

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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 on 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	<div> <div>10%</div> <div>66%12%22%</div> </div>
1	B	336	<div> <div>4%</div> <div>71%10%19%</div> </div>
1	C	336	<div> <div>3%</div> <div>69%12%19%</div> </div>
1	D	336	<div> <div>6%</div> <div>62%16%22%</div> </div>
1	E	336	<div> <div>4%</div> <div>39%10%51%</div> </div>
1	F	336	<div> <div>10%</div> <div>49%5%46%</div> </div>

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:

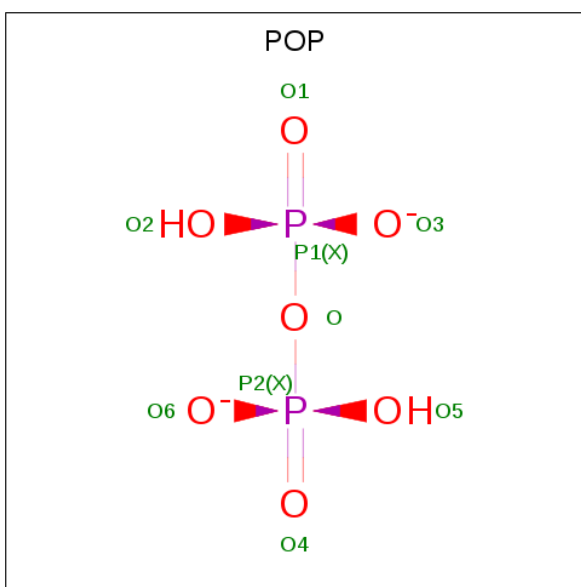
Chain	Residue	Modelled	Actual	Comment	Reference
A	236	HIS	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
B	236	HIS	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
C	236	HIS	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
D	236	HIS	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
E	236	HIS	ARG	ENGINEERED MUTATION	UNP Q8NBZ7
F	236	HIS	ARG	ENGINEERED MUTATION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

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 3 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



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 (three-letter code: SO4) (formula: O₄S).



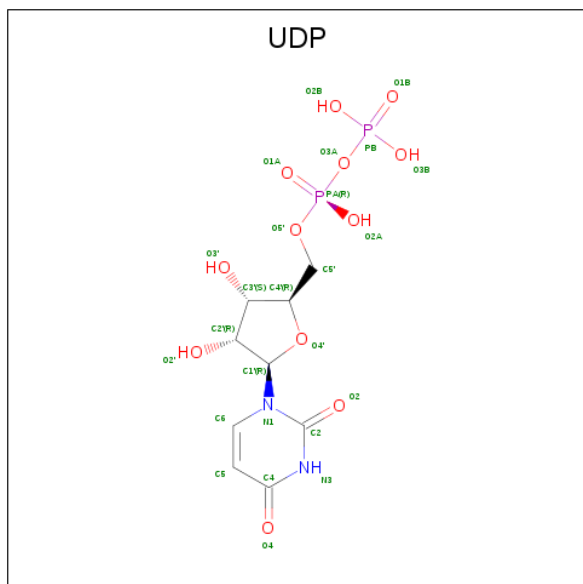
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

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

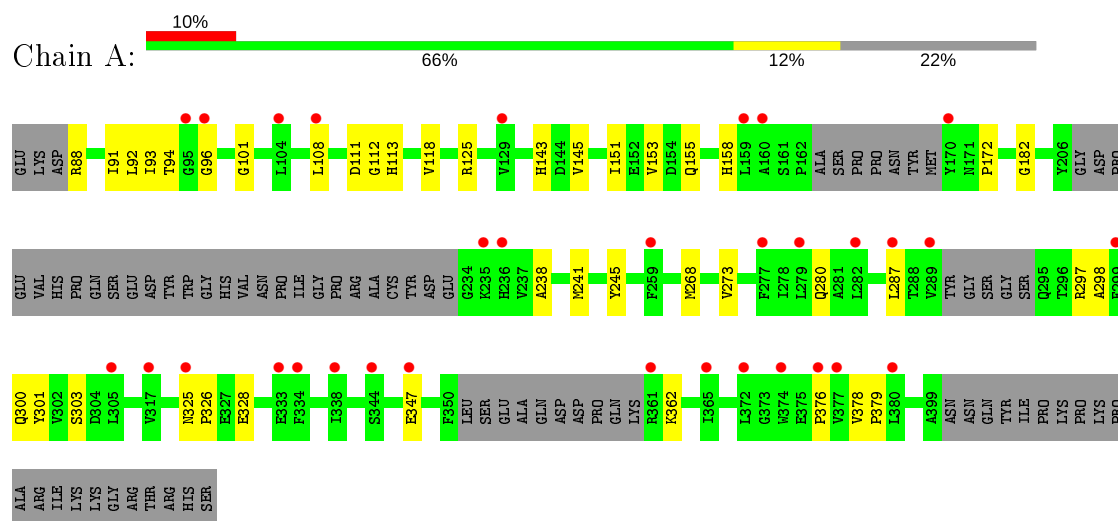
- Molecule 5 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



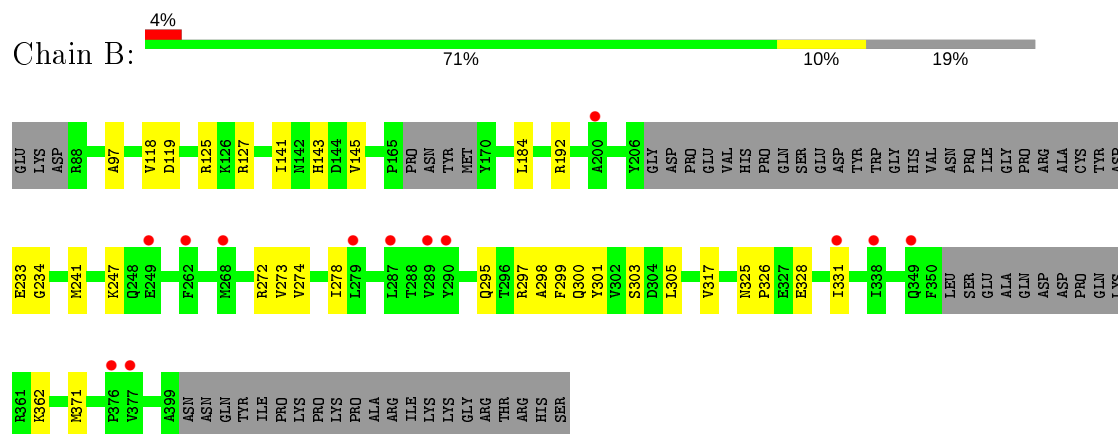
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

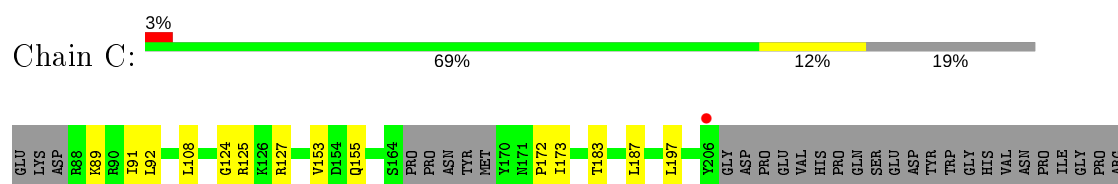
• Molecule 1: UDP-glucuronic acid decarboxylase 1

