



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:00 am BST

PDB ID : 3E5R  
Title : Crystal structure and Functional Analysis of Glyceraldehyde-3-phosphate Dehydrogenase from Oryza Sativa  
Authors : Tien, Y.C.; Lin, Y.H.; Chang, S.L.; Chen, C.J.  
Deposited on : 2008-08-14  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

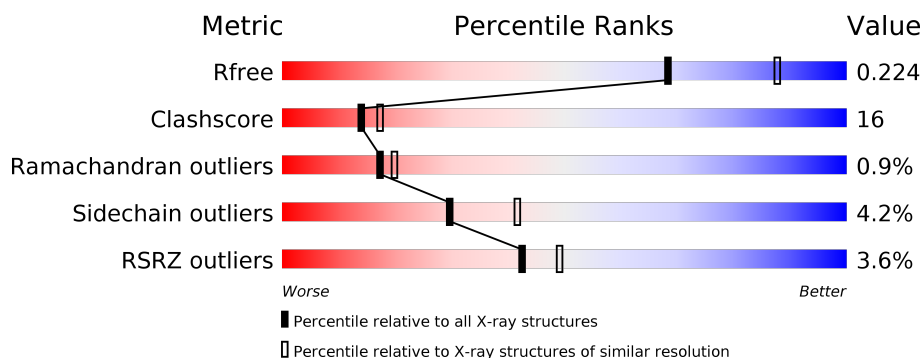
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	337	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>•</div> </div> </div>
1	B	337	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>•</div> </div> </div>
1	C	337	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>•</div> </div> </div>
1	O	337	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>•</div> </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	B	5465	X	-	-	-
2	NAD	O	5463	-	-	X	X

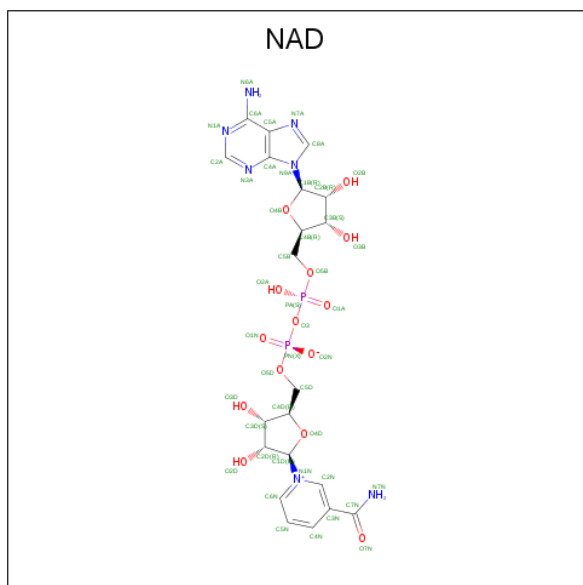


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	336	Total 2553	C 1621	N 432	O 491	S 9	0	0	0
1	A	336	Total 2553	C 1621	N 432	O 491	S 9	0	0	0
1	B	336	Total 2553	C 1621	N 432	O 491	S 9	0	0	0
1	C	336	Total 2553	C 1621	N 432	O 491	S 9	0	0	0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



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

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

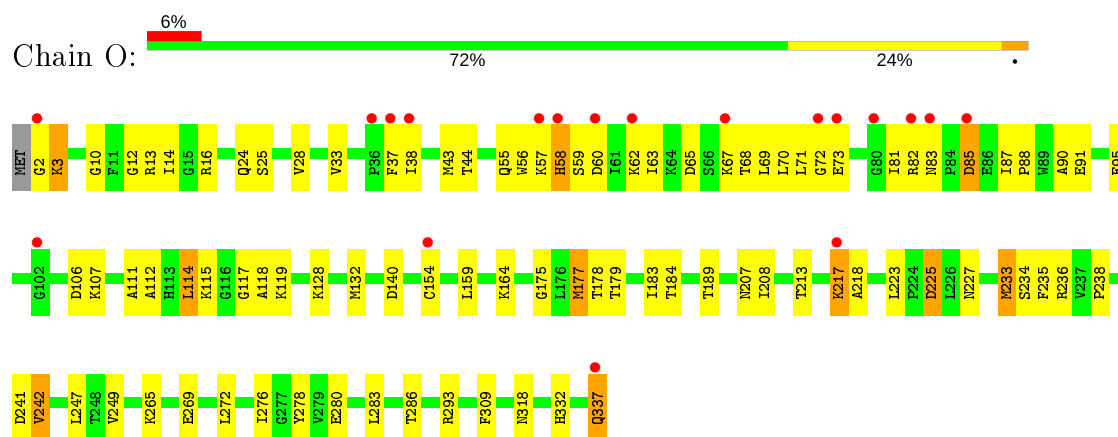
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	233	Total	O	0	0
			233	233		
3	A	194	Total	O	0	0
			194	194		
3	B	204	Total	O	0	0
			204	204		
3	C	212	Total	O	0	0
			212	212		

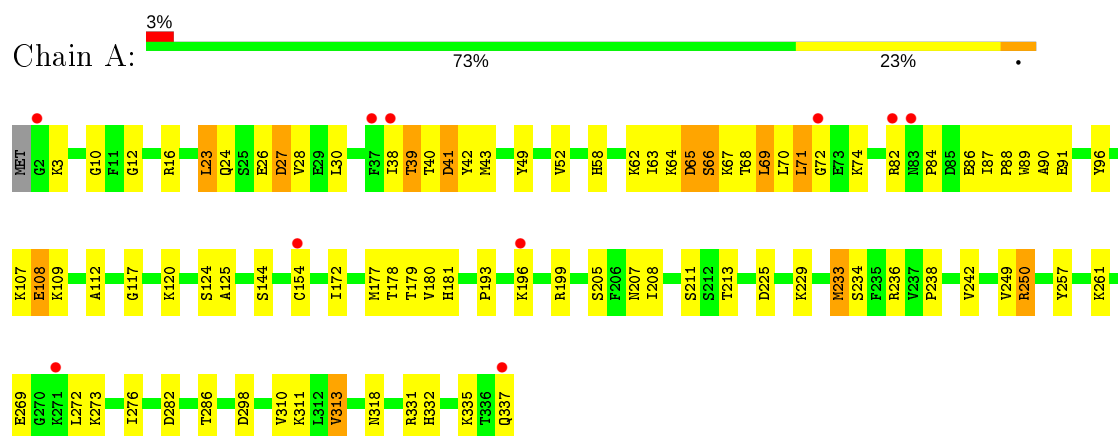
### 3 Residue-property plots [i](#)

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

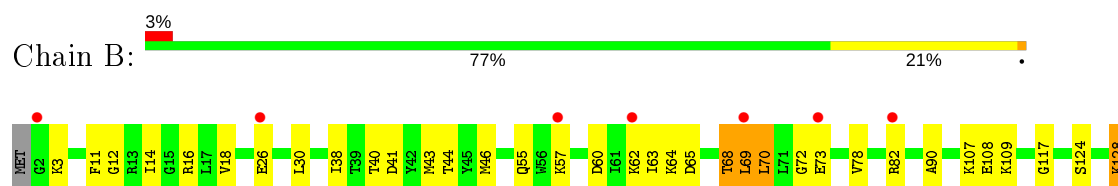
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, cytosolic

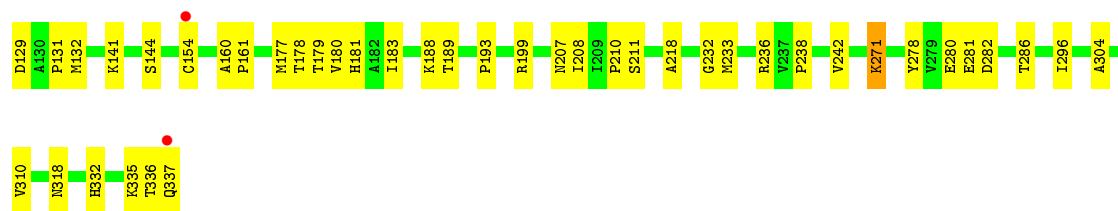


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, cytosolic

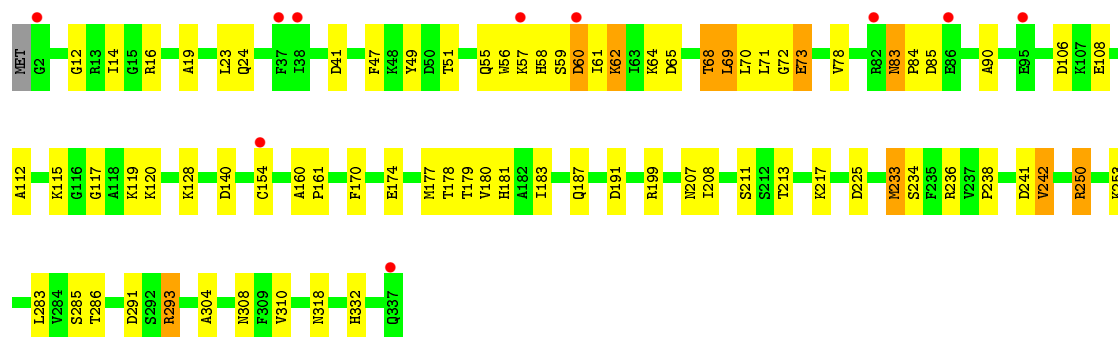
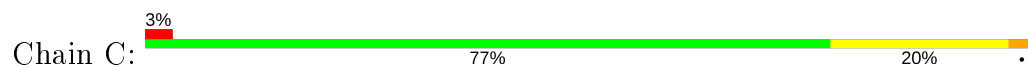


