



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 12:27 pm BST

PDB ID : 3DMT  
Title : Structure of Glycosomal Glyceraldehyde-3-Phosphate Dehydrogenase from Trypanosoma cruzi in complex with the irreversible iodoacetate inhibitor  
Authors : Guido, R.V.C.; Balliano, T.L.; Andricopulo, A.D.; Oliva, G.  
Deposited on : 2008-07-01  
Resolution : 2.30 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](mailto: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.

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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

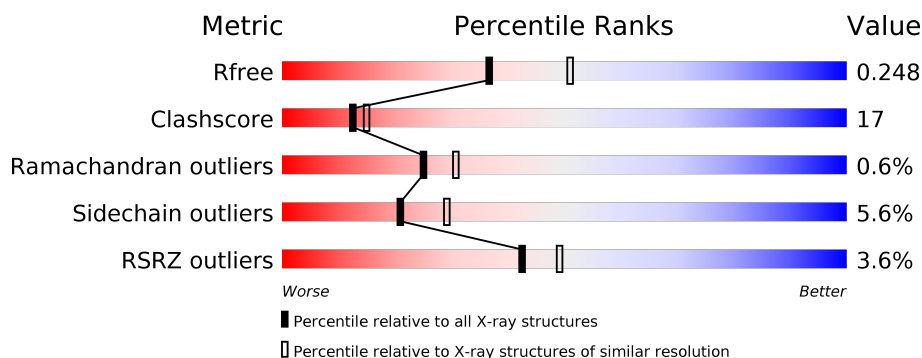
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	359	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>29%</div> <div>.</div> </div> </div>
1	B	359	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div>.</div> </div> </div>
1	D	359	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>.</div> </div> </div>
2	C	359	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>30%</div> <div>.</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	C	361	-	-	X	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 12123 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.

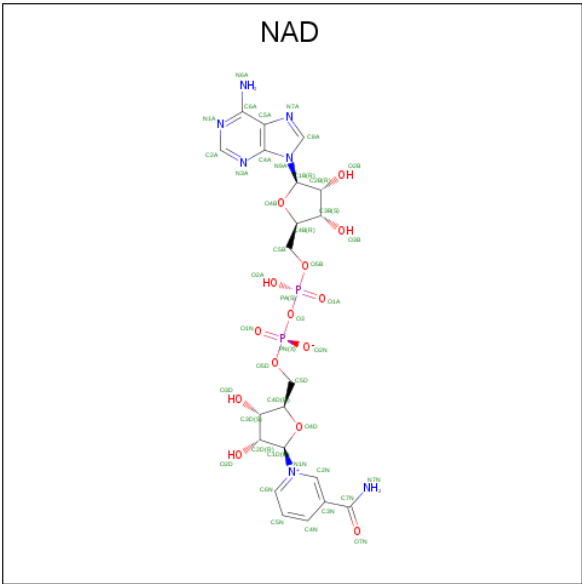
- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase, glycosomal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2733	1717	483	520	13			
1	B	359	Total	C	N	O	S	0	0	0
			2733	1717	483	520	13			
1	D	359	Total	C	N	O	S	0	0	0
			2733	1717	483	520	13			

- Molecule 2 is a protein called Glyceraldehyde-3-phosphate dehydrogenase, glycosomal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	359	Total	C	N	O	S	0	0	0
			2737	1719	483	522	13			

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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 GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		

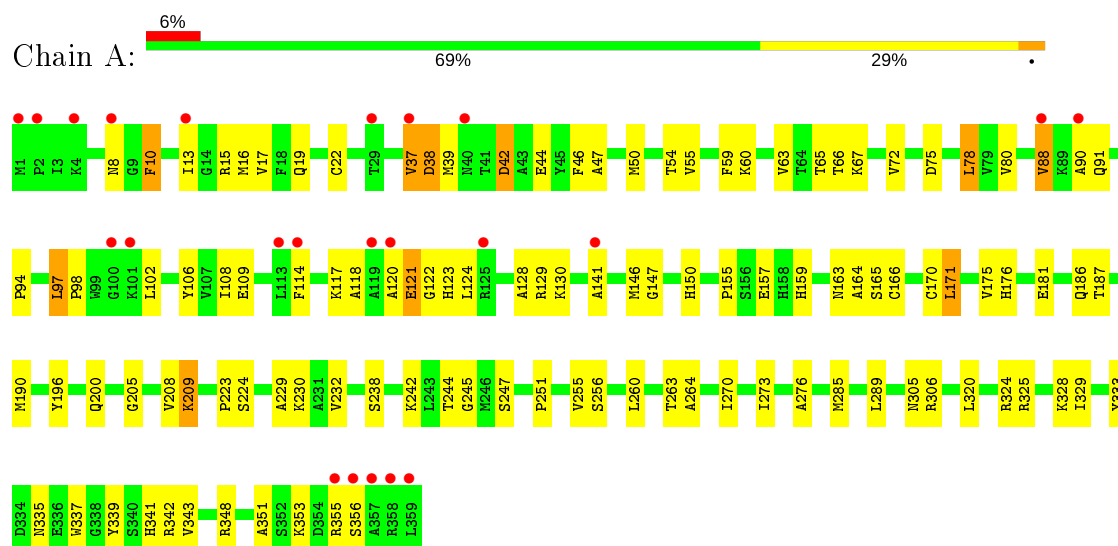
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	195	Total	O	0	0
			195	195		
5	B	294	Total	O	0	0
			294	294		
5	C	297	Total	O	0	0
			297	297		
5	D	219	Total	O	0	0
			219	219		

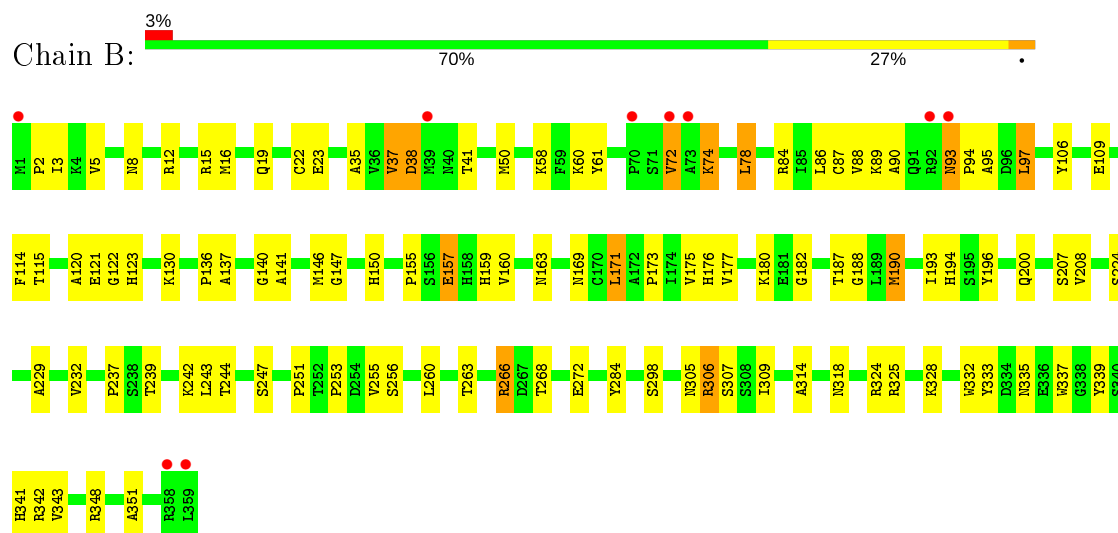
### 3 Residue-property plots [i](#)

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.

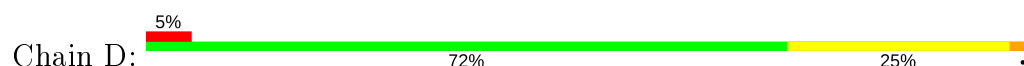
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, glycosomal

