Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2023 – 04:23 AM EDT

PDB ID	:	2PD4
Title	:	Crystal Structure of the Helicobacter pylori Enoyl-Acyl Carrier Protein Reductase in Complex with Hydroxydiphenyl Ether Compounds, Triclosan and Diclosan
Authors	:	Lee, H.H.; Moon, J.H.; Suh, S.W.
Deposited on	:	2007-03-31
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

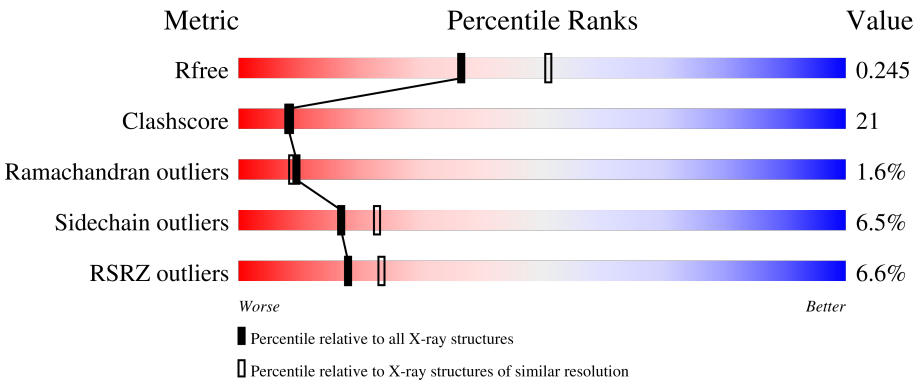
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	275	7% 66% 29% 5%
1	B	275	5% 65% 30% • •
1	C	275	6% 67% 28% •
1	D	275	7% 65% 29% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	D	4780	X	-	-	-

2 Entry composition (i)

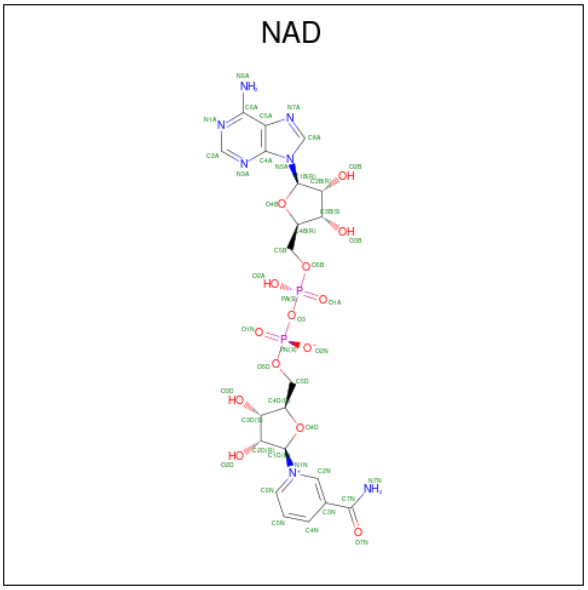
There are 4 unique types of molecules in this entry. The entry contains 8866 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	2102	1341	354	399	8	0	0	0
1	B	274	2102	1341	354	399	8	0	0	0
1	C	274	2102	1341	354	399	8	0	0	0
1	D	274	2102	1341	354	399	8	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
			Total	C	N	O	P		
2	A	1	44	21	7	14	2	0	0
2	B	1	44	21	7	14	2	0	0

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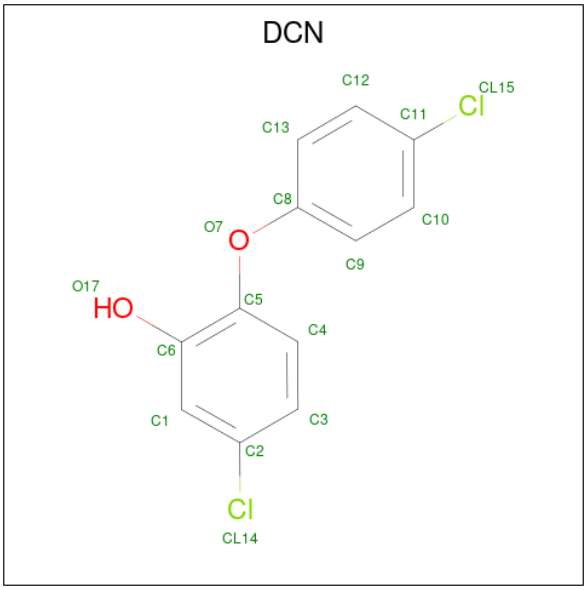
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
2	D	1	44	21	7	14	2	0	0

- Molecule 3 is DICLOSAN (three-letter code: DCN) (formula: $C_{12}H_8Cl_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Cl	O		
3	A	1	16	12	2	2	0	0
			Total	C	Cl	O		
3	B	1	16	12	2	2	0	0
			Total	C	Cl	O		
3	C	1	16	12	2	2	0	0
			Total	C	Cl	O		
3	D	1	16	12	2	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	54	54	54	0	0
			Total	O		
4	B	61	61	61	0	0
			Total	O		
4	C	60	60	60	0	0

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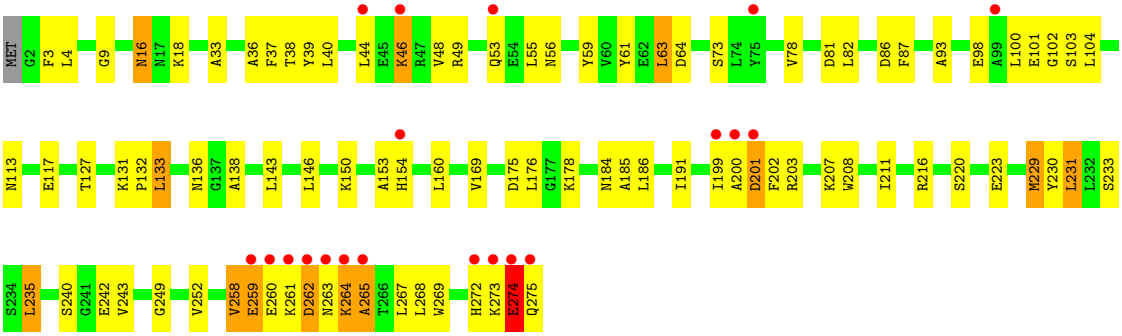
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	43	43	43	0	0

3 Residue-property plots (i)

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

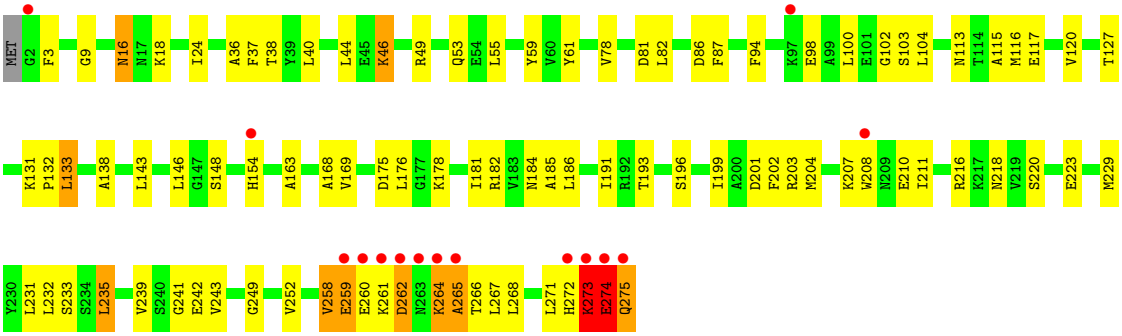
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain A: 7% 66% 29% 5%



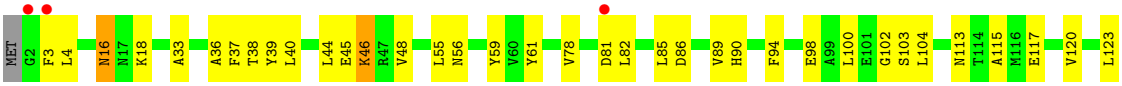
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

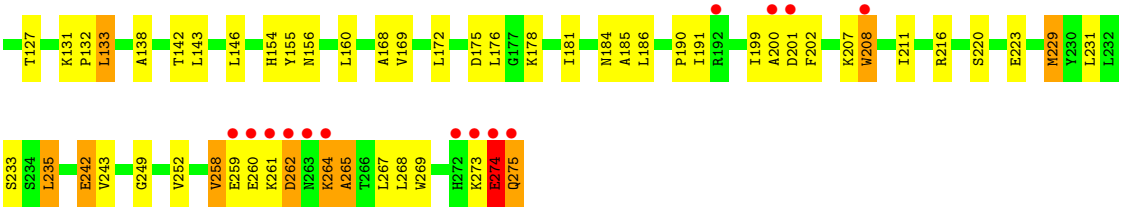
Chain B: 5% 65% 30%



• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

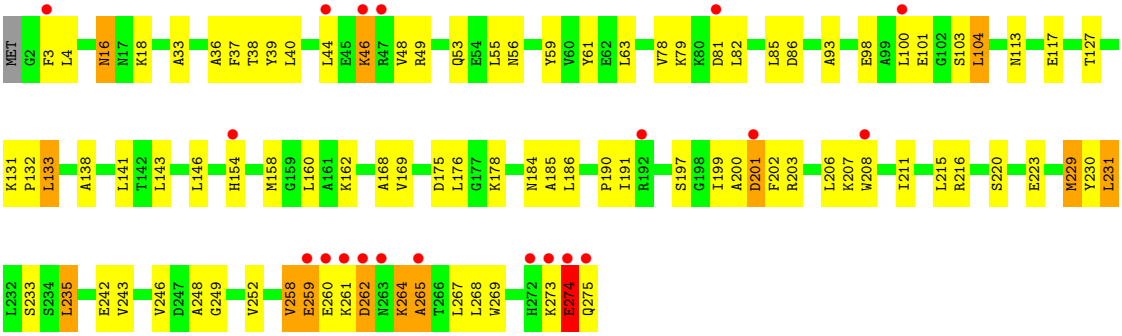
Chain C: 6% 67% 28%





- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.25Å 95.07Å 75.02Å 90.00° 106.53° 90.00°	Depositor
Resolution (Å)	28.95 – 2.30 29.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.7 (28.95-2.30) 89.8 (29.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.36 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.248 0.221 , 0.245	Depositor DCC
R_{free} test set	3908 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8866	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8951e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: DCN, 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	0.35	0/2140	0.60	0/2890
1	B	0.51	3/2140 (0.1%)	0.67	2/2890 (0.1%)
1	C	0.36	0/2140	0.60	0/2890
1	D	0.36	0/2140	0.60	0/2890
All	All	0.40	3/8560 (0.0%)	0.62	2/11560 (0.0%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	274	GLU	CB-CG	-14.18	1.25	1.52
1	B	274	GLU	C-N	-7.83	1.16	1.34
1	B	273	LYS	C-N	5.52	1.46	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	274	GLU	CA-CB-CG	10.72	136.98	113.40
1	B	273	LYS	C-N-CA	6.30	137.44	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	273	LYS	Peptide

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	2102	0	2125	102	0
1	B	2102	0	2124	101	0
1	C	2102	0	2125	106	0
1	D	2102	0	2125	101	0
2	A	44	0	26	5	0
2	B	44	0	26	1	0
2	C	44	0	26	3	0
2	D	44	0	26	3	0
3	A	16	0	7	5	0
3	B	16	0	7	4	0
3	C	16	0	7	4	0
3	D	16	0	7	5	0
4	A	54	0	0	6	0
4	B	61	0	0	6	0
4	C	60	0	0	10	0
4	D	43	0	0	4	0
All	All	8866	0	8631	367	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 21.

