



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:26 PM UTC

PDB ID : 2PD4 / pdb_00002pd4
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

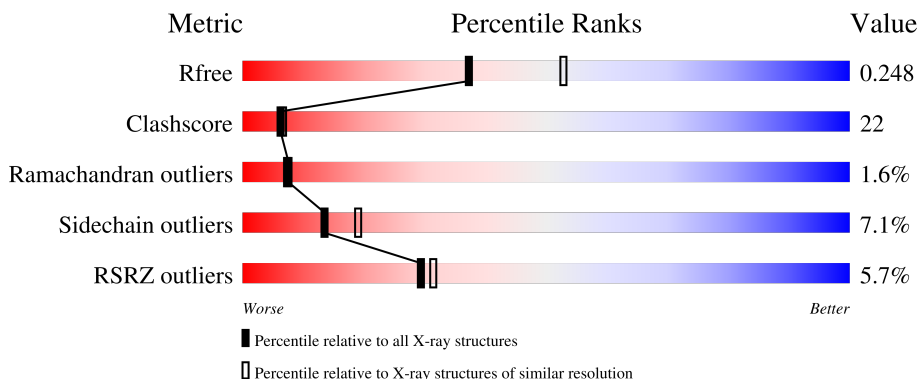
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	275	 6% 64% 30% 5% .
1	B	275	 5% 63% 32% . .
1	C	275	 6% 65% 29% . .
1	D	275	 6% 64% 31% . .

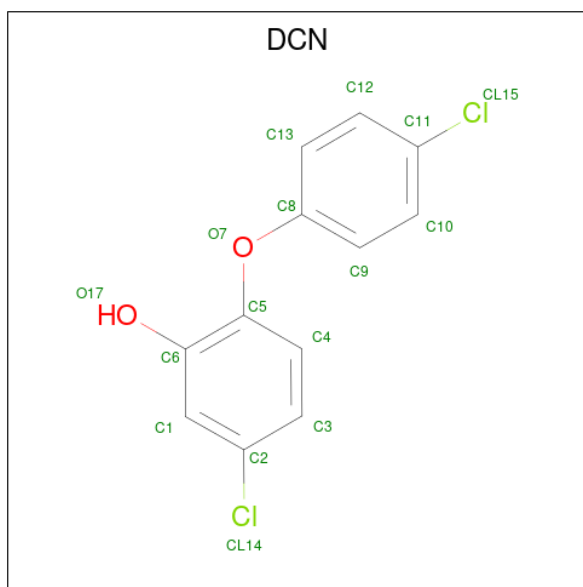
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

Continued from previous page...

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

- Molecule 3 is DICLOSAN (CCD ID: DCN) (formula: C₁₂H₈Cl₂O₂).



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

- Molecule 4 is water.

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

Continued on next page...

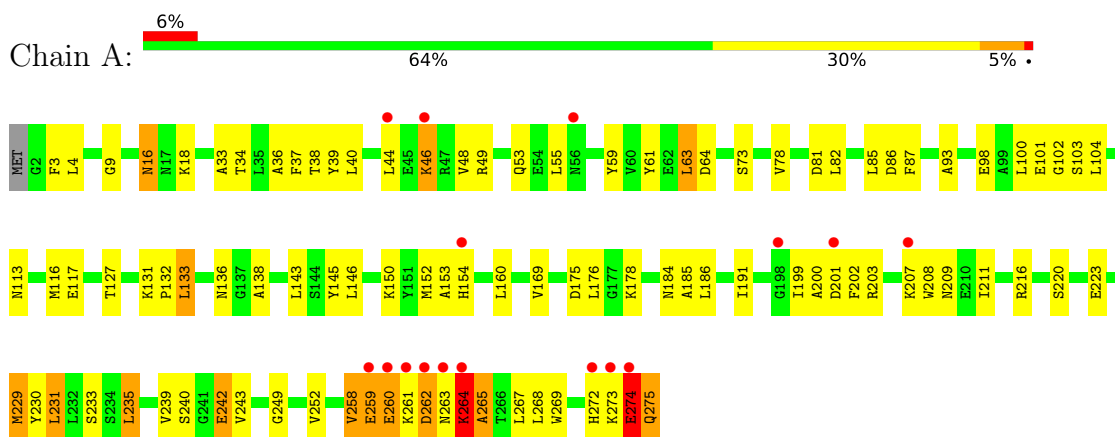
Continued from previous page...