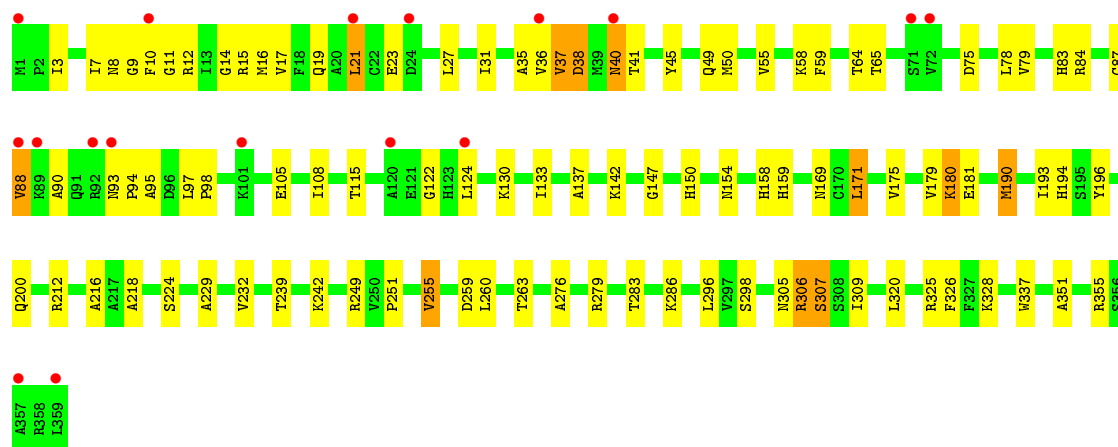


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, glycosomal

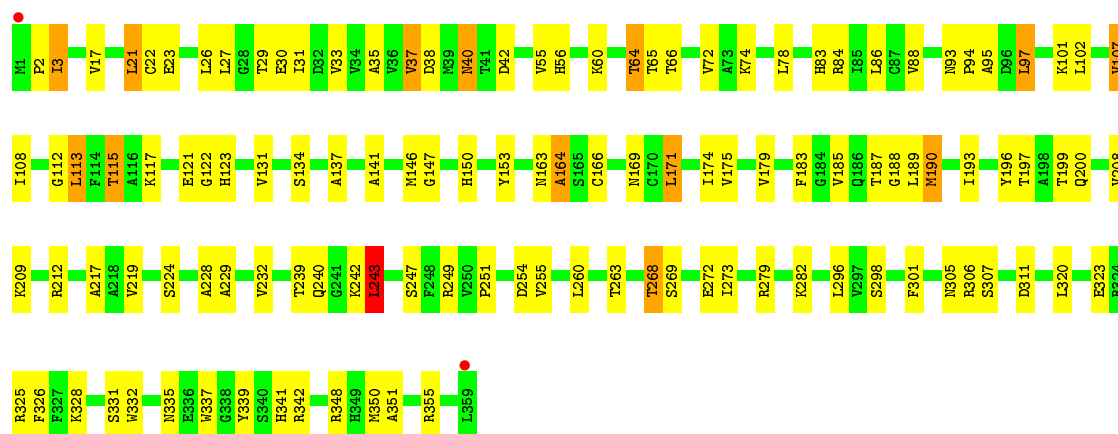


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, glycosomal





- Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase, glycosomal



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.75Å 83.71Å 105.61Å 90.00° 96.44° 90.00°	Depositor
Resolution (Å)	38.10 – 2.30 38.09 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.5 (38.10-2.30) 96.5 (38.09-2.30)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.62 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.186 , 0.252 0.185 , 0.248	Depositor DCC
$R_{free}$ test set	2987 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.8	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12123	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, CCS, 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	0.56	1/2786 (0.0%)	0.67	0/3778
1	B	0.57	0/2786	0.70	0/3778
1	D	0.54	0/2786	0.66	1/3778 (0.0%)
2	C	0.60	1/2779 (0.0%)	0.73	3/3767 (0.1%)
All	All	0.57	2/11137 (0.0%)	0.69	4/15101 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	22	CYS	CB-SG	-7.58	1.69	1.82
1	A	22	CYS	CB-SG	-5.99	1.72	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	243	LEU	CA-CB-CG	5.97	129.04	115.30
2	C	113	LEU	CA-CB-CG	5.46	127.85	115.30
2	C	279	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	D	21	LEU	CA-CB-CG	5.17	127.18	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2733	0	2721	86	0
1	B	2733	0	2722	89	0
1	D	2733	0	2722	88	0
2	C	2737	0	2723	115	0
3	A	44	0	26	4	0
3	B	44	0	26	3	0
3	C	44	0	26	7	0
3	D	44	0	26	3	0
4	C	6	0	8	5	0
5	A	195	0	0	13	0
5	B	294	0	0	15	0
5	C	297	0	0	19	0
5	D	219	0	0	10	0
All	All	12123	0	11000	364	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 17.