All (367) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ARG:HH22	1:C:260:GLU:HB2	1.18	1.07
1:A:216:ARG:HH22	1:A:260:GLU:HB2	1.20	1.01
1:D:216:ARG:HH22	1:D:260:GLU:HB2	1.26	1.01
1:B:216:ARG:HH22	1:B:260:GLU:HB2	1.26	0.99
1:A:100:LEU:HD21	3:A:2414:DCN:H12	1.59	0.84
1:B:211:ILE:HD11	1:B:273:LYS:HB2	1.59	0.84
1:A:261:LYS:HB2	4:A:2425:HOH:O	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:LYS:O	1:C:274:GLU:HB2	1.76	0.82
1:A:16:ASN:ND2	1:A:18:LYS:H	1.78	0.82
1:C:100:LEU:HD21	3:C:4414:DCN:H12	1.61	0.81
1:D:100:LEU:HD21	3:D:5414:DCN:H12	1.63	0.81
1:B:16:ASN:ND2	1:B:18:LYS:H	1.81	0.79
1:D:274:GLU:O	1:D:275:GLN:HG3	1.84	0.78
1:B:184:ASN:HD22	1:B:242:GLU:H	1.31	0.78
1:B:207:LYS:HB3	1:B:273:LYS:HD3	1.65	0.77
1:D:184:ASN:HD22	1:D:242:GLU:H	1.32	0.77
1:C:40:LEU:HB3	1:C:44:LEU:CD1	2.14	0.77
1:A:184:ASN:HD22	1:A:242:GLU:H	1.30	0.77
1:C:216:ARG:NH2	1:C:260:GLU:HB2	1.99	0.77
1:B:100:LEU:HD21	3:B:3414:DCN:H12	1.64	0.76
1:C:169:VAL:HA	4:C:4449:HOH:O	1.84	0.76
1:D:16:ASN:ND2	1:D:18:LYS:H	1.84	0.76
1:B:259:GLU:HB3	4:B:3454:HOH:O	1.86	0.76
1:A:40:LEU:HB3	1:A:44:LEU:CD1	2.16	0.75
1:B:40:LEU:HB3	1:B:44:LEU:CD1	2.16	0.75
1:C:184:ASN:HD22	1:C:242:GLU:H	1.35	0.74
1:A:273:LYS:O	1:A:274:GLU:HB2	1.84	0.74
1:B:16:ASN:C	1:B:16:ASN:HD22	1.90	0.74
1:D:273:LYS:O	1:D:274:GLU:HB2	1.86	0.74
1:D:16:ASN:C	1:D:16:ASN:HD22	1.91	0.74
1:B:184:ASN:ND2	1:B:242:GLU:H	1.86	0.73
1:D:40:LEU:HB3	1:D:44:LEU:CD1	2.19	0.72
1:B:24:ILE:HD12	4:B:3475:HOH:O	1.88	0.72
1:A:216:ARG:NH2	1:A:260:GLU:HB2	2.02	0.71
1:B:211:ILE:CD1	1:B:273:LYS:HB2	2.19	0.71
1:A:16:ASN:C	1:A:16:ASN:HD22	1.95	0.71
1:C:16:ASN:ND2	1:C:18:LYS:H	1.89	0.70
1:A:211:ILE:HD11	1:A:273:LYS:HB2	1.71	0.70
1:C:172:LEU:HD12	4:C:4449:HOH:O	1.91	0.70
1:C:16:ASN:C	1:C:16:ASN:HD22	1.95	0.69
1:D:207:LYS:HB3	1:D:273:LYS:HD3	1.74	0.68
1:D:216:ARG:NH2	1:D:260:GLU:HB2	2.05	0.68
1:D:38:THR:HA	1:D:61:TYR:O	1.93	0.68
1:A:3:PHE:CE1	1:C:3:PHE:HE1	2.13	0.67
1:B:3:PHE:HE1	1:D:3:PHE:HE1	1.42	0.67
1:D:113:ASN:O	1:D:117:GLU:HG3	1.93	0.66
1:B:3:PHE:CE1	1:D:3:PHE:HE1	2.13	0.66
1:A:3:PHE:HE1	1:C:3:PHE:HE1	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:PHE:HE1	1:D:3:PHE:CE1	2.14	0.66
1:C:46:LYS:O	1:C:46:LYS:HD3	1.97	0.65
1:A:131:LYS:HB3	1:A:132:PRO:HD3	1.79	0.64
1:D:184:ASN:ND2	1:D:242:GLU:H	1.94	0.64
1:B:38:THR:HA	1:B:61:TYR:O	1.98	0.64
1:D:197:SER:HA	4:D:5444:HOH:O	1.96	0.64
1:A:3:PHE:HE1	1:C:3:PHE:CE1	2.16	0.64
1:D:78:VAL:CG2	1:D:133:LEU:HD23	2.28	0.64
1:A:211:ILE:CD1	1:A:273:LYS:HB2	2.27	0.64
1:B:78:VAL:HG23	1:B:133:LEU:HD23	1.79	0.64
1:D:78:VAL:HG23	1:D:133:LEU:HD23	1.79	0.64
1:B:127:THR:HG21	1:B:176:LEU:HD11	1.79	0.63
1:C:127:THR:HG21	1:C:176:LEU:HD11	1.79	0.63
1:D:127:THR:HG21	1:D:176:LEU:HD11	1.81	0.63
1:C:207:LYS:HB3	1:C:273:LYS:HD3	1.80	0.63
1:A:184:ASN:ND2	1:A:242:GLU:H	1.97	0.63
1:B:46:LYS:O	1:B:46:LYS:HD3	1.97	0.63
1:C:211:ILE:HD11	1:C:273:LYS:HB2	1.80	0.63
1:A:269:TRP:O	1:A:274:GLU:HB3	1.99	0.62
1:B:249:GLY:O	1:B:252:VAL:HG22	1.99	0.62
1:A:38:THR:HA	1:A:61:TYR:O	1.99	0.62
1:C:261:LYS:N	1:C:261:LYS:HD2	2.14	0.62
1:A:258:VAL:HA	1:A:268:LEU:HD13	1.82	0.62
1:A:261:LYS:N	1:A:261:LYS:HD2	2.14	0.62
1:A:249:GLY:O	1:A:252:VAL:HG22	1.99	0.62
1:A:143:LEU:HD13	1:A:186:LEU:HB3	1.81	0.62
1:B:216:ARG:NH2	1:B:260:GLU:HB2	2.07	0.61
1:B:82:LEU:HD13	4:B:3446:HOH:O	1.99	0.61
1:C:78:VAL:HG23	1:C:133:LEU:HD23	1.82	0.61
1:A:127:THR:HG21	1:A:176:LEU:HD11	1.80	0.61
1:A:100:LEU:CD2	3:A:2414:DCN:H12	2.31	0.61
1:C:258:VAL:HA	1:C:268:LEU:HD13	1.81	0.61
1:C:38:THR:HA	1:C:61:TYR:O	2.01	0.61
1:C:40:LEU:HB3	1:C:44:LEU:HD12	1.82	0.61
1:A:261:LYS:CB	4:A:2425:HOH:O	2.42	0.60
1:C:184:ASN:ND2	1:C:242:GLU:H	1.98	0.60
1:A:46:LYS:O	1:A:46:LYS:HD3	2.01	0.60
1:C:143:LEU:HD22	4:C:4441:HOH:O	2.00	0.60
1:C:199:ILE:HD11	3:C:4414:DCN:H13	1.83	0.60
1:A:78:VAL:HG23	1:A:133:LEU:HD23	1.82	0.60
1:A:264:LYS:HE2	1:D:201:ASP:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ILE:CD1	1:C:273:LYS:HB2	2.31	0.60
1:D:199:ILE:HD11	3:D:5414:DCN:H13	1.84	0.59
1:A:199:ILE:HD11	3:A:2414:DCN:H13	1.83	0.59
1:A:175:ASP:O	1:A:178:LYS:HE2	2.03	0.59
1:A:264:LYS:HE3	1:A:264:LYS:HA	1.83	0.59
1:C:143:LEU:HD13	1:C:186:LEU:HB3	1.83	0.59
1:B:78:VAL:CG2	1:B:133:LEU:HD23	2.31	0.59
1:A:40:LEU:HB3	1:A:44:LEU:HD13	1.84	0.59
1:B:201:ASP:HB3	1:C:264:LYS:HE2	1.84	0.59
1:A:59:TYR:CE1	1:A:81:ASP:HB3	2.38	0.59
1:A:78:VAL:CG2	1:A:133:LEU:HD23	2.32	0.58
1:C:100:LEU:CD2	3:C:4414:DCN:H12	2.31	0.58
1:B:261:LYS:HD2	1:B:261:LYS:N	2.17	0.58
1:C:89:VAL:HG12	4:C:4442:HOH:O	2.03	0.58
1:D:249:GLY:O	1:D:252:VAL:HG22	2.03	0.58
1:D:131:LYS:HB3	1:D:132:PRO:HD3	1.84	0.58
1:C:86:ASP:O	1:C:138:ALA:HA	2.02	0.58
1:B:3:PHE:CE1	1:D:3:PHE:CE1	2.92	0.58
1:D:203:ARG:O	1:D:207:LYS:HG3	2.04	0.58
1:D:264:LYS:HE3	1:D:264:LYS:HA	1.85	0.58
1:C:274:GLU:O	1:C:275:GLN:HG3	2.03	0.58
1:B:40:LEU:HB3	1:B:44:LEU:HD12	1.84	0.58
1:B:40:LEU:HB3	1:B:44:LEU:HD13	1.84	0.58
1:B:262:ASP:OD1	1:C:154:HIS:NE2	2.37	0.57
1:C:264:LYS:HA	1:C:264:LYS:HE3	1.86	0.57
1:B:154:HIS:NE2	1:C:262:ASP:OD1	2.37	0.57
1:C:103:SER:HB2	1:D:175:ASP:CG	2.24	0.57
1:D:40:LEU:HB3	1:D:44:LEU:HD13	1.84	0.57
1:B:264:LYS:HE3	1:B:264:LYS:HA	1.86	0.57
1:C:78:VAL:CG2	1:C:133:LEU:HD23	2.34	0.57
1:B:178:LYS:HD3	1:D:259:GLU:HG3	1.86	0.56
1:D:267:LEU:HD13	4:D:5422:HOH:O	2.04	0.56
1:A:261:LYS:HD2	1:A:261:LYS:H	1.70	0.56
1:B:59:TYR:CE1	1:B:81:ASP:HB3	2.40	0.56
1:B:100:LEU:CD2	3:B:3414:DCN:H12	2.34	0.56
1:D:100:LEU:CD2	3:D:5414:DCN:H12	2.34	0.56
1:D:211:ILE:HD11	1:D:273:LYS:HB2	1.87	0.56
1:A:262:ASP:OD1	1:D:154:HIS:NE2	2.39	0.56
1:C:40:LEU:HB3	1:C:44:LEU:HD13	1.87	0.56
1:B:86:ASP:O	1:B:138:ALA:HA	2.05	0.56
1:B:199:ILE:HD11	3:B:3414:DCN:H13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:LYS:O	1:D:46:LYS:HD3	2.05	0.56
1:B:207:LYS:HG2	1:B:273:LYS:HE3	1.87	0.56
1:D:258:VAL:HA	1:D:268:LEU:HD13	1.88	0.56
1:A:40:LEU:HB3	1:A:44:LEU:HD12	1.86	0.56
1:B:258:VAL:HA	1:B:268:LEU:HD13	1.87	0.56
1:A:274:GLU:O	1:A:275:GLN:HG3	2.06	0.56
1:D:261:LYS:HD2	1:D:261:LYS:N	2.21	0.56
1:A:4:LEU:HB3	1:A:33:ALA:HB2	1.87	0.56
1:B:169:VAL:HG21	1:B:185:ALA:HB2	1.88	0.56
1:B:274:GLU:OE1	1:C:274:GLU:OE1	2.24	0.56
1:A:98:GLU:CD	1:A:98:GLU:H	2.09	0.55
1:B:220:SER:OG	1:B:223:GLU:HG3	2.06	0.55
1:A:207:LYS:HB3	1:A:273:LYS:HD3	1.88	0.55
1:A:16:ASN:HD22	1:A:18:LYS:H	1.51	0.55
1:A:136:ASN:HB3	4:A:2462:HOH:O	2.06	0.55
1:A:261:LYS:N	4:A:2425:HOH:O	2.30	0.55
1:C:260:GLU:HB3	1:C:261:LYS:HD2	1.88	0.55
1:D:53:GLN:HB3	4:D:5447:HOH:O	2.05	0.55
1:C:160:LEU:HD11	1:D:168:ALA:HA	1.88	0.54
1:A:113:ASN:O	1:A:117:GLU:HG3	2.08	0.54
1:B:184:ASN:HD22	1:B:242:GLU:N	2.04	0.54
1:A:3:PHE:CE1	1:C:3:PHE:CE1	2.92	0.53
1:D:220:SER:OG	1:D:223:GLU:HG3	2.08	0.53
1:A:259:GLU:HG3	1:C:178:LYS:HD3	1.89	0.53
1:B:16:ASN:ND2	1:B:16:ASN:C	2.61	0.53
1:D:191:ILE:N	2:D:4780:NAD:O7N	2.38	0.53
1:B:272:HIS:O	1:B:273:LYS:C	2.47	0.53
1:C:229:MET:HE2	1:C:233:SER:HB3	1.89	0.53
1:A:36:ALA:HB2	1:A:82:LEU:HD11	1.91	0.53
1:D:16:ASN:ND2	1:D:16:ASN:C	2.61	0.53
1:B:178:LYS:HG2	1:D:216:ARG:CZ	2.39	0.52
1:B:143:LEU:HD13	1:B:186:LEU:HB3	1.90	0.52
1:C:207:LYS:HG2	1:C:273:LYS:CE	2.40	0.52
1:D:36:ALA:HB2	1:D:82:LEU:HD11	1.91	0.52
1:D:211:ILE:CD1	1:D:273:LYS:HB2	2.40	0.52
1:B:116:MET:HE3	1:B:120:VAL:HG21	1.91	0.52
1:B:207:LYS:CB	1:B:273:LYS:HD3	2.37	0.52
1:C:242:GLU:HG3	1:C:243:VAL:N	2.24	0.52
1:D:269:TRP:O	1:D:274:GLU:HB3	2.09	0.52
1:B:218:ASN:HB3	4:B:3420:HOH:O	2.09	0.52
1:D:59:TYR:CE1	1:D:81:ASP:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:LEU:HD21	1:D:246:VAL:CG2	2.40	0.52
1:A:9:GLY:HA3	1:A:87:PHE:CE1	2.45	0.51
1:A:201:ASP:HB3	1:D:264:LYS:HE2	1.91	0.51
1:B:264:LYS:HG3	1:B:264:LYS:O	2.11	0.51
1:C:207:LYS:HG2	1:C:273:LYS:HE3	1.92	0.51
1:A:229:MET:HE2	1:A:233:SER:HB3	1.93	0.51
1:B:36:ALA:HB2	1:B:82:LEU:HD11	1.93	0.51
1:A:154:HIS:NE2	1:D:262:ASP:OD1	2.43	0.51
1:B:265:ALA:HB3	1:C:201:ASP:OD2	2.10	0.51
1:D:37:PHE:HZ	1:D:55:LEU:HD12	1.75	0.51
1:C:59:TYR:CE1	1:C:81:ASP:HB3	2.46	0.51
1:C:131:LYS:HB3	1:C:132:PRO:HD3	1.93	0.51
1:C:267:LEU:HD13	4:C:4423:HOH:O	2.11	0.51
1:B:262:ASP:CG	1:C:154:HIS:HE2	2.14	0.50
1:C:269:TRP:O	1:C:274:GLU:HB3	2.10	0.50
