



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 03:04 am BST

PDB ID : 3IWK  
Title : Crystal structure of aminoaldehyde dehydrogenase 1 from Pisum sativum (PsAMADH1)  
Authors : Kopecny, D.; Morera, S.; Briozzo, P.  
Deposited on : 2009-09-02  
Resolution : 2.40 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

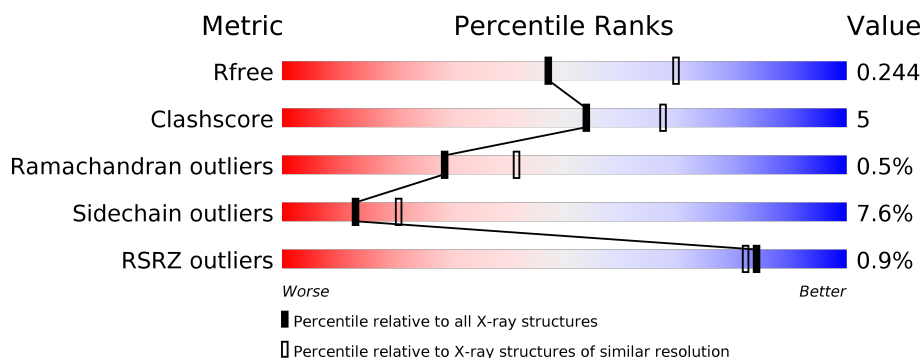
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	503	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>..</div> </div> </div>
1	B	503	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>..</div> </div> </div>
1	C	503	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>
1	D	503	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>..</div> </div> </div>
1	E	503	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>..</div> </div> </div>
1	F	503	<div> <div></div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	503	<div><div><div>%</div><div><div></div></div><div>82%</div><div>14%</div><div>..</div></div></div>
1	H	503	<div><div><div>%</div><div><div></div></div><div>82%</div><div>15%</div><div>..</div></div></div>
1	I	503	<div><div><div>%</div><div><div></div></div><div>82%</div><div>14%</div><div>..</div></div></div>
1	J	503	<div><div><div>%</div><div><div></div></div><div>84%</div><div>12%</div><div>..</div></div></div>
1	K	503	<div><div><div>%</div><div><div></div></div><div>84%</div><div>13%</div><div>..</div></div></div>
1	L	503	<div><div><div>%</div><div><div></div></div><div>84%</div><div>13%</div><div>..</div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 48369 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 Aminoaldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	1	0
			3811	2430	639	726	16			
1	B	496	Total	C	N	O	S	0	1	0
			3813	2432	641	724	16			
1	C	495	Total	C	N	O	S	0	0	0
			3797	2421	637	723	16			
1	D	496	Total	C	N	O	S	0	0	0
			3806	2427	639	724	16			
1	E	496	Total	C	N	O	S	0	0	0
			3806	2427	639	724	16			
1	F	495	Total	C	N	O	S	0	1	0
			3804	2426	639	723	16			
1	G	496	Total	C	N	O	S	0	0	0
			3806	2427	639	724	16			
1	H	497	Total	C	N	O	S	0	1	0
			3820	2435	643	726	16			
1	I	496	Total	C	N	O	S	0	2	0
			3821	2437	644	724	16			
1	J	497	Total	C	N	O	S	0	0	0
			3812	2430	640	726	16			
1	K	496	Total	C	N	O	S	0	2	0
			3821	2437	644	724	16			
1	L	496	Total	C	N	O	S	0	1	0
			3810	2429	640	725	16			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

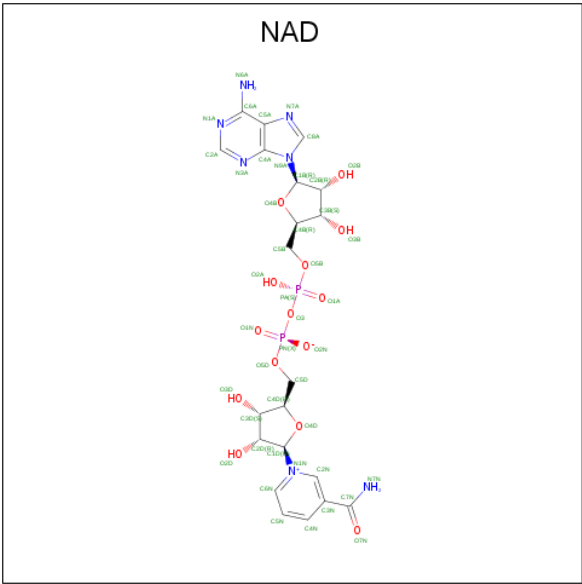
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Na	0	0
			1	1		
2	J	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Na	0	0
			1	1		
2	K	1	Total	Na	0	0
			1	1		
2	E	1	Total	Na	0	0
			1	1		
2	H	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	I	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		
2	L	1	Total	Na	0	0
			1	1		
2	F	1	Total	Na	0	0
			1	1		

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



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

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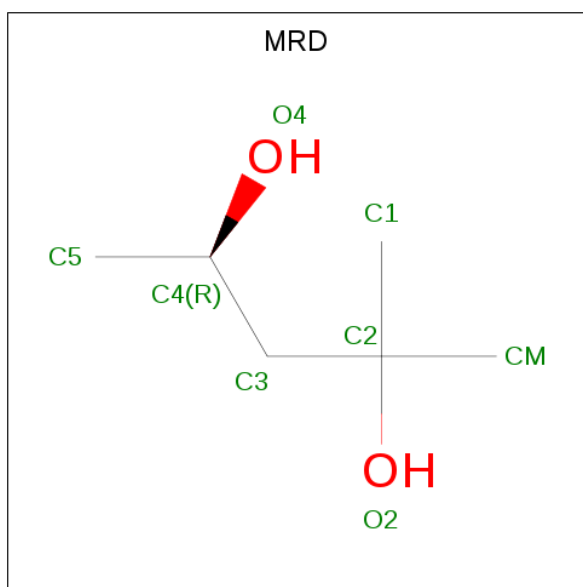
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	J	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	K	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	L	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		
4	K	1	Total	C	O	0	0
			6	3	3		
4	K	1	Total	C	O	0	0
			6	3	3		
4	K	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	145	Total	O	0	0
			145	145		
6	B	134	Total	O	0	0
			134	134		
6	C	148	Total	O	0	0
			148	148		
6	D	117	Total	O	0	0
			117	117		
6	E	154	Total	O	0	0
			154	154		
6	F	160	Total	O	0	0
			160	160		
6	G	180	Total	O	0	0
			180	180		
6	H	197	Total	O	0	0
			197	197		
6	I	199	Total	O	0	0
			199	199		
6	J	170	Total	O	0	0
			170	170		
6	K	195	Total	O	0	0
			195	195		

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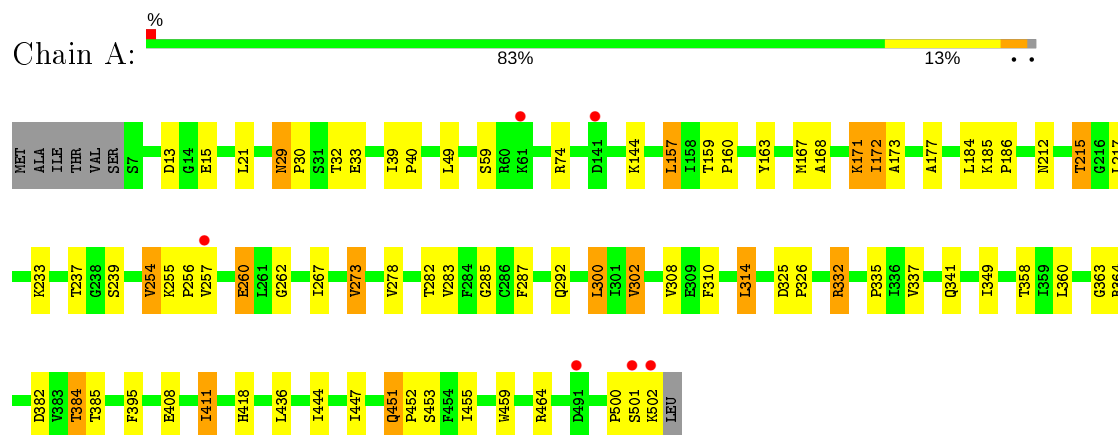
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	198	Total 198	O 198	0	0

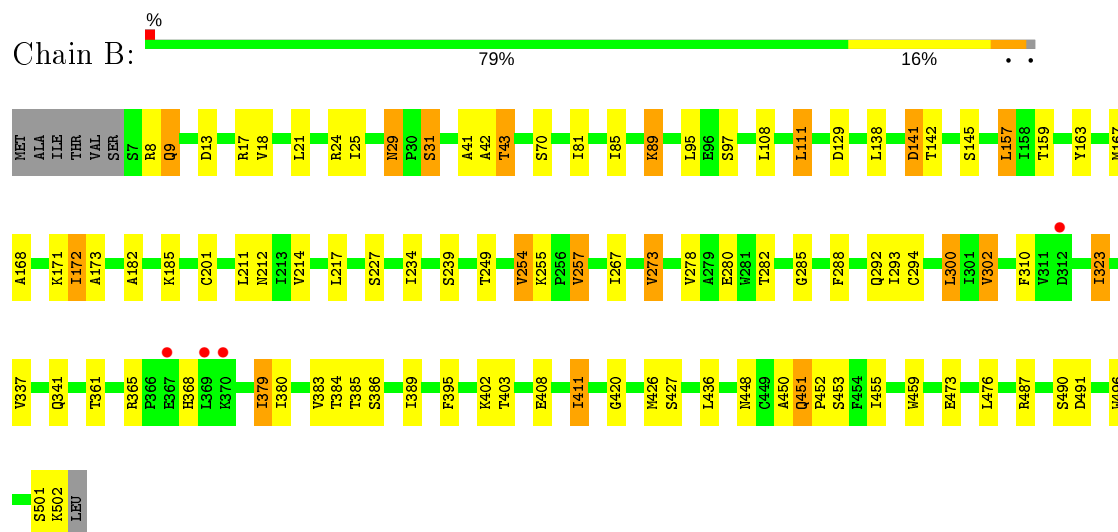
### 3 Residue-property plots [i](#)

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

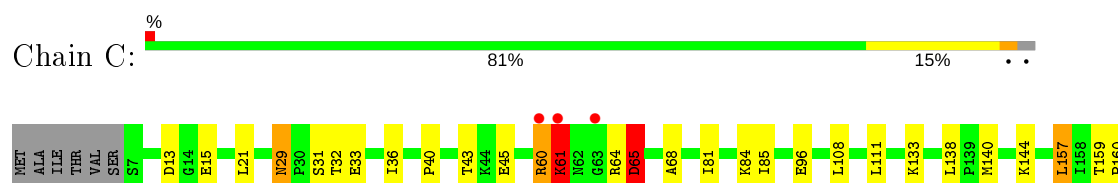
#### • Molecule 1: Aminoaldehyde dehydrogenase

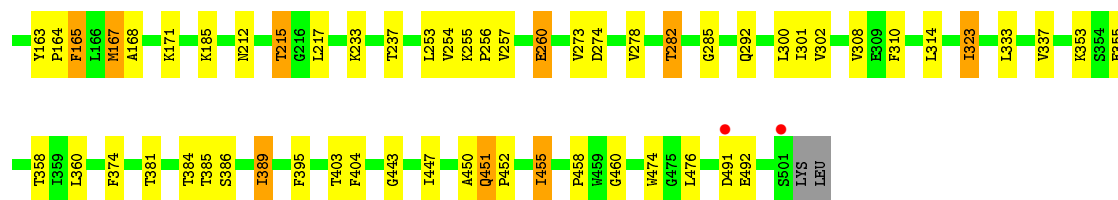


#### • Molecule 1: Aminoaldehyde dehydrogenase

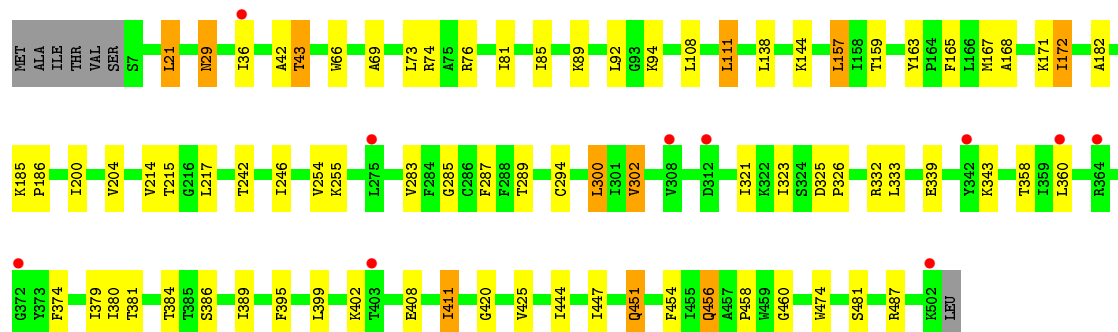
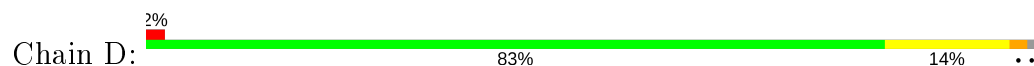


#### • Molecule 1: Aminoaldehyde dehydrogenase

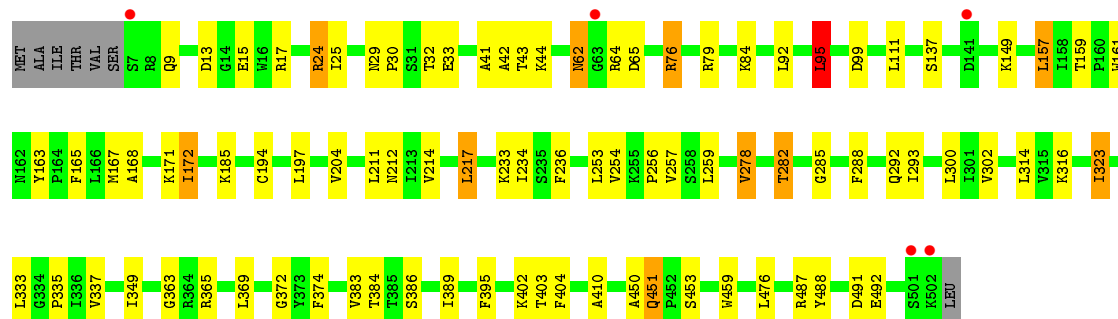
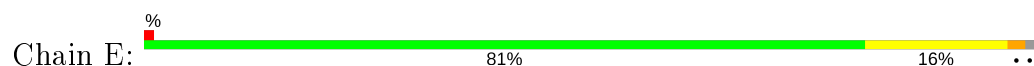




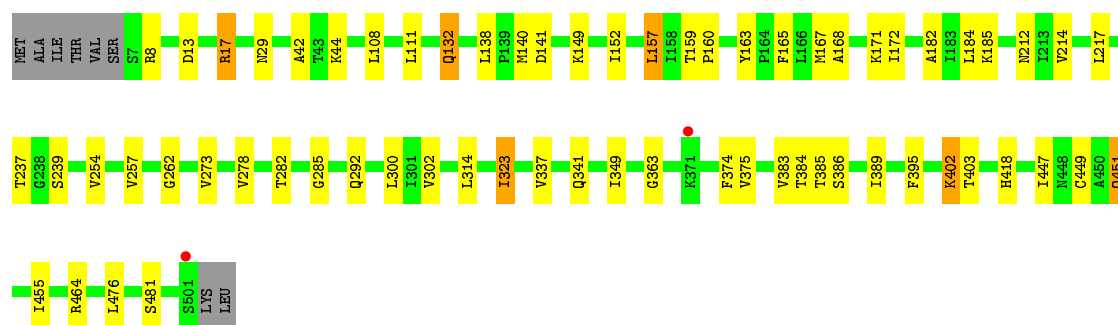
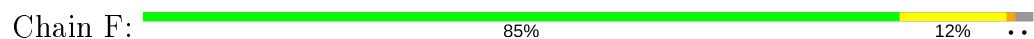
• Molecule 1: Aminoaldehyde dehydrogenase




• Molecule 1: Aminoaldehyde dehydrogenase

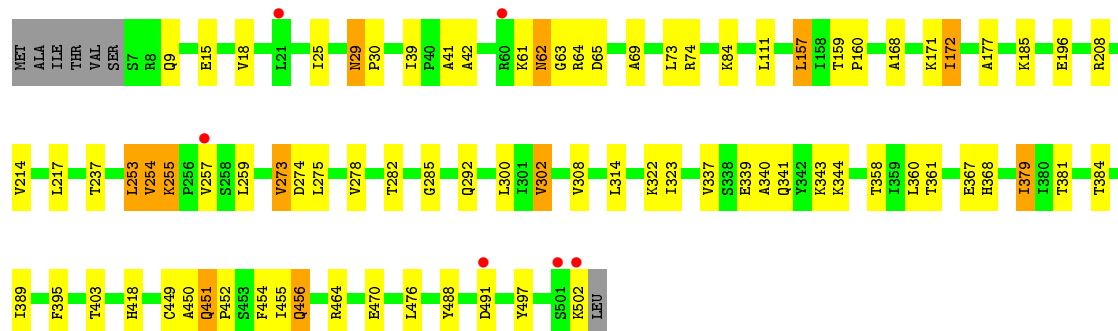


• Molecule 1: Aminoaldehyde dehydrogenase




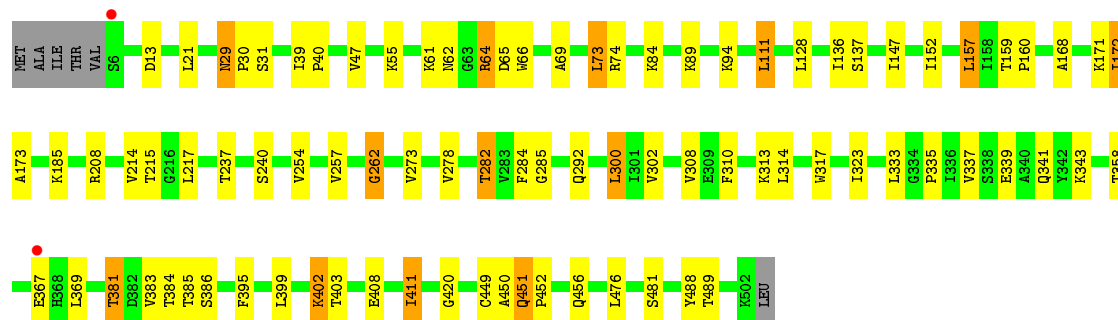
• Molecule 1: Aminoaldehyde dehydrogenase

Chain G:  82% 14% ..




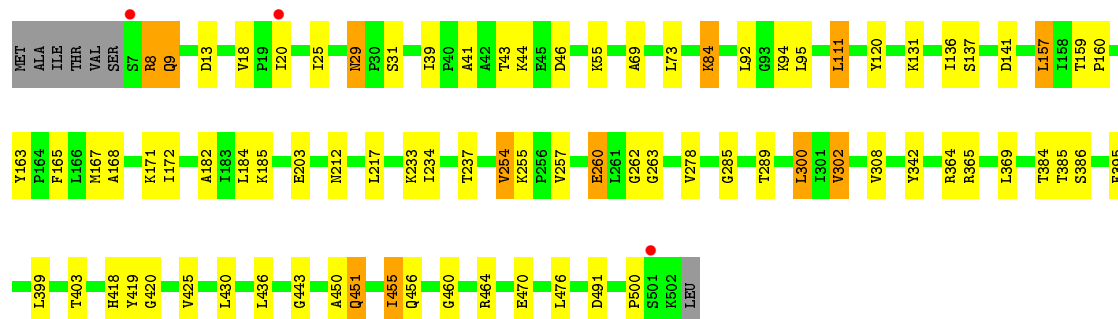
• Molecule 1: Aminoaldehyde dehydrogenase

Chain H:  82% 15% ..




• Molecule 1: Aminoaldehyde dehydrogenase

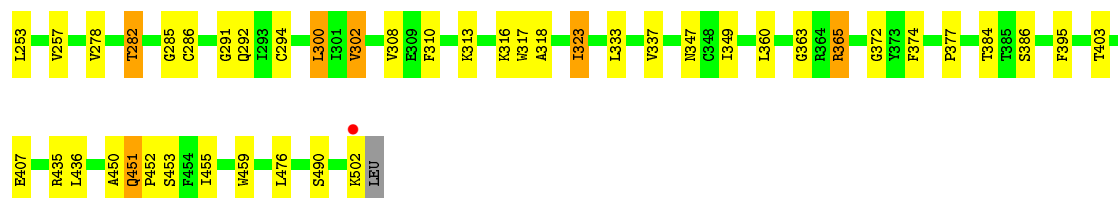
Chain I:  82% 14% ..



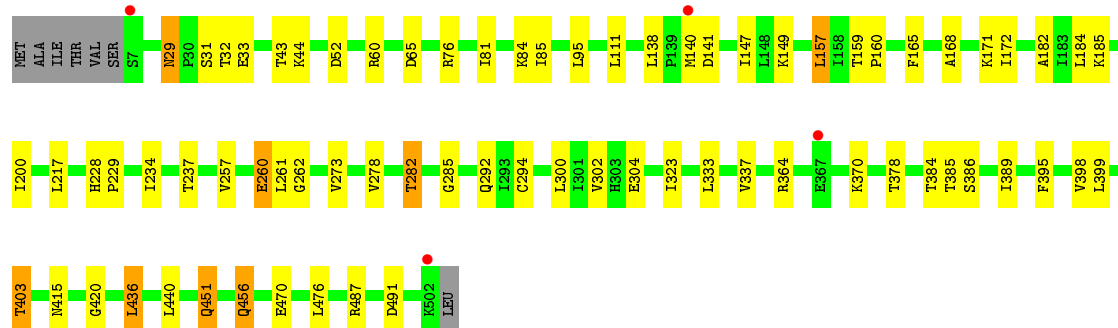
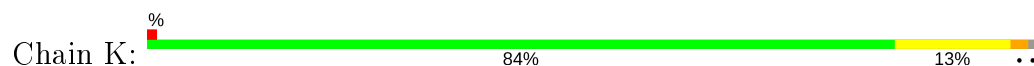
• Molecule 1: Aminoaldehyde dehydrogenase

Chain J:  84% 12% ..