All (364) 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:A:16:MET:HG2	5:A:435:HOH:O	1.41	1.18
1:B:37:VAL:HG22	3:B:360:NAD:H2A	1.40	0.99
1:A:305:ASN:HB3	5:A:535:HOH:O	1.72	0.88
1:D:37:VAL:HG22	3:D:360:NAD:H2A	1.57	0.83
1:A:47:ALA:HA	1:A:50:MET:HE3	1.61	0.82
1:A:66:THR:HG22	5:A:480:HOH:O	1.80	0.82
2:C:311:ASP:HB2	5:C:445:HOH:O	1.79	0.81
1:A:147:GLY:H	1:A:150:HIS:HD2	1.29	0.80
1:D:16:MET:HG2	5:D:471:HOH:O	1.80	0.79
1:B:19:GLN:HG3	5:B:375:HOH:O	1.83	0.79
2:C:3:ILE:HG22	2:C:355:ARG:HH21	1.47	0.78
2:C:37:VAL:HG22	3:C:360:NAD:H2A	1.64	0.78
1:D:8:ASN:HA	1:D:37:VAL:HG13	1.66	0.77
2:C:147:GLY:H	2:C:150:HIS:HD2	1.31	0.77
2:C:171:LEU:HD13	2:C:232:VAL:HG21	1.67	0.77
1:A:190:MET:HG2	1:A:229:ALA:HB2	1.68	0.76
2:C:190:MET:HG2	2:C:229:ALA:HB2	1.66	0.76
1:B:2:PRO:HB3	5:B:531:HOH:O	1.86	0.76
1:A:186:GLN:HB2	1:A:263:THR:HG23	1.68	0.76
2:C:239:THR:HA	2:C:242:LYS:HE2	1.68	0.75
2:C:147:GLY:H	2:C:150:HIS:CD2	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:101:LYS:HG3	5:C:430:HOH:O	1.86	0.75
1:A:176:HIS:HD2	5:A:425:HOH:O	1.68	0.74
1:B:190:MET:HG2	1:B:229:ALA:HB2	1.68	0.74
2:C:26:LEU:HD22	2:C:30:GLU:HG3	1.68	0.74
1:D:147:GLY:H	1:D:150:HIS:CD2	2.06	0.74
1:B:37:VAL:CG2	3:B:360:NAD:H2A	2.17	0.74
1:B:176:HIS:HE1	5:B:411:HOH:O	1.72	0.73
2:C:188:GLY:HA3	2:C:243:LEU:HD13	1.70	0.73
1:A:147:GLY:H	1:A:150:HIS:CD2	2.05	0.73
1:A:238:SER:O	1:A:242:LYS:HE2	1.89	0.72
1:A:171:LEU:HD13	1:A:232:VAL:HG21	1.72	0.71
2:C:37:VAL:HB	2:C:88:VAL:HG22	1.71	0.71
2:C:107:VAL:HG11	2:C:123:HIS:HB3	1.71	0.71
1:B:348:ARG:HD2	5:B:510:HOH:O	1.91	0.71
2:C:199:THR:HG23	4:C:361:GOL:H32	1.71	0.70
2:C:268:THR:HG22	2:C:269:SER:H	1.54	0.70
1:B:115:THR:HG23	1:B:136:PRO:O	1.92	0.70
1:A:171:LEU:HG	1:A:190:MET:HE2	1.75	0.69
1:D:37:VAL:CG2	3:D:360:NAD:H2A	2.23	0.68
2:C:174:ILE:HD11	2:C:331:SER:HB2	1.74	0.68
1:A:190:MET:HG3	1:A:245:GLY:HA3	1.76	0.68
1:A:263:THR:HA	1:A:325:ARG:O	1.95	0.66
2:C:94:PRO:HA	2:C:97:LEU:HD22	1.78	0.66
1:D:21:LEU:HD11	1:D:31:ILE:HD13	1.78	0.65
2:C:331:SER:HA	5:C:445:HOH:O	1.96	0.65
1:D:38:ASP:O	1:D:90:ALA:HB2	1.96	0.65
1:D:171:LEU:HD22	1:D:175:VAL:HG23	1.80	0.64
1:A:42:ASP:O	1:A:46:PHE:HD1	1.80	0.64
1:B:74:LYS:HG3	5:B:410:HOH:O	1.97	0.64
1:B:182:GLY:O	1:B:266:ARG:HD3	1.97	0.64
1:A:171:LEU:HD22	1:A:175:VAL:HG23	1.80	0.64
1:D:93:ASN:OD1	1:D:95:ALA:HB3	1.98	0.63
1:B:171:LEU:HD22	1:B:175:VAL:HG23	1.81	0.63
2:C:117:LYS:O	2:C:121:GLU:HG3	1.98	0.63
2:C:23:GLU:OE1	5:C:650:HOH:O	2.16	0.63
1:B:157:GLU:HG3	5:B:459:HOH:O	1.99	0.63
1:A:8:ASN:HA	1:A:37:VAL:HG13	1.80	0.62
1:B:78:LEU:HD22	1:B:87:CYS:SG	2.38	0.62
1:B:171:LEU:HD13	1:B:232:VAL:HG21	1.81	0.62
1:A:114:PHE:O	1:A:120:ALA:HB2	2.00	0.62
1:A:117:LYS:HG3	1:A:141:ALA:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:239:THR:HB	2:C:243:LEU:HD23	1.82	0.61
1:D:169:ASN:O	1:D:307:SER:HB2	1.99	0.61
2:C:196:TYR:HA	2:C:200:GLN:NE2	2.15	0.61
2:C:171:LEU:HD22	2:C:175:VAL:HG23	1.82	0.61
1:A:47:ALA:HA	1:A:50:MET:CE	2.31	0.61
1:D:181:GLU:HG3	1:D:276:ALA:HB1	1.84	0.60
1:B:147:GLY:H	1:B:150:HIS:CD2	2.20	0.60
1:B:23:GLU:OE2	1:B:341:HIS:CE1	2.55	0.59
1:D:19:GLN:HG3	1:D:59:PHE:CE1	2.37	0.59
1:A:285:MET:HB3	1:A:289:LEU:HB3	1.84	0.59
1:D:171:LEU:HD13	1:D:232:VAL:HG21	1.85	0.59
2:C:341:HIS:HE1	5:C:650:HOH:O	1.85	0.59
1:A:50:MET:HE1	1:A:63:VAL:HG11	1.84	0.59
2:C:84:ARG:NH2	5:C:498:HOH:O	2.34	0.59
1:D:306:ARG:HB2	1:D:309:ILE:CD1	2.33	0.58
1:B:306:ARG:HB2	1:B:309:ILE:CD1	2.32	0.58
1:D:45:TYR:O	1:D:49:GLN:HG3	2.04	0.58
1:A:38:ASP:O	1:A:90:ALA:HB2	2.03	0.58
1:D:283:THR:O	1:D:286:LYS:HB2	2.04	0.58
2:C:185:VAL:O	2:C:242:LYS:HE3	2.03	0.58
1:B:137:ALA:HB3	1:B:141:ALA:HB3	1.85	0.58
1:D:224:SER:HB2	1:D:249:ARG:NH2	2.20	0.57
2:C:94:PRO:HA	2:C:97:LEU:CD2	2.35	0.57
1:D:147:GLY:H	1:D:150:HIS:HD2	1.53	0.57
1:D:64:THR:HG22	1:D:65:THR:H	1.69	0.57
2:C:107:VAL:HG11	2:C:123:HIS:CB	2.35	0.57
1:D:190:MET:HG2	1:D:229:ALA:HB2	1.87	0.56
2:C:260:LEU:O	2:C:328:LYS:HA	2.05	0.56
1:B:207:SER:HB2	5:B:542:HOH:O	2.05	0.56
1:B:266:ARG:NH2	1:B:272:GLU:OE1	2.36	0.56
2:C:351:ALA:O	2:C:355:ARG:HG2	2.06	0.56
1:B:38:ASP:O	1:B:90:ALA:HB2	2.06	0.56
2:C:196:TYR:HA	2:C:200:GLN:HE22	1.71	0.56
1:A:15:ARG:O	1:A:19:GLN:HG3	2.07	0.55
1:D:64:THR:HG22	1:D:65:THR:N	2.21	0.55
1:D:84:ARG:NH2	5:D:444:HOH:O	2.39	0.55
2:C:112:GLY:HA2	3:C:360:NAD:O3D	2.07	0.55
1:B:306:ARG:HB2	1:B:309:ILE:HD11	1.88	0.54
1:A:17:VAL:HG11	1:A:108:ILE:HD13	1.90	0.54
1:A:320:LEU:HD13	1:B:187:THR:HG23	1.89	0.54
2:C:197:THR:OG1	4:C:361:GOL:H11	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:HIS:HE1	5:B:471:HOH:O	1.89	0.54
1:B:86:LEU:HD23	1:B:88:VAL:HG12	1.89	0.54
1:A:348:ARG:HD2	5:A:422:HOH:O	2.08	0.54
2:C:171:LEU:HD12	2:C:229:ALA:HA	1.89	0.54
2:C:21:LEU:HD11	2:C:31:ILE:HD13	1.89	0.54
1:A:165:SER:HB2	5:A:511:HOH:O	2.07	0.54
1:A:260:LEU:O	1:A:328:LYS:HA	2.08	0.54
2:C:197:THR:OG1	4:C:361:GOL:H31	2.08	0.54
1:B:94:PRO:HA	1:B:97:LEU:HD22	1.90	0.54
1:A:196:TYR:HA	1:A:200:GLN:NE2	2.22	0.54
1:A:166:CYS:HB3	3:A:360:NAD:H5N	1.90	0.53
1:A:171:LEU:CG	1:A:190:MET:HE2	2.38	0.53
2:C:174:ILE:HD11	2:C:331:SER:CB	2.38	0.53
2:C:183:PHE:CD1	2:C:268:THR:HG21	2.44	0.53
2:C:282:LYS:HE2	5:C:580:HOH:O	2.08	0.53
1:A:118:ALA:O	1:A:121:GLU:HB2	2.09	0.53
1:A:124:LEU:HA	1:A:128:ALA:O	2.09	0.53
1:B:239:THR:HA	1:B:242:LYS:HD2	1.91	0.53
1:A:251:PRO:HB2	1:B:251:PRO:HB2	1.91	0.53
2:C:146:MET:HB2	2:C:342:ARG:HD3	1.90	0.53
1:A:130:LYS:NZ	1:A:159:HIS:HD2	2.07	0.52
2:C:35:ALA:HB1	2:C:88:VAL:HG13	1.90	0.52
3:A:360:NAD:N7N	3:A:360:NAD:O2N	2.43	0.52
2:C:55:VAL:HG22	2:C:56:HIS:CD2	2.43	0.52
1:D:196:TYR:HA	1:D:200:GLN:NE2	2.24	0.52
1:B:196:TYR:HA	1:B:200:GLN:NE2	2.25	0.52
2:C:2:PRO:HB3	2:C:29:THR:O	2.10	0.52
1:A:320:LEU:HG	1:B:244:THR:HG22	1.90	0.52
1:D:159:HIS:HE1	5:D:485:HOH:O	1.91	0.52
1:A:273:ILE:HG21	1:A:329:ILE:HD11	1.92	0.52
2:C:337:TRP:O	2:C:341:HIS:HD2	1.93	0.52
1:B:188:GLY:HA3	1:B:243:LEU:HD23	1.92	0.52
1:A:16:MET:SD	1:A:337:TRP:HZ3	2.33	0.52
1:D:351:ALA:O	1:D:355:ARG:HD3	2.10	0.51
2:C:320:LEU:HB2	2:C:323:GLU:HB2	1.92	0.51
1:B:84:ARG:NH2	5:B:495:HOH:O	2.42	0.51
2:C:72:VAL:HG12	2:C:74:LYS:O	2.11	0.51
1:D:78:LEU:HD22	1:D:87:CYS:SG	2.50	0.51
1:A:229:ALA:HB3	1:A:244:THR:HA	1.92	0.51
1:A:339:TYR:O	1:A:343:VAL:HG23	2.11	0.51
2:C:323:GLU:HG2	2:C:326:PHE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:17:VAL:HG11	2:C:108:ILE:HD13	1.92	0.51
2:C:208:VAL:HG23	5:C:408:HOH:O	2.10	0.51
2:C:166:CCS:HD2	3:C:360:NAD:C4N	2.40	0.51
2:C:326:PHE:HE1	1:D:326:PHE:CE1	2.29	0.51
1:B:208:VAL:HG22	5:B:446:HOH:O	2.11	0.51
1:B:260:LEU:O	1:B:328:LYS:HA	2.11	0.51
2:C:263:THR:HA	2:C:325:ARG:O	2.11	0.51
1:B:58:LYS:HG3	5:D:451:HOH:O	2.12	0.50
3:D:360:NAD:O2N	3:D:360:NAD:N7N	2.44	0.50
2:C:268:THR:HG22	2:C:272:GLU:HB3	1.93	0.50
2:C:193:ILE:HD12	1:D:193:ILE:HG13	1.93	0.50
2:C:33:VAL:H	2:C:83:HIS:HE1	1.58	0.50
1:B:169:ASN:O	1:B:307:SER:HB3	2.11	0.50
2:C:153:TYR:CE2	2:C:350:MET:HA	2.46	0.50
1:A:230:LYS:HE2	5:A:388:HOH:O	2.11	0.50
1:D:181:GLU:OE2	1:D:279:ARG:NH2	2.45	0.49
1:B:194:HIS:HA	1:B:256:SER:HB3	1.94	0.49
1:D:19:GLN:HG3	1:D:59:PHE:CD1	2.47	0.49
1:D:224:SER:HB2	1:D:249:ARG:CZ	2.43	0.49
1:A:121:GLU:O	1:A:124:LEU:HB2	2.13	0.49
1:D:40:ASN:ND2	1:D:40:ASN:H	2.09	0.49
1:A:50:MET:HE1	1:A:78:LEU:HG	1.94	0.49
1:A:91:GLN:HG2	1:A:97:LEU:HD13	1.95	0.49
1:B:314:ALA:O	1:B:318:ASN:ND2	2.41	0.49
2:C:296:LEU:O	1:D:212:ARG:HD3	2.12	0.49
1:D:159:HIS:CE1	5:D:485:HOH:O	2.66	0.49
1:B:146:MET:HB2	1:B:342:ARG:HD3	1.93	0.49
2:C:224:SER:HB3	2:C:247:SER:HB3	1.95	0.49
1:B:266:ARG:NH1	5:B:477:HOH:O	2.46	0.48
3:C:360:NAD:O2N	3:C:360:NAD:N7N	2.44	0.48
2:C:326:PHE:CE1	1:D:326:PHE:CE1	3.02	0.48
2:C:240:GLN:NE2	5:C:485:HOH:O	2.47	0.48
2:C:301:PHE:CZ	2:C:332:TRP:CD1	3.02	0.48
1:B:193:ILE:HD12	1:B:193:ILE:N	2.28	0.48
1:B:94:PRO:HB3	1:B:123:HIS:CE1	2.48	0.48
1:B:130:LYS:NZ	1:B:159:HIS:HD2	2.11	0.48
2:C:35:ALA:HB1	2:C:88:VAL:CG1	2.43	0.48
1:A:337:TRP:O	1:A:341:HIS:HD2	1.96	0.48
1:A:106:TYR:OH	1:A:351:ALA:HA	2.14	0.48
1:A:205:GLY:HA2	5:A:515:HOH:O	2.14	0.48
