



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 07:09 PM EDT

PDB ID : 1O01  
Title : Human mitochondrial aldehyde dehydrogenase complexed with crotonaldehyde, NAD(H) and Mg<sup>2+</sup>  
Authors : Perez-Miller, S.J.; Hurley, T.D.  
Deposited on : 2003-02-20  
Resolution : 2.15 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

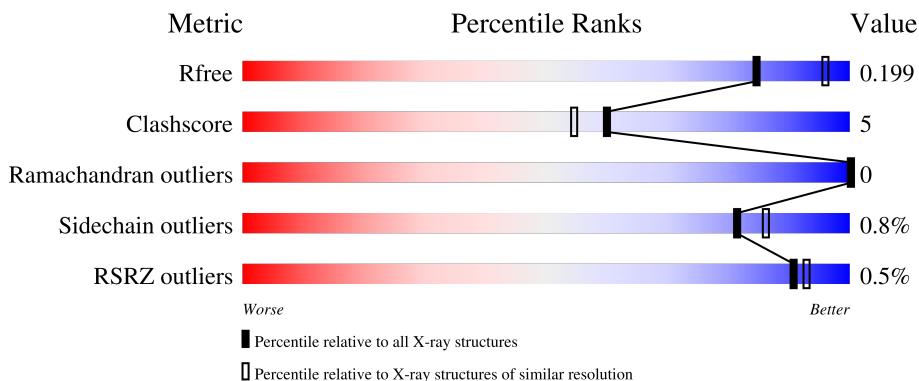
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	500	91% 8% .
1	B	500	89% 10% .
1	C	500	87% 12% .
1	D	500	88% 10% .
1	E	500	91% 8% .

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	500	 89% 10%
1	G	500	 87% 11%
1	H	500	 86% 13%

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
6	CRD	B	4512	-	-	X	X
6	CRD	C	4513	-	-	X	X
6	CRD	D	4514	-	-	X	X
6	CRD	E	4515	-	-	X	-
6	CRD	F	4516	-	-	X	-
6	CRD	G	4517	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 34568 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	494	3804	2418	649	718	19	0	1	0
1	B	494	3804	2418	649	718	19	0	1	0
1	C	495	3813	2423	651	720	19	0	1	0
1	D	494	3804	2418	649	718	19	0	1	0
1	E	494	3804	2418	649	718	19	0	1	0
1	F	494	3804	2418	649	718	19	0	1	0
1	G	494	3804	2418	649	718	19	0	1	0
1	H	494	3804	2418	649	718	19	0	1	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0
2	E	1	Total 1	Mg 1	0	0
2	F	1	Total 1	Mg 1	0	0

*Continued on next page...*

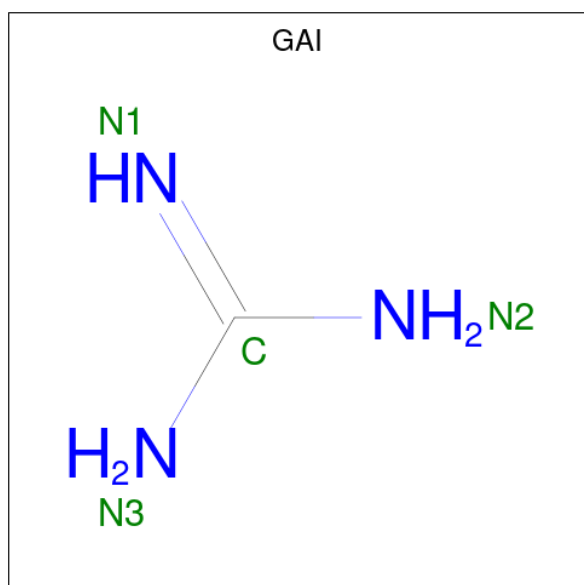
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

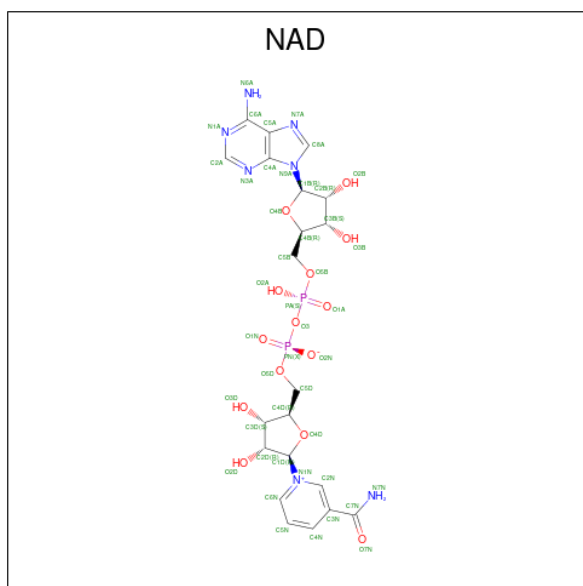
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	E	1	Total Na 1 1	0	0
3	F	1	Total Na 1 1	0	0
3	G	1	Total Na 1 1	0	0
3	H	1	Total Na 1 1	0	0

- Molecule 4 is GUANIDINE (three-letter code: GAI) (formula: CH<sub>5</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			4	1	3		
4	B	1	Total	C	N	0	0
			4	1	3		
4	C	1	Total	C	N	0	0
			4	1	3		
4	D	1	Total	C	N	0	0
			4	1	3		
4	E	1	Total	C	N	0	0
			4	1	3		
4	F	1	Total	C	N	0	0
			4	1	3		
4	G	1	Total	C	N	0	0
			4	1	3		
4	H	1	Total	C	N	0	0
			4	1	3		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



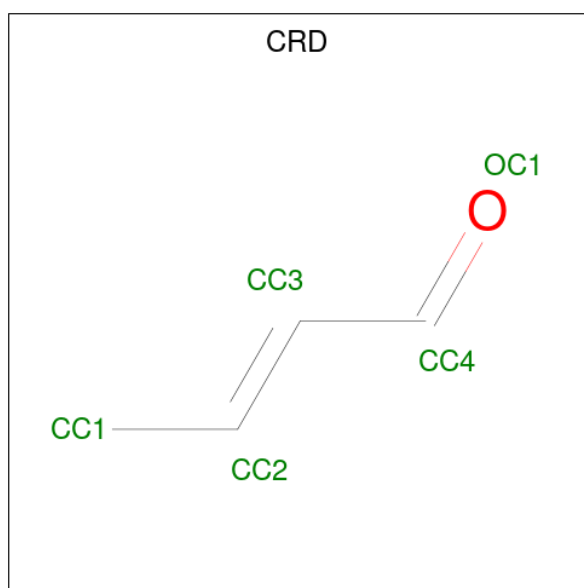
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

*Continued on next page...*

Continued from previous page...

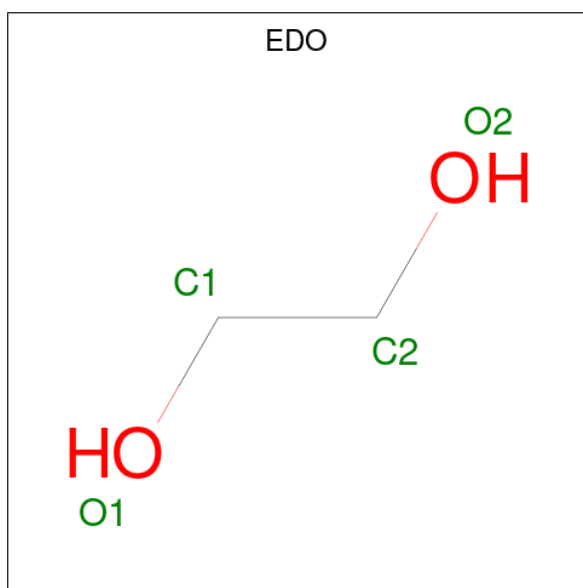
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 6 is (2E)-BUT-2-ENAL (three-letter code: CRD) (formula: C<sub>4</sub>H<sub>6</sub>O).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	C O	0	0
			5	4 1		
6	C	1	Total	C O	0	0
			5	4 1		
6	D	1	Total	C O	0	0
			5	4 1		
6	E	1	Total	C O	0	0
			5	4 1		
6	F	1	Total	C O	0	0
			5	4 1		
6	G	1	Total	C O	0	0
			5	4 1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	G	1	Total C O 4 2 2	0	0
7	H	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	454	Total O 454 454	0	0
8	B	514	Total O 514 514	0	0
8	C	488	Total O 488 488	0	0

*Continued on next page...*



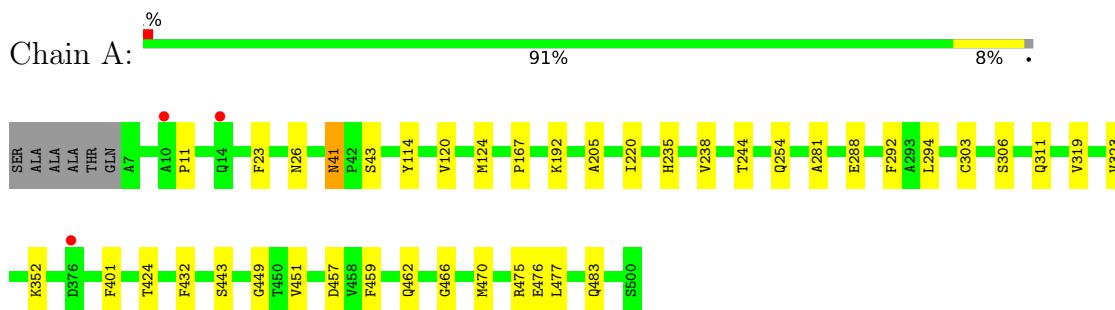
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
8	D	458	Total 458	O 458	0	0
8	E	449	Total 449	O 449	0	0
8	F	480	Total 480	O 480	0	0
8	G	440	Total 440	O 440	0	0
8	H	382	Total 382	O 382	0	0

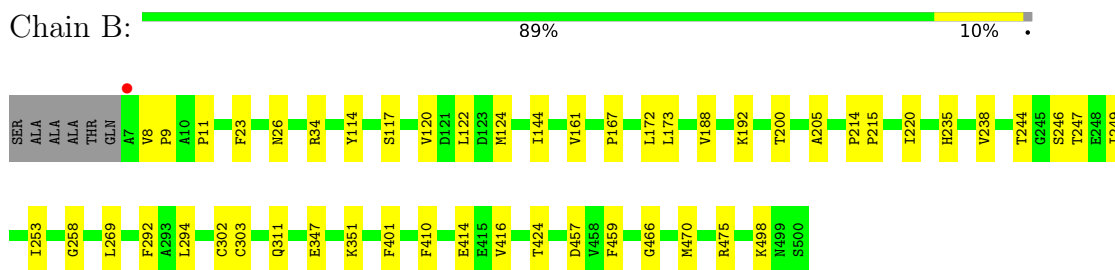
### 3 Residue-property plots [i](#)

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

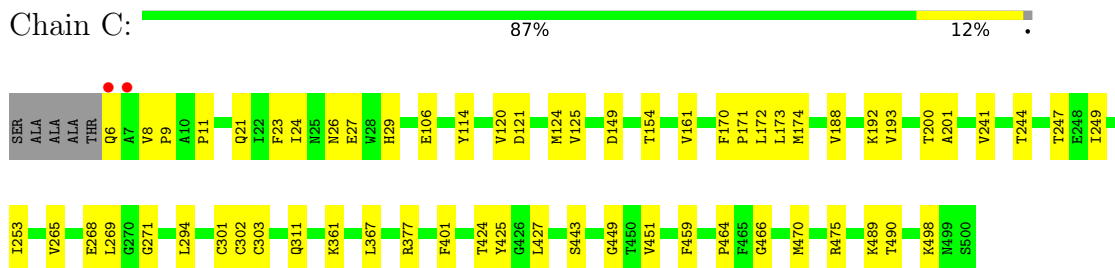
- Molecule 1: Aldehyde dehydrogenase



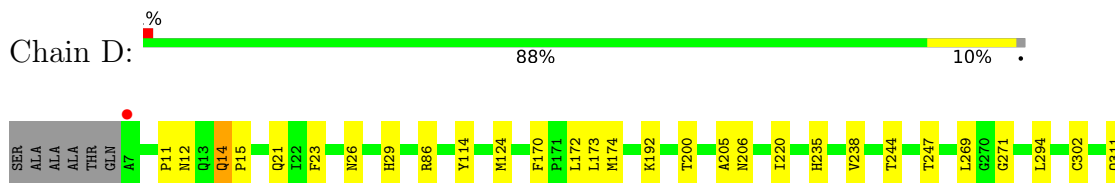
- Molecule 1: Aldehyde dehydrogenase

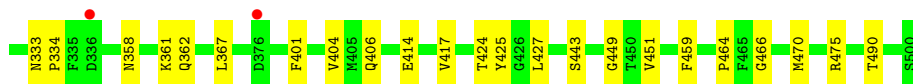


- Molecule 1: Aldehyde dehydrogenase

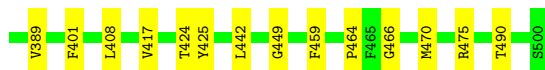


- Molecule 1: Aldehyde dehydrogenase

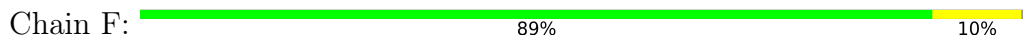




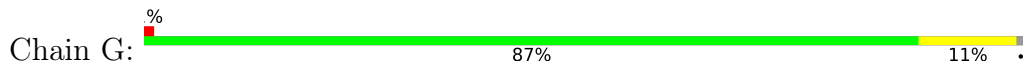
- Molecule 1: Aldehyde dehydrogenase



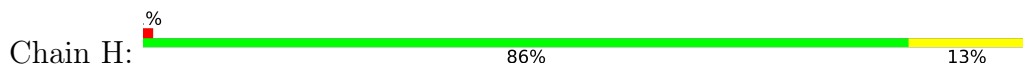
- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.13Å 150.57Å 176.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.84 – 2.15 40.24 – 2.14	Depositor EDS
% Data completeness (in resolution range)	91.1 (34.84-2.15) 90.4 (40.24-2.14)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.79 (at 2.14Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.170 , 0.206 0.162 , 0.199	Depositor DCC
$R_{free}$ test set	9472 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.6	Xtrriage
Anisotropy	1.212	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	34568	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6010e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: EDO, GAI, MG, NA, CRD, 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	0.33	0/3888	0.58	0/5275
1	B	0.34	0/3888	0.58	0/5275
1	C	0.34	0/3897	0.59	0/5287
1	D	0.33	0/3888	0.59	0/5275
1	E	0.34	0/3888	0.58	0/5275
1	F	0.33	0/3888	0.59	0/5275
1	G	0.33	0/3888	0.57	0/5275
1	H	0.33	0/3888	0.57	0/5275
All	All	0.33	0/31113	0.58	0/42212