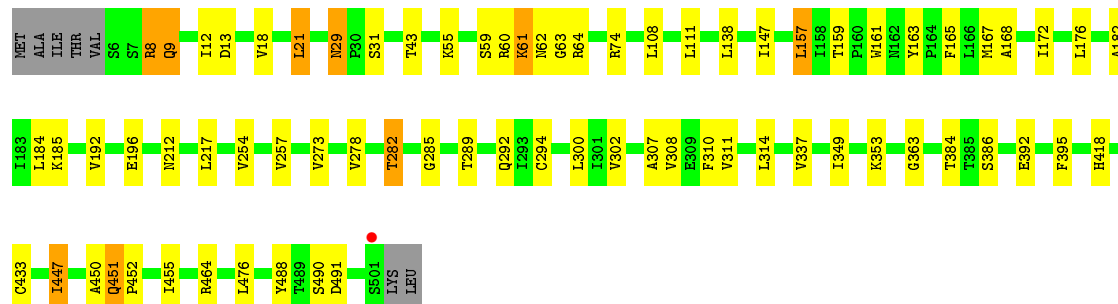
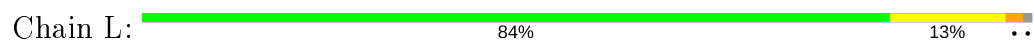




• Molecule 1: Aminoaldehyde dehydrogenase



• Molecule 1: Aminoaldehyde dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.41Å 216.87Å 205.76Å 90.00° 98.02° 90.00°	Depositor
Resolution (Å)	47.84 – 2.40 46.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.84-2.40) 99.8 (46.81-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.61 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.200 , 0.244 0.200 , 0.244	Depositor DCC
$R_{free}$ test set	14543 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	48369	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, GOL, NAD, NA

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	0.38	0/3894	0.53	0/5286
1	B	0.38	0/3897	0.53	0/5290
1	C	0.37	0/3877	0.54	0/5264
1	D	0.36	0/3886	0.54	0/5275
1	E	0.39	0/3886	0.56	1/5275 (0.0%)
1	F	0.39	0/3888	0.53	0/5279
1	G	0.38	0/3886	0.54	1/5275 (0.0%)
1	H	0.38	0/3903	0.56	1/5297 (0.0%)
1	I	0.38	0/3908	0.55	0/5304
1	J	0.38	0/3892	0.53	0/5283
1	K	0.38	0/3908	0.54	0/5304
1	L	0.39	0/3894	0.55	0/5287
All	All	0.38	0/46719	0.54	3/63419 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	73	LEU	CA-CB-CG	6.92	131.21	115.30
1	E	95	LEU	CA-CB-CG	6.09	129.30	115.30
1	G	302	VAL	CB-CA-C	-5.15	101.61	111.40