1:A:256:SER:HB2	1:A:333:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:PHE:CE1	1:D:36:VAL:HG11	2.49	0.48
1:A:129:ARG:HG3	1:A:130:LYS:HG2	1.96	0.47
1:B:23:GLU:HA	1:B:60:LYS:HD3	1.96	0.47
1:B:8:ASN:HA	1:B:37:VAL:HG13	1.95	0.47
1:A:37:VAL:HB	1:A:88:VAL:HG22	1.96	0.47
1:B:130:LYS:NZ	1:B:155:PRO:O	2.47	0.47
2:C:95:ALA:HA	2:C:122:GLY:O	2.13	0.47
1:A:94:PRO:HB2	1:A:122:GLY:HA3	1.95	0.47
2:C:268:THR:HG23	2:C:272:GLU:OE2	2.15	0.47
2:C:341:HIS:CE1	5:C:650:HOH:O	2.64	0.47
1:A:37:VAL:HG22	3:A:360:NAD:H2A	1.97	0.47
1:B:176:HIS:CD2	5:B:647:HOH:O	2.68	0.47
1:A:263:THR:HG21	5:A:476:HOH:O	2.14	0.47
1:D:298:SER:HB2	5:D:445:HOH:O	2.14	0.47
1:D:37:VAL:O	1:D:37:VAL:HG22	2.15	0.47
1:B:224:SER:HB3	1:B:247:SER:HB3	1.97	0.46
2:C:197:THR:HG21	4:C:361:GOL:H11	1.97	0.46
1:A:209:LYS:HE3	1:A:209:LYS:HA	1.95	0.46
1:B:50:MET:HG2	5:B:375:HOH:O	2.15	0.46
1:D:65:THR:HB	1:D:75:ASP:HB3	1.98	0.46
1:A:10:PHE:CE2	1:A:15:ARG:HG2	2.50	0.46
1:B:23:GLU:OE2	1:B:341:HIS:HE1	1.97	0.46
1:B:93:ASN:C	1:B:93:ASN:HD22	2.18	0.46
2:C:134:SER:O	3:C:360:NAD:H6N	2.16	0.46
2:C:115:THR:HG22	5:C:461:HOH:O	2.16	0.46
1:B:58:LYS:HE3	5:D:451:HOH:O	2.16	0.46
1:D:11:GLY:O	1:D:15:ARG:HB2	2.16	0.46
1:B:12:ARG:HH11	1:B:15:ARG:NH2	2.13	0.46
2:C:339:TYR:CG	3:C:360:NAD:H5N	2.50	0.46
1:A:155:PRO:HG3	1:A:353:LYS:O	2.16	0.46
2:C:40:ASN:HD22	2:C:40:ASN:C	2.20	0.46
1:D:130:LYS:NZ	1:D:159:HIS:HD2	2.13	0.46
1:D:94:PRO:HA	1:D:97:LEU:HD23	1.98	0.46
1:B:121:GLU:HG3	1:B:160:VAL:HG21	1.97	0.45
2:C:239:THR:HB	2:C:243:LEU:CD2	2.46	0.45
1:B:16:MET:SD	1:B:337:TRP:HZ3	2.40	0.45
1:B:106:TYR:OH	1:B:351:ALA:HA	2.16	0.45
1:D:298:SER:CB	5:D:445:HOH:O	2.64	0.45
2:C:187:THR:HG23	1:D:320:LEU:CD1	2.47	0.45
1:A:98:PRO:HG2	1:A:102:LEU:HD22	1.98	0.45
1:D:17:VAL:O	1:D:21:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:THR:HA	1:B:325:ARG:O	2.17	0.45
1:D:17:VAL:HG11	1:D:108:ILE:HD13	1.99	0.45
1:A:223:PRO:CG	1:B:332:TRP:HZ2	2.29	0.45
1:D:196:TYR:HA	1:D:200:GLN:HE22	1.81	0.45
1:A:54:THR:HG21	1:D:216:ALA:HB3	1.99	0.45
1:A:181:GLU:HG3	1:A:276:ALA:HB1	1.98	0.45
2:C:183:PHE:CE1	2:C:268:THR:HG21	2.51	0.45
1:A:170:CYS:HG	1:A:333:TYR:HD1	1.64	0.45
1:B:93:ASN:C	1:B:93:ASN:ND2	2.70	0.45
1:A:50:MET:O	1:A:59:PHE:HB2	2.16	0.45
2:C:348:ARG:HD2	5:C:503:HOH:O	2.17	0.45
1:A:176:HIS:CD2	5:A:425:HOH:O	2.55	0.45
1:B:3:ILE:HG22	1:B:5:VAL:HG23	1.99	0.45
2:C:137:ALA:HB3	2:C:141:ALA:HB3	1.99	0.44
2:C:188:GLY:O	2:C:243:LEU:HA	2.17	0.44
2:C:93:ASN:HD22	2:C:94:PRO:HD2	1.82	0.44
1:D:130:LYS:NZ	1:D:159:HIS:CD2	2.86	0.44
1:A:109:GLU:OE2	1:A:123:HIS:NE2	2.48	0.44
1:A:320:LEU:CD1	1:B:187:THR:CG2	2.95	0.44
1:D:21:LEU:HD11	1:D:31:ILE:CD1	2.46	0.44
1:B:16:MET:SD	1:B:337:TRP:CZ3	3.11	0.44
2:C:187:THR:HG21	1:D:326:PHE:HB3	2.00	0.44
1:D:21:LEU:CD1	1:D:31:ILE:HD13	2.46	0.44
1:D:50:MET:O	1:D:59:PHE:HB2	2.17	0.44
1:D:171:LEU:HD21	1:D:260:LEU:HD13	2.00	0.44
1:D:190:MET:HG3	1:D:190:MET:O	2.16	0.44
2:C:187:THR:CG2	1:D:320:LEU:CD1	2.96	0.44
1:B:196:TYR:HA	1:B:200:GLN:HE22	1.82	0.44
1:D:263:THR:HA	1:D:325:ARG:O	2.16	0.44
1:B:12:ARG:HH11	1:B:15:ARG:HH21	1.65	0.44
2:C:115:THR:CG2	5:C:461:HOH:O	2.66	0.44
2:C:200:GLN:HB3	2:C:217:ALA:HB2	1.99	0.44
1:D:259:ASP:OD1	1:D:328:LYS:HE3	2.18	0.44
1:D:23:GLU:OE1	1:D:337:TRP:CZ2	2.70	0.44
1:A:171:LEU:CD1	1:A:190:MET:HE2	2.48	0.44
1:A:320:LEU:CD1	1:B:187:THR:HG23	2.47	0.44
1:B:256:SER:HB2	1:B:333:TYR:CZ	2.53	0.44
2:C:27:LEU:HB2	5:C:469:HOH:O	2.17	0.44
1:A:130:LYS:NZ	1:A:159:HIS:CD2	2.85	0.44
1:A:13:ILE:O	1:A:17:VAL:HG23	2.18	0.44
1:A:196:TYR:HA	1:A:200:GLN:HE22	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ALA:O	1:D:251:PRO:HB3	2.18	0.44
1:A:176:HIS:HE1	5:A:451:HOH:O	2.00	0.43
1:B:114:PHE:O	1:B:120:ALA:HB2	2.17	0.43
2:C:40:ASN:ND2	2:C:42:ASP:H	2.16	0.43
2:C:163:ASN:O	2:C:164:ALA:HB3	2.17	0.43
1:D:255:VAL:HG11	1:D:298:SER:O	2.19	0.43
2:C:212:ARG:HD3	1:D:296:LEU:O	2.18	0.43
1:A:63:VAL:HG22	1:A:80:VAL:HG22	2.01	0.43
1:D:11:GLY:O	1:D:12:ARG:C	2.56	0.43
1:B:93:ASN:HD22	1:B:94:PRO:HD2	1.83	0.43
2:C:30:GLU:OE2	2:C:348:ARG:NH1	2.51	0.43
1:A:335:ASN:O	3:A:360:NAD:H4N	2.18	0.43
1:D:260:LEU:O	1:D:328:LYS:HA	2.18	0.43
2:C:107:VAL:HG13	2:C:131:VAL:HG22	2.00	0.43
1:A:130:LYS:HZ1	1:A:159:HIS:HD2	1.66	0.43
1:B:298:SER:HB3	1:B:332:TRP:HZ3	1.84	0.43
1:D:180:LYS:N	1:D:180:LYS:HD2	2.32	0.43
2:C:64:THR:CG2	2:C:65:THR:N	2.81	0.43
1:A:190:MET:O	1:A:245:GLY:HA3	2.19	0.42
1:A:67:LYS:HB3	1:A:72:VAL:HG22	2.01	0.42
2:C:55:VAL:HG21	2:C:254:ASP:CB	2.49	0.42
2:C:268:THR:CG2	2:C:269:SER:H	2.23	0.42
2:C:305:ASN:HB3	5:C:393:HOH:O	2.19	0.42
2:C:335:ASN:O	3:C:360:NAD:H4N	2.18	0.42
2:C:101:LYS:HE3	5:C:430:HOH:O	2.19	0.42
2:C:298:SER:HB3	2:C:332:TRP:HZ3	1.84	0.42
1:A:44:GLU:HG2	5:A:429:HOH:O	2.19	0.42
1:A:65:THR:HB	1:A:75:ASP:HB3	2.01	0.42
1:B:140:GLY:HA2	5:B:636:HOH:O	2.19	0.42
1:B:237:PRO:HD2	5:B:551:HOH:O	2.19	0.42
2:C:183:PHE:CD1	2:C:273:ILE:HD13	2.54	0.42
2:C:298:SER:HB3	2:C:332:TRP:CZ3	2.54	0.42
1:B:109:GLU:OE2	1:B:123:HIS:NE2	2.37	0.42
1:B:337:TRP:O	1:B:341:HIS:HD2	2.02	0.42
2:C:83:HIS:HD2	5:C:433:HOH:O	2.02	0.42
1:D:10:PHE:CE2	1:D:15:ARG:HG3	2.55	0.42
1:B:22:CYS:O	1:B:61:TYR:HE1	2.03	0.42
1:B:180:LYS:HE2	1:B:284:TYR:CE2	2.55	0.42
1:B:41:THR:HG21	1:B:89:LYS:HG2	2.02	0.42
2:C:190:MET:HE2	2:C:228:ALA:HB3	2.02	0.42
1:D:239:THR:HA	1:D:242:LYS:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:HIS:HB2	5:D:546:HOH:O	2.20	0.42
1:B:339:TYR:O	1:B:343:VAL:HG23	2.20	0.41
2:C:175:VAL:O	2:C:179:VAL:HG23	2.19	0.41
2:C:209:LYS:HE2	5:C:525:HOH:O	2.20	0.41
1:D:142:LYS:HB2	1:D:158:HIS:CD2	2.55	0.41
1:A:16:MET:SD	1:A:337:TRP:CZ3	3.13	0.41
2:C:174:ILE:CD1	2:C:331:SER:HB2	2.45	0.41
1:D:79:VAL:HA	1:D:83:HIS:O	2.20	0.41
1:A:146:MET:HB2	1:A:342:ARG:HD3	2.01	0.41
2:C:115:THR:HB	5:C:484:HOH:O	2.18	0.41
1:D:35:ALA:HB1	1:D:88:VAL:HG22	2.02	0.41
2:C:200:GLN:NE2	2:C:249:ARG:HD2	2.36	0.41
1:D:175:VAL:O	1:D:179:VAL:HG23	2.19	0.41
2:C:94:PRO:HB3	2:C:123:HIS:CE1	2.55	0.41
2:C:169:ASN:O	2:C:307:SER:HB3	2.21	0.41
1:A:224:SER:HB3	1:A:247:SER:HB3	2.02	0.41
1:A:324:ARG:HG2	5:A:492:HOH:O	2.20	0.41
1:B:163:ASN:O	1:B:169:ASN:ND2	2.48	0.41
2:C:33:VAL:H	2:C:83:HIS:CE1	2.37	0.41
1:D:115:THR:HA	1:D:133:ILE:HG21	2.02	0.41
1:D:306:ARG:HB2	1:D:309:ILE:HD11	2.02	0.41
2:C:189:LEU:HD13	1:D:328:LYS:HB2	2.02	0.41
1:A:270:ILE:HD12	1:A:270:ILE:HA	1.90	0.41
1:B:253:PRO:HG3	2:C:219:VAL:HG11	2.02	0.41
1:B:335:ASN:O	3:B:360:NAD:H4N	2.21	0.41
2:C:35:ALA:HA	2:C:86:LEU:O	2.20	0.41
1:D:124:LEU:HD21	1:D:159:HIS:HB3	2.01	0.41
1:D:21:LEU:CD1	1:D:31:ILE:CD1	2.99	0.41
1:B:35:ALA:HB1	1:B:88:VAL:HG13	2.01	0.41
1:D:23:GLU:OE1	1:D:337:TRP:HZ2	2.02	0.41
1:D:64:THR:HG21	5:D:460:HOH:O	2.21	0.41
1:B:175:VAL:CG1	1:B:239:THR:HG21	2.51	0.41
1:D:7:ILE:HB	1:D:36:VAL:HG12	2.03	0.41
1:D:9:GLY:O	1:D:14:GLY:HA3	2.21	0.41
1:B:268:THR:O	1:B:324:ARG:HA	2.21	0.41
2:C:196:TYR:CD2	2:C:251:PRO:HA	2.56	0.41
1:A:163:ASN:O	1:A:164:ALA:HB3	2.21	0.40
1:B:93:ASN:HD22	1:B:94:PRO:N	2.19	0.40
2:C:342:ARG:NE	2:C:342:ARG:HA	2.36	0.40
1:D:16:MET:SD	1:D:337:TRP:CZ3	3.14	0.40
1:B:86:LEU:CD2	1:B:88:VAL:HG12	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:200:GLN:CD	2:C:249:ARG:HD2	2.42	0.40
1:D:200:GLN:NE2	1:D:249:ARG:HD2	2.37	0.40
1:A:186:GLN:HG3	1:A:264:ALA:O	2.21	0.40
1:B:173:PRO:O	1:B:177:VAL:HG23	2.22	0.40
2:C:196:TYR:CE2	2:C:251:PRO:HA	2.55	0.40
2:C:3:ILE:HD12	2:C:351:ALA:HB2	2.04	0.40
1:D:95:ALA:HA	1:D:122:GLY:O	2.21	0.40
1:D:194:HIS:O	1:D:249:ARG:HA	2.22	0.40
1:B:196:TYR:CE2	1:B:251:PRO:HA	2.56	0.40
1:B:95:ALA:HA	1:B:122:GLY:O	2.22	0.40
1:B:196:TYR:CD2	1:B:251:PRO:HA	2.57	0.40
2:C:197:THR:CB	4:C:361:GOL:H31	2.52	0.40
1:D:115:THR:O	1:D:137:ALA:HA	2.21	0.40
1:D:130:LYS:HZ1	1:D:159:HIS:CD2	2.39	0.40
1:D:97:LEU:HA	1:D:98:PRO:HD3	1.92	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	357/359 (99%)	337 (94%)	17 (5%)	3 (1%)	19	23
1	B	357/359 (99%)	341 (96%)	14 (4%)	2 (1%)	25	31
1	D	357/359 (99%)	337 (94%)	19 (5%)	1 (0%)	41	50
2	C	356/359 (99%)	337 (95%)	17 (5%)	2 (1%)	25	31
All	All	1427/1436 (99%)	1352 (95%)	67 (5%)	8 (1%)	25	31