1:D:98:GLU:CD	1:D:98:GLU:H	2.14	0.50
1:D:207:LYS:HG2	1:D:273:LYS:HE3	1.94	0.50
1:A:260:GLU:HB3	1:A:261:LYS:HD2	1.93	0.50
1:C:220:SER:OG	1:C:223:GLU:HG3	2.12	0.50
1:B:207:LYS:HG2	1:B:273:LYS:CE	2.42	0.50
1:C:113:ASN:O	1:C:117:GLU:HG3	2.11	0.50
1:C:229:MET:CE	1:C:233:SER:HB3	2.42	0.50
1:C:261:LYS:O	1:C:265:ALA:HA	2.12	0.50
1:D:40:LEU:HB3	1:D:44:LEU:HD12	1.92	0.50
1:D:143:LEU:HD13	1:D:186:LEU:HB3	1.93	0.50
1:B:16:ASN:HD22	1:B:18:LYS:H	1.54	0.49
1:A:220:SER:OG	1:A:223:GLU:HG3	2.13	0.49
1:B:37:PHE:CZ	1:B:55:LEU:HD12	2.48	0.49
1:D:37:PHE:CZ	1:D:55:LEU:HD12	2.47	0.49
1:A:40:LEU:HD13	2:A:1780:NAD:C6A	2.42	0.49
1:C:258:VAL:CA	1:C:268:LEU:HD13	2.42	0.49
1:D:86:ASP:O	1:D:138:ALA:HA	2.12	0.49
1:A:207:LYS:HG2	1:A:273:LYS:CE	2.43	0.49
1:B:260:GLU:HB3	1:B:261:LYS:HD2	1.95	0.49
1:A:191:ILE:N	2:A:1780:NAD:O7N	2.42	0.49
1:A:100:LEU:HD23	1:A:199:ILE:HG12	1.94	0.49
1:D:16:ASN:HD22	1:D:18:LYS:H	1.60	0.49
1:C:249:GLY:O	1:C:252:VAL:HG22	2.14	0.48
1:D:4:LEU:HB3	1:D:33:ALA:HB2	1.95	0.48
1:B:201:ASP:OD2	1:C:265:ALA:HB3	2.14	0.48
1:B:210:GLU:OE2	1:B:273:LYS:HE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ASN:ND2	1:C:16:ASN:C	2.65	0.48
1:B:267:LEU:HD13	4:B:3428:HOH:O	2.14	0.48
1:C:143:LEU:CD1	1:C:186:LEU:HB3	2.43	0.48
1:C:175:ASP:OD2	1:D:103:SER:HB2	2.14	0.48
1:C:4:LEU:HB3	1:C:33:ALA:HB2	1.94	0.48
1:D:258:VAL:HG12	1:D:267:LEU:HA	1.96	0.48
1:B:262:ASP:OD2	1:C:154:HIS:NE2	2.44	0.48
1:D:200:ALA:O	1:D:201:ASP:OD1	2.32	0.48
1:B:242:GLU:HG3	1:B:243:VAL:N	2.29	0.47
1:C:120:VAL:N	4:C:4473:HOH:O	2.46	0.47
1:D:39:TYR:HB3	1:D:48:VAL:HG21	1.96	0.47
1:D:175:ASP:O	1:D:178:LYS:HE2	2.14	0.47
1:D:207:LYS:HG2	1:D:273:LYS:CE	2.44	0.47
1:C:172:LEU:HD23	4:C:4426:HOH:O	2.13	0.47
1:C:261:LYS:HD2	1:C:261:LYS:H	1.78	0.47
1:B:98:GLU:H	1:B:98:GLU:CD	2.18	0.47
1:D:260:GLU:HB3	1:D:261:LYS:HD2	1.96	0.47
1:B:176:LEU:HB3	1:B:181:ILE:HB	1.96	0.47
1:B:258:VAL:CA	1:B:268:LEU:HD13	2.44	0.47
1:A:230:TYR:HD1	1:A:231:LEU:HD13	1.80	0.47
1:A:203:ARG:O	1:A:207:LYS:HG3	2.15	0.47
1:B:127:THR:CG2	1:B:176:LEU:HD11	2.45	0.47
1:B:203:ARG:O	1:B:207:LYS:HG3	2.15	0.47
1:B:264:LYS:HE2	1:C:201:ASP:HB3	1.96	0.46
1:C:98:GLU:CD	1:C:98:GLU:H	2.18	0.46
1:A:86:ASP:O	1:A:138:ALA:HA	2.15	0.46
1:B:154:HIS:HE2	1:C:262:ASP:CG	2.19	0.46
1:D:169:VAL:HG21	1:D:185:ALA:HB2	1.96	0.46
1:B:94:PHE:O	1:B:115:ALA:HA	2.15	0.46
1:B:37:PHE:HZ	1:B:55:LEU:HD12	1.79	0.46
1:B:100:LEU:HD23	1:B:199:ILE:HG12	1.97	0.46
1:A:127:THR:CG2	1:A:176:LEU:HD11	2.44	0.46
1:A:229:MET:CE	1:A:233:SER:HB3	2.46	0.46
1:A:37:PHE:CZ	1:A:55:LEU:HD12	2.50	0.46
1:A:160:LEU:HD11	1:B:168:ALA:HA	1.98	0.46
1:A:169:VAL:HG21	1:A:185:ALA:HB2	1.98	0.46
1:A:202:PHE:CE2	3:A:2414:DCN:H3	2.51	0.46
1:C:36:ALA:HB2	1:C:82:LEU:HD11	1.96	0.46
1:A:37:PHE:HZ	1:A:55:LEU:HD12	1.80	0.46
1:A:49:ARG:HG2	1:A:49:ARG:HH11	1.81	0.46
1:A:103:SER:HB2	1:B:175:ASP:CG	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:THR:H	1:B:196:SER:HG	1.63	0.45
1:B:204:MET:SD	1:C:267:LEU:HD11	2.56	0.45
1:A:258:VAL:CA	1:A:268:LEU:HD13	2.44	0.45
1:D:184:ASN:HD22	1:D:242:GLU:N	2.09	0.45
1:A:260:GLU:HG3	1:A:261:LYS:NZ	2.32	0.45
1:C:175:ASP:CG	1:D:103:SER:HB2	2.37	0.45
1:A:230:TYR:CD1	1:A:231:LEU:HD13	2.51	0.45
1:C:16:ASN:HD22	1:C:18:LYS:H	1.65	0.45
1:B:131:LYS:HB3	1:B:132:PRO:HD3	1.99	0.45
4:C:4426:HOH:O	1:D:104:LEU:CB	2.65	0.45
1:D:275:GLN:HE21	1:D:275:GLN:HB2	1.62	0.45
1:C:233:SER:OG	1:C:235:LEU:HB2	2.17	0.45
1:D:93:ALA:O	3:D:5414:DCN:H10	2.17	0.45
1:A:39:TYR:HB3	1:A:48:VAL:HG21	1.98	0.44
1:A:272:HIS:O	1:A:273:LYS:C	2.56	0.44
1:B:233:SER:OG	1:B:235:LEU:HB2	2.18	0.44
1:C:102:GLY:N	1:C:154:HIS:HD2	2.15	0.44
1:C:176:LEU:HB3	1:C:181:ILE:HB	1.99	0.44
1:D:258:VAL:CA	1:D:268:LEU:HD13	2.46	0.44
1:C:175:ASP:O	1:C:178:LYS:HE2	2.17	0.44
1:A:175:ASP:CG	1:B:103:SER:HB2	2.38	0.44
1:B:202:PHE:CE2	3:B:3414:DCN:H3	2.52	0.44
2:A:1780:NAD:H2N	2:A:1780:NAD:O2N	2.17	0.44
1:C:169:VAL:HG21	1:C:185:ALA:HB2	1.99	0.44
1:A:49:ARG:O	1:A:53:GLN:HG3	2.17	0.44
1:A:184:ASN:HD21	1:A:240:SER:HA	1.81	0.44
1:C:168:ALA:HA	1:D:160:LEU:HD11	2.00	0.44
1:A:261:LYS:CA	4:A:2425:HOH:O	2.63	0.44
1:C:184:ASN:HD22	1:C:242:GLU:N	2.11	0.43
1:A:260:GLU:HG3	1:A:261:LYS:HZ2	1.84	0.43
1:B:261:LYS:O	1:B:265:ALA:HA	2.18	0.43
1:C:59:TYR:CD1	1:C:81:ASP:HB3	2.53	0.43
1:D:49:ARG:O	1:D:53:GLN:HG3	2.18	0.43
1:A:16:ASN:ND2	1:A:16:ASN:C	2.66	0.43
1:B:113:ASN:O	1:B:117:GLU:HG3	2.19	0.43
1:C:190:PRO:HA	2:C:3780:NAD:O7N	2.18	0.43
1:D:261:LYS:O	1:D:265:ALA:HA	2.19	0.43
1:A:59:TYR:CD1	1:A:81:ASP:HB3	2.53	0.43
1:D:59:TYR:CD1	1:D:81:ASP:HB3	2.54	0.43
1:A:93:ALA:O	3:A:2414:DCN:H10	2.18	0.43
1:B:102:GLY:N	1:B:154:HIS:HD2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ASP:CG	1:C:154:HIS:NE2	2.72	0.43
1:B:266:THR:HG23	4:B:3428:HOH:O	2.17	0.43
1:A:262:ASP:CG	1:D:154:HIS:HE2	2.22	0.43
1:D:16:ASN:ND2	4:D:5419:HOH:O	2.51	0.43
1:B:59:TYR:CD1	1:B:81:ASP:HB3	2.54	0.43
1:C:39:TYR:CD2	1:C:45:GLU:HB2	2.54	0.43
1:C:127:THR:CG2	1:C:176:LEU:HD11	2.48	0.43
1:C:260:GLU:HG3	1:C:261:LYS:NZ	2.34	0.43
1:A:64:ASP:HA	2:A:1780:NAD:N1A	2.34	0.43
1:A:264:LYS:HE3	1:A:264:LYS:CA	2.48	0.43
1:B:241:GLY:HA3	1:D:252:VAL:HG11	2.00	0.42
1:C:155:TYR:O	1:C:156:ASN:C	2.58	0.42
1:C:191:ILE:N	2:C:3780:NAD:O7N	2.50	0.42
1:C:264:LYS:O	1:C:264:LYS:HG3	2.19	0.42
1:A:3:PHE:CE1	1:A:235:LEU:HD21	2.54	0.42
1:B:9:GLY:HA2	1:B:87:PHE:O	2.20	0.42
1:C:39:TYR:HB3	1:C:48:VAL:HG21	2.00	0.42
1:D:264:LYS:HE3	1:D:264:LYS:CA	2.49	0.42
1:A:269:TRP:NE1	1:D:267:LEU:HD22	2.35	0.42
1:A:259:GLU:HA	1:A:259:GLU:OE2	2.20	0.42
1:C:202:PHE:CE2	3:C:4414:DCN:H3	2.55	0.42
1:D:233:SER:OG	1:D:235:LEU:HB2	2.19	0.42
1:B:182:ARG:HD2	1:B:239:VAL:O	2.19	0.42
1:C:274:GLU:O	1:C:275:GLN:CG	2.68	0.42
1:D:261:LYS:HD2	1:D:261:LYS:H	1.84	0.42
1:A:102:GLY:N	1:A:154:HIS:HD2	2.18	0.42
1:D:215:LEU:HD12	1:D:248:ALA:HA	2.00	0.42
1:D:141:LEU:HD11	1:D:186:LEU:HB2	2.02	0.42
1:B:154:HIS:NE2	1:C:262:ASP:OD2	2.48	0.42
1:B:193:THR:N	1:B:196:SER:HG	2.18	0.42
1:C:37:PHE:CZ	1:C:55:LEU:HD12	2.54	0.42
1:C:200:ALA:O	1:C:201:ASP:OD1	2.38	0.42
1:B:148:SER:HB2	1:B:163:ALA:HA	2.02	0.42
1:D:79:LYS:HB2	1:D:133:LEU:HD21	2.02	0.42
1:D:158:MET:O	1:D:162:LYS:HG2	2.19	0.42
1:B:154:HIS:NE2	1:C:262:ASP:CG	2.74	0.41
1:B:261:LYS:HD2	1:B:261:LYS:H	1.81	0.41
1:D:190:PRO:HA	2:D:4780:NAD:O7N	2.20	0.41
1:A:98:GLU:O	1:A:101:GLU:HG2	2.20	0.41
1:A:242:GLU:HG3	1:A:243:VAL:N	2.36	0.41
1:A:258:VAL:HG12	1:A:267:LEU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:GLU:O	1:D:101:GLU:HG2	2.21	0.41
1:D:230:TYR:CD1	1:D:231:LEU:HD13	2.55	0.41
1:A:73:SER:HB2	4:A:2448:HOH:O	2.20	0.41
1:B:49:ARG:O	1:B:53:GLN:HG3	2.20	0.41
1:B:216:ARG:NH2	1:B:268:LEU:HD21	2.36	0.41
4:C:4426:HOH:O	1:D:104:LEU:HB3	2.20	0.41
1:D:40:LEU:HD13	2:D:4780:NAD:C6A	2.50	0.41
1:D:229:MET:CE	1:D:233:SER:HB3	2.51	0.41
1:B:271:LEU:O	1:B:275:GLN:OE1	2.38	0.41
1:D:186:LEU:HD21	1:D:246:VAL:HG21	2.02	0.41
1:A:9:GLY:HA2	1:A:87:PHE:O	2.21	0.41
1:C:211:ILE:HD11	1:C:273:LYS:HD2	2.02	0.41
1:A:200:ALA:O	1:A:201:ASP:OD1	2.39	0.41
1:A:262:ASP:O	1:A:263:ASN:C	2.58	0.41
1:B:87:PHE:HB2	1:B:232:LEU:HD22	2.02	0.41
1:C:40:LEU:HD13	2:C:3780:NAD:C6A	2.50	0.41
1:C:94:PHE:O	1:C:115:ALA:HA	2.21	0.41
1:C:258:VAL:HG12	1:C:267:LEU:HA	2.02	0.41
1:D:202:PHE:O	1:D:206:LEU:HB2	2.20	0.41
1:D:242:GLU:HG3	1:D:243:VAL:N	2.35	0.41
1:A:154:HIS:HE2	1:D:262:ASP:CG	2.24	0.41
1:A:265:ALA:HB3	1:D:201:ASP:OD2	2.21	0.40
1:C:123:LEU:HD21	4:C:4449:HOH:O	2.21	0.40
1:A:264:LYS:O	1:A:265:ALA:HB3	2.22	0.40
1:B:267:LEU:HD21	1:C:208:TRP:CD1	2.57	0.40
1:D:202:PHE:CE2	3:D:5414:DCN:H3	2.56	0.40
1:A:150:LYS:HA	1:A:150:LYS:HD3	1.94	0.40
1:B:191:ILE:N	2:B:2780:NAD:O7N	2.52	0.40
1:C:90:HIS:O	1:C:142:THR:HA	2.21	0.40
1:A:63:LEU:O	2:A:1780:NAD:H2A	2.22	0.40
1:B:267:LEU:HD22	1:C:269:TRP:NE1	2.37	0.40
1:D:229:MET:HE2	1:D:233:SER:HB3	2.04	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	272/275 (99%)	252 (93%)	15 (6%)	5 (2%)	8 7
1	B	272/275 (99%)	254 (93%)	14 (5%)	4 (2%)	10 10
1	C	272/275 (99%)	252 (93%)	16 (6%)	4 (2%)	10 10
1	D	272/275 (99%)	253 (93%)	15 (6%)	4 (2%)	10 10
All	All	1088/1100 (99%)	1011 (93%)	60 (6%)	17 (2%)	9 9