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	3811	0	3841	44	0
1	B	3813	0	3844	59	0
1	C	3797	0	3824	50	0
1	D	3806	0	3837	44	0
1	E	3806	0	3837	48	0
1	F	3804	0	3831	34	0
1	G	3806	0	3837	39	0
1	H	3820	0	3855	41	0
1	I	3821	0	3857	38	0
1	J	3812	0	3842	35	0
1	K	3821	0	3857	36	0
1	L	3810	0	3836	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
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	44	0	26	5	0
3	B	44	0	26	2	0
3	C	44	0	26	0	0
3	D	27	0	12	0	0
3	E	44	0	26	1	0
3	F	44	0	26	3	0
3	G	44	0	26	2	0
3	H	44	0	26	2	0
3	I	44	0	26	2	0
3	J	44	0	26	1	0
3	K	44	0	26	2	0
3	L	44	0	26	2	0
4	B	12	0	16	2	0
4	C	6	0	8	0	0
4	F	6	0	8	0	0
4	G	18	0	24	0	0
4	H	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	6	0	8	0	0
4	J	12	0	16	1	0
4	K	18	0	24	2	0
4	L	30	0	40	3	0
5	D	8	0	14	2	0
6	A	145	0	0	1	0
6	B	134	0	0	1	0
6	C	148	0	0	2	0
6	D	117	0	0	1	0
6	E	154	0	0	0	0
6	F	160	0	0	3	0
6	G	180	0	0	3	0
6	H	197	0	0	1	0
6	I	199	0	0	0	0
6	J	170	0	0	0	0
6	K	195	0	0	3	0
6	L	198	0	0	0	0
All	All	48369	0	46562	490	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 (490) 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:J:323:ILE:HD11	1:J:374:PHE:HD2	1.19	1.07
1:I:456:GLN:HB3	1:J:136:ILE:HD11	1.39	1.05
1:E:24:ARG:HH11	1:E:24:ARG:HG3	1.29	0.97
1:E:323:ILE:HD11	1:E:374:PHE:HD2	1.34	0.92
1:J:323:ILE:HD11	1:J:374:PHE:CD2	2.03	0.92
1:C:323:ILE:HD11	1:C:374:PHE:HD2	1.35	0.91
1:L:60:ARG:HG2	4:L:2005:GOL:H12	1.53	0.91
1:B:361:THR:HG22	1:B:379:ILE:HG22	1.56	0.88
1:F:132:GLN:HE22	1:F:149:LYS:H	1.17	0.88
1:F:323:ILE:HD11	1:F:374:PHE:HD2	1.43	0.82
1:F:132:GLN:NE2	1:F:149:LYS:H	1.80	0.80
1:B:278:VAL:HG23	1:B:310:PHE:HE1	1.46	0.79
1:D:254:VAL:HG12	1:D:254:VAL:O	1.80	0.79
1:J:278:VAL:O	1:J:282:THR:HG22	1.85	0.75
1:E:323:ILE:HD11	1:E:374:PHE:CD2	2.20	0.75
1:E:254:VAL:HG12	1:E:254:VAL:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:282:THR:HG21	1:L:310:PHE:HZ	1.51	0.75
1:A:447:ILE:HB	1:B:487:ARG:HB3	1.69	0.73
1:C:254:VAL:HG12	1:C:254:VAL:O	1.86	0.73
1:H:254:VAL:O	1:H:254:VAL:HG12	1.87	0.73
1:B:384:THR:HG22	1:B:386:SER:H	1.54	0.72
1:F:254:VAL:O	1:F:254:VAL:HG12	1.88	0.72
1:B:157:LEU:HD23	1:B:172:ILE:HG22	1.72	0.71
1:I:163:TYR:HB2	1:I:167:MET:HG2	1.71	0.71
1:D:389:ILE:HD12	1:D:389:ILE:H	1.57	0.70
1:F:383:VAL:O	1:F:402:LYS:HD3	1.92	0.70
1:H:13:ASP:OD1	1:H:208:ARG:HG2	1.91	0.70
1:C:282:THR:HG21	1:C:310:PHE:HZ	1.56	0.69
1:E:24:ARG:HH11	1:E:24:ARG:CG	2.05	0.69
1:G:159:THR:HG21	1:G:168:ALA:HA	1.74	0.69
1:E:278:VAL:O	1:E:282:THR:HG23	1.92	0.69
1:K:43:THR:HG22	1:K:44:LYS:H	1.56	0.69
1:G:29:ASN:HD22	1:G:30:PRO:HD2	1.58	0.68
1:D:85:ILE:HD13	1:D:200:ILE:HD13	1.73	0.68
1:K:81:ILE:O	1:K:85:ILE:HG12	1.93	0.68
1:B:383:VAL:O	1:B:402:LYS:HD3	1.93	0.68
1:K:29:ASN:HD22	1:K:31:SER:H	1.41	0.68
1:A:237:THR:HG23	1:A:260:GLU:HG2	1.76	0.68
1:L:433:CYS:SG	1:L:447:ILE:HD13	2.34	0.68
1:F:384:THR:HG22	1:F:386:SER:H	1.57	0.67
1:E:76:ARG:HH12	1:E:79:ARG:HD2	1.59	0.67
1:A:418:HIS:HB3	1:A:464:ARG:HG3	1.76	0.67
1:K:261:LEU:HD11	1:L:254:VAL:HG21	1.77	0.67
1:G:64:ARG:O	6:G:980:HOH:O	2.13	0.67
1:C:403:THR:HG23	6:C:516:HOH:O	1.95	0.66
1:A:332:ARG:NH1	1:B:496:TRP:O	2.29	0.66
1:I:43:THR:HG22	1:I:44:LYS:H	1.60	0.66
1:I:456:GLN:CB	1:J:136:ILE:HD11	2.23	0.66
1:I:29:ASN:HD22	1:I:31:SER:H	1.43	0.66
1:L:278:VAL:HG23	1:L:310:PHE:HE1	1.60	0.66
1:B:278:VAL:HG23	1:B:310:PHE:CE1	2.29	0.66
1:G:74:ARG:NH1	1:G:177:ALA:O	2.28	0.66
1:J:29:ASN:HD22	1:J:30:PRO:HD2	1.60	0.65
1:A:157:LEU:HD23	1:A:172:ILE:HG22	1.79	0.65
1:E:383:VAL:O	1:E:402:LYS:HD3	1.97	0.65
1:E:62:ASN:HD22	1:E:64:ARG:H	1.45	0.65
1:E:168:ALA:O	1:E:172:ILE:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:278:VAL:O	1:H:282:THR:HG23	1.96	0.65
1:I:159:THR:HG21	1:I:168:ALA:HA	1.79	0.65
1:K:147:ILE:HD12	1:K:149:LYS:HD3	1.78	0.64
1:E:384:THR:HG22	1:E:386:SER:H	1.62	0.64
1:J:384:THR:HG22	1:J:386:SER:H	1.62	0.64
1:F:278:VAL:O	1:F:282:THR:HG23	1.98	0.64
1:D:157:LEU:HD23	1:D:172:ILE:HG22	1.80	0.63
1:J:157:LEU:HG	1:J:171:LYS:HB2	1.80	0.63
1:C:447:ILE:HB	1:D:487:ARG:HG3	1.78	0.63
1:H:172:ILE:HG13	1:H:173:ALA:N	2.12	0.63
1:D:294:CYS:H	5:D:2004:MRD:HMC2	1.63	0.63
1:L:278:VAL:O	1:L:282:THR:HG22	1.99	0.63
1:B:81:ILE:O	1:B:85:ILE:HG12	1.98	0.62
1:E:30:PRO:HB2	1:E:335:PRO:HG2	1.80	0.62
1:D:21:LEU:HD22	1:D:43:THR:HG21	1.81	0.62
1:G:278:VAL:O	1:G:282:THR:HG23	1.99	0.62
1:A:30:PRO:HB2	1:A:335:PRO:HG2	1.82	0.62
1:B:239:SER:HB3	3:B:505:NAD:H1D	1.81	0.62
1:C:65:ASP:HB3	1:C:68:ALA:HB3	1.82	0.62
1:I:254:VAL:O	1:I:254:VAL:HG13	1.99	0.62
1:K:487:ARG:HG3	1:L:447:ILE:HG13	1.83	0.61
1:G:418:HIS:HB3	1:G:464:ARG:HG3	1.83	0.61
1:K:384:THR:HG22	1:K:386:SER:H	1.64	0.61
1:C:81:ILE:O	1:C:85:ILE:HG12	2.01	0.61
1:G:403:THR:HG22	6:G:1348:HOH:O	2.00	0.61
1:K:323:ILE:HD12	1:K:333:LEU:HD23	1.83	0.61
1:G:168:ALA:O	1:G:172:ILE:HG23	2.00	0.60
1:L:278:VAL:HG23	1:L:310:PHE:CE1	2.36	0.60
1:A:254:VAL:HG13	1:A:254:VAL:O	2.02	0.60
1:C:323:ILE:HD11	1:C:374:PHE:CD2	2.26	0.60
1:L:12:ILE:HA	1:L:212:ASN:HD22	1.67	0.59
1:G:292:GLN:HE22	1:G:337:VAL:H	1.49	0.59
1:B:29:ASN:HD22	1:B:31:SER:H	1.50	0.59
1:A:157:LEU:HG	1:A:171:LYS:HB2	1.83	0.59
1:D:73:LEU:HD13	1:D:76:ARG:NH1	2.18	0.59
1:E:365:ARG:NH2	1:E:372:GLY:O	2.35	0.59
1:F:323:ILE:HD11	1:F:374:PHE:CD2	2.31	0.59
1:I:92:LEU:HB2	1:I:111:LEU:HD21	1.83	0.59
1:B:254:VAL:CG1	1:B:254:VAL:O	2.50	0.59
1:E:233:LYS:HG2	1:E:256:PRO:HG2	1.85	0.59
1:D:254:VAL:CG1	1:D:254:VAL:O	2.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:341:GLN:NE2	3:H:505:NAD:H3D	2.18	0.58
1:G:454:PHE:HB3	1:G:456:GLN:HE21	1.68	0.58
1:E:157:LEU:HG	1:E:171:LYS:HB3	1.85	0.58
1:G:254:VAL:CG1	1:G:254:VAL:O	2.51	0.58
1:I:384:THR:HG22	1:I:386:SER:H	1.68	0.58
1:G:157:LEU:HG	1:G:171:LYS:HB3	1.84	0.58
1:H:157:LEU:HG	1:H:171:LYS:HB3	1.86	0.58
1:L:63:GLY:O	1:L:64:ARG:HB2	2.02	0.58
1:C:274:ASP:O	1:C:278:VAL:HG12	2.03	0.57
1:G:340:ALA:O	1:G:344:LYS:HG2	2.04	0.57
1:B:368:HIS:H	1:B:368:HIS:CD2	2.23	0.57
1:L:282:THR:HG21	1:L:310:PHE:CZ	2.38	0.57
1:A:453:SER:HB3	1:A:459:TRP:CZ3	2.39	0.57
1:I:254:VAL:O	1:I:254:VAL:CG1	2.52	0.57
1:J:294:CYS:H	4:J:2014:GOL:HO3	1.52	0.57
1:A:160:PRO:HD3	1:A:237:THR:HB	1.87	0.57
1:B:138:LEU:HD11	1:B:145:SER:HB2	1.86	0.56
1:D:81:ILE:O	1:D:85:ILE:HG12	2.05	0.56
1:F:285:GLY:HA2	1:F:451:GLN:HG2	1.86	0.56
1:C:278:VAL:O	1:C:282:THR:HG22	2.06	0.56
1:J:282:THR:HG21	1:J:310:PHE:HZ	1.70	0.56
1:K:159:THR:HG21	1:K:168:ALA:HA	1.88	0.56
1:B:163:TYR:HB2	1:B:167:MET:HG2	1.88	0.56
1:J:159:THR:HG21	1:J:168:ALA:HA	1.86	0.56
1:L:13:ASP:H	1:L:212:ASN:ND2	2.03	0.56
1:L:159:THR:HG21	1:L:168:ALA:HA	1.88	0.56
1:A:254:VAL:CG1	1:A:254:VAL:O	2.54	0.56
1:C:358:THR:HB	1:C:381:THR:CG2	2.35	0.56
1:E:62:ASN:HB3	1:E:65:ASP:HB3	1.87	0.55
1:B:285:GLY:HA2	1:B:451:GLN:HG2	1.88	0.55
1:F:163:TYR:HB2	1:F:167:MET:HG2	1.89	0.55
1:I:157:LEU:HG	1:I:171:LYS:HB3	1.88	0.55
1:L:285:GLY:HA2	1:L:451:GLN:HG2	1.88	0.55
1:G:341:GLN:NE2	3:G:505:NAD:H3D	2.21	0.55
1:A:13:ASP:H	1:A:212:ASN:ND2	2.04	0.55
1:E:285:GLY:HA2	1:E:451:GLN:HG2	1.89	0.55
1:H:282:THR:HG21	1:H:310:PHE:HZ	1.70	0.55
1:A:285:GLY:HA2	1:A:451:GLN:HG2	1.88	0.55
1:B:157:LEU:HD22	1:B:182:ALA:HB1	1.89	0.55
1:D:168:ALA:O	1:D:172:ILE:HG23	2.07	0.55
1:H:168:ALA:O	1:H:172:ILE:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:ALA:CB	1:D:214:VAL:HG13	2.36	0.55
1:I:20:ILE:HD12	1:I:46:ASP:OD2	2.07	0.55
1:L:61:LYS:HD2	1:L:61:LYS:N	2.22	0.55
1:F:254:VAL:O	1:F:254:VAL:CG1	2.53	0.55
1:J:163:TYR:HB2	1:J:167:MET:HG2	1.89	0.55
1:A:233:LYS:HG3	1:A:256:PRO:HG2	1.89	0.54
1:B:21:LEU:HD22	1:B:43:THR:HG21	1.89	0.54
1:D:163:TYR:HB2	1:D:167:MET:HG2	1.89	0.54
1:I:157:LEU:HD22	1:I:182:ALA:HB1	1.88	0.54
1:D:444:ILE:HD11	1:D:460:GLY:H	1.72	0.54
1:A:278:VAL:O	1:A:282:THR:HG23	2.07	0.54
1:B:8:ARG:O	1:B:24:ARG:NH2	2.38	0.54
1:J:300:LEU:HD22	1:J:302:VAL:HG22	1.90	0.54
1:H:384:THR:HG22	1:H:386:SER:H	1.72	0.54
1:I:262:GLY:HA3	3:I:505:NAD:H72N	1.72	0.54
1:D:157:LEU:HG	1:D:171:LYS:HB3	1.89	0.53
1:E:159:THR:HG21	1:E:168:ALA:HA	1.88	0.53
1:K:157:LEU:HG	1:K:171:LYS:HB3	1.90	0.53
1:K:85:ILE:HD13	1:K:200:ILE:HD13	1.90	0.53
1:B:267:ILE:HD13	1:B:282:THR:HG22	1.90	0.53
1:E:453:SER:HB3	1:E:459:TRP:CZ3	2.42	0.53
1:K:262:GLY:HA2	3:K:505:NAD:H72N	1.74	0.53
1:K:304:GLU:HB3	1:K:403:THR:HG23	1.89	0.53
1:E:161:TRP:NE1	3:E:505:NAD:H6N	2.24	0.53
1:H:358:THR:HB	1:H:381:THR:HG22	1.89	0.53
1:I:69:ALA:HB1	1:I:73:LEU:HD23	1.91	0.52
1:H:89:LYS:HA	1:H:111:LEU:HD22	1.92	0.52
1:J:282:THR:HG21	1:J:310:PHE:CZ	2.45	0.52
1:L:418[B]:HIS:HB3	1:L:464:ARG:HG3	1.91	0.52
1:A:408:GLU:O	1:A:411:ILE:HD13	2.09	0.52
1:C:301:ILE:HG22	1:C:404:PHE:CD2	2.44	0.52
1:F:282:THR:OG1	1:F:314:LEU:HD11	2.09	0.52
1:J:285:GLY:HA2	1:J:451:GLN:HG2	1.92	0.52
1:L:163:TYR:HB2	1:L:167:MET:HG2	1.92	0.52
1:C:323:ILE:HD12	1:C:333:LEU:O	2.10	0.52
1:D:159:THR:HG21	1:D:168:ALA:HA	1.92	0.52
1:D:323:ILE:HD13	1:D:333:LEU:HD23	1.92	0.52
1:E:163:TYR:HB2	1:E:167:MET:HG2	1.90	0.52
1:I:263:GLY:HA2	1:I:419:TYR:CD2	2.45	0.52
1:A:237:THR:HG23	1:A:260:GLU:CG	2.40	0.51
1:H:323:ILE:HD12	1:H:333:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:418[B]:HIS:HB2	1:I:464:ARG:HG3	1.92	0.51
1:H:262:GLY:HA2	3:H:505:NAD:H72N	1.74	0.51
1:A:163:TYR:HB2	1:A:167:MET:HG2	1.93	0.51
1:I:9:GLN:HG3	1:I:18:VAL:HA	1.92	0.51
1:K:60:ARG:NH2	6:K:527:HOH:O	2.41	0.51
1:B:288:PHE:HB3	1:B:293:ILE:HD11	1.93	0.51
1:C:140:MET:HG3	1:D:454:PHE:HE2	1.76	0.51
1:H:61:LYS:HD3	1:H:65:ASP:OD2	2.10	0.51
1:I:263:GLY:HA2	1:I:419:TYR:CG	2.45	0.51
1:L:307:ALA:O	1:L:311:VAL:HG23	2.11	0.51
1:B:168:ALA:O	1:B:172:ILE:HG23	2.11	0.51
1:E:323:ILE:HD12	1:E:333:LEU:O	2.11	0.50
1:H:339:GLU:HG2	1:H:343:LYS:HE2	1.93	0.50
1:K:415:ASN:HB2	4:K:2018:GOL:H2	1.91	0.50
1:C:254:VAL:O	1:C:254:VAL:CG1	2.55	0.50
1:H:292:GLN:HE22	1:H:337:VAL:H	1.58	0.50
1:H:66:TRP:CH2	1:H:74:ARG:HG2	2.47	0.50
1:L:450:ALA:O	1:L:451:GLN:HB2	2.11	0.50
1:C:282:THR:HG21	1:C:310:PHE:CZ	2.43	0.50
1:D:323:ILE:HD11	1:D:374:PHE:HD2	1.77	0.50
1:D:425:VAL:HB	1:D:447:ILE:HG22	1.92	0.50
1:F:403:THR:HG22	6:F:545:HOH:O	2.10	0.50
1:C:384:THR:HG22	1:C:386:SER:H	1.77	0.50
1:G:361:THR:HG22	1:G:379:ILE:HG23	1.94	0.50
1:J:313:LYS:HA	1:J:316:LYS:HE3	1.93	0.50
1:L:9:GLN:HG3	1:L:18:VAL:HA	1.93	0.50
1:B:254:VAL:HG13	1:B:254:VAL:O	2.11	0.50
1:D:487:ARG:NH2	6:D:1288:HOH:O	2.43	0.50
1:K:278:VAL:O	1:K:282:THR:HG23	2.12	0.50
1:E:92:LEU:HA	1:E:95:LEU:HD22	1.93	0.50
1:I:43:THR:HG22	1:I:44:LYS:N	2.26	0.50
1:C:21:LEU:HD13	1:C:43:THR:HG21	1.93	0.50
1:J:185:LYS:C	1:J:185:LYS:HD2	2.32	0.50
1:L:418[A]:HIS:HB2	1:L:464:ARG:HG3	1.94	0.50
1:A:278:VAL:HG23	1:A:310:PHE:CE1	2.47	0.50
1:H:383:VAL:O	1:H:402:LYS:HD3	2.10	0.50
1:H:40:PRO:O	1:H:215:THR:HG22	2.11	0.49
1:J:13:ASP:H	1:J:212:ASN:ND2	2.11	0.49
1:B:25:ILE:HG13	1:B:41:ALA:HB2	1.94	0.49
1:E:42:ALA:CB	1:E:214:VAL:HG13	2.42	0.49
1:E:76:ARG:NH1	1:E:79:ARG:HD2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:408:GLU:O	1:H:411:ILE:HD13	2.11	0.49
1:H:450:ALA:C	1:H:452:PRO:HD3	2.33	0.49
1:B:234:ILE:HB	1:B:257:VAL:HG23	1.95	0.49
1:B:450:ALA:C	1:B:452:PRO:HD3	2.33	0.49
1:B:361:THR:HG22	1:B:379:ILE:CG2	2.36	0.49
1:G:470:GLU:HG2	6:G:526:HOH:O	2.13	0.49
1:G:488:TYR:HB2	1:H:449:CYS:HB3	1.95	0.49
1:A:349:ILE:HD13	1:A:363:GLY:HA2	1.95	0.49
1:E:487:ARG:HG3	1:F:447:ILE:HB	1.95	0.49
1:E:349:ILE:HD13	1:E:363:GLY:HA2	1.95	0.48
1:G:69:ALA:HB1	1:G:73:LEU:HD23	1.95	0.48
1:K:172:ILE:HD11	1:K:184:LEU:HD22	1.95	0.48
1:K:43:THR:HG22	1:K:44:LYS:N	2.27	0.48
1:D:384:THR:HG22	1:D:386:SER:H	1.78	0.48
1:F:13:ASP:H	1:F:212:ASN:ND2	2.11	0.48
1:D:285:GLY:HA2	1:D:451:GLN:HG2	1.95	0.48
1:H:285:GLY:HA2	1:H:451:GLN:HG2	1.94	0.48
1:I:425:VAL:HG11	1:I:436:LEU:HB3	1.94	0.48
1:G:449:CYS:HB3	1:H:488:TYR:HB2	1.96	0.48
1:B:13:ASP:H	1:B:212:ASN:ND2	2.11	0.48
1:B:17:ARG:HH21	1:C:355:GLU:HB3	1.79	0.48
1:K:32:THR:O	1:K:33:GLU:HB2	2.14	0.48
1:G:323:ILE:O	1:G:368:HIS:HE1	1.97	0.48
1:A:168:ALA:O	1:A:172:ILE:HG23	2.14	0.48
1:A:451:GLN:N	1:A:452:PRO:HD2	2.29	0.48
1:J:292:GLN:HE22	1:J:337:VAL:H	1.60	0.48
1:F:172:ILE:HD11	1:F:184:LEU:HD22	1.95	0.47
1:G:61:LYS:O	1:G:62:ASN:C	2.53	0.47
1:I:418[A]:HIS:HB3	1:I:464:ARG:HG3	1.95	0.47
1:K:76:ARG:HG2	6:K:914:HOH:O	2.14	0.47
1:D:283:VAL:HG13	1:D:287:PHE:HD1	1.80	0.47
1:C:285:GLY:HA2	1:C:451:GLN:HG2	1.96	0.47
1:K:234:ILE:HB	1:K:257:VAL:HG23	1.96	0.47
1:L:294:CYS:HB2	4:L:2008:GOL:O2	2.14	0.47
1:E:254:VAL:CG1	1:E:254:VAL:O	2.57	0.47
1:F:159:THR:HG21	1:F:168:ALA:HA	1.96	0.47
1:I:13:ASP:H	1:I:212:ASN:HD22	1.62	0.47
1:A:282:THR:OG1	1:A:314:LEU:HD11	2.14	0.47
1:B:172:ILE:HG13	1:B:173:ALA:N	2.29	0.47
1:B:273:VAL:HG23	1:B:427:SER:HA	1.97	0.47
1:B:323:ILE:O	1:B:323:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:29:ASN:ND2	1:I:31:SER:H	2.10	0.47
1:G:157:LEU:HD23	1:G:172:ILE:HG22	1.96	0.47
1:B:273:VAL:HG11	1:B:278:VAL:HG21	1.97	0.47
1:B:402:LYS:HD2	6:B:559:HOH:O	2.14	0.47
1:F:341:GLN:NE2	3:F:505:NAD:H3D	2.30	0.47
1:D:157:LEU:HD22	1:D:182:ALA:HB1	1.97	0.47
1:E:25:ILE:HG13	1:E:41:ALA:HB2	1.97	0.47
1:B:89:LYS:HA	1:B:111:LEU:HD22	1.97	0.47
1:B:42:ALA:HB3	1:B:214:VAL:HG13	1.96	0.47
1:C:458:PRO:HB3	1:C:474:TRP:CD1	2.50	0.47
1:B:157:LEU:HG	1:B:171:LYS:HB3	1.96	0.46
1:B:302:VAL:HG11	1:B:310:PHE:CD2	2.50	0.46
1:J:29:ASN:HD22	1:J:30:PRO:CD	2.25	0.46
1:B:292:GLN:HE22	1:B:337:VAL:H	1.63	0.46
1:G:339:GLU:HG2	1:G:343:LYS:HE2	1.97	0.46
1:H:300:LEU:HB2	1:H:399:LEU:HD11	1.97	0.46
1:J:157:LEU:HD22	1:J:182:ALA:HB1	1.96	0.46
1:D:294:CYS:HB2	5:D:2004:MRD:H1C1	1.97	0.46
1:E:25:ILE:HD13	1:E:217:LEU:HD13	1.97	0.46
1:J:160:PRO:HB2	3:J:505:NAD:H5N	1.98	0.46
1:K:157:LEU:HD22	1:K:182:ALA:HB1	1.96	0.46
1:K:378:THR:HB	1:K:398:VAL:HG22	1.96	0.46
1:L:8:ARG:HD2	1:L:196:GLU:OE2	2.15	0.46
1:J:43:THR:CG2	1:J:44:LYS:N	2.79	0.46
1:D:408:GLU:HA	1:D:411:ILE:CD1	2.45	0.46
1:A:273:VAL:HG11	1:A:278:VAL:HG21	1.97	0.46
1:C:358:THR:HB	1:C:381:THR:HG22	1.97	0.46
1:L:294:CYS:SG	3:L:505:NAD:O7N	2.68	0.46
1:C:278:VAL:O	1:C:282:THR:CG2	2.64	0.46
1:E:450:ALA:O	1:E:451:GLN:HB2	2.16	0.46
1:B:142:THR:HG22	1:B:490:SER:HB2	1.98	0.46
1:B:159:THR:HG21	1:B:168:ALA:HA	1.98	0.46
1:B:201:CYS:SG	1:B:211:LEU:HD23	2.56	0.46
1:E:288:PHE:HB3	1:E:293:ILE:HD11	1.98	0.46
1:E:292:GLN:HE22	1:E:337:VAL:H	1.64	0.46
1:G:62:ASN:O	1:G:64:ARG:N	2.49	0.46
1:B:70:SER:HB2	1:B:129:ASP:OD2	2.16	0.45
1:C:29:ASN:HD22	1:C:29:ASN:C	2.19	0.45
1:E:234:ILE:HB	1:E:257:VAL:HG22	1.97	0.45
1:C:237:THR:HA	1:C:260:GLU:O	2.16	0.45
1:F:132:GLN:HE22	1:F:149:LYS:N	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:450:ALA:O	1:G:451:GLN:HB2	2.15	0.45
1:K:29:ASN:ND2	1:K:31:SER:H	2.09	0.45
1:K:160:PRO:HB2	3:K:505:NAD:H5N	1.99	0.45
1:D:73:LEU:HD13	1:D:76:ARG:HH11	1.79	0.45
1:I:450:ALA:O	1:I:451:GLN:HB2	2.16	0.45
1:E:43:THR:HG22	1:E:44:LYS:N	2.32	0.45
1:H:29:ASN:HD22	1:H:31:SER:H	1.65	0.45
1:L:21:LEU:HD22	1:L:43:THR:HG21	1.99	0.45
1:A:159:THR:HG21	1:A:168:ALA:HA	1.99	0.45
1:C:358:THR:HB	1:C:381:THR:HG23	1.97	0.45
1:G:253:LEU:HB3	1:G:255:LYS:HE3	1.99	0.45
1:K:228:HIS:HA	1:K:229:PRO:HD3	1.85	0.45
1:A:384:THR:HG23	6:A:713:HOH:O	2.16	0.45
1:B:141:ASP:N	1:B:141:ASP:OD2	2.49	0.45
1:D:69:ALA:HB1	1:D:73:LEU:HD23	1.98	0.45
1:F:160:PRO:HD3	1:F:237:THR:HB	1.98	0.45
1:G:254:VAL:HG12	1:G:254:VAL:O	2.17	0.45
1:G:25:ILE:HG13	1:G:41:ALA:HB2	1.98	0.45
1:J:318:ALA:HB1	1:J:377:PRO:HB2	1.98	0.45
1:J:349:ILE:HD13	1:J:363:GLY:HA2	1.98	0.45
1:B:42:ALA:CB	1:B:214:VAL:HG13	2.46	0.45
1:J:160:PRO:HD3	1:J:237:THR:HB	1.99	0.45
1:L:488:TYR:CZ	1:L:490:SER:HB3	2.52	0.45
1:L:74:ARG:HD3	1:L:176:LEU:O	2.17	0.45
1:B:17:ARG:NH2	1:C:355:GLU:O	2.50	0.44
1:E:32:THR:O	1:E:33:GLU:HB2	2.17	0.44
1:H:69:ALA:O	1:H:74:ARG:NH2	2.50	0.44
1:A:283:VAL:HG13	1:A:287:PHE:HD1	1.82	0.44
1:B:9:GLN:HG2	1:B:18:VAL:HA	2.00	0.44
1:F:262:GLY:HA2	3:F:505:NAD:H72N	1.82	0.44
1:J:407:GLU:OE1	1:J:435:ARG:HD2	2.18	0.44
1:K:294:CYS:HB2	4:K:2016:GOL:H32	1.98	0.44
1:L:161:TRP:NE1	3:L:505:NAD:H6N	2.31	0.44
1:C:29:ASN:ND2	1:C:31:SER:H	2.15	0.44
1:A:172:ILE:HG13	1:A:173:ALA:N	2.32	0.44
1:A:292:GLN:HE22	1:A:337:VAL:H	1.64	0.44
1:A:239:SER:HB3	3:A:505:NAD:H1D	2.00	0.44
1:F:157:LEU:HD22	1:F:182:ALA:HB1	1.99	0.44
1:G:274:ASP:O	1:G:278:VAL:HG13	2.17	0.44
1:A:262:GLY:HA2	3:A:505:NAD:H72N	1.82	0.44
1:C:85:ILE:HD12	1:C:165:PHE:HZ	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ASP:CB	1:C:68:ALA:HB3	2.48	0.44
1:C:96:GLU:OE1	1:C:164:PRO:HD2	2.17	0.44
1:G:9:GLN:HE21	1:G:18:VAL:HA	1.82	0.44
1:I:285:GLY:HA2	1:I:451:GLN:HG2	2.00	0.44
1:J:365:ARG:NH2	1:J:372:GLY:O	2.51	0.44
1:K:292:GLN:HE22	1:K:337:VAL:H	1.66	0.44
1:F:152:ILE:HD12	1:F:481:SER:HB2	1.99	0.44
1:H:152:ILE:HD12	1:H:481:SER:HB3	1.99	0.44
1:H:159:THR:HG21	1:H:168:ALA:HA	1.99	0.44
1:K:29:ASN:ND2	1:K:31:SER:HB3	2.33	0.44
1:E:13:ASP:HB3	1:E:17:ARG:HH12	1.81	0.44
1:I:84:LYS:HD3	1:I:203:GLU:OE1	2.18	0.44
1:I:300:LEU:HD13	1:I:302:VAL:HG22	2.00	0.44
1:L:172:ILE:HD11	1:L:184:LEU:HD22	1.99	0.44
1:L:278:VAL:O	1:L:282:THR:CG2	2.64	0.44
1:L:59:SER:O	1:L:62:ASN:HB3	2.18	0.44
1:C:85:ILE:HD12	1:C:165:PHE:CZ	2.53	0.44
1:C:29:ASN:HD22	1:C:31:SER:H	1.64	0.44
1:C:43:THR:HG23	1:C:45:GLU:H	1.83	0.44
1:E:404:PHE:CD1	1:E:410:ALA:HB2	2.53	0.44
1:B:389:ILE:H	1:B:389:ILE:HG13	1.61	0.43
1:H:313:LYS:O	1:H:317:TRP:HD1	2.01	0.43
1:D:85:ILE:CD1	1:D:200:ILE:HD13	2.46	0.43
1:D:66:TRP:CZ3	1:D:74:ARG:HG2	2.53	0.43
1:G:497:TYR:HE2	1:H:284:PHE:HA	1.83	0.43
1:D:300:LEU:HD22	1:D:302:VAL:HG22	2.00	0.43
1:L:450:ALA:C	1:L:452:PRO:HD3	2.39	0.43
1:C:32:THR:O	1:C:33:GLU:HB2	2.17	0.43
1:D:29:ASN:C	1:D:29:ASN:HD22	2.22	0.43
1:D:456:GLN:NE2	1:D:456:GLN:H	2.17	0.43
1:E:236:PHE:HB3	1:E:259:LEU:HD23	1.99	0.43
1:D:321:ILE:HG23	1:D:332:ARG:HB3	2.01	0.43
1:G:450:ALA:C	1:G:452:PRO:HD3	2.38	0.43
1:C:13:ASP:H	1:C:212:ASN:ND2	2.16	0.43
1:E:389:ILE:H	1:E:389:ILE:HG13	1.70	0.43
1:L:384:THR:HG22	1:L:386:SER:H	1.84	0.43
1:B:29:ASN:ND2	1:B:31:SER:H	2.15	0.43
1:B:341:GLN:NE2	3:B:505:NAD:H3D	2.33	0.43
1:C:159:THR:HG21	1:C:168:ALA:HA	1.99	0.43
1:C:389:ILE:H	1:C:389:ILE:HG13	1.66	0.43
1:E:204:VAL:CG1	1:E:204:VAL:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:160:PRO:HB2	3:I:505:NAD:H5N	2.00	0.43
1:K:237:THR:HG23	1:K:260:GLU:HB3	2.01	0.43
1:L:9:GLN:CG	1:L:18:VAL:HA	2.49	0.43
1:C:163:TYR:O	1:C:167:MET:HB2	2.19	0.43
1:L:157:LEU:HD22	1:L:182:ALA:HB1	2.01	0.43
1:E:13:ASP:H	1:E:212:ASN:ND2	2.16	0.43
1:E:172:ILE:HD13	1:E:211:LEU:HD22	2.00	0.43
1:G:358:THR:HB	1:G:381:THR:HG23	2.00	0.43
1:H:39:ILE:HB	1:H:215:THR:HG21	2.01	0.43
1:K:436:LEU:O	1:K:440:LEU:HG	2.19	0.43
1:A:160:PRO:CB	3:A:505:NAD:H5N	2.49	0.42
1:B:453:SER:HB3	1:B:459:TRP:CZ3	2.53	0.42
1:D:36:ILE:O	1:D:36:ILE:HG13	2.19	0.42
1:H:30:PRO:HB2	1:H:335:PRO:HG2	2.00	0.42
1:C:160:PRO:HD3	1:C:237:THR:HB	2.00	0.42
1:F:13:ASP:H	1:F:212:ASN:HD22	1.65	0.42
1:C:292:GLN:HE22	1:C:337:VAL:H	1.65	0.42
1:I:120:TYR:CD2	1:I:455:ILE:HD12	2.55	0.42
1:K:65:ASP:HB2	6:K:976:HOH:O	2.17	0.42
1:L:29:ASN:ND2	1:L:31:SER:H	2.17	0.42
1:C:60:ARG:HH12	1:C:61:LYS:HD2	1.84	0.42
1:A:184:LEU:HG	1:A:186:PRO:HD3	2.00	0.42
1:A:40:PRO:HG2	1:A:215:THR:CG2	2.49	0.42
1:C:447:ILE:CG2	1:D:487:ARG:HG3	2.50	0.42
1:D:339:GLU:HG2	1:D:343:LYS:HE2	2.00	0.42
1:F:157:LEU:HG	1:F:171:LYS:HB3	2.00	0.42
1:A:29:ASN:HD22	1:A:29:ASN:C	2.22	0.42
1:I:234:ILE:HB	1:I:257:VAL:HG23	2.02	0.42
1:A:341:GLN:NE2	3:A:505:NAD:H3D	2.35	0.42
1:F:349:ILE:HD13	1:F:363:GLY:HA2	2.01	0.42
1:G:273:VAL:HG12	1:G:275:LEU:HD12	2.02	0.42
1:D:92:LEU:HB2	1:D:111:LEU:HD21	2.01	0.42
1:B:294:CYS:H	4:B:2002:GOL:HO1	1.67	0.42
1:D:186:PRO:HG2	1:D:215:THR:HG22	2.01	0.42
1:E:24:ARG:NH1	1:E:24:ARG:HG3	2.10	0.42
1:F:292:GLN:HE22	1:F:337:VAL:H	1.68	0.42
1:G:285:GLY:HA2	1:G:451:GLN:HG2	2.01	0.42
1:H:136:ILE:HD13	1:H:147:ILE:HG23	2.01	0.42
1:H:308:VAL:HG12	6:H:1177:HOH:O	2.19	0.42
1:I:342:TYR:OH	1:I:365:ARG:NH1	2.53	0.42
1:A:325:ASP:HA	1:A:326:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:ILE:HG23	1:B:300:LEU:HD23	2.02	0.41
1:B:426:MET:SD	1:B:448:ASN:HA	2.59	0.41
1:I:25:ILE:HG13	1:I:41:ALA:HB2	2.01	0.41
1:J:453:SER:HB3	1:J:459:TRP:CZ3	2.55	0.41
1:F:17:ARG:HD2	6:F:1341:HOH:O	2.21	0.41
1:F:273:VAL:HB	1:F:278:VAL:HG21	2.02	0.41
1:A:40:PRO:HG2	1:A:215:THR:HG23	2.02	0.41
1:D:458:PRO:HB3	1:D:474:TRP:CD1	2.55	0.41
1:H:254:VAL:CG1	1:H:254:VAL:O	2.59	0.41
1:H:64[A]:ARG:HA	1:H:64[A]:ARG:HD2	1.90	0.41
1:K:389:ILE:HG13	1:K:389:ILE:H	1.65	0.41
1:A:300:LEU:HD22	1:A:302:VAL:HG22	2.02	0.41
1:E:488:TYR:HB2	1:F:449:CYS:HB3	2.03	0.41
1:G:42:ALA:CB	1:G:214:VAL:HG13	2.50	0.41
1:H:29:ASN:HD22	1:H:29:ASN:C	2.22	0.41
1:I:500:PRO:HD3	1:J:317:TRP:CE2	2.56	0.41
1:J:43:THR:HG22	1:J:45:GLU:H	1.84	0.41
1:K:285:GLY:HA2	1:K:451:GLN:HG2	2.03	0.41
1:C:233:LYS:HG2	1:C:256:PRO:HG2	2.02	0.41
1:D:325:ASP:HA	1:D:326:PRO:HD3	1.94	0.41
1:G:259:LEU:HD12	1:H:254:VAL:HG13	2.02	0.41
1:I:13:ASP:H	1:I:212:ASN:ND2	2.18	0.41
1:C:450:ALA:C	1:C:452:PRO:HD3	2.41	0.41
1:K:456:GLN:H	1:K:456:GLN:NE2	2.18	0.41
1:L:292:GLN:HE22	1:L:337:VAL:H	1.67	0.41
1:C:15:GLU:HB2	6:C:523:HOH:O	2.21	0.41
1:F:418[A]:HIS:HB3	1:F:464:ARG:HG3	2.03	0.41
1:I:237:THR:HG23	1:I:260:GLU:HG3	2.02	0.41
1:J:323:ILE:HB	1:J:333:LEU:HD23	2.01	0.41
1:L:349:ILE:HD13	1:L:363:GLY:HA2	2.03	0.41
1:L:60:ARG:HG2	4:L:2005:GOL:C1	2.38	0.41
1:A:74:ARG:NH1	1:A:177:ALA:O	2.54	0.41
1:B:227:SER:HB3	1:B:249:THR:CG2	2.51	0.41
1:C:443:GLY:HA3	1:C:460:GLY:O	2.20	0.41
1:H:47:VAL:HG22	1:H:214:VAL:HG11	2.03	0.41
1:J:286:CYS:O	1:J:291:GLY:HA2	2.21	0.41
1:J:450:ALA:C	1:J:452:PRO:HD3	2.41	0.41
1:E:95:LEU:O	1:E:99:ASP:HB2	2.21	0.41
1:F:402:LYS:HD2	6:F:545:HOH:O	2.20	0.41
1:G:160:PRO:HD3	1:G:237:THR:HB	2.02	0.41
1:I:443:GLY:HA3	1:I:460:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:60:ARG:C	1:L:62:ASN:H	2.23	0.41
1:F:239:SER:HB3	3:F:505:NAD:H1D	2.03	0.41
1:J:227:SER:HB3	1:J:249:THR:HG21	2.02	0.41
1:A:32:THR:O	1:A:33:GLU:HB2	2.21	0.41
1:E:194:CYS:O	1:E:197:LEU:HB3	2.21	0.41
1:B:408:GLU:O	1:B:411:ILE:HD13	2.21	0.40
1:D:242:THR:O	1:D:246:ILE:HG12	2.20	0.40
1:E:43:THR:CG2	1:E:44:LYS:N	2.83	0.40
1:F:42:ALA:CB	1:F:214:VAL:HG13	2.52	0.40
1:A:160:PRO:HB2	3:A:505:NAD:H5N	2.03	0.40
1:G:341:GLN:HE22	3:G:505:NAD:H3D	1.86	0.40
1:A:358:THR:OG1	1:A:382:ASP:OD1	2.33	0.40
1:C:40:PRO:HG2	1:C:215:THR:CG2	2.51	0.40
1:D:358:THR:HB	1:D:381:THR:HG23	2.03	0.40
1:H:160:PRO:HD3	1:H:237:THR:HB	2.03	0.40
1:A:267:ILE:HD13	1:A:282:THR:HG22	2.04	0.40
1:B:13:ASP:H	1:B:212:ASN:HD22	1.69	0.40
1:B:167:MET:HE1	4:B:2002:GOL:H31	2.04	0.40
1:B:501:SER:HA	1:B:502:LYS:HA	1.87	0.40
1:C:455:ILE:H	1:C:455:ILE:HD13	1.86	0.40
1:K:273:VAL:HB	1:K:278:VAL:HG21	2.03	0.40
1:C:157:LEU:HG	1:C:171:LYS:HB3	2.04	0.40
1:I:172:ILE:HD11	1:I:184:LEU:HD22	2.03	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	495/503 (98%)	472 (95%)	20 (4%)	3 (1%)	25 36
1	B	495/503 (98%)	473 (96%)	20 (4%)	2 (0%)	34 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	493/503 (98%)	471 (96%)	18 (4%)	4 (1%)	19	29
1	D	494/503 (98%)	472 (96%)	20 (4%)	2 (0%)	34	48
1	E	494/503 (98%)	476 (96%)	17 (3%)	1 (0%)	47	62
1	F	494/503 (98%)	477 (97%)	16 (3%)	1 (0%)	47	62
1	G	494/503 (98%)	473 (96%)	17 (3%)	4 (1%)	19	29
1	H	496/503 (99%)	477 (96%)	15 (3%)	4 (1%)	19	29
1	I	496/503 (99%)	478 (96%)	15 (3%)	3 (1%)	25	36
1	J	495/503 (98%)	474 (96%)	19 (4%)	2 (0%)	34	48
1	K	496/503 (99%)	475 (96%)	19 (4%)	2 (0%)	34	48
1	L	495/503 (98%)	480 (97%)	14 (3%)	1 (0%)	47	62
All	All	5937/6036 (98%)	5698 (96%)	210 (4%)	29 (0%)	29	41

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	GLN
1	B	451	GLN
1	C	60	ARG
1	C	61	LYS
1	C	65	ASP
1	C	451	GLN
1	D	451	GLN
1	E	451	GLN
1	F	451	GLN
1	G	451	GLN
1	H	451	GLN
1	I	451	GLN
1	J	451	GLN
1	K	451	GLN
1	L	451	GLN
1	G	62	ASN
1	G	63	GLY
1	I	8	ARG
1	J	64	ARG
1	A	500	PRO
1	A	501	SER
1	G	65	ASP
1	H	262	GLY