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	SER
1	A	255	VAL
1	B	255	VAL
2	C	255	VAL
1	D	255	VAL
1	A	42	ASP
1	B	72	VAL
2	C	164	ALA

### 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	293/296 (99%)	276 (94%)	17 (6%)	20	27
1	B	293/296 (99%)	280 (96%)	13 (4%)	28	39
1	D	293/296 (99%)	276 (94%)	17 (6%)	20	27
2	C	292/295 (99%)	273 (94%)	19 (6%)	17	23
All	All	1171/1183 (99%)	1105 (94%)	66 (6%)	21	29

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PHE
1	A	37	VAL
1	A	38	ASP
1	A	39	MET
1	A	55	VAL
1	A	60	LYS
1	A	78	LEU
1	A	88	VAL
1	A	97	LEU
1	A	121	GLU
1	A	157	GLU
1	A	171	LEU
1	A	187	THR
1	A	208	VAL

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Mol	Chain	Res	Type
1	A	209	LYS
1	A	306	ARG
1	A	355	ARG
1	B	37	VAL
1	B	38	ASP
1	B	72	VAL
1	B	74	LYS
1	B	78	LEU
1	B	93	ASN
1	B	97	LEU
1	B	157	GLU
1	B	171	LEU
1	B	190	MET
1	B	266	ARG
1	B	305	ASN
1	B	306	ARG
2	C	3	ILE
2	C	21	LEU
2	C	37	VAL
2	C	38	ASP
2	C	40	ASN
2	C	60	LYS
2	C	64	THR
2	C	66	THR
2	C	78	LEU
2	C	97	LEU
2	C	102	LEU
2	C	107	VAL
2	C	113	LEU
2	C	115	THR
2	C	171	LEU
2	C	190	MET
2	C	243	LEU
2	C	268	THR
2	C	306	ARG
1	D	3	ILE
1	D	27	LEU
1	D	37	VAL
1	D	38	ASP
1	D	40	ASN
1	D	41	THR
1	D	55	VAL

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Mol	Chain	Res	Type
1	D	58	LYS
1	D	88	VAL
1	D	105	GLU
1	D	154	ASN
1	D	171	LEU
1	D	180	LYS
1	D	190	MET
1	D	305	ASN
1	D	306	ARG
1	D	307	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	150	HIS
1	A	159	HIS
1	A	176	HIS
1	A	186	GLN
1	A	200	GLN
1	B	8	ASN
1	B	83	HIS
1	B	93	ASN
1	B	150	HIS
1	B	151	HIS
1	B	159	HIS
1	B	176	HIS
1	B	200	GLN
1	B	305	ASN
1	B	341	HIS
2	C	19	GLN
2	C	40	ASN
2	C	83	HIS
2	C	93	ASN
2	C	150	HIS
2	C	151	HIS
2	C	176	HIS
2	C	200	GLN
2	C	240	GLN
2	C	341	HIS
1	D	8	ASN
1	D	150	HIS

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Mol	Chain	Res	Type
1	D	154	ASN
1	D	159	HIS
1	D	200	GLN
1	D	305	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CCS	C	166	2	5,9,10	1.76	1 (20%)	3,10,12	1.38	1 (33%)

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	CCS	C	166	2	-	0/4/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	166	CCS	CD-SG	-3.59	1.76	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	166	CCS	CB-SG-CD	2.07	105.65	101.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	166	CCS	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAD	C	360	-	42,48,48	1.09	3 (7%)	50,73,73	1.40	6 (12%)
3	NAD	D	360	-	42,48,48	1.17	3 (7%)	50,73,73	1.25	4 (8%)
3	NAD	A	360	-	42,48,48	1.09	2 (4%)	50,73,73	1.20	3 (6%)
3	NAD	B	360	-	42,48,48	1.07	2 (4%)	50,73,73	1.29	7 (14%)
4	GOL	C	361	-	5,5,5	0.31	0	5,5,5	0.25	0

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	C	360	-	-	6/26/62/62	0/5/5/5
3	NAD	D	360	-	-	11/26/62/62	0/5/5/5
3	NAD	A	360	-	-	7/26/62/62	0/5/5/5
3	NAD	B	360	-	-	6/26/62/62	0/5/5/5
4	GOL	C	361	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	360	NAD	C2N-N1N	4.58	1.40	1.35
3	A	360	NAD	C2N-N1N	4.23	1.40	1.35
3	B	360	NAD	C2N-N1N	3.94	1.39	1.35
3	D	360	NAD	C2N-N1N	3.49	1.39	1.35
3	D	360	NAD	O4B-C1B	3.41	1.45	1.41
3	B	360	NAD	O4D-C1D	2.76	1.44	1.41
3	D	360	NAD	O4D-C1D	2.62	1.44	1.41
3	A	360	NAD	O4D-C1D	2.51	1.44	1.41
3	C	360	NAD	C6N-N1N	2.26	1.40	1.35
3	C	360	NAD	O4B-C1B	2.07	1.44	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	360	NAD	N3A-C2A-N1A	-4.95	120.94	128.68
3	D	360	NAD	N3A-C2A-N1A	-4.78	121.21	128.68
3	A	360	NAD	N3A-C2A-N1A	-4.24	122.06	128.68
3	B	360	NAD	N3A-C2A-N1A	-4.02	122.40	128.68
3	A	360	NAD	PN-O3-PA	-3.36	121.28	132.83
3	C	360	NAD	O4B-C1B-C2B	-3.14	102.33	106.93
3	D	360	NAD	C3N-C7N-N7N	-3.07	114.06	117.75
3	C	360	NAD	O4D-C1D-C2D	-2.90	102.68	106.93
3	D	360	NAD	O4B-C1B-C2B	-2.77	102.88	106.93
3	B	360	NAD	C3N-C7N-N7N	-2.76	114.44	117.75
3	B	360	NAD	C4A-C5A-N7A	-2.71	106.57	109.40
3	B	360	NAD	PN-O3-PA	-2.69	123.61	132.83
3	A	360	NAD	C6N-N1N-C2N	-2.63	119.58	121.97
3	C	360	NAD	PN-O3-PA	-2.51	124.23	132.83
3	B	360	NAD	O4D-C1D-C2D	-2.25	103.64	106.93
3	C	360	NAD	O4D-C4D-C5D	-2.20	102.13	109.37
3	B	360	NAD	C5B-C4B-C3B	-2.14	107.15	115.18
3	B	360	NAD	O4B-C1B-C2B	-2.07	103.90	106.93
3	C	360	NAD	C4A-C5A-N7A	-2.03	107.28	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	360	NAD	PN-O3-PA	-2.02	125.90	132.83

There are no chirality outliers.

