



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:50 am BST

PDB ID : 3ZWM  
Title : Crystal structure of ADP ribosyl cyclase complexed with substrate NAD and product cADPR  
Authors : Kotaka, M.; Graeff, R.; Zhang, L.H.; Lee, H.C.; Hao, Q.  
Deposited on : 2011-08-02  
Resolution : 2.50 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

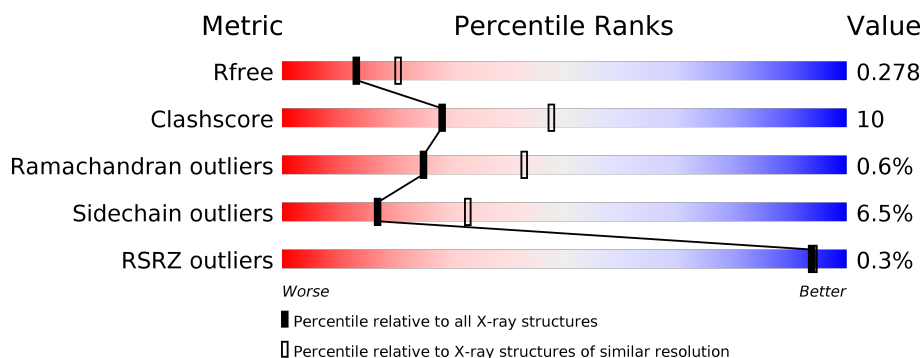
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	260	<div> <div>72%</div> <div>23%</div> <div>• •</div> </div>
1	B	260	<div> <div>75%</div> <div>18%</div> <div>• •</div> </div>
1	C	260	<div> <div>%</div> <div>78%</div> <div>18%</div> <div>• •</div> </div>
1	D	260	<div> <div>76%</div> <div>18%</div> <div>• •</div> </div>
1	E	260	<div> <div>73%</div> <div>23%</div> <div>• •</div> </div>
1	F	260	<div> <div>%</div> <div>73%</div> <div>20%</div> <div>5%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	260	
1	H	260	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CXR	F	303	X	-	X	-
3	CXR	H	303	X	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16762 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 ADP-RIBOSYL CYLCASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	1
			2018	1291	344	369	14			
1	B	252	Total	C	N	O	S	0	0	1
			2010	1285	343	368	14			
1	C	254	Total	C	N	O	S	0	0	1
			2023	1294	345	370	14			
1	D	251	Total	C	N	O	S	0	0	1
			2005	1282	342	367	14			
1	E	254	Total	C	N	O	S	0	0	1
			2023	1294	345	370	14			
1	F	254	Total	C	N	O	S	0	0	1
			2023	1294	345	370	14			
1	G	251	Total	C	N	O	S	0	0	1
			2008	1285	342	367	14			
1	H	254	Total	C	N	O	S	0	0	1
			2023	1294	345	370	14			

There are 16 discrepancies between the modelled and reference sequences:

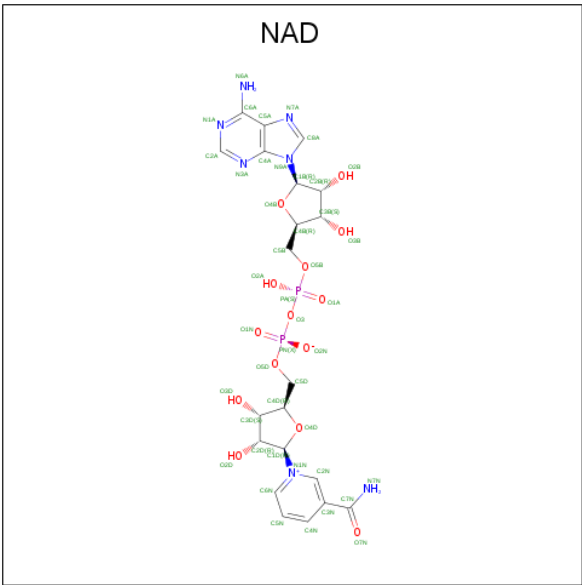
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP P29241
A	0	ALA	-	expression tag	UNP P29241
B	-1	ALA	-	expression tag	UNP P29241
B	0	ALA	-	expression tag	UNP P29241
C	-1	ALA	-	expression tag	UNP P29241
C	0	ALA	-	expression tag	UNP P29241
D	-1	ALA	-	expression tag	UNP P29241
D	0	ALA	-	expression tag	UNP P29241
E	-1	ALA	-	expression tag	UNP P29241
E	0	ALA	-	expression tag	UNP P29241
F	-1	ALA	-	expression tag	UNP P29241
F	0	ALA	-	expression tag	UNP P29241
G	-1	ALA	-	expression tag	UNP P29241

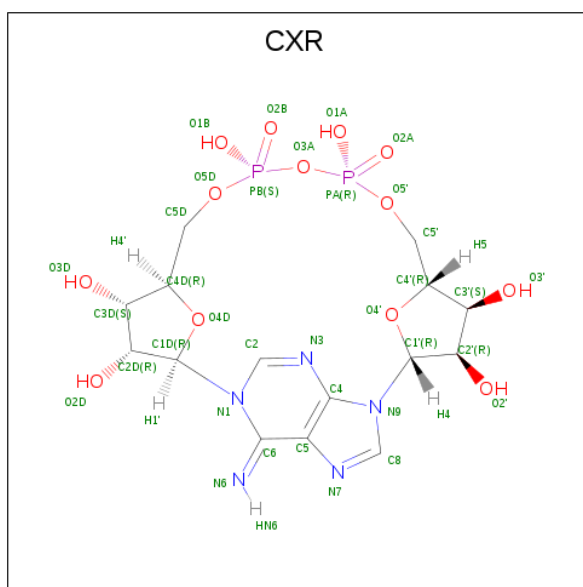
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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	ALA	-	expression tag	UNP P29241
H	-1	ALA	-	expression tag	UNP P29241
H	0	ALA	-	expression tag	UNP P29241

- Molecule 2 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	F	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	H	1	Total	C	N	O	P	0	0
			35	15	5	13	2		

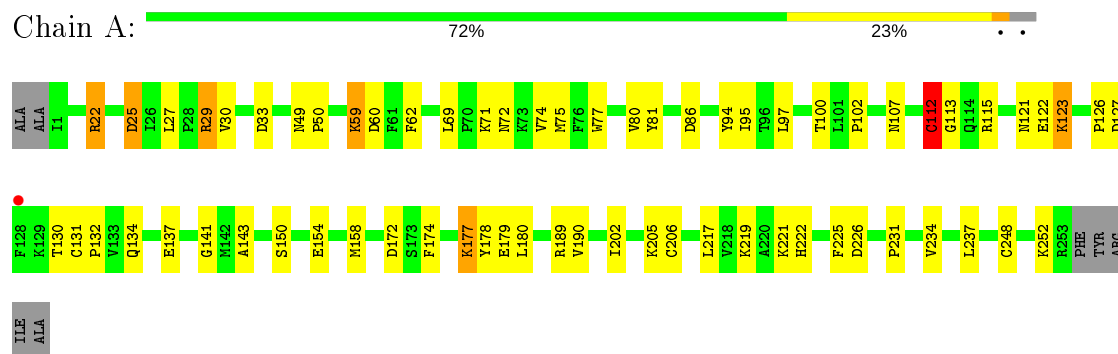
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total	O	0	0
			25	25		
4	B	52	Total	O	0	0
			52	52		
4	C	41	Total	O	0	0
			41	41		
4	D	52	Total	O	0	0
			52	52		
4	E	43	Total	O	0	0
			43	43		
4	F	18	Total	O	0	0
			18	18		
4	G	36	Total	O	0	0
			36	36		
4	H	28	Total	O	0	0
			28	28		

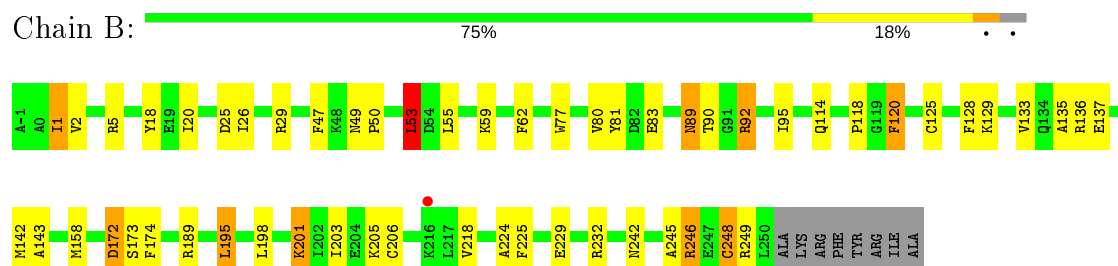
### 3 Residue-property plots

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.

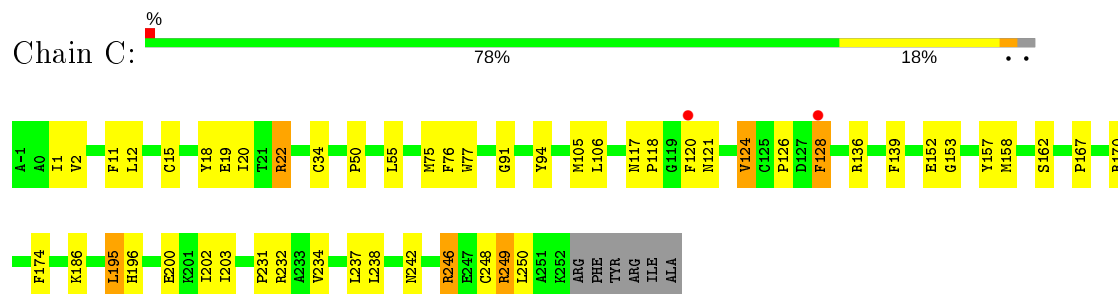
#### • Molecule 1: ADP-RIBOSYL CYLCASE



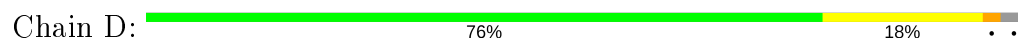
#### • Molecule 1: ADP-RIBOSYL CYLCASE

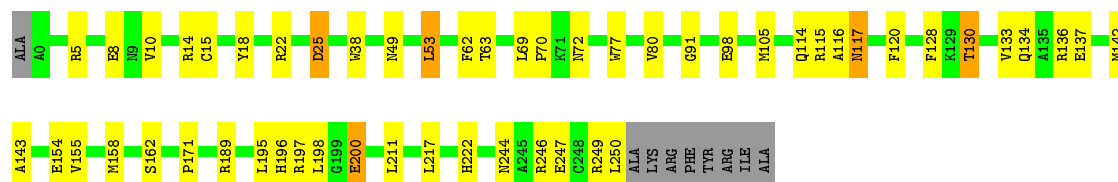


#### • Molecule 1: ADP-RIBOSYL CYLCASE

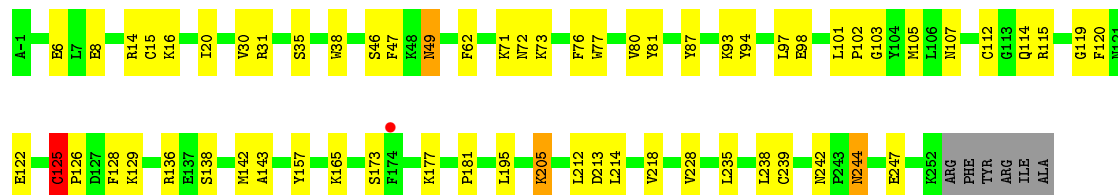


#### • Molecule 1: ADP-RIBOSYL CYLCASE

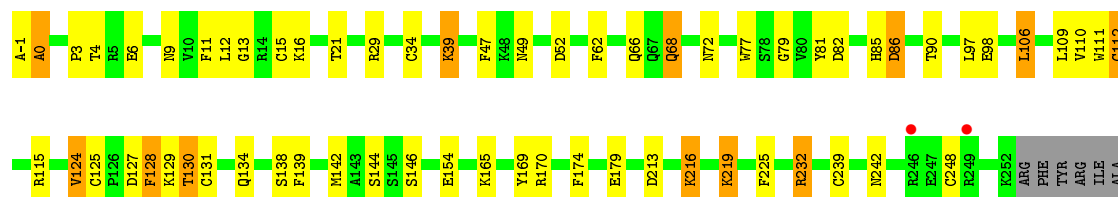




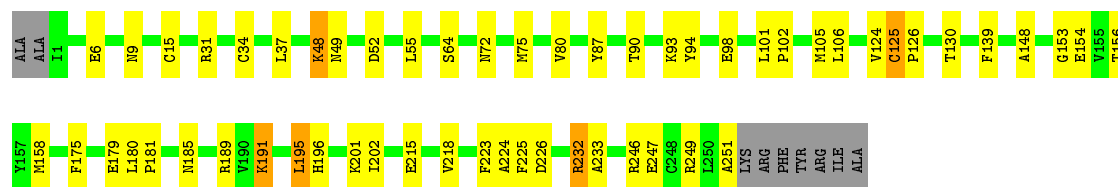
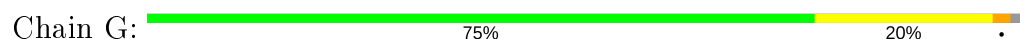
• Molecule 1: ADP-RIBOSYL CYLCASE



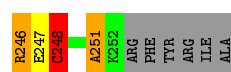
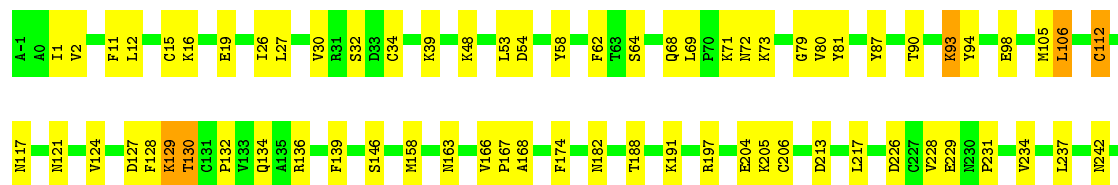
• Molecule 1: ADP-RIBOSYL CYLCASE