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3804	0	3749	27	0
1	B	3804	0	3749	35	0
1	C	3813	0	3757	45	0
1	D	3804	0	3749	38	0
1	E	3804	0	3749	29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3804	0	3749	35	0
1	G	3804	0	3749	43	0
1	H	3804	0	3749	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	4	0	5	0	0
4	B	4	0	5	0	0
4	C	4	0	4	0	0
4	D	4	0	5	0	0
4	E	4	0	4	0	0
4	F	4	0	5	0	0
4	G	4	0	4	0	0
4	H	4	0	5	0	0
5	A	44	0	26	0	0
5	B	44	0	26	1	0
5	C	44	0	26	0	0
5	D	44	0	26	0	0
5	E	44	0	26	0	0
5	F	44	0	26	0	0
5	G	44	0	26	0	0
5	H	44	0	26	0	0
6	B	5	0	6	4	0
6	C	5	0	6	6	0
6	D	5	0	6	5	0
6	E	5	0	6	4	0
6	F	5	0	6	8	0
6	G	5	0	6	9	0
7	C	8	0	12	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	8	0	12	0	0
7	E	4	0	6	0	0
7	F	4	0	6	0	0
7	G	4	0	6	0	0
7	H	4	0	6	0	0
8	A	454	0	0	4	0
8	B	514	0	0	2	0
8	C	488	0	0	2	0
8	D	458	0	0	3	0
8	E	449	0	0	3	0
8	F	480	0	0	0	0
8	G	440	0	0	3	0
8	H	382	0	0	0	0
All	All	34568	0	30329	284	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 5.

All (284) 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:C:302:CYS:SG	6:C:4513:CRD:HC4	1.38	1.64
1:G:302:CYS:SG	6:G:4517:CRD:HC4	1.50	1.52
1:F:302:CYS:SG	6:F:4516:CRD:HC4	1.56	1.46
1:C:302:CYS:SG	6:C:4513:CRD:CC4	2.13	1.37
1:G:302:CYS:SG	6:G:4517:CRD:CC4	2.17	1.32
1:F:302:CYS:SG	6:F:4516:CRD:CC4	2.17	1.30
1:E:302:CYS:SG	6:E:4515:CRD:HC4	1.87	1.13
1:C:302:CYS:HG	6:C:4513:CRD:CC4	1.54	1.09
1:C:27:GLU:HG3	1:C:29:HIS:NE2	1.82	0.93
1:E:302:CYS:SG	6:E:4515:CRD:CC4	2.57	0.92
1:D:302:CYS:SG	6:D:4514:CRD:CC4	2.61	0.88
1:C:174:MET:HE2	1:C:244:THR:HG21	1.55	0.86
1:F:302:CYS:HG	6:F:4516:CRD:CC4	1.85	0.85
1:C:302:CYS:HG	6:C:4513:CRD:HC4	1.03	0.84
1:C:24:ILE:O	1:C:27:GLU:HG2	1.80	0.81
1:G:302:CYS:CB	6:G:4517:CRD:HC4	2.11	0.79
1:F:301[B]:CYS:SG	6:F:4516:CRD:HC12	2.23	0.79
1:E:361:LYS:HE2	1:E:367:LEU:HD22	1.66	0.78
1:G:301[B]:CYS:SG	6:G:4517:CRD:HC3	2.28	0.73
1:D:174:MET:CE	1:D:244:THR:HG21	2.18	0.72