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	GLU
1	C	274	GLU
1	D	274	GLU
1	A	259	GLU
1	B	259	GLU
1	B	274	GLU
1	C	259	GLU
1	D	259	GLU
1	B	265	ALA
1	A	265	ALA
1	C	265	ALA
1	D	265	ALA
1	A	153	ALA
1	D	258	VAL
1	A	258	VAL
1	B	258	VAL
1	C	258	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/227 (100%)	211 (93%)	15 (7%)	16	22
1	B	226/227 (100%)	214 (95%)	12 (5%)	22	31
1	C	226/227 (100%)	210 (93%)	16 (7%)	14	19
1	D	226/227 (100%)	210 (93%)	16 (7%)	14	19
All	All	904/908 (100%)	845 (94%)	59 (6%)	17	23

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	46	LYS
1	A	56	ASN
1	A	63	LEU
1	A	104	LEU
1	A	133	LEU
1	A	146	LEU
1	A	201	ASP
1	A	208	TRP
1	A	229	MET
1	A	231	LEU
1	A	235	LEU
1	A	262	ASP
1	A	264	LYS
1	A	274	GLU
1	B	16	ASN
1	B	46	LYS
1	B	104	LEU
1	B	133	LEU
1	B	146	LEU
1	B	208	TRP
1	B	229	MET
1	B	231	LEU
1	B	235	LEU
1	B	262	ASP
1	B	264	LYS
1	B	275	GLN
1	C	16	ASN
1	C	46	LYS
1	C	56	ASN
1	C	85	LEU
1	C	104	LEU
1	C	133	LEU

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Mol	Chain	Res	Type
1	C	146	LEU
1	C	208	TRP
1	C	229	MET
1	C	231	LEU
1	C	235	LEU
1	C	242	GLU
1	C	262	ASP
1	C	264	LYS
1	C	274	GLU
1	C	275	GLN
1	D	16	ASN
1	D	46	LYS
1	D	56	ASN
1	D	63	LEU
1	D	85	LEU
1	D	104	LEU
1	D	133	LEU
1	D	146	LEU
1	D	201	ASP
1	D	208	TRP
1	D	229	MET
1	D	231	LEU
1	D	235	LEU
1	D	262	ASP
1	D	264	LYS
1	D	274	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	30	ASN
1	A	53	GLN
1	A	56	ASN
1	A	76	ASN
1	A	156	ASN
1	A	184	ASN
1	A	226	ASN
1	A	275	GLN
1	B	16	ASN
1	B	30	ASN
1	B	53	GLN

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Mol	Chain	Res	Type
1	B	56	ASN
1	B	76	ASN
1	B	156	ASN
1	B	184	ASN
1	B	226	ASN
1	B	275	GLN
1	C	16	ASN
1	C	30	ASN
1	C	56	ASN
1	C	76	ASN
1	C	156	ASN
1	C	184	ASN
1	C	226	ASN
1	C	275	GLN
1	D	16	ASN
1	D	30	ASN
1	D	53	GLN
1	D	56	ASN
1	D	76	ASN
1	D	128	ASN
1	D	156	ASN
1	D	184	ASN
1	D	226	ASN
1	D	275	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	D	4780	-	42,48,48	1.76	3 (7%)	50,73,73	1.39	5 (10%)
3	DCN	C	4414	-	17,17,17	3.12	13 (76%)	23,23,23	0.96	1 (4%)
2	NAD	C	3780	-	42,48,48	1.81	4 (9%)	50,73,73	1.38	7 (14%)
3	DCN	D	5414	-	17,17,17	3.07	13 (76%)	23,23,23	0.97	1 (4%)
3	DCN	A	2414	-	17,17,17	3.06	13 (76%)	23,23,23	0.98	1 (4%)
2	NAD	B	2780	-	42,48,48	1.77	5 (11%)	50,73,73	1.33	6 (12%)
3	DCN	B	3414	-	17,17,17	3.09	14 (82%)	23,23,23	0.96	1 (4%)
2	NAD	A	1780	-	42,48,48	1.73	5 (11%)	50,73,73	1.31	4 (8%)

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	D	4780	-	1/1/11/11	13/26/62/62	0/5/5/5
3	DCN	C	4414	-	-	0/4/4/4	0/2/2/2
2	NAD	C	3780	-	-	5/26/62/62	0/5/5/5
3	DCN	D	5414	-	-	0/4/4/4	0/2/2/2
3	DCN	A	2414	-	-	0/4/4/4	0/2/2/2
2	NAD	B	2780	-	-	2/26/62/62	0/5/5/5
3	DCN	B	3414	-	-	0/4/4/4	0/2/2/2
2	NAD	A	1780	-	-	8/26/62/62	0/5/5/5