• Molecule 1: ADP-RIBOSYL CYLCASE



• Molecule 1: ADP-RIBOSYL CYLCASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.58Å 76.66Å 140.32Å 87.78° 89.19° 89.24°	Depositor
Resolution (Å)	30.00 – 2.50 28.04 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-2.50) 90.6 (28.04-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.215 , 0.285 0.208 , 0.278	Depositor DCC
$R_{free}$ test set	3953 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 16.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.118 for h,-k,-l 0.011 for -h,k,-l 0.009 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16762	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CXR, 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	0.78	2/2070 (0.1%)	0.84	3/2802 (0.1%)
1	B	0.85	1/2062 (0.0%)	0.87	2/2791 (0.1%)
1	C	0.82	1/2075 (0.0%)	0.80	1/2809 (0.0%)
1	D	0.85	0/2057	0.84	1/2784 (0.0%)
1	E	0.84	0/2075	0.87	1/2809 (0.0%)
1	F	0.68	0/2075	0.74	1/2809 (0.0%)
1	G	0.87	1/2060 (0.0%)	0.88	1/2788 (0.0%)
1	H	0.72	3/2075 (0.1%)	0.79	2/2809 (0.1%)
All	All	0.81	8/16549 (0.0%)	0.83	12/22401 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	112	CYS	CB-SG	-9.06	1.66	1.82
1	A	112	CYS	CB-SG	-7.56	1.69	1.82
1	B	248	CYS	CB-SG	-6.42	1.71	1.82
1	H	248	CYS	CB-SG	-5.88	1.72	1.81
1	A	206	CYS	CB-SG	5.78	1.92	1.82
1	G	34	CYS	CB-SG	5.15	1.91	1.82
1	C	200	GLU	CG-CD	5.13	1.59	1.51
1	H	251	ALA	C-N	-5.02	1.22	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	125	CYS	CA-CB-SG	-11.70	92.94	114.00
1	G	125	CYS	CA-CB-SG	-10.59	94.94	114.00
1	A	112	CYS	CB-CA-C	-7.87	94.67	110.40
1	B	53	LEU	CA-CB-CG	6.50	130.24	115.30
1	H	206	CYS	CA-CB-SG	-6.48	102.33	114.00
1	F	106	LEU	CA-CB-CG	-6.14	101.18	115.30
1	H	106	LEU	CA-CB-CG	-5.90	101.73	115.30
1	D	53	LEU	CA-CB-CG	5.54	128.05	115.30
1	A	112	CYS	CA-CB-SG	5.45	123.82	114.00
1	A	22	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	B	172	ASP	CB-CG-OD1	5.19	122.97	118.30
1	C	22	ARG	NE-CZ-NH2	-5.09	117.75	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	249	ARG	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2018	0	1970	35	0
1	B	2010	0	1962	39	0
1	C	2023	0	1978	34	0
1	D	2005	0	1957	39	0
1	E	2023	0	1978	41	0
1	F	2023	0	1980	41	0
1	G	2008	0	1963	38	0
1	H	2023	0	1980	43	0
2	A	44	0	26	5	0
2	B	44	0	26	3	0
2	C	44	0	26	2	0
2	D	44	0	26	5	0
2	E	44	0	26	10	0
2	G	44	0	26	1	0
3	F	35	0	18	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	35	0	18	11	0
4	A	25	0	0	1	0
4	B	52	0	0	6	0
4	C	41	0	0	2	0
4	D	52	0	0	4	0
4	E	43	0	0	0	0
4	F	18	0	0	2	0
4	G	36	0	0	1	0
4	H	28	0	0	1	0
All	All	16762	0	15960	317	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 10.