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:CYS:SG	6:D:4514:CRD:OC1	2.52	0.68
1:F:347:GLU:HG2	1:F:351:LYS:HD3	1.76	0.68
1:D:174:MET:HE2	1:D:244:THR:HG21	1.75	0.67
1:G:366:LYS:HG3	8:G:3035:HOH:O	1.95	0.67
1:C:174:MET:CE	1:C:244:THR:HG21	2.25	0.67
1:F:302:CYS:CB	6:F:4516:CRD:HC4	2.25	0.66
1:G:349:GLN:NE2	1:G:401:PHE:HB3	2.11	0.66
1:C:247:THR:HA	1:C:269:LEU:HD13	1.78	0.64
1:D:174:MET:HE1	8:D:5877:HOH:O	1.98	0.64
1:H:205:ALA:HB2	1:H:220:ILE:HD12	1.80	0.63
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.34	0.62
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.34	0.62
1:B:311:GLN:HG3	8:B:5679:HOH:O	2.00	0.61
1:G:258:GLY:CA	1:H:254:GLN:HG2	2.32	0.60
1:F:292:PHE:HE1	1:F:457:ASP:HB2	1.67	0.59
1:D:170:PHE:CE1	6:D:4514:CRD:HC3	2.38	0.59
1:G:148:GLY:O	1:G:498:LYS:HE3	2.02	0.59
1:D:459:PHE:CE1	6:D:4514:CRD:HC11	2.38	0.59
1:D:247:THR:HA	1:D:269:LEU:HD13	1.85	0.59
1:D:362:GLN:HE21	1:D:362:GLN:HA	1.67	0.59
1:E:459:PHE:CE1	6:E:4515:CRD:HC11	2.37	0.59
1:C:424:THR:CG2	1:C:470:MET:SD	2.92	0.58
1:A:311:GLN:HG3	8:A:5755:HOH:O	2.02	0.58
1:B:424:THR:CG2	1:B:470:MET:SD	2.92	0.58
1:B:466:GLY:HA3	1:B:475:ARG:HD3	1.85	0.58
1:D:170:PHE:O	1:D:174:MET:HG2	2.04	0.57
1:G:483:GLN:HB3	8:G:2790:HOH:O	2.03	0.57
1:B:303:CYS:SG	1:B:459:PHE:HZ	2.27	0.57
1:E:29:HIS:HD2	8:E:5743:HOH:O	1.88	0.57
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.39	0.57
1:C:170:PHE:O	1:C:174:MET:HG2	2.05	0.56
1:D:174:MET:HE1	1:D:244:THR:HG21	1.87	0.56
1:F:424:THR:HG21	1:F:470:MET:SD	2.46	0.56
1:F:170:PHE:CE1	6:F:4516:CRD:HC3	2.40	0.56
1:F:15:PRO:HD2	1:F:108:LEU:HD22	1.88	0.56
1:F:424:THR:CG2	1:F:470:MET:SD	2.94	0.56
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.41	0.56
1:D:459:PHE:CZ	6:D:4514:CRD:HC11	2.40	0.55
1:G:466:GLY:HA3	1:G:475:ARG:HD3	1.89	0.55
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.41	0.55
1:G:11:PRO:HB3	1:G:114:TYR:CZ	2.41	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:499:ASN:HD21	1:G:73:GLY:H	1.55	0.55
1:D:404:VAL:HG12	1:D:406:GLN:HE22	1.71	0.54
1:B:205:ALA:HB2	1:B:220:ILE:HD12	1.88	0.54
1:E:490:THR:OG1	1:F:464:PRO:HG2	2.08	0.54
1:A:41:ASN:C	1:A:41:ASN:HD22	2.10	0.54
1:B:172:LEU:HD21	1:B:200:THR:HB	1.90	0.54
1:C:172:LEU:HD21	1:C:200:THR:HB	1.88	0.54
1:H:311:GLN:NE2	1:H:312:GLU:HG2	2.24	0.53
1:H:271:GLY:HA2	1:H:425:TYR:CG	2.44	0.53
1:G:424:THR:CG2	1:G:470:MET:SD	2.96	0.53
1:F:499:ASN:ND2	1:G:73:GLY:H	2.06	0.53
1:G:161:VAL:HA	1:G:188:VAL:HG23	1.90	0.53
1:G:247:THR:HA	1:G:269:LEU:HD13	1.89	0.53
1:A:352:LYS:HD3	8:A:5937:HOH:O	2.08	0.53
1:B:11:PRO:HB3	1:B:114:TYR:CZ	2.44	0.53
1:A:41:ASN:ND2	1:A:43:SER:H	2.07	0.52
1:B:235:HIS:HB3	1:B:238:VAL:HG23	1.91	0.52
1:G:424:THR:HG22	1:G:470:MET:HB2	1.90	0.52
1:E:271:GLY:HA2	1:E:425:TYR:CG	2.44	0.52
1:C:490:THR:OG1	1:D:464:PRO:HG2	2.09	0.52
1:D:361:LYS:HD3	1:D:367:LEU:HD22	1.91	0.52
1:C:249:ILE:O	1:C:253:ILE:HG12	2.10	0.51
1:D:358:ASN:O	1:D:362:GLN:HG2	2.10	0.51
1:E:170:PHE:CE1	6:E:4515:CRD:HC3	2.45	0.51
1:A:254:GLN:HG2	1:B:258:GLY:CA	2.40	0.51
1:C:174:MET:HE2	1:C:244:THR:CG2	2.33	0.51
1:B:120:VAL:HG12	1:B:124:MET:HE1	1.92	0.51
1:H:198:PRO:O	1:H:202:LEU:HG	2.10	0.51
1:D:466:GLY:HA3	1:D:475:ARG:HD3	1.93	0.51
1:A:41:ASN:HD22	1:A:43:SER:H	1.57	0.51
1:F:301[B]:CYS:SG	6:F:4516:CRD:CC1	2.96	0.51
1:H:284:ASP:OD1	1:H:321:ARG:NH1	2.44	0.51
1:A:205:ALA:HB2	1:A:220:ILE:HD12	1.93	0.51
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.45	0.51
1:G:172:LEU:HD21	1:G:200:THR:HB	1.92	0.50
1:H:424:THR:CG2	1:H:470:MET:SD	2.99	0.50
1:C:11:PRO:HB3	1:C:114:TYR:CZ	2.46	0.50
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.46	0.50
1:D:21:GLN:HB3	1:D:29:HIS:O	2.11	0.50
1:B:347:GLU:HG2	1:B:351:LYS:HE2	1.93	0.50
1:C:361:LYS:HD3	1:C:367:LEU:HD22	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ALA:HB2	1:D:220:ILE:HD12	1.94	0.50
1:C:124:MET:HE3	1:C:173:LEU:HD22	1.93	0.50
1:H:271:GLY:HA2	1:H:425:TYR:CD2	2.46	0.50
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.46	0.50
1:F:466:GLY:HA3	1:F:475:ARG:HD3	1.93	0.50
1:G:408:LEU:N	1:G:408:LEU:HD12	2.27	0.49
1:C:464:PRO:HG2	1:D:490:THR:OG1	2.12	0.49
1:E:11:PRO:HB3	1:E:114:TYR:CZ	2.47	0.49
1:E:424:THR:CG2	1:E:470:MET:SD	3.00	0.49
1:C:303:CYS:SG	1:C:459:PHE:HZ	2.35	0.49
1:E:466:GLY:HA3	1:E:475:ARG:HD3	1.95	0.49
1:H:12:ASN:O	1:H:15:PRO:HD3	2.12	0.49
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.47	0.49
1:H:466:GLY:HA3	1:H:475:ARG:HD3	1.95	0.49
1:B:124:MET:HE3	1:B:173:LEU:HD22	1.94	0.49
1:E:449:GLY:HA3	1:E:466:GLY:O	2.13	0.49
1:D:362:GLN:HA	1:D:362:GLN:NE2	2.28	0.49
1:D:302:CYS:SG	1:D:427:LEU:HD21	2.53	0.48
1:D:11:PRO:HB3	1:D:114:TYR:CZ	2.48	0.48
1:E:244:THR:HA	1:E:268:GLU:O	2.14	0.48
1:F:443:SER:HA	1:F:451:VAL:HG11	1.96	0.48
1:A:483:GLN:HB3	8:A:5884:HOH:O	2.13	0.48
1:H:303:CYS:SG	1:H:459:PHE:HZ	2.37	0.48
1:H:389:VAL:HB	1:H:408:LEU:HG	1.95	0.48
1:C:241:VAL:CG1	1:C:265:VAL:HG22	2.43	0.48
1:C:443:SER:HA	1:C:451:VAL:HG11	1.96	0.48
1:C:311:GLN:HG3	8:C:5573:HOH:O	2.13	0.48
1:H:247:THR:HA	1:H:269:LEU:HD13	1.95	0.48
1:D:271:GLY:HA2	1:D:425:TYR:CG	2.49	0.48
1:F:449:GLY:HA3	1:F:466:GLY:O	2.14	0.48
1:B:117:SER:O	1:B:122:LEU:HD23	2.14	0.47
1:B:302:CYS:SG	6:B:4512:CRD:HC4	2.55	0.47
1:H:166:ILE:HD11	1:H:193:VAL:HG12	1.96	0.47
1:A:443:SER:HA	1:A:451:VAL:HG11	1.96	0.47
1:G:12:ASN:O	1:G:15:PRO:HD3	2.14	0.47
1:G:258:GLY:HA3	1:H:254:GLN:HG2	1.96	0.47
1:G:490:THR:OG1	1:H:464:PRO:HG2	2.14	0.47
1:H:161:VAL:HA	1:H:188:VAL:HG23	1.96	0.47
1:E:170:PHE:HB3	1:E:173:LEU:HB3	1.96	0.47
1:H:424:THR:HG22	1:H:470:MET:HB2	1.95	0.47
1:H:443:SER:HA	1:H:451:VAL:HG11	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:377:ARG:HH11	1:G:377:ARG:HG2	1.80	0.47
1:E:424:THR:HG22	1:E:470:MET:HB2	1.95	0.47
1:B:124:MET:HE3	1:B:173:LEU:CD2	2.45	0.46
1:A:292:PHE:HE1	1:A:457:ASP:HB2	1.80	0.46
1:B:302:CYS:HG	6:B:4512:CRD:CC4	2.29	0.46
1:F:247:THR:HA	1:F:269:LEU:HD13	1.98	0.46
1:B:161:VAL:HA	1:B:188:VAL:HG23	1.98	0.46
1:D:449:GLY:HA3	1:D:466:GLY:O	2.15	0.46
1:F:359:THR:O	1:F:363:GLU:HG3	2.15	0.46
1:G:449:GLY:HA3	1:G:466:GLY:O	2.16	0.46
1:A:294:LEU:HD23	1:A:306:SER:HA	1.97	0.46
1:D:235:HIS:HB3	1:D:238:VAL:HG23	1.98	0.46
1:D:311:GLN:HG3	8:D:5857:HOH:O	2.14	0.46
1:F:294:LEU:HD13	1:F:294:LEU:C	2.36	0.46
1:B:302:CYS:SG	6:B:4512:CRD:CC4	3.04	0.46
1:G:166:ILE:HD11	1:G:193:VAL:HG12	1.97	0.46
1:F:303:CYS:SG	1:F:459:PHE:HZ	2.39	0.45
1:H:408:LEU:HD12	1:H:408:LEU:N	2.30	0.45
1:E:11:PRO:HB3	1:E:114:TYR:CE1	2.51	0.45
1:E:464:PRO:HG2	1:F:490:THR:OG1	2.16	0.45
1:A:424:THR:CG2	1:A:470:MET:SD	3.04	0.45
1:G:249:ILE:O	1:G:253:ILE:HG12	2.16	0.45
1:H:244:THR:HA	1:H:268:GLU:O	2.16	0.45
1:D:12:ASN:O	1:D:15:PRO:HD3	2.16	0.45
1:E:389:VAL:HB	1:E:408:LEU:HG	1.98	0.45
1:H:170:PHE:HB3	1:H:173:LEU:HB3	1.99	0.45
1:C:120:VAL:HG12	1:C:124:MET:HE1	1.99	0.45
1:C:294:LEU:HD13	1:C:294:LEU:C	2.37	0.45
1:C:449:GLY:HA3	1:C:466:GLY:O	2.16	0.45
1:G:205:ALA:HB2	1:G:220:ILE:HD12	1.99	0.45
1:C:466:GLY:HA3	1:C:475:ARG:HD3	1.98	0.45
1:D:124:MET:HE3	1:D:173:LEU:HD22	1.97	0.45
1:C:193:VAL:HG11	1:C:201:ALA:CB	2.47	0.45
1:D:294:LEU:HD13	1:D:294:LEU:C	2.37	0.45
1:H:424:THR:HG21	1:H:470:MET:SD	2.57	0.45
1:G:303:CYS:SG	1:G:459:PHE:HZ	2.40	0.45
1:A:167:PRO:HD3	1:A:244:THR:HB	1.99	0.45
1:D:172:LEU:HD21	1:D:200:THR:HB	1.98	0.45
1:F:161:VAL:HA	1:F:188:VAL:HG23	1.98	0.45
1:H:172:LEU:HD21	1:H:200:THR:HB	1.99	0.45
1:A:466:GLY:HA3	1:A:475:ARG:HD3	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:302:CYS:N	6:G:4517:CRD:HC4	2.32	0.44
1:H:449:GLY:HA3	1:H:466:GLY:O	2.17	0.44
1:C:301[B]:CYS:SG	6:C:4513:CRD:HC12	2.58	0.44
1:D:424:THR:CG2	1:D:470:MET:SD	3.06	0.44
1:G:271:GLY:HA2	1:G:425:TYR:CD2	2.53	0.44
1:B:292:PHE:HE1	1:B:457:ASP:HB2	1.81	0.44
1:F:271:GLY:HA2	1:F:425:TYR:CG	2.52	0.44
1:B:424:THR:HG22	1:B:470:MET:HB2	1.98	0.44
1:G:38:PRO:HB3	1:G:50:GLN:HE22	1.83	0.44
1:B:249:ILE:O	1:B:253:ILE:HG12	2.18	0.44
1:C:174:MET:HE1	8:C:5817:HOH:O	2.17	0.44
1:C:302:CYS:SG	1:C:427:LEU:HD21	2.58	0.44
1:E:12:ASN:O	1:E:15:PRO:HD3	2.18	0.43
1:H:358:ASN:O	1:H:362:GLN:HG2	2.18	0.43
1:B:294:LEU:C	1:B:294:LEU:HD13	2.38	0.43
1:A:462:GLN:HB3	1:B:144:ILE:CG2	2.47	0.43
1:B:167:PRO:HD3	1:B:244:THR:HB	2.00	0.43
1:G:111:GLY:O	1:G:343:PRO:HD2	2.19	0.43
1:E:121:ASP:O	1:E:125:VAL:HG23	2.17	0.43
1:B:410:PHE:CD1	1:B:416:VAL:HB	2.54	0.43
1:A:288:GLU:HG2	8:A:5952:HOH:O	2.18	0.43
1:B:214:PRO:HA	1:B:215:PRO:HD3	1.92	0.43
1:C:244:THR:HA	1:C:268:GLU:O	2.18	0.43
1:C:424:THR:HG22	1:C:470:MET:HB2	1.99	0.43
1:F:249:ILE:O	1:F:253:ILE:HG12	2.18	0.43
1:C:161:VAL:HA	1:C:188:VAL:HG23	2.01	0.42
1:G:236:GLU:HB2	8:G:1646:HOH:O	2.20	0.42
1:H:167:PRO:HD3	1:H:244:THR:HB	2.01	0.42
1:A:476:GLU:O	1:A:477:LEU:HB2	2.18	0.42
1:E:115:VAL:HG23	8:E:5703:HOH:O	2.19	0.42
1:B:11:PRO:HB3	1:B:114:TYR:CE2	2.53	0.42
1:C:424:THR:HG21	1:C:470:MET:SD	2.60	0.42
1:G:275:ASN:ND2	1:G:430:ALA:HB3	2.34	0.42
1:E:167:PRO:HD3	1:E:244:THR:HB	2.00	0.42
1:G:8:VAL:HA	1:G:9:PRO:HD3	1.90	0.42
1:A:449:GLY:HA3	1:A:466:GLY:O	2.20	0.42
1:E:107:THR:HG23	1:E:112:LYS:O	2.20	0.42
1:D:14:GLN:HE21	1:D:14:GLN:HA	1.84	0.42
1:D:86:ARG:HD3	8:D:5586:HOH:O	2.20	0.42
1:F:244:THR:HA	1:F:268:GLU:O	2.19	0.42
1:A:120:VAL:HG12	1:A:124:MET:CE	2.50	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:GLU:HB3	8:B:5740:HOH:O	2.20	0.42
1:D:333:ASN:HA	1:D:334:PRO:HD2	1.92	0.42
1:F:214:PRO:HA	1:F:215:PRO:HD3	1.98	0.42
1:H:249:ILE:O	1:H:253:ILE:HG12	2.18	0.42
1:C:170:PHE:CZ	6:C:4513:CRD:HC13	2.55	0.41
1:A:235:HIS:HB3	1:A:238:VAL:HG23	2.01	0.41
1:H:8:VAL:HA	1:H:9:PRO:HD3	1.95	0.41
1:H:148:GLY:O	1:H:498:LYS:HE3	2.20	0.41
1:H:185:THR:HG23	1:H:482:LEU:HD22	2.01	0.41
1:E:21:GLN:HB3	1:E:29:HIS:O	2.20	0.41
1:F:413:ILE:O	1:F:417:VAL:HG23	2.19	0.41
1:G:193:VAL:HG11	1:G:201:ALA:CB	2.50	0.41
1:G:347:GLU:HG2	1:G:351:LYS:HE2	2.03	0.41
1:H:120:VAL:HG12	1:H:124:MET:HE2	2.02	0.41
1:H:167:PRO:HD3	1:H:244:THR:O	2.20	0.41
1:D:443:SER:HA	1:D:451:VAL:HG11	2.03	0.41
1:A:424:THR:HG22	1:A:470:MET:HB2	2.03	0.41
1:B:8:VAL:HA	1:B:9:PRO:HD3	1.95	0.41
1:G:319:VAL:O	1:G:323:VAL:HG23	2.21	0.41
1:C:106:GLU:OE2	1:C:171:PRO:HB2	2.21	0.41
1:C:121:ASP:O	1:C:125:VAL:HG23	2.20	0.41
1:F:63:VAL:HG11	1:F:235:HIS:CE1	2.56	0.41
1:A:303:CYS:SG	1:A:459:PHE:HZ	2.44	0.41
1:A:319:VAL:O	1:A:323:VAL:HG23	2.21	0.41
1:B:459:PHE:CE1	6:B:4512:CRD:HC12	2.55	0.41
1:C:170:PHE:HB3	1:C:173:LEU:HB3	2.03	0.41
1:C:271:GLY:HA2	1:C:425:TYR:CG	2.56	0.41
1:E:294:LEU:C	1:E:294:LEU:HD13	2.41	0.41
1:G:131:TYR:CE1	1:G:462:GLN:HG3	2.56	0.41
1:H:120:VAL:HG12	1:H:124:MET:CE	2.50	0.41
1:H:214:PRO:HA	1:H:215:PRO:HD3	1.92	0.41
1:B:246:SER:HB3	5:B:5502:NAD:O4D	2.21	0.41
1:C:149:ASP:HA	1:C:498:LYS:HB2	2.03	0.41
1:F:167:PRO:HD3	1:F:244:THR:O	2.21	0.41
1:H:121:ASP:O	1:H:125:VAL:HG23	2.21	0.40
1:B:120:VAL:CG1	1:B:124:MET:HE1	2.50	0.40
1:B:247:THR:HA	1:B:269:LEU:HD13	2.02	0.40
1:C:8:VAL:HA	1:C:9:PRO:HD3	1.95	0.40
1:C:21:GLN:HB3	1:C:29:HIS:O	2.22	0.40
1:C:154:THR:HA	1:C:489:LYS:O	2.21	0.40
1:F:11:PRO:HB3	1:F:114:TYR:CZ	2.56	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:271:GLY:HA2	1:G:425:TYR:CG	2.57	0.40
1:H:292:PHE:HE1	1:H:457:ASP:HB2	1.86	0.40
1:E:298:GLN:HA	8:E:5696:HOH:O	2.20	0.40
1:F:301[B]:CYS:SG	6:F:4516:CRD:CC2	3.09	0.40
1:H:107:THR:HG23	1:H:112:LYS:O	2.21	0.40
1:A:11:PRO:HB3	1:A:114:TYR:CE1	2.56	0.40
1:A:281:ALA:HB2	1:A:432:PHE:O	2.22	0.40
1:E:111:GLY:O	1:E:343:PRO:HD2	2.22	0.40
1:G:464:PRO:HG2	1:H:490:THR:OG1	2.21	0.40
1:B:424:THR:HG21	1:B:470:MET:SD	2.61	0.40
1:D:414:GLU:O	1:D:417:VAL:HG12	2.21	0.40
1:E:417:VAL:HG22	1:E:442:LEU:HD23	2.04	0.40
1:F:193:VAL:HG11	1:F:201:ALA:CB	2.51	0.40
1:G:377:ARG:HG2	1:G:377:ARG:NH1	2.36	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	493/500 (99%)	477 (97%)	16 (3%)	0	100	100
1	B	493/500 (99%)	476 (97%)	17 (3%)	0	100	100
1	C	494/500 (99%)	477 (97%)	17 (3%)	0	100	100
1	D	493/500 (99%)	475 (96%)	18 (4%)	0	100	100
1	E	493/500 (99%)	476 (97%)	17 (3%)	0	100	100
1	F	493/500 (99%)	476 (97%)	17 (3%)	0	100	100
1	G	493/500 (99%)	471 (96%)	22 (4%)	0	100	100
1	H	493/500 (99%)	474 (96%)	19 (4%)	0	100	100
All	All	3945/4000 (99%)	3802 (96%)	143 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	400/402 (100%)	397 (99%)	3 (1%)	81	86
1	B	400/402 (100%)	396 (99%)	4 (1%)	76	81
1	C	401/402 (100%)	397 (99%)	4 (1%)	76	81
1	D	400/402 (100%)	396 (99%)	4 (1%)	76	81
1	E	400/402 (100%)	398 (100%)	2 (0%)	88	92
1	F	400/402 (100%)	396 (99%)	4 (1%)	76	81
1	G	400/402 (100%)	398 (100%)	2 (0%)	88	92
1	H	400/402 (100%)	396 (99%)	4 (1%)	76	81
All	All	3201/3216 (100%)	3174 (99%)	27 (1%)	81	86

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	192	LYS
1	A	401	PHE
1	B	34	ARG
1	B	192	LYS
1	B	401	PHE
1	B	498	LYS
1	C	6	GLN
1	C	192	LYS
1	C	377	ARG
1	C	401	PHE
1	D	14	GLN
1	D	192	LYS
1	D	206	ASN
1	D	401	PHE
1	E	192	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	401	PHE
1	F	192	LYS
1	F	206	ASN
1	F	377	ARG
1	F	401	PHE
1	G	192	LYS
1	G	401	PHE
1	H	192	LYS
1	H	254	GLN
1	H	275	ASN
1	H	401	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	50	GLN
1	A	175	GLN
1	B	71	GLN
1	C	175	GLN
1	C	254	GLN
1	C	440	ASN
1	D	14	GLN
1	D	26	ASN
1	D	362	GLN
1	D	406	GLN
1	E	26	ASN
1	E	254	GLN
1	E	275	ASN
1	E	362	GLN
1	F	14	GLN
1	F	89	ASN
1	F	497	GLN
1	F	499	ASN
1	G	13	GLN
1	G	14	GLN
1	G	50	GLN
1	G	89	ASN
1	G	275	ASN
1	G	289	GLN
1	G	349	GLN
1	G	440	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	H	50	GLN
1	H	71	GLN
1	H	275	ASN
1	H	358	ASN
1	H	362	GLN
1	H	483	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 16 are monoatomic - leaving 30 for Mogul analysis.