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, cytosolic





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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.44Å 129.56Å 77.58Å 90.00° 117.40° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 23.43 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.00-2.30) 100.0 (23.43-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.199 , 0.239 0.226 , 0.224	Depositor DCC
$R_{free}$ test set	5246 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.2	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 30.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.046 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11231	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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: 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	0.38	1/2600 (0.0%)	0.70	3/3522 (0.1%)
1	B	0.36	0/2600	0.67	2/3522 (0.1%)
1	C	0.36	0/2600	0.70	3/3522 (0.1%)
1	O	0.39	0/2600	0.84	11/3522 (0.3%)
All	All	0.37	1/10400 (0.0%)	0.73	19/14088 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	LYS	CD-CE	5.39	1.64	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	67	LYS	N-CA-C	-8.92	86.92	111.00
1	O	68	THR	N-CA-C	8.18	133.09	111.00
1	O	57	LYS	C-N-CA	-7.39	103.23	121.70
1	A	3	LYS	CD-CE-NZ	7.15	128.15	111.70
1	O	85	ASP	N-CA-CB	-6.98	98.03	110.60
1	O	67	LYS	CB-CA-C	6.44	123.28	110.40
1	O	208	ILE	N-CA-C	-6.28	94.03	111.00
1	O	67	LYS	CA-CB-CG	6.21	127.06	113.40
1	O	85	ASP	CB-CG-OD2	6.14	123.82	118.30
1	B	208	ILE	N-CA-C	-5.97	94.89	111.00
1	B	180	VAL	N-CA-C	-5.83	95.25	111.00
1	A	208	ILE	N-CA-C	-5.82	95.29	111.00
1	C	208	ILE	N-CA-C	-5.82	95.30	111.00
1	O	85	ASP	CB-CG-OD1	-5.68	113.18	118.30
1	C	180	VAL	N-CA-C	-5.63	95.81	111.00
1	O	67	LYS	O-C-N	-5.12	114.51	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	58	HIS	O-C-N	5.09	130.85	122.70
1	C	60	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	180	VAL	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2553	0	2576	88	1
1	B	2553	0	2576	73	0
1	C	2553	0	2576	68	0
1	O	2553	0	2576	116	0
2	A	44	0	26	9	0
2	B	44	0	24	6	0
2	C	44	0	26	10	0
2	O	44	0	26	21	0
3	A	194	0	0	11	9
3	B	204	0	0	6	2
3	C	212	0	0	17	3
3	O	233	0	0	13	9
All	All	11231	0	10406	326	12

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 16.