All (317) 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)
3:H:303:CXR:C2	3:H:303:CXR:H12	1.70	1.21
3:H:303:CXR:H3	3:H:303:CXR:C5D	1.86	1.06
1:A:174:PHE:CE2	2:A:301:NAD:H5N	2.02	0.95
1:G:191:LYS:HD2	1:G:226:ASP:OD2	1.65	0.94
1:F:77:TRP:O	3:F:303:CXR:H11	1.68	0.94
2:E:301:NAD:H6N	2:E:301:NAD:O5D	1.71	0.91
3:H:303:CXR:H3	3:H:303:CXR:H12	0.93	0.90
1:H:15:CYS:HG	1:H:34:CYS:HG	0.94	0.86
1:H:246:ARG:C	1:H:248:CYS:H	1.79	0.86
3:F:303:CXR:H3	3:F:303:CXR:O5D	1.77	0.84
1:F:213:ASP:O	1:F:216:LYS:HD3	1.77	0.83
1:A:127:ASP:O	1:A:130:THR:HG22	1.80	0.82
1:B:205:LYS:HG3	1:B:229:GLU:OE2	1.78	0.82
2:B:301:NAD:N6A	4:B:2035:HOH:O	2.12	0.81
1:B:205:LYS:CG	1:B:229:GLU:OE2	2.28	0.80
1:D:246:ARG:HB3	4:D:2051:HOH:O	1.81	0.80
1:E:98:GLU:OE2	2:E:301:NAD:N7N	2.14	0.80
1:C:195:LEU:HD11	1:C:238:LEU:HD21	1.62	0.80
1:E:173:SER:O	1:E:177:LYS:HG3	1.83	0.79
2:E:301:NAD:H6N	2:E:301:NAD:C5D	2.13	0.78
1:H:246:ARG:O	1:H:248:CYS:N	2.17	0.77
1:E:120:PHE:CE2	1:E:122:GLU:HG2	2.20	0.76
1:E:8:GLU:HG3	1:E:38:TRP:CE2	2.20	0.76
1:C:1:ILE:HG12	1:C:128:PHE:HE1	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:168:ALA:H	1:H:204:GLU:HG3	1.52	0.74
1:A:121:ASN:OD1	1:A:123:LYS:HG3	1.89	0.73
1:B:189:ARG:NH1	1:B:224:ALA:HB1	2.05	0.71
1:D:117:ASN:HD22	1:D:117:ASN:H	1.38	0.71
1:B:83:GLU:HG2	1:B:195:LEU:HD21	1.73	0.71
1:A:50:PRO:HG3	1:A:113:GLY:O	1.92	0.70
1:F:106:LEU:HD13	1:F:139:PHE:CZ	2.27	0.70
1:D:62:PHE:CZ	1:D:143:ALA:HB2	2.27	0.69
1:H:174:PHE:HE1	3:H:303:CXR:H9	1.58	0.69
1:B:29:ARG:N	1:B:29:ARG:HD2	2.06	0.69
1:F:174:PHE:HB2	3:F:303:CXR:O5D	1.93	0.69
1:E:97:LEU:HD23	2:E:301:NAD:H2N	1.75	0.69
1:D:128:PHE:HD2	1:D:136:ARG:HD3	1.59	0.68
1:H:246:ARG:C	1:H:248:CYS:N	2.47	0.68
1:B:80:VAL:HG21	1:B:158:MET:HG2	1.76	0.68
1:D:98:GLU:OE2	2:D:301:NAD:N7N	2.25	0.68
1:D:25:ASP:N	1:D:25:ASP:OD1	2.27	0.68
1:E:125:CYS:SG	1:E:126:PRO:HD2	2.35	0.67
1:C:34:CYS:HB2	4:C:2005:HOH:O	1.93	0.67
1:E:101:LEU:HB3	1:E:102:PRO:HD3	1.75	0.67
3:F:303:CXR:H3	3:F:303:CXR:C5D	2.24	0.66
1:H:174:PHE:CE1	3:H:303:CXR:H9	2.31	0.66
2:E:301:NAD:C6N	2:E:301:NAD:C5D	2.75	0.65
1:G:180:LEU:HB3	1:G:181:PRO:HD3	1.79	0.64
1:E:125:CYS:SG	1:E:126:PRO:CD	2.85	0.64
1:H:174:PHE:HD1	3:H:303:CXR:O1B	1.81	0.64
1:B:205:LYS:HG2	1:B:229:GLU:OE2	1.97	0.64
1:F:3:PRO:HA	1:F:110:VAL:HB	1.79	0.63
1:H:11:PHE:HD1	1:H:12:LEU:HD23	1.63	0.63
1:G:15:CYS:HB2	1:G:105:MET:SD	2.39	0.63
1:F:174:PHE:HE2	3:F:303:CXR:H10	1.46	0.63
1:D:130:THR:O	1:E:181:PRO:HB3	1.98	0.62
1:G:101:LEU:HG	1:G:105:MET:HE3	1.81	0.62
1:E:120:PHE:HE2	1:E:122:GLU:HG2	1.61	0.62
1:D:171:PRO:HG3	1:E:129:LYS:HD2	1.80	0.62
1:F:81:TYR:O	1:F:85:HIS:HD2	1.82	0.62
1:G:72:ASN:OD1	1:G:153:GLY:HA3	1.99	0.62
1:G:196:HIS:CG	1:G:202:ILE:HD12	2.34	0.62
1:F:219:LYS:HE2	1:F:225:PHE:HB3	1.83	0.61
1:G:101:LEU:HD11	1:G:105:MET:HE2	1.81	0.61
1:B:218:VAL:HG11	1:B:225:PHE:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:GLU:HG2	1:C:20:ILE:HD13	1.83	0.60
1:F:4:THR:HG21	1:F:109:LEU:HD22	1.81	0.60
1:A:174:PHE:CZ	2:A:301:NAD:H5N	2.37	0.60
1:B:201:LYS:O	4:B:2040:HOH:O	2.17	0.60
1:C:167:PRO:HD2	1:C:170:ARG:HD3	1.84	0.60
1:G:90:THR:HG22	1:G:90:THR:O	2.02	0.59
1:A:80:VAL:HG21	1:A:158:MET:HG2	1.83	0.59
1:D:133:VAL:HA	1:D:136:ARG:HG2	1.84	0.59
1:H:15:CYS:HG	1:H:34:CYS:CB	2.15	0.59
1:E:205:LYS:NZ	1:E:205:LYS:HB3	2.18	0.58
1:G:175:PHE:HA	1:G:179:GLU:HB2	1.85	0.58
1:A:27:LEU:O	1:A:29:ARG:NH1	2.37	0.58
1:C:196:HIS:CE1	1:C:202:ILE:HG23	2.38	0.58
1:C:1:ILE:HG12	1:C:128:PHE:CE1	2.37	0.58
1:A:49:ASN:OD1	1:A:115:ARG:HG3	2.03	0.58
1:A:72:ASN:HA	1:A:154:GLU:O	2.04	0.58
1:G:48:LYS:NZ	4:G:2009:HOH:O	2.37	0.58
3:H:303:CXR:C2	3:H:303:CXR:C5D	2.62	0.58
1:B:246:ARG:NH1	4:B:2051:HOH:O	2.37	0.57
1:C:246:ARG:O	1:C:249:ARG:HG3	2.04	0.57
1:A:69:LEU:HD12	1:A:150:SER:HB2	1.86	0.57
2:E:301:NAD:H3B	2:E:301:NAD:C8A	2.35	0.57
1:H:58:TYR:O	1:H:62:PHE:CD2	2.58	0.57
1:H:87:TYR:CE2	1:H:94:TYR:HE2	2.23	0.57
1:E:235:LEU:O	1:E:238:LEU:HB2	2.05	0.57
1:D:222:HIS:HD2	4:D:2045:HOH:O	1.88	0.56
1:A:59:LYS:HG2	1:A:60:ASP:N	2.19	0.56
1:B:53:LEU:HD12	1:B:135:ALA:HB1	1.87	0.56
1:A:27:LEU:HD11	1:A:95:ILE:HD11	1.88	0.56
1:A:177:LYS:HD2	1:A:178:TYR:CZ	2.41	0.56
1:D:114:GLN:NE2	1:D:116:ALA:O	2.30	0.56
1:H:127:ASP:O	1:H:128:PHE:C	2.44	0.56
1:F:62:PHE:O	1:F:66:GLN:HB2	2.06	0.56
1:E:98:GLU:H	1:E:98:GLU:CD	2.09	0.55
1:A:221:LYS:O	1:A:222:HIS:HB2	2.06	0.55
1:A:22:ARG:O	1:A:29:ARG:NH2	2.40	0.55
1:B:246:ARG:C	1:B:248:CYS:H	2.10	0.55
1:C:91:GLY:HA2	1:C:94:TYR:O	2.06	0.55
2:E:301:NAD:H52N	2:E:301:NAD:C6N	2.36	0.55
1:E:77:TRP:O	2:E:301:NAD:H51N	2.07	0.55
1:G:87:TYR:OH	1:G:93:LYS:HE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:VAL:HG13	1:G:223:PHE:HB2	1.89	0.55
1:B:92:ARG:NH1	4:B:2026:HOH:O	2.39	0.55
1:C:50:PRO:HB2	1:C:126:PRO:HG3	1.89	0.55
1:H:121:ASN:HD21	1:H:124:VAL:HG12	1.72	0.54
1:A:25:ASP:N	1:A:25:ASP:OD1	2.34	0.54
1:G:87:TYR:CZ	1:G:93:LYS:HE2	2.42	0.54
2:D:301:NAD:H52A	2:D:301:NAD:PN	2.47	0.54
1:E:77:TRP:CH2	1:E:81:TYR:HD2	2.26	0.54
1:F:72:ASN:HA	1:F:154:GLU:O	2.08	0.54
1:F:111:TRP:C	1:F:112:CYS:SG	2.86	0.54
1:D:15:CYS:HB2	1:D:105:MET:SD	2.48	0.53
1:H:87:TYR:CZ	1:H:93:LYS:HE2	2.44	0.53
1:B:189:ARG:NH1	1:B:224:ALA:CB	2.72	0.53
1:H:1:ILE:HG13	1:H:2:VAL:N	2.24	0.53
1:F:124:VAL:O	1:F:125:CYS:SG	2.67	0.53
1:F:179:GLU:OE1	3:F:303:CXR:H4'	2.09	0.53
1:C:196:HIS:NE2	1:C:202:ILE:HG23	2.24	0.53
1:D:8:GLU:HG3	1:D:38:TRP:CE2	2.44	0.53
1:C:121:ASN:ND2	1:C:124:VAL:O	2.42	0.53
1:F:106:LEU:HD23	1:F:109:LEU:HD12	1.91	0.53
1:C:15:CYS:HB2	1:C:105:MET:SD	2.50	0.52
1:H:121:ASN:ND2	1:H:124:VAL:HG12	2.25	0.52
1:C:250:LEU:HD22	1:D:250:LEU:N	2.24	0.52
1:B:55:LEU:O	1:B:142:MET:HG3	2.09	0.52
1:A:174:PHE:CG	2:A:301:NAD:H6N	2.45	0.52
1:F:165:LYS:HE3	1:G:202:ILE:HD11	1.91	0.52
1:E:128:PHE:O	1:E:136:ARG:HD2	2.10	0.51
1:F:138:SER:O	4:F:2008:HOH:O	2.19	0.51
1:D:117:ASN:HD22	1:D:117:ASN:N	2.06	0.51
1:F:128:PHE:O	1:F:130:THR:N	2.44	0.51
1:B:62:PHE:CZ	1:B:143:ALA:HB2	2.46	0.51
1:G:72:ASN:HA	1:G:154:GLU:O	2.11	0.51
1:E:6:GLU:OE1	1:F:16:LYS:HE2	2.10	0.50
1:F:134:GLN:OE1	1:F:134:GLN:N	2.35	0.50
1:A:137:GLU:O	1:A:141:GLY:HA3	2.10	0.50
1:C:76:PHE:O	1:C:157:TYR:HA	2.12	0.50
1:D:77:TRP:CE2	2:D:301:NAD:H3D	2.46	0.50
1:E:46:SER:HA	1:E:119:GLY:O	2.11	0.50
1:F:79:GLY:N	3:F:303:CXR:O2A	2.34	0.50
1:B:245:ALA:O	1:B:248:CYS:HB3	2.12	0.50
1:F:15:CYS:HB3	1:F:34:CYS:SG	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:TRP:CE2	2:C:301:NAD:H3D	2.47	0.49
1:G:93:LYS:HG2	1:G:94:TYR:CD2	2.46	0.49
1:H:58:TYR:O	1:H:62:PHE:HD2	1.94	0.49
1:B:25:ASP:OD1	1:B:25:ASP:N	2.44	0.49
1:H:106:LEU:HD13	1:H:139:PHE:CZ	2.48	0.49
1:B:128:PHE:HB2	1:B:136:ARG:HB2	1.93	0.49
1:F:-1:ALA:O	1:F:0:ALA:HB2	2.12	0.49
1:F:142:MET:HB2	4:F:2008:HOH:O	2.11	0.49
1:H:205:LYS:HE3	1:H:229:GLU:OE1	2.13	0.49
1:G:37:LEU:HD13	1:G:105:MET:HE1	1.94	0.49
1:B:133:VAL:HA	1:B:136:ARG:HG2	1.95	0.48
1:E:49:ASN:ND2	1:E:115:ARG:HE	2.11	0.48
1:C:174:PHE:CE2	2:C:301:NAD:H5N	2.48	0.48
1:F:174:PHE:HE2	3:F:303:CXR:O2'	1.95	0.48
1:C:11:PHE:HD2	1:C:12:LEU:HD23	1.78	0.48
1:E:103:GLY:O	1:E:107:ASN:HB2	2.13	0.48
1:A:131:CYS:HB3	1:A:132:PRO:HD2	1.95	0.48
1:H:242:ASN:ND2	4:H:2025:HOH:O	2.43	0.48
1:H:98:GLU:CD	1:H:98:GLU:H	2.16	0.48
1:B:49:ASN:HB3	1:B:50:PRO:HD2	1.95	0.48
1:H:80:VAL:HG21	1:H:158:MET:HG2	1.96	0.48
1:H:79:GLY:N	3:H:303:CXR:O2A	2.44	0.48
1:F:68:GLN:HG2	1:F:68:GLN:H	1.52	0.47
1:H:128:PHE:HB2	1:H:129:LYS:HD3	1.96	0.47
1:A:231:PRO:HD2	1:A:234:VAL:HB	1.96	0.47
1:E:235:LEU:CD2	1:E:239:CYS:SG	3.02	0.47
3:F:303:CXR:C5D	3:F:303:CXR:C2	2.90	0.47
1:C:196:HIS:CE1	1:C:202:ILE:CG2	2.98	0.47
1:B:18:TYR:O	1:B:29:ARG:NH2	2.48	0.47
1:F:47:PHE:HA	1:F:115:ARG:HA	1.96	0.47
1:D:72:ASN:HA	1:D:154:GLU:O	2.15	0.47
1:C:153:GLY:N	1:C:186:LYS:O	2.44	0.46
1:H:191:LYS:HG2	1:H:226:ASP:OD2	2.15	0.46
1:C:246:ARG:NH1	4:C:2041:HOH:O	2.48	0.46
1:G:125:CYS:SG	1:G:126:PRO:HD2	2.56	0.46
1:C:75:MET:HG2	1:C:76:PHE:N	2.31	0.46
1:D:246:ARG:HE	1:D:249:ARG:NH2	2.13	0.46
2:E:301:NAD:C8A	2:E:301:NAD:C3B	2.91	0.46
1:G:196:HIS:NE2	1:G:202:ILE:HG23	2.31	0.46
1:E:214:LEU:O	1:E:218:VAL:HG23	2.16	0.46
1:E:238:LEU:HA	1:E:238:LEU:HD23	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:301:NAD:H3B	2:E:301:NAD:H8A	1.98	0.46
1:E:16:LYS:HG2	1:F:9:ASN:HB3	1.97	0.46
3:F:303:CXR:H12	3:F:303:CXR:C2	2.45	0.46
1:G:125:CYS:SG	1:G:126:PRO:CD	3.04	0.46
1:C:248:CYS:O	1:C:249:ARG:HG2	2.16	0.46
2:D:301:NAD:H52A	2:D:301:NAD:O5D	2.16	0.46
1:C:117:ASN:HA	1:C:118:PRO:HA	1.58	0.45
1:D:198:LEU:HD22	1:D:247:GLU:HG2	1.98	0.45
1:G:6:GLU:O	1:G:9:ASN:HB2	2.16	0.45
1:D:197:ARG:HB2	1:D:200:GLU:HG3	1.98	0.45
1:H:71:LYS:O	1:H:73:LYS:HG2	2.17	0.45
1:G:215:GLU:HG3	1:G:225:PHE:CD2	2.52	0.45
1:G:75:MET:HA	1:G:156:THR:O	2.17	0.45
1:E:87:TYR:CE2	1:E:94:TYR:HE2	2.35	0.45
1:F:49:ASN:HB2	1:F:52:ASP:HB2	1.99	0.45
1:B:62:PHE:CE1	1:B:143:ALA:HA	2.51	0.45
1:H:48:LYS:HB2	1:H:48:LYS:HE2	1.76	0.45
1:B:77:TRP:CH2	1:B:81:TYR:HD2	2.34	0.44
1:A:100:THR:OG1	1:A:102:PRO:HD2	2.17	0.44
1:F:98:GLU:OE1	1:F:98:GLU:N	2.50	0.44
1:B:20:ILE:HG22	1:B:20:ILE:O	2.18	0.44
1:B:245:ALA:O	1:B:248:CYS:CB	2.65	0.44
1:H:127:ASP:OD1	1:H:130:THR:OG1	2.33	0.44
1:B:26:ILE:HG22	1:B:95:ILE:HD11	2.00	0.44
1:D:49:ASN:OD1	1:D:115:ARG:HG3	2.17	0.44
1:D:80:VAL:HG21	1:D:158:MET:HG2	1.98	0.44
1:H:16:LYS:NZ	1:H:19:GLU:OE2	2.47	0.44
1:G:189:ARG:HA	1:G:224:ALA:O	2.17	0.44
1:A:190:VAL:O	1:A:225:PHE:HA	2.17	0.44
1:C:18:TYR:HA	1:C:22:ARG:CG	2.47	0.44
2:B:301:NAD:H5N	4:B:2052:HOH:O	2.18	0.44
1:C:231:PRO:HD2	1:C:234:VAL:HB	1.98	0.44
1:G:124:VAL:O	1:G:125:CYS:SG	2.76	0.44
1:E:214:LEU:O	1:E:214:LEU:HG	2.17	0.44
1:F:82:ASP:O	1:F:86:ASP:HB2	2.18	0.43
1:D:155:VAL:HG22	1:D:189:ARG:O	2.17	0.43
1:G:49:ASN:HB3	1:G:52:ASP:HB2	2.00	0.43
1:B:89:ASN:HD22	1:B:89:ASN:C	2.21	0.43
1:D:217:LEU:HD21	1:E:129:LYS:HE2	1.99	0.43
1:A:74:VAL:HA	1:A:95:ILE:HG22	2.01	0.43
1:B:118:PRO:HG2	1:B:120:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:LEU:HG	1:C:139:PHE:CZ	2.54	0.43
1:E:30:VAL:HG22	1:E:31:ARG:N	2.34	0.43
1:E:62:PHE:CZ	1:E:143:ALA:HB2	2.53	0.43
1:H:174:PHE:HE1	3:H:303:CXR:C2'	2.30	0.43
1:F:12:LEU:O	1:F:13:GLY:C	2.56	0.43
1:B:198:LEU:HD13	1:B:245:ALA:CB	2.49	0.43
1:C:128:PHE:CD1	1:C:128:PHE:N	2.85	0.43
1:C:232:ARG:HH22	1:D:244:ASN:CG	2.21	0.43
1:E:14:ARG:HH21	1:F:21:THR:CB	2.32	0.43
1:E:76:PHE:O	1:E:157:TYR:HA	2.20	0.42
1:A:75:MET:HE3	1:A:94:TYR:HB2	2.01	0.42
1:H:213:ASP:O	1:H:217:LEU:HG	2.18	0.42
1:E:73:LYS:HD3	1:E:93:LYS:O	2.19	0.42
1:G:249:ARG:HG2	1:H:251:ALA:HB3	2.02	0.42
1:B:136:ARG:HG3	1:B:137:GLU:HG3	2.01	0.42
1:B:47:PHE:HA	1:B:114:GLN:O	2.19	0.42
1:F:39:LYS:HD3	1:F:39:LYS:HA	1.70	0.42
1:G:101:LEU:N	1:G:102:PRO:HD2	2.33	0.42
1:A:62:PHE:CZ	1:A:143:ALA:HB2	2.55	0.42
1:G:232:ARG:O	1:G:233:ALA:C	2.57	0.42
1:A:71:LYS:HG2	1:A:72:ASN:ND2	2.34	0.42
1:B:174:PHE:HZ	4:B:2034:HOH:O	2.02	0.42
1:D:211:LEU:HD23	1:D:211:LEU:HA	1.82	0.42
1:E:212:LEU:O	1:E:213:ASP:C	2.56	0.42
1:E:47:PHE:HA	1:E:114:GLN:O	2.19	0.42
1:D:222:HIS:CD2	4:D:2045:HOH:O	2.69	0.42
1:D:198:LEU:HD22	1:D:247:GLU:CG	2.50	0.42
1:H:174:PHE:CD1	3:H:303:CXR:O1B	2.66	0.42
1:A:179:GLU:O	1:A:180:LEU:C	2.58	0.42
1:B:128:PHE:CE2	1:B:129:LYS:HG3	2.55	0.42
1:C:162:SER:HA	1:C:203:ILE:HG12	2.01	0.42
1:D:18:TYR:HA	1:D:22:ARG:CG	2.50	0.42
1:E:81:TYR:CD1	1:E:81:TYR:C	2.93	0.42
1:G:158:MET:SD	1:G:195:LEU:HD12	2.60	0.42
1:D:91:GLY:N	4:D:2030:HOH:O	2.50	0.41
1:F:12:LEU:O	1:F:15:CYS:N	2.53	0.41
1:B:1:ILE:HB	1:B:125:CYS:O	2.20	0.41
1:A:154:GLU:OE2	1:A:189:ARG:HD2	2.20	0.41
1:H:166:VAL:HA	1:H:167:PRO:HD2	1.87	0.41
1:E:71:LYS:HG2	1:E:72:ASN:ND2	2.35	0.41
1:E:8:GLU:HG3	1:E:38:TRP:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:106:LEU:HG	1:G:139:PHE:CZ	2.55	0.41
1:H:197:ARG:NH1	1:H:197:ARG:HG2	2.34	0.41
1:H:174:PHE:HZ	3:H:303:CXR:H10	1.67	0.41
1:B:173:SER:HB2	2:B:301:NAD:O1N	2.20	0.41
1:C:250:LEU:HB3	1:D:249:ARG:O	2.20	0.41
2:D:301:NAD:N3A	2:D:301:NAD:H51A	2.35	0.41
1:F:144:SER:HB3	1:F:179:GLU:HG2	2.01	0.41
1:H:231:PRO:HD2	1:H:234:VAL:HB	2.02	0.41
1:B:218:VAL:HG21	1:B:225:PHE:HD2	1.84	0.41
1:D:69:LEU:HA	1:D:70:PRO:HD3	1.90	0.41
1:G:98:GLU:OE2	2:G:301:NAD:H2N	2.20	0.41
1:A:174:PHE:CD2	2:A:301:NAD:H6N	2.56	0.41
1:A:80:VAL:O	1:A:81:TYR:C	2.58	0.41
1:C:55:LEU:HA	1:C:55:LEU:HD12	1.69	0.41
1:A:122:GLU:HG3	4:A:2014:HOH:O	2.19	0.41
1:A:77:TRP:CZ3	2:A:301:NAD:H52A	2.56	0.41
1:D:133:VAL:HG13	1:D:134:GLN:N	2.36	0.41
1:G:148:ALA:CB	1:G:179:GLU:HA	2.51	0.41
1:H:105:MET:C	1:H:106:LEU:HG	2.41	0.41
1:H:1:ILE:HG13	1:H:2:VAL:H	1.85	0.41
1:H:228:VAL:HG13	1:H:231:PRO:HG3	2.03	0.41
1:A:112:CYS:SG	1:A:126:PRO:HD2	2.61	0.41
1:E:15:CYS:HB2	1:E:105:MET:SD	2.61	0.41
1:E:20:ILE:CD1	1:F:6:GLU:HB2	2.51	0.41
1:F:11:PHE:C	1:F:11:PHE:CD1	2.94	0.41
1:G:55:LEU:H	1:G:55:LEU:HG	1.74	0.41
1:G:251:ALA:N	1:H:251:ALA:HB2	2.36	0.41
1:B:120:PHE:N	1:B:120:PHE:CD1	2.89	0.40
1:G:189:ARG:HB2	1:G:224:ALA:HB3	2.02	0.40
1:C:77:TRP:HA	1:C:158:MET:O	2.20	0.40
1:D:62:PHE:O	1:D:63:THR:C	2.59	0.40
1:E:247:GLU:OE1	1:E:247:GLU:N	2.32	0.40
1:F:106:LEU:HD13	1:F:139:PHE:HZ	1.82	0.40
1:F:232:ARG:HE	1:F:232:ARG:HB2	1.59	0.40
1:A:49:ASN:HA	1:A:50:PRO:HD3	1.89	0.40
1:D:136:ARG:HG3	1:D:137:GLU:HG3	2.03	0.40
1:A:202:ILE:HG21	1:A:205:LYS:HE3	2.03	0.40
1:D:18:TYR:HA	1:D:22:ARG:HB2	2.03	0.40
1:F:169:TYR:CG	1:F:170:ARG:N	2.89	0.40
1:H:71:LYS:O	1:H:72:ASN:HB2	2.21	0.40
1:B:205:LYS:HG2	1:B:206:CYS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:TYR:HA	1:C:22:ARG:HG2	2.03	0.40
1:D:120:PHE:N	1:D:120:PHE:CD1	2.90	0.40
1:D:10:VAL:O	1:D:14:ARG:HG3	2.22	0.40
1:D:162:SER:OG	1:D:196:HIS:HA	2.22	0.40
1:G:201:LYS:HG3	1:G:202:ILE:N	2.37	0.40
1:G:93:LYS:HG2	1:G:94:TYR:CE2	2.57	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	251/260 (96%)	230 (92%)	20 (8%)	1 (0%)	34	54
1	B	250/260 (96%)	235 (94%)	15 (6%)	0	100	100
1	C	252/260 (97%)	230 (91%)	22 (9%)	0	100	100
1	D	249/260 (96%)	239 (96%)	10 (4%)	0	100	100
1	E	252/260 (97%)	238 (94%)	12 (5%)	2 (1%)	19	35
1	F	252/260 (97%)	226 (90%)	22 (9%)	4 (2%)	9	17
1	G	249/260 (96%)	232 (93%)	15 (6%)	2 (1%)	19	35
1	H	252/260 (97%)	229 (91%)	19 (8%)	4 (2%)	9	17
All	All	2007/2080 (96%)	1859 (93%)	135 (7%)	13 (1%)	25	43