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
6	CRD	C	4513	-	4,4,4	0.44	0	2,3,3	1.72	1 (50%)
6	CRD	D	4514	-	4,4,4	0.36	0	2,3,3	2.14	2 (100%)
7	EDO	D	4901	-	3,3,3	0.44	0	2,2,2	0.38	0
5	NAD	B	5502	2	42,48,48	2.30	9 (21%)	50,73,73	1.40	10 (20%)
4	GAI	A	4801	-	3,3,3	1.53	1 (33%)	3,3,3	0.99	0
7	EDO	G	4907	-	3,3,3	0.51	0	2,2,2	0.32	0
7	EDO	E	4905	-	3,3,3	0.48	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	CRD	E	4515	-	4,4,4	0.41	0	2,3,3	1.96	1 (50%)
5	NAD	C	5503	2	42,48,48	2.15	9 (21%)	50,73,73	1.45	10 (20%)
5	NAD	F	5506	2	42,48,48	2.15	9 (21%)	50,73,73	1.46	7 (14%)
4	GAI	B	4802	-	3,3,3	1.29	1 (33%)	3,3,3	0.83	0
6	CRD	G	4517	-	4,4,4	0.33	0	2,3,3	2.22	1 (50%)
7	EDO	C	4902	-	3,3,3	0.49	0	2,2,2	0.32	0
6	CRD	B	4512	-	4,4,4	0.38	0	2,3,3	1.92	1 (50%)
4	GAI	C	4803	-	3,3,3	1.18	1 (33%)	3,3,3	0.93	0
4	GAI	G	4807	-	3,3,3	1.16	0	3,3,3	0.88	0
5	NAD	A	5501	2	42,48,48	2.18	8 (19%)	50,73,73	1.51	9 (18%)
7	EDO	F	4906	-	3,3,3	0.46	0	2,2,2	0.37	0
5	NAD	G	5507	2	42,48,48	2.23	8 (19%)	50,73,73	1.30	8 (16%)
6	CRD	F	4516	-	4,4,4	0.28	0	2,3,3	2.00	1 (50%)
4	GAI	D	4804	-	3,3,3	1.42	1 (33%)	3,3,3	0.93	0
4	GAI	H	4808	-	3,3,3	1.50	1 (33%)	3,3,3	0.91	0
5	NAD	H	5508	2	42,48,48	2.20	9 (21%)	50,73,73	1.54	9 (18%)
4	GAI	F	4806	-	3,3,3	1.59	1 (33%)	3,3,3	0.96	0
5	NAD	E	5505	2	42,48,48	2.10	9 (21%)	50,73,73	1.61	8 (16%)
7	EDO	C	4903	-	3,3,3	0.50	0	2,2,2	0.29	0
5	NAD	D	5504	2	42,48,48	2.09	9 (21%)	50,73,73	1.65	10 (20%)
7	EDO	H	4908	-	3,3,3	0.43	0	2,2,2	0.38	0
7	EDO	D	4904	-	3,3,3	0.45	0	2,2,2	0.30	0
4	GAI	E	4805	-	3,3,3	1.22	1 (33%)	3,3,3	0.94	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
6	CRD	C	4513	-	-	1/2/2/2	-
6	CRD	D	4514	-	-	1/2/2/2	-
7	EDO	D	4901	-	-	0/1/1/1	-
5	NAD	B	5502	2	-	2/26/62/62	0/5/5/5
7	EDO	G	4907	-	-	0/1/1/1	-
7	EDO	E	4905	-	-	0/1/1/1	-
6	CRD	E	4515	-	-	1/2/2/2	-
5	NAD	C	5503	2	-	3/26/62/62	0/5/5/5

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAD	F	5506	2	-	0/26/62/62	0/5/5/5
6	CRD	G	4517	-	-	1/2/2/2	-
7	EDO	C	4902	-	-	0/1/1/1	-
6	CRD	B	4512	-	-	1/2/2/2	-
5	NAD	A	5501	2	-	2/26/62/62	0/5/5/5
7	EDO	F	4906	-	-	0/1/1/1	-
5	NAD	G	5507	2	-	0/26/62/62	0/5/5/5
6	CRD	F	4516	-	-	1/2/2/2	-
5	NAD	H	5508	2	-	0/26/62/62	0/5/5/5
5	NAD	E	5505	2	-	2/26/62/62	0/5/5/5
7	EDO	C	4903	-	-	0/1/1/1	-
5	NAD	D	5504	2	-	1/26/62/62	0/5/5/5
7	EDO	H	4908	-	-	0/1/1/1	-
7	EDO	D	4904	-	-	0/1/1/1	-

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	5507	NAD	C3N-C7N	-10.83	1.34	1.50
5	B	5502	NAD	C3N-C7N	-10.66	1.34	1.50
5	A	5501	NAD	C3N-C7N	-10.18	1.35	1.50
5	C	5503	NAD	C3N-C7N	-10.15	1.35	1.50
5	H	5508	NAD	C3N-C7N	-10.06	1.35	1.50
5	F	5506	NAD	C3N-C7N	-10.02	1.35	1.50
5	E	5505	NAD	C3N-C7N	-9.55	1.36	1.50
5	D	5504	NAD	C3N-C7N	-9.05	1.37	1.50
5	B	5502	NAD	C2A-N3A	5.12	1.40	1.32
5	H	5508	NAD	C2A-N3A	5.02	1.40	1.32
5	D	5504	NAD	C2A-N3A	4.73	1.39	1.32
5	F	5506	NAD	C2A-N3A	4.65	1.39	1.32
5	G	5507	NAD	C2A-N3A	4.62	1.39	1.32
5	C	5503	NAD	C2A-N3A	4.59	1.39	1.32
5	E	5505	NAD	C2A-N3A	4.42	1.39	1.32
5	A	5501	NAD	C2A-N3A	4.41	1.39	1.32
5	D	5504	NAD	C2A-N1A	3.51	1.40	1.33
5	H	5508	NAD	C2A-N1A	3.43	1.40	1.33
5	C	5503	NAD	C2A-N1A	3.40	1.40	1.33
5	B	5502	NAD	C2A-N1A	3.37	1.40	1.33
5	F	5506	NAD	C2A-N1A	3.34	1.40	1.33
5	D	5504	NAD	C8A-N7A	3.32	1.40	1.34
5	A	5501	NAD	C2A-N1A	3.30	1.40	1.33
5	E	5505	NAD	O4D-C1D	3.23	1.45	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	5505	NAD	C2A-N1A	3.20	1.39	1.33
5	G	5507	NAD	C4N-C3N	-3.13	1.33	1.39
5	B	5502	NAD	C4N-C3N	-3.08	1.34	1.39
5	A	5501	NAD	C4N-C3N	-3.08	1.34	1.39
5	E	5505	NAD	C4N-C3N	-3.08	1.34	1.39
5	A	5501	NAD	C8A-N7A	3.05	1.40	1.34
5	G	5507	NAD	C2A-N1A	3.03	1.39	1.33
5	B	5502	NAD	C8A-N7A	3.03	1.40	1.34
5	F	5506	NAD	C2N-C3N	-2.97	1.34	1.39
5	B	5502	NAD	O4D-C1D	2.93	1.45	1.41
5	H	5508	NAD	C4N-C3N	-2.92	1.34	1.39
5	C	5503	NAD	C2N-C3N	-2.91	1.34	1.39
5	F	5506	NAD	C4N-C3N	-2.90	1.34	1.39
5	D	5504	NAD	C4N-C3N	-2.85	1.34	1.39
5	H	5508	NAD	C5N-C4N	-2.82	1.33	1.38
5	B	5502	NAD	C4A-N3A	2.79	1.39	1.35
4	F	4806	GAI	C-N1	2.72	1.36	1.30
5	G	5507	NAD	C8A-N7A	2.72	1.39	1.34
5	F	5506	NAD	O4D-C1D	2.72	1.44	1.41
5	B	5502	NAD	C2N-C3N	-2.71	1.34	1.39
5	A	5501	NAD	C2N-C3N	-2.70	1.34	1.39
5	A	5501	NAD	O4D-C1D	2.69	1.44	1.41
5	B	5502	NAD	C5N-C4N	-2.66	1.33	1.38
4	A	4801	GAI	C-N1	2.64	1.36	1.30
5	D	5504	NAD	C2N-C3N	-2.64	1.34	1.39
5	H	5508	NAD	C8A-N7A	2.63	1.39	1.34
5	G	5507	NAD	C2N-C3N	-2.61	1.35	1.39
5	G	5507	NAD	C5N-C4N	-2.60	1.33	1.38
5	H	5508	NAD	C4A-N3A	2.59	1.39	1.35
5	A	5501	NAD	C5N-C4N	-2.59	1.33	1.38
4	H	4808	GAI	C-N1	2.59	1.36	1.30
5	D	5504	NAD	O4D-C1D	2.59	1.44	1.41
5	C	5503	NAD	C4N-C3N	-2.57	1.34	1.39
5	H	5508	NAD	O4D-C1D	2.54	1.44	1.41
5	H	5508	NAD	C2N-C3N	-2.49	1.35	1.39
5	C	5503	NAD	C5N-C4N	-2.47	1.33	1.38
5	G	5507	NAD	O4D-C1D	2.39	1.44	1.41
4	D	4804	GAI	C-N1	2.39	1.35	1.30
5	D	5504	NAD	C5N-C4N	-2.38	1.33	1.38
5	E	5505	NAD	C8A-N7A	2.37	1.38	1.34
5	C	5503	NAD	O4D-C1D	2.36	1.44	1.41
5	F	5506	NAD	C4A-N3A	2.35	1.38	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	5505	NAD	C5N-C4N	-2.35	1.34	1.38
5	F	5506	NAD	C5N-C4N	-2.34	1.34	1.38
5	F	5506	NAD	C8A-N7A	2.30	1.38	1.34
5	C	5503	NAD	C8A-N7A	2.30	1.38	1.34
5	C	5503	NAD	C4A-N3A	2.24	1.38	1.35
4	B	4802	GAI	C-N1	2.20	1.35	1.30
5	E	5505	NAD	C4A-N3A	2.18	1.38	1.35
5	E	5505	NAD	C2N-C3N	-2.09	1.35	1.39
4	E	4805	GAI	C-N1	2.08	1.35	1.30
5	D	5504	NAD	C4A-N3A	2.07	1.38	1.35
4	C	4803	GAI	C-N1	2.03	1.34	1.30

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	5504	NAD	O7N-C7N-N7N	-5.39	114.92	122.58
5	E	5505	NAD	C3N-C7N-N7N	4.70	123.39	117.75
5	E	5505	NAD	O7N-C7N-N7N	-4.61	116.03	122.58
5	E	5505	NAD	N3A-C2A-N1A	-4.18	122.15	128.68
5	H	5508	NAD	N3A-C2A-N1A	-4.07	122.32	128.68
5	F	5506	NAD	O7N-C7N-N7N	-3.94	116.98	122.58
5	D	5504	NAD	N3A-C2A-N1A	-3.87	122.64	128.68
5	C	5503	NAD	O7N-C7N-N7N	-3.76	117.24	122.58
5	A	5501	NAD	C3N-C7N-N7N	3.73	122.23	117.75
5	F	5506	NAD	C3N-C7N-N7N	3.69	122.18	117.75
5	F	5506	NAD	O4B-C1B-C2B	-3.69	101.54	106.93
5	A	5501	NAD	N3A-C2A-N1A	-3.67	122.94	128.68
5	A	5501	NAD	O7N-C7N-N7N	-3.65	117.39	122.58
5	C	5503	NAD	O4B-C1B-C2B	-3.64	101.61	106.93
5	F	5506	NAD	N3A-C2A-N1A	-3.62	123.01	128.68
5	H	5508	NAD	O7N-C7N-N7N	-3.57	117.50	122.58
5	D	5504	NAD	O7N-C7N-C3N	3.57	123.90	119.63
5	A	5501	NAD	O4B-C1B-C2B	-3.42	101.93	106.93
5	H	5508	NAD	C3N-C7N-N7N	3.38	121.80	117.75
5	C	5503	NAD	N3A-C2A-N1A	-3.25	123.59	128.68
5	G	5507	NAD	C3N-C7N-N7N	3.24	121.64	117.75
5	B	5502	NAD	N3A-C2A-N1A	-3.18	123.71	128.68
5	G	5507	NAD	N3A-C2A-N1A	-3.06	123.90	128.68
5	D	5504	NAD	PN-O3-PA	-3.05	122.38	132.83
5	C	5503	NAD	C3N-C7N-N7N	3.04	121.39	117.75
5	D	5504	NAD	O4D-C4D-C3D	-2.97	99.23	105.11
5	B	5502	NAD	O4D-C4D-C3D	-2.95	99.28	105.11