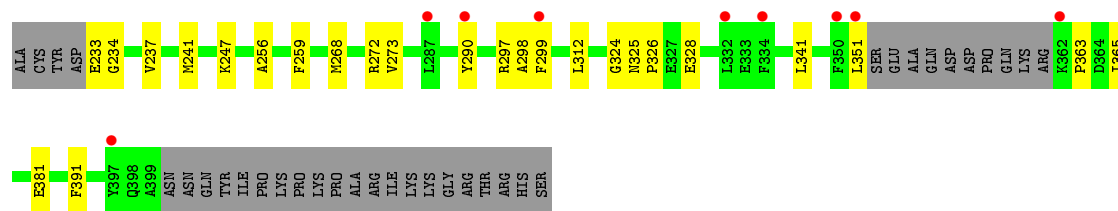


• Molecule 1: UDP-glucuronic acid decarboxylase 1

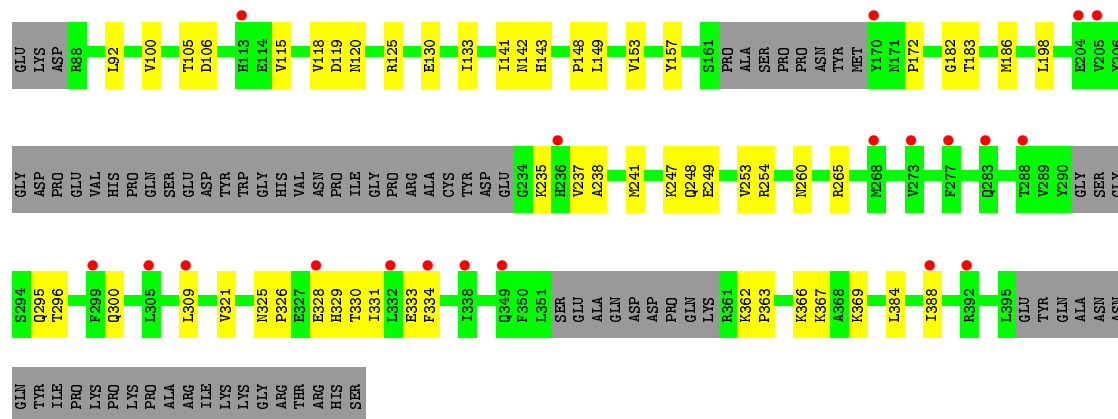


• Molecule 1: UDP-glucuronic acid decarboxylase 1

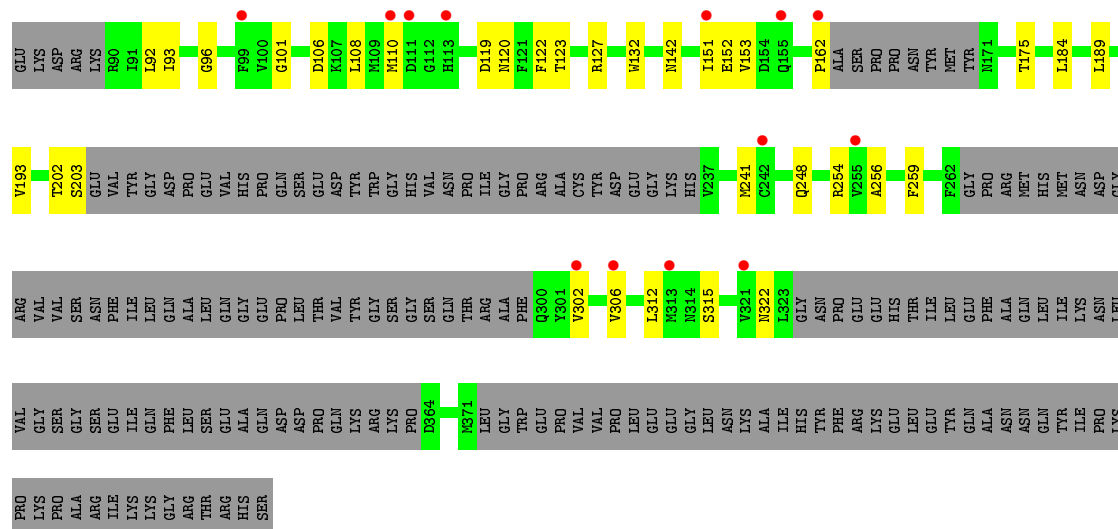
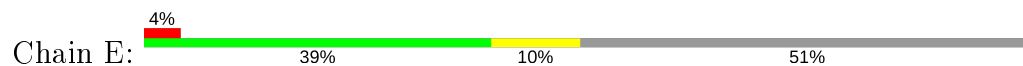




• Molecule 1: UDP-glucuronic acid decarboxylase 1

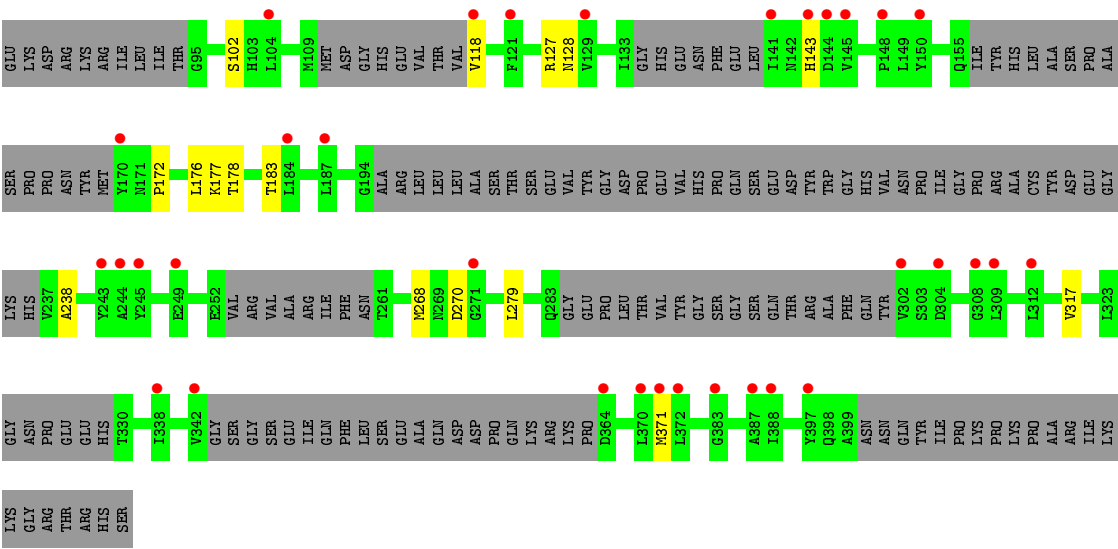


• Molecule 1: UDP-glucuronic acid decarboxylase 1



• 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 48.22 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.31-2.86) 100.0 (48.22-2.86)	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 0.241 , 0.296	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 , 79.6	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: UDP, SO4, NAD, POP

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	0.37	0/2125	0.51	0/2868
1	B	0.50	0/2187	0.59	0/2954
1	C	0.51	0/2176	0.59	0/2939
1	D	0.42	0/2108	0.54	0/2844
1	E	0.37	0/1299	0.51	0/1752
1	F	0.34	0/1448	0.46	0/1946
All	All	0.43	0/11343	0.54	0/15303

There are no bond length outliers.

There are no bond angle outliers.

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	26	0
1	B	2145	0	2149	25	0
1	C	2135	0	2140	27	0
1	D	2070	0	2090	36	0
1	E	1281	0	1301	24	0
1	F	1429	0	1445	11	0
2	A	44	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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	139	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 6.

All (139) 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:A:172:PRO:HG3	1:B:247:LYS:HE3	1.79	0.64
1:D:238:ALA:HA	1:D:241:MET:HE2	1.79	0.64
1:A:326:PRO:O	1:A:362:LYS:NZ	2.31	0.64
1:C:233:GLU:HG2	1:C:234:GLY:H	1.62	0.63
1:B:272:ARG:HD3	1:B:299:PHE:HE1	1.63	0.63
1:A:301:TYR:HD2	1:A:303:SER:HG	1.47	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
1:B:233:GLU:HG2	1:B:234:GLY:H	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ARG:HB3	1:C:299:PHE:HE2	1.68	0.57
1:A:238:ALA:HA	1:A:241:MET:HE2	1.85	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:F:268:MET:HE2	1:F:279:LEU:HD21	1.90	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: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:E:119:ASP:OD1	1:E:120:ASN:N	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:145:VAL:HG22	2:B:501:NAD:N1A	2.29	0.47
1:A:145:VAL:O	1:A:182:GLY:HA2	2.15	0.47
1:A:94:THR:OG1	1:A:158:HIS:HA	2.14	0.47
1:B:273:VAL:HG21	1:B:331:ILE:HD12	1.97	0.47
1:C:183:THR:HB	1:C:241:MET:HE1	1.96	0.47
1:F:183:THR:HG21	1:F:238:ALA:HB1	1.97	0.47
1:B:301:TYR:HD2	1:B:303:SER:HG	1.59	0.46
1:E:151:ILE:HG12	1:E:152:GLU:H	1.79	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:D:183:THR:HB	1:D:241:MET:HE1	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:N	1:F:270:ASP:OD1	2.48	0.45
1:D:141:ILE:HG22	1:D:143:HIS:HB2	2.00	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:ILE:HD11	1:E:108:LEU:HD12	1.99	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: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: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:E:119:ASP:OD2	2:E:800:NAD:O3B	2.27	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: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:C:268:MET:HE2	1:C:391:PHE:CD2	2.55	0.41
1:B:118:VAL:HG22	1:B:141:ILE:HB	2.01	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:HB3	1:D:235:LYS:HE3	1.84	0.41
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: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: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%)	91	96
1	D	226/290 (78%)	225 (100%)	1 (0%)	91	96
1	E	142/290 (49%)	142 (100%)	0	100	100
1	F	157/290 (54%)	157 (100%)	0	100	100
All	All	1217/1740 (70%)	1215 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	237	VAL
1	D	237	VAL

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates 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	$\# Z > 2$
2	NAD	C	501	-	42,48,48	0.85	1 (2%)	50,73,73	1.33	5 (10%)
5	UDP	D	502	-	11,13,26	0.97	0	15,19,40	1.06	1 (6%)
2	NAD	A	501	-	42,48,48	0.83	1 (2%)	50,73,73	1.18	5 (10%)
3	POP	A	502	-	6,8,8	0.64	0	13,13,13	1.32	2 (15%)
3	POP	C	502	-	6,8,8	0.71	0	13,13,13	1.19	2 (15%)
2	NAD	E	800	-	42,48,48	0.93	3 (7%)	50,73,73	1.26	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	D	501	-	42,48,48	0.81	2 (4%)	50,73,73	1.29	7 (14%)
2	NAD	B	501	-	42,48,48	1.06	3 (7%)	50,73,73	1.38	9 (18%)
5	UDP	B	502	-	20,26,26	1.09	1 (5%)	25,40,40	0.98	2 (8%)
4	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.09	0
4	SO4	B	503	-	4,4,4	0.14	0	6,6,6	0.18	0
4	SO4	C	503	-	4,4,4	0.11	0	6,6,6	0.18	0
2	NAD	F	800	-	42,48,48	0.78	1 (2%)	50,73,73	1.28	5 (10%)

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	NAD	C	501	-	-	9/26/62/62	0/5/5/5
5	UDP	D	502	-	-	4/14/14/32	-
2	NAD	A	501	-	-	9/26/62/62	0/5/5/5
3	POP	A	502	-	-	1/6/6/6	-
3	POP	C	502	-	-	2/6/6/6	-
2	NAD	E	800	-	-	8/26/62/62	0/5/5/5
2	NAD	D	501	-	-	8/26/62/62	0/5/5/5
2	NAD	B	501	-	-	3/26/62/62	0/5/5/5
5	UDP	B	502	-	-	3/14/32/32	0/2/2/2
2	NAD	F	800	-	-	5/26/62/62	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	C2A-N3A	3.13	1.37	1.32
2	B	501	NAD	C5A-C4A	3.11	1.49	1.40
5	B	502	UDP	C4-N3	3.00	1.38	1.33
2	E	800	NAD	C5A-C4A	2.56	1.47	1.40
2	D	501	NAD	C5A-C4A	2.50	1.47	1.40
2	E	800	NAD	C2A-N3A	2.49	1.36	1.32
2	A	501	NAD	C5A-C4A	2.47	1.47	1.40
2	B	501	NAD	O4B-C1B	2.35	1.44	1.41
2	F	800	NAD	C5A-C4A	2.32	1.47	1.40
2	C	501	NAD	C5A-C4A	2.27	1.46	1.40
2	E	800	NAD	O4D-C1D	2.26	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	NAD	O4D-C1D	2.01	1.43	1.41