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	LYS
1	F	128	PHE
1	H	247	GLU
1	F	0	ALA

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Mol	Chain	Res	Type
1	F	129	LYS
1	H	132	PRO
1	F	127	ASP
1	G	247	GLU
1	E	244	ASN
1	H	81	TYR
1	G	80	VAL
1	H	117	ASN
1	E	80	VAL

### 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	220/226 (97%)	202 (92%)	18 (8%)	11	22
1	B	219/226 (97%)	202 (92%)	17 (8%)	12	24
1	C	220/226 (97%)	210 (96%)	10 (4%)	27	51
1	D	219/226 (97%)	211 (96%)	8 (4%)	34	60
1	E	220/226 (97%)	208 (94%)	12 (6%)	21	41
1	F	220/226 (97%)	203 (92%)	17 (8%)	13	25
1	G	220/226 (97%)	211 (96%)	9 (4%)	30	55
1	H	220/226 (97%)	196 (89%)	24 (11%)	6	12
All	All	1758/1808 (97%)	1643 (94%)	115 (6%)	17	33

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASP
1	A	29	ARG
1	A	30	VAL
1	A	33	ASP
1	A	59	LYS
1	A	86	ASP

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Mol	Chain	Res	Type
1	A	97	LEU
1	A	107	ASN
1	A	112	CYS
1	A	123	LYS
1	A	134	GLN
1	A	172	ASP
1	A	177	LYS
1	A	217	LEU
1	A	219	LYS
1	A	226	ASP
1	A	237	LEU
1	A	248	CYS
1	B	1	ILE
1	B	2	VAL
1	B	5	ARG
1	B	53	LEU
1	B	59	LYS
1	B	89	ASN
1	B	90	THR
1	B	92	ARG
1	B	120	PHE
1	B	172	ASP
1	B	195	LEU
1	B	201	LYS
1	B	203	ILE
1	B	232	ARG
1	B	242	ASN
1	B	246	ARG
1	B	249	ARG
1	C	2	VAL
1	C	120	PHE
1	C	124	VAL
1	C	128	PHE
1	C	136	ARG
1	C	152	GLU
1	C	195	LEU
1	C	237	LEU
1	C	242	ASN
1	C	246	ARG
1	D	5	ARG
1	D	25	ASP
1	D	53	LEU

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Mol	Chain	Res	Type
1	D	117	ASN
1	D	130	THR
1	D	142	MET
1	D	195	LEU
1	D	200	GLU
1	E	35	SER
1	E	49	ASN
1	E	112	CYS
1	E	125	CYS
1	E	138	SER
1	E	142	MET
1	E	165	LYS
1	E	195	LEU
1	E	205	LYS
1	E	228	VAL
1	E	242	ASN
1	E	244	ASN
1	F	29	ARG
1	F	39	LYS
1	F	68	GLN
1	F	86	ASP
1	F	90	THR
1	F	97	LEU
1	F	112	CYS
1	F	124	VAL
1	F	130	THR
1	F	131	CYS
1	F	146	SER
1	F	216	LYS
1	F	219	LYS
1	F	232	ARG
1	F	239	CYS
1	F	242	ASN
1	F	248	CYS
1	G	31	ARG
1	G	48	LYS
1	G	64	SER
1	G	130	THR
1	G	185	ASN
1	G	191	LYS
1	G	195	LEU
1	G	232	ARG

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Mol	Chain	Res	Type
1	G	246	ARG
1	H	26	ILE
1	H	27	LEU
1	H	30	VAL
1	H	32	SER
1	H	39	LYS
1	H	53	LEU
1	H	54	ASP
1	H	64	SER
1	H	68	GLN
1	H	69	LEU
1	H	90	THR
1	H	93	LYS
1	H	112	CYS
1	H	129	LYS
1	H	130	THR
1	H	134	GLN
1	H	136	ARG
1	H	146	SER
1	H	163	ASN
1	H	182	ASN
1	H	188	THR
1	H	237	LEU
1	H	246	ARG
1	H	248	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	107	ASN
1	B	89	ASN
1	B	242	ASN
1	C	242	ASN
1	D	89	ASN
1	D	117	ASN
1	D	196	HIS
1	E	49	ASN
1	E	242	ASN
1	F	85	HIS
1	F	242	ASN
1	G	89	ASN

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Mol	Chain	Res	Type
1	G	185	ASN
1	G	242	ASN
1	H	117	ASN
1	H	163	ASN
1	H	196	HIS
1	H	242	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAD	B	301	-	42,48,48	1.93	4 (9%)	50,73,73	1.69	9 (18%)
2	NAD	D	301	-	42,48,48	1.83	4 (9%)	50,73,73	1.55	7 (14%)
3	CXR	H	303	-	30,39,39	1.64	3 (10%)	37,62,62	1.66	5 (13%)
2	NAD	C	301	-	42,48,48	1.88	5 (11%)	50,73,73	1.66	8 (16%)
3	CXR	F	303	-	30,39,39	1.57	4 (13%)	37,62,62	1.46	5 (13%)
2	NAD	E	301	-	42,48,48	2.03	6 (14%)	50,73,73	1.98	12 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	G	301	-	42,48,48	2.01	7 (16%)	50,73,73	1.72	10 (20%)
2	NAD	A	301	-	42,48,48	2.00	5 (11%)	50,73,73	1.63	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	B	301	-	-	12/26/62/62	0/5/5/5
2	NAD	D	301	-	-	11/26/62/62	0/5/5/5
3	CXR	H	303	-	1/1/10/10	6/20/58/58	0/3/5/5
2	NAD	C	301	-	-	8/26/62/62	0/5/5/5
3	CXR	F	303	-	1/1/10/10	6/20/58/58	0/3/5/5
2	NAD	E	301	-	-	5/26/62/62	0/5/5/5
2	NAD	G	301	-	-	5/26/62/62	0/5/5/5
2	NAD	A	301	-	-	4/26/62/62	0/5/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAD	O7N-C7N	9.86	1.43	1.24
2	E	301	NAD	O7N-C7N	9.49	1.42	1.24
2	B	301	NAD	O7N-C7N	9.41	1.42	1.24
2	D	301	NAD	O7N-C7N	9.29	1.41	1.24
2	G	301	NAD	O7N-C7N	9.24	1.41	1.24
2	C	301	NAD	O7N-C7N	8.83	1.41	1.24
3	H	303	CXR	O4'-C1'	6.01	1.49	1.41
3	F	303	CXR	O4'-C1'	4.85	1.47	1.41
2	E	301	NAD	C2A-N3A	4.74	1.39	1.32
2	A	301	NAD	C2A-N3A	4.69	1.39	1.32
2	B	301	NAD	C2A-N3A	4.67	1.39	1.32
2	G	301	NAD	C2A-N3A	4.55	1.39	1.32
2	C	301	NAD	C2A-N3A	4.52	1.39	1.32
2	D	301	NAD	C2A-N3A	4.37	1.39	1.32
3	F	303	CXR	O4D-C1D	4.35	1.47	1.41
3	H	303	CXR	C2-N1	3.62	1.43	1.35
2	E	301	NAD	C2N-N1N	3.60	1.39	1.35
2	C	301	NAD	C2N-N1N	3.60	1.39	1.35
2	G	301	NAD	C2N-N1N	3.38	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	303	CXR	C2-N1	3.31	1.42	1.35
2	B	301	NAD	C2N-N1N	3.30	1.39	1.35
2	A	301	NAD	C2N-N1N	3.12	1.38	1.35
2	A	301	NAD	C2A-N1A	2.96	1.39	1.33
2	E	301	NAD	C2A-N1A	2.92	1.39	1.33
2	G	301	NAD	C2A-N1A	2.90	1.39	1.33
2	E	301	NAD	C2N-C3N	2.81	1.43	1.39
2	B	301	NAD	C2A-N1A	2.74	1.39	1.33
2	D	301	NAD	C2A-N1A	2.70	1.38	1.33
2	C	301	NAD	C2A-N1A	2.70	1.38	1.33
2	D	301	NAD	C2N-N1N	2.52	1.38	1.35
2	G	301	NAD	C2N-C3N	2.49	1.42	1.39
3	H	303	CXR	O4D-C1D	2.48	1.44	1.41
2	A	301	NAD	C2N-C3N	2.46	1.42	1.39
2	C	301	NAD	C2N-C3N	2.45	1.42	1.39
2	G	301	NAD	O4D-C1D	2.44	1.44	1.41
2	E	301	NAD	O4D-C1D	2.32	1.44	1.41
2	G	301	NAD	O4B-C1B	2.23	1.44	1.41
3	F	303	CXR	C2D-C1D	2.04	1.56	1.53