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Mol	Chain	Res	Type
1	H	62	ASN
1	B	420	GLY
1	H	420	GLY
1	I	420	GLY
1	K	420	GLY
1	D	420	GLY

### 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	411/416 (99%)	378 (92%)	33 (8%)	12	18
1	B	411/416 (99%)	377 (92%)	34 (8%)	11	17
1	C	409/416 (98%)	372 (91%)	37 (9%)	9	14
1	D	410/416 (99%)	382 (93%)	28 (7%)	16	25
1	E	410/416 (99%)	380 (93%)	30 (7%)	14	22
1	F	410/416 (99%)	385 (94%)	25 (6%)	18	30
1	G	410/416 (99%)	378 (92%)	32 (8%)	12	19
1	H	412/416 (99%)	379 (92%)	33 (8%)	12	18
1	I	412/416 (99%)	375 (91%)	37 (9%)	9	14
1	J	411/416 (99%)	381 (93%)	30 (7%)	14	22
1	K	412/416 (99%)	385 (93%)	27 (7%)	16	26
1	L	411/416 (99%)	381 (93%)	30 (7%)	14	22
All	All	4929/4992 (99%)	4553 (92%)	376 (8%)	13	20

All (376) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	21	LEU
1	A	29	ASN
1	A	39	ILE

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Mol	Chain	Res	Type
1	A	49	LEU
1	A	59	SER
1	A	144	LYS
1	A	157	LEU
1	A	171	LYS
1	A	172	ILE
1	A	185	LYS
1	A	215	THR
1	A	217	LEU
1	A	254	VAL
1	A	255	LYS
1	A	257	VAL
1	A	260	GLU
1	A	273	VAL
1	A	300	LEU
1	A	302	VAL
1	A	308	VAL
1	A	314	LEU
1	A	332	ARG
1	A	360	LEU
1	A	364	ARG
1	A	384	THR
1	A	385	THR
1	A	395	PHE
1	A	411	ILE
1	A	436	LEU
1	A	444	ILE
1	A	455	ILE
1	A	502	LYS
1	B	9	GLN
1	B	29	ASN
1	B	31	SER
1	B	43	THR
1	B	89	LYS
1	B	95	LEU
1	B	97	SER
1	B	108	LEU
1	B	111	LEU
1	B	141	ASP
1	B	157	LEU
1	B	172	ILE
1	B	185	LYS

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Mol	Chain	Res	Type
1	B	217	LEU
1	B	254	VAL
1	B	255	LYS
1	B	257	VAL
1	B	273	VAL
1	B	280	GLU
1	B	300	LEU
1	B	302	VAL
1	B	323	ILE
1	B	365	ARG
1	B	379	ILE
1	B	380	ILE
1	B	385	THR
1	B	395	PHE
1	B	403	THR
1	B	411	ILE
1	B	436	LEU
1	B	455	ILE
1	B	473	GLU
1	B	476	LEU
1	B	491	ASP
1	C	29	ASN
1	C	36	ILE
1	C	61	LYS
1	C	64	ARG
1	C	65	ASP
1	C	84	LYS
1	C	108	LEU
1	C	111	LEU
1	C	133	LYS
1	C	138	LEU
1	C	144	LYS
1	C	157	LEU
1	C	165	PHE
1	C	167	MET
1	C	185	LYS
1	C	215	THR
1	C	217	LEU
1	C	253	LEU
1	C	255	LYS
1	C	257	VAL
1	C	260	GLU

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Mol	Chain	Res	Type
1	C	273	VAL
1	C	282	THR
1	C	300	LEU
1	C	302	VAL
1	C	308	VAL
1	C	314	LEU
1	C	323	ILE
1	C	353	LYS
1	C	360	LEU
1	C	385	THR
1	C	389	ILE
1	C	395	PHE
1	C	455	ILE
1	C	476	LEU
1	C	491	ASP
1	C	492	GLU
1	D	21	LEU
1	D	29	ASN
1	D	43	THR
1	D	89	LYS
1	D	94	LYS
1	D	108	LEU
1	D	111	LEU
1	D	138	LEU
1	D	144	LYS
1	D	157	LEU
1	D	165	PHE
1	D	172	ILE
1	D	185	LYS
1	D	204	VAL
1	D	217	LEU
1	D	255	LYS
1	D	289	THR
1	D	300	LEU
1	D	302	VAL
1	D	360	LEU
1	D	379	ILE
1	D	380	ILE
1	D	395	PHE
1	D	399	LEU
1	D	402	LYS
1	D	411	ILE

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Mol	Chain	Res	Type
1	D	456	GLN
1	D	481	SER
1	E	9	GLN
1	E	15	GLU
1	E	24	ARG
1	E	29	ASN
1	E	62	ASN
1	E	76	ARG
1	E	84	LYS
1	E	95	LEU
1	E	111	LEU
1	E	137	SER
1	E	149	LYS
1	E	157	LEU
1	E	165	PHE
1	E	172	ILE
1	E	185	LYS
1	E	217	LEU
1	E	253	LEU
1	E	278	VAL
1	E	282	THR
1	E	300	LEU
1	E	302	VAL
1	E	314	LEU
1	E	316	LYS
1	E	323	ILE
1	E	369	LEU
1	E	395	PHE
1	E	403	THR
1	E	476	LEU
1	E	491	ASP
1	E	492	GLU
1	F	8	ARG
1	F	17	ARG
1	F	29	ASN
1	F	44	LYS
1	F	108	LEU
1	F	111	LEU
1	F	132	GLN
1	F	138	LEU
1	F	140	MET
1	F	141	ASP

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Mol	Chain	Res	Type
1	F	157	LEU
1	F	165	PHE
1	F	185	LYS
1	F	217	LEU
1	F	257	VAL
1	F	300	LEU
1	F	302	VAL
1	F	323	ILE
1	F	375	VAL
1	F	385	THR
1	F	389	ILE
1	F	395	PHE
1	F	402	LYS
1	F	455	ILE
1	F	476	LEU
1	G	15	GLU
1	G	29	ASN
1	G	39	ILE
1	G	84	LYS
1	G	111	LEU
1	G	157	LEU
1	G	172	ILE
1	G	185	LYS
1	G	196	GLU
1	G	208	ARG
1	G	217	LEU
1	G	253	LEU
1	G	254	VAL
1	G	255	LYS
1	G	257	VAL
1	G	273	VAL
1	G	300	LEU
1	G	302	VAL
1	G	308	VAL
1	G	314	LEU
1	G	322	LYS
1	G	360	LEU
1	G	367	GLU
1	G	379	ILE
1	G	384	THR
1	G	389	ILE
1	G	395	PHE

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Mol	Chain	Res	Type
1	G	455	ILE
1	G	456	GLN
1	G	476	LEU
1	G	491	ASP
1	G	502	LYS
1	H	21	LEU
1	H	29	ASN
1	H	55	LYS
1	H	64[A]	ARG
1	H	64[B]	ARG
1	H	73	LEU
1	H	84	LYS
1	H	94	LYS
1	H	111	LEU
1	H	128	LEU
1	H	137	SER
1	H	157	LEU
1	H	172	ILE
1	H	185	LYS
1	H	217	LEU
1	H	240	SER
1	H	257	VAL
1	H	273	VAL
1	H	282	THR
1	H	300	LEU
1	H	302	VAL
1	H	314	LEU
1	H	367	GLU
1	H	369	LEU
1	H	381	THR
1	H	385	THR
1	H	395	PHE
1	H	402	LYS
1	H	403	THR
1	H	411	ILE
1	H	456	GLN
1	H	476	LEU
1	H	489	THR
1	I	8	ARG
1	I	9	GLN
1	I	29	ASN
1	I	39	ILE

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Mol	Chain	Res	Type
1	I	55	LYS
1	I	84	LYS
1	I	94	LYS
1	I	95	LEU
1	I	111	LEU
1	I	131	LYS
1	I	136	ILE
1	I	137	SER
1	I	141	ASP
1	I	157	LEU
1	I	165	PHE
1	I	185	LYS
1	I	217	LEU
1	I	233	LYS
1	I	254	VAL
1	I	255	LYS
1	I	260	GLU
1	I	278	VAL
1	I	289	THR
1	I	300	LEU
1	I	302	VAL
1	I	308	VAL
1	I	364	ARG
1	I	369	LEU
1	I	385	THR
1	I	395	PHE
1	I	399	LEU
1	I	403	THR
1	I	430	LEU
1	I	455	ILE
1	I	470	GLU
1	I	476	LEU
1	I	491	ASP
1	J	29	ASN
1	J	43	THR
1	J	55	LYS
1	J	95	LEU
1	J	108	LEU
1	J	111	LEU
1	J	124	LEU
1	J	136	ILE
1	J	157	LEU

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Mol	Chain	Res	Type
1	J	171	LYS
1	J	185	LYS
1	J	204	VAL
1	J	217	LEU
1	J	253	LEU
1	J	257	VAL
1	J	282	THR
1	J	300	LEU
1	J	302	VAL
1	J	308	VAL
1	J	323	ILE
1	J	347	ASN
1	J	360	LEU
1	J	365	ARG
1	J	395	PHE
1	J	403	THR
1	J	436	LEU
1	J	455	ILE
1	J	476	LEU
1	J	490	SER
1	J	502	LYS
1	K	29	ASN
1	K	52	ASP
1	K	84	LYS
1	K	95	LEU
1	K	111	LEU
1	K	138	LEU
1	K	140	MET
1	K	141	ASP
1	K	157	LEU
1	K	165	PHE
1	K	185	LYS
1	K	217	LEU
1	K	260	GLU
1	K	282	THR
1	K	300	LEU
1	K	302	VAL
1	K	364	ARG
1	K	370	LYS
1	K	385	THR
1	K	395	PHE
1	K	399	LEU

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Mol	Chain	Res	Type
1	K	403	THR
1	K	436	LEU
1	K	456	GLN
1	K	470	GLU
1	K	476	LEU
1	K	491	ASP
1	L	8	ARG
1	L	9	GLN
1	L	21	LEU
1	L	29	ASN
1	L	55	LYS
1	L	61	LYS
1	L	108	LEU
1	L	111	LEU
1	L	138	LEU
1	L	147	ILE
1	L	157	LEU
1	L	165	PHE
1	L	185	LYS
1	L	192	VAL
1	L	217	LEU
1	L	257	VAL
1	L	273	VAL
1	L	282	THR
1	L	289	THR
1	L	300	LEU
1	L	302	VAL
1	L	308	VAL
1	L	314	LEU
1	L	353	LYS
1	L	392	GLU
1	L	395	PHE
1	L	447	ILE
1	L	455	ILE
1	L	476	LEU
1	L	491	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	29	ASN

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Mol	Chain	Res	Type
1	A	212	ASN
1	A	292	GLN
1	A	341	GLN
1	A	368	HIS
1	B	29	ASN
1	B	212	ASN
1	B	219	HIS
1	B	292	GLN
1	B	341	GLN
1	B	368	HIS
1	C	29	ASN
1	C	212	ASN
1	C	292	GLN
1	C	341	GLN
1	C	368	HIS
1	C	484	GLN
1	C	498	GLN
1	D	29	ASN
1	D	456	GLN
1	E	29	ASN
1	E	62	ASN
1	E	212	ASN
1	E	292	GLN
1	E	341	GLN
1	F	29	ASN
1	F	132	GLN
1	F	212	ASN
1	F	292	GLN
1	F	341	GLN
1	G	9	GLN
1	G	29	ASN
1	G	292	GLN
1	G	341	GLN
1	G	368	HIS
1	G	456	GLN
1	H	29	ASN
1	H	292	GLN
1	H	341	GLN
1	H	456	GLN
1	I	29	ASN
1	I	212	ASN
1	I	219	HIS

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Mol	Chain	Res	Type
1	I	341	GLN
1	J	29	ASN
1	J	62	ASN
1	J	212	ASN
1	J	292	GLN
1	J	341	GLN
1	J	347	ASN
1	K	29	ASN
1	K	219	HIS
1	K	292	GLN
1	K	341	GLN
1	K	347	ASN
1	K	456	GLN
1	K	478	ASN
1	L	29	ASN
1	L	212	ASN
1	L	292	GLN
1	L	347	ASN
1	L	368	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 12 are monoatomic - leaving 32 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	$\# Z  > 2$
4	GOL	G	2009	-	5,5,5	0.37	0	5,5,5	0.51	0
4	GOL	G	2007	-	5,5,5	0.36	0	5,5,5	0.23	0
4	GOL	B	2001	-	5,5,5	0.39	0	5,5,5	0.28	0
3	NAD	A	505	-	42,48,48	2.71	8 (19%)	50,73,73	1.90	6 (12%)
4	GOL	L	2008	-	5,5,5	0.41	0	5,5,5	0.24	0
3	NAD	K	505	-	42,48,48	2.72	8 (19%)	50,73,73	1.92	7 (14%)
4	GOL	J	2013	-	5,5,5	0.39	0	5,5,5	0.30	0
4	GOL	K	2016	-	5,5,5	0.36	0	5,5,5	0.42	0
3	NAD	H	505	-	42,48,48	2.71	8 (19%)	50,73,73	1.95	8 (16%)
4	GOL	C	2003	-	5,5,5	0.39	0	5,5,5	0.24	0
4	GOL	J	2014	-	5,5,5	0.37	0	5,5,5	0.39	0
4	GOL	K	2019	-	5,5,5	0.35	0	5,5,5	0.30	0
4	GOL	F	2006	-	5,5,5	0.41	0	5,5,5	0.18	0
3	NAD	I	505	-	42,48,48	2.73	8 (19%)	50,73,73	1.92	6 (12%)
3	NAD	B	505	-	42,48,48	2.73	9 (21%)	50,73,73	1.87	6 (12%)
4	GOL	I	2012	-	5,5,5	0.31	0	5,5,5	0.50	0
5	MRD	D	2004	-	7,7,7	0.27	0	9,10,10	0.45	0
3	NAD	J	505	-	42,48,48	2.70	8 (19%)	50,73,73	1.90	6 (12%)
4	GOL	L	2015	-	5,5,5	0.38	0	5,5,5	0.18	0
3	NAD	G	505	-	42,48,48	2.74	9 (21%)	50,73,73	1.91	7 (14%)
4	GOL	G	2011	-	5,5,5	0.40	0	5,5,5	0.24	0
4	GOL	B	2002	-	5,5,5	0.38	0	5,5,5	0.26	0
4	GOL	H	2010	-	5,5,5	0.37	0	5,5,5	0.51	0
4	GOL	L	2017	-	5,5,5	0.36	0	5,5,5	0.30	0
3	NAD	C	505	-	42,48,48	2.69	8 (19%)	50,73,73	1.96	6 (12%)
3	NAD	D	505	-	24,29,48	3.37	6 (25%)	29,45,73	2.26	3 (10%)
4	GOL	L	2000	-	5,5,5	0.37	0	5,5,5	0.21	0
3	NAD	L	505	-	42,48,48	2.74	8 (19%)	50,73,73	1.88	6 (12%)
4	GOL	L	2005	-	5,5,5	0.41	0	5,5,5	0.31	0
4	GOL	K	2018	-	5,5,5	0.36	0	5,5,5	0.21	0
3	NAD	F	505	-	42,48,48	2.66	8 (19%)	50,73,73	1.94	7 (14%)
3	NAD	E	505	-	42,48,48	2.69	8 (19%)	50,73,73	1.99	8 (16%)

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
4	GOL	G	2009	-	-	2/4/4/4	-
4	GOL	G	2007	-	-	0/4/4/4	-
4	GOL	B	2001	-	-	1/4/4/4	-
3	NAD	A	505	-	-	10/26/62/62	0/5/5/5
4	GOL	L	2008	-	-	2/4/4/4	-
3	NAD	K	505	-	-	11/26/62/62	0/5/5/5
4	GOL	J	2013	-	-	4/4/4/4	-
4	GOL	K	2016	-	-	2/4/4/4	-
3	NAD	H	505	-	-	8/26/62/62	0/5/5/5
4	GOL	C	2003	-	-	0/4/4/4	-
4	GOL	J	2014	-	-	2/4/4/4	-
4	GOL	K	2019	-	-	3/4/4/4	-
4	GOL	F	2006	-	-	2/4/4/4	-
3	NAD	I	505	-	-	12/26/62/62	0/5/5/5
3	NAD	B	505	-	-	8/26/62/62	0/5/5/5
4	GOL	I	2012	-	-	2/4/4/4	-
5	MRD	D	2004	-	-	1/5/5/5	-
3	NAD	J	505	-	-	12/26/62/62	0/5/5/5
4	GOL	L	2015	-	-	2/4/4/4	-
3	NAD	G	505	-	-	6/26/62/62	0/5/5/5
4	GOL	G	2011	-	-	1/4/4/4	-
4	GOL	B	2002	-	-	3/4/4/4	-
4	GOL	H	2010	-	-	4/4/4/4	-
4	GOL	L	2017	-	-	2/4/4/4	-
3	NAD	C	505	-	-	12/26/62/62	0/5/5/5
3	NAD	D	505	-	-	5/12/32/62	0/3/3/5
4	GOL	L	2000	-	-	2/4/4/4	-
3	NAD	L	505	-	-	12/26/62/62	0/5/5/5
4	GOL	L	2005	-	-	0/4/4/4	-
4	GOL	K	2018	-	-	4/4/4/4	-
3	NAD	F	505	-	-	12/26/62/62	0/5/5/5
3	NAD	E	505	-	-	10/26/62/62	0/5/5/5

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	505	NAD	C2A-N3A	10.66	1.49	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	505	NAD	C2A-N3A	10.65	1.49	1.32
3	D	505	NAD	C2A-N3A	10.60	1.49	1.32
3	E	505	NAD	C2A-N3A	10.52	1.49	1.32
3	F	505	NAD	C2A-N3A	10.47	1.49	1.32
3	B	505	NAD	C2A-N3A	10.40	1.48	1.32
3	J	505	NAD	C2A-N3A	10.39	1.48	1.32
3	H	505	NAD	C2A-N3A	10.39	1.48	1.32
3	G	505	NAD	C2A-N3A	10.37	1.48	1.32
3	L	505	NAD	C2A-N3A	10.37	1.48	1.32
3	C	505	NAD	C2A-N3A	10.34	1.48	1.32
3	A	505	NAD	C2A-N3A	10.34	1.48	1.32
3	L	505	NAD	C2A-N1A	8.24	1.49	1.33
3	E	505	NAD	C2A-N1A	8.23	1.49	1.33
3	G	505	NAD	C2A-N1A	8.22	1.49	1.33
3	B	505	NAD	C2A-N1A	8.22	1.49	1.33
3	A	505	NAD	C2A-N1A	8.21	1.49	1.33
3	D	505	NAD	C2A-N1A	8.20	1.49	1.33
3	H	505	NAD	C2A-N1A	8.15	1.49	1.33
3	K	505	NAD	C2A-N1A	8.14	1.49	1.33
3	I	505	NAD	C2A-N1A	8.10	1.49	1.33
3	C	505	NAD	C2A-N1A	8.08	1.48	1.33
3	J	505	NAD	C2A-N1A	8.03	1.48	1.33
3	F	505	NAD	C2A-N1A	7.98	1.48	1.33
3	C	505	NAD	C8A-N7A	7.05	1.47	1.34
3	A	505	NAD	C8A-N7A	7.04	1.47	1.34
3	I	505	NAD	C8A-N7A	6.98	1.47	1.34
3	H	505	NAD	C8A-N7A	6.96	1.47	1.34
3	J	505	NAD	C8A-N7A	6.94	1.47	1.34
3	G	505	NAD	C8A-N7A	6.93	1.47	1.34
3	E	505	NAD	C8A-N7A	6.88	1.46	1.34
3	D	505	NAD	C8A-N7A	6.81	1.46	1.34
3	B	505	NAD	C8A-N7A	6.77	1.46	1.34
3	F	505	NAD	C8A-N7A	6.73	1.46	1.34
3	K	505	NAD	C8A-N7A	6.72	1.46	1.34
3	L	505	NAD	C8A-N7A	6.64	1.46	1.34
3	B	505	NAD	C2N-N1N	5.36	1.41	1.35
3	L	505	NAD	C2N-N1N	5.32	1.41	1.35
3	K	505	NAD	C2N-N1N	5.19	1.41	1.35
3	G	505	NAD	C2N-N1N	5.12	1.41	1.35
3	A	505	NAD	C2N-N1N	5.09	1.41	1.35
3	I	505	NAD	C2N-N1N	5.03	1.41	1.35
3	J	505	NAD	C2N-N1N	5.01	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	505	NAD	C2N-N1N	4.96	1.41	1.35
3	F	505	NAD	C2N-N1N	4.89	1.40	1.35
3	H	505	NAD	C2N-N1N	4.66	1.40	1.35
3	E	505	NAD	C2N-N1N	4.44	1.40	1.35
3	I	505	NAD	C4A-N3A	4.26	1.41	1.35
3	D	505	NAD	C4A-N3A	4.22	1.41	1.35
3	E	505	NAD	C4A-N3A	4.21	1.41	1.35
3	G	505	NAD	C4A-N3A	4.18	1.41	1.35
3	H	505	NAD	C4A-N3A	4.16	1.41	1.35
3	A	505	NAD	C4A-N3A	4.16	1.41	1.35
3	L	505	NAD	C4A-N3A	4.05	1.41	1.35
3	C	505	NAD	C4A-N3A	4.05	1.41	1.35
3	J	505	NAD	C4A-N3A	3.96	1.41	1.35
3	B	505	NAD	C4A-N3A	3.84	1.41	1.35
3	K	505	NAD	C4A-N3A	3.81	1.40	1.35
3	F	505	NAD	C4A-N3A	3.78	1.40	1.35
3	L	505	NAD	O4D-C1D	3.52	1.46	1.41
3	B	505	NAD	O4B-C1B	3.44	1.45	1.41
3	J	505	NAD	O4B-C1B	3.33	1.45	1.41
3	H	505	NAD	O4B-C1B	3.31	1.45	1.41
3	D	505	NAD	O4B-C1B	3.31	1.45	1.41
3	K	505	NAD	O4B-C1B	3.22	1.45	1.41
3	L	505	NAD	O4B-C1B	3.22	1.45	1.41
3	G	505	NAD	O4B-C1B	3.20	1.45	1.41
3	I	505	NAD	O4B-C1B	3.03	1.45	1.41
3	A	505	NAD	O4B-C1B	3.01	1.45	1.41
3	C	505	NAD	O4D-C1D	3.00	1.45	1.41
3	H	505	NAD	O4D-C1D	2.97	1.45	1.41
3	F	505	NAD	O4D-C1D	2.88	1.45	1.41
3	E	505	NAD	O4D-C1D	2.84	1.45	1.41
3	K	505	NAD	O4D-C1D	2.83	1.45	1.41
3	J	505	NAD	O4D-C1D	2.82	1.45	1.41
3	E	505	NAD	O4B-C1B	2.79	1.45	1.41
3	F	505	NAD	O4B-C1B	2.78	1.45	1.41
3	I	505	NAD	O4D-C1D	2.74	1.44	1.41
3	B	505	NAD	O4D-C1D	2.72	1.44	1.41
3	G	505	NAD	C6N-N1N	2.61	1.41	1.35
3	G	505	NAD	C3N-C7N	2.54	1.54	1.50
3	C	505	NAD	C6N-N1N	2.50	1.41	1.35
3	C	505	NAD	O4B-C1B	2.49	1.44	1.41
3	H	505	NAD	C6N-N1N	2.48	1.41	1.35
3	G	505	NAD	O4D-C1D	2.48	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	505	NAD	C6N-N1N	2.42	1.41	1.35
3	L	505	NAD	C6N-N1N	2.40	1.41	1.35
3	I	505	NAD	C6N-N1N	2.39	1.41	1.35
3	E	505	NAD	C6N-N1N	2.39	1.41	1.35
3	K	505	NAD	C6N-N1N	2.36	1.41	1.35
3	F	505	NAD	C6N-N1N	2.35	1.41	1.35
3	A	505	NAD	O4D-C1D	2.30	1.44	1.41
3	J	505	NAD	C6N-N1N	2.28	1.41	1.35
3	A	505	NAD	C6N-N1N	2.27	1.41	1.35
3	B	505	NAD	C3N-C7N	2.15	1.53	1.50
3	D	505	NAD	PN-O5D	2.15	1.63	1.54