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NAD	N3A-C2A-N1A	-4.03	122.38	128.68
2	F	800	NAD	N3A-C2A-N1A	-3.65	122.97	128.68
2	F	800	NAD	C3D-C2D-C1D	3.47	106.20	100.98
2	A	501	NAD	N3A-C2A-N1A	-3.43	123.31	128.68
2	B	501	NAD	O4B-C1B-C2B	-3.32	102.07	106.93
2	C	501	NAD	N3A-C2A-N1A	-3.16	123.74	128.68
2	C	501	NAD	C1B-N9A-C4A	-3.15	121.10	126.64
5	D	502	UDP	PA-O3A-PB	-3.14	122.06	132.83
2	E	800	NAD	N3A-C2A-N1A	-3.07	123.88	128.68
2	A	501	NAD	C3D-C2D-C1D	2.94	105.40	100.98
3	A	502	POP	P2-O-P1	-2.93	122.77	132.83
2	C	501	NAD	C4A-C5A-N7A	-2.88	106.40	109.40
2	B	501	NAD	C5D-C4D-C3D	-2.86	104.48	115.18
2	A	501	NAD	C4A-C5A-N7A	-2.67	106.62	109.40
2	D	501	NAD	C2A-N1A-C6A	2.65	123.28	118.75
2	B	501	NAD	O2N-PN-O1N	2.63	125.27	112.24
2	B	501	NAD	C2N-C3N-C4N	2.62	121.23	118.26
2	B	501	NAD	PN-O3-PA	-2.62	123.85	132.83
2	C	501	NAD	PN-O3-PA	-2.59	123.95	132.83
2	F	800	NAD	C4A-C5A-N7A	-2.54	106.75	109.40
3	C	502	POP	P2-O-P1	-2.52	124.17	132.83
2	D	501	NAD	PN-O3-PA	-2.51	124.20	132.83
2	E	800	NAD	C3D-C2D-C1D	2.51	104.76	100.98
5	B	502	UDP	PA-O3A-PB	-2.44	124.46	132.83
5	B	502	UDP	C3'-C2'-C1'	2.42	104.63	100.98
2	B	501	NAD	C3D-C2D-C1D	2.41	104.61	100.98
2	D	501	NAD	C1B-N9A-C4A	-2.39	122.44	126.64
2	E	800	NAD	C1B-N9A-C4A	-2.36	122.49	126.64
2	E	800	NAD	PN-O3-PA	-2.34	124.78	132.83
2	D	501	NAD	C3D-C2D-C1D	2.32	104.47	100.98
2	F	800	NAD	PN-O3-PA	-2.30	124.94	132.83
2	C	501	NAD	C3N-C7N-N7N	2.29	120.49	117.75
2	E	800	NAD	C4A-C5A-N7A	-2.27	107.03	109.40
2	B	501	NAD	O4B-C4B-C5B	2.22	116.66	109.37
2	E	800	NAD	C2D-C3D-C4D	2.21	106.93	102.64
2	F	800	NAD	C2A-N1A-C6A	2.19	122.50	118.75
3	A	502	POP	O6-P2-O	2.16	111.86	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAD	C5N-C4N-C3N	-2.14	117.81	120.34
2	B	501	NAD	C4A-C5A-N7A	-2.14	107.17	109.40
2	A	501	NAD	C2A-N1A-C6A	2.10	122.35	118.75
2	A	501	NAD	O2N-PN-O1N	2.10	122.61	112.24
2	E	800	NAD	O2N-PN-O1N	2.09	122.59	112.24
3	C	502	POP	O6-P2-O	2.07	111.57	104.64
2	E	800	NAD	O2A-PA-O1A	2.04	122.34	112.24
2	D	501	NAD	C5D-C4D-C3D	-2.02	107.60	115.18
2	D	501	NAD	C2D-C3D-C4D	2.01	106.54	102.64

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	NAD	C5B-O5B-PA-O2A
2	C	501	NAD	C5D-O5D-PN-O1N
2	C	501	NAD	C5D-O5D-PN-O2N
5	D	502	UDP	O3'-C3'-C4'-C5'
2	A	501	NAD	C5B-O5B-PA-O2A
2	A	501	NAD	C5D-O5D-PN-O1N
2	A	501	NAD	C5D-O5D-PN-O2N
3	C	502	POP	P1-O-P2-O5
3	C	502	POP	P1-O-P2-O6
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	D	501	NAD	C5B-O5B-PA-O2A
2	D	501	NAD	C5D-O5D-PN-O1N
2	B	501	NAD	C5D-O5D-PN-O1N
5	B	502	UDP	O4'-C1'-N1-C6
2	F	800	NAD	C5D-O5D-PN-O1N
2	F	800	NAD	C5D-O5D-PN-O2N
2	E	800	NAD	C4N-C3N-C7N-O7N
2	E	800	NAD	C4N-C3N-C7N-N7N
2	A	501	NAD	O4B-C4B-C5B-O5B
5	D	502	UDP	O3'-C3'-C4'-O4'
2	A	501	NAD	C3B-C4B-C5B-O5B
2	D	501	NAD	O4B-C4B-C5B-O5B
2	C	501	NAD	C5B-O5B-PA-O3
2	C	501	NAD	C5D-O5D-PN-O3
2	A	501	NAD	C5B-O5B-PA-O3
2	E	800	NAD	C5D-O5D-PN-O3

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

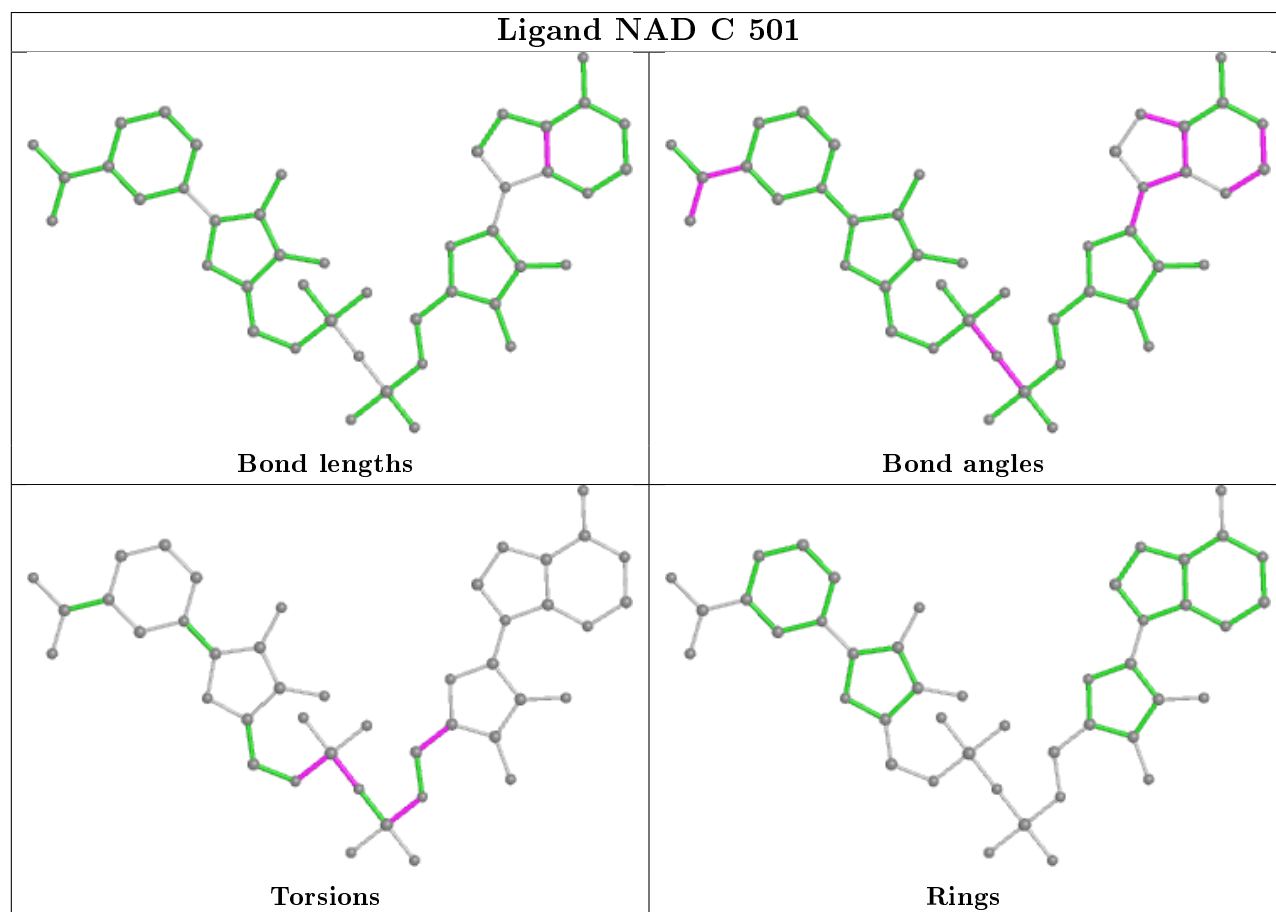
There are no ring outliers.