All (32) torsion outliers are listed below:

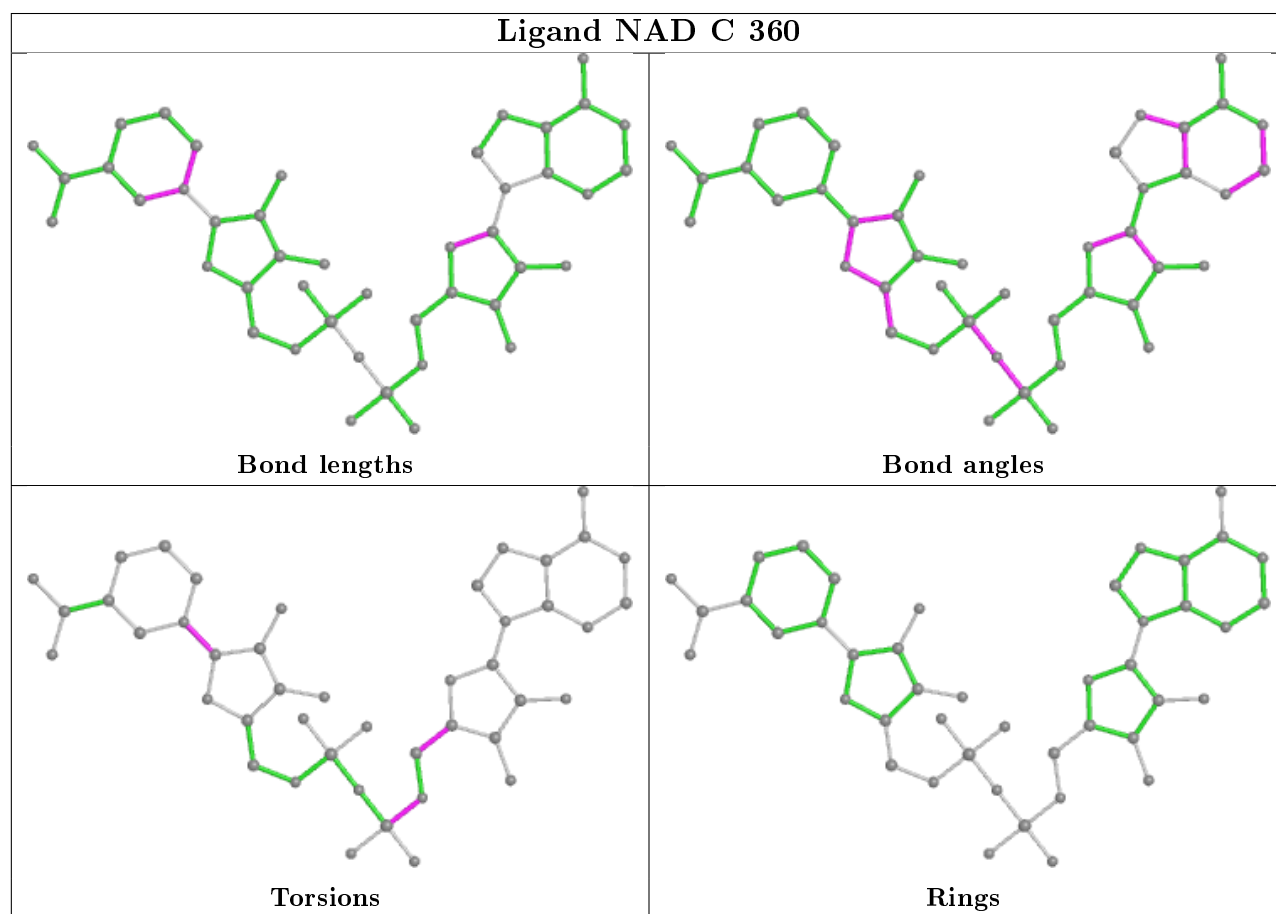
Mol	Chain	Res	Type	Atoms
3	C	360	NAD	C5B-O5B-PA-O1A
3	C	360	NAD	O4D-C1D-N1N-C2N
3	C	360	NAD	O4D-C1D-N1N-C6N
3	C	360	NAD	C2D-C1D-N1N-C2N
3	C	360	NAD	C2D-C1D-N1N-C6N
3	D	360	NAD	C5B-O5B-PA-O1A
3	D	360	NAD	O4D-C1D-N1N-C2N
3	D	360	NAD	O4D-C1D-N1N-C6N
3	D	360	NAD	C2D-C1D-N1N-C2N
3	D	360	NAD	C2D-C1D-N1N-C6N
3	A	360	NAD	C5B-O5B-PA-O1A
3	A	360	NAD	O4D-C1D-N1N-C2N
3	A	360	NAD	O4D-C1D-N1N-C6N
3	A	360	NAD	C2D-C1D-N1N-C6N
3	B	360	NAD	O4D-C1D-N1N-C2N
3	B	360	NAD	O4D-C1D-N1N-C6N
3	B	360	NAD	C2D-C1D-N1N-C2N
3	B	360	NAD	C2D-C1D-N1N-C6N
4	C	361	GOL	C1-C2-C3-O3
4	C	361	GOL	O2-C2-C3-O3
3	D	360	NAD	C5B-O5B-PA-O3
3	D	360	NAD	C5B-O5B-PA-O2A
3	D	360	NAD	O4B-C4B-C5B-O5B
3	D	360	NAD	C4B-C5B-O5B-PA
3	C	360	NAD	O4B-C4B-C5B-O5B
3	A	360	NAD	C2D-C1D-N1N-C2N
3	B	360	NAD	C5D-O5D-PN-O3
3	D	360	NAD	O4D-C4D-C5D-O5D
3	A	360	NAD	O4D-C4D-C5D-O5D
3	B	360	NAD	O4B-C4B-C5B-O5B
3	D	360	NAD	PA-O3-PN-O2N
3	A	360	NAD	O4B-C4B-C5B-O5B

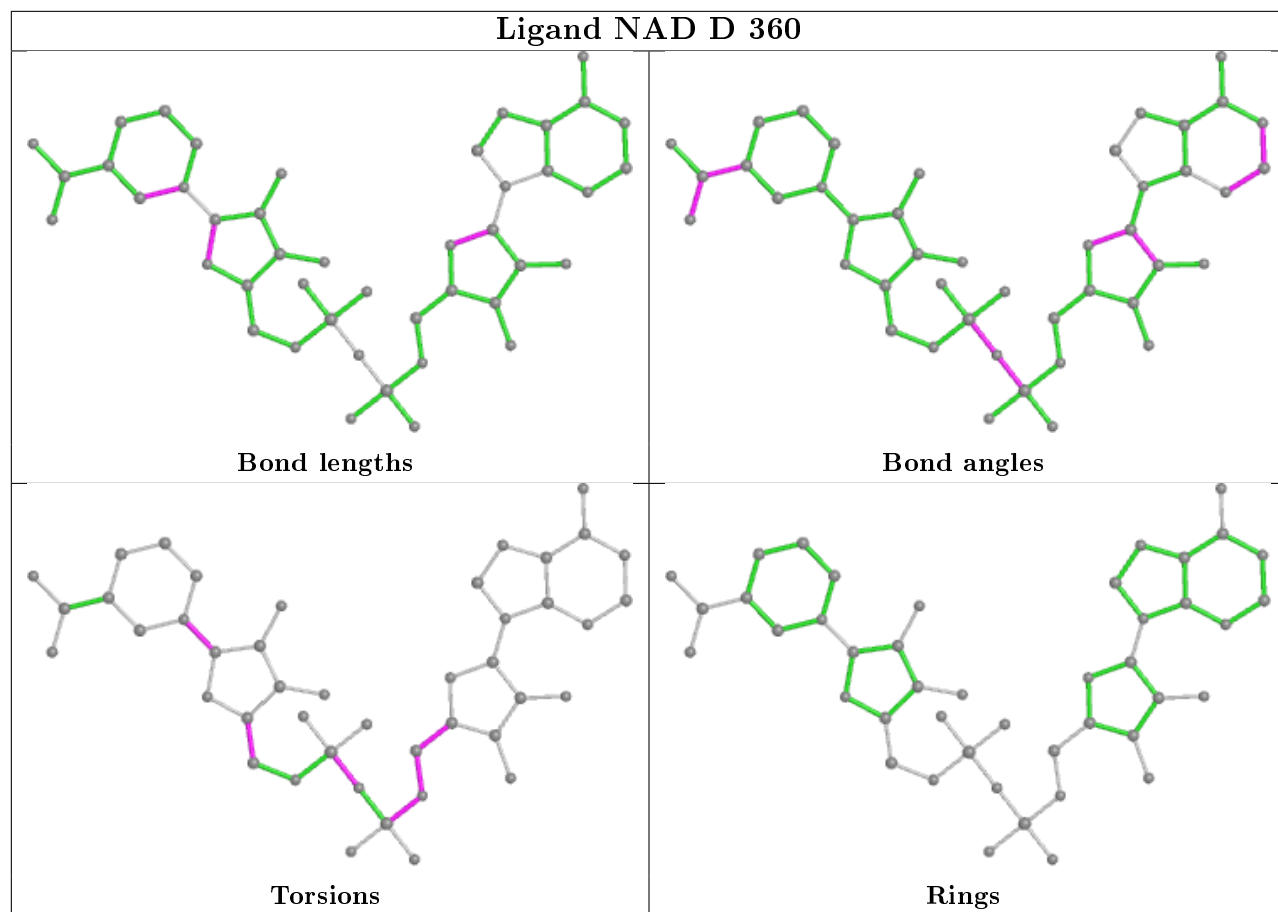
There are no ring outliers.