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAD	N3A-C2A-N1A	-6.13	119.10	128.68
2	G	301	NAD	N3A-C2A-N1A	-6.01	119.29	128.68
2	E	301	NAD	N3A-C2A-N1A	-6.00	119.30	128.68
2	A	301	NAD	N3A-C2A-N1A	-5.98	119.33	128.68
2	C	301	NAD	N3A-C2A-N1A	-5.98	119.34	128.68
2	B	301	NAD	N3A-C2A-N1A	-5.69	119.79	128.68
2	E	301	NAD	C6N-N1N-C2N	-5.61	116.86	121.97
2	C	301	NAD	C6N-N1N-C2N	-5.09	117.33	121.97
3	H	303	CXR	O4D-C1D-C2D	-5.07	99.52	106.93
3	H	303	CXR	PA-O3A-PB	-4.58	117.11	132.83
2	B	301	NAD	C6N-N1N-C2N	-4.50	117.87	121.97
2	G	301	NAD	C6N-N1N-C2N	-4.34	118.02	121.97
2	E	301	NAD	C3D-C2D-C1D	3.99	106.99	100.98
2	E	301	NAD	O4B-C1B-C2B	-3.94	101.17	106.93
2	B	301	NAD	C3D-C2D-C1D	3.92	106.88	100.98
2	E	301	NAD	O4D-C1D-C2D	-3.91	101.21	106.93
3	F	303	CXR	O4D-C1D-C2D	-3.89	101.23	106.93
2	G	301	NAD	O5B-C5B-C4B	3.74	121.86	108.99
3	F	303	CXR	C3D-C2D-C1D	3.54	106.31	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	303	CXR	C2-N3-C4	3.54	121.00	116.58
2	A	301	NAD	C2N-N1N-C1D	3.51	126.95	119.14
2	G	301	NAD	C2N-N1N-C1D	3.50	126.93	119.14
2	C	301	NAD	C2N-N1N-C1D	3.48	126.89	119.14
2	A	301	NAD	C6N-N1N-C2N	-3.45	118.83	121.97
3	H	303	CXR	C5D-C4D-C3D	-3.41	102.38	115.18
3	F	303	CXR	C2-N3-C4	3.32	120.73	116.58
2	C	301	NAD	C3D-C2D-C1D	3.29	105.94	100.98
3	F	303	CXR	PA-O3A-PB	-3.26	121.63	132.83
2	G	301	NAD	C3D-C2D-C1D	3.16	105.74	100.98
2	A	301	NAD	C3N-C7N-N7N	3.16	121.54	117.75
2	D	301	NAD	C3B-C2B-C1B	3.00	105.49	100.98
2	D	301	NAD	C4N-C3N-C7N	-2.99	113.04	121.04
2	A	301	NAD	C4N-C3N-C7N	-2.90	113.29	121.04
2	A	301	NAD	O7N-C7N-C3N	-2.88	116.19	119.63
2	D	301	NAD	C2N-N1N-C1D	2.86	125.51	119.14
2	A	301	NAD	C3B-C2B-C1B	2.86	105.28	100.98
2	D	301	NAD	C3D-C2D-C1D	2.84	105.25	100.98
2	G	301	NAD	C3N-C7N-N7N	2.81	121.12	117.75
2	B	301	NAD	C2N-N1N-C1D	2.80	125.38	119.14
2	B	301	NAD	PN-O3-PA	-2.76	123.34	132.83
2	A	301	NAD	C3D-C2D-C1D	2.75	105.11	100.98
2	E	301	NAD	O7N-C7N-N7N	-2.74	118.69	122.58
2	E	301	NAD	C3N-C7N-N7N	2.71	121.01	117.75
2	E	301	NAD	C2N-N1N-C1D	2.71	125.17	119.14
2	E	301	NAD	PN-O3-PA	-2.52	124.18	132.83
2	E	301	NAD	C5N-C6N-N1N	2.47	123.94	120.40
2	E	301	NAD	C4N-C3N-C7N	-2.45	114.49	121.04
2	E	301	NAD	C5D-C4D-C3D	-2.38	106.27	115.18
2	C	301	NAD	O7N-C7N-N7N	-2.37	119.21	122.58
2	C	301	NAD	C3B-C2B-C1B	2.36	104.53	100.98
2	B	301	NAD	C5N-C6N-N1N	2.35	123.77	120.40
2	C	301	NAD	C3N-C7N-N7N	2.33	120.55	117.75
2	G	301	NAD	C5N-C6N-N1N	2.32	123.73	120.40
2	A	301	NAD	C2N-C3N-C7N	2.28	126.09	119.46
3	F	303	CXR	C4-C5-N7	-2.25	107.05	109.40
2	D	301	NAD	C3N-C7N-N7N	2.22	120.42	117.75
2	C	301	NAD	PN-O3-PA	-2.14	125.48	132.83
3	H	303	CXR	C3D-C2D-C1D	2.12	104.18	100.98
2	G	301	NAD	C4N-C3N-C7N	-2.11	115.40	121.04
2	B	301	NAD	C3B-C2B-C1B	2.11	104.15	100.98
2	D	301	NAD	C6N-N1N-C2N	-2.10	120.06	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAD	C2N-C3N-C4N	2.09	120.62	118.26
2	G	301	NAD	C2N-C3N-C7N	2.06	125.43	119.46
2	G	301	NAD	O2A-PA-O5B	2.05	117.27	107.75
2	B	301	NAD	C4N-C3N-C7N	-2.04	115.58	121.04

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	H	303	CXR	N1
3	F	303	CXR	N1

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	NAD	C5B-O5B-PA-O1A
2	B	301	NAD	C5B-O5B-PA-O2A
2	B	301	NAD	O4B-C4B-C5B-O5B
2	B	301	NAD	C3B-C4B-C5B-O5B
2	B	301	NAD	C5D-O5D-PN-O3
2	B	301	NAD	C5D-O5D-PN-O1N
2	B	301	NAD	C5D-O5D-PN-O2N
2	B	301	NAD	C2D-C1D-N1N-C2N
2	B	301	NAD	C2D-C1D-N1N-C6N
2	D	301	NAD	C5B-O5B-PA-O1A
2	D	301	NAD	C5B-O5B-PA-O3
2	D	301	NAD	C2D-C1D-N1N-C2N
2	D	301	NAD	C2D-C1D-N1N-C6N
3	H	303	CXR	C5D-O5D-PB-O2B
3	H	303	CXR	C5D-O5D-PB-O3A
3	H	303	CXR	C5D-O5D-PB-O1B
3	H	303	CXR	C3D-C4D-C5D-O5D
2	C	301	NAD	C5B-O5B-PA-O2A
2	C	301	NAD	C5B-O5B-PA-O3
2	C	301	NAD	C2D-C1D-N1N-C2N
2	C	301	NAD	C2D-C1D-N1N-C6N
3	F	303	CXR	C5'-O5'-PA-O2A
3	F	303	CXR	C5'-O5'-PA-O1A
2	G	301	NAD	C2D-C1D-N1N-C2N
2	G	301	NAD	C2D-C1D-N1N-C6N
2	A	301	NAD	PN-O3-PA-O5B
2	A	301	NAD	C2D-C1D-N1N-C2N
2	A	301	NAD	C2D-C1D-N1N-C6N

*Continued on next page...*

*Continued from previous page...*

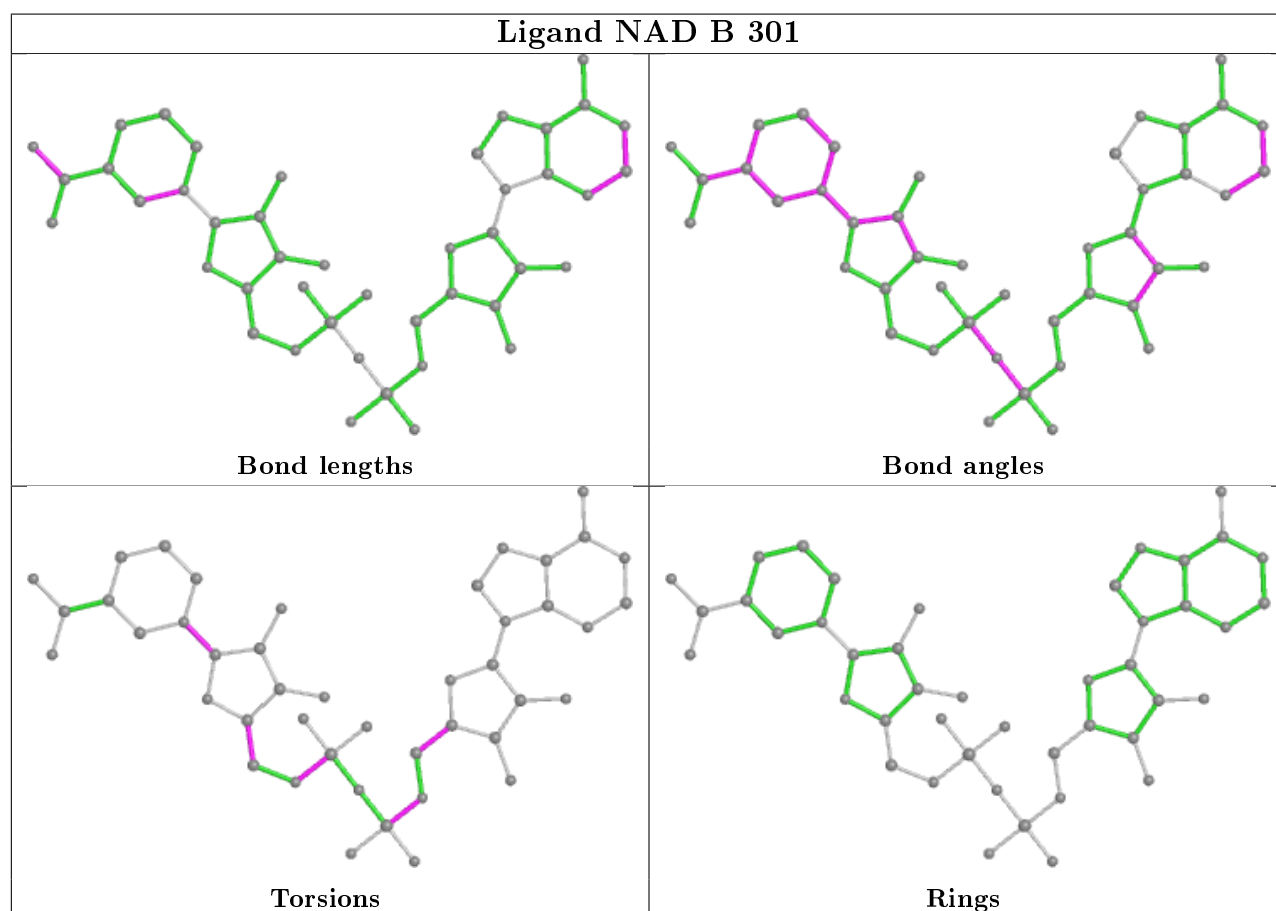
Mol	Chain	Res	Type	Atoms
2	B	301	NAD	C3D-C4D-C5D-O5D
2	D	301	NAD	O4B-C4B-C5B-O5B
2	E	301	NAD	C4N-C3N-C7N-N7N
3	H	303	CXR	O4D-C4D-C5D-O5D
2	E	301	NAD	C4N-C3N-C7N-O7N
2	B	301	NAD	O4D-C4D-C5D-O5D
2	E	301	NAD	C4D-C5D-O5D-PN
2	D	301	NAD	C4D-C5D-O5D-PN
2	D	301	NAD	PN-O3-PA-O5B
2	C	301	NAD	PA-O3-PN-O5D
2	E	301	NAD	PN-O3-PA-O5B
2	A	301	NAD	C4D-C5D-O5D-PN
3	F	303	CXR	C5'-O5'-PA-O3A
2	C	301	NAD	PN-O3-PA-O1A
2	G	301	NAD	PA-O3-PN-O2N
2	D	301	NAD	C4B-C5B-O5B-PA
2	C	301	NAD	C4D-C5D-O5D-PN
2	D	301	NAD	PA-O3-PN-O1N
2	D	301	NAD	PA-O3-PN-O2N
3	F	303	CXR	PB-O3A-PA-O1A
2	E	301	NAD	C4B-C5B-O5B-PA
2	G	301	NAD	C4D-C5D-O5D-PN
3	F	303	CXR	C3D-C4D-C5D-O5D
2	C	301	NAD	PN-O3-PA-O5B
2	B	301	NAD	C5B-O5B-PA-O3
3	F	303	CXR	PB-O3A-PA-O2A
2	D	301	NAD	C5B-O5B-PA-O2A
3	H	303	CXR	C5'-O5'-PA-O2A
2	G	301	NAD	C5B-O5B-PA-O1A

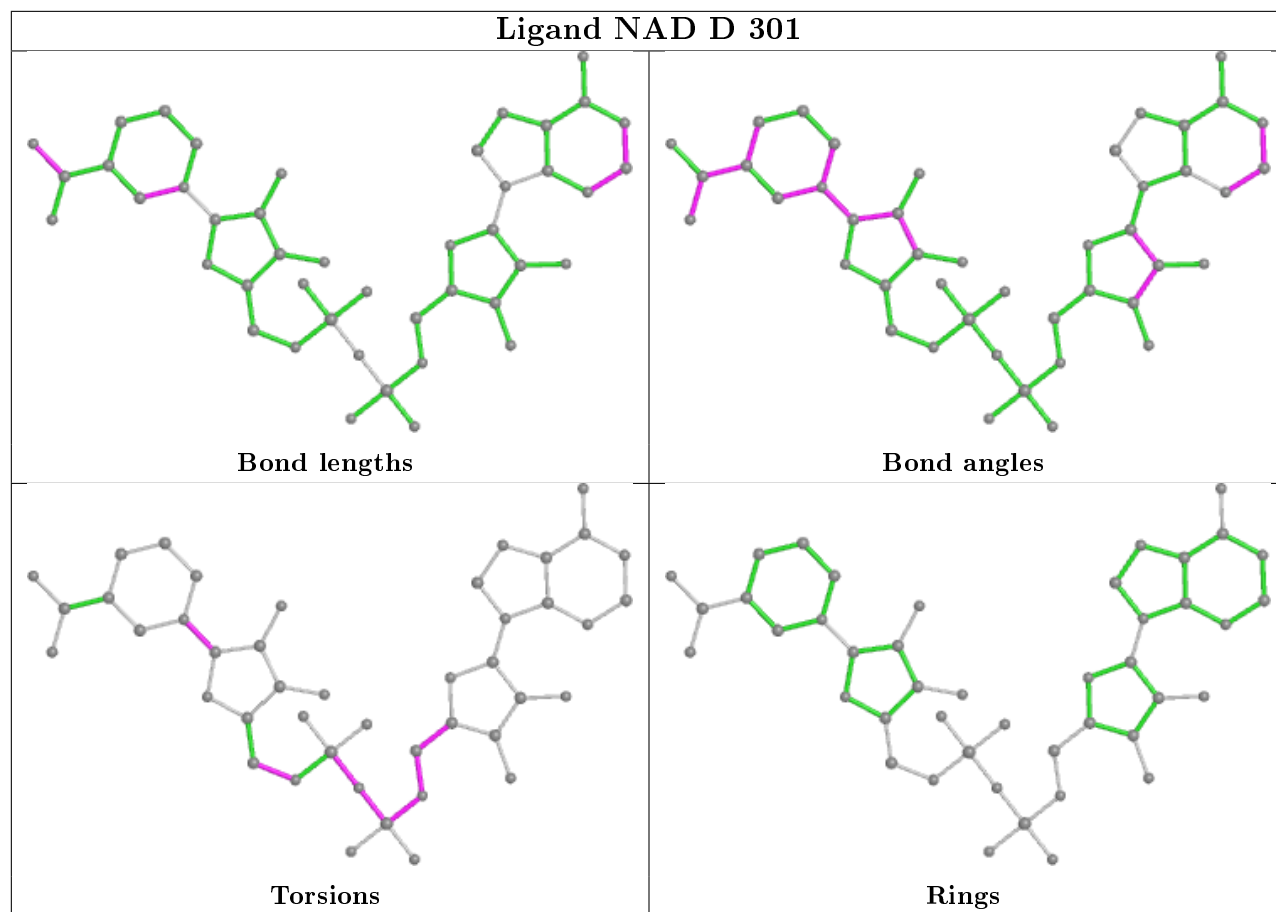
There are no ring outliers.