All (326) 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:O:12:GLY:HA3	2:O:5463:NAD:O5B	1.32	1.29
1:O:38:ILE:HD11	1:O:43:MET:CE	1.81	1.08
1:B:107:LYS:NZ	1:B:108:GLU:OE1	1.91	1.04
1:O:12:GLY:HA3	2:O:5463:NAD:C5B	1.88	1.03
1:O:184:THR:HG23	1:O:236:ARG:HH22	1.21	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:VAL:HB	3:C:5782:HOH:O	1.57	1.03
1:O:83:ASN:OD1	1:O:85:ASP:HB3	1.62	0.98
1:B:69:LEU:O	1:B:70:LEU:HB2	1.63	0.97
1:O:13:ARG:N	2:O:5463:NAD:O1A	1.98	0.96
1:O:38:ILE:HD11	1:O:43:MET:HE2	1.47	0.95
1:A:64:LYS:HB2	1:A:70:LEU:HD23	1.47	0.94
1:A:107:LYS:HB3	3:A:5581:HOH:O	1.69	0.92
1:C:56:TRP:CD1	1:C:61:ILE:HD11	2.06	0.90
1:O:184:THR:CG2	1:O:236:ARG:HH22	1.85	0.89
1:A:67:LYS:HD2	3:A:5715:HOH:O	1.72	0.89
1:B:12:GLY:HA3	2:B:5465:NAD:H51A	1.55	0.88
1:A:64:LYS:HB2	1:A:70:LEU:CD2	2.06	0.86
1:O:184:THR:HG23	1:O:236:ARG:NH2	1.92	0.85
2:C:5467:NAD:H2N	2:C:5467:NAD:H51N	1.57	0.85
1:A:88:PRO:HB2	1:A:91:GLU:HG3	1.60	0.84
1:B:271:LYS:H	1:B:271:LYS:HD2	1.42	0.83
1:O:12:GLY:CA	2:O:5463:NAD:C5B	2.55	0.83
1:C:225:ASP:HB3	3:C:5599:HOH:O	1.80	0.82
1:A:82:ARG:HB2	1:A:82:ARG:NH2	1.97	0.80
1:B:40:THR:OG1	1:B:78:VAL:HG21	1.82	0.79
1:O:12:GLY:N	2:O:5463:NAD:H4B	1.97	0.79
1:A:65:ASP:O	1:A:66:SER:HB2	1.79	0.79
1:B:109:LYS:HD2	3:B:5639:HOH:O	1.81	0.79
1:O:38:ILE:HD11	1:O:43:MET:HE3	1.64	0.79
1:A:108:GLU:HG3	1:A:109:LYS:N	1.96	0.79
1:O:38:ILE:HD12	1:O:43:MET:HB2	1.65	0.78
1:O:164:LYS:HE2	3:O:5609:HOH:O	1.84	0.78
1:O:2:GLY:O	1:O:3:LYS:HB2	1.83	0.77
1:O:272:LEU:HB3	1:O:276:ILE:HG22	1.66	0.77
1:C:179:THR:HG21	3:C:5709:HOH:O	1.84	0.76
1:O:179:THR:HG21	3:O:5616:HOH:O	1.86	0.75
1:O:88:PRO:HB2	1:O:91:GLU:HG3	1.67	0.75
1:C:115:LYS:HB3	3:C:5755:HOH:O	1.85	0.75
1:O:107:LYS:HE3	3:O:5615:HOH:O	1.86	0.74
1:B:318:ASN:HD22	2:B:5465:NAD:H72N	1.36	0.73
1:O:13:ARG:H	2:O:5463:NAD:PA	2.12	0.73
1:O:13:ARG:HG2	2:O:5463:NAD:O1A	1.87	0.73
1:A:12:GLY:HA3	2:A:5466:NAD:O5B	1.89	0.73
1:O:13:ARG:HB2	2:O:5463:NAD:O1N	1.89	0.72
1:C:55:GLN:HB2	3:C:5734:HOH:O	1.87	0.72
1:O:38:ILE:HG13	1:O:38:ILE:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:PRO:HB2	3:B:5586:HOH:O	1.89	0.71
1:O:24:GLN:OE1	1:O:58:HIS:CG	2.44	0.71
1:O:24:GLN:OE1	1:O:58:HIS:CB	2.39	0.71
1:O:12:GLY:HA3	2:O:5463:NAD:PA	2.31	0.70
2:C:5467:NAD:C2N	2:C:5467:NAD:H51N	2.22	0.69
1:O:38:ILE:CD1	1:O:43:MET:HE3	2.23	0.69
1:A:58:HIS:HB2	3:A:5690:HOH:O	1.92	0.69
1:C:211:SER:HB2	3:C:5771:HOH:O	1.94	0.68
1:C:64:LYS:HE2	3:C:5752:HOH:O	1.94	0.68
1:O:159:LEU:HD22	1:O:177:MET:HE1	1.75	0.68
1:A:82:ARG:HB2	1:A:82:ARG:HH21	1.58	0.67
1:O:72:GLY:O	1:O:73:GLU:HG3	1.94	0.67
1:O:95:GLU:HG2	3:O:5571:HOH:O	1.94	0.67
1:A:144:SER:HB3	1:A:337:GLN:O	1.94	0.67
1:O:38:ILE:HD12	1:O:43:MET:CB	2.24	0.66
1:A:38:ILE:O	1:A:38:ILE:HG13	1.93	0.66
1:A:298:ASP:HB3	1:A:313:VAL:HG22	1.76	0.66
1:A:282:ASP:HB3	1:B:199:ARG:HG2	1.77	0.66
1:C:12:GLY:HA3	2:C:5467:NAD:C5B	2.27	0.65
1:A:318:ASN:HD22	2:A:5466:NAD:H72N	1.44	0.65
1:C:55:GLN:NE2	1:C:57:LYS:HE2	2.12	0.64
1:O:217:LYS:HB2	1:O:217:LYS:NZ	2.11	0.64
1:A:124:SER:O	2:A:5466:NAD:H1D	1.97	0.64
1:C:181:HIS:HB3	1:C:236:ARG:HD3	1.78	0.64
1:O:44:THR:HG21	1:O:63:ILE:HD11	1.79	0.64
1:A:63:ILE:N	1:A:63:ILE:HD12	2.13	0.64
1:A:335:LYS:HE3	3:A:5621:HOH:O	1.97	0.64
1:C:85:ASP:OD1	1:C:115:LYS:HD2	1.97	0.63
1:B:177:MET:HG2	1:B:178:THR:N	2.14	0.63
1:C:12:GLY:HA3	2:C:5467:NAD:H51A	1.81	0.62
1:O:318:ASN:HD22	2:O:5463:NAD:H72N	1.46	0.62
1:O:62:LYS:HG3	1:O:70:LEU:HB3	1.81	0.62
1:B:12:GLY:CA	2:B:5465:NAD:H51A	2.30	0.61
1:B:90:ALA:HB2	1:B:117:GLY:HA3	1.81	0.61
1:O:178:THR:HG23	1:O:233:MET:HE1	1.83	0.61
1:B:62:LYS:HE3	1:B:70:LEU:HD23	1.82	0.61
1:O:83:ASN:CG	1:O:85:ASP:HB3	2.21	0.61
1:C:24:GLN:NE2	3:C:5796:HOH:O	2.33	0.61
1:B:278:TYR:CE2	1:B:280:GLU:HG3	2.36	0.61
1:O:38:ILE:CD1	1:O:43:MET:CE	2.67	0.61
1:A:90:ALA:HB2	1:A:117:GLY:HA3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:265:LYS:O	1:O:269:GLU:HG3	2.02	0.60
1:A:181:HIS:HB3	1:A:236:ARG:HD3	1.83	0.60
1:B:271:LYS:H	1:B:271:LYS:CD	2.05	0.60
1:C:177:MET:HG2	1:C:178:THR:N	2.16	0.60
1:O:115:LYS:NZ	3:O:5575:HOH:O	2.34	0.60
1:O:213:THR:HG22	1:O:233:MET:HA	1.82	0.60
1:O:25:SER:OG	1:O:28:VAL:HG22	2.01	0.60
1:O:10:GLY:HA2	2:O:5463:NAD:N3A	2.17	0.60
1:O:140:ASP:HB2	3:O:5610:HOH:O	2.02	0.60
1:B:107:LYS:CE	1:B:108:GLU:OE1	2.50	0.59
1:C:108:GLU:HG3	3:C:5661:HOH:O	2.02	0.59
1:B:72:GLY:O	1:B:73:GLU:HB2	2.03	0.59
1:C:318:ASN:O	2:C:5467:NAD:H4N	2.03	0.59
1:O:159:LEU:HD22	1:O:177:MET:CE	2.32	0.59
1:A:207:ASN:ND2	1:B:286:THR:HG23	2.18	0.59
1:B:69:LEU:O	1:B:70:LEU:CB	2.48	0.58
1:O:207:ASN:ND2	1:C:286:THR:HG23	2.18	0.58
1:B:64:LYS:HB3	1:B:68:THR:OG1	2.03	0.58
1:B:65:ASP:OD1	1:B:68:THR:HG23	2.02	0.58
1:A:229:LYS:HE2	3:A:5611:HOH:O	2.03	0.58
1:C:250:ARG:HD3	1:C:308:ASN:O	2.04	0.58
1:O:12:GLY:CA	2:O:5463:NAD:H51A	2.34	0.58
1:C:83:ASN:HD22	1:C:84:PRO:HD2	1.69	0.58
1:O:14:ILE:HD11	2:O:5463:NAD:C3N	2.34	0.58
1:B:271:LYS:N	1:B:271:LYS:HD2	2.17	0.57
1:A:310:VAL:HG22	1:A:311:LYS:N	2.17	0.57
1:O:183:ILE:HD12	1:B:189:THR:HB	1.86	0.57
1:O:217:LYS:HD3	3:O:5683:HOH:O	2.05	0.57
1:O:63:ILE:N	1:O:63:ILE:HD12	2.18	0.57
1:B:12:GLY:HA3	2:B:5465:NAD:C5B	2.32	0.56
1:O:12:GLY:CA	2:O:5463:NAD:H4B	2.36	0.56
1:O:154:CYS:HB3	2:O:5463:NAD:H5N	1.87	0.56
1:C:90:ALA:HB2	1:C:117:GLY:HA3	1.87	0.56
1:O:177:MET:HG2	1:O:178:THR:N	2.20	0.56
1:A:12:GLY:HA3	2:A:5466:NAD:C5B	2.36	0.56
1:A:211:SER:HB3	1:A:234:SER:OG	2.06	0.56
1:A:65:ASP:OD1	1:A:66:SER:O	2.23	0.56
1:B:60:ASP:OD1	1:B:72:GLY:HA2	2.06	0.55
1:O:55:GLN:NE2	3:O:5594:HOH:O	2.16	0.55
1:A:272:LEU:HD13	1:A:276:ILE:CD1	2.36	0.55
1:A:269:GLU:HA	1:A:273:LYS:CE	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:278:TYR:CE2	1:O:280:GLU:HG3	2.42	0.55
1:B:141:LYS:HG3	3:B:5480:HOH:O	2.05	0.54
1:B:124:SER:O	2:B:5465:NAD:H1D	2.08	0.53
1:O:112:ALA:HA	1:O:115:LYS:HD2	1.89	0.53
1:B:129:ASP:N	1:B:129:ASP:OD1	2.42	0.53
1:C:119:LYS:O	1:C:120:LYS:HD2	2.07	0.53
1:O:132:MET:HE1	1:O:218:ALA:HB1	1.90	0.53
1:A:179:THR:CG2	1:A:234:SER:HB3	2.39	0.53
1:A:207:ASN:HD22	1:B:286:THR:H	1.57	0.53
1:O:114:LEU:HD12	1:O:118:ALA:O	2.08	0.53
1:A:39:THR:CG2	1:A:40:THR:N	2.72	0.53
1:B:63:ILE:HD12	1:B:63:ILE:N	2.24	0.53
1:A:23:LEU:HD12	3:A:5702:HOH:O	2.08	0.53
1:A:39:THR:HG22	1:A:41:ASP:N	2.24	0.53
1:A:39:THR:HG22	1:A:42:TYR:H	1.74	0.53
1:C:304:ALA:CB	1:C:310:VAL:HG12	2.39	0.52
1:B:181:HIS:HB3	1:B:236:ARG:HD3	1.92	0.52
1:O:24:GLN:OE1	1:O:58:HIS:CD2	2.62	0.52
1:A:207:ASN:ND2	1:B:286:THR:H	2.07	0.52
1:C:160:ALA:HB3	1:C:161:PRO:HD3	1.92	0.52
1:B:199:ARG:HD2	1:B:210:PRO:HG2	1.90	0.52
1:O:83:ASN:OD1	1:O:85:ASP:CB	2.48	0.52
1:C:62:LYS:NZ	1:C:62:LYS:CB	2.73	0.52
1:O:88:PRO:HB2	1:O:91:GLU:CG	2.37	0.52
1:C:72:GLY:O	1:C:73:GLU:HB2	2.10	0.51
1:A:125:ALA:CB	2:A:5466:NAD:O2D	2.58	0.51
1:A:82:ARG:CB	1:A:82:ARG:HH21	2.22	0.51
1:O:111:ALA:O	1:O:114:LEU:HD22	2.09	0.51
1:O:72:GLY:O	1:O:73:GLU:CG	2.59	0.51
1:O:189:THR:HB	1:B:183:ILE:HD12	1.92	0.51
1:O:44:THR:HG21	1:O:63:ILE:CD1	2.40	0.51
1:A:177:MET:HG2	1:A:178:THR:N	2.25	0.51
1:C:291:ASP:OD1	1:C:293:ARG:HD3	2.11	0.50
1:O:164:LYS:CE	3:O:5609:HOH:O	2.53	0.50
1:O:207:ASN:HD22	1:C:286:THR:H	1.58	0.50
1:O:38:ILE:CD1	1:O:43:MET:HG3	2.42	0.50
1:O:159:LEU:HB2	1:O:177:MET:CE	2.42	0.50
1:C:16:ARG:O	1:C:19:ALA:HB3	2.12	0.50
1:O:12:GLY:HA2	2:O:5463:NAD:H51A	1.93	0.50
1:B:12:GLY:O	1:B:16:ARG:HG3	2.11	0.50
1:A:12:GLY:O	1:A:16:ARG:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:SER:CB	1:A:337:GLN:O	2.60	0.50