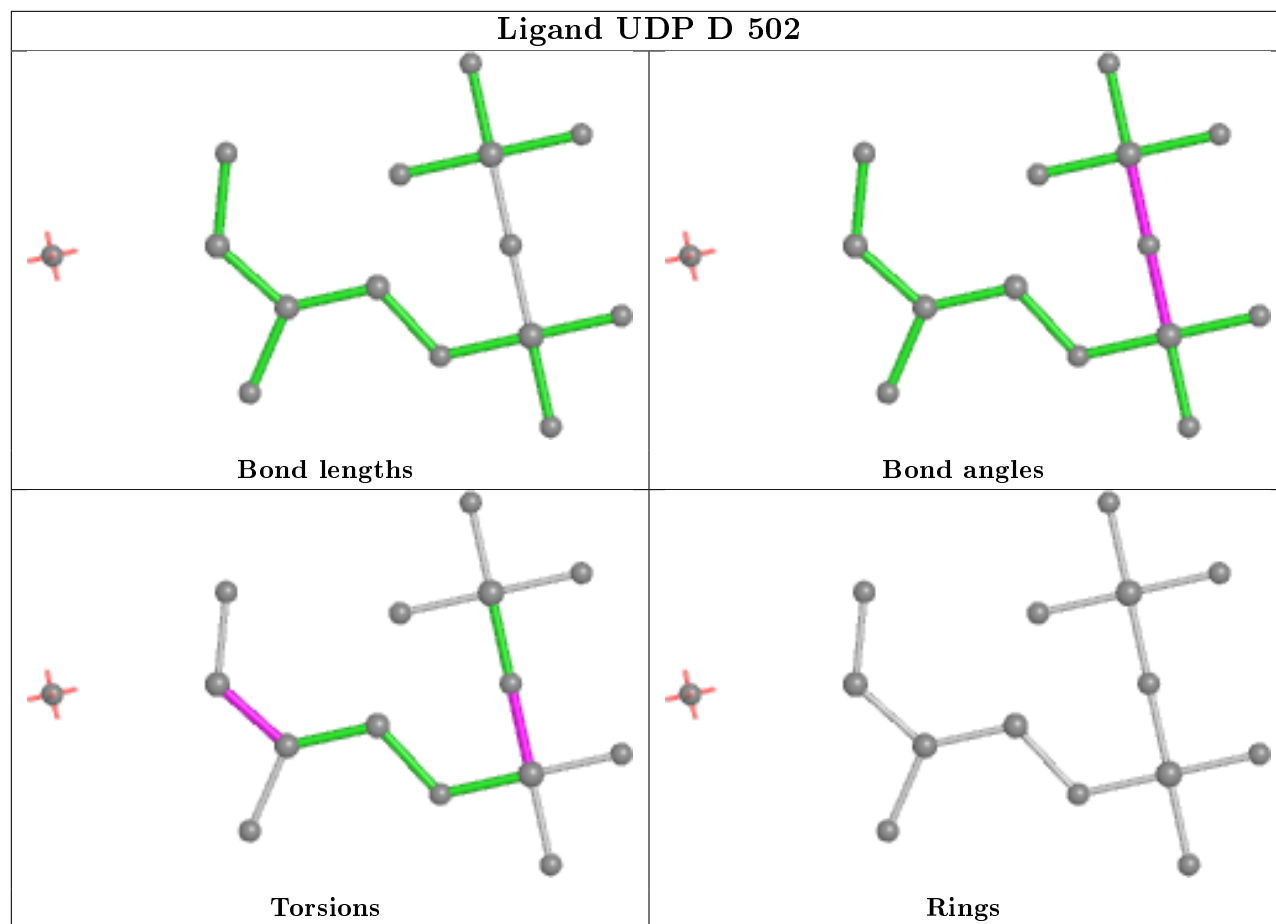
9 monomers are involved in 9 short contacts:

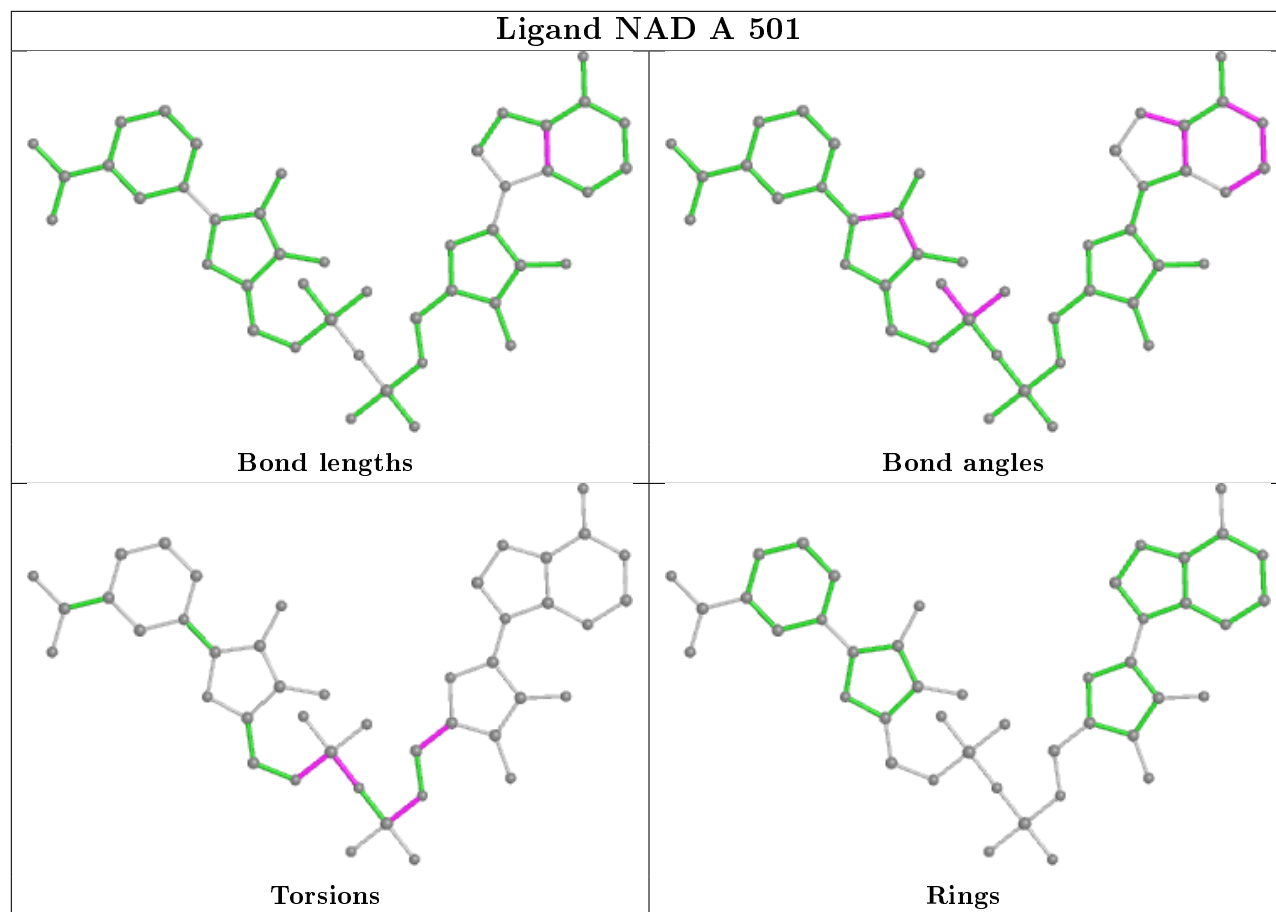
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	502	UDP	1	0
2	A	501	NAD	1	0
3	A	502	POP	1	0
2	E	800	NAD	1	0
2	D	501	NAD	1	0
2	B	501	NAD	1	0
5	B	502	UDP	1	0
4	A	503	SO4	1	0
2	F	800	NAD	1	0

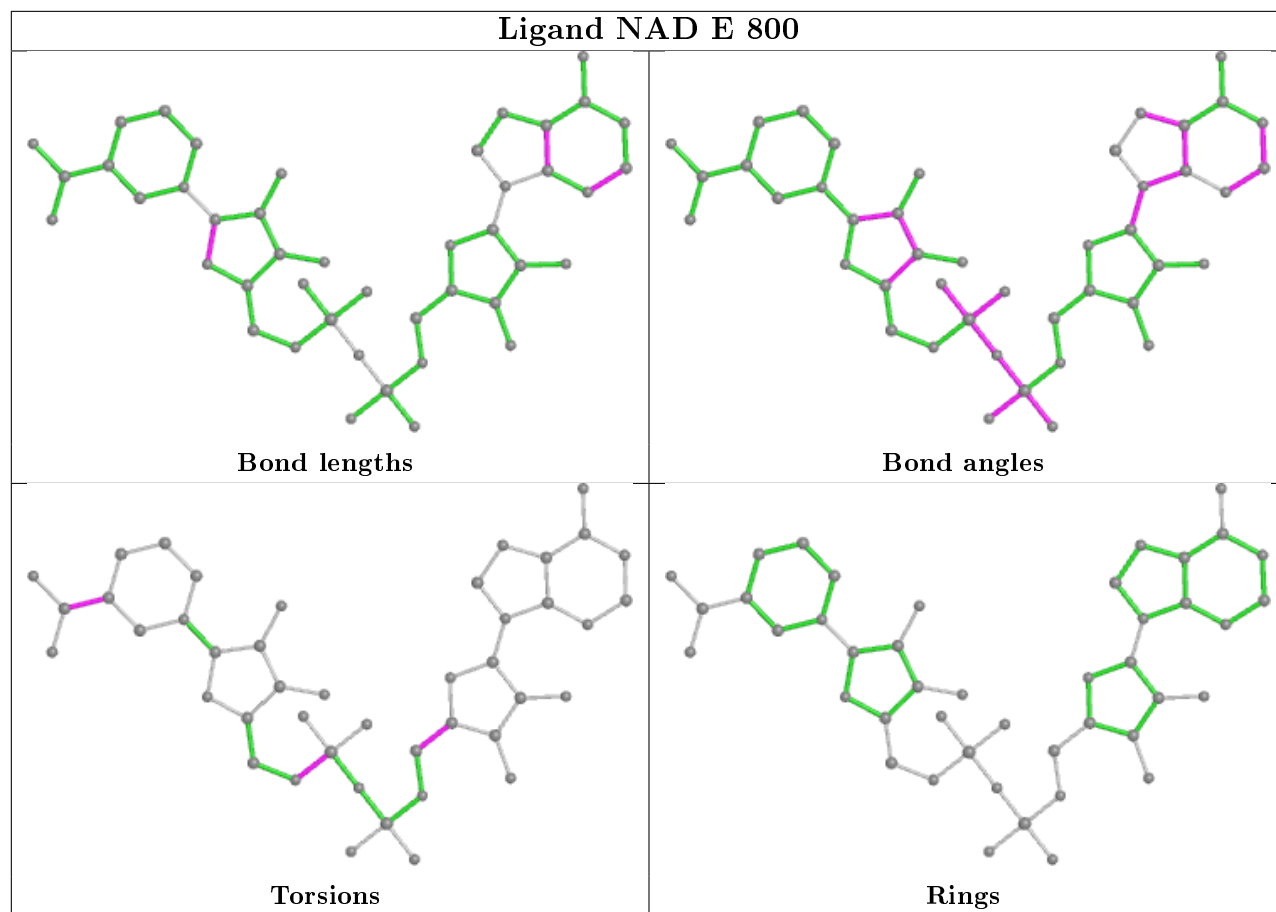
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