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3780	NAD	O7N-C7N	8.59	1.40	1.24
2	D	4780	NAD	O7N-C7N	8.36	1.40	1.24
2	B	2780	NAD	O7N-C7N	8.27	1.40	1.24
2	A	1780	NAD	O7N-C7N	8.13	1.39	1.24
3	D	5414	DCN	C9-C8	5.75	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3414	DCN	C9-C8	5.61	1.49	1.38
3	A	2414	DCN	C9-C8	5.55	1.49	1.38
3	C	4414	DCN	C9-C8	5.53	1.49	1.38
3	A	2414	DCN	C6-C5	5.02	1.49	1.40
3	C	4414	DCN	C10-C11	4.78	1.47	1.38
3	D	5414	DCN	C6-C5	4.68	1.48	1.40
3	B	3414	DCN	C3-C2	4.62	1.46	1.38
3	C	4414	DCN	C6-C5	4.47	1.48	1.40
3	C	4414	DCN	C3-C2	4.46	1.46	1.38
3	D	5414	DCN	C10-C11	4.42	1.46	1.38
3	D	5414	DCN	C3-C2	4.40	1.46	1.38
3	A	2414	DCN	C10-C11	4.40	1.46	1.38
3	B	3414	DCN	C10-C11	4.40	1.46	1.38
3	B	3414	DCN	C6-C5	4.29	1.48	1.40
3	A	2414	DCN	C3-C2	4.24	1.46	1.38
3	B	3414	DCN	C1-C6	3.79	1.44	1.38
2	C	3780	NAD	C2A-N3A	3.40	1.37	1.32
3	C	4414	DCN	C9-C10	3.34	1.44	1.38
3	C	4414	DCN	C1-C6	3.30	1.43	1.38
2	D	4780	NAD	C2A-N3A	3.26	1.37	1.32
3	D	5414	DCN	C13-C12	3.17	1.44	1.38
3	A	2414	DCN	C9-C10	3.08	1.44	1.38
3	D	5414	DCN	C1-C6	3.07	1.43	1.38
3	B	3414	DCN	C9-C10	3.06	1.44	1.38
2	B	2780	NAD	C2A-N3A	2.99	1.36	1.32
2	A	1780	NAD	C2A-N3A	2.95	1.36	1.32
3	D	5414	DCN	C9-C10	2.94	1.44	1.38
3	C	4414	DCN	C13-C12	2.93	1.44	1.38
3	C	4414	DCN	C12-C11	2.90	1.43	1.38
3	A	2414	DCN	C12-C11	2.86	1.43	1.38
3	A	2414	DCN	C13-C12	2.85	1.43	1.38
3	B	3414	DCN	C13-C12	2.84	1.43	1.38
3	B	3414	DCN	C12-C11	2.74	1.43	1.38
3	D	5414	DCN	C12-C11	2.72	1.43	1.38
3	A	2414	DCN	C1-C6	2.70	1.42	1.38
3	B	3414	DCN	O17-C6	-2.51	1.31	1.36
3	A	2414	DCN	C4-C5	2.47	1.44	1.39
3	A	2414	DCN	C3-C4	2.43	1.43	1.38
3	C	4414	DCN	O17-C6	-2.38	1.31	1.36
3	C	4414	DCN	C4-C5	2.37	1.44	1.39
2	C	3780	NAD	PN-O2N	-2.35	1.44	1.55
2	A	1780	NAD	PN-O2N	-2.33	1.44	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5414	DCN	O17-C6	-2.32	1.31	1.36
3	B	3414	DCN	C3-C4	2.31	1.43	1.38
3	D	5414	DCN	C4-C5	2.30	1.44	1.39
3	A	2414	DCN	O17-C6	-2.29	1.31	1.36
3	C	4414	DCN	C3-C4	2.28	1.42	1.38
2	B	2780	NAD	PN-O2N	-2.27	1.44	1.55
2	A	1780	NAD	C2B-C1B	-2.25	1.50	1.53
3	C	4414	DCN	C13-C8	2.24	1.43	1.38
3	D	5414	DCN	C3-C4	2.23	1.42	1.38
2	D	4780	NAD	PN-O2N	-2.23	1.44	1.55
3	D	5414	DCN	C13-C8	2.22	1.43	1.38
3	A	2414	DCN	C1-C2	2.20	1.41	1.38
3	B	3414	DCN	C4-C5	2.19	1.44	1.39
3	A	2414	DCN	C13-C8	2.16	1.43	1.38
3	D	5414	DCN	C1-C2	2.16	1.41	1.38
2	B	2780	NAD	C2B-C1B	-2.14	1.50	1.53
3	B	3414	DCN	C13-C8	2.13	1.42	1.38
2	B	2780	NAD	O4B-C4B	-2.13	1.40	1.45
3	C	4414	DCN	C1-C2	2.11	1.41	1.38
3	B	3414	DCN	C1-C2	2.09	1.41	1.38
2	C	3780	NAD	C2B-C1B	-2.06	1.50	1.53
3	B	3414	DCN	O7-C8	2.05	1.44	1.39
2	A	1780	NAD	PA-O1A	-2.05	1.43	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2780	NAD	N3A-C2A-N1A	-5.49	120.10	128.68
2	D	4780	NAD	N3A-C2A-N1A	-5.36	120.31	128.68
2	A	1780	NAD	N3A-C2A-N1A	-4.96	120.93	128.68
2	C	3780	NAD	N3A-C2A-N1A	-4.47	121.69	128.68
2	A	1780	NAD	C6N-N1N-C2N	-3.43	118.84	121.97
2	D	4780	NAD	C1B-N9A-C4A	-3.06	121.26	126.64
2	B	2780	NAD	C5D-C4D-C3D	-2.91	104.28	115.18
2	D	4780	NAD	PN-O3-PA	-2.72	123.50	132.83
2	C	3780	NAD	C6N-N1N-C2N	-2.71	119.50	121.97
3	B	3414	DCN	C5-O7-C8	2.68	124.67	118.00
3	C	4414	DCN	C5-O7-C8	2.66	124.64	118.00
3	D	5414	DCN	C5-O7-C8	2.66	124.64	118.00
3	A	2414	DCN	C5-O7-C8	2.65	124.61	118.00
2	C	3780	NAD	C4A-C5A-N7A	-2.65	106.64	109.40
2	C	3780	NAD	PN-O3-PA	-2.58	123.96	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4780	NAD	O4B-C4B-C5B	2.52	117.67	109.37
2	D	4780	NAD	C6N-N1N-C2N	-2.27	119.90	121.97
2	C	3780	NAD	C5D-C4D-C3D	-2.24	106.78	115.18
2	A	1780	NAD	C4A-C5A-N7A	-2.21	107.10	109.40
2	B	2780	NAD	PN-O3-PA	-2.21	125.24	132.83
2	B	2780	NAD	O2N-PN-O1N	2.19	123.06	112.24
2	B	2780	NAD	C1B-N9A-C4A	-2.17	122.83	126.64
2	C	3780	NAD	C1B-N9A-C4A	-2.14	122.88	126.64
2	C	3780	NAD	C3N-C7N-N7N	2.11	120.28	117.75
2	B	2780	NAD	O4B-C4B-C3B	2.05	109.17	105.11
2	A	1780	NAD	C1B-N9A-C4A	-2.02	123.10	126.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	4780	NAD	C4B

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1780	NAD	C5D-O5D-PN-O3
2	A	1780	NAD	O4D-C4D-C5D-O5D
2	A	1780	NAD	C3D-C4D-C5D-O5D
2	C	3780	NAD	C5D-O5D-PN-O3
2	D	4780	NAD	C5B-O5B-PA-O3
2	D	4780	NAD	O4B-C4B-C5B-O5B
2	D	4780	NAD	C5D-O5D-PN-O3
2	D	4780	NAD	C5D-O5D-PN-O1N
2	D	4780	NAD	C5D-O5D-PN-O2N
2	D	4780	NAD	O4D-C4D-C5D-O5D
2	D	4780	NAD	C3D-C4D-C5D-O5D
2	D	4780	NAD	O4D-C1D-N1N-C2N
2	C	3780	NAD	C3D-C4D-C5D-O5D
2	C	3780	NAD	O4D-C4D-C5D-O5D
2	A	1780	NAD	PN-O3-PA-O1A
2	D	4780	NAD	C3B-C4B-C5B-O5B
2	B	2780	NAD	O4B-C4B-C5B-O5B
2	D	4780	NAD	PA-O3-PN-O1N
2	A	1780	NAD	C5D-O5D-PN-O1N
2	A	1780	NAD	C5D-O5D-PN-O2N
2	D	4780	NAD	C5B-O5B-PA-O1A
2	D	4780	NAD	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	D	4780	NAD	PN-O3-PA-O2A
2	A	1780	NAD	PN-O3-PA-O2A
2	C	3780	NAD	O4B-C4B-C5B-O5B
2	A	1780	NAD	O4B-C4B-C5B-O5B
2	C	3780	NAD	C5D-O5D-PN-O1N
2	B	2780	NAD	C3D-C4D-C5D-O5D

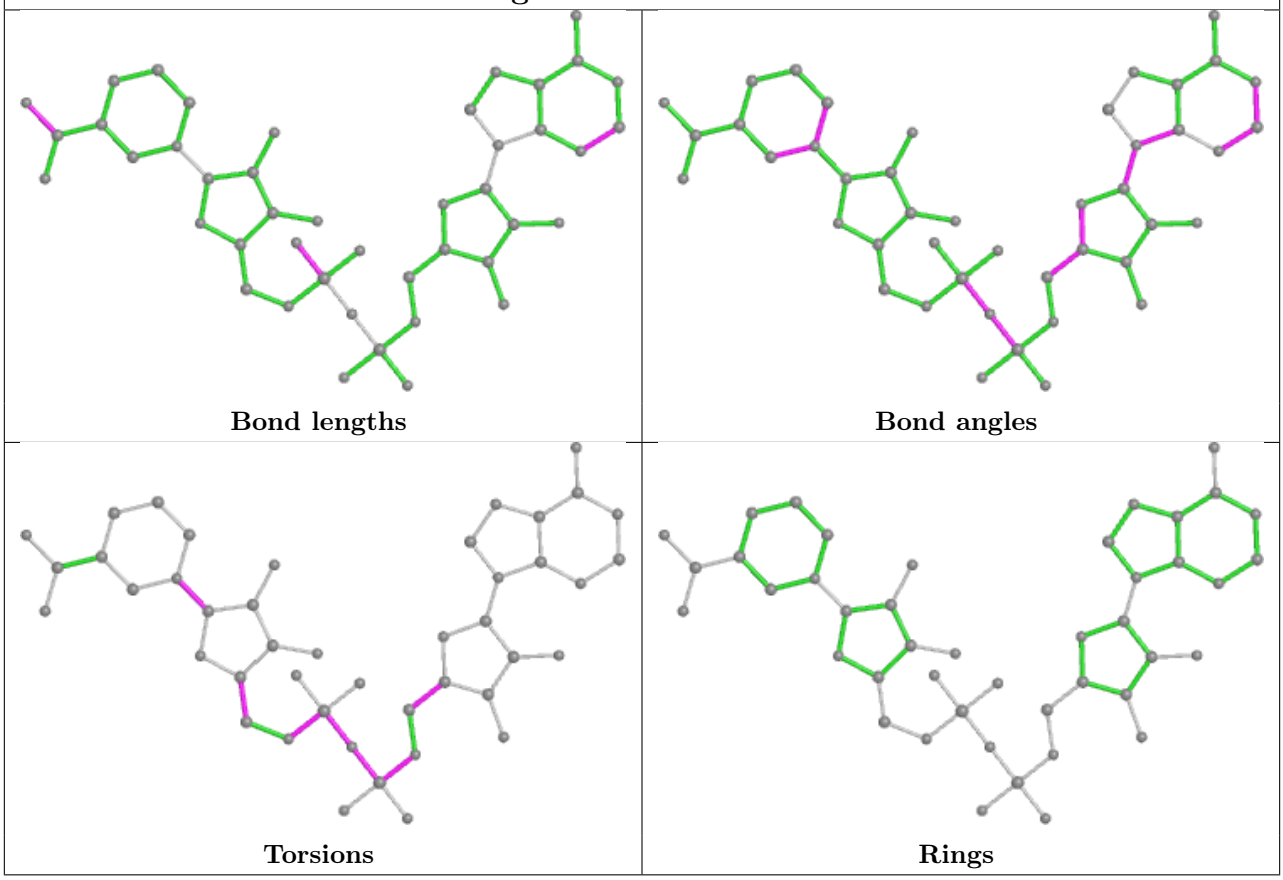
There are no ring outliers.