1:A:84:PRO:HB2	1:A:112:ALA:HB3	1.94	0.50
1:B:199:ARG:CD	1:B:210:PRO:HG2	2.42	0.50
1:B:55:GLN:O	1:B:57:LYS:HG2	2.11	0.50
1:B:281:GLU:OE2	1:C:49:TYR:OH	2.28	0.50
1:C:64:LYS:O	1:C:65:ASP:CG	2.50	0.50
1:A:125:ALA:HB2	2:A:5466:NAD:O2D	2.12	0.50
1:A:272:LEU:HB3	1:A:276:ILE:HG13	1.94	0.50
1:O:81:ILE:HD12	1:O:87:ILE:HA	1.92	0.50
1:B:160:ALA:HB3	1:B:161:PRO:HD3	1.94	0.49
1:C:69:LEU:HD22	1:C:78:VAL:CG2	2.42	0.49
1:B:336:THR:HG22	1:B:337:GLN:HG2	1.94	0.49
1:B:14:ILE:O	1:B:18:VAL:HG23	2.13	0.48
1:O:332:HIS:HE1	3:O:5604:HOH:O	1.95	0.48
1:C:83:ASN:HD22	1:C:84:PRO:CD	2.27	0.48
1:B:296:ILE:N	1:B:296:ILE:HD12	2.29	0.48
1:C:14:ILE:HG12	2:C:5467:NAD:O2N	2.13	0.48
1:B:107:LYS:NZ	1:B:108:GLU:CD	2.66	0.48
1:O:12:GLY:CA	2:O:5463:NAD:C4B	2.92	0.48
1:O:217:LYS:HB2	1:O:217:LYS:HZ2	1.77	0.48
1:O:247:LEU:HG	1:O:249:VAL:HG13	1.95	0.48
1:O:13:ARG:CB	2:O:5463:NAD:O1N	2.61	0.48
1:B:82:ARG:HH11	1:B:82:ARG:HG3	1.79	0.48
1:O:309:PHE:CE2	1:C:174:GLU:HG3	2.49	0.48
1:O:178:THR:HG23	1:O:233:MET:CE	2.43	0.48
1:A:332:HIS:HE1	3:A:5666:HOH:O	1.96	0.48
1:O:2:GLY:O	1:O:3:LYS:CB	2.60	0.48
1:C:56:TRP:CZ2	1:C:58:HIS:HB3	2.49	0.47
1:C:24:GLN:HG3	1:C:58:HIS:CD2	2.48	0.47
1:O:33:VAL:HG21	1:O:43:MET:SD	2.55	0.47
2:O:5463:NAD:H2N	2:O:5463:NAD:H52N	1.96	0.47
1:C:318:ASN:HD22	2:C:5467:NAD:H72N	1.62	0.47
1:O:233:MET:HE2	1:O:233:MET:C	2.34	0.47
2:A:5466:NAD:H2N	2:A:5466:NAD:H52N	1.96	0.47
1:B:304:ALA:CB	1:B:310:VAL:HG12	2.45	0.47
1:A:64:LYS:HB2	1:A:70:LEU:HD21	1.94	0.47
1:C:170:PHE:HD1	1:C:253:LYS:HE2	1.80	0.47
1:A:172:ILE:HG23	1:A:249:VAL:HG23	1.97	0.47
1:A:335:LYS:HG3	3:A:5621:HOH:O	2.14	0.47
1:B:154:CYS:HB3	2:B:5465:NAD:H5N	1.95	0.47
1:A:179:THR:HG22	1:A:234:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ARG:HG3	3:C:5634:HOH:O	2.15	0.47
1:C:293:ARG:NH1	3:C:5635:HOH:O	2.47	0.46
1:A:96:TYR:CD1	1:A:120:LYS:HB2	2.50	0.46
1:B:278:TYR:HE2	1:B:280:GLU:HG3	1.79	0.46
1:A:172:ILE:HG23	1:A:249:VAL:CG2	2.46	0.46
1:A:74:LYS:HG3	1:A:74:LYS:O	2.15	0.46
1:O:332:HIS:CE1	3:O:5604:HOH:O	2.67	0.46
1:O:337:GLN:CD	1:O:337:GLN:H	2.19	0.46
1:A:213:THR:HG22	1:A:233:MET:HA	1.98	0.46
1:B:336:THR:O	1:B:337:GLN:HB2	2.16	0.46
1:A:69:LEU:C	1:A:70:LEU:HD22	2.36	0.46
1:A:24:GLN:NE2	3:A:5693:HOH:O	2.49	0.46
1:B:335:LYS:O	1:B:335:LYS:HG2	2.16	0.46
1:O:81:ILE:HD12	1:O:88:PRO:HD2	1.98	0.46
1:A:39:THR:HG23	1:A:40:THR:N	2.31	0.45
1:O:286:THR:H	1:C:207:ASN:HD22	1.62	0.45
1:O:238:PRO:HB2	1:C:238:PRO:HB2	1.99	0.45
1:C:106:ASP:CG	1:C:128:LYS:HE2	2.37	0.45
1:O:207:ASN:ND2	1:C:286:THR:H	2.15	0.45
1:O:63:ILE:CD1	1:O:63:ILE:N	2.79	0.45
1:A:27:ASP:CG	1:A:331:ARG:HE	2.20	0.45
1:C:154:CYS:HB3	2:C:5467:NAD:H5N	1.97	0.45
1:O:184:THR:CB	1:O:236:ARG:HH22	2.27	0.45
1:C:179:THR:HG22	1:C:234:SER:HB2	1.98	0.45
1:A:65:ASP:C	1:A:66:SER:O	2.54	0.45
1:C:217:LYS:HE3	3:C:5701:HOH:O	2.16	0.45
1:O:283:LEU:HD21	1:A:49:TYR:CZ	2.51	0.45
1:O:38:ILE:CD1	1:O:43:MET:CG	2.94	0.45
1:A:310:VAL:CG2	1:A:311:LYS:N	2.79	0.45
1:C:304:ALA:HB1	1:C:310:VAL:HG12	1.99	0.45
1:O:106:ASP:OD1	1:O:128:LYS:HE2	2.17	0.45
1:O:72:GLY:C	1:O:73:GLU:HG3	2.37	0.45
1:A:286:THR:HG23	1:B:207:ASN:ND2	2.31	0.45
1:O:111:ALA:O	1:O:114:LEU:CD2	2.65	0.45
1:O:119:LYS:HB2	3:O:5571:HOH:O	2.16	0.45
1:O:56:TRP:CD1	1:O:59:SER:O	2.70	0.45
1:A:10:GLY:HA2	2:A:5466:NAD:N3A	2.32	0.44
1:A:193:PRO:HD3	3:C:5794:HOH:O	2.16	0.44
1:A:38:ILE:HD11	1:A:43:MET:HG3	1.99	0.44
1:O:13:ARG:N	2:O:5463:NAD:O3	2.51	0.44
1:B:69:LEU:HA	1:B:69:LEU:HD23	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:HIS:HD2	3:C:5792:HOH:O	2.01	0.44
1:A:199:ARG:HG2	1:B:282:ASP:HB3	1.99	0.44
1:A:74:LYS:HE3	3:A:5694:HOH:O	2.17	0.44
1:B:278:TYR:CE2	1:B:280:GLU:CG	3.01	0.44
1:C:241:ASP:O	1:C:242:VAL:HB	2.17	0.44
1:A:154:CYS:HB3	2:A:5466:NAD:H5N	1.99	0.44
1:B:144:SER:OG	1:B:337:GLN:NE2	2.51	0.44
1:O:233:MET:HE1	1:O:235:PHE:CE2	2.53	0.44
1:A:286:THR:H	1:B:207:ASN:ND2	2.16	0.44
1:A:74:LYS:HE3	1:A:74:LYS:HB2	1.85	0.44
1:B:38:ILE:HD13	1:B:46:MET:SD	2.57	0.44
1:A:65:ASP:O	1:A:66:SER:CB	2.54	0.43
1:A:286:THR:H	1:B:207:ASN:HD22	1.65	0.43
1:C:23:LEU:HD13	1:C:71:LEU:HD22	1.99	0.43
1:O:286:THR:H	1:C:207:ASN:ND2	2.16	0.43
1:A:257:TYR:CE2	1:A:261:LYS:HD2	2.53	0.43
1:A:282:ASP:HB3	1:B:199:ARG:CG	2.46	0.43
1:B:286:THR:HG21	1:C:51:THR:HG23	2.00	0.43
1:B:336:THR:O	1:B:337:GLN:CB	2.66	0.43
1:B:11:PHE:CE2	1:B:43:MET:HG2	2.53	0.43
1:B:177:MET:CE	1:B:179:THR:HG23	2.48	0.43
1:B:332:HIS:HE1	3:B:5554:HOH:O	2.00	0.43
1:A:249:VAL:HG22	1:A:250:ARG:N	2.34	0.43
1:A:272:LEU:HD13	1:A:276:ILE:HD11	2.00	0.43
1:C:84:PRO:HB2	1:C:112:ALA:HB3	2.01	0.43
1:C:68:THR:HG22	3:C:5746:HOH:O	2.19	0.43
1:O:175:GLY:HA3	1:O:249:VAL:HG12	2.01	0.43
1:A:269:GLU:HA	1:A:273:LYS:HE3	2.01	0.42
1:B:178:THR:HA	1:B:233:MET:O	2.19	0.42
1:B:44:THR:HG22	1:B:69:LEU:HD22	2.01	0.42
1:C:115:LYS:HG3	3:C:5754:HOH:O	2.19	0.42
1:C:62:LYS:NZ	1:C:62:LYS:HB3	2.33	0.42
1:O:90:ALA:HB2	1:O:117:GLY:HA3	2.01	0.42
1:A:62:LYS:NZ	1:A:72:GLY:H	2.17	0.42
1:B:177:MET:O	1:B:232:GLY:HA3	2.18	0.42
1:C:213:THR:HG22	1:C:233:MET:HA	2.00	0.42
1:O:24:GLN:OE1	1:O:58:HIS:HB2	2.16	0.42
1:O:82:ARG:HB3	1:O:82:ARG:HE	1.50	0.42
1:B:141:LYS:CG	3:B:5480:HOH:O	2.67	0.42
1:A:66:SER:C	1:A:68:THR:H	2.22	0.42
1:B:188:LYS:HE3	1:B:193:PRO:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:SER:HB3	3:B:5659:HOH:O	2.20	0.42
1:O:12:GLY:O	1:O:16:ARG:HG3	2.19	0.42
1:B:70:LEU:HD12	1:B:70:LEU:HA	1.89	0.42
1:C:115:LYS:CG	3:C:5754:HOH:O	2.68	0.41
1:O:73:GLU:OE2	1:O:73:GLU:C	2.57	0.41
1:C:12:GLY:CA	2:C:5467:NAD:H51A	2.48	0.41
1:C:70:LEU:HA	1:C:70:LEU:HD12	1.90	0.41
1:A:196:LYS:HG2	1:A:196:LYS:O	2.21	0.41
1:A:66:SER:O	1:A:68:THR:N	2.53	0.41
1:A:87:ILE:HG21	1:A:89:TRP:CZ2	2.55	0.41
1:O:179:THR:CG2	1:O:234:SER:HB2	2.51	0.41
1:O:241:ASP:O	1:O:242:VAL:HB	2.20	0.41
1:C:106:ASP:OD2	1:C:128:LYS:HE2	2.20	0.41
1:O:38:ILE:HD11	1:O:43:MET:CG	2.50	0.41
1:C:12:GLY:HA3	2:C:5467:NAD:O5B	2.20	0.41
1:O:38:ILE:CD1	1:O:43:MET:CB	2.95	0.41
1:A:87:ILE:HG21	1:A:89:TRP:CE2	2.56	0.41
1:C:47:PHE:HD1	1:C:61:ILE:HD13	1.86	0.41
1:A:63:ILE:CD1	1:A:63:ILE:N	2.83	0.41
1:C:183:ILE:HA	1:C:187:GLN:OE1	2.21	0.41
1:A:39:THR:CG2	1:A:41:ASP:H	2.33	0.41
1:A:64:LYS:O	1:A:65:ASP:HB3	2.19	0.41
1:A:205:SER:HA	1:A:238:PRO:HB3	2.03	0.41
1:B:128:LYS:HE3	1:B:128:LYS:HB3	1.46	0.41
1:A:86:GLU:CD	3:A:5661:HOH:O	2.59	0.41
1:B:132:MET:HE1	1:B:218:ALA:HB1	2.03	0.41
1:O:13:ARG:CG	2:O:5463:NAD:O1N	2.69	0.41
1:B:63:ILE:H	1:B:63:ILE:HD12	1.85	0.40
1:O:225:ASP:HB3	3:O:5678:HOH:O	2.22	0.40
1:O:286:THR:HG23	1:C:207:ASN:ND2	2.36	0.40
1:O:38:ILE:HD11	1:O:43:MET:HG3	2.02	0.40
1:A:71:LEU:CD2	1:A:71:LEU:N	2.84	0.40
1:O:37:PHE:N	1:O:37:PHE:CD2	2.89	0.40
1:O:207:ASN:HA	1:C:285:SER:OG	2.22	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:5500:HOH:O	3:A:5665:HOH:O[1_556]	1.92	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:5659:HOH:O	3:C:5630:HOH:O[2_645]	1.94	0.26
3:O:5615:HOH:O	3:A:5764:HOH:O[1_556]	1.95	0.25
3:O:5601:HOH:O	3:A:5736:HOH:O[1_556]	2.02	0.18
3:A:5700:HOH:O	3:C:5800:HOH:O[2_645]	2.08	0.12
3:O:5502:HOH:O	3:B:5586:HOH:O[1_656]	2.08	0.12
1:A:225:ASP:OD1	3:O:5600:HOH:O[1_554]	2.10	0.10
3:O:5629:HOH:O	3:B:5679:HOH:O[1_656]	2.14	0.06
3:O:5603:HOH:O	3:A:5728:HOH:O[1_556]	2.15	0.05
3:A:5659:HOH:O	3:C:5606:HOH:O[2_645]	2.15	0.05
3:O:5602:HOH:O	3:A:5765:HOH:O[1_556]	2.17	0.03
3:O:5569:HOH:O	3:A:5715:HOH:O[1_455]	2.19	0.01