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

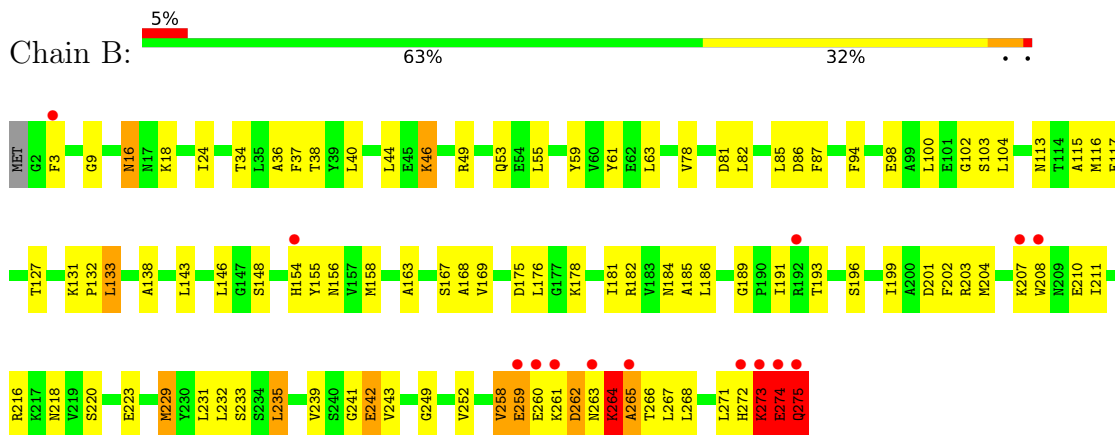
3 Residue-property plots [i](#)

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.

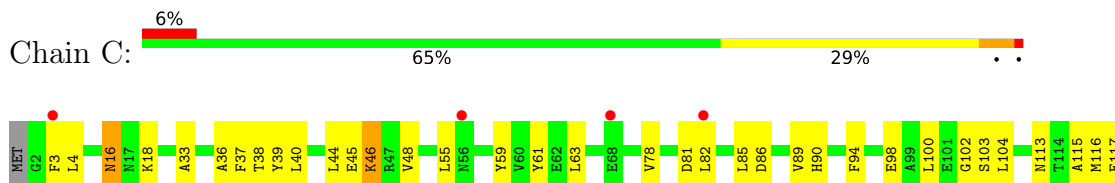
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

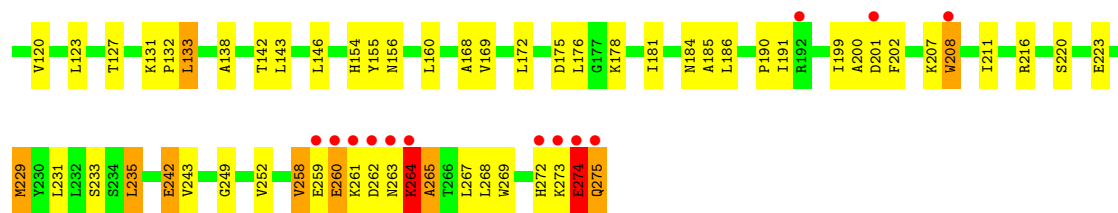


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

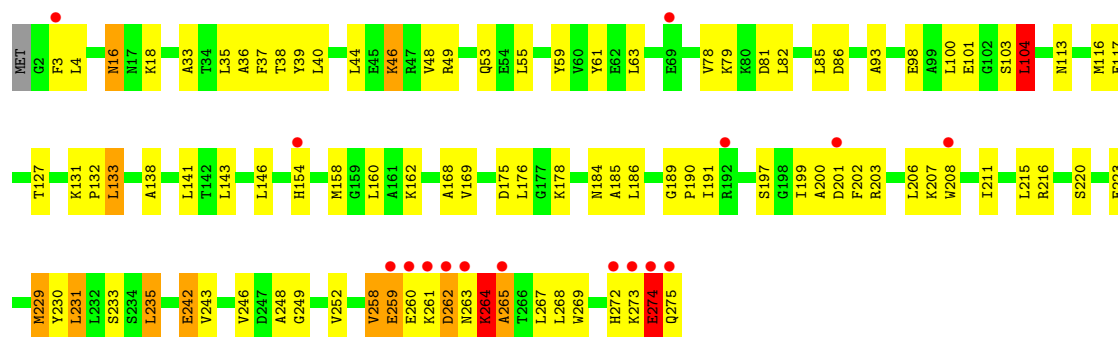


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]