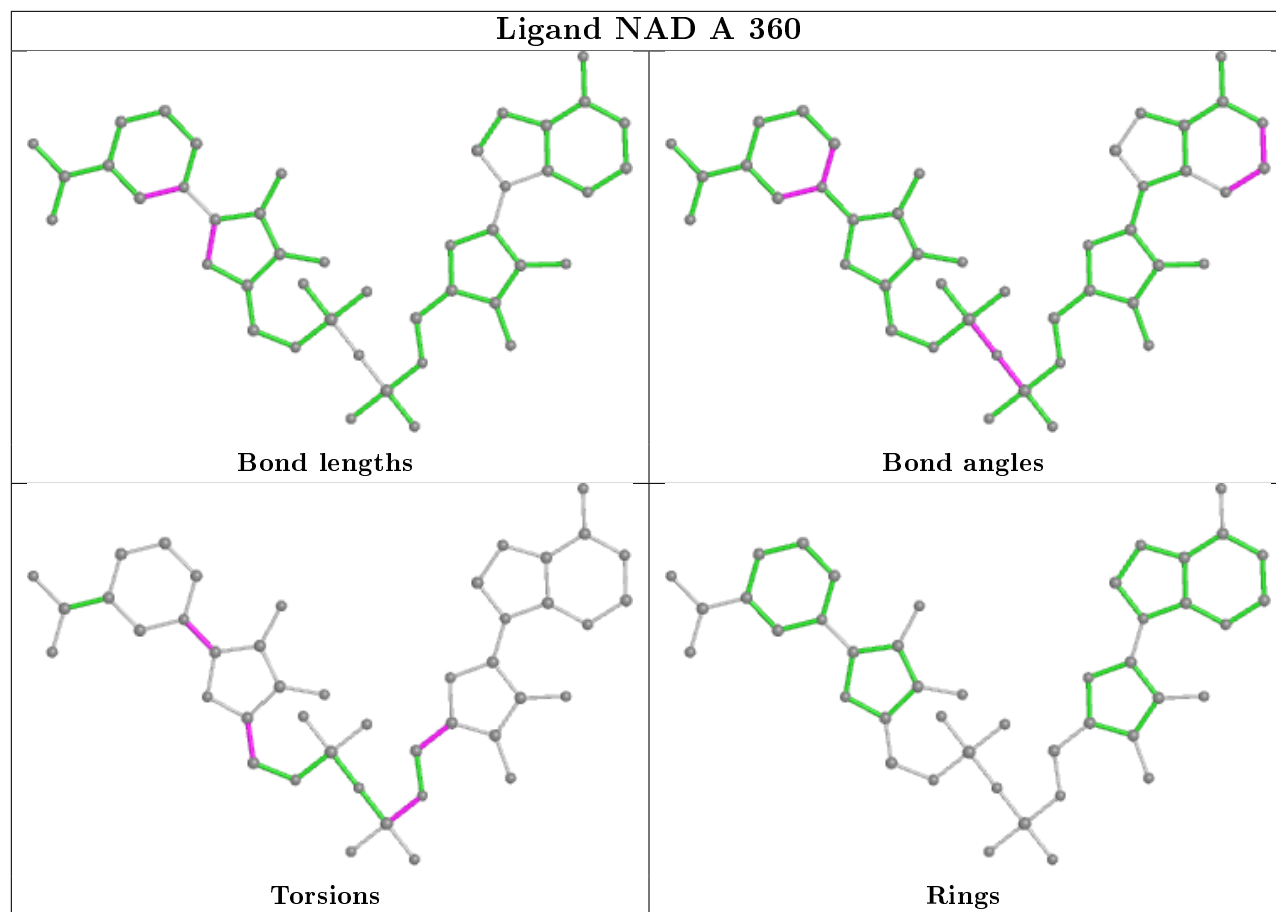
5 monomers are involved in 22 short contacts:

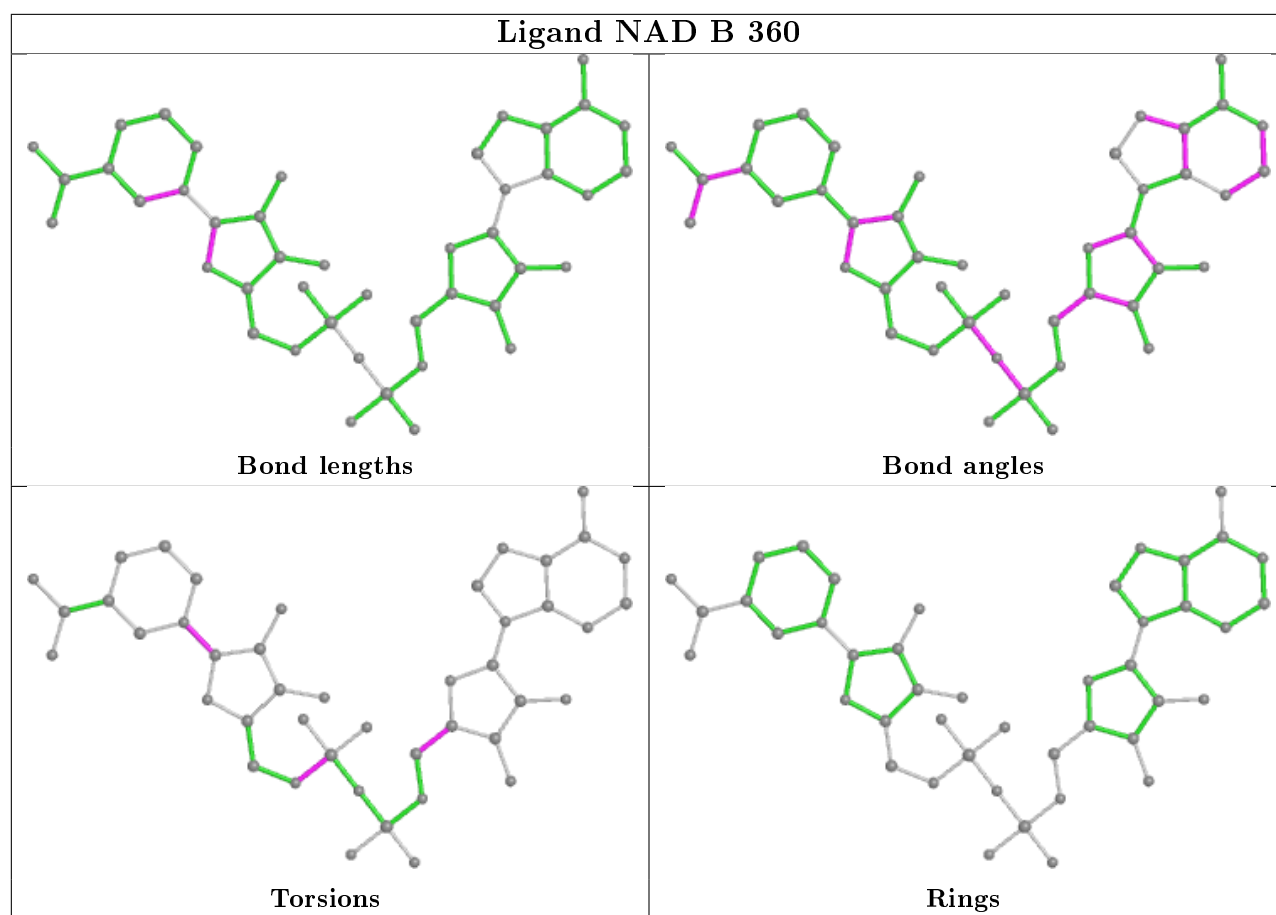
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	360	NAD	7	0
3	D	360	NAD	3	0
3	A	360	NAD	4	0
3	B	360	NAD	3	0
4	C	361	GOL	5	0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	359/359 (100%)	0.42	23 (6%) 19 25	6, 19, 38, 43	24 (6%)
1	B	359/359 (100%)	0.03	9 (2%) 57 64	6, 16, 28, 39	7 (1%)
1	D	359/359 (100%)	0.31	17 (4%) 31 38	8, 20, 40, 48	14 (3%)
2	C	358/359 (99%)	-0.17	2 (0%) 89 92	7, 16, 28, 51	3 (0%)
All	All	1435/1436 (99%)	0.15	51 (3%) 42 49	6, 17, 38, 51	48 (3%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	359	LEU	44.6
1	A	1	MET	27.0
1	D	72	VAL	26.9
1	A	2	PRO	21.0
1	A	357	ALA	20.2
1	A	356	SER	19.9
1	B	358	ARG	19.8
1	A	359	LEU	14.5
1	A	358	ARG	9.5
1	A	355	ARG	8.4
1	D	1	MET	6.1
1	B	72	VAL	5.4
1	D	357	ALA	4.4
2	C	359	LEU	4.0
1	B	92	ARG	3.9
1	A	37	VAL	3.7
1	D	92	ARG	3.4
1	B	73	ALA	3.4
1	A	141	ALA	3.2
1	D	359	LEU	3.2
1	D	24	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	36	VAL	2.9
1	A	100	GLY	2.9
2	C	1	MET	2.9
1	D	21	LEU	2.7
1	A	114	PHE	2.7
1	A	113	LEU	2.7
1	A	8	ASN	2.7
1	D	88	VAL	2.7
1	A	13	ILE	2.6
1	A	90	ALA	2.6
1	A	119	ALA	2.6
1	A	29	THR	2.6
1	B	1	MET	2.5
1	B	70	PRO	2.4
1	B	39	MET	2.4
1	A	125	ARG	2.4
1	D	40	ASN	2.4
1	A	40	ASN	2.2
1	A	120	ALA	2.2
1	D	120	ALA	2.2
1	A	101	LYS	2.1
1	D	71	SER	2.1
1	A	88	VAL	2.1
1	D	89	LYS	2.1
1	D	10	PHE	2.1
1	D	124	LEU	2.0
1	D	93	ASN	2.0
1	A	4	LYS	2.0
1	D	101	LYS	2.0
1	B	93	ASN	2.0

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CCS	C	166	10/11	0.97	0.14	12,12,16,18	0