## 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	334/337 (99%)	309 (92%)	23 (7%)	2 (1%)	25	31
1	B	334/337 (99%)	311 (93%)	18 (5%)	5 (2%)	10	10
1	C	334/337 (99%)	319 (96%)	13 (4%)	2 (1%)	25	31
1	O	334/337 (99%)	313 (94%)	18 (5%)	3 (1%)	17	20
All	All	1336/1348 (99%)	1252 (94%)	72 (5%)	12 (1%)	17	20

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ASP
1	B	3	LYS
1	B	70	LEU
1	O	3	LYS
1	C	242	VAL
1	O	242	VAL

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Mol	Chain	Res	Type
1	A	242	VAL
1	B	242	VAL
1	B	69	LEU
1	O	65	ASP
1	C	191	ASP
1	B	238	PRO

### 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	276/277 (100%)	261 (95%)	15 (5%)	22	30
1	B	276/277 (100%)	270 (98%)	6 (2%)	52	69
1	C	276/277 (100%)	263 (95%)	13 (5%)	26	37
1	O	276/277 (100%)	264 (96%)	12 (4%)	29	40
All	All	1104/1108 (100%)	1058 (96%)	46 (4%)	30	42

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	60	ASP
1	O	69	LEU
1	O	71	LEU
1	O	114	LEU
1	O	177	MET
1	O	217	LYS
1	O	223	LEU
1	O	225	ASP
1	O	227	ASN
1	O	233	MET
1	O	293	ARG
1	O	337	GLN
1	A	23	LEU
1	A	26	GLU
1	A	27	ASP

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Mol	Chain	Res	Type
1	A	28	VAL
1	A	30	LEU
1	A	39	THR
1	A	41	ASP
1	A	52	VAL
1	A	66	SER
1	A	69	LEU
1	A	71	LEU
1	A	108	GLU
1	A	233	MET
1	A	250	ARG
1	A	313	VAL
1	B	26	GLU
1	B	30	LEU
1	B	41	ASP
1	B	68	THR
1	B	128	LYS
1	B	271	LYS
1	C	41	ASP
1	C	59	SER
1	C	60	ASP
1	C	62	LYS
1	C	68	THR
1	C	69	LEU
1	C	73	GLU
1	C	83	ASN
1	C	140	ASP
1	C	233	MET
1	C	250	ARG
1	C	283	LEU
1	C	293	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	207	ASN
1	O	227	ASN
1	O	318	ASN
1	O	332	HIS
1	A	24	GLN
1	A	83	ASN
1	A	207	ASN

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Mol	Chain	Res	Type
1	A	318	ASN
1	A	332	HIS
1	B	24	GLN
1	B	58	HIS
1	B	207	ASN
1	B	318	ASN
1	B	332	HIS
1	C	24	GLN
1	C	55	GLN
1	C	58	HIS
1	C	83	ASN
1	C	207	ASN
1	C	332	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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAD	C	5467	-	42,48,48	2.48	16 (38%)	50,73,73	3.50	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	B	5465	-	42,48,48	2.15	10 (23%)	50,73,73	3.83	20 (40%)
2	NAD	A	5466	-	42,48,48	1.50	4 (9%)	50,73,73	2.62	20 (40%)
2	NAD	O	5463	-	42,48,48	1.41	5 (11%)	50,73,73	2.62	18 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	C	5467	-	-	5/26/62/62	0/5/5/5
2	NAD	B	5465	-	1/1/11/11	5/26/62/62	0/5/5/5
2	NAD	A	5466	-	-	4/26/62/62	0/5/5/5
2	NAD	O	5463	-	-	5/26/62/62	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	5467	NAD	O4D-C1D	7.78	1.51	1.41
2	B	5465	NAD	C2D-C1D	7.42	1.65	1.53
2	C	5467	NAD	O4D-C4D	5.35	1.57	1.45
2	A	5466	NAD	O4B-C1B	5.17	1.48	1.41
2	B	5465	NAD	O4B-C1B	5.04	1.48	1.41
2	C	5467	NAD	O4B-C1B	4.53	1.47	1.41
2	O	5463	NAD	O4B-C1B	4.40	1.47	1.41
2	B	5465	NAD	PN-O5D	4.35	1.76	1.59
2	O	5463	NAD	O4D-C1D	4.30	1.47	1.41
2	A	5466	NAD	O4D-C1D	4.25	1.47	1.41
2	C	5467	NAD	O3D-C3D	4.21	1.52	1.43
2	C	5467	NAD	O5B-C5B	-4.02	1.29	1.44
2	B	5465	NAD	O3D-C3D	-4.00	1.33	1.43
2	C	5467	NAD	C5D-C4D	-3.47	1.40	1.51
2	B	5465	NAD	C5D-C4D	-3.40	1.41	1.51
2	B	5465	NAD	C2D-C3D	3.39	1.62	1.53
2	C	5467	NAD	C2B-C3B	-3.36	1.44	1.53
2	C	5467	NAD	PN-O1N	3.31	1.62	1.50
2	O	5463	NAD	C2N-C3N	3.12	1.43	1.39
2	A	5466	NAD	C2N-C3N	3.09	1.43	1.39
2	B	5465	NAD	O5D-C5D	2.96	1.56	1.44
2	C	5467	NAD	C3B-C4B	-2.84	1.45	1.53
2	C	5467	NAD	PN-O5D	2.73	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5465	NAD	O4B-C4B	2.54	1.50	1.45
2	A	5466	NAD	C2N-N1N	2.48	1.38	1.35
2	C	5467	NAD	C8A-N7A	-2.47	1.30	1.34
2	C	5467	NAD	C5B-C4B	-2.47	1.43	1.51
2	C	5467	NAD	C3D-C4D	2.28	1.58	1.53
2	B	5465	NAD	C2N-N1N	-2.28	1.32	1.35
2	O	5463	NAD	C2N-N1N	2.26	1.37	1.35
2	C	5467	NAD	C2A-N3A	2.22	1.35	1.32
2	C	5467	NAD	C4N-C3N	2.17	1.43	1.39
2	B	5465	NAD	C3D-C4D	-2.12	1.47	1.53
2	C	5467	NAD	C6A-N6A	2.05	1.41	1.34
2	O	5463	NAD	C2A-N3A	2.04	1.35	1.32