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



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 28.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.7 (28.95-2.30) 89.8 (28.95-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.36 (at 2.31Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.248 0.222 , 0.248	Depositor DCC
R_{free} test set	3908 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtrriage
Anisotropy	0.292	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for l,-k,h	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.42	0/2140	0.90	3/2890 (0.1%)
1	B	0.58	3/2140 (0.1%)	0.99	10/2890 (0.3%)
1	C	0.43	0/2140	0.90	1/2890 (0.0%)
1	D	0.42	0/2140	0.90	4/2890 (0.1%)
All	All	0.47	3/8560 (0.0%)	0.92	18/11560 (0.2%)

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	C-N	-12.37	1.16	1.33
1	B	273	LYS	C-N	9.33	1.46	1.33
1	B	274	GLU	CB-CG	-9.08	1.25	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	GLU	CA-CB-CG	11.44	136.98	114.10
1	B	275	GLN	OE1-CD-NE2	-8.90	113.69	122.60
1	B	273	LYS	CA-C-N	8.32	137.44	121.54
1	B	273	LYS	C-N-CA	8.32	137.44	121.54
1	D	264	LYS	N-CA-C	-6.87	103.30	113.61
1	C	264	LYS	N-CA-C	-6.48	103.89	113.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	GLN	CG-CD-NE2	6.48	126.12	116.40
1	B	264	LYS	N-CA-C	-6.26	104.00	113.89
1	A	264	LYS	N-CA-C	-6.19	104.32	113.61
1	A	239	VAL	N-CA-C	5.73	116.11	107.80
1	D	189	GLY	N-CA-C	-5.62	105.18	112.10
1	B	167	SER	N-CA-C	-5.53	105.34	111.36
1	B	189	GLY	N-CA-C	-5.47	105.37	112.10
1	A	34	THR	N-CA-C	-5.22	100.66	108.96
1	D	104	LEU	N-CA-C	-5.15	105.74	111.36
1	D	35	LEU	N-CA-C	5.14	118.11	110.14
1	B	158	MET	N-CA-C	-5.14	106.27	112.54
1	B	34	THR	N-CA-C	-5.09	100.87	108.96

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	108	0
1	B	2102	0	2124	107	0
1	C	2102	0	2125	112	0
1	D	2102	0	2125	109	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	60	0	0	10	0
4	D	43	0	0	4	0
All	All	8866	0	8631	386	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 22.

All (386) 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:116:MET:HE2	1:B:116:MET:HE2	1.36	1.03
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:C:116:MET:HE2	1:D:116:MET:HE2	1.55	0.85
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
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:B:16:ASN:C	1:B:16:ASN:HD22	1.90	0.79
1:D:16:ASN:C	1:D:16:ASN:HD22	1.91	0.78
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:16:ASN:C	1:A:16:ASN:HD22	1.95	0.75
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LYS:O	1:A:274:GLU:HB2	1.84	0.74
1:D:273:LYS:O	1:D:274:GLU:HB2	1.86	0.74
1:C:16:ASN:C	1:C:16:ASN:HD22	1.95	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: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:A:116:MET:CE	1:B:116:MET:HE2	2.20	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
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:A:116:MET:HE2	1:B:116:MET:CE	2.21	0.63
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:THR:HA	1:A:61:TYR:O	1.99	0.62
1:C:229:MET:HE2	1:C:233:SER:HB3	1.82	0.62
1:C:261:LYS:N	1:C:261:LYS:HD2	2.14	0.62
1:C:103:SER:HB2	1:D:175:ASP:CG	2.24	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:C:116:MET:