8 monomers are involved in 30 short contacts:

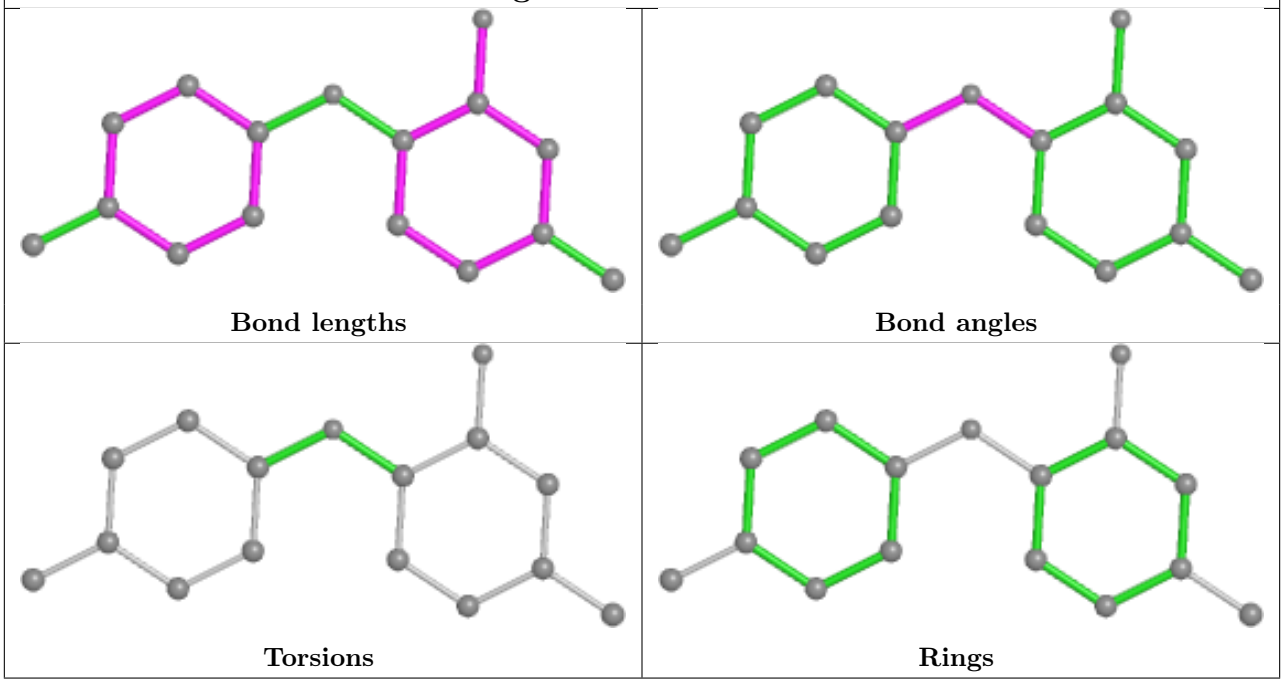
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4780	NAD	3	0
3	C	4414	DCN	4	0
2	C	3780	NAD	3	0
3	D	5414	DCN	5	0
3	A	2414	DCN	5	0
2	B	2780	NAD	1	0
3	B	3414	DCN	4	0
2	A	1780	NAD	5	0