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5465	NAD	C5D-C4D-C3D	15.45	173.06	115.18
2	B	5465	NAD	O4D-C4D-C5D	-11.18	72.58	109.37
2	C	5467	NAD	O4D-C4D-C5D	-11.05	73.03	109.37
2	C	5467	NAD	O4D-C4D-C3D	-10.34	84.66	105.11
2	C	5467	NAD	O5D-C5D-C4D	-9.02	77.96	108.99
2	A	5466	NAD	O2N-PN-O1N	-8.24	71.51	112.24
2	C	5467	NAD	C2D-C3D-C4D	8.14	118.45	102.64
2	O	5463	NAD	O2N-PN-O1N	-8.10	72.19	112.24
2	B	5465	NAD	O5D-PN-O1N	-7.94	78.05	109.07
2	B	5465	NAD	PN-O3-PA	-7.49	107.13	132.83
2	O	5463	NAD	PN-O3-PA	-6.84	109.34	132.83
2	A	5466	NAD	PN-O3-PA	-6.67	109.95	132.83
2	A	5466	NAD	O5D-PN-O1N	6.61	134.88	109.07
2	O	5463	NAD	O5D-PN-O1N	6.47	134.36	109.07
2	B	5465	NAD	O3D-C3D-C4D	5.84	127.94	111.05
2	C	5467	NAD	C5D-C4D-C3D	5.69	136.50	115.18
2	C	5467	NAD	O4B-C4B-C5B	5.49	127.42	109.37
2	B	5465	NAD	PA-O5B-C5B	-5.41	89.97	121.68
2	B	5465	NAD	O2D-C2D-C1D	4.96	129.15	110.85
2	C	5467	NAD	O5B-PA-O1A	4.82	127.88	109.07
2	A	5466	NAD	O2N-PN-O5D	-4.74	85.73	107.75
2	O	5463	NAD	O2N-PN-O5D	-4.73	85.78	107.75
2	O	5463	NAD	N3A-C2A-N1A	-4.68	121.36	128.68
2	A	5466	NAD	N3A-C2A-N1A	-4.65	121.41	128.68
2	B	5465	NAD	N3A-C2A-N1A	-4.58	121.52	128.68
2	C	5467	NAD	N3A-C2A-N1A	-4.45	121.73	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5467	NAD	PA-O5B-C5B	-4.17	97.23	121.68
2	B	5465	NAD	O5B-C5B-C4B	4.17	123.34	108.99
2	O	5463	NAD	O4B-C1B-C2B	-4.16	100.84	106.93
2	A	5466	NAD	O4B-C1B-C2B	-4.12	100.91	106.93
2	B	5465	NAD	O4D-C1D-C2D	-4.02	101.05	106.93
2	C	5467	NAD	O5B-C5B-C4B	4.00	122.77	108.99
2	A	5466	NAD	PA-O5B-C5B	-3.99	98.27	121.68
2	O	5463	NAD	PA-O5B-C5B	-3.92	98.68	121.68
2	C	5467	NAD	C5B-C4B-C3B	-3.76	101.10	115.18
2	B	5465	NAD	O2N-PN-O5D	-3.73	90.40	107.75
2	C	5467	NAD	O4D-C1D-C2D	-3.64	101.61	106.93
2	O	5463	NAD	PN-O5D-C5D	-3.42	101.61	121.68
2	B	5465	NAD	O4B-C4B-C5B	3.25	120.08	109.37
2	B	5465	NAD	O5B-PA-O1A	3.22	121.66	109.07
2	A	5466	NAD	PN-O5D-C5D	-3.14	103.25	121.68
2	O	5463	NAD	O5B-PA-O1A	3.06	121.02	109.07
2	B	5465	NAD	O4B-C1B-C2B	-3.01	102.52	106.93
2	A	5466	NAD	O4B-C4B-C5B	2.82	118.65	109.37
2	A	5466	NAD	C5D-C4D-C3D	-2.81	104.65	115.18
2	A	5466	NAD	C3D-C2D-C1D	2.80	105.19	100.98
2	O	5463	NAD	C5D-C4D-C3D	-2.79	104.72	115.18
2	C	5467	NAD	O4B-C1B-C2B	-2.76	102.90	106.93
2	O	5463	NAD	C3D-C2D-C1D	2.74	105.11	100.98
2	O	5463	NAD	O4B-C4B-C5B	2.71	118.30	109.37
2	C	5467	NAD	O4B-C4B-C3B	2.69	110.44	105.11
2	A	5466	NAD	O5B-PA-O1A	2.68	119.53	109.07
2	O	5463	NAD	C2D-C3D-C4D	2.66	107.81	102.64
2	O	5463	NAD	C5B-C4B-C3B	-2.65	105.25	115.18
2	C	5467	NAD	O7N-C7N-N7N	-2.64	118.83	122.58
2	A	5466	NAD	O7N-C7N-N7N	-2.58	118.91	122.58
2	A	5466	NAD	O2A-PA-O1A	2.56	124.88	112.24
2	A	5466	NAD	C5B-C4B-C3B	-2.53	105.72	115.18
2	B	5465	NAD	C5B-C4B-C3B	-2.52	105.73	115.18
2	B	5465	NAD	O2A-PA-O1A	2.51	124.65	112.24
2	C	5467	NAD	PN-O5D-C5D	-2.51	106.98	121.68
2	C	5467	NAD	O2D-C2D-C3D	2.50	119.92	111.82
2	A	5466	NAD	C2D-C3D-C4D	2.50	107.50	102.64
2	B	5465	NAD	C6N-N1N-C2N	2.47	124.22	121.97
2	O	5463	NAD	O7N-C7N-N7N	-2.42	119.14	122.58
2	B	5465	NAD	O4B-C4B-C3B	2.35	109.76	105.11
2	C	5467	NAD	C4A-C5A-N7A	-2.30	107.00	109.40
2	O	5463	NAD	O2A-PA-O1A	2.26	123.43	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5466	NAD	O5B-C5B-C4B	2.24	116.70	108.99
2	O	5463	NAD	O5D-C5D-C4D	2.22	116.63	108.99
2	A	5466	NAD	O5D-C5D-C4D	2.21	116.59	108.99
2	B	5465	NAD	C3D-C2D-C1D	2.18	104.26	100.98
2	B	5465	NAD	O2N-PN-O1N	2.13	122.78	112.24
2	A	5466	NAD	O4D-C1D-C2D	2.09	109.97	106.93
2	A	5466	NAD	C4A-C5A-N7A	-2.06	107.25	109.40
2	O	5463	NAD	O4D-C1D-C2D	2.00	109.85	106.93

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	5465	NAD	C4D

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	5467	NAD	C5B-O5B-PA-O1A
2	C	5467	NAD	C3D-C4D-C5D-O5D
2	C	5467	NAD	O4D-C1D-N1N-C2N
2	O	5463	NAD	C5B-O5B-PA-O2A
2	O	5463	NAD	C5D-O5D-PN-O1N
2	A	5466	NAD	C5B-O5B-PA-O2A
2	A	5466	NAD	C5D-O5D-PN-O1N
2	B	5465	NAD	C5B-O5B-PA-O1A
2	C	5467	NAD	O4D-C4D-C5D-O5D
2	B	5465	NAD	O4D-C4D-C5D-O5D
2	B	5465	NAD	O4B-C4B-C5B-O5B
2	C	5467	NAD	C5B-O5B-PA-O2A
2	O	5463	NAD	C5B-O5B-PA-O1A
2	A	5466	NAD	C5B-O5B-PA-O1A
2	B	5465	NAD	C5B-O5B-PA-O2A
2	O	5463	NAD	PN-O3-PA-O2A
2	A	5466	NAD	PN-O3-PA-O2A
2	O	5463	NAD	PN-O3-PA-O1A
2	B	5465	NAD	C3B-C4B-C5B-O5B

There are no ring outliers.

4 monomers are involved in 46 short contacts:

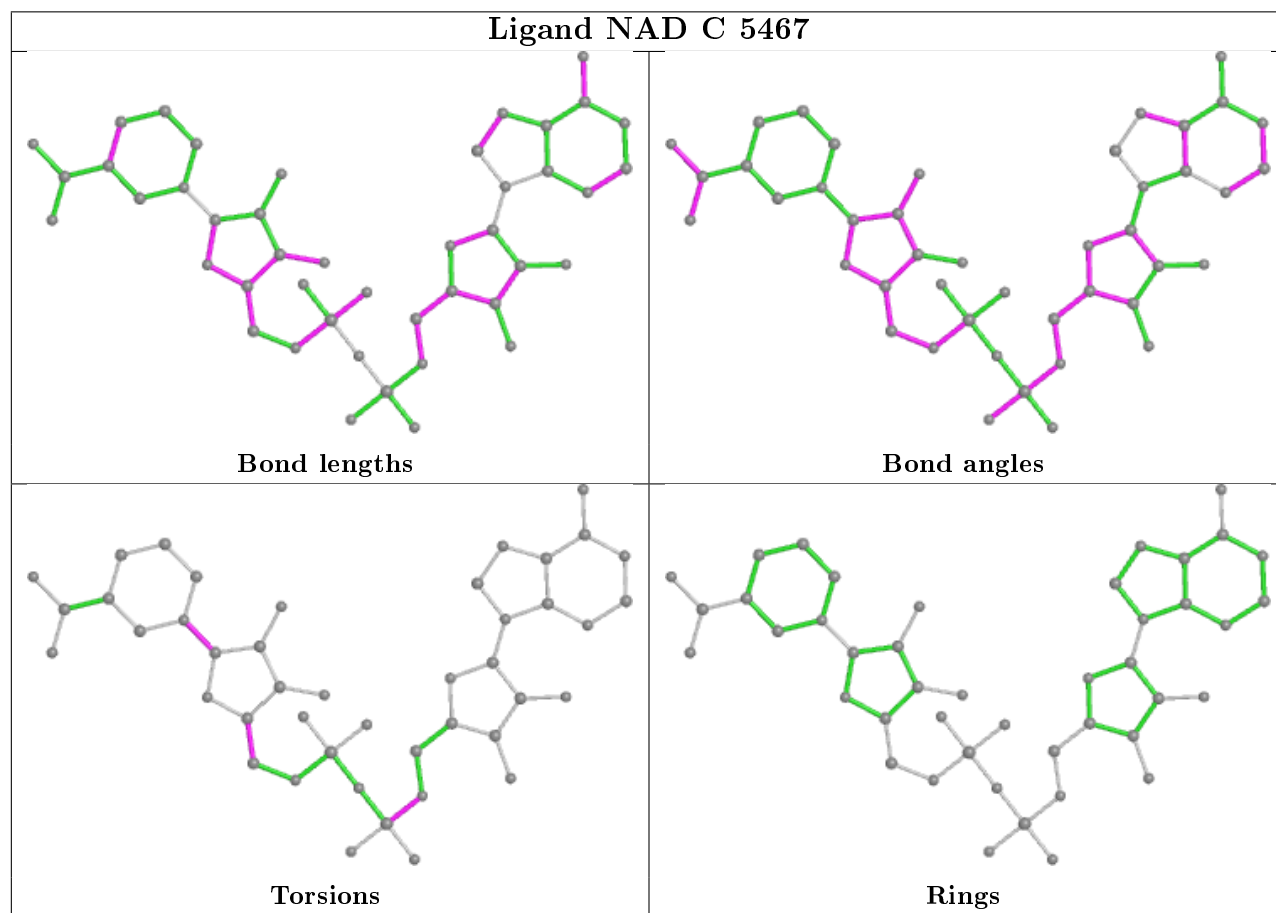
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	5467	NAD	10	0