8 monomers are involved in 47 short contacts:

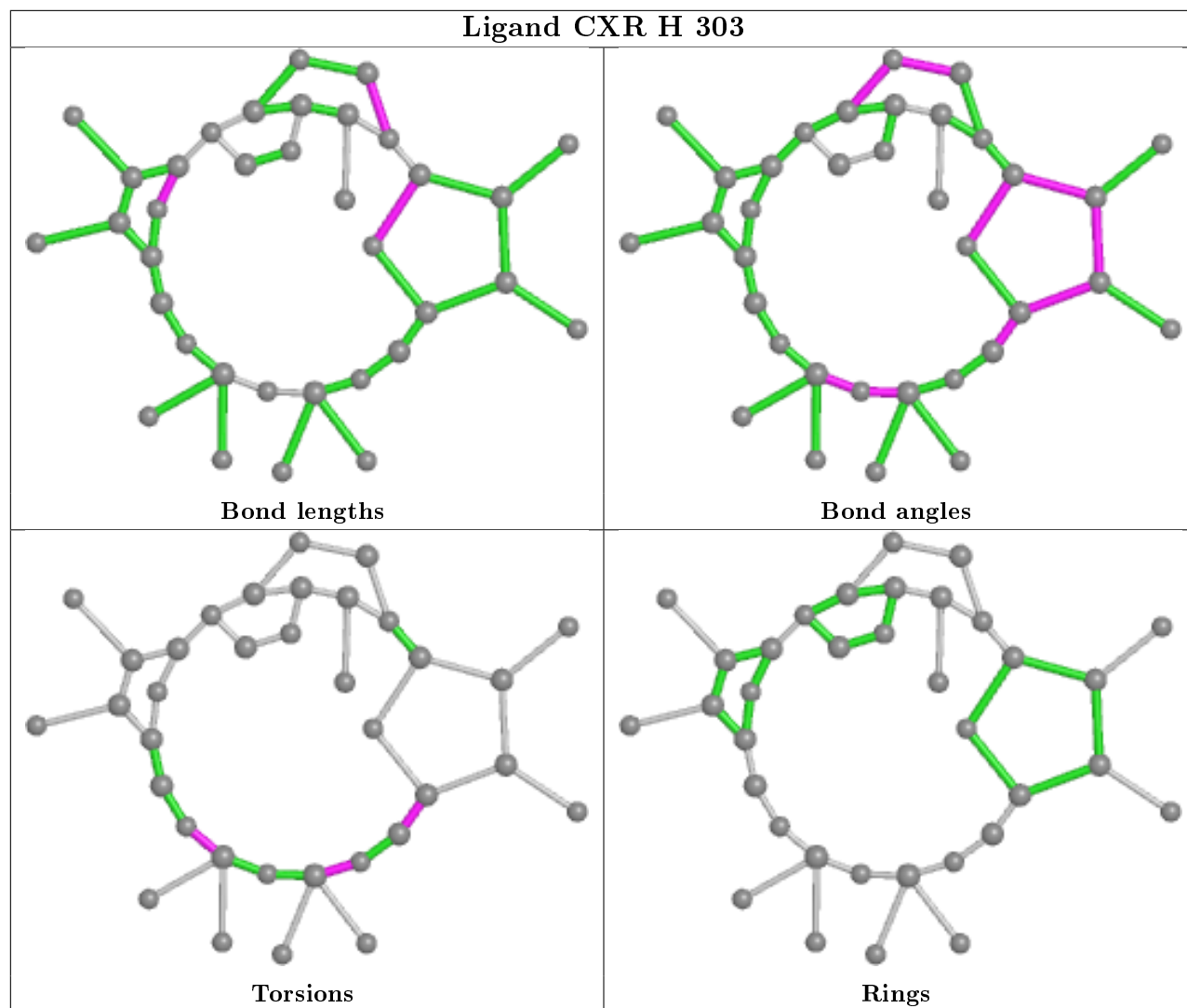
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	NAD	3	0
2	D	301	NAD	5	0
3	H	303	CXR	11	0
2	C	301	NAD	2	0
3	F	303	CXR	10	0
2	E	301	NAD	10	0
2	G	301	NAD	1	0
2	A	301	NAD	5	0

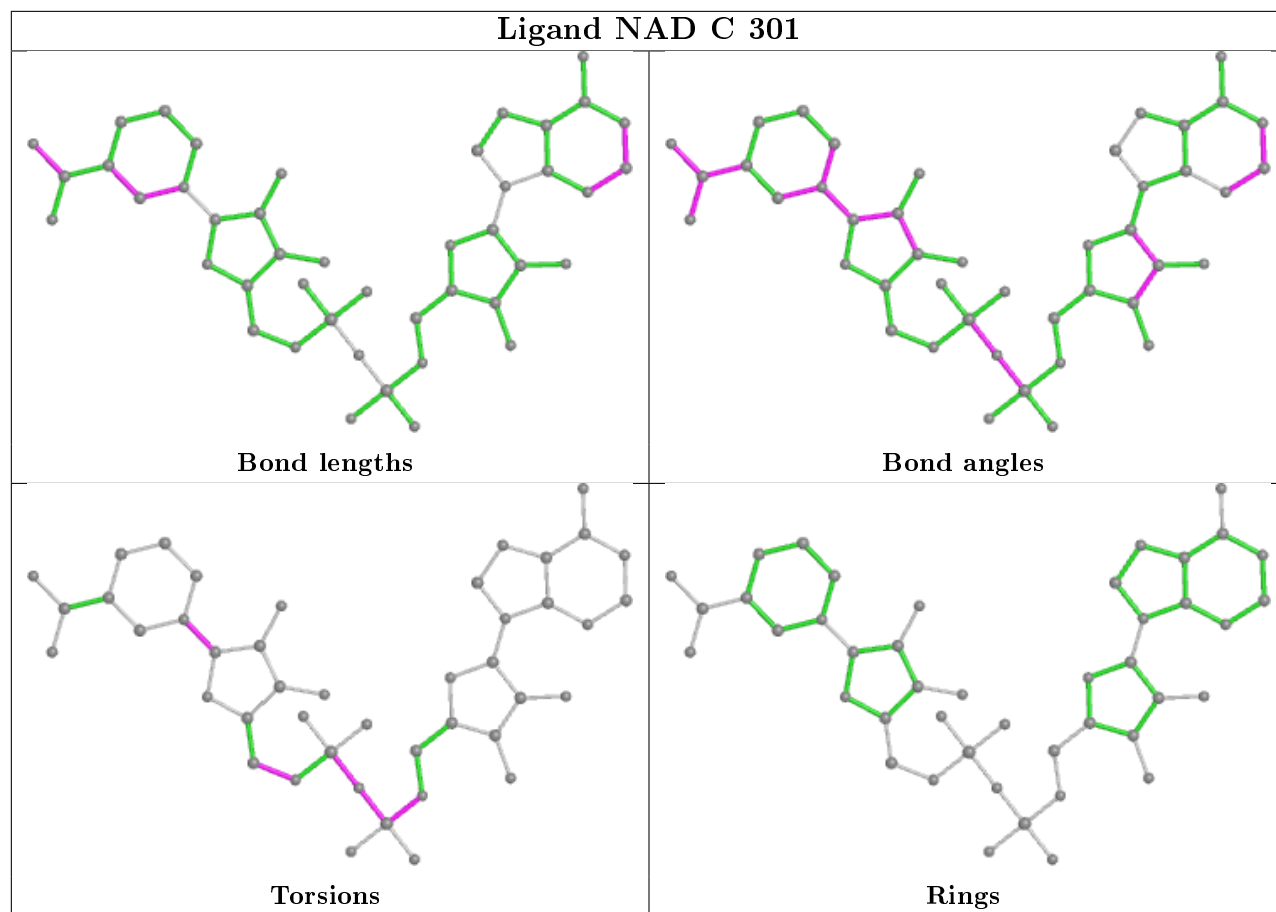
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