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	505	NAD	N3A-C2A-N1A	-10.79	111.82	128.68
3	C	505	NAD	N3A-C2A-N1A	-10.77	111.85	128.68
3	E	505	NAD	N3A-C2A-N1A	-10.71	111.94	128.68
3	A	505	NAD	N3A-C2A-N1A	-10.69	111.96	128.68
3	J	505	NAD	N3A-C2A-N1A	-10.65	112.04	128.68
3	I	505	NAD	N3A-C2A-N1A	-10.62	112.08	128.68
3	L	505	NAD	N3A-C2A-N1A	-10.61	112.09	128.68
3	F	505	NAD	N3A-C2A-N1A	-10.61	112.10	128.68
3	D	505	NAD	N3A-C2A-N1A	-10.57	112.15	128.68
3	G	505	NAD	N3A-C2A-N1A	-10.55	112.19	128.68
3	K	505	NAD	N3A-C2A-N1A	-10.48	112.31	128.68
3	B	505	NAD	N3A-C2A-N1A	-10.47	112.32	128.68
3	J	505	NAD	PN-O3-PA	-4.37	117.82	132.83
3	G	505	NAD	PN-O3-PA	-4.31	118.02	132.83
3	E	505	NAD	PN-O3-PA	-4.06	118.88	132.83
3	K	505	NAD	PN-O3-PA	-4.02	119.03	132.83
3	F	505	NAD	PN-O3-PA	-3.97	119.21	132.83
3	E	505	NAD	O4D-C1D-C2D	-3.95	101.15	106.93
3	F	505	NAD	O4D-C1D-C2D	-3.93	101.18	106.93
3	K	505	NAD	O4D-C1D-C2D	-3.80	101.37	106.93
3	A	505	NAD	PN-O3-PA	-3.80	119.78	132.83
3	C	505	NAD	PN-O3-PA	-3.80	119.80	132.83
3	I	505	NAD	PN-O3-PA	-3.76	119.91	132.83
3	D	505	NAD	PA-O3-PN	-3.70	120.12	132.83
3	B	505	NAD	O4D-C1D-C2D	-3.67	101.56	106.93
3	B	505	NAD	PN-O3-PA	-3.67	120.24	132.83
3	A	505	NAD	O4D-C1D-C2D	-3.59	101.68	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	505	NAD	O4D-C1D-C2D	-3.56	101.72	106.93
3	H	505	NAD	PN-O3-PA	-3.34	121.37	132.83
3	G	505	NAD	O4D-C1D-C2D	-3.24	102.19	106.93
3	H	505	NAD	O4D-C1D-C2D	-3.17	102.29	106.93
3	C	505	NAD	O4D-C1D-C2D	-3.14	102.34	106.93
3	C	505	NAD	C3N-C7N-N7N	-3.08	114.05	117.75
3	L	505	NAD	PN-O3-PA	-3.04	122.41	132.83
3	J	505	NAD	O4D-C1D-C2D	-2.96	102.61	106.93
3	L	505	NAD	O4D-C1D-C2D	-2.90	102.69	106.93
3	L	505	NAD	C6N-N1N-C2N	-2.88	119.34	121.97
3	H	505	NAD	C3N-C7N-N7N	-2.70	114.51	117.75
3	I	505	NAD	C3N-C7N-N7N	-2.64	114.58	117.75
3	E	505	NAD	C3N-C7N-N7N	-2.64	114.58	117.75
3	H	505	NAD	C6N-N1N-C2N	-2.64	119.57	121.97
3	K	505	NAD	C3N-C7N-N7N	-2.61	114.61	117.75
3	H	505	NAD	C2A-N1A-C6A	2.60	123.20	118.75
3	A	505	NAD	C3N-C7N-N7N	-2.59	114.64	117.75
3	B	505	NAD	C6N-N1N-C2N	-2.56	119.64	121.97
3	C	505	NAD	C2A-N1A-C6A	2.53	123.08	118.75
3	E	505	NAD	C6N-N1N-C2N	-2.51	119.68	121.97
3	A	505	NAD	C2A-N1A-C6A	2.51	123.04	118.75
3	F	505	NAD	C3N-C7N-N7N	-2.49	114.77	117.75
3	L	505	NAD	C2A-N1A-C6A	2.47	122.98	118.75
3	C	505	NAD	C6N-N1N-C2N	-2.46	119.73	121.97
3	E	505	NAD	C2A-N1A-C6A	2.45	122.94	118.75
3	G	505	NAD	C2A-N1A-C6A	2.44	122.93	118.75
3	L	505	NAD	C3N-C7N-N7N	-2.40	114.86	117.75
3	H	505	NAD	C3B-C2B-C1B	2.35	104.52	100.98
3	I	505	NAD	C2A-N1A-C6A	2.34	122.75	118.75
3	G	505	NAD	C6N-N1N-C2N	-2.31	119.86	121.97
3	J	505	NAD	C2A-N1A-C6A	2.31	122.71	118.75
3	F	505	NAD	C2A-N1A-C6A	2.29	122.68	118.75
3	J	505	NAD	C3N-C7N-N7N	-2.29	115.00	117.75
3	K	505	NAD	C6N-N1N-C2N	-2.29	119.89	121.97
3	I	505	NAD	C6N-N1N-C2N	-2.28	119.90	121.97
3	B	505	NAD	C2A-N1A-C6A	2.26	122.63	118.75
3	E	505	NAD	C5B-C4B-C3B	-2.24	106.78	115.18
3	K	505	NAD	C3B-C2B-C1B	2.21	104.30	100.98
3	D	505	NAD	C2A-N1A-C6A	2.21	122.53	118.75
3	F	505	NAD	C6N-N1N-C2N	-2.20	119.97	121.97
3	A	505	NAD	C6N-N1N-C2N	-2.19	119.98	121.97
3	F	505	NAD	C5B-C4B-C3B	-2.18	107.00	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	505	NAD	O4B-C1B-C2B	-2.17	103.75	106.93
3	H	505	NAD	C5B-C4B-C3B	-2.12	107.23	115.18
3	B	505	NAD	C3N-C7N-N7N	-2.12	115.21	117.75
3	K	505	NAD	C2A-N1A-C6A	2.11	122.37	118.75
3	J	505	NAD	C6N-N1N-C2N	-2.06	120.09	121.97
3	G	505	NAD	C3B-C2B-C1B	2.02	104.02	100.98
3	G	505	NAD	C3N-C7N-N7N	-2.01	115.34	117.75

There are no chirality outliers.

All (157) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	2009	GOL	O1-C1-C2-C3
3	C	505	NAD	O4B-C4B-C5B-O5B
3	C	505	NAD	C3B-C4B-C5B-O5B
3	C	505	NAD	PA-O3-PN-O5D
3	C	505	NAD	C5D-O5D-PN-O3
3	C	505	NAD	C5D-O5D-PN-O2N
3	C	505	NAD	C4D-C5D-O5D-PN
3	C	505	NAD	O4D-C4D-C5D-O5D
3	C	505	NAD	C3D-C4D-C5D-O5D
3	A	505	NAD	O4B-C4B-C5B-O5B
3	A	505	NAD	C5D-O5D-PN-O3
3	A	505	NAD	C5D-O5D-PN-O2N
3	A	505	NAD	C4D-C5D-O5D-PN
3	A	505	NAD	O4D-C4D-C5D-O5D
3	A	505	NAD	C3D-C4D-C5D-O5D
3	K	505	NAD	O4B-C4B-C5B-O5B
3	K	505	NAD	C4D-C5D-O5D-PN
3	K	505	NAD	O4D-C4D-C5D-O5D
3	K	505	NAD	C3D-C4D-C5D-O5D
3	H	505	NAD	O4B-C4B-C5B-O5B
3	H	505	NAD	C5D-O5D-PN-O3
3	H	505	NAD	C5D-O5D-PN-O1N
3	H	505	NAD	C5D-O5D-PN-O2N
3	H	505	NAD	C3D-C4D-C5D-O5D
4	J	2014	GOL	C1-C2-C3-O3
3	I	505	NAD	PA-O3-PN-O5D
3	I	505	NAD	C5D-O5D-PN-O3
3	I	505	NAD	C5D-O5D-PN-O2N
3	I	505	NAD	C4D-C5D-O5D-PN
3	B	505	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	B	505	NAD	C5D-O5D-PN-O3
3	B	505	NAD	C5D-O5D-PN-O2N
3	B	505	NAD	C4D-C5D-O5D-PN
3	B	505	NAD	O4D-C4D-C5D-O5D
3	B	505	NAD	C3D-C4D-C5D-O5D
3	J	505	NAD	O4B-C4B-C5B-O5B
3	J	505	NAD	PA-O3-PN-O5D
3	J	505	NAD	C4D-C5D-O5D-PN
3	J	505	NAD	C3D-C4D-C5D-O5D
3	G	505	NAD	O4B-C4B-C5B-O5B
3	G	505	NAD	C5D-O5D-PN-O3
3	G	505	NAD	C5D-O5D-PN-O1N
3	G	505	NAD	C5D-O5D-PN-O2N
4	B	2002	GOL	O1-C1-C2-C3
4	H	2010	GOL	O1-C1-C2-C3
4	L	2017	GOL	C1-C2-C3-O3
4	L	2017	GOL	O2-C2-C3-O3
3	D	505	NAD	C5B-O5B-PA-O1A
4	L	2000	GOL	C1-C2-C3-O3
4	L	2000	GOL	O2-C2-C3-O3
3	L	505	NAD	C5B-O5B-PA-O3
3	L	505	NAD	C4D-C5D-O5D-PN
3	L	505	NAD	C3D-C4D-C5D-O5D
4	K	2019	GOL	O1-C1-C2-C3
4	K	2018	GOL	C1-C2-C3-O3
4	K	2018	GOL	O2-C2-C3-O3
3	F	505	NAD	O4B-C4B-C5B-O5B
3	F	505	NAD	PA-O3-PN-O5D
3	F	505	NAD	C5D-O5D-PN-O3
3	F	505	NAD	C5D-O5D-PN-O2N
3	F	505	NAD	C4D-C5D-O5D-PN
3	F	505	NAD	C3D-C4D-C5D-O5D
3	E	505	NAD	O4B-C4B-C5B-O5B
3	E	505	NAD	C3B-C4B-C5B-O5B
3	E	505	NAD	C5D-O5D-PN-O3
3	E	505	NAD	C5D-O5D-PN-O2N
3	E	505	NAD	C4D-C5D-O5D-PN
3	K	505	NAD	C2N-C3N-C7N-N7N
3	A	505	NAD	C3B-C4B-C5B-O5B
3	K	505	NAD	C3B-C4B-C5B-O5B
3	H	505	NAD	C3B-C4B-C5B-O5B
3	I	505	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	I	505	NAD	C3B-C4B-C5B-O5B
3	I	505	NAD	O4D-C4D-C5D-O5D
3	I	505	NAD	C3D-C4D-C5D-O5D
3	B	505	NAD	C3B-C4B-C5B-O5B
3	J	505	NAD	C3B-C4B-C5B-O5B
3	J	505	NAD	O4D-C4D-C5D-O5D
3	G	505	NAD	C3B-C4B-C5B-O5B
3	L	505	NAD	O4D-C4D-C5D-O5D
3	F	505	NAD	O4D-C4D-C5D-O5D
3	E	505	NAD	O4D-C4D-C5D-O5D
3	E	505	NAD	C3D-C4D-C5D-O5D
3	H	505	NAD	C4D-C5D-O5D-PN
3	K	505	NAD	C4N-C3N-C7N-N7N
3	K	505	NAD	C2N-C3N-C7N-O7N
3	J	505	NAD	C2N-C3N-C7N-O7N
3	J	505	NAD	C2N-C3N-C7N-N7N
3	F	505	NAD	C2N-C3N-C7N-O7N
3	K	505	NAD	C4N-C3N-C7N-O7N
3	J	505	NAD	C4N-C3N-C7N-N7N
3	J	505	NAD	C4N-C3N-C7N-O7N
3	F	505	NAD	C2N-C3N-C7N-N7N
3	F	505	NAD	C4N-C3N-C7N-N7N
4	I	2012	GOL	O2-C2-C3-O3
4	L	2015	GOL	O2-C2-C3-O3
3	H	505	NAD	O4D-C4D-C5D-O5D
3	D	505	NAD	O4B-C4B-C5B-O5B
3	F	505	NAD	C3B-C4B-C5B-O5B
3	F	505	NAD	C4N-C3N-C7N-O7N
3	L	505	NAD	C2N-C3N-C7N-N7N
3	L	505	NAD	C4N-C3N-C7N-N7N
3	L	505	NAD	C2N-C3N-C7N-O7N
3	L	505	NAD	C4N-C3N-C7N-O7N
4	K	2016	GOL	C1-C2-C3-O3
4	L	2008	GOL	C1-C2-C3-O3
4	J	2013	GOL	O1-C1-C2-C3
4	J	2013	GOL	C1-C2-C3-O3
4	I	2012	GOL	C1-C2-C3-O3
4	F	2006	GOL	O1-C1-C2-C3
4	L	2015	GOL	C1-C2-C3-O3
4	H	2010	GOL	C1-C2-C3-O3
4	G	2009	GOL	O1-C1-C2-O2
4	J	2013	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	J	2014	GOL	O2-C2-C3-O3
4	B	2002	GOL	O1-C1-C2-O2
4	H	2010	GOL	O1-C1-C2-O2
4	H	2010	GOL	O2-C2-C3-O3
3	D	505	NAD	C3B-C4B-C5B-O5B
3	G	505	NAD	C4D-C5D-O5D-PN
3	C	505	NAD	C4N-C3N-C7N-O7N
3	C	505	NAD	C4N-C3N-C7N-N7N
3	C	505	NAD	C2N-C3N-C7N-O7N
4	J	2013	GOL	O1-C1-C2-O2
4	K	2019	GOL	O1-C1-C2-O2
3	A	505	NAD	PA-O3-PN-O5D
3	L	505	NAD	PA-O3-PN-O5D
3	E	505	NAD	PA-O3-PN-O5D
3	C	505	NAD	C2N-C3N-C7N-N7N
4	K	2016	GOL	O2-C2-C3-O3
4	F	2006	GOL	O1-C1-C2-O2
3	D	505	NAD	C5B-O5B-PA-O3
3	L	505	NAD	C5D-O5D-PN-O3
3	E	505	NAD	C5B-O5B-PA-O3
4	K	2018	GOL	O1-C1-C2-C3
3	K	505	NAD	C5D-O5D-PN-O2N
3	J	505	NAD	C5D-O5D-PN-O2N
3	D	505	NAD	C5B-O5B-PA-O2A
3	L	505	NAD	C5B-O5B-PA-O1A
3	E	505	NAD	C5B-O5B-PA-O1A
3	I	505	NAD	C4N-C3N-C7N-O7N
3	I	505	NAD	C4N-C3N-C7N-N7N
4	B	2001	GOL	C1-C2-C3-O3
4	G	2011	GOL	O1-C1-C2-C3
4	B	2002	GOL	C1-C2-C3-O3
3	A	505	NAD	C4N-C3N-C7N-N7N
3	A	505	NAD	C4N-C3N-C7N-O7N
4	K	2019	GOL	C1-C2-C3-O3
5	D	2004	MRD	O2-C2-C3-C4
3	L	505	NAD	PN-O3-PA-O5B
3	I	505	NAD	C2N-C3N-C7N-O7N
4	L	2008	GOL	O2-C2-C3-O3
3	K	505	NAD	C5D-O5D-PN-O3
3	J	505	NAD	C5D-O5D-PN-O3
4	K	2018	GOL	O1-C1-C2-O2
3	I	505	NAD	C2N-C3N-C7N-N7N

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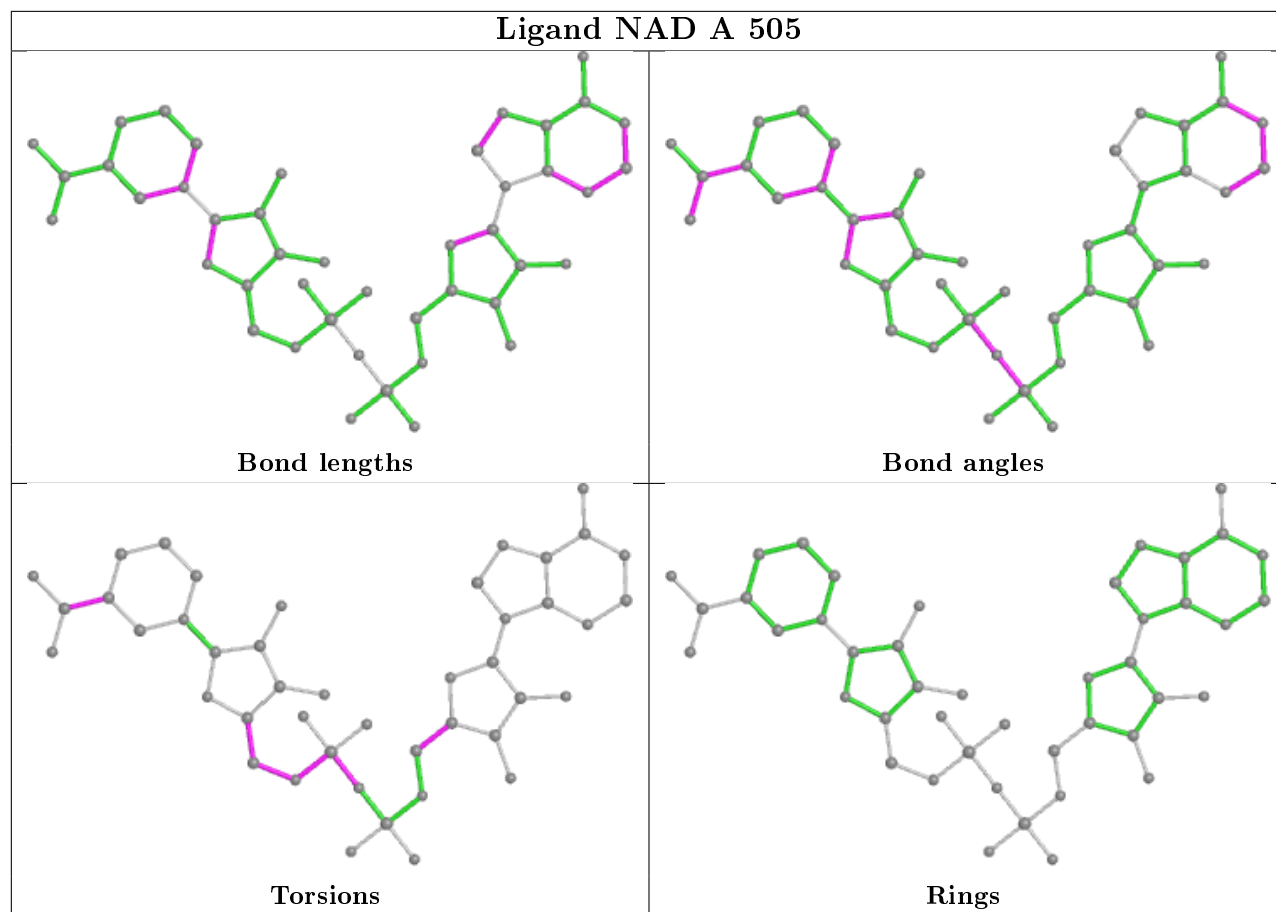
Mol	Chain	Res	Type	Atoms
3	B	505	NAD	C4N-C3N-C7N-O7N

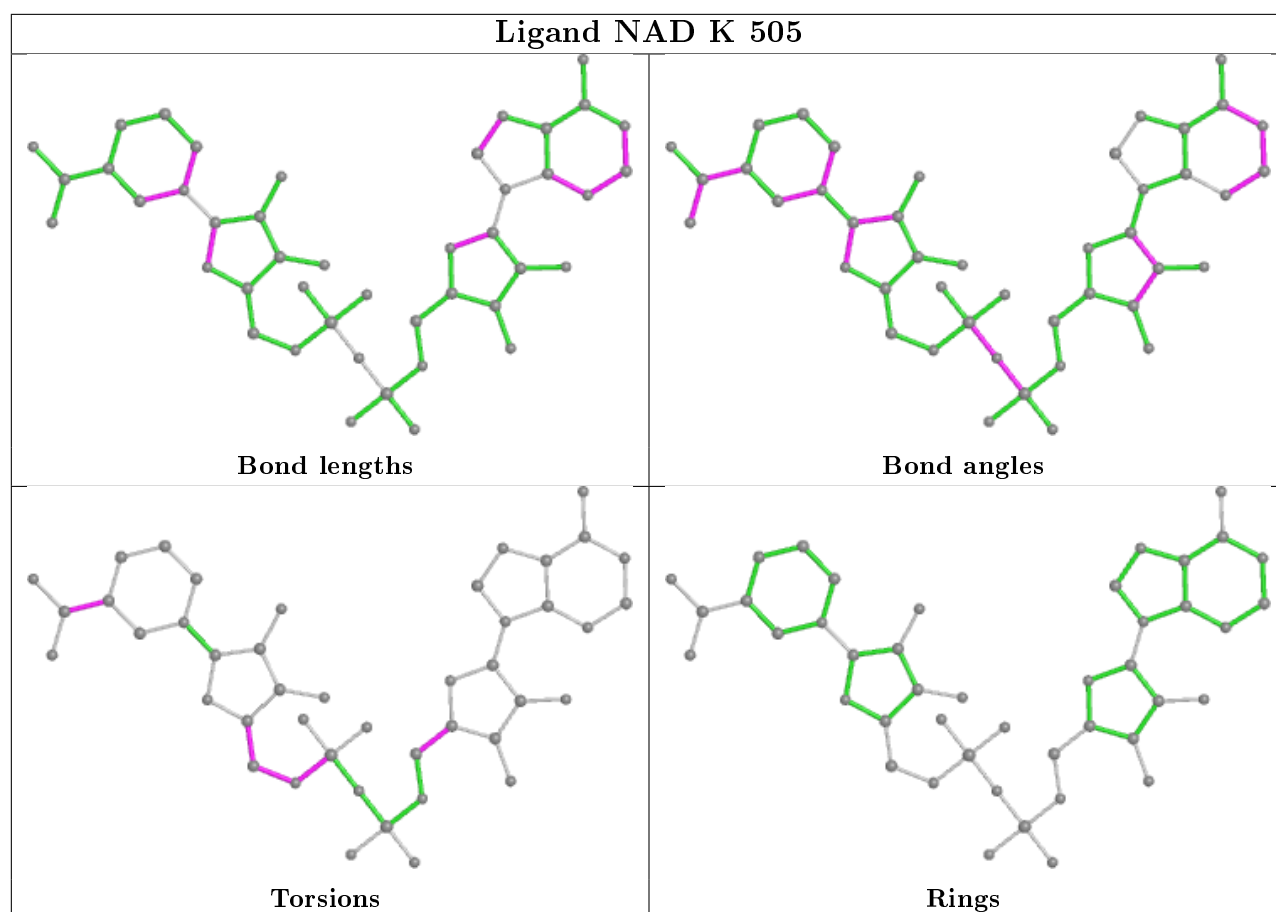
There are no ring outliers.