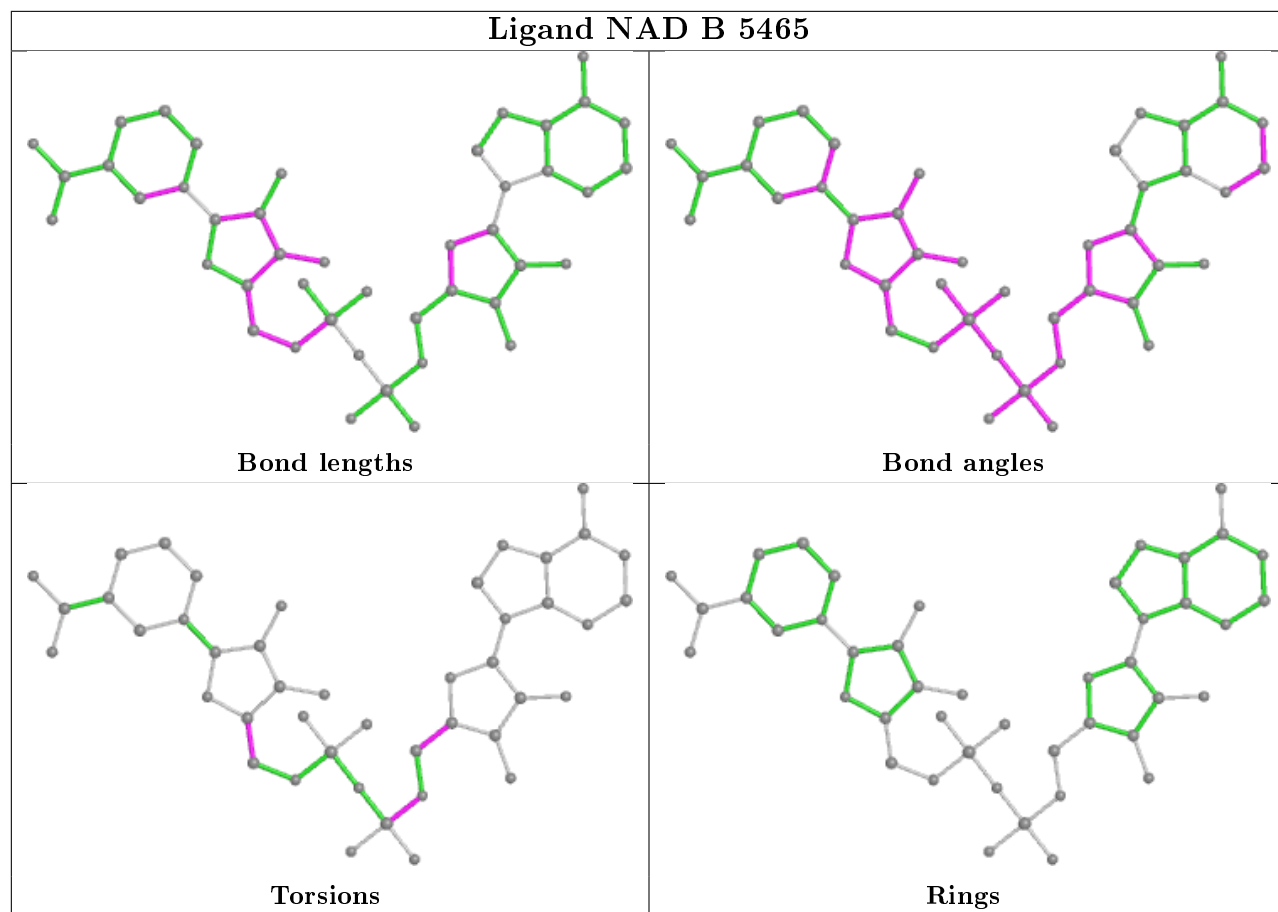
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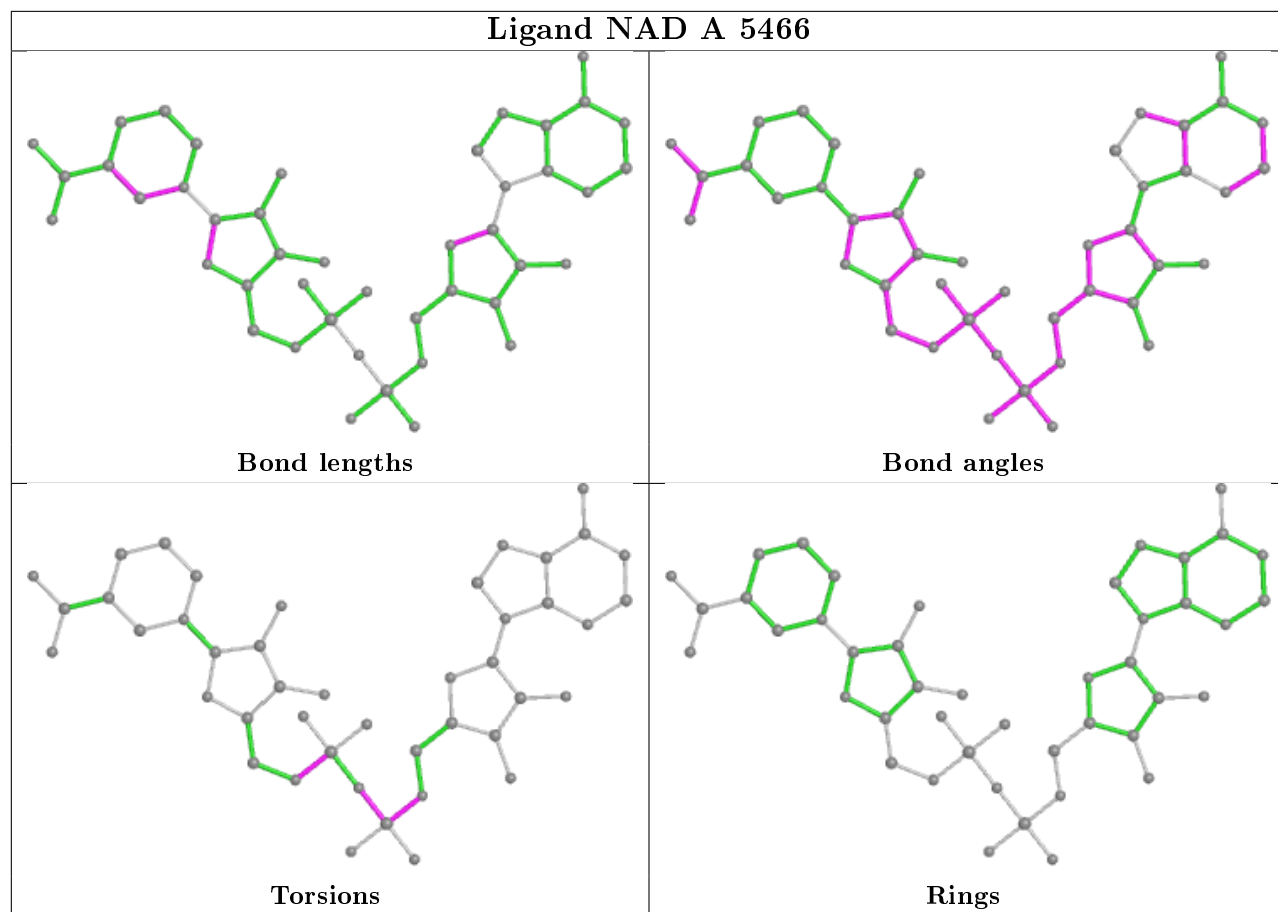
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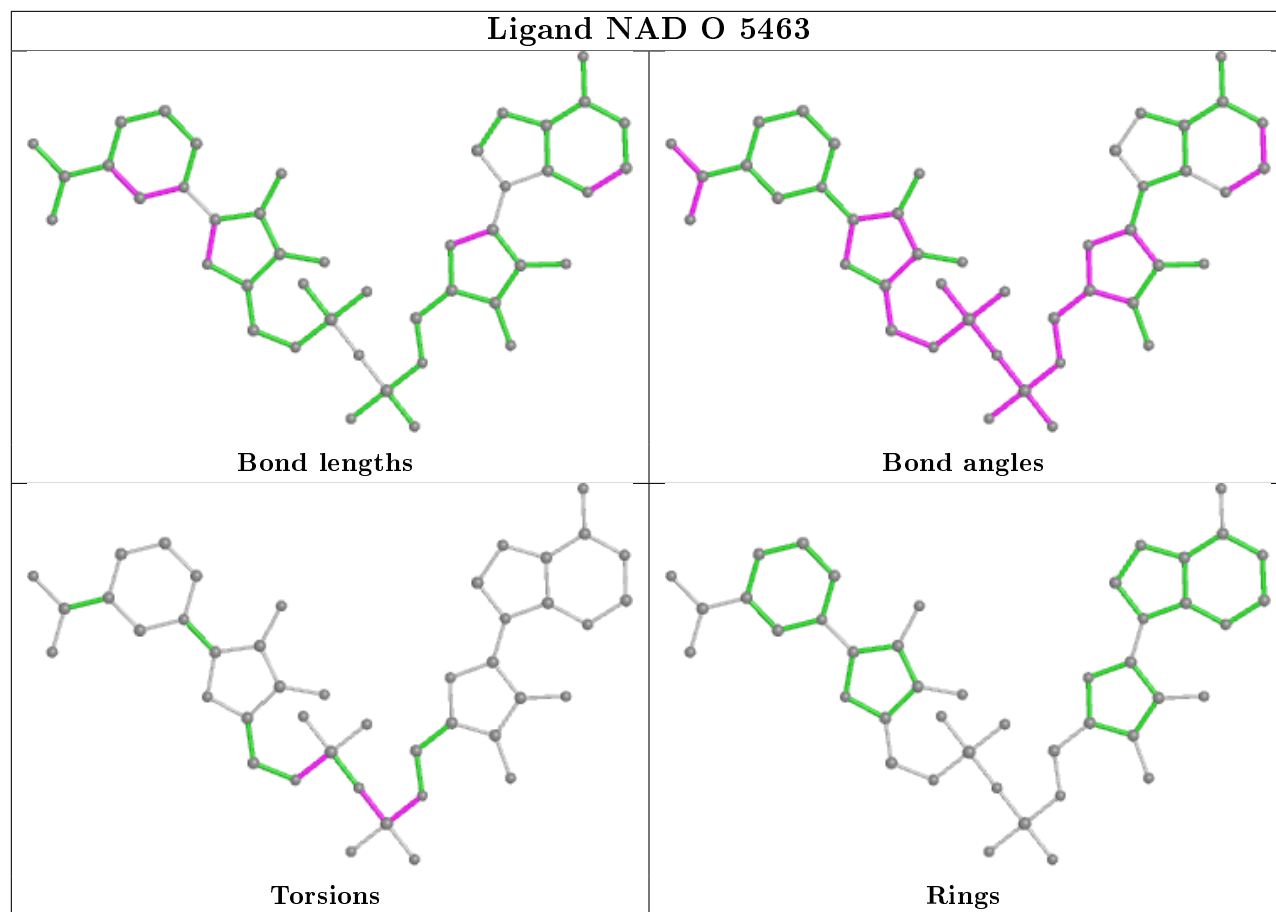
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5465	NAD	6	0
2	A	5466	NAD	9	0
2	O	5463	NAD	21	0