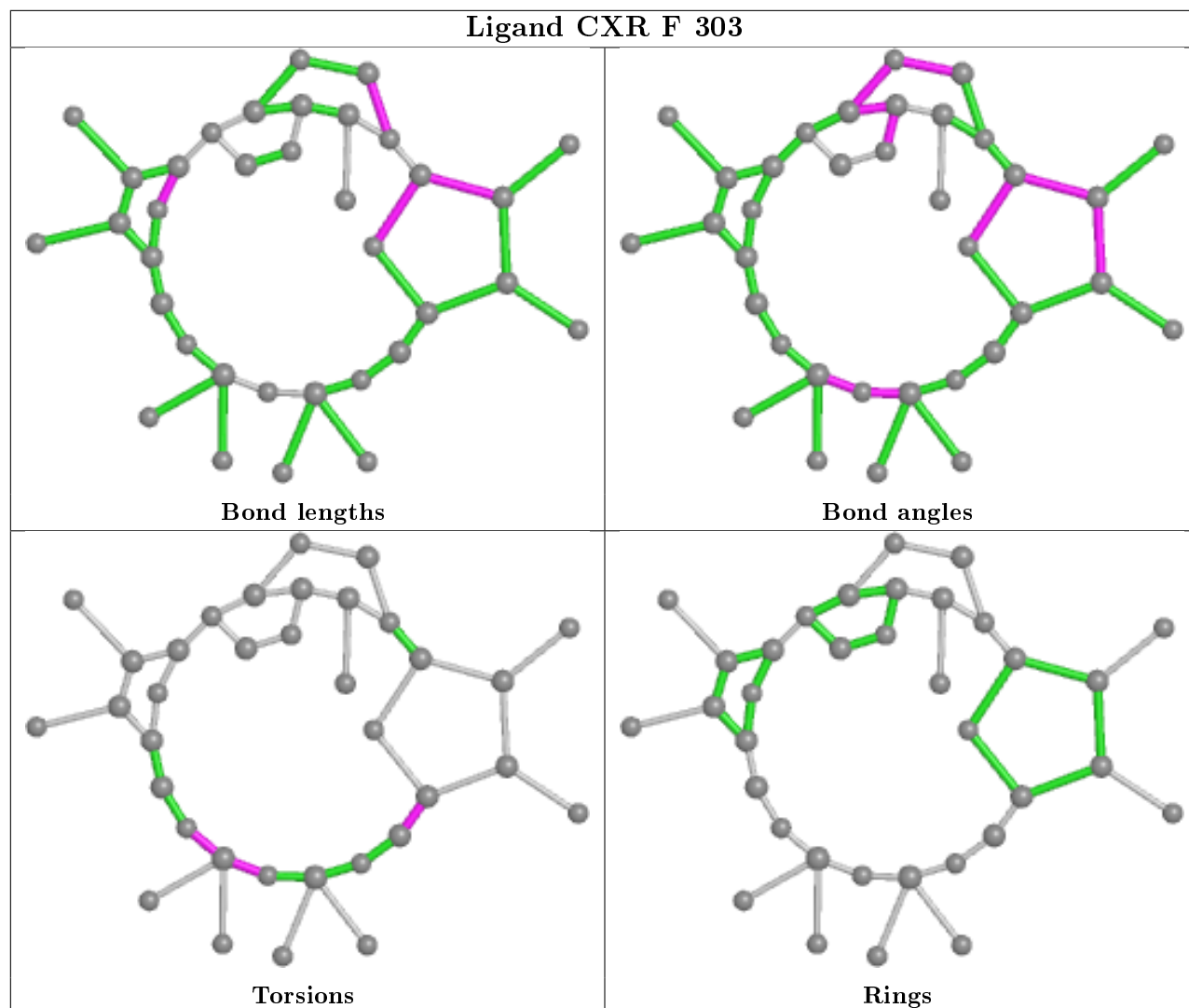


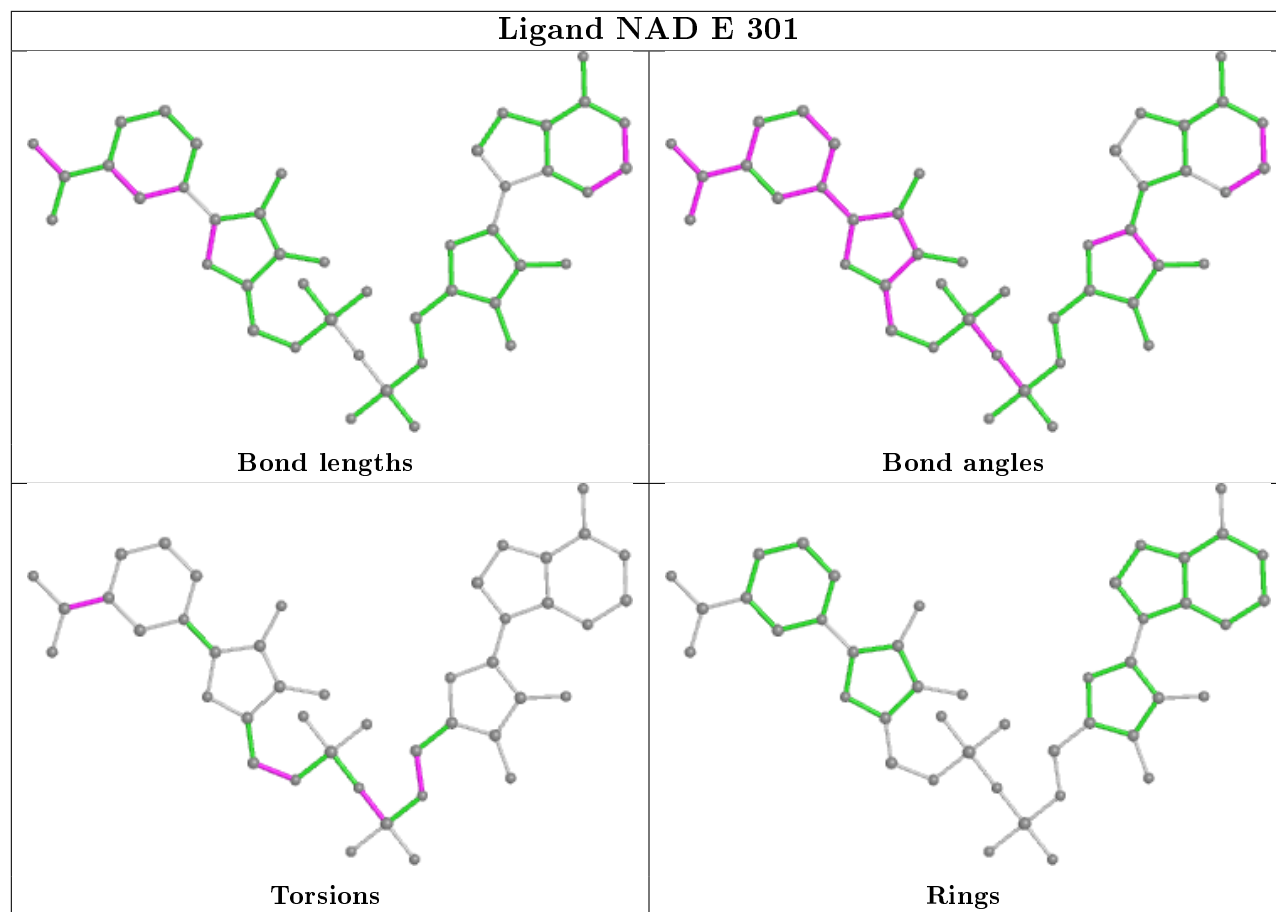


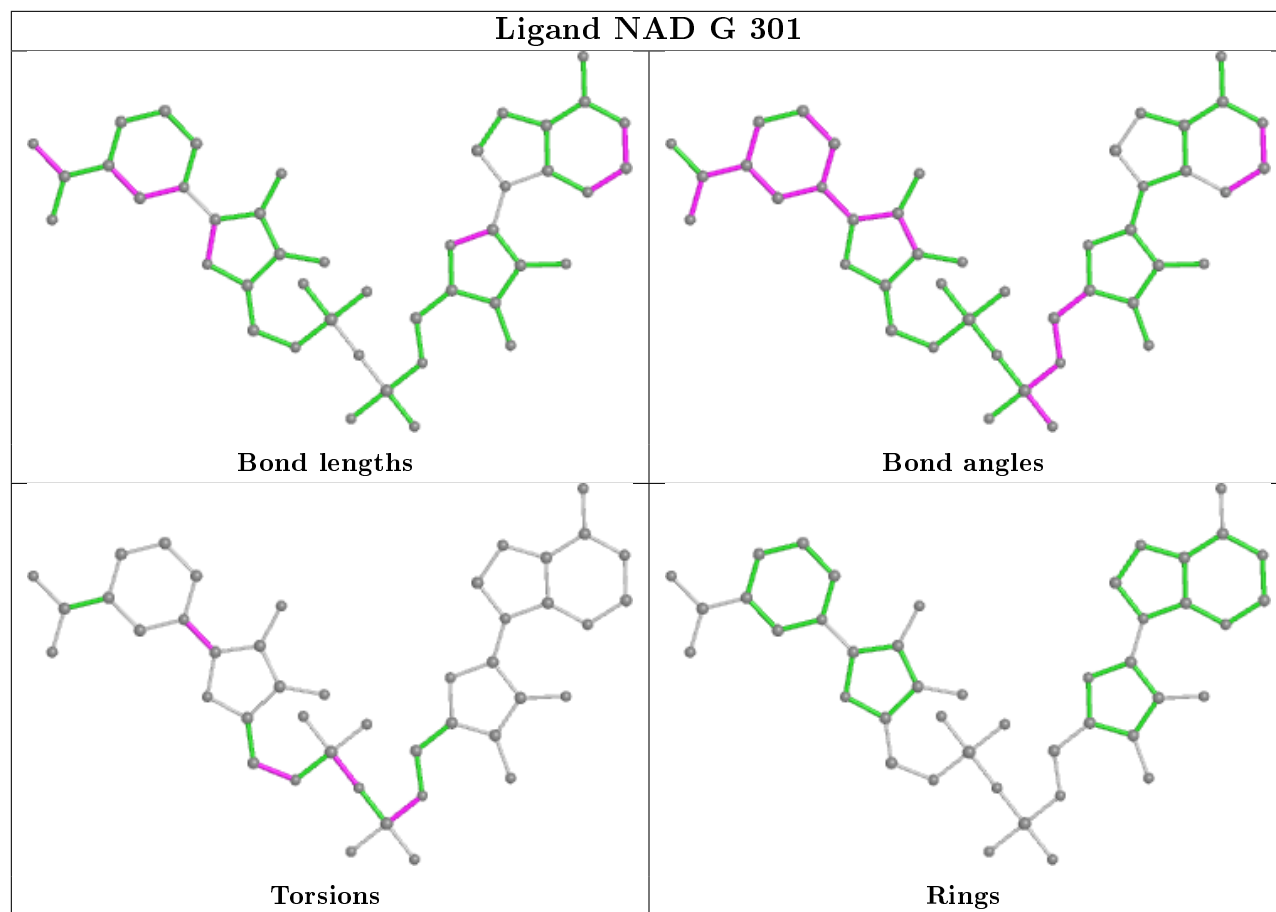


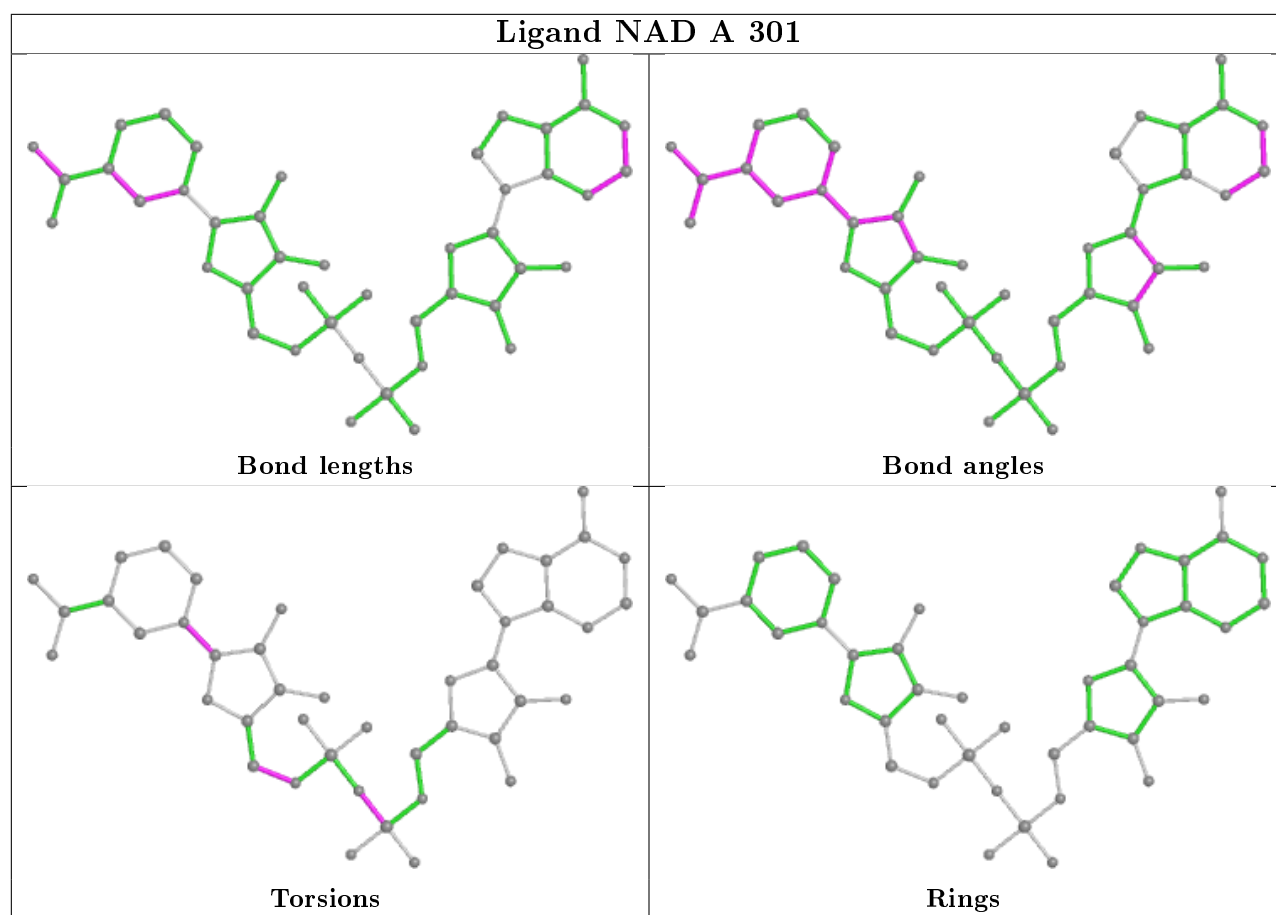


## Ligand CXR F 303









## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	253/260 (97%)	-0.49	1 (0%) 92 93	44, 62, 86, 99	0
1	B	252/260 (96%)	-0.49	1 (0%) 92 93	40, 55, 75, 94	0
1	C	254/260 (97%)	-0.50	2 (0%) 86 87	42, 60, 86, 97	0
1	D	251/260 (96%)	-0.49	0 100 100	40, 56, 75, 87	0
1	E	254/260 (97%)	-0.40	1 (0%) 92 93	43, 59, 78, 89	0
1	F	254/260 (97%)	-0.33	2 (0%) 86 87	54, 75, 95, 102	0
1	G	251/260 (96%)	-0.41	0 100 100	43, 58, 77, 92	0
1	H	254/260 (97%)	-0.35	0 100 100	55, 80, 98, 118	0
All	All	2023/2080 (97%)	-0.43	7 (0%) 94 94	40, 62, 90, 118	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	PHE	5.6
1	C	128	PHE	3.4
1	E	174	PHE	3.1
1	F	249	ARG	2.3
1	B	216	LYS	2.3
1	F	246	ARG	2.2
1	C	120	PHE	2.2

### 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

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.

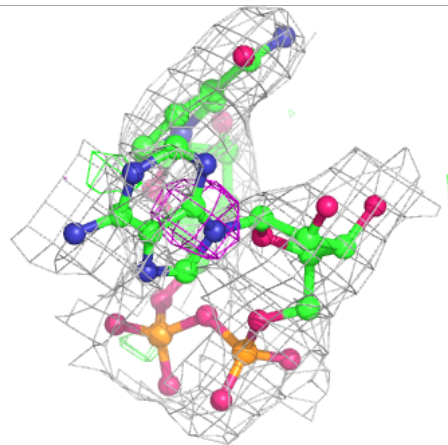
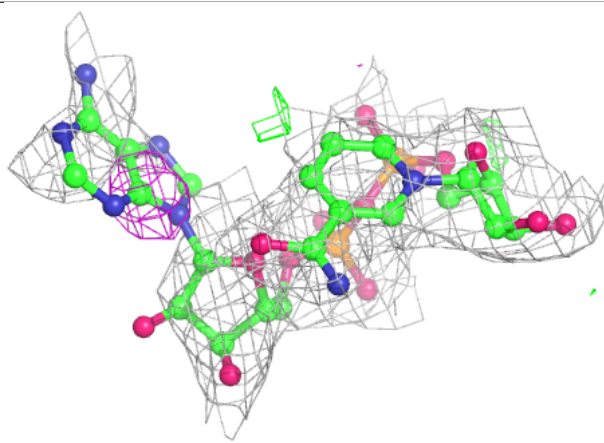
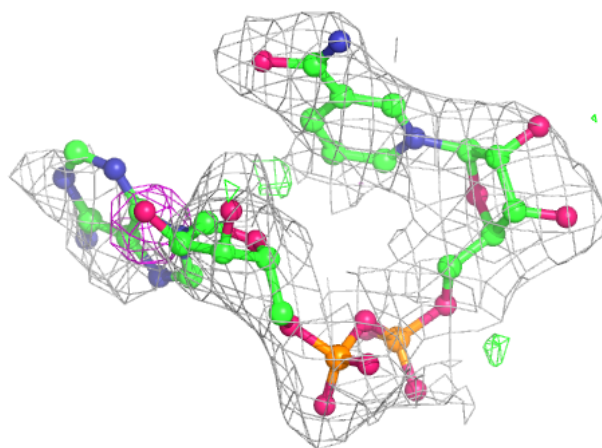
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	B	301	44/44	0.87	0.16	86,108,129,130	0
2	NAD	G	301	44/44	0.87	0.20	75,91,118,119	0
3	CXR	H	303	35/35	0.90	0.16	90,101,108,111	0
2	NAD	C	301	44/44	0.90	0.19	84,113,142,145	0
2	NAD	D	301	44/44	0.90	0.15	84,89,119,119	0
3	CXR	F	303	35/35	0.91	0.14	85,94,101,102	0
2	NAD	A	301	44/44	0.91	0.17	66,91,125,127	0
2	NAD	E	301	44/44	0.93	0.20	68,86,116,116	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.