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

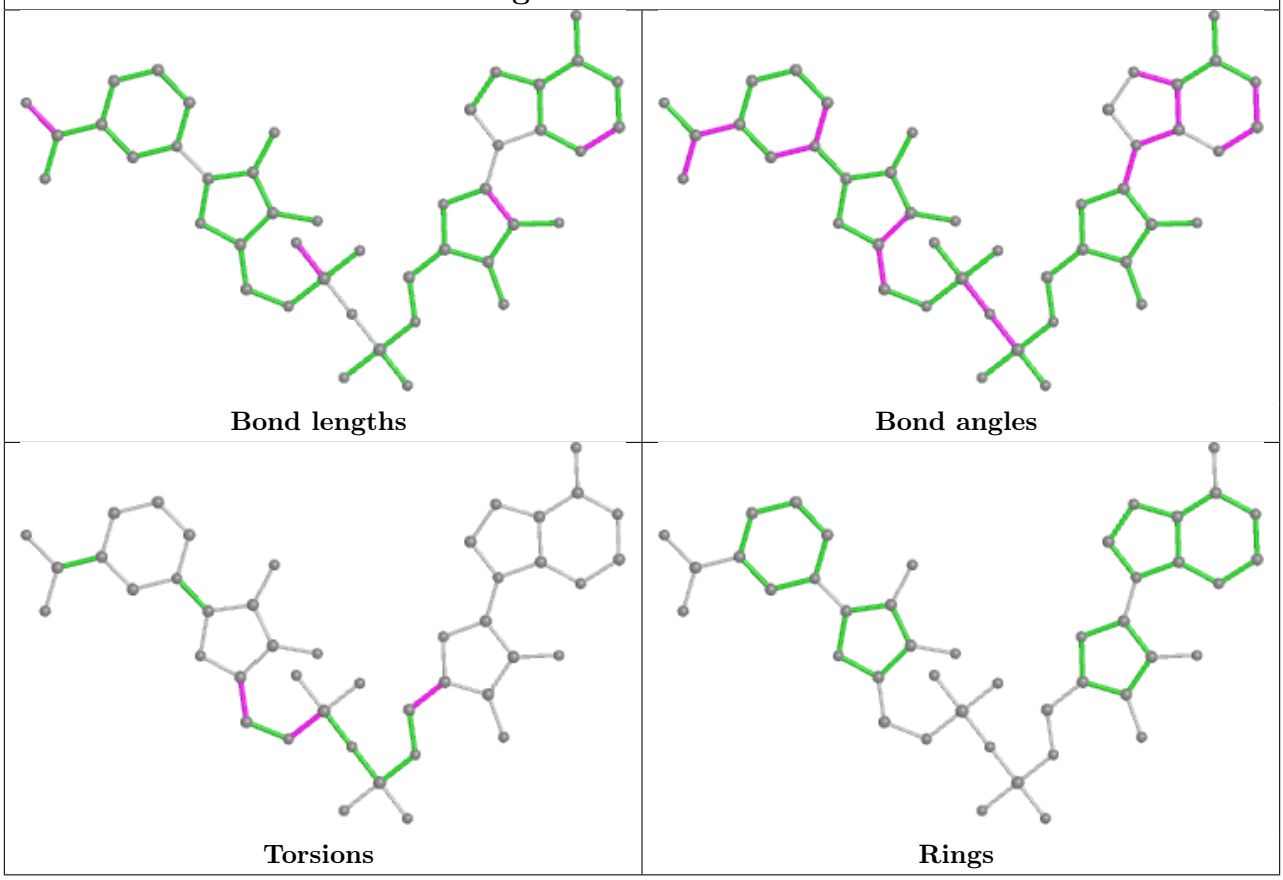
Ligand NAD D 4780



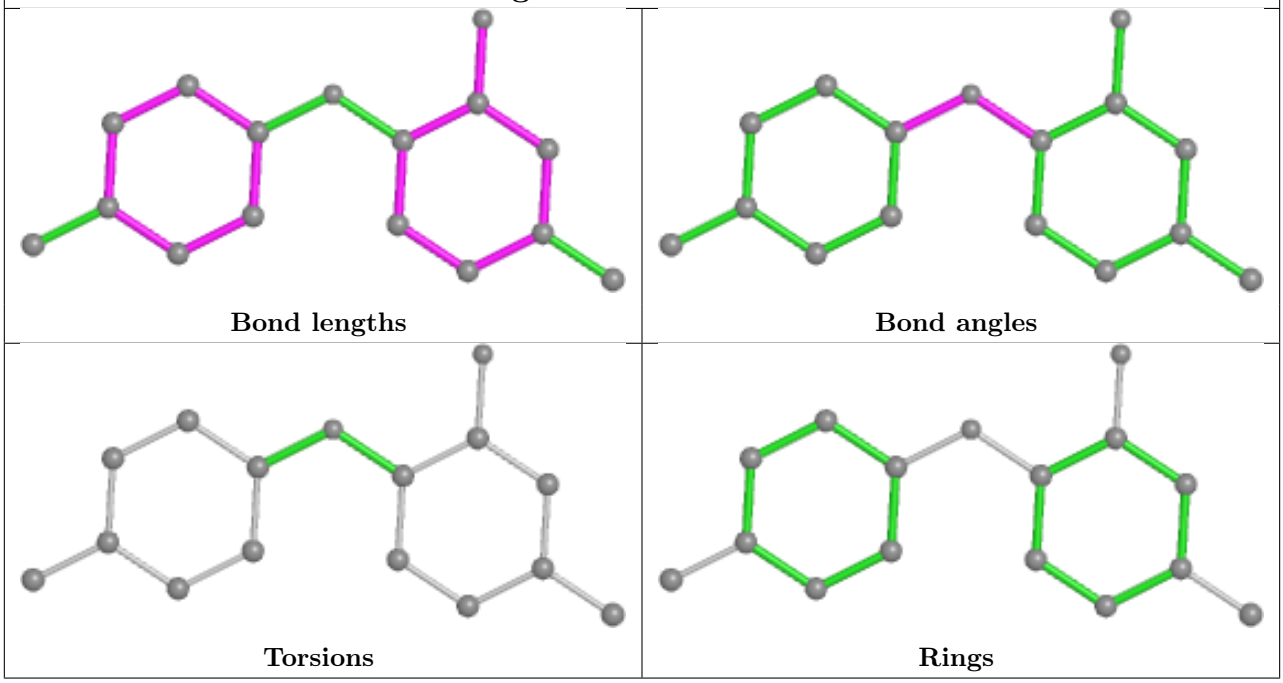
Ligand DCN C 4414



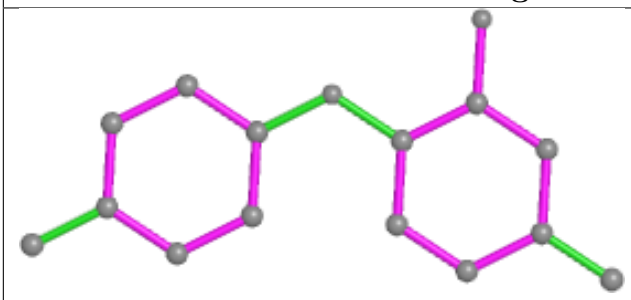
Ligand NAD C 3780



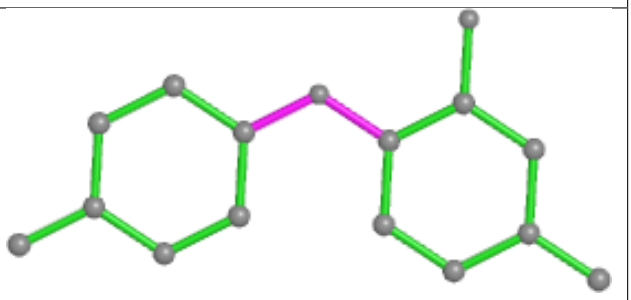
Ligand DCN D 5414



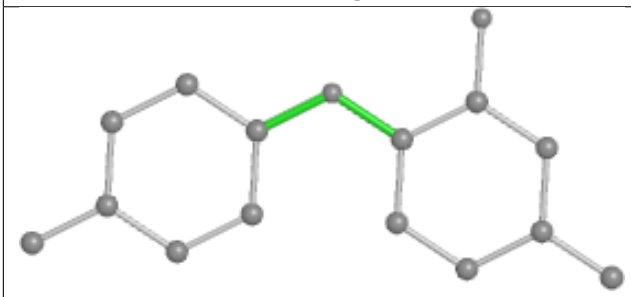
Ligand DCN A 2414



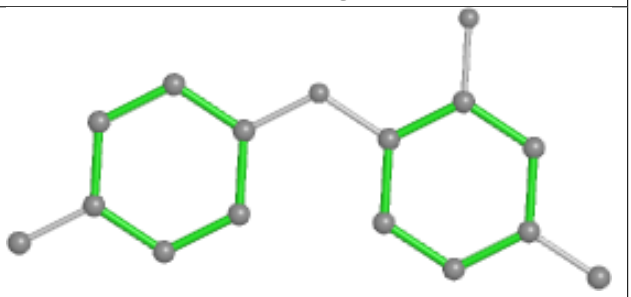
Bond lengths



Bond angles

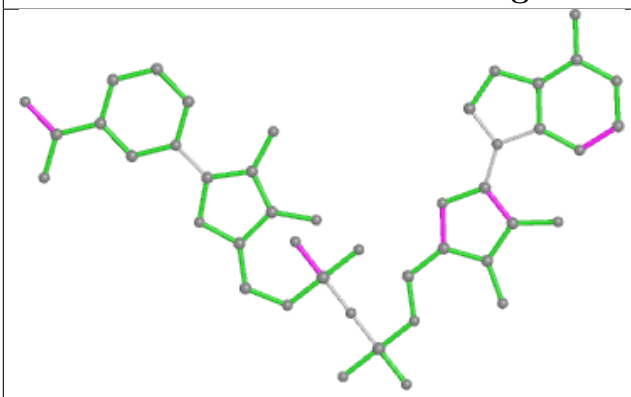


Torsions

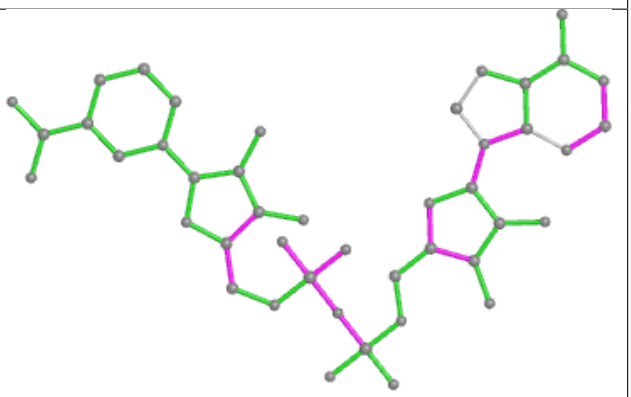


Rings

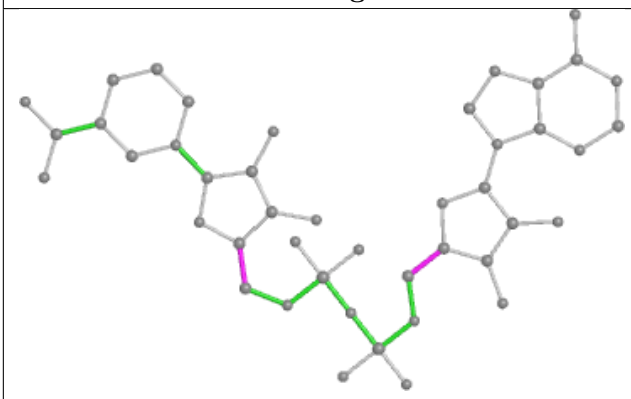
Ligand NAD B 2780



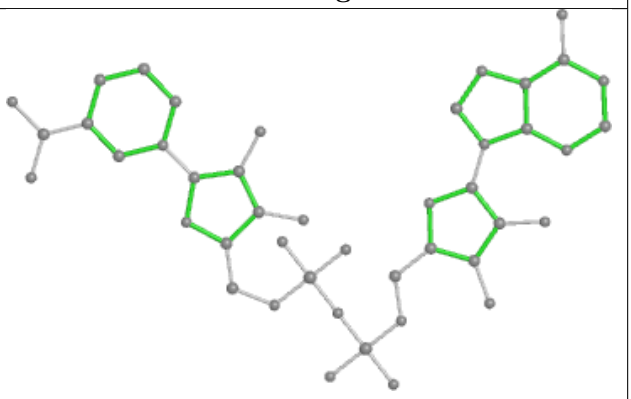
Bond lengths



Bond angles

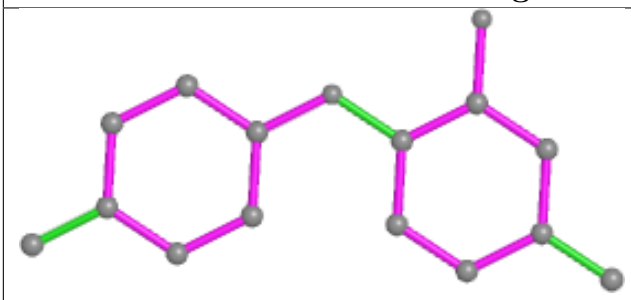


Torsions

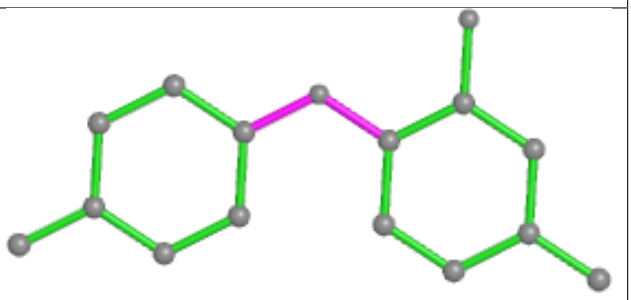


Rings

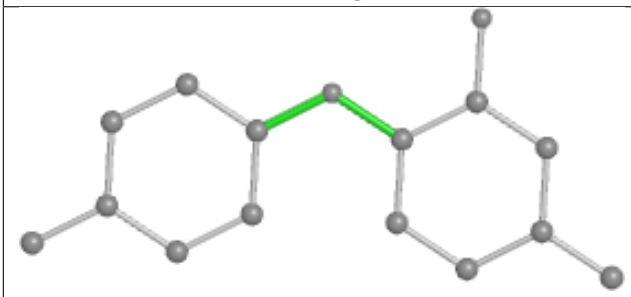
Ligand DCN B 3414



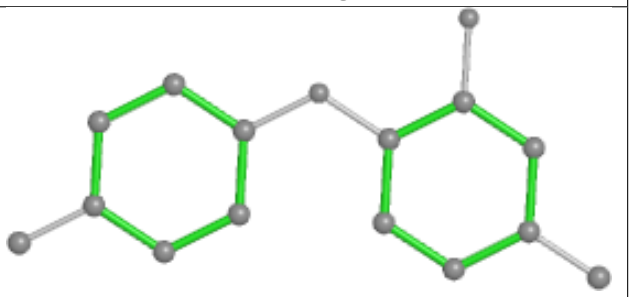
Bond lengths



Bond angles

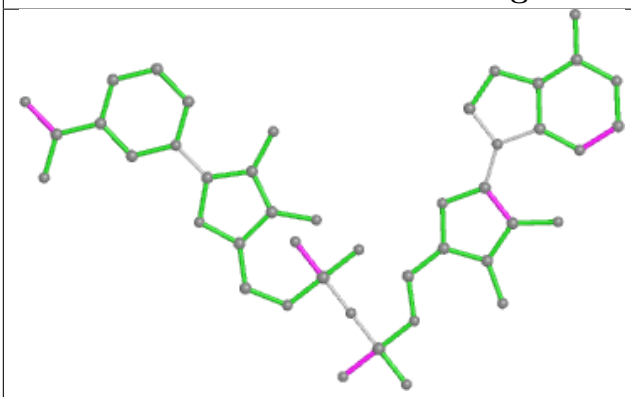


Torsions

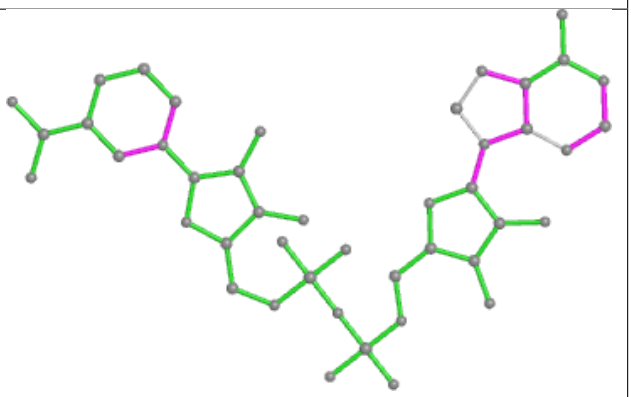


Rings

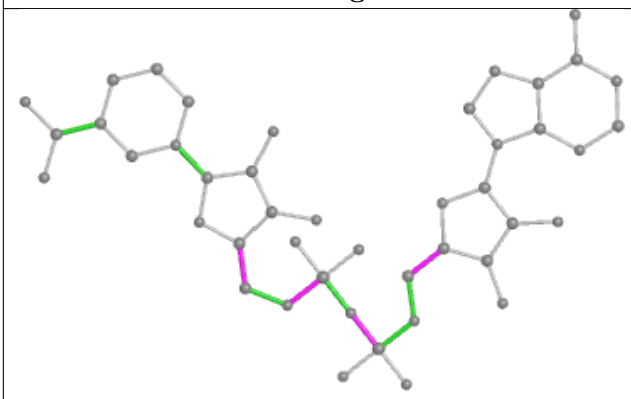
Ligand NAD A 1780



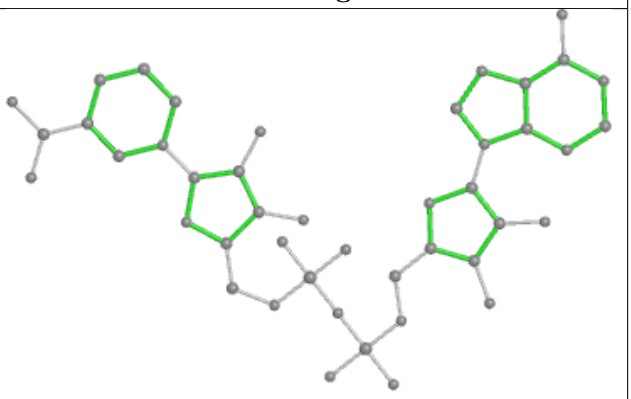
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	274:GLU	C	275:GLN	N	1.16

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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^2)	Q<0.9
1	A	274/275 (99%)	0.42	20 (7%)	15	20	16, 31, 51, 90	0
1	B	274/275 (99%)	0.30	15 (5%)	25	31	14, 28, 49, 90	0
1	C	274/275 (99%)	0.41	17 (6%)	20	26	14, 29, 51, 89	0
1	D	274/275 (99%)	0.34	20 (7%)	15	20	17, 30, 49, 89	0
All	All	1096/1100 (99%)	0.37	72 (6%)	18	23	14, 29, 51, 90	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	275	GLN	7.1
1	A	260	GLU	7.0
1	B	260	GLU	7.0
1	D	275	GLN	6.8
1	A	275	GLN	6.6
1	C	259	GLU	6.3
1	A	264	LYS	6.3
1	C	260	GLU	5.8
1	A	259	GLU	5.7
1	B	259	GLU	5.1
1	B	261	LYS	5.1
1	C	272	HIS	5.0
1	C	273	LYS	5.0
1	A	261	LYS	5.0
1	D	259	GLU	4.9
1	D	261	LYS	4.9
1	B	272	HIS	4.8
1	D	260	GLU	4.7
1	C	201	ASP	4.7
1	A	272	HIS	4.6
1	C	264	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	263	ASN	4.3
1	B	263	ASN	4.2
1	D	263	ASN	4.0
1	D	274	GLU	4.0
1	B	274	GLU	4.0
1	A	201	ASP	4.0
1	C	275	GLN	3.9
1	A	262	ASP	3.9
1	C	274	GLU	3.9
1	B	262	ASP	3.8
1	C	262	ASP	3.8
1	C	261	LYS	3.7
1	C	3	PHE	3.6
1	D	154	HIS	3.4
1	D	44	LEU	3.4
1	D	273	LYS	3.3
1	D	46	LYS	3.3
1	B	273	LYS	3.2
1	B	154	HIS	3.2
1	D	262	ASP	3.2
1	A	274	GLU	3.1
1	A	263	ASN	3.0
1	C	200	ALA	3.0
1	A	46	LYS	3.0
1	D	265	ALA	2.9
1	A	44	LEU	2.9
1	B	264	LYS	2.9
1	A	154	HIS	2.8
1	B	208	TRP	2.6
1	B	97	LYS	2.6
1	A	273	LYS	2.6
1	D	3	PHE	2.6
1	A	199	ILE	2.6
1	A	200	ALA	2.5
1	B	265	ALA	2.5
1	C	2	GLY	2.5
1	C	208	TRP	2.5
1	D	201	ASP	2.4
1	C	81	ASP	2.4
1	D	100	LEU	2.4
1	D	192	ARG	2.3
1	D	272	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	208	TRP	2.2
1	B	2	GLY	2.2
1	A	265	ALA	2.2
1	A	75	TYR	2.1
1	D	81	ASP	2.1
1	A	53	GLN	2.1
1	A	99	ALA	2.0
1	C	192	ARG	2.0
1	D	47	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

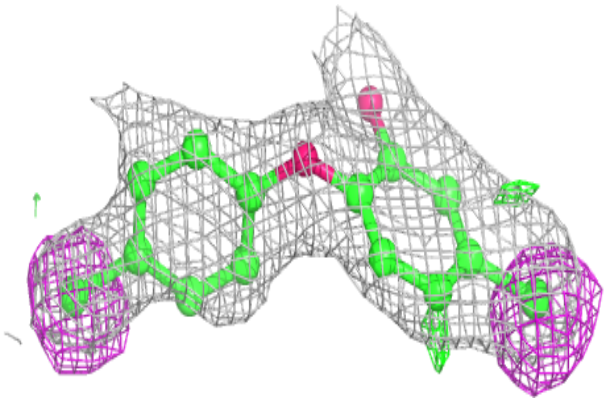
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

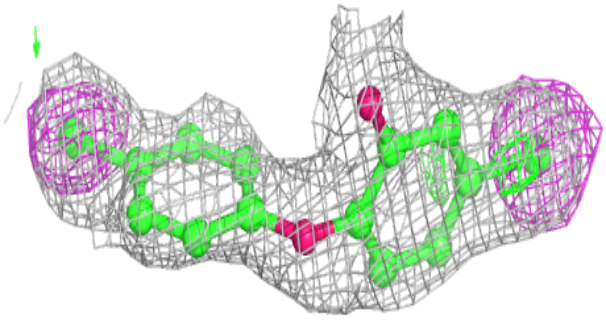
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DCN	A	2414	16/16	0.82	0.20	11,28,33,33	0
3	DCN	B	3414	16/16	0.82	0.19	6,26,29,30	0
3	DCN	C	4414	16/16	0.82	0.23	11,26,29,30	0
3	DCN	D	5414	16/16	0.83	0.23	6,26,30,32	0
2	NAD	A	1780	44/44	0.93	0.13	20,28,31,34	0
2	NAD	D	4780	44/44	0.94	0.12	18,27,31,32	0
2	NAD	C	3780	44/44	0.95	0.12	18,23,27,28	0
2	NAD	B	2780	44/44	0.95	0.12	16,24,28,30	0