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	5501	NAD	C2B-C3B-C4B	-2.91	96.99	102.64
5	B	5502	NAD	O7N-C7N-N7N	-2.90	118.46	122.58
5	E	5505	NAD	PN-O3-PA	-2.86	123.01	132.83
5	D	5504	NAD	C3N-C7N-N7N	2.85	121.18	117.75
5	B	5502	NAD	O4B-C1B-C2B	-2.83	102.79	106.93
5	G	5507	NAD	PN-O3-PA	-2.82	123.14	132.83
5	H	5508	NAD	PN-O3-PA	-2.78	123.28	132.83
5	C	5503	NAD	PN-O3-PA	-2.78	123.28	132.83
5	E	5505	NAD	O4B-C1B-C2B	-2.77	102.88	106.93
5	F	5506	NAD	C2B-C3B-C4B	-2.74	97.31	102.64
5	B	5502	NAD	C3N-C7N-N7N	2.68	120.96	117.75
5	H	5508	NAD	C6N-C5N-C4N	-2.59	115.67	119.44
5	A	5501	NAD	PN-O3-PA	-2.55	124.07	132.83
5	D	5504	NAD	O4B-C1B-C2B	-2.53	103.23	106.93
5	B	5502	NAD	C2B-C3B-C4B	-2.51	97.77	102.64
6	G	4517	CRD	CC1-CC2-CC3	-2.49	119.29	125.55
5	E	5505	NAD	C2D-C3D-C4D	-2.49	97.81	102.64
5	G	5507	NAD	O7N-C7N-N7N	-2.47	119.07	122.58
5	D	5504	NAD	C5N-C4N-C3N	2.47	123.26	120.34
5	H	5508	NAD	C2B-C3B-C4B	-2.46	97.87	102.64
5	H	5508	NAD	O4D-C4D-C3D	-2.42	100.32	105.11
5	B	5502	NAD	PN-O3-PA	-2.42	124.51	132.83
5	D	5504	NAD	C6N-C5N-C4N	-2.38	115.97	119.44
5	B	5502	NAD	C6N-C5N-C4N	-2.36	116.01	119.44
5	C	5503	NAD	O4D-C4D-C3D	-2.36	100.45	105.11
5	A	5501	NAD	C6N-C5N-C4N	-2.32	116.07	119.44
5	G	5507	NAD	O4B-C1B-C2B	-2.26	103.62	106.93
5	H	5508	NAD	C6N-N1N-C2N	-2.21	119.96	121.97
5	A	5501	NAD	C5N-C4N-C3N	2.19	122.94	120.34
6	D	4514	CRD	OC1-CC4-CC3	-2.19	118.19	125.67
5	D	5504	NAD	C3D-C2D-C1D	-2.19	97.68	100.98
5	C	5503	NAD	C3D-C2D-C1D	-2.19	97.69	100.98
6	E	4515	CRD	CC1-CC2-CC3	-2.18	120.08	125.55
5	A	5501	NAD	O4D-C4D-C3D	-2.18	100.81	105.11
5	E	5505	NAD	C2B-C3B-C4B	-2.17	98.43	102.64
5	G	5507	NAD	C6N-C5N-C4N	-2.17	116.29	119.44
5	C	5503	NAD	C6N-C5N-C4N	-2.16	116.30	119.44
5	F	5506	NAD	C6N-C5N-C4N	-2.14	116.32	119.44
5	B	5502	NAD	C2N-C3N-C4N	2.11	120.65	118.26
6	D	4514	CRD	CC1-CC2-CC3	-2.09	120.29	125.55
6	C	4513	CRD	CC1-CC2-CC3	-2.08	120.31	125.55
5	E	5505	NAD	C6N-C5N-C4N	-2.08	116.41	119.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	5502	NAD	C3D-C2D-C1D	-2.08	97.84	100.98
5	G	5507	NAD	C6N-N1N-C2N	-2.07	120.09	121.97
6	B	4512	CRD	CC1-CC2-CC3	-2.05	120.41	125.55
5	C	5503	NAD	C2B-C3B-C4B	-2.04	98.68	102.64
5	G	5507	NAD	C2N-C3N-C4N	2.03	120.56	118.26
5	F	5506	NAD	C6N-N1N-C2N	-2.02	120.14	121.97
5	H	5508	NAD	C2N-C3N-C4N	2.02	120.55	118.26
6	F	4516	CRD	OC1-CC4-CC3	-2.01	118.81	125.67
5	C	5503	NAD	C5A-C6A-N6A	2.00	123.39	120.35

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	4512	CRD	CC2-CC3-CC4-OC1
6	C	4513	CRD	CC2-CC3-CC4-OC1
6	D	4514	CRD	CC2-CC3-CC4-OC1
6	E	4515	CRD	CC2-CC3-CC4-OC1
6	F	4516	CRD	CC2-CC3-CC4-OC1
6	G	4517	CRD	CC2-CC3-CC4-OC1
5	A	5501	NAD	C5B-O5B-PA-O3
5	A	5501	NAD	C5B-O5B-PA-O2A
5	B	5502	NAD	C5B-O5B-PA-O2A
5	C	5503	NAD	PN-O3-PA-O1A
5	D	5504	NAD	PN-O3-PA-O1A
5	C	5503	NAD	C4N-C3N-C7N-O7N
5	C	5503	NAD	C4N-C3N-C7N-N7N
5	B	5502	NAD	C5B-O5B-PA-O3
5	E	5505	NAD	C5B-O5B-PA-O3
5	E	5505	NAD	C5B-O5B-PA-O2A

There are no ring outliers.

7 monomers are involved in 37 short contacts:

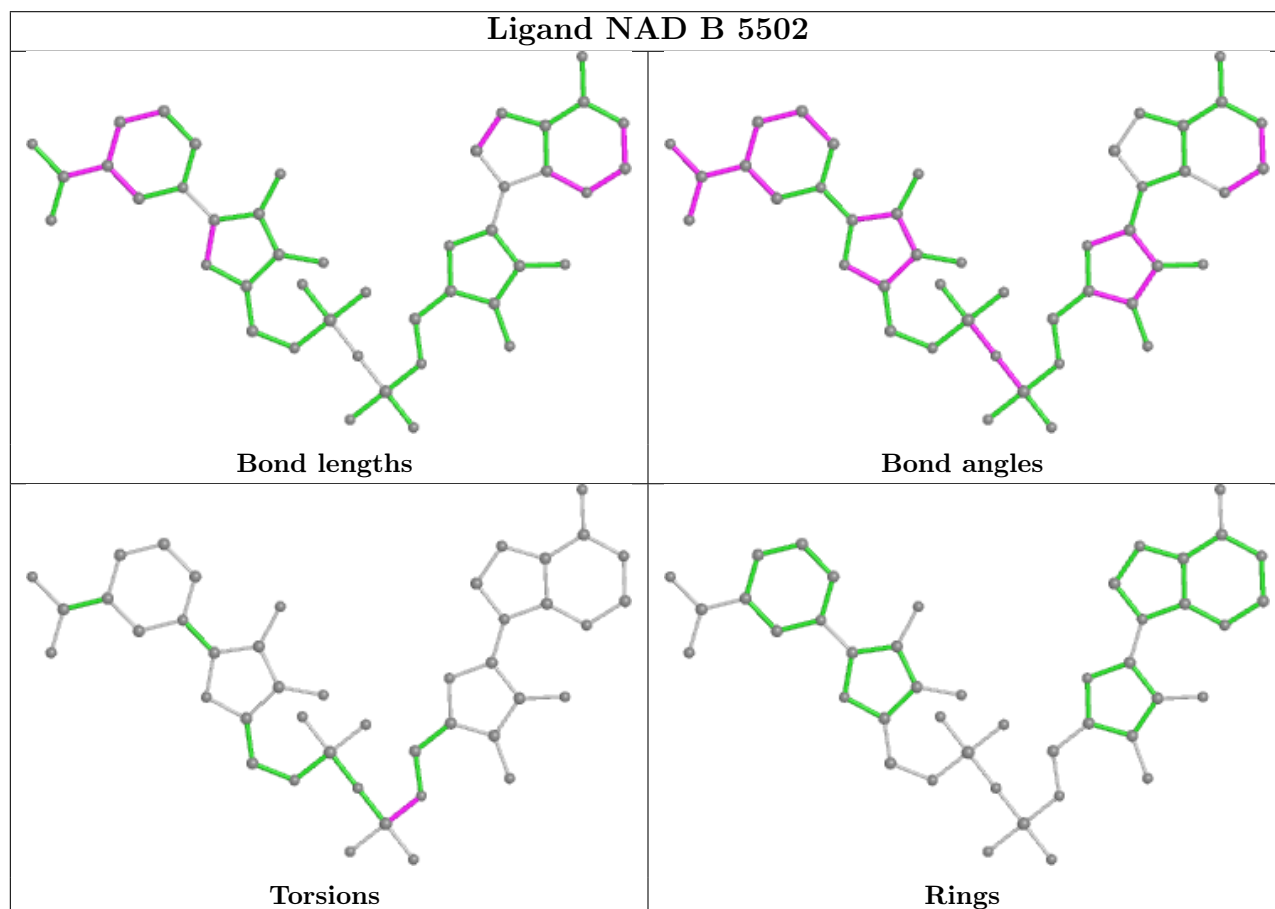
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	4513	CRD	6	0
6	D	4514	CRD	5	0
5	B	5502	NAD	1	0
6	E	4515	CRD	4	0
6	G	4517	CRD	9	0
6	B	4512	CRD	4	0