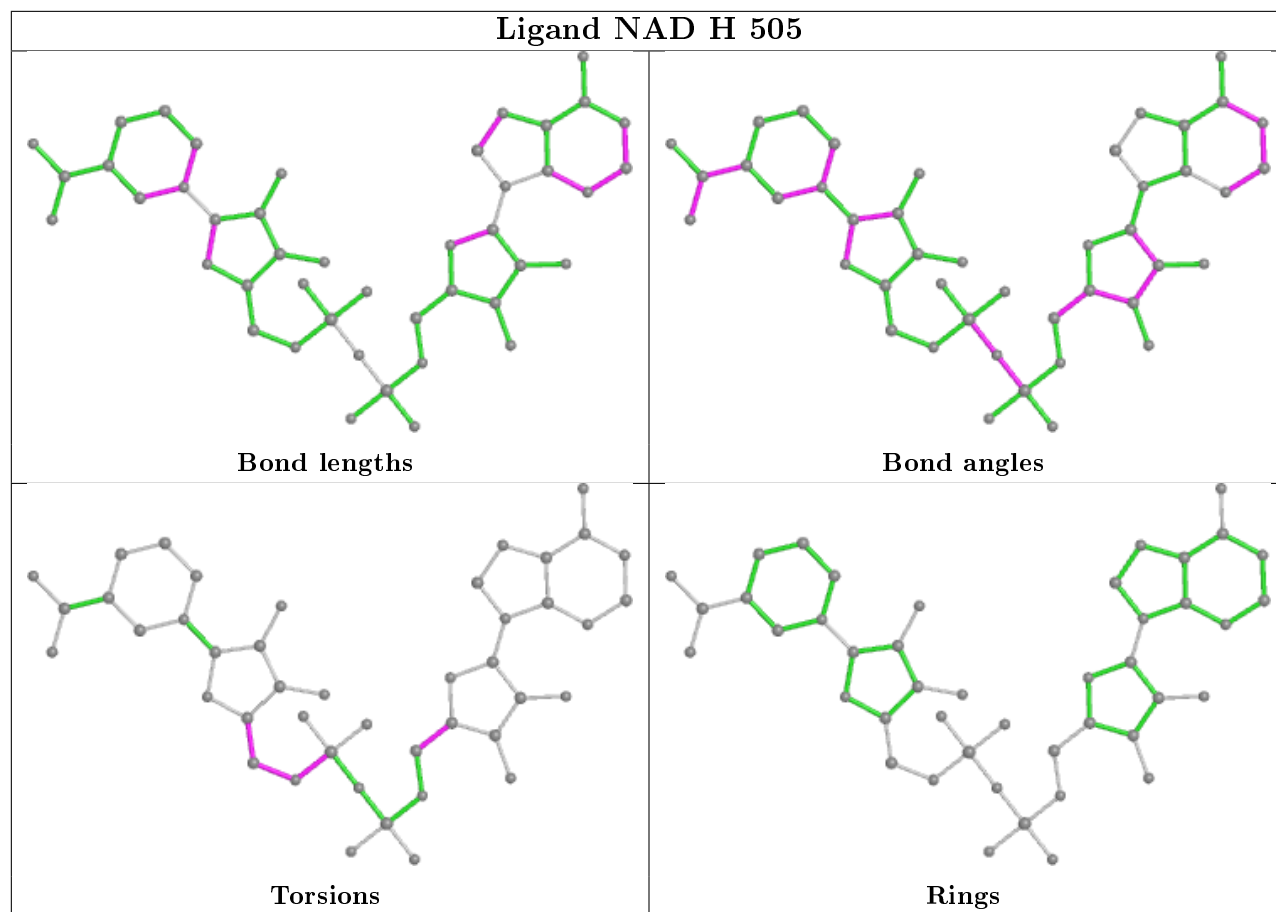
17 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	505	NAD	5	0
4	L	2008	GOL	1	0
3	K	505	NAD	2	0
4	K	2016	GOL	1	0
3	H	505	NAD	2	0
4	J	2014	GOL	1	0
3	I	505	NAD	2	0
3	B	505	NAD	2	0
5	D	2004	MRD	2	0
3	J	505	NAD	1	0
3	G	505	NAD	2	0
4	B	2002	GOL	2	0
3	L	505	NAD	2	0
4	L	2005	GOL	2	0
4	K	2018	GOL	1	0
3	F	505	NAD	3	0
3	E	505	NAD	1	0

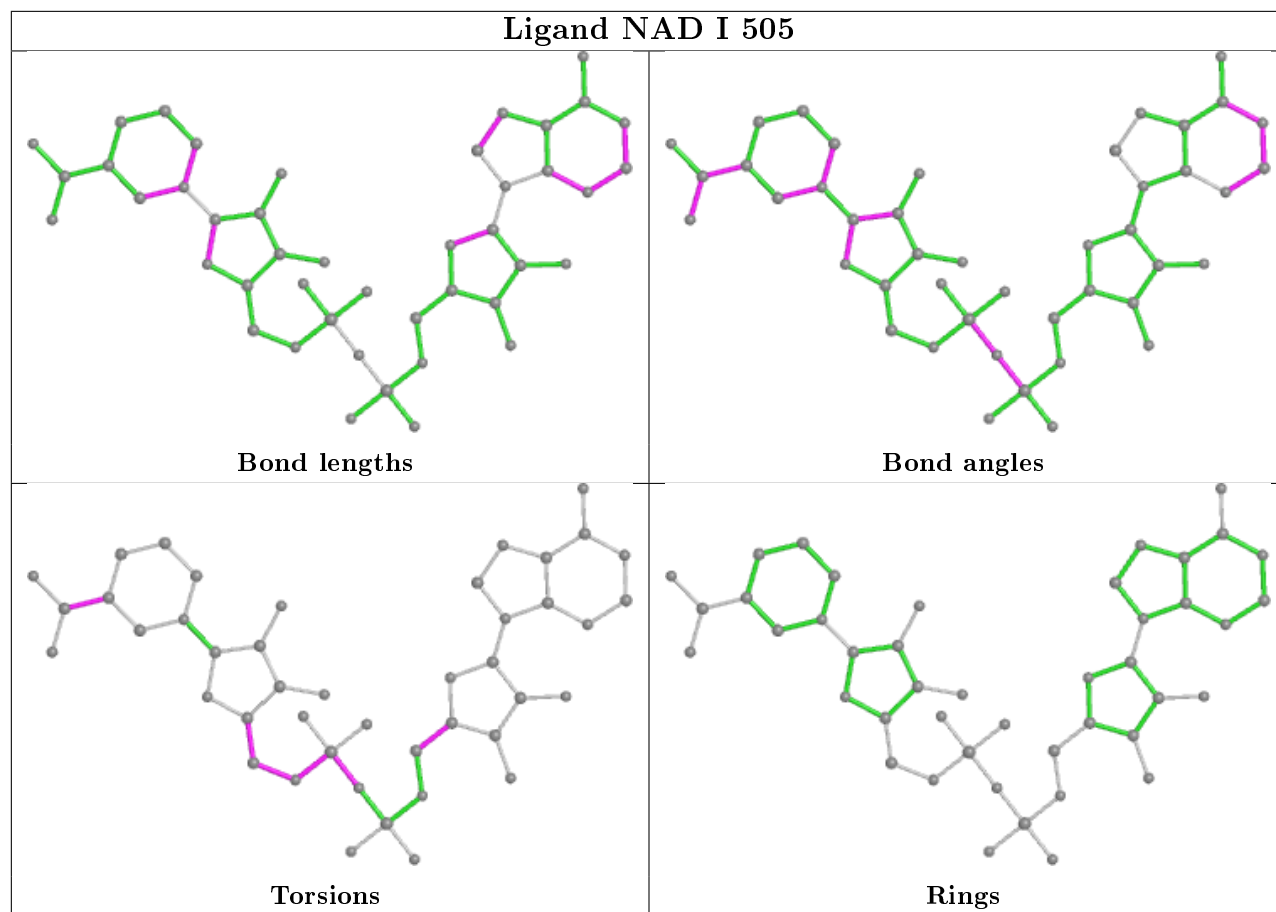
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