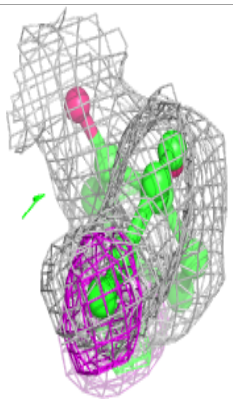
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DCN A 2414:

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

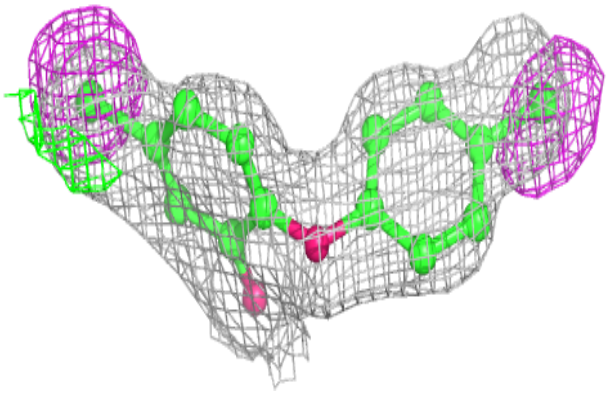


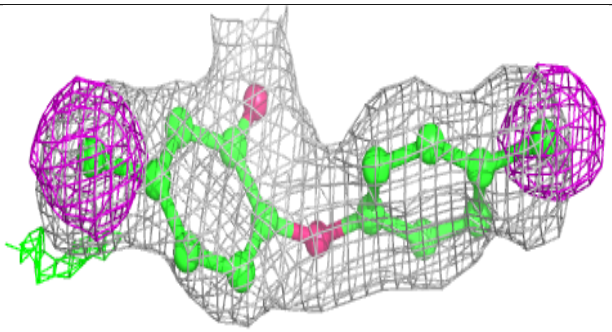


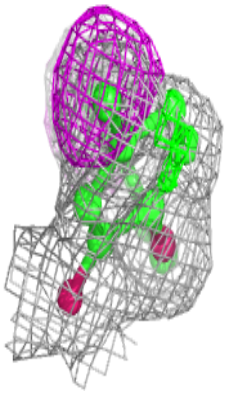


Electron density around DCN B 3414:

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

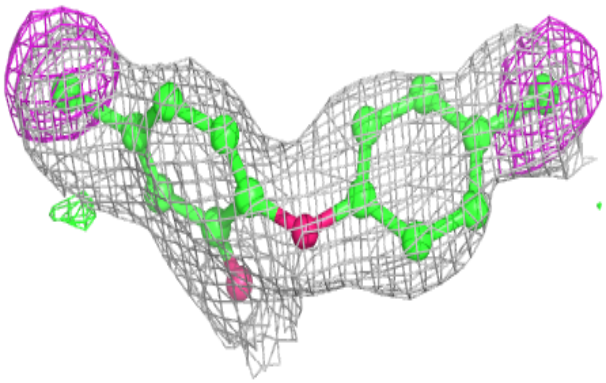


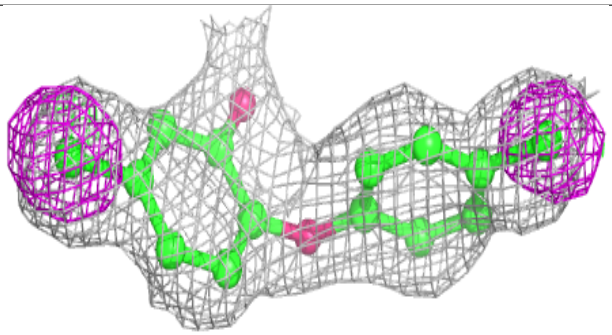


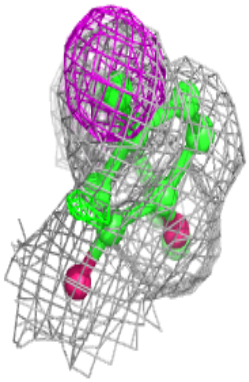


Electron density around DCN C 4414:

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

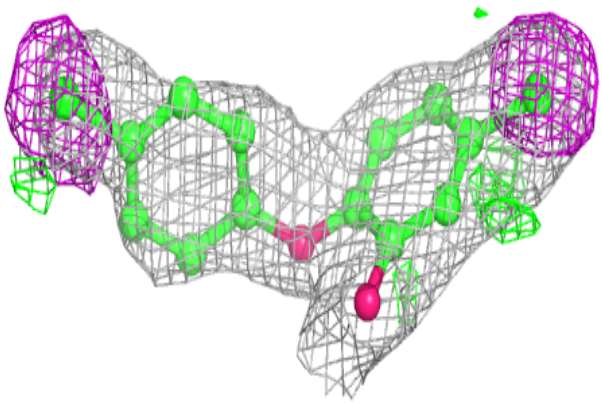


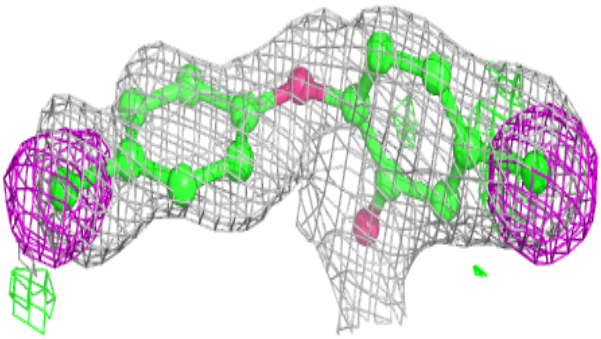


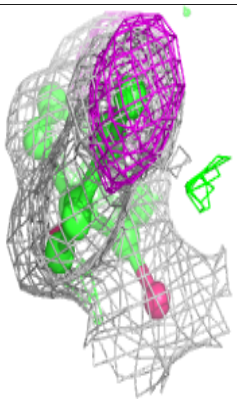


Electron density around DCN D 5414:

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

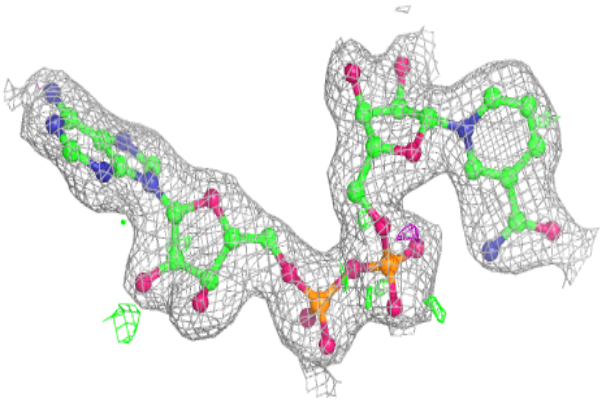


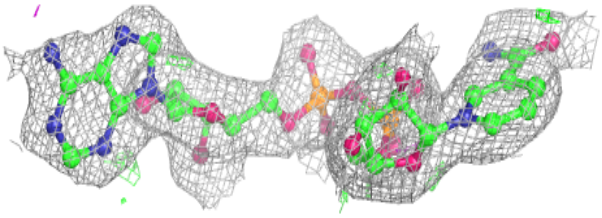


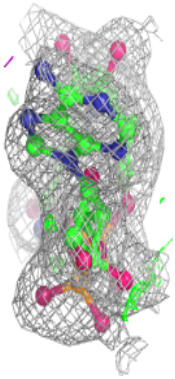


Electron density around NAD A 1780:

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

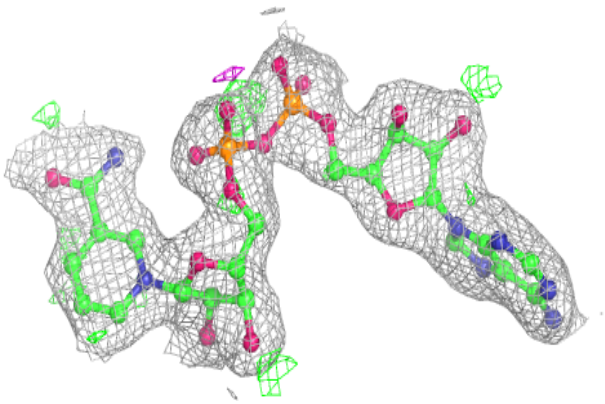


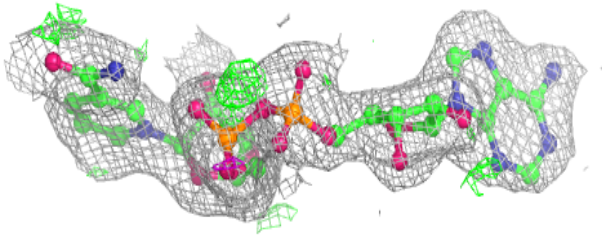


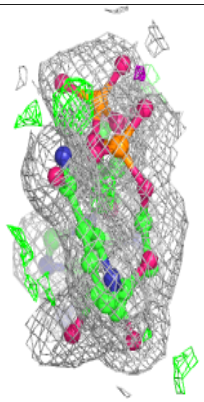


Electron density around NAD D 4780:

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

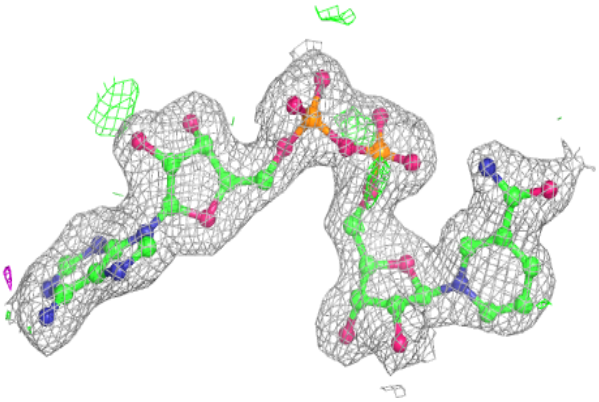


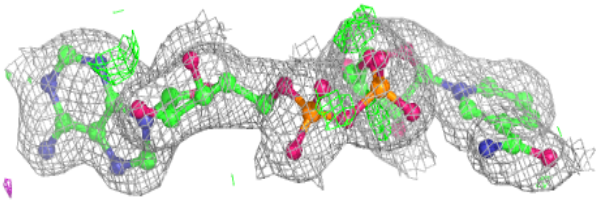


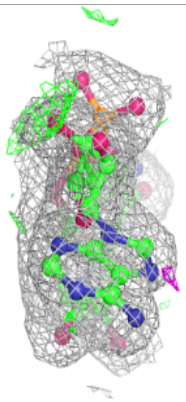


Electron density around NAD C 3780:

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

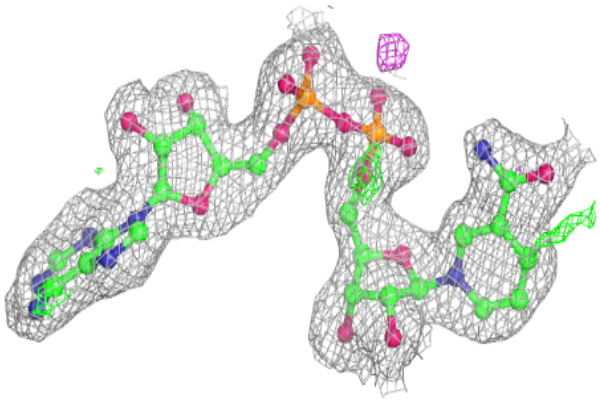


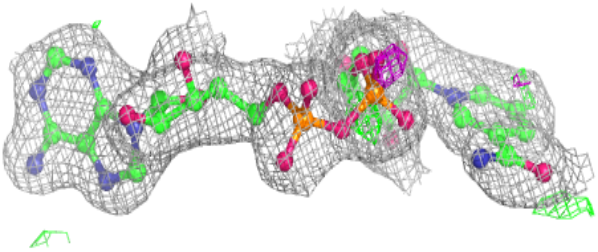


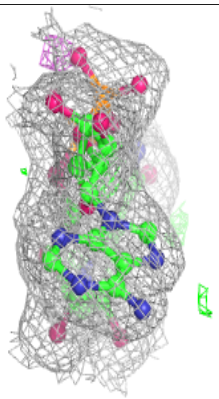


Electron density around NAD B 2780:

$2mF_o$-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.