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	336/337 (99%)	0.13	10 (2%) 50 57	0, 0, 0, 1	2 (0%)
1	B	336/337 (99%)	0.11	9 (2%) 54 62	0, 0, 0, 1	2 (0%)
1	C	336/337 (99%)	0.12	10 (2%) 50 57	0, 0, 0, 0	2 (0%)
1	O	336/337 (99%)	0.20	19 (5%) 23 30	0, 0, 0, 1	2 (0%)
All	All	1344/1348 (99%)	0.14	48 (3%) 42 49	0, 0, 0, 1	8 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	154	CYS	13.9
1	C	154	CYS	13.5
1	B	154	CYS	12.4
1	A	154	CYS	11.5
1	O	2	GLY	6.3
1	B	2	GLY	5.4
1	A	337	GLN	5.2
1	C	82	ARG	4.5
1	O	337	GLN	4.5
1	A	37	PHE	4.2
1	A	271	LYS	4.1
1	O	38	ILE	4.0
1	A	2	GLY	3.9
1	B	57	LYS	3.7
1	C	2	GLY	3.7
1	O	82	ARG	3.4
1	O	37	PHE	3.4
1	C	37	PHE	3.2
1	B	73	GLU	3.1
1	O	83	ASN	3.0
1	O	57	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	O	73	GLU	2.8
1	O	60	ASP	2.7
1	O	67	LYS	2.7
1	O	72	GLY	2.7
1	B	69	LEU	2.7
1	A	82	ARG	2.6
1	O	85	ASP	2.6
1	O	80	GLY	2.5
1	B	62	LYS	2.5
1	B	337	GLN	2.5
1	A	83	ASN	2.4
1	O	102	GLY	2.4
1	O	36	PRO	2.3
1	B	26	GLU	2.3
1	C	60	ASP	2.3
1	A	196	LYS	2.2
1	B	82	ARG	2.2
1	C	38	ILE	2.2
1	C	95	GLU	2.2
1	O	217	LYS	2.2
1	C	86	GLU	2.1
1	C	337	GLN	2.1
1	O	58	HIS	2.1
1	A	38	ILE	2.1
1	C	57	LYS	2.1
1	O	62	LYS	2.1
1	A	72	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



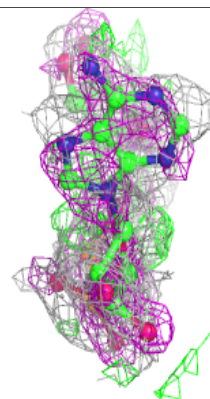
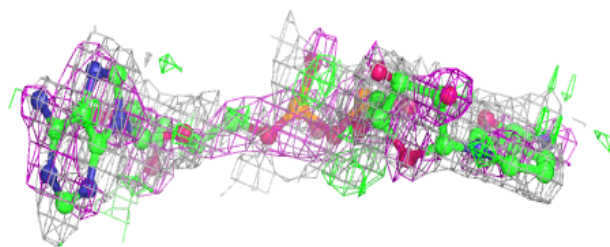
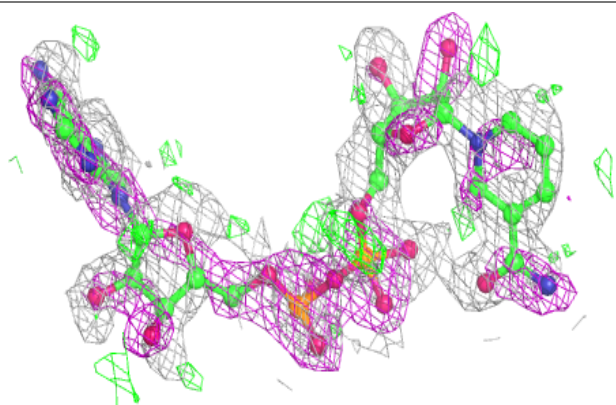
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	O	5463	44/44	0.62	0.45	0,0,0,0	0
2	NAD	A	5466	44/44	0.79	0.32	0,0,0,0	0
2	NAD	C	5467	44/44	0.84	0.26	0,0,0,0	0
2	NAD	B	5465	44/44	0.85	0.18	0,0,0,0	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.

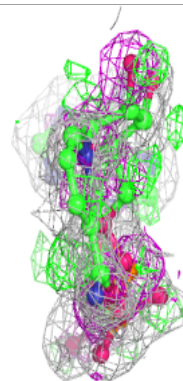
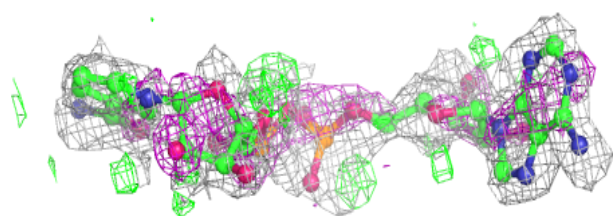
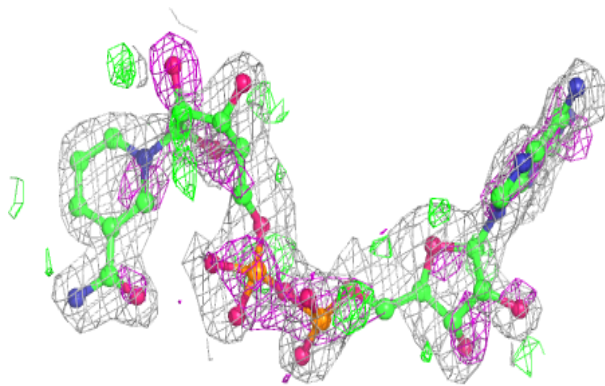
**Electron density around NAD O 5463:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

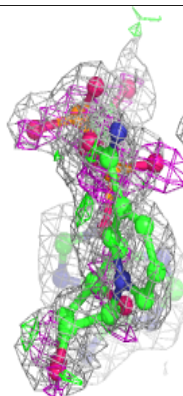
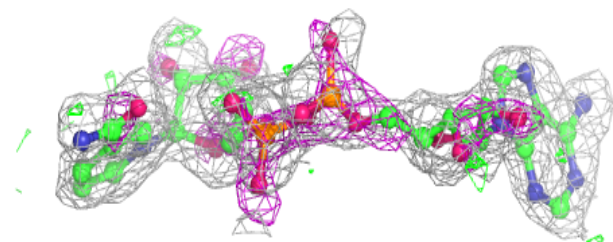
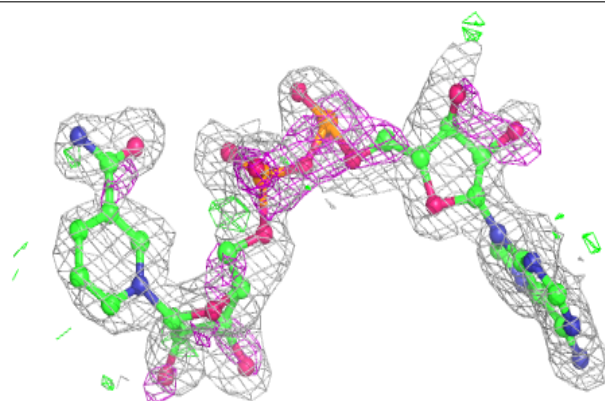


**Electron density around NAD A 5466:**

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

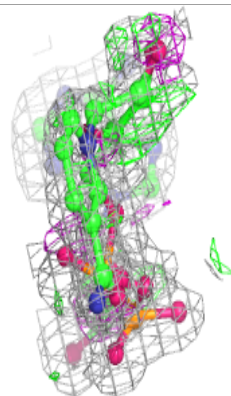
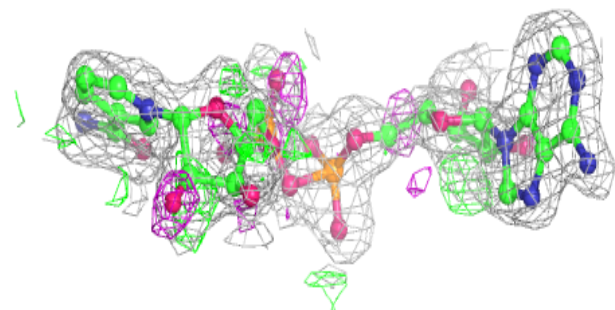
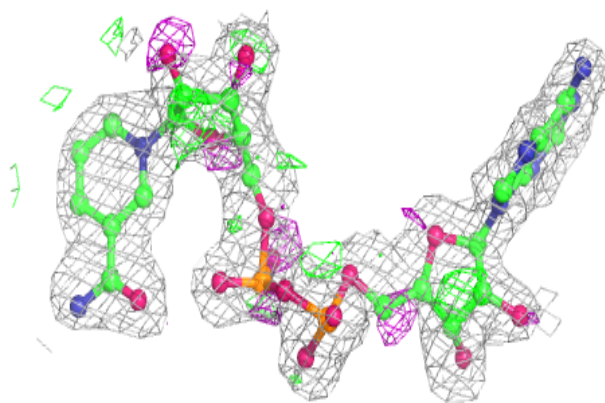
**Electron density around NAD C 5467:**

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



**Electron density around NAD B 5465:**

$2mF_o-DF_c$  (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.