*Continued on next page...*

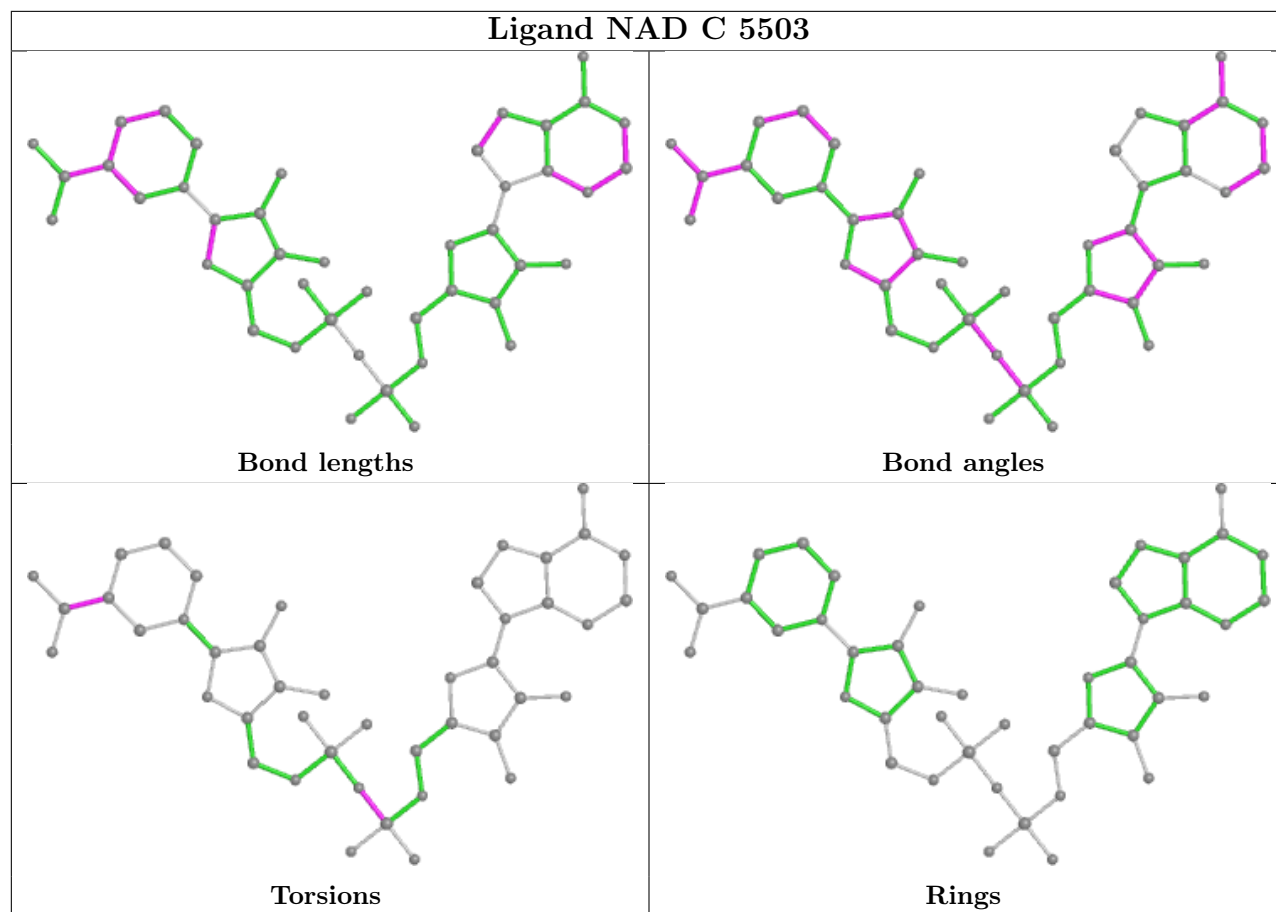
*Continued from previous page...*

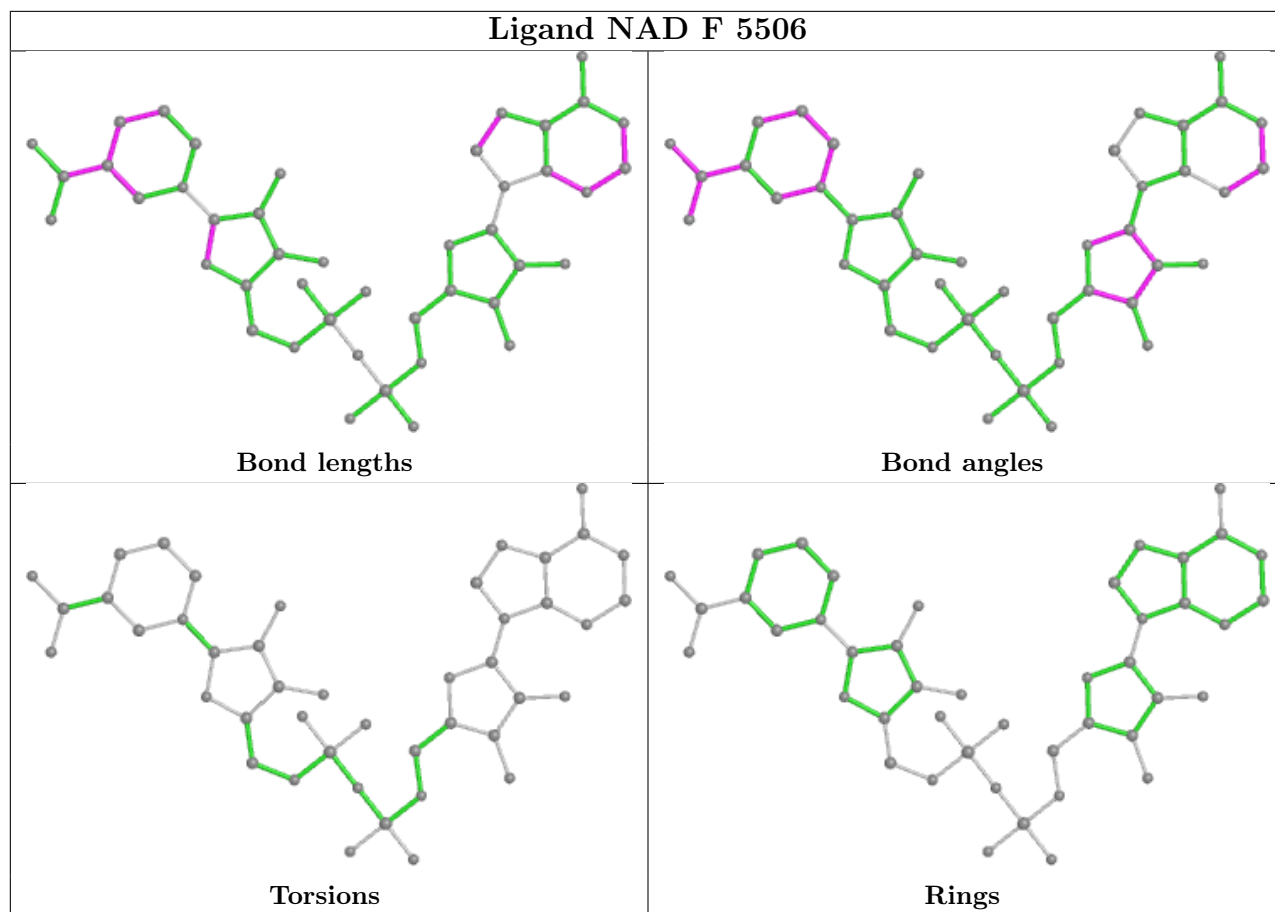
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	4516	CRD	8	0

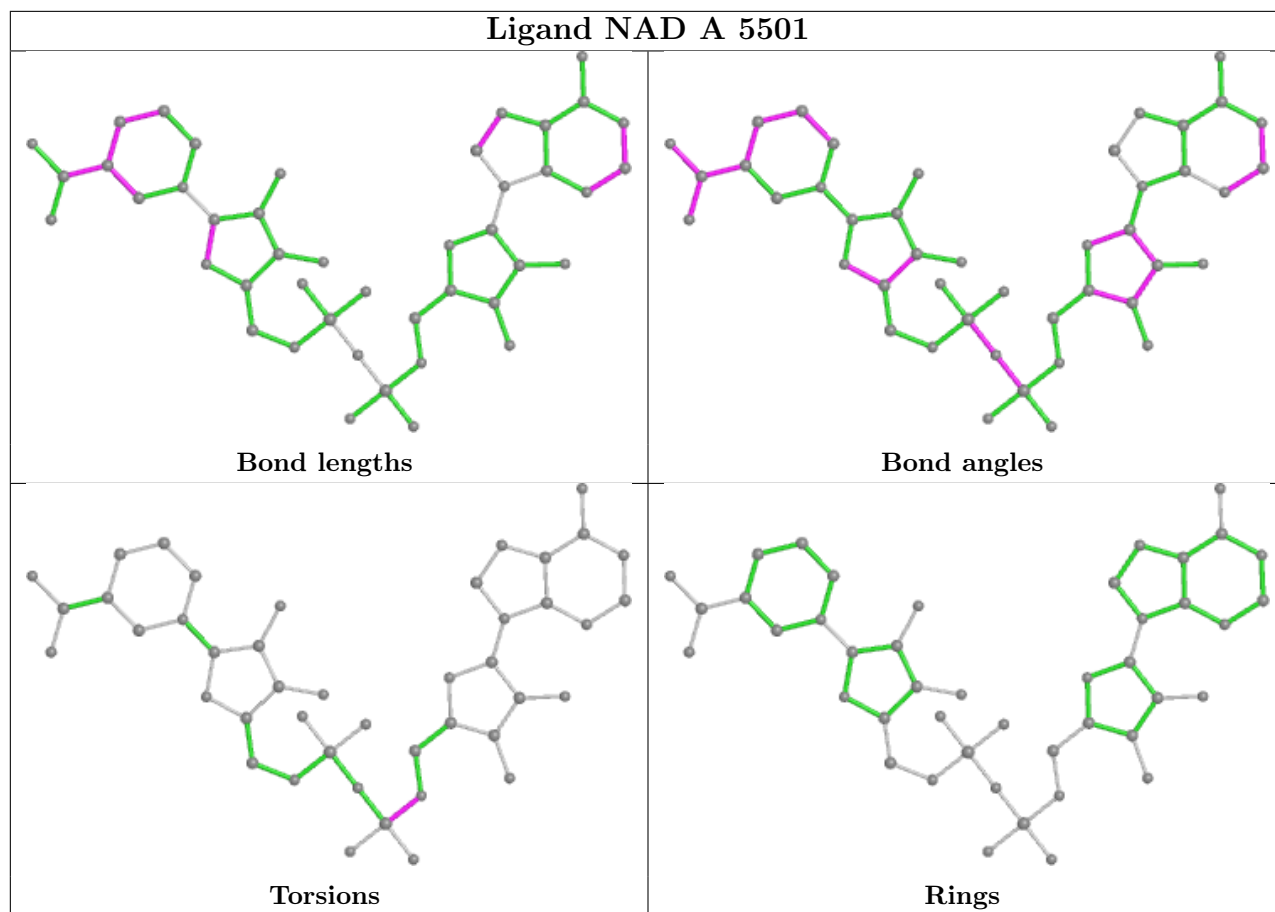
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