## 6.3 Carbohydrates [i](#)

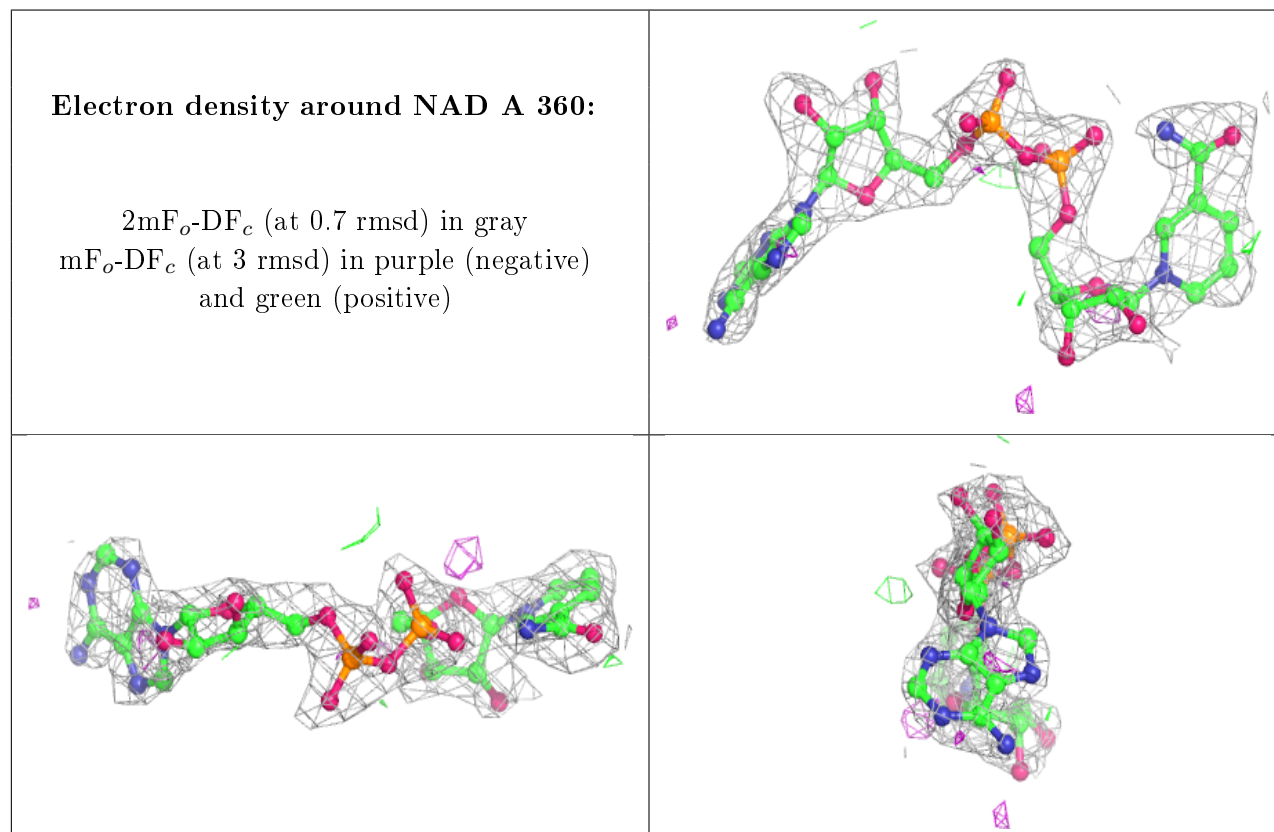
There are no carbohydrates in this entry.

## 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, 95<sup>th</sup> 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.

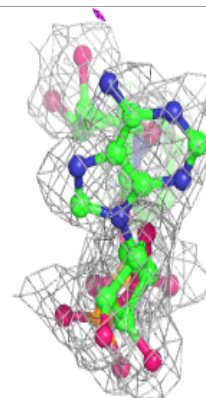
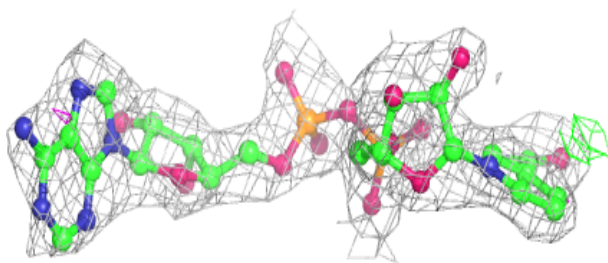
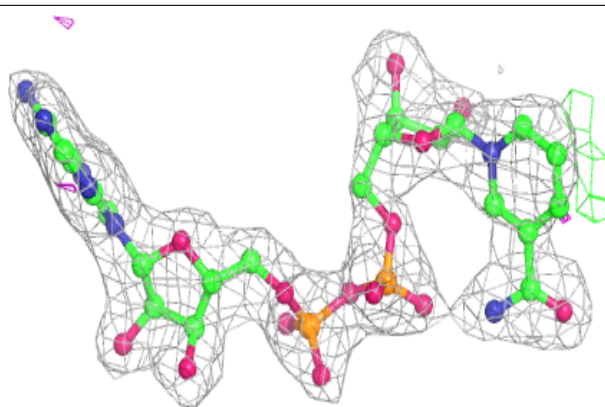
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	C	361	6/6	0.74	1.02	43,47,48,49	6
3	NAD	A	360	44/44	0.90	0.23	20,31,33,33	0
3	NAD	D	360	44/44	0.92	0.14	16,24,31,32	0
3	NAD	B	360	44/44	0.95	0.14	18,23,29,29	0
3	NAD	C	360	44/44	0.97	0.10	10,13,17,20	0

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.

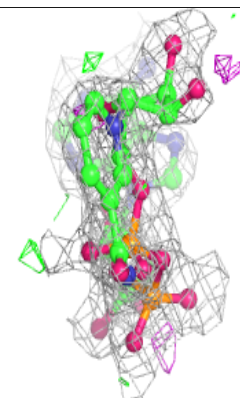
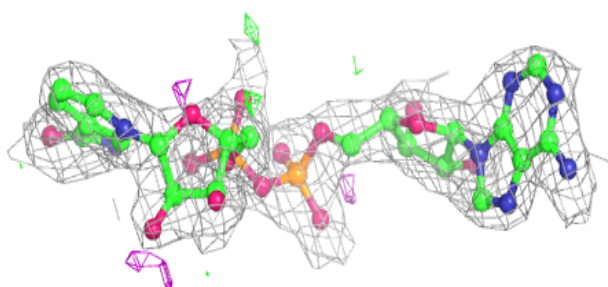
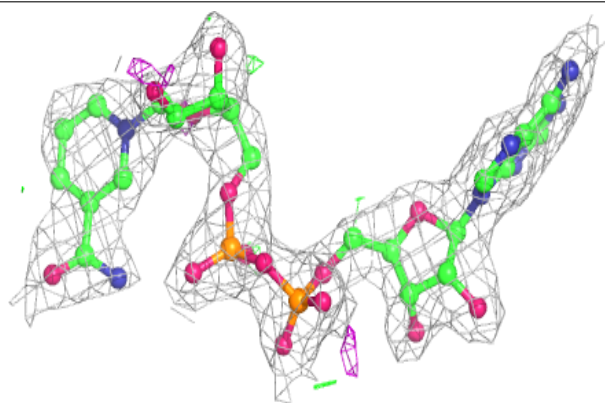


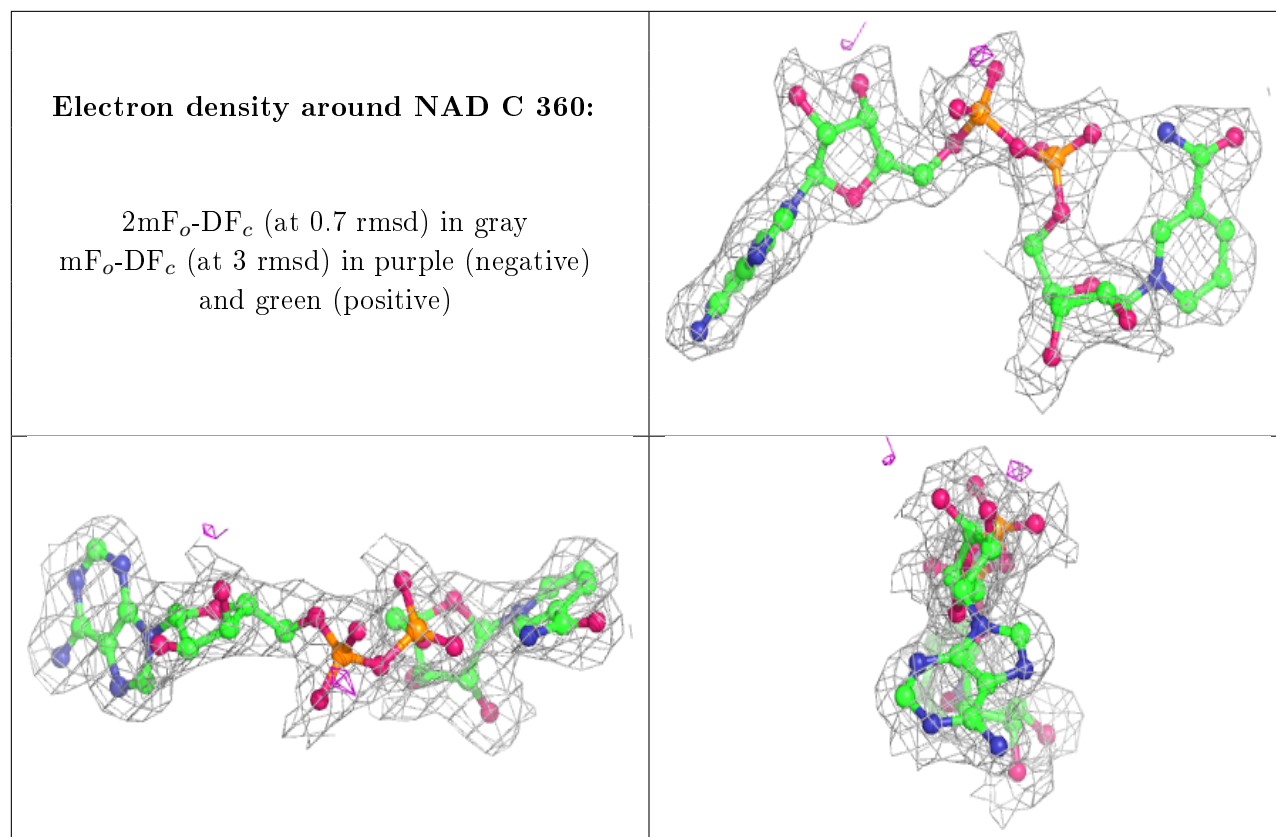
**Electron density around NAD D 360:**

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

**Electron density around NAD B 360:**

$2mF_o-DF_c$  (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.