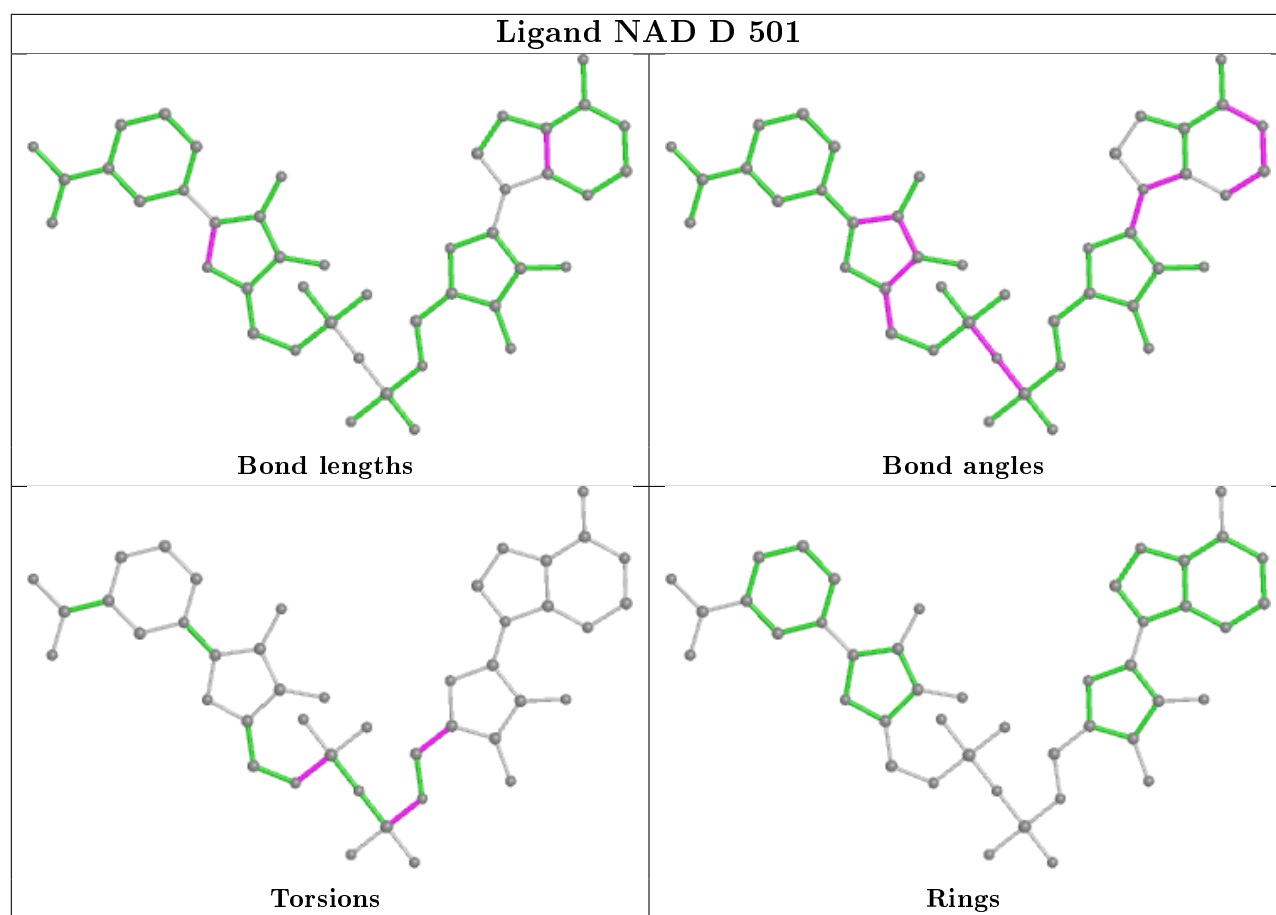
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

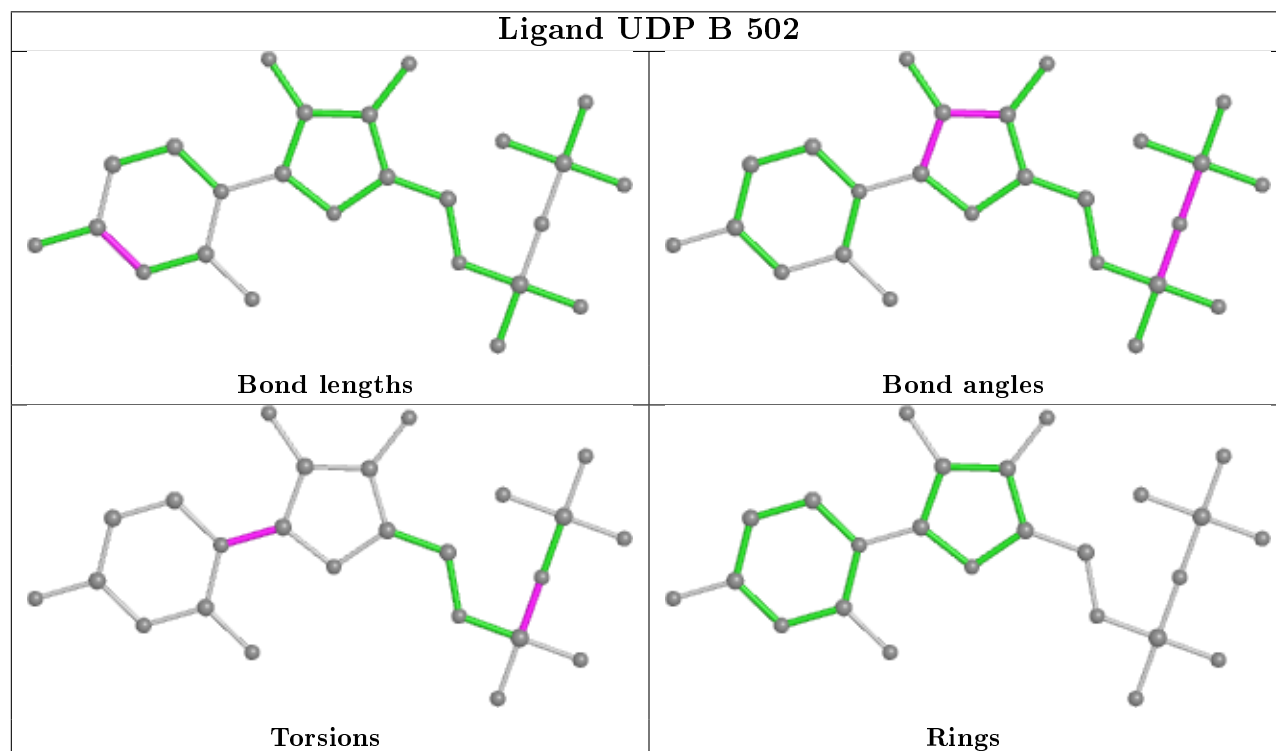
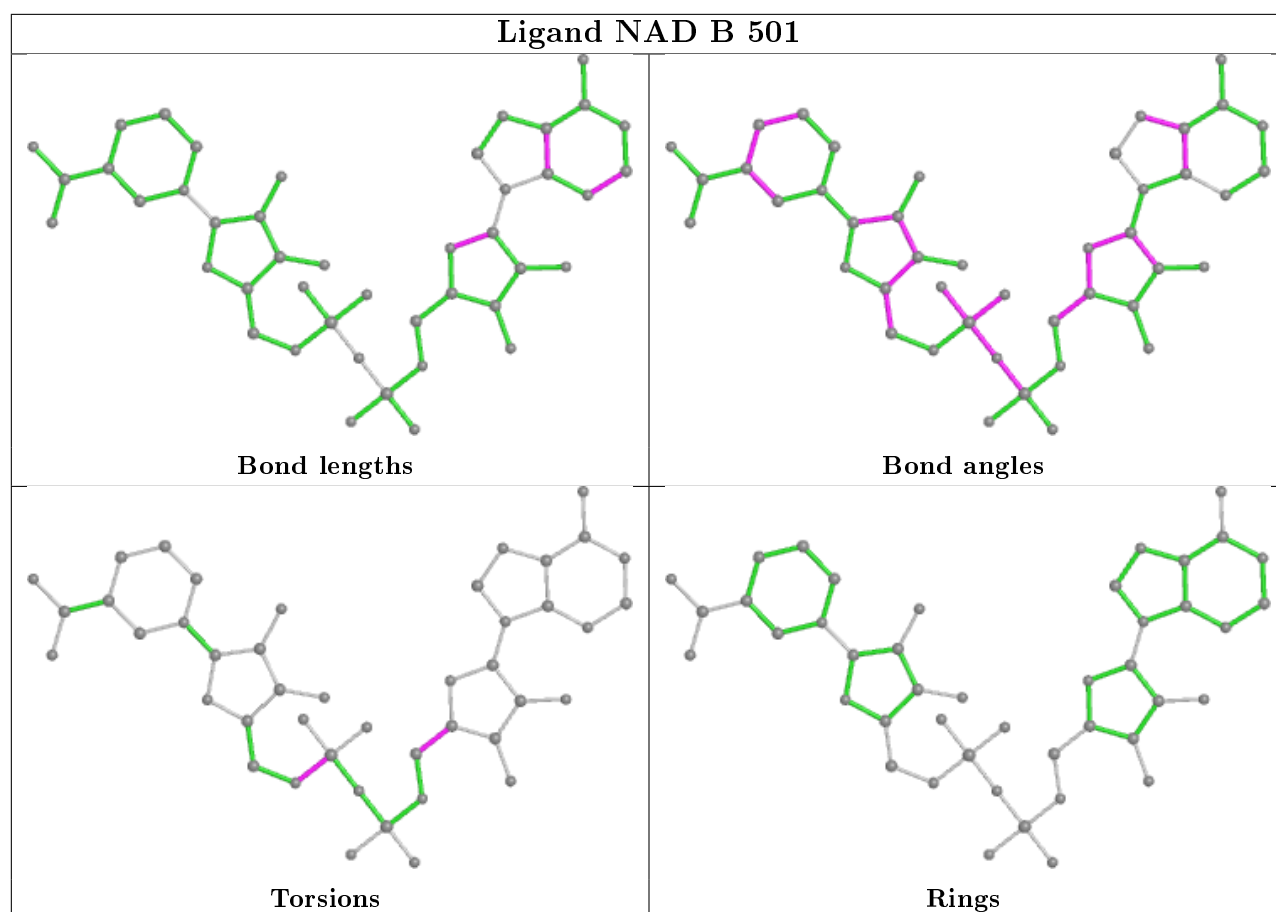