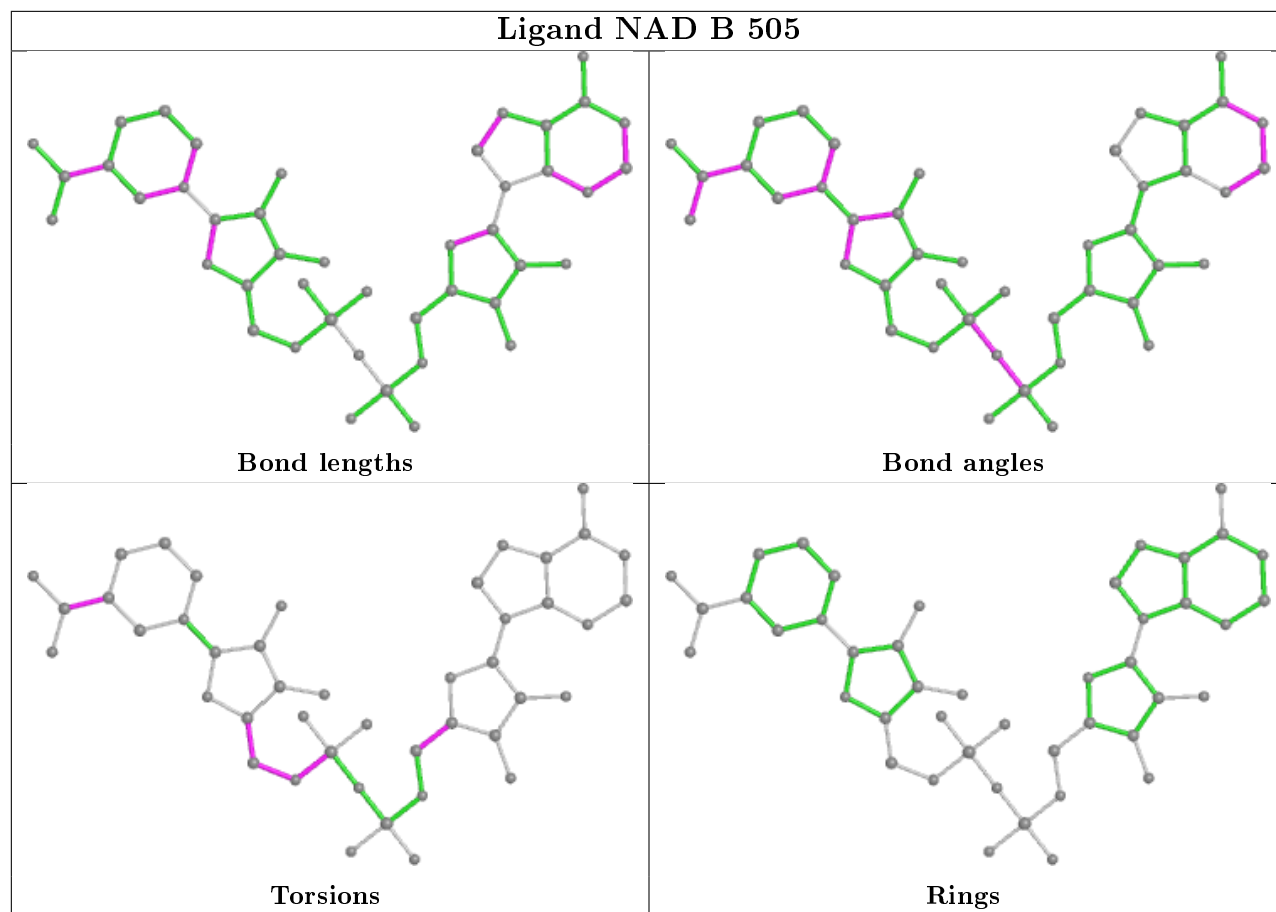


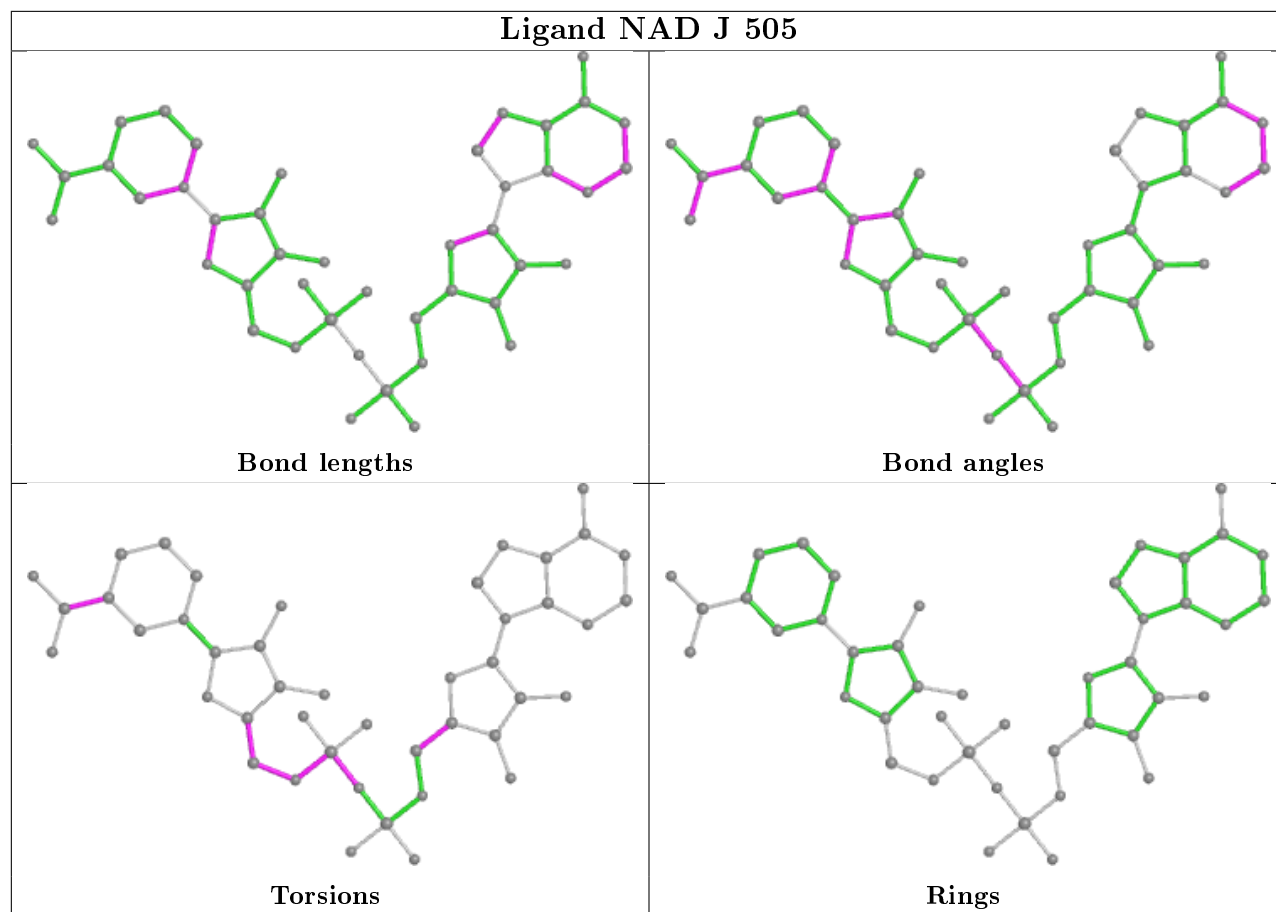


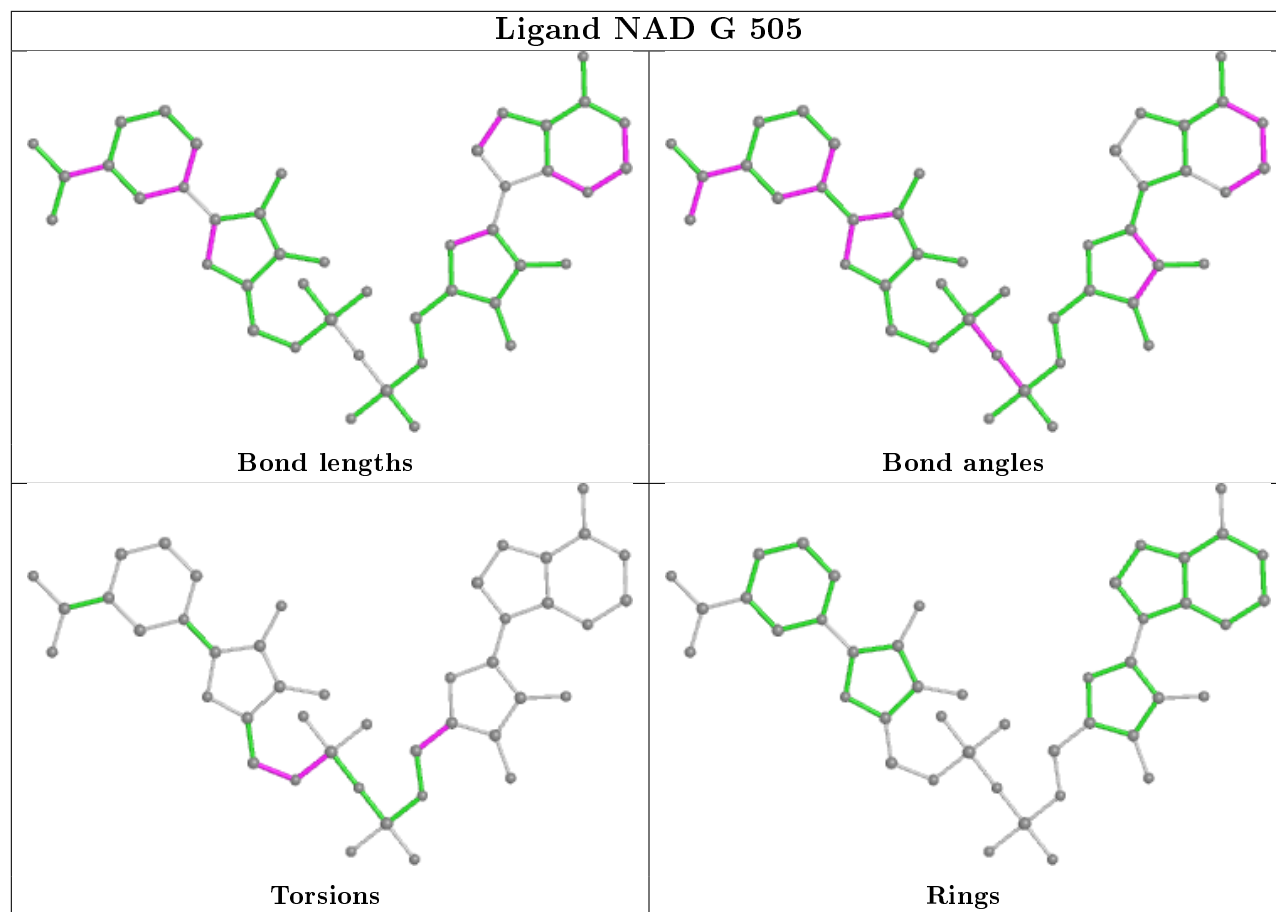


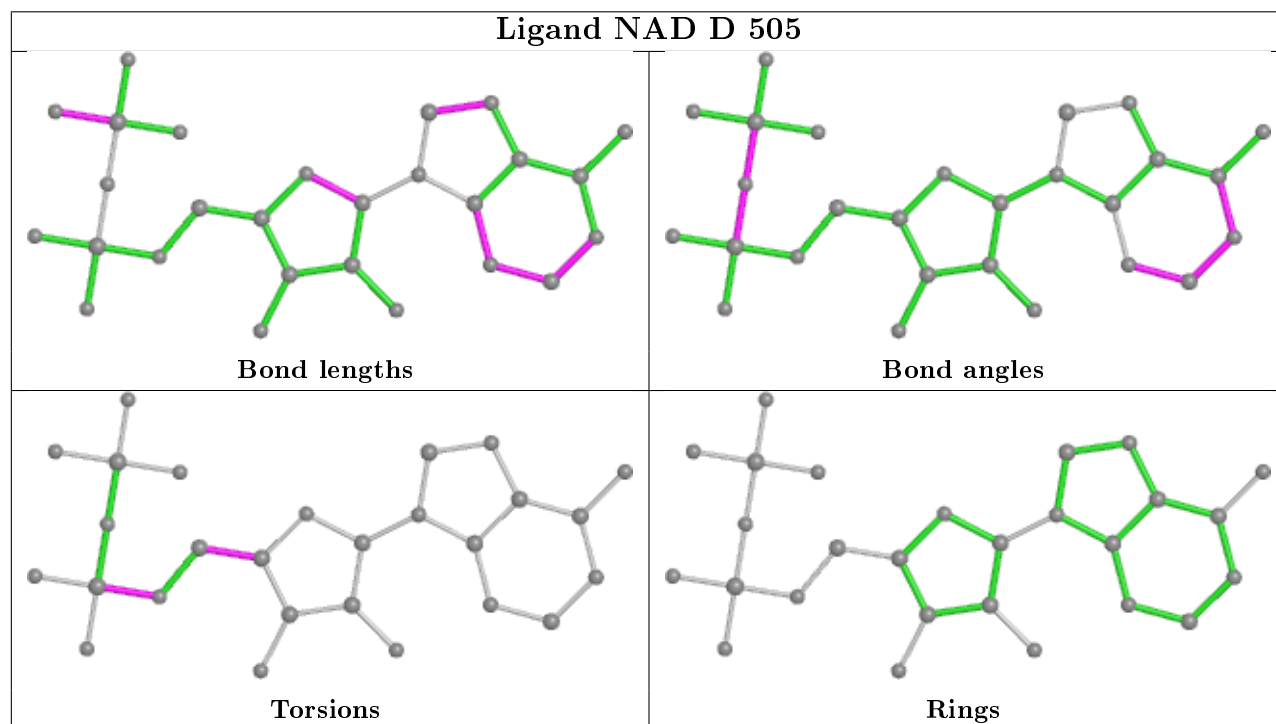
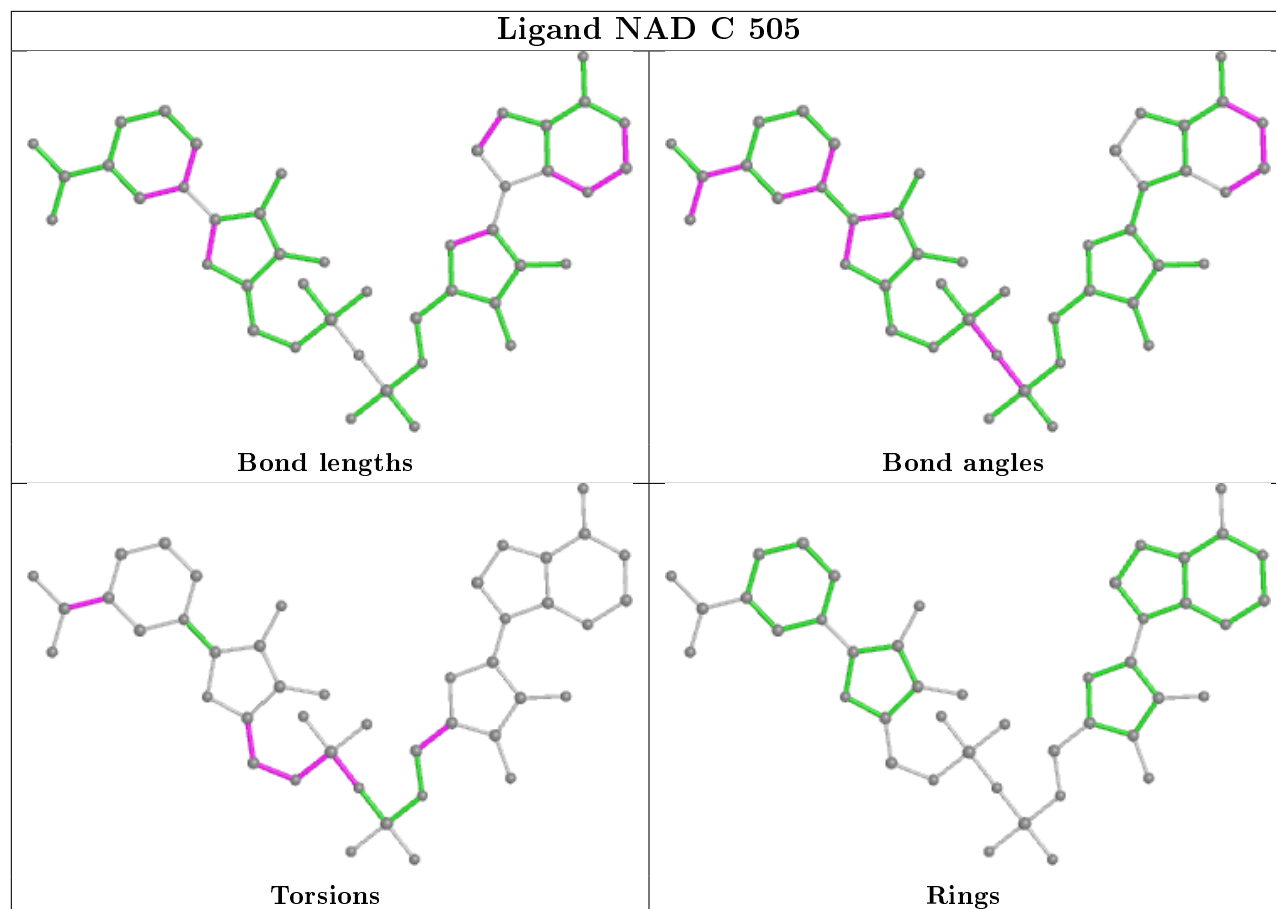


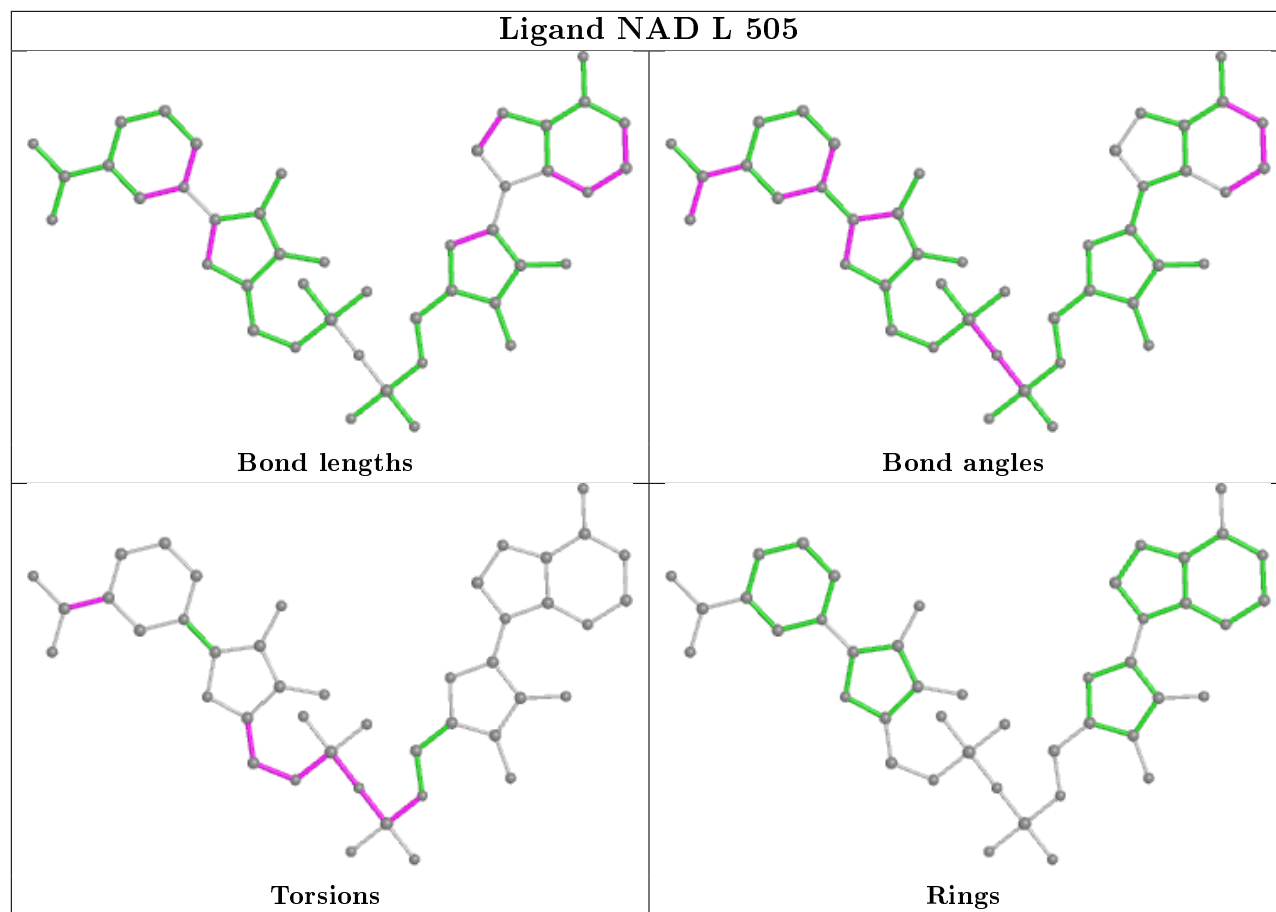


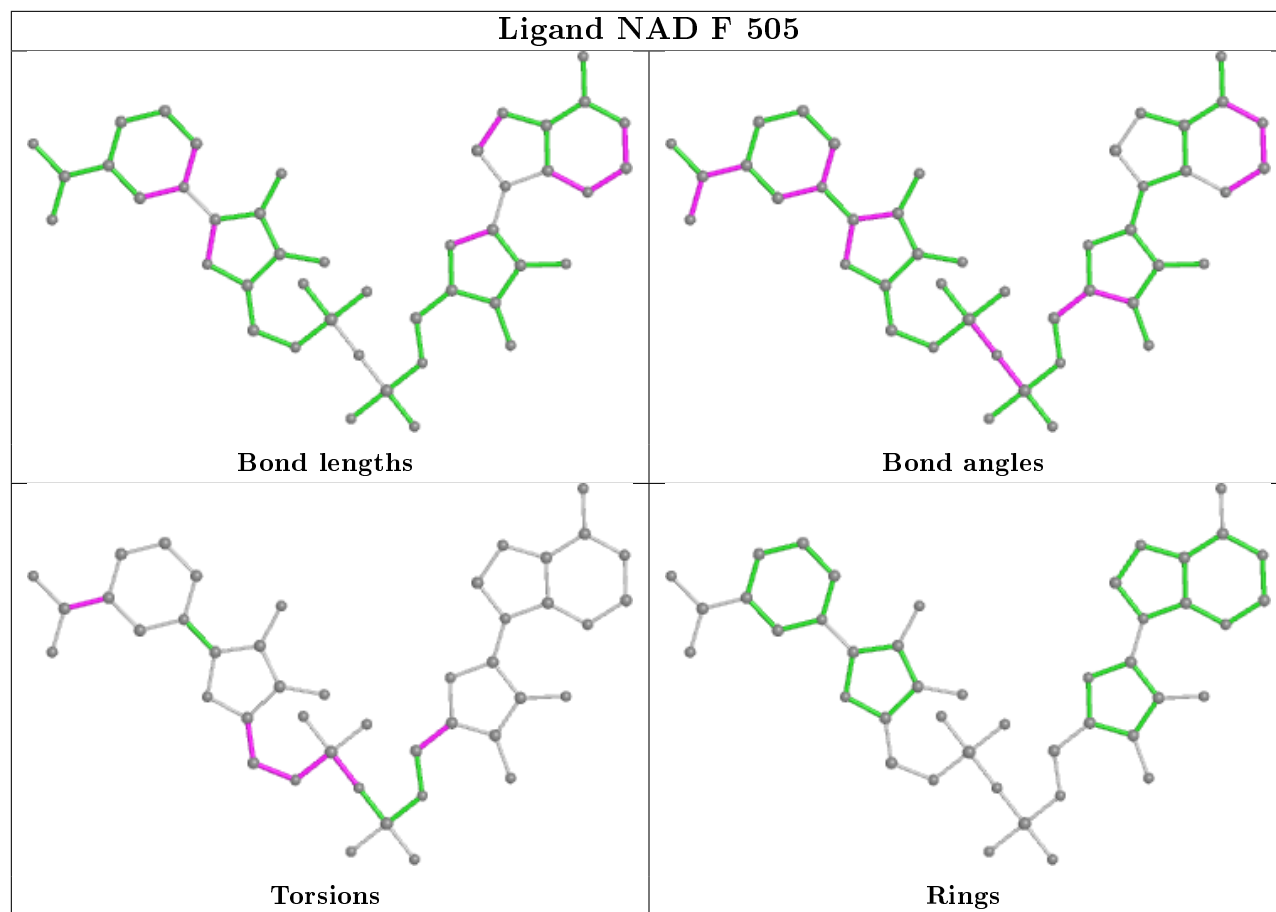


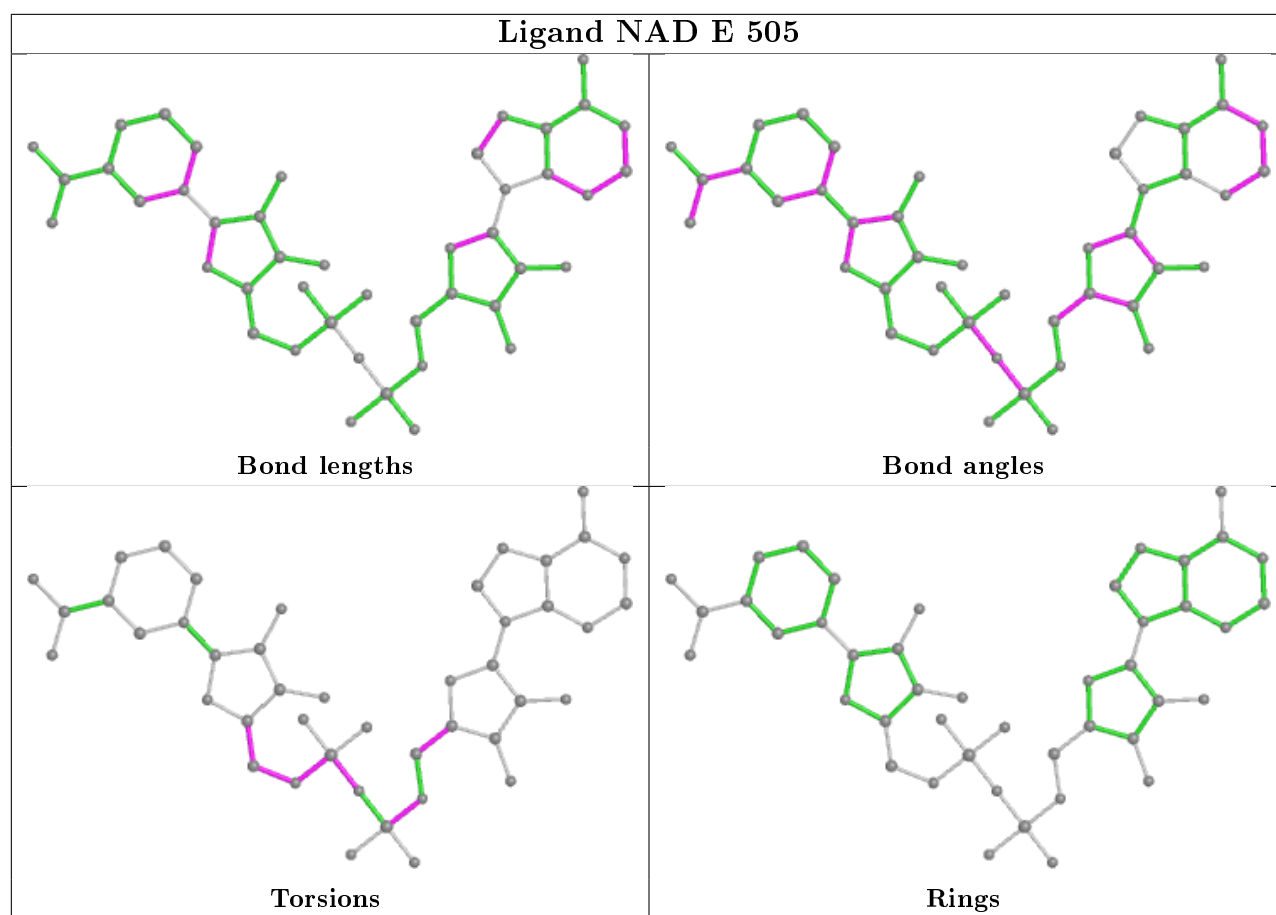












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	496/503 (98%)	-0.16	6 (1%) 79 77	24, 34, 50, 65	0
1	B	496/503 (98%)	-0.28	4 (0%) 86 84	21, 34, 50, 60	0
1	C	495/503 (98%)	-0.27	5 (1%) 82 80	20, 32, 51, 65	0
1	D	496/503 (98%)	-0.03	10 (2%) 65 63	22, 40, 65, 71	0
1	E	496/503 (98%)	-0.26	5 (1%) 82 80	22, 33, 47, 56	0
1	F	495/503 (98%)	-0.39	2 (0%) 92 91	21, 32, 44, 52	0
1	G	496/503 (98%)	-0.22	6 (1%) 79 77	21, 31, 45, 55	0
1	H	497/503 (98%)	-0.32	2 (0%) 92 91	20, 31, 42, 51	0
1	I	496/503 (98%)	-0.36	3 (0%) 89 88	19, 31, 44, 51	0
1	J	497/503 (98%)	-0.31	5 (1%) 82 80	21, 33, 50, 58	0
1	K	496/503 (98%)	-0.30	4 (0%) 86 84	19, 32, 45, 51	0
1	L	496/503 (98%)	-0.42	1 (0%) 95 94	19, 30, 45, 50	0
All	All	5952/6036 (98%)	-0.28	53 (0%) 84 82	19, 32, 49, 71	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	6	SER	4.8
1	C	501	SER	4.8
1	J	63	GLY	4.8
1	K	502	LYS	4.3
1	A	502	LYS	4.3
1	L	501	SER	4.1
1	D	372	GLY	3.6
1	E	502	LYS	3.5
1	E	141	ASP	3.4
1	E	63	GLY	3.3
1	C	60	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	61	LYS	3.1
1	D	364	ARG	3.1
1	I	501	SER	3.0
1	F	501	SER	2.9
1	I	20	ILE	2.9
1	D	502	LYS	2.8
1	D	360	LEU	2.8
1	G	257	VAL	2.8
1	D	308	VAL	2.7
1	G	502	LYS	2.7
1	D	312	ASP	2.7
1	J	62	ASN	2.6
1	D	275	LEU	2.6
1	E	501	SER	2.6
1	J	64	ARG	2.6
1	G	21	LEU	2.6
1	E	7	SER	2.5
1	K	7	SER	2.5
1	B	369	LEU	2.5
1	I	7	SER	2.4
1	B	370	LYS	2.4
1	K	140	MET	2.4
1	G	491	ASP	2.3
1	A	141	ASP	2.2
1	A	491	ASP	2.2
1	K	367	GLU	2.2
1	B	367	GLU	2.2
1	B	312	ASP	2.2
1	C	491	ASP	2.2
1	D	403	THR	2.2
1	G	501	SER	2.1
1	H	367	GLU	2.1
1	F	371	LYS	2.1
1	A	257	VAL	2.1
1	D	36	ILE	2.1
1	A	61	LYS	2.1
1	G	60	ARG	2.1
1	A	501	SER	2.0
1	J	6	SER	2.0
1	C	63	GLY	2.0
1	J	502	LYS	2.0
1	D	342	TYR	2.0

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

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

## 6.3 Carbohydrates ⓘ

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.

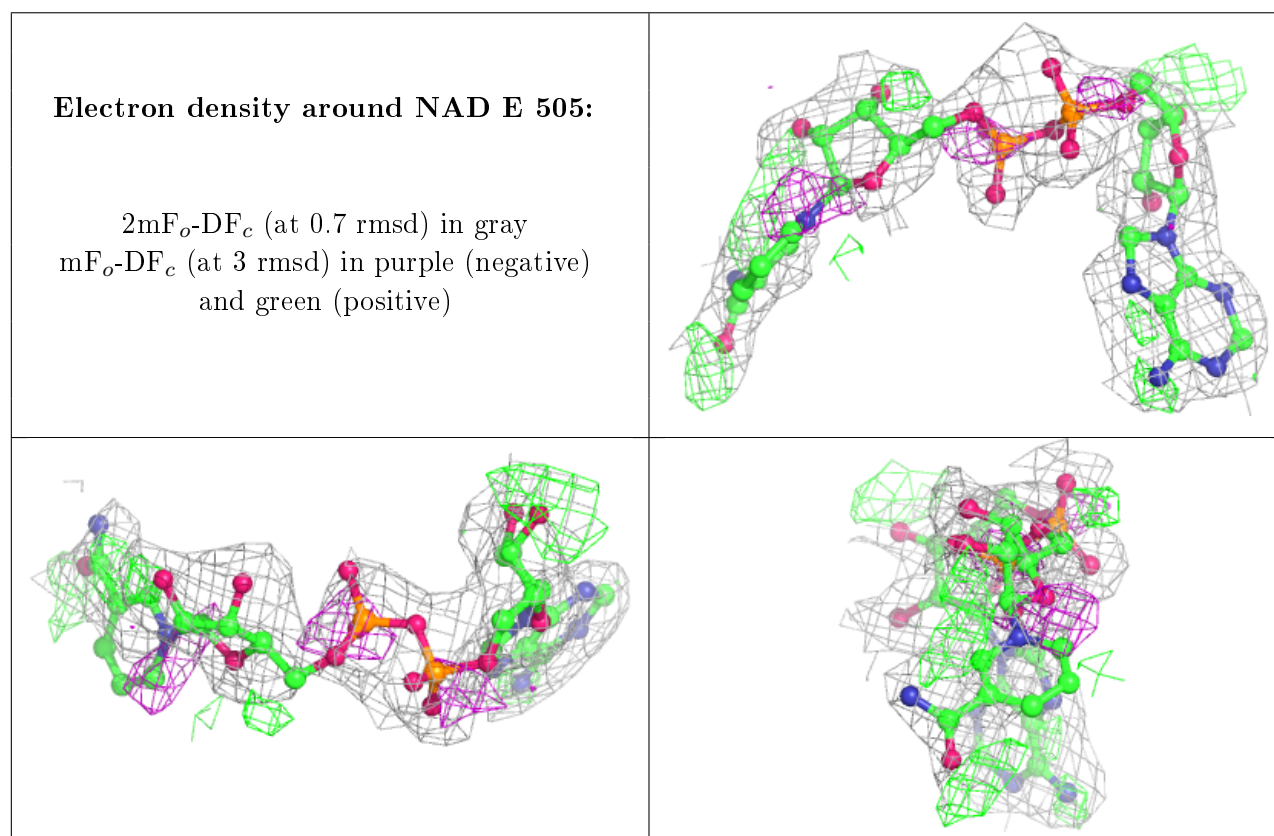
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	L	2015	6/6	0.52	0.19	61,62,62,62	0
2	NA	I	504	1/1	0.54	0.23	61,61,61,61	0
2	NA	C	504	1/1	0.65	0.34	65,65,65,65	0
4	GOL	L	2000	6/6	0.71	0.26	66,66,66,67	0
3	NAD	E	505	44/44	0.73	0.24	58,75,78,78	0
2	NA	L	504	1/1	0.75	0.15	61,61,61,61	0
3	NAD	F	505	44/44	0.77	0.23	61,76,79,79	0
4	GOL	L	2017	6/6	0.77	0.24	63,64,64,64	0
3	NAD	D	505	27/44	0.78	0.23	67,73,79,79	0
3	NAD	B	505	44/44	0.78	0.21	58,75,79,79	0
3	NAD	A	505	44/44	0.78	0.22	53,71,73,73	0
3	NAD	K	505	44/44	0.78	0.22	60,73,76,77	0
3	NAD	C	505	44/44	0.78	0.22	61,74,79,79	0
3	NAD	I	505	44/44	0.79	0.23	67,81,86,86	0
4	GOL	G	2011	6/6	0.79	0.32	65,65,66,66	0
4	GOL	G	2007	6/6	0.80	0.17	61,62,62,62	0
3	NAD	H	505	44/44	0.80	0.24	46,69,76,77	0
4	GOL	C	2003	6/6	0.80	0.27	50,52,52,53	0
5	MRD	D	2004	8/8	0.80	0.37	54,55,55,55	0
4	GOL	K	2019	6/6	0.81	0.20	56,56,57,57	0
3	NAD	J	505	44/44	0.81	0.20	65,77,79,79	0
3	NAD	G	505	44/44	0.81	0.20	57,69,73,74	0
3	NAD	L	505	44/44	0.81	0.18	47,66,68,68	0
4	GOL	B	2001	6/6	0.82	0.18	58,59,59,60	0
4	GOL	K	2018	6/6	0.84	0.36	48,49,49,50	0
4	GOL	H	2010	6/6	0.84	0.38	59,60,60,60	0
4	GOL	G	2009	6/6	0.85	0.27	43,46,46,47	0

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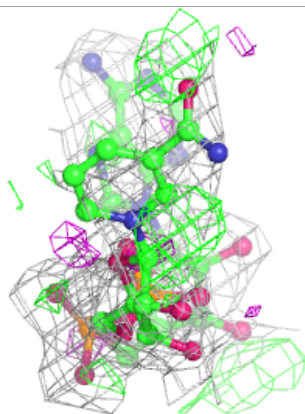
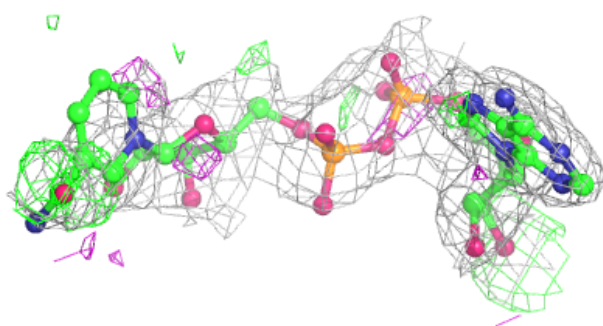
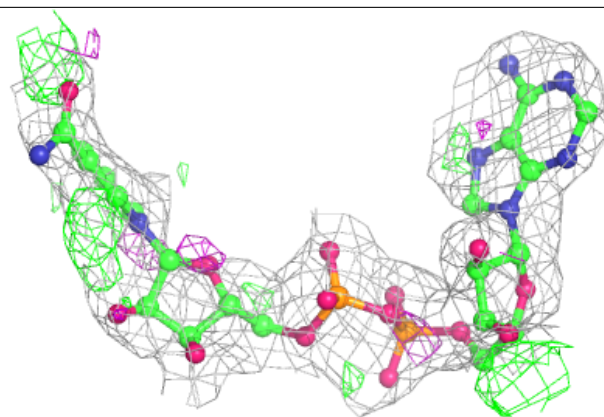
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	K	2016	6/6	0.85	0.30	45,46,46,46	0
4	GOL	J	2013	6/6	0.86	0.18	58,58,59,59	0
2	NA	D	504	1/1	0.87	0.09	43,43,43,43	0
4	GOL	J	2014	6/6	0.87	0.27	54,55,55,56	0
4	GOL	I	2012	6/6	0.87	0.27	47,47,47,47	0
2	NA	A	504	1/1	0.88	0.19	60,60,60,60	0
4	GOL	L	2008	6/6	0.89	0.18	46,46,47,47	0
2	NA	K	504	1/1	0.89	0.07	37,37,37,37	0
4	GOL	F	2006	6/6	0.89	0.27	50,50,51,51	0
2	NA	E	504	1/1	0.89	0.23	47,47,47,47	0
4	GOL	B	2002	6/6	0.89	0.27	60,61,61,61	0
4	GOL	L	2005	6/6	0.92	0.21	66,66,67,67	0
2	NA	G	504	1/1	0.95	0.14	43,43,43,43	0
2	NA	B	504	1/1	0.96	0.06	41,41,41,41	0
2	NA	J	504	1/1	0.96	0.09	41,41,41,41	0
2	NA	F	504	1/1	0.97	0.05	34,34,34,34	0
2	NA	H	504	1/1	0.97	0.09	30,30,30,30	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.