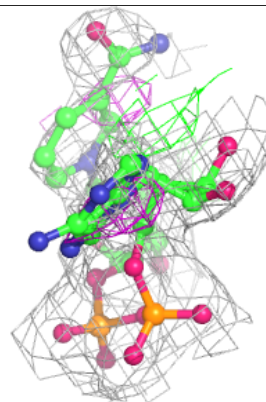
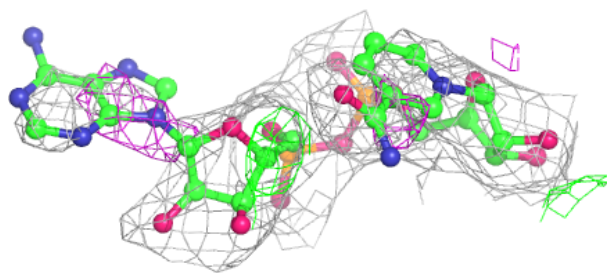
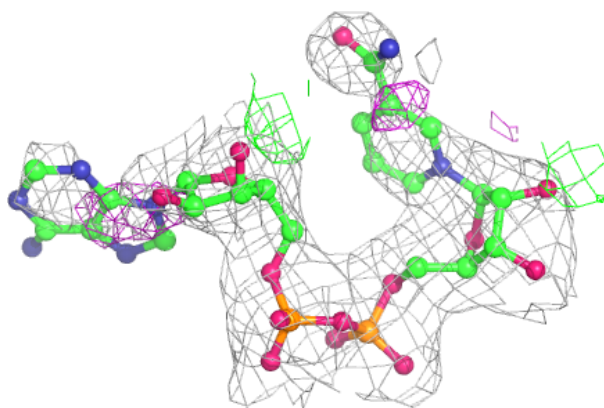
**Electron density around NAD B 301:**

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



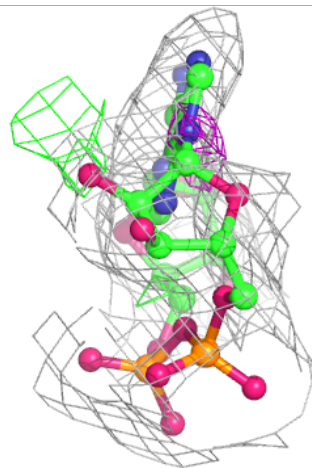
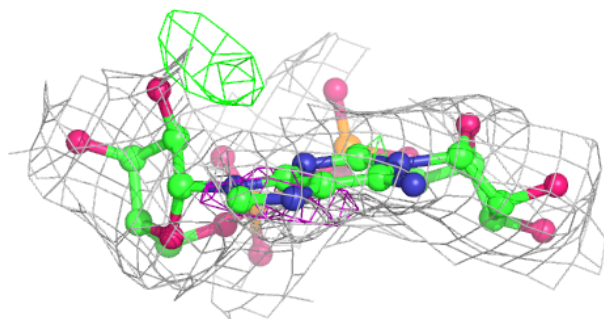
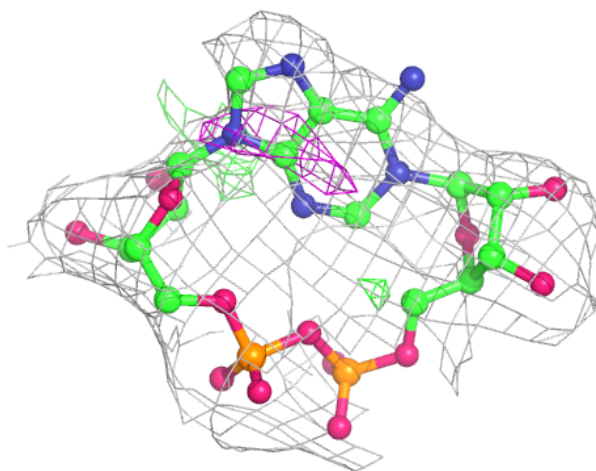
**Electron density around NAD G 301:**

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



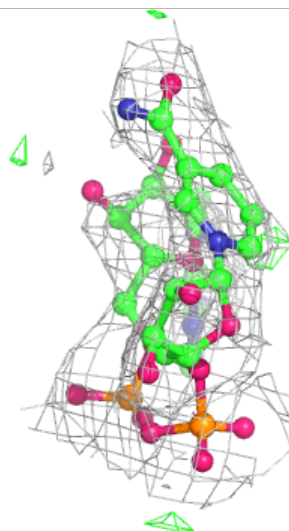
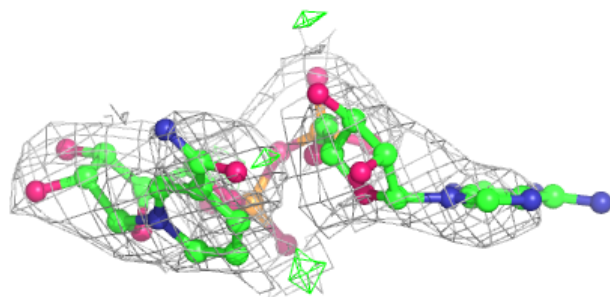
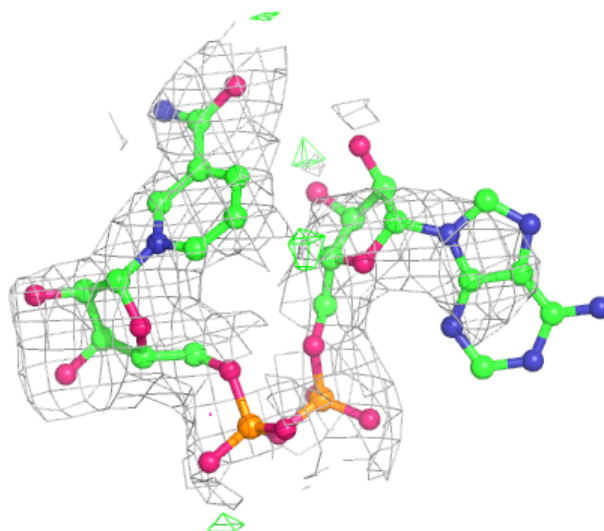
**Electron density around CXR H 303:**

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



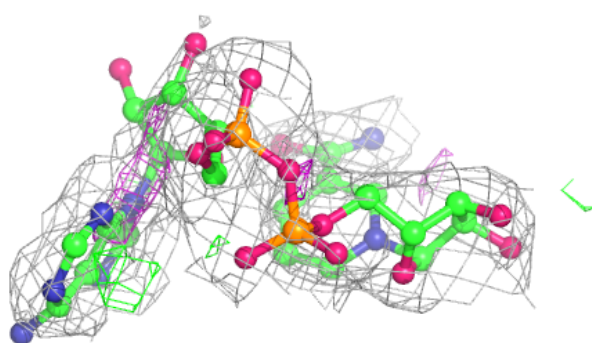
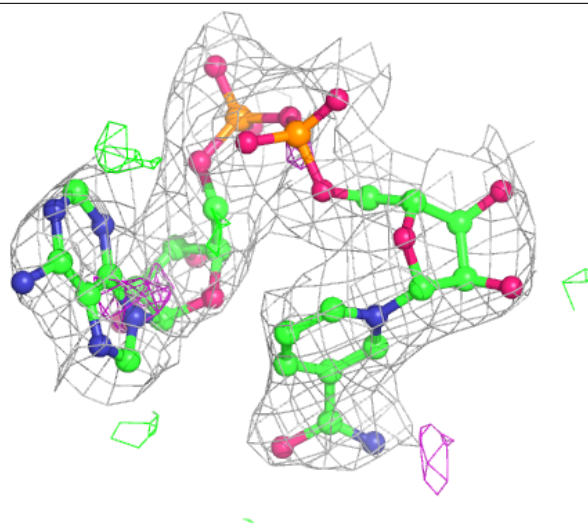
**Electron density around NAD C 301:**

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



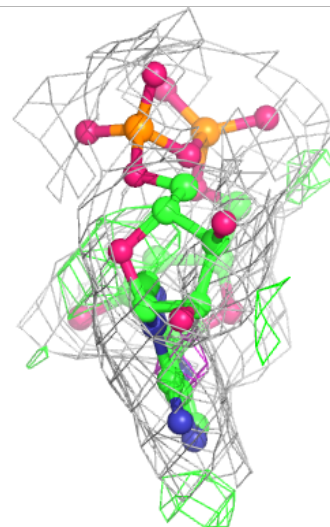
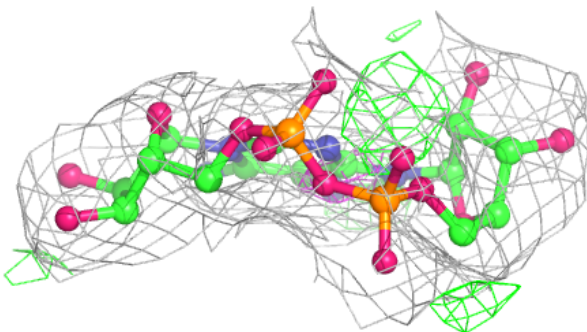
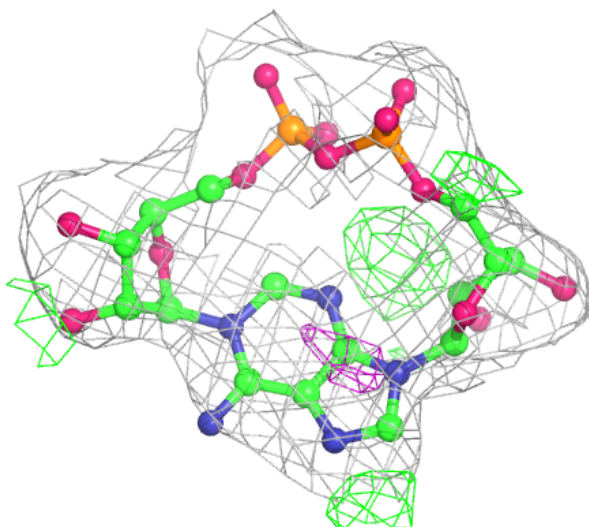
**Electron density around NAD D 301:**

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



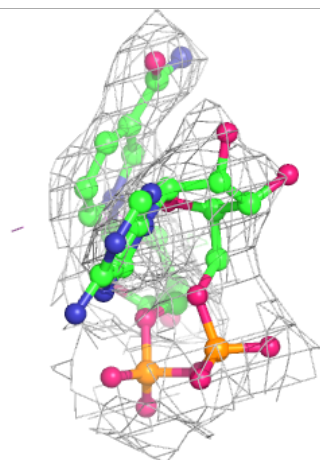
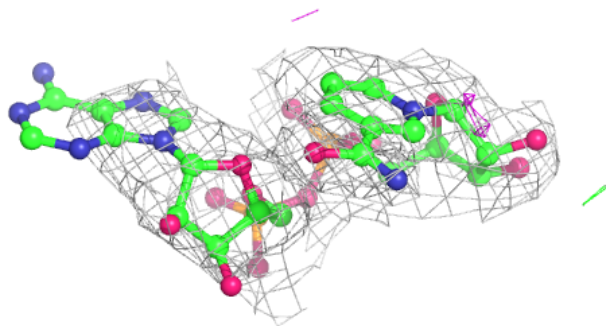
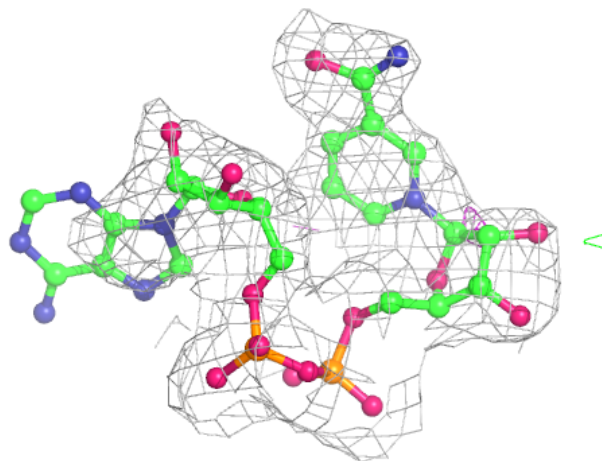
**Electron density around CXR F 303:**

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



**Electron density around NAD A 301:**

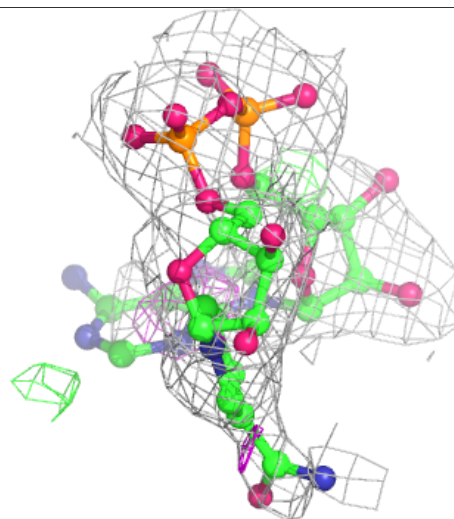
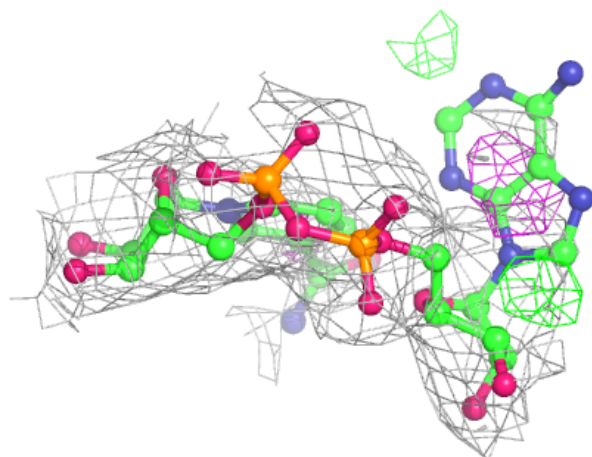
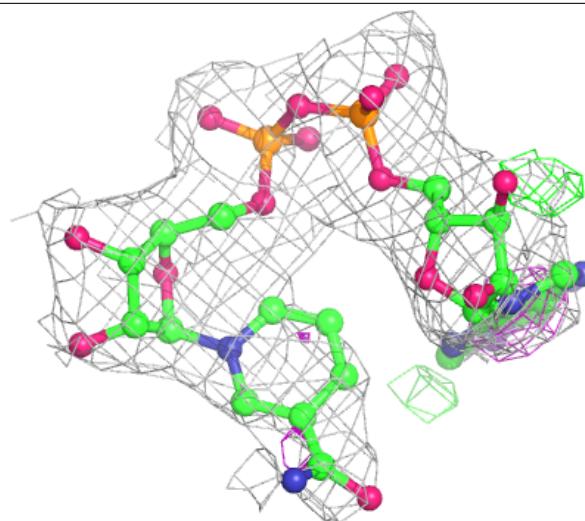
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around NAD E 301:**

$2mF_o-DF_c$  (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.