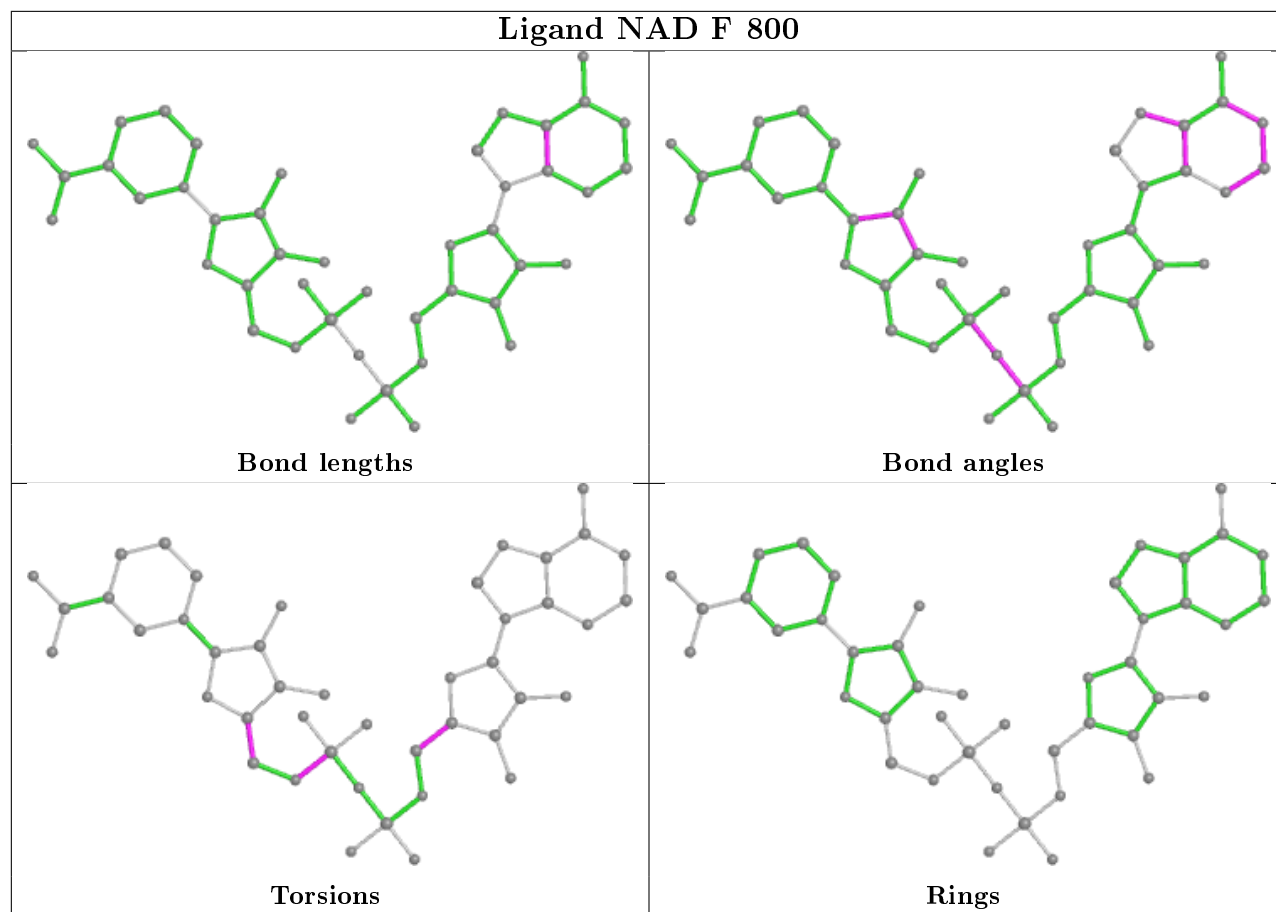












5.7 Other polymers [i](#)

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%)	0.82	32 (12%) 4 2	52, 131, 173, 208	0
1	B	272/336 (80%)	0.53	13 (4%) 30 26	47, 88, 152, 174	0
1	C	271/336 (80%)	0.53	10 (3%) 41 36	47, 91, 143, 169	0
1	D	261/336 (77%)	0.64	20 (7%) 13 10	47, 110, 182, 212	0
1	E	164/336 (48%)	0.60	13 (7%) 12 9	84, 125, 169, 205	0
1	F	181/336 (53%)	0.94	33 (18%) 1 1	85, 142, 175, 184	0
All	All	1412/2016 (70%)	0.66	121 (8%) 10 7	47, 112, 170, 212	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	290	TYR	7.2
1	F	309	LEU	6.4
1	C	351	LEU	6.1
1	A	376	PRO	6.0
1	F	364	ASP	5.4
1	F	397	TYR	4.4
1	A	334	PHE	4.3
1	F	243	TYR	4.3
1	D	283	GLN	4.2
1	A	338	ILE	4.2
1	F	104	LEU	3.9
1	A	289	VAL	3.8
1	A	333	GLU	3.8
1	E	151	ILE	3.7
1	A	299	PHE	3.6
1	F	372	LEU	3.6
1	D	277	PHE	3.5
1	D	388	ILE	3.4
1	D	392	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	289	VAL	3.3
1	F	371	MET	3.3
1	F	244	ALA	3.2
1	F	150	TYR	3.1
1	F	245	TYR	3.1
1	A	377	VAL	3.1
1	F	370	LEU	3.0
1	F	308	GLY	3.0
1	F	302	VAL	3.0
1	D	328	GLU	3.0
1	A	365	ILE	3.0
1	B	349	GLN	3.0
1	E	99	PHE	2.9
1	D	204	GLU	2.9
1	D	338	ILE	2.9
1	E	111	ASP	2.9
1	A	108	LEU	2.9
1	E	242	CYS	2.9
1	F	338	ILE	2.9
1	D	205	VAL	2.8
1	F	144	ASP	2.8
1	C	299	PHE	2.8
1	A	325	ASN	2.8
1	A	317	VAL	2.8
1	E	113	HIS	2.7
1	D	299	PHE	2.7
1	B	376	PRO	2.7
1	F	148	PRO	2.7
1	A	372	LEU	2.7
1	F	187	LEU	2.7
1	A	305	LEU	2.7
1	B	290	TYR	2.7
1	B	262	PHE	2.7
1	D	349	GLN	2.7
1	A	170	TYR	2.7
1	B	279	LEU	2.7
1	A	96	GLY	2.7
1	A	160	ALA	2.6
1	E	162	PRO	2.6
1	A	236	HIS	2.6
1	A	361	ARG	2.6
1	F	388	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	206	TYR	2.6
1	B	200	ALA	2.6
1	C	334	PHE	2.6
1	D	268	MET	2.5
1	A	104	LEU	2.5
1	F	145	VAL	2.5
1	F	304	ASP	2.5
1	F	312	LEU	2.5
1	A	235	LYS	2.5
1	E	155	GLN	2.5
1	D	334	PHE	2.5
1	A	374	TRP	2.5
1	F	170	TYR	2.5
1	A	282	LEU	2.4
1	F	118	VAL	2.4
1	D	113	HIS	2.4
1	B	377	VAL	2.4
1	D	288	THR	2.4
1	F	387	ALA	2.4
1	A	129	VAL	2.4
1	E	110	MET	2.4
1	B	287	LEU	2.3
1	F	141	ILE	2.3
1	A	344	SER	2.3
1	D	273	VAL	2.3
1	A	277	PHE	2.3
1	F	383	GLY	2.3
1	C	350	PHE	2.3
1	D	170	TYR	2.3
1	F	129	VAL	2.2
1	B	249	GLU	2.2
1	A	347	GLU	2.2
1	B	268	MET	2.2
1	C	397	TYR	2.2
1	D	332	LEU	2.2
1	E	313	MET	2.2
1	F	121	PHE	2.2
1	F	271	GLY	2.2
1	B	331	ILE	2.2
1	A	380	LEU	2.1
1	F	184	LEU	2.1
1	B	338	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	249	GLU	2.1
1	C	287	LEU	2.1
1	D	236	HIS	2.1
1	E	255	VAL	2.1
1	A	95	GLY	2.1
1	A	259	PHE	2.1
1	F	342	VAL	2.1
1	A	159	LEU	2.1
1	C	362	LYS	2.1
1	F	143	HIS	2.0
1	E	302	VAL	2.0
1	C	332	LEU	2.0
1	A	279	LEU	2.0
1	E	321	VAL	2.0
1	A	287	LEU	2.0
1	E	306	VAL	2.0
1	D	305	LEU	2.0
1	D	309	LEU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