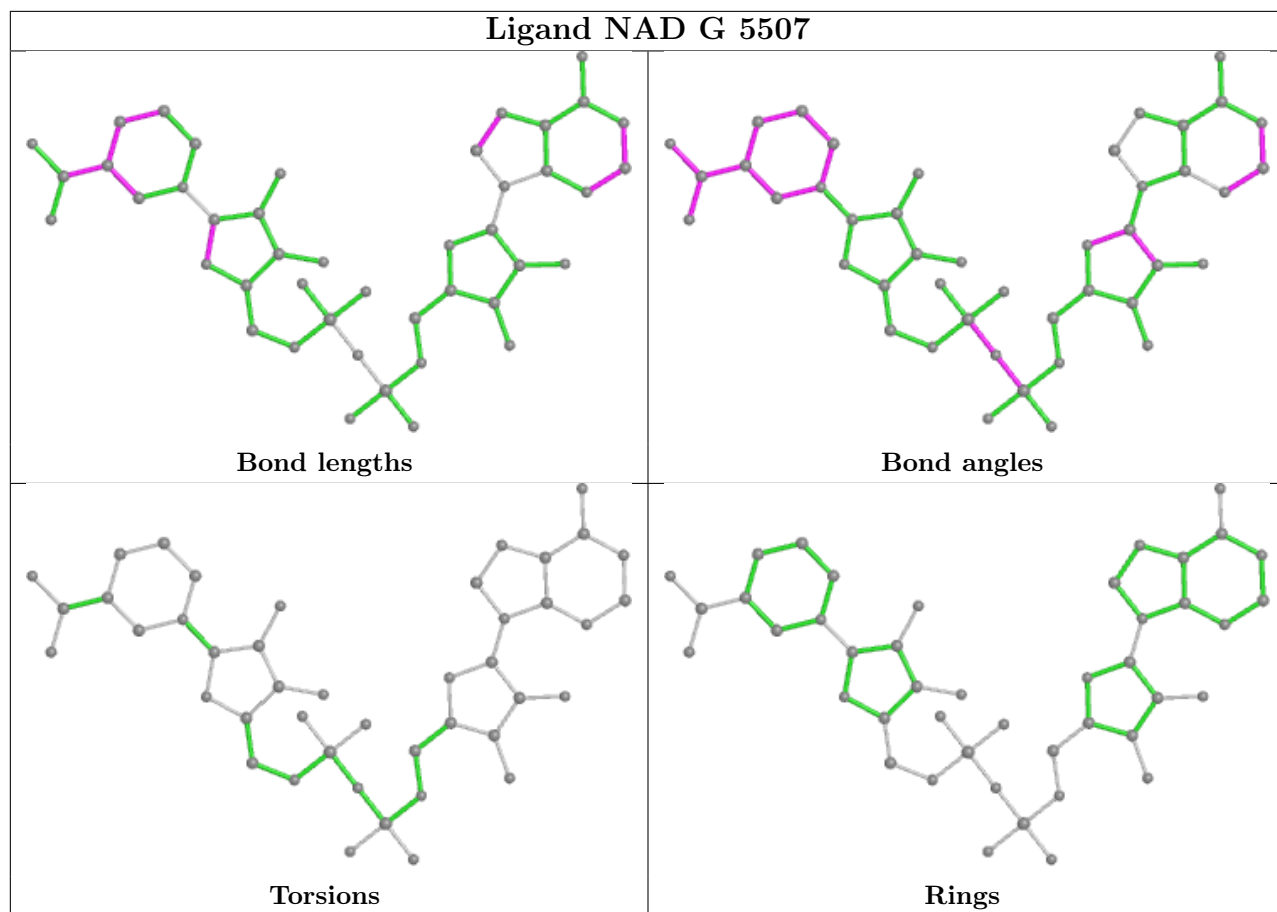


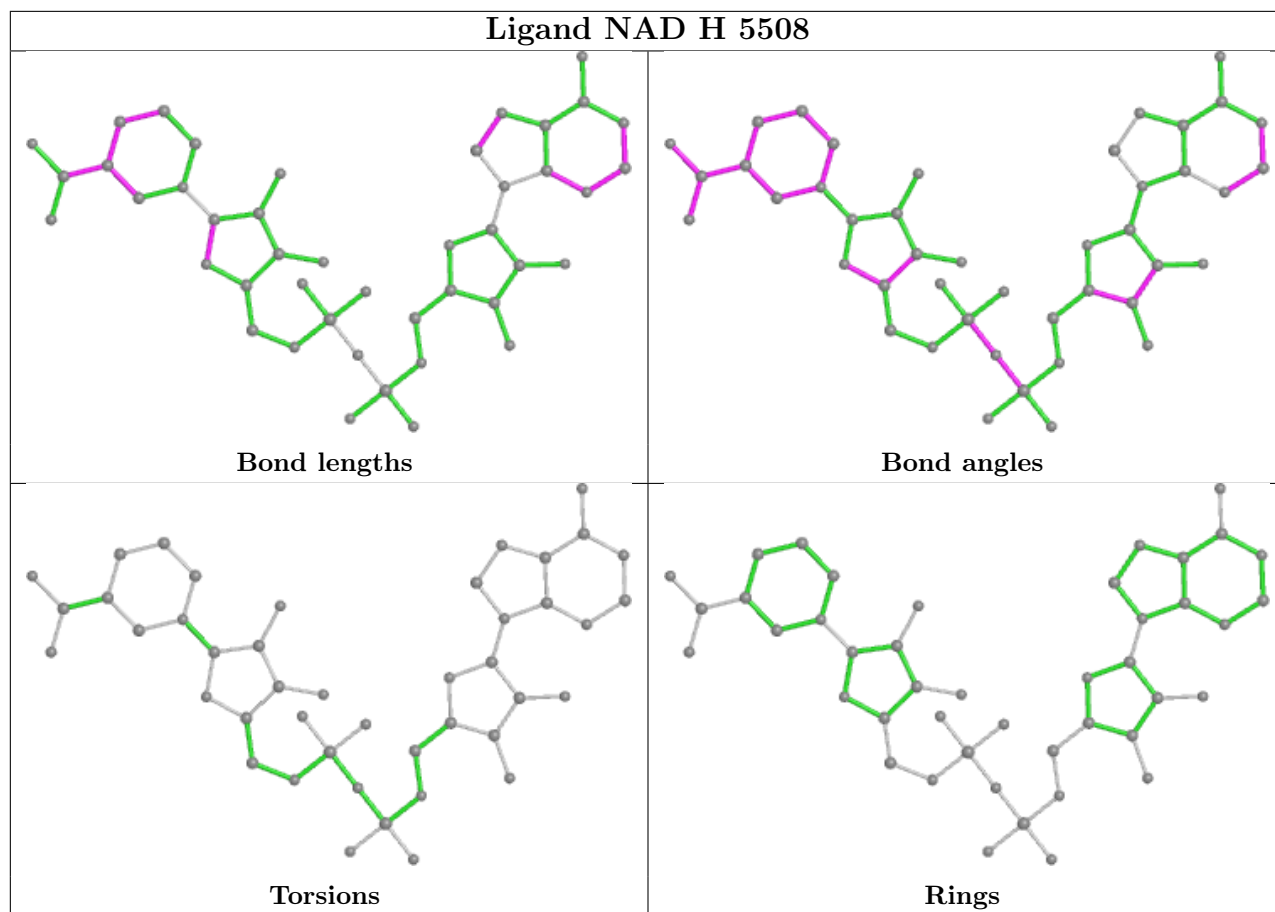


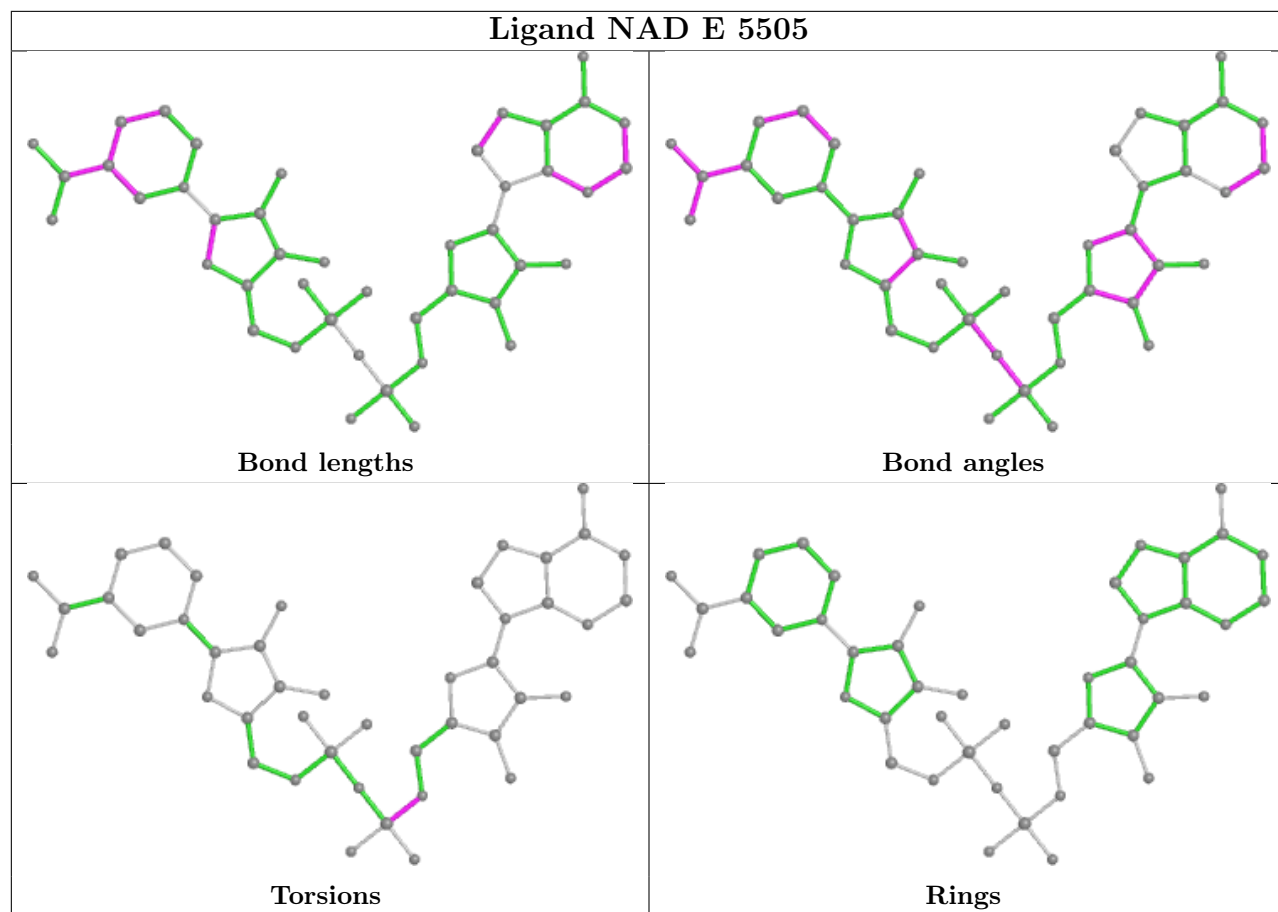


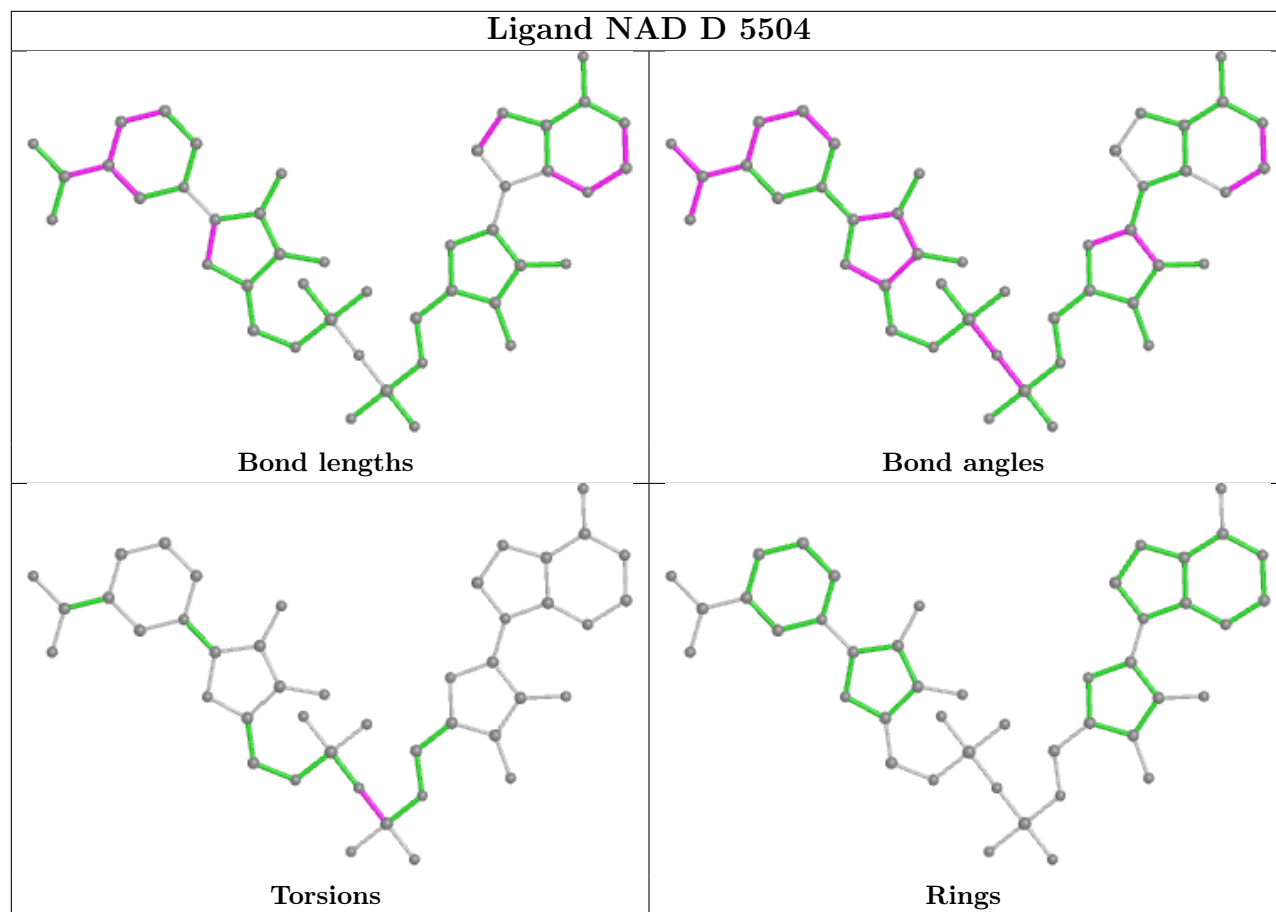












## 5.7 Other polymers [i](#)

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	494/500 (98%)	-0.34	3 (0%) 89 91	8, 18, 31, 47	0
1	B	494/500 (98%)	-0.52	1 (0%) 95 96	9, 15, 24, 39	0
1	C	495/500 (99%)	-0.53	2 (0%) 92 94	9, 15, 24, 42	1 (0%)
1	D	494/500 (98%)	-0.45	3 (0%) 89 91	9, 16, 28, 48	0
1	E	494/500 (98%)	-0.44	1 (0%) 95 96	9, 16, 28, 51	0
1	F	494/500 (98%)	-0.56	0 100 100	8, 15, 25, 36	0
1	G	494/500 (98%)	-0.37	3 (0%) 89 91	12, 18, 31, 53	0
1	H	494/500 (98%)	-0.15	7 (1%) 75 80	11, 21, 36, 53	0
All	All	3953/4000 (98%)	-0.42	20 (0%) 91 93	8, 17, 30, 53	1 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	376	ASP	5.3
1	G	7	ALA	4.4
1	B	7	ALA	4.2
1	H	7	ALA	3.9
1	H	10	ALA	3.5
1	E	376	ASP	3.5
1	D	7	ALA	2.9
1	H	34	ARG	2.6
1	G	14	GLN	2.6
1	C	7	ALA	2.5
1	D	376	ASP	2.5
1	A	10	ALA	2.4
1	C	6	GLN	2.4
1	H	377	ARG	2.3
1	A	376	ASP	2.3
1	H	350	PHE	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	336	ASP	2.2
1	A	14	GLN	2.1
1	G	11	PRO	2.1
1	H	375	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å <sup>2</sup> )	Q<0.9
6	CRD	G	4517	5/5	0.65	0.40	41,42,46,48	0
6	CRD	D	4514	5/5	0.69	0.43	47,47,48,48	0
2	MG	A	4601	1/1	0.74	0.10	47,47,47,47	0
2	MG	E	4605	1/1	0.75	0.19	48,48,48,48	0
6	CRD	C	4513	5/5	0.75	0.47	44,46,47,49	0
6	CRD	B	4512	5/5	0.76	0.44	44,46,47,48	0
2	MG	B	4602	1/1	0.77	0.18	37,37,37,37	0
2	MG	F	4606	1/1	0.80	0.31	40,40,40,40	0
6	CRD	E	4515	5/5	0.81	0.41	48,49,50,53	0
2	MG	C	4603	1/1	0.83	0.27	39,39,39,39	0
2	MG	D	4604	1/1	0.85	0.25	43,43,43,43	0
6	CRD	F	4516	5/5	0.87	0.35	44,44,46,47	0
3	NA	E	4705	1/1	0.87	0.13	27,27,27,27	0
3	NA	A	4701	1/1	0.88	0.08	31,31,31,31	0
4	GAI	A	4801	4/4	0.89	0.13	15,16,18,20	0
4	GAI	H	4808	4/4	0.89	0.14	22,23,25,25	0
7	EDO	H	4908	4/4	0.89	0.14	24,27,27,27	0
5	NAD	H	5508	44/44	0.90	0.13	19,34,43,44	0
4	GAI	D	4804	4/4	0.91	0.13	13,18,20,21	0

*Continued on next page...*

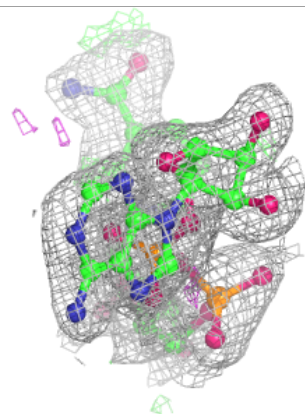
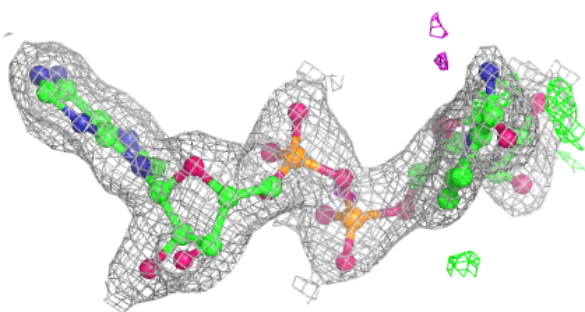
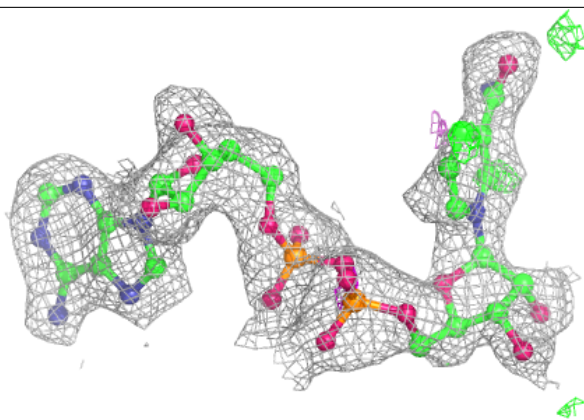
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	G	4607	1/1	0.91	0.23	45,45,45,45	0
4	GAI	F	4806	4/4	0.92	0.11	18,18,19,20	0
4	GAI	B	4802	4/4	0.93	0.11	17,19,20,21	0
5	NAD	D	5504	44/44	0.93	0.12	11,22,35,36	0
2	MG	H	4608	1/1	0.93	0.09	32,32,32,32	0
4	GAI	E	4805	4/4	0.93	0.11	20,20,22,23	0
3	NA	D	4704	1/1	0.93	0.10	24,24,24,24	0
5	NAD	G	5507	44/44	0.94	0.12	16,30,39,40	0
5	NAD	A	5501	44/44	0.94	0.11	14,24,37,37	0
5	NAD	E	5505	44/44	0.94	0.11	13,23,34,34	0
5	NAD	C	5503	44/44	0.95	0.11	9,23,31,32	0
4	GAI	C	4803	4/4	0.95	0.08	17,18,19,20	0
3	NA	H	4708	1/1	0.95	0.09	27,27,27,27	0
7	EDO	C	4902	4/4	0.95	0.10	18,22,24,24	0
7	EDO	F	4906	4/4	0.95	0.11	20,23,23,23	0
5	NAD	B	5502	44/44	0.95	0.09	15,26,33,34	0
7	EDO	D	4901	4/4	0.96	0.12	20,21,24,24	0
7	EDO	D	4904	4/4	0.96	0.11	14,16,17,18	0
4	GAI	G	4807	4/4	0.96	0.10	21,22,23,24	0
3	NA	C	4703	1/1	0.96	0.07	18,18,18,18	0
3	NA	B	4702	1/1	0.97	0.10	18,18,18,18	0
3	NA	G	4707	1/1	0.97	0.06	19,19,19,19	0
7	EDO	E	4905	4/4	0.97	0.12	18,22,22,23	0
5	NAD	F	5506	44/44	0.97	0.09	8,19,29,30	0
7	EDO	G	4907	4/4	0.97	0.09	22,22,23,24	0
7	EDO	C	4903	4/4	0.97	0.07	16,16,17,17	0
3	NA	F	4706	1/1	0.98	0.14	21,21,21,21	0