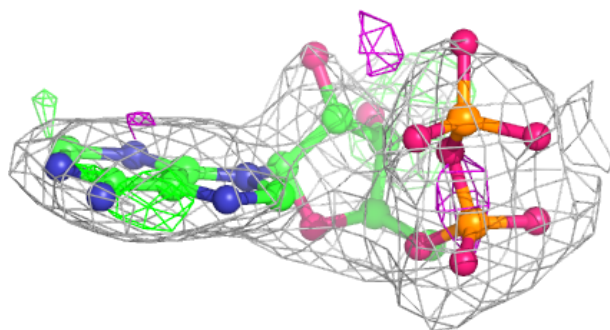
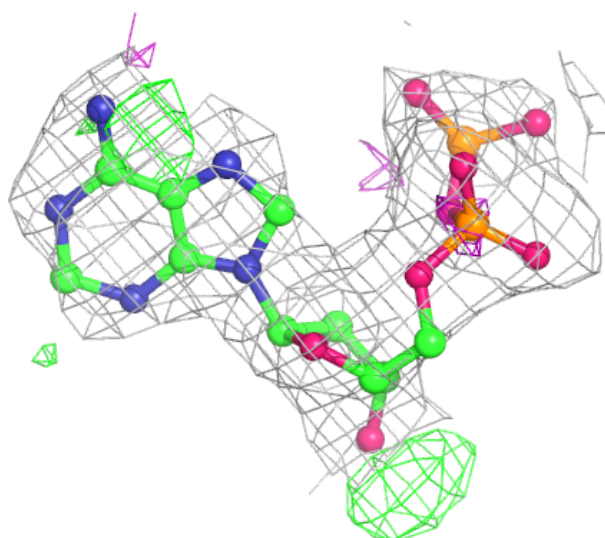
**Electron density around NAD F 505:**

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



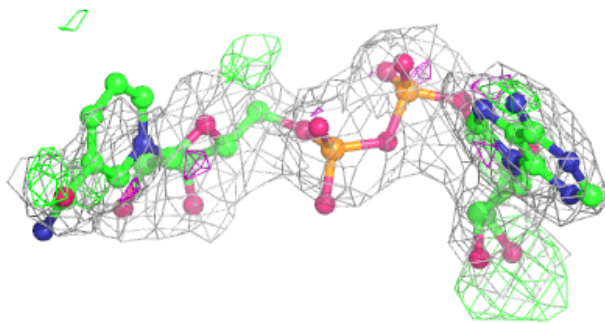
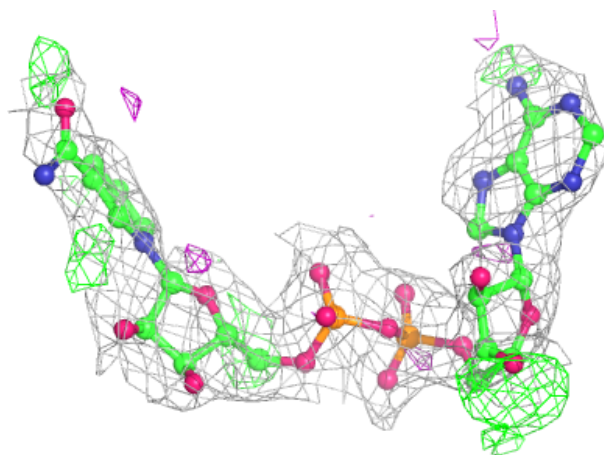
**Electron density around NAD D 505:**

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



**Electron density around NAD B 505:**

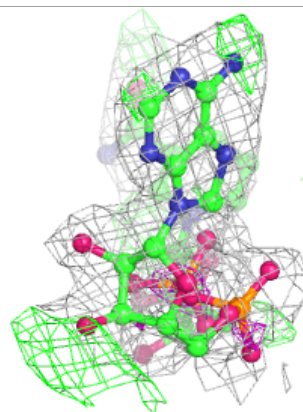
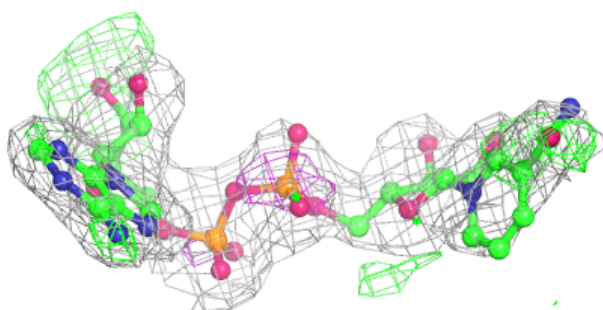
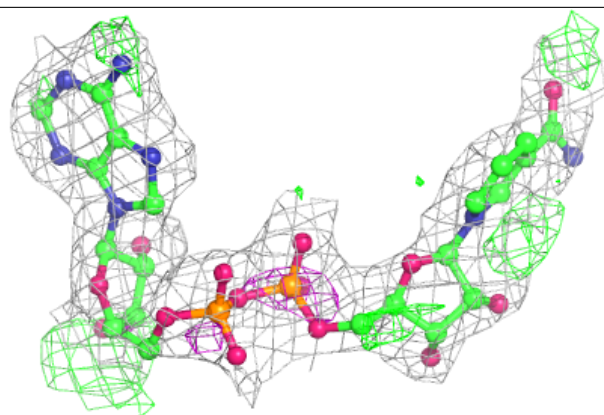
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



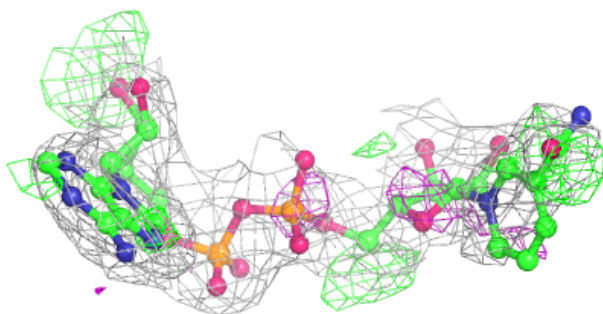
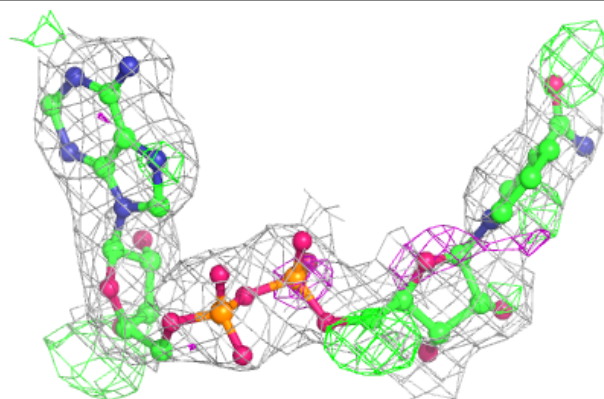


**Electron density around NAD A 505:**

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

**Electron density around NAD K 505:**

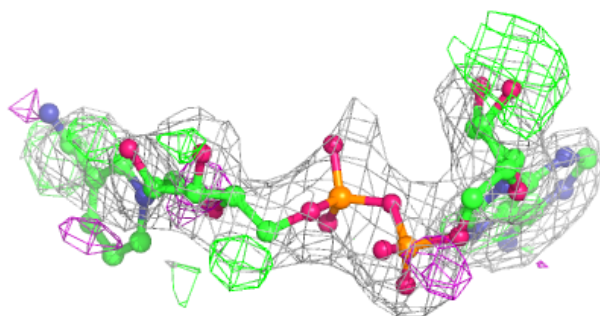
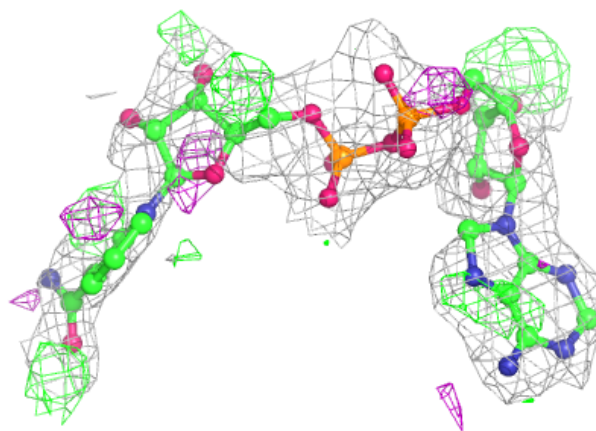
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



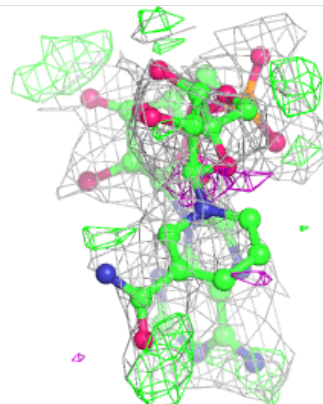
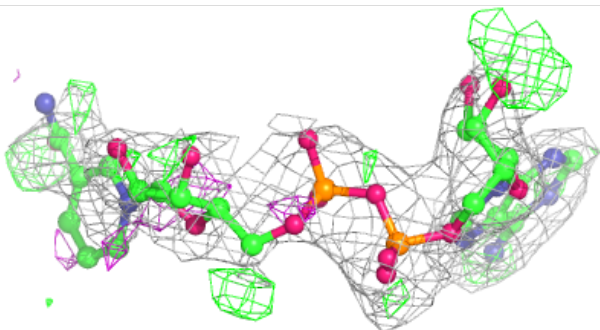
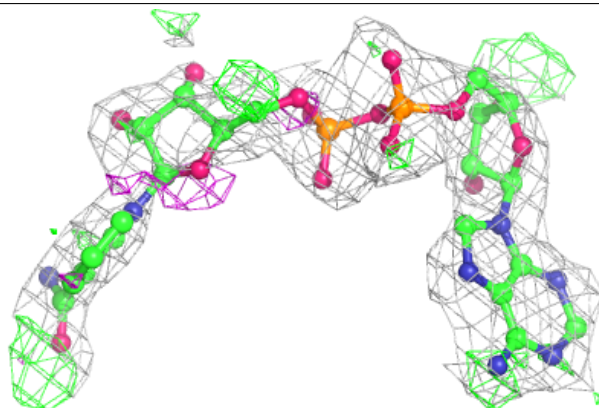


**Electron density around NAD C 505:**

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

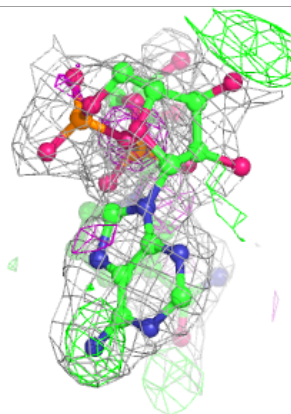
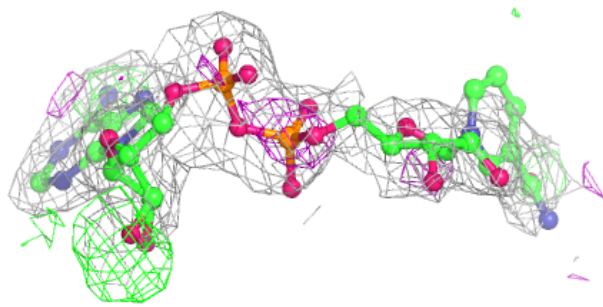
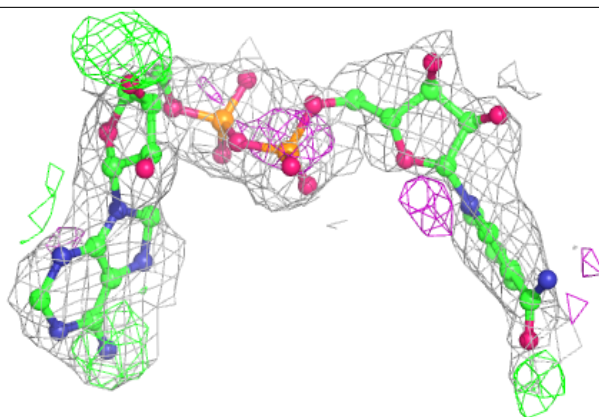
**Electron density around NAD I 505:**

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

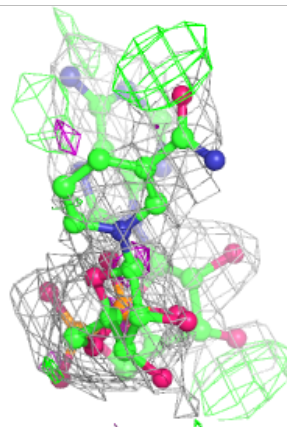
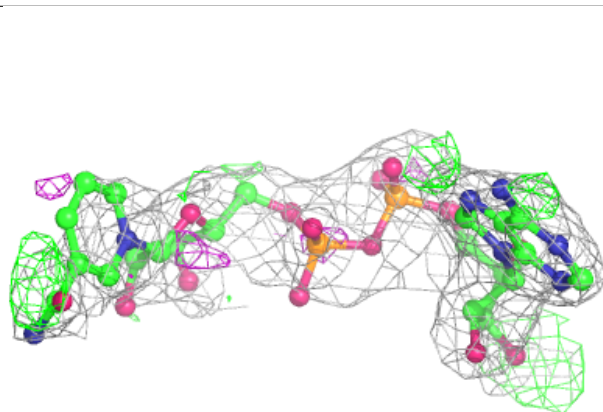
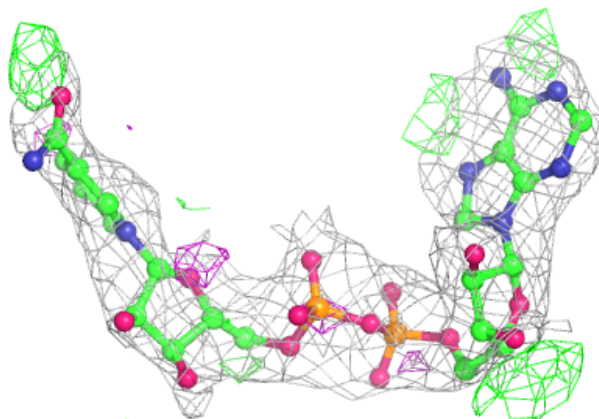


**Electron density around NAD H 505:**

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

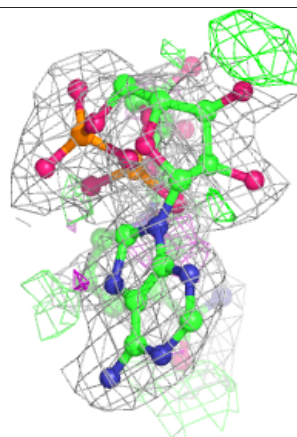
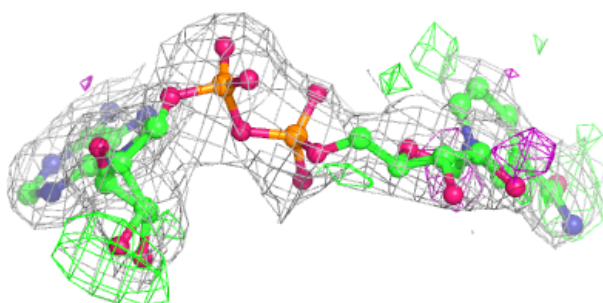
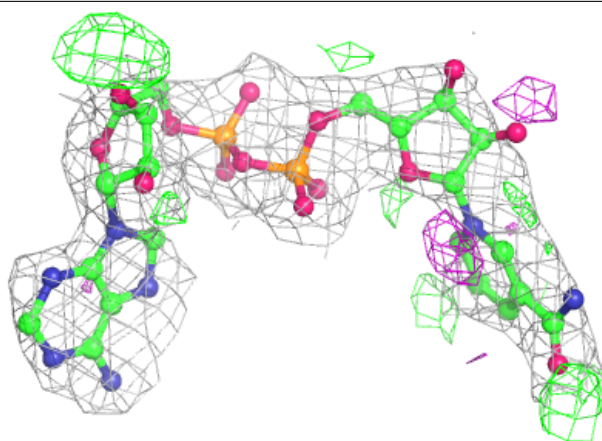
**Electron density around NAD J 505:**

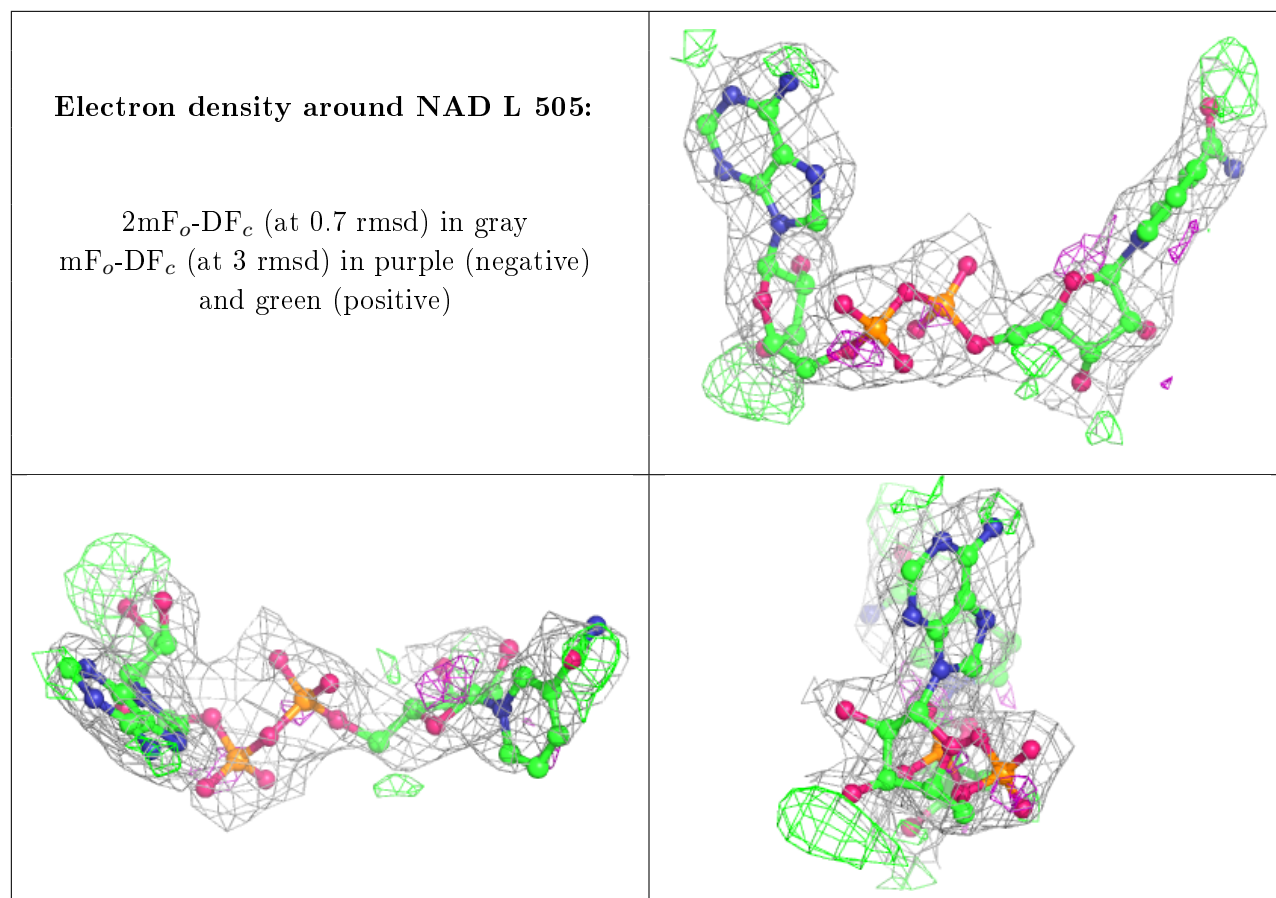
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around NAD G 505:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.