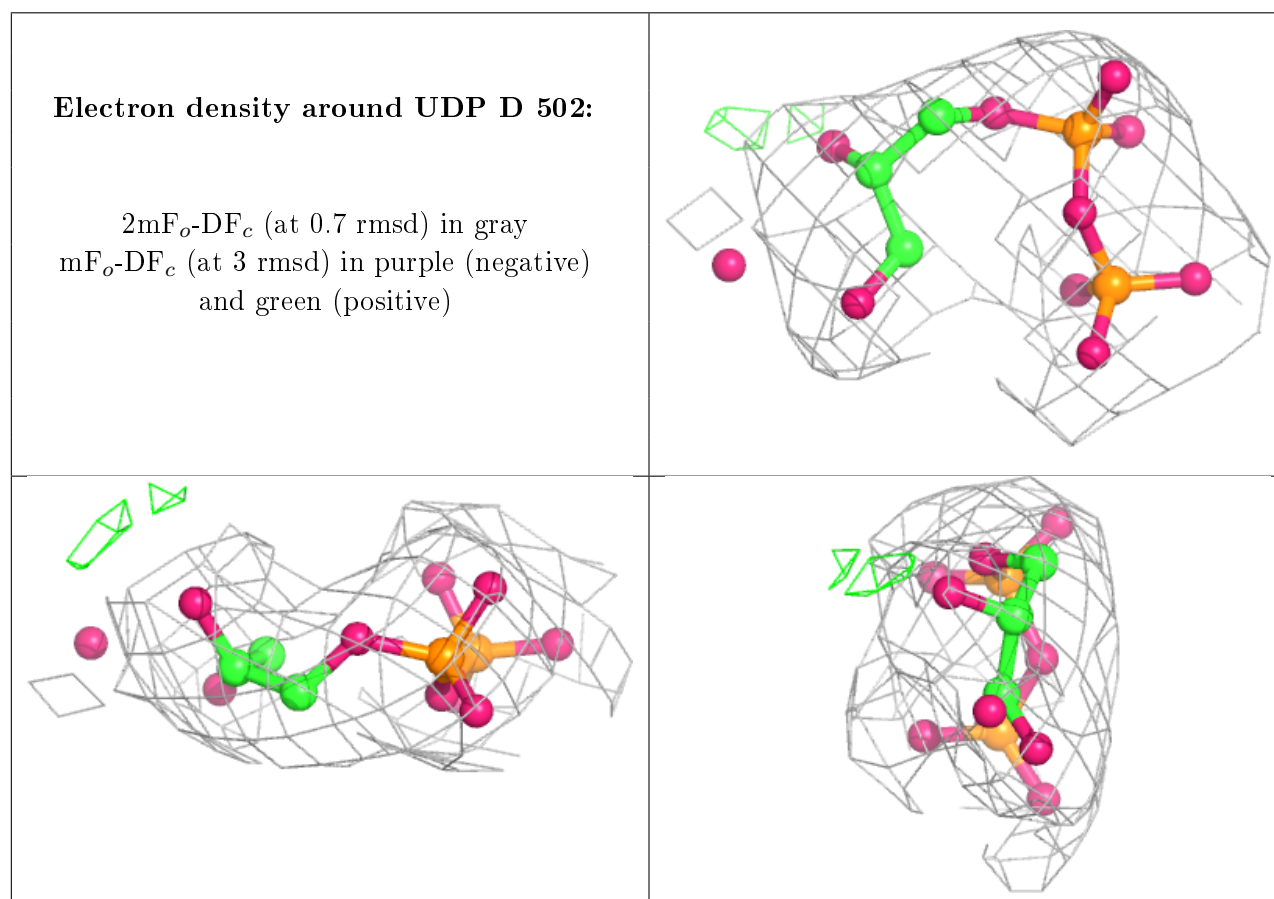
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	POP	A	502	9/9	0.85	0.15	111,120,154,274	1
5	UDP	D	502	15/25	0.89	0.15	100,135,199,289	0
3	POP	C	502	9/9	0.89	0.30	103,111,174,175	1
4	SO4	C	503	5/5	0.90	0.16	131,133,138,146	0
2	NAD	E	800	44/44	0.91	0.20	70,125,168,299	0

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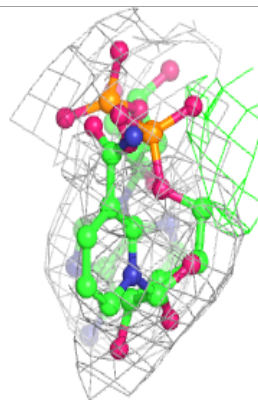
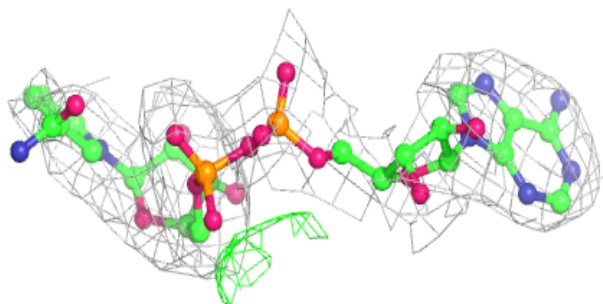
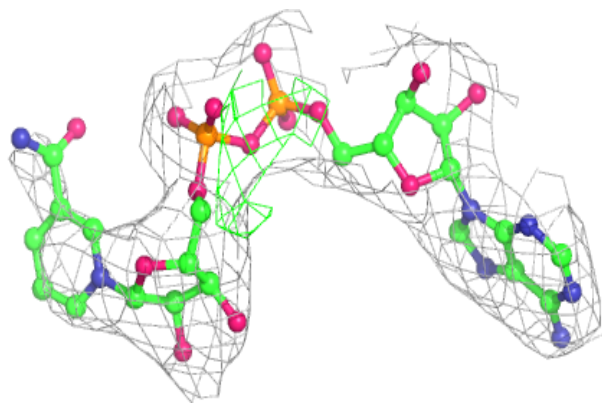
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	B	503	5/5	0.91	0.20	125,131,133,141	0
2	NAD	F	800	44/44	0.92	0.19	82,123,143,153	0
5	UDP	B	502	25/25	0.93	0.30	101,130,171,323	0
2	NAD	D	501	44/44	0.95	0.18	63,99,118,122	0
4	SO4	A	503	5/5	0.95	0.17	164,165,168,168	0
2	NAD	A	501	44/44	0.96	0.18	52,107,118,120	0
2	NAD	C	501	44/44	0.97	0.19	49,76,95,183	0
2	NAD	B	501	44/44	0.97	0.20	43,72,87,276	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.

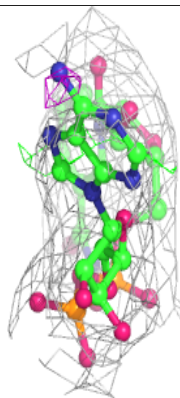
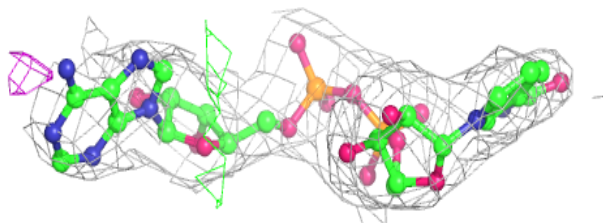
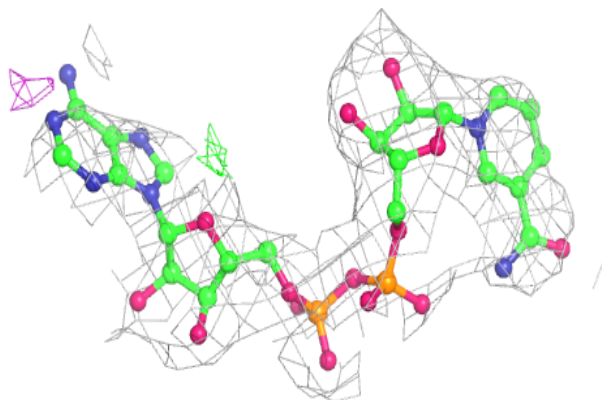


Electron density around NAD E 800:

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

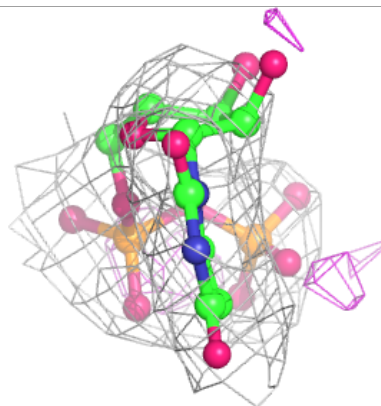
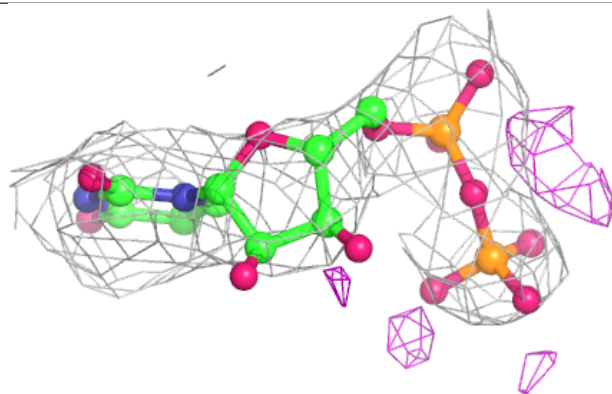
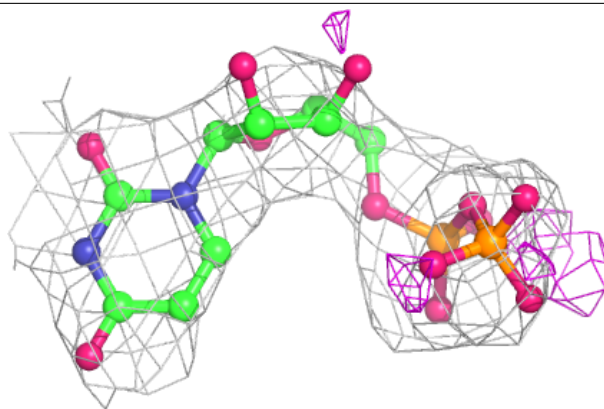
**Electron density around NAD F 800:**

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

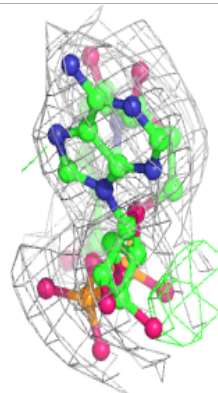
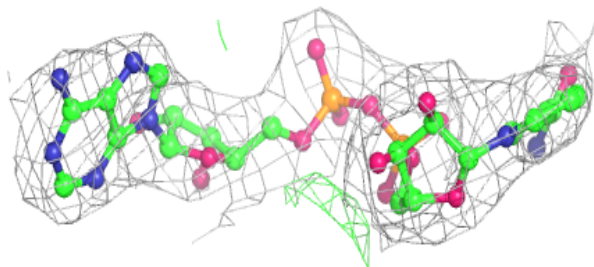
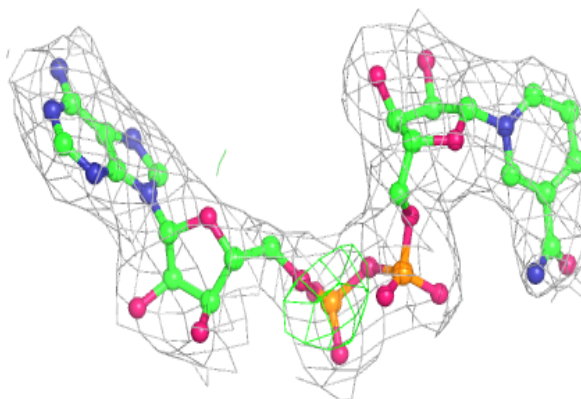


Electron density around UDP B 502:

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

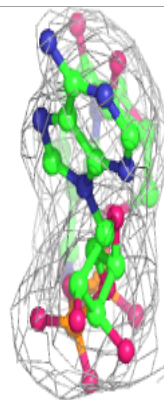
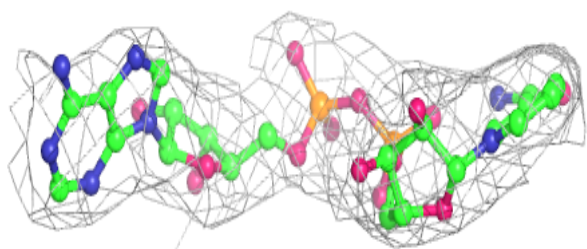
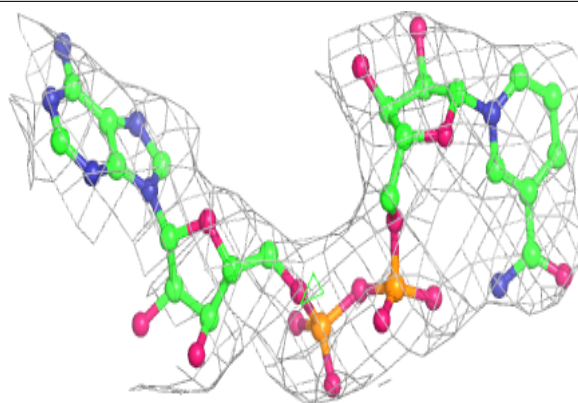
**Electron density around NAD D 501:**

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

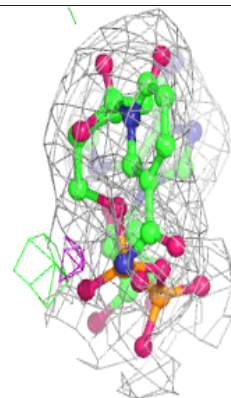
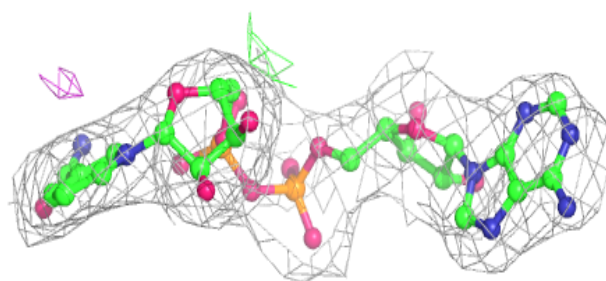
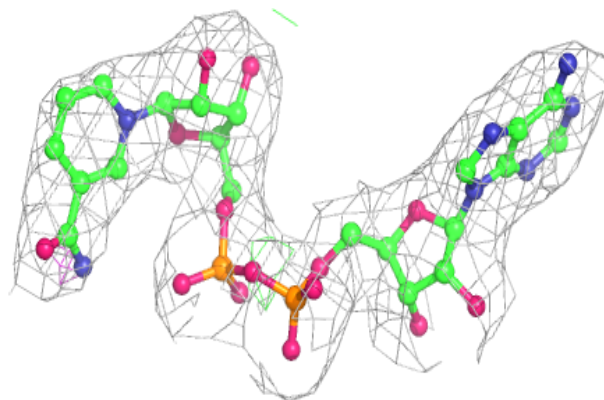


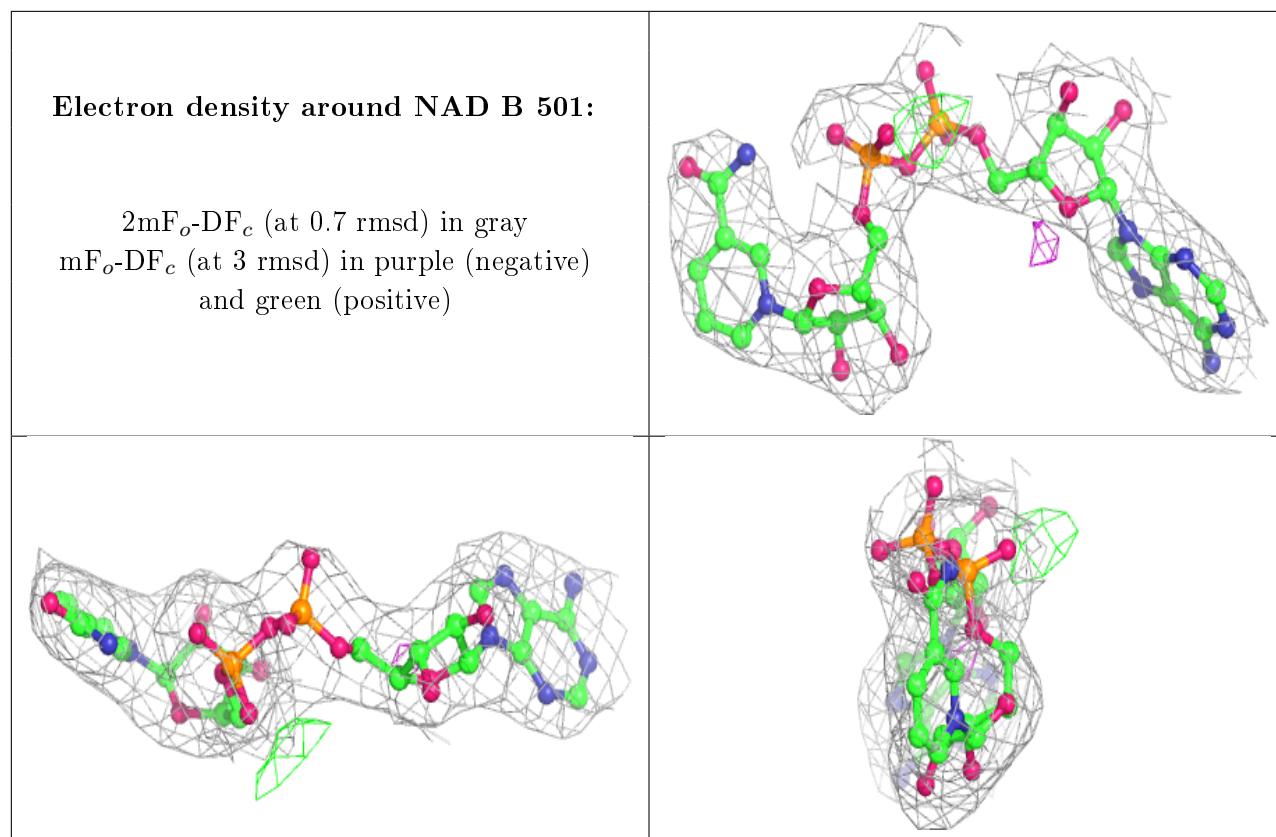
Electron density around NAD A 501:

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

**Electron density around NAD 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 [i](#)

There are no such residues in this entry.