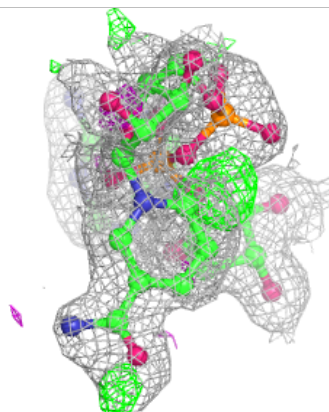
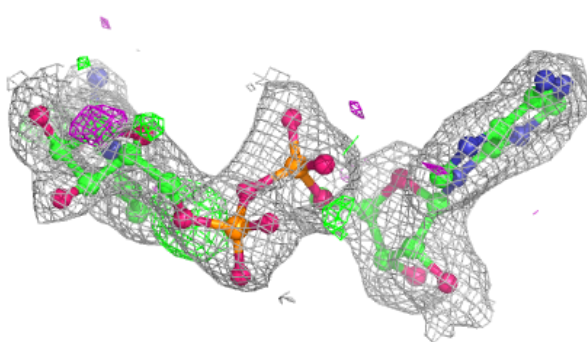
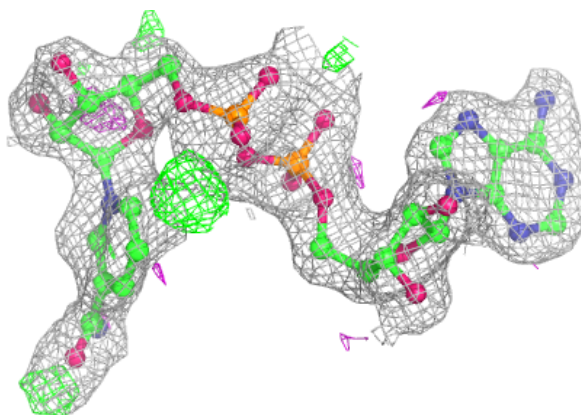
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAD H 5508:**

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

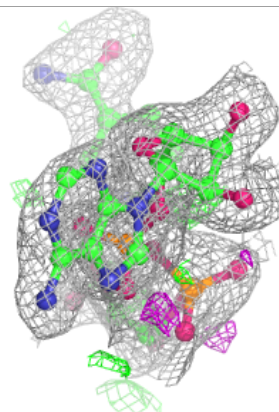
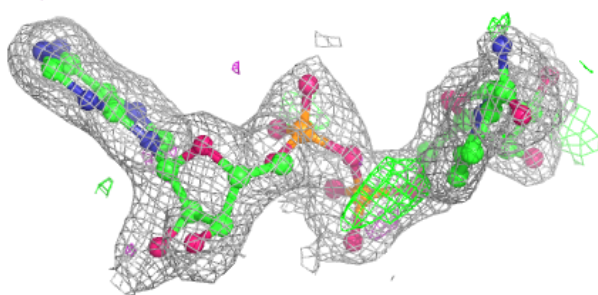
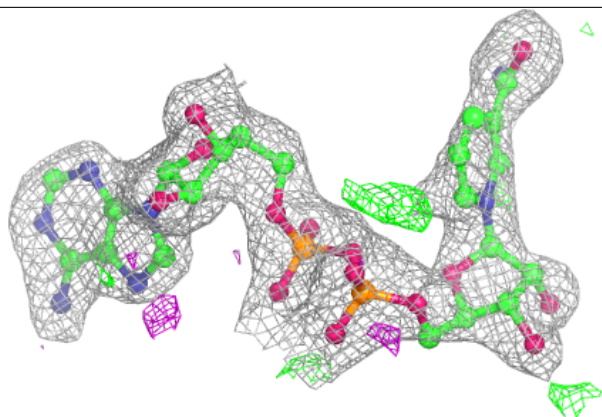
**Electron density around NAD D 5504:**

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

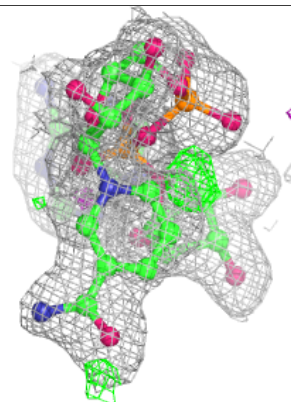
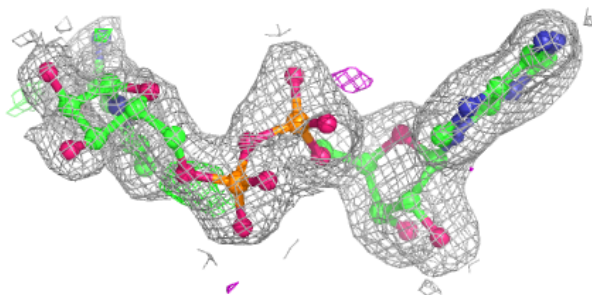
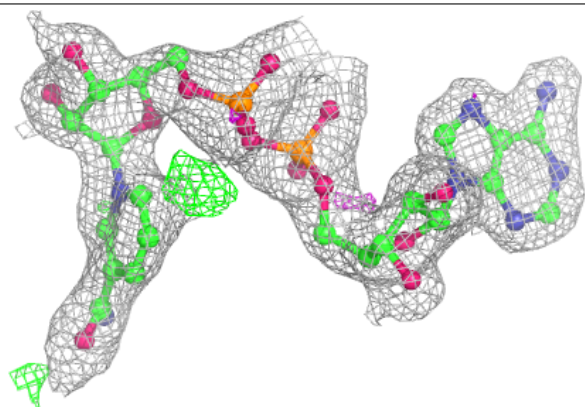


**Electron density around NAD G 5507:**

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

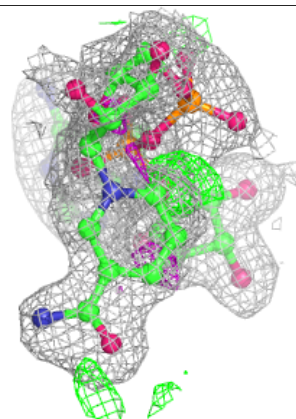
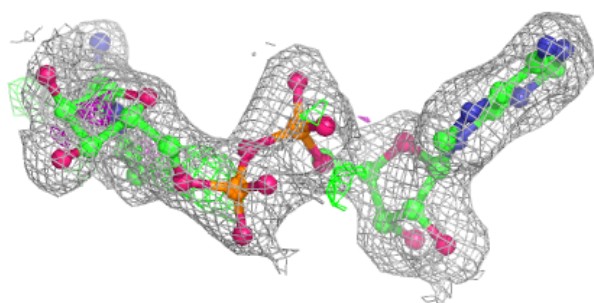
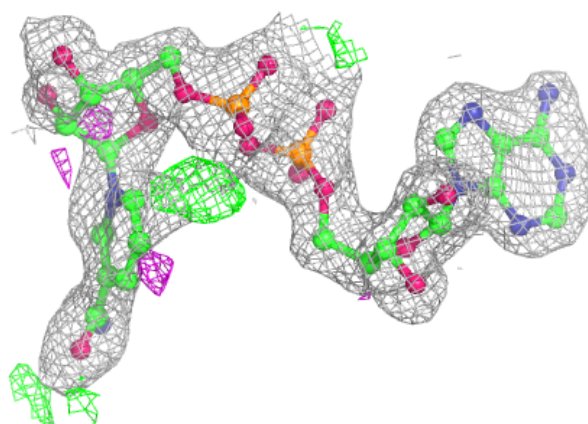
**Electron density around NAD A 5501:**

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

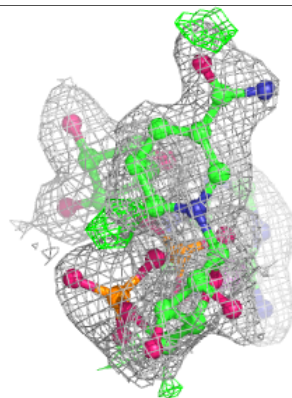
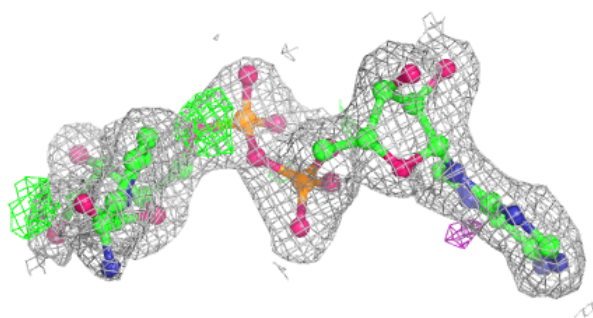
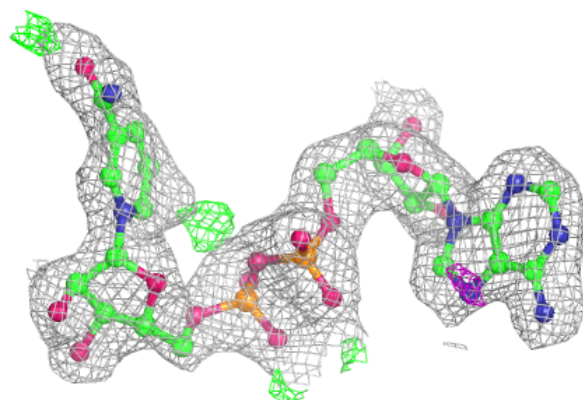


**Electron density around NAD E 5505:**

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

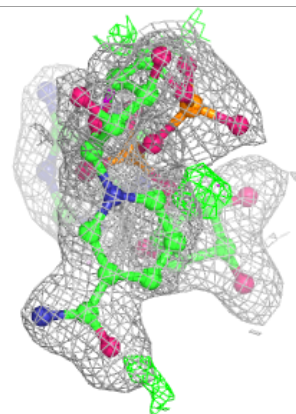
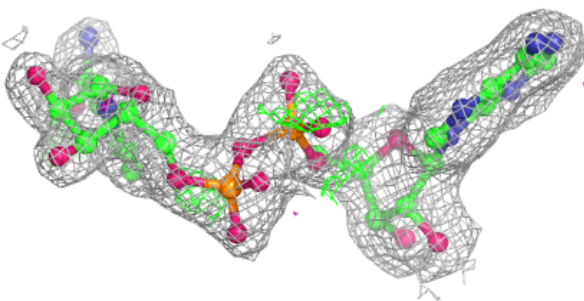
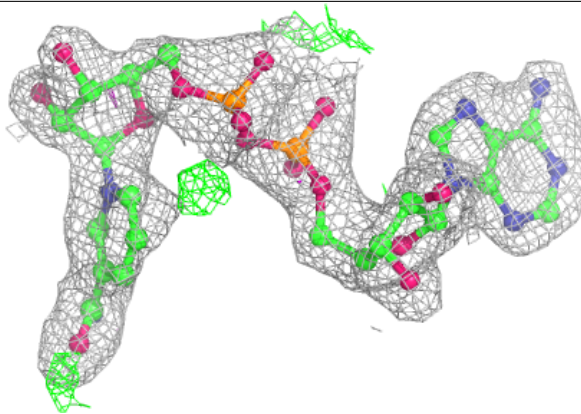
**Electron density around NAD C 5503:**

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

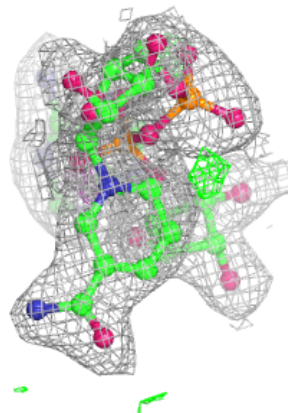
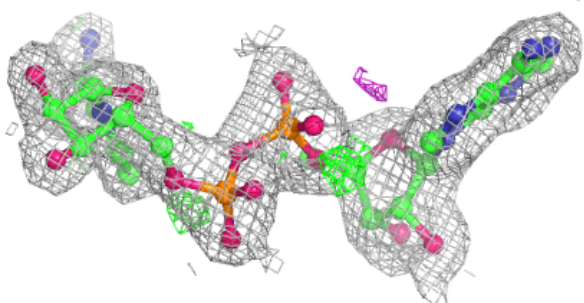
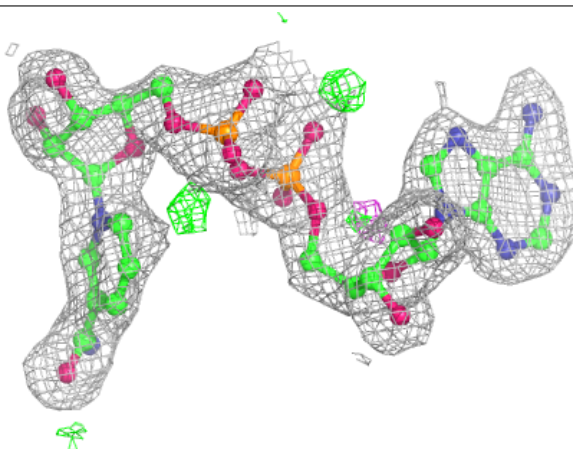


**Electron density around NAD B 5502:**

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

**Electron density around NAD F 5506:**

$2mF_o-DF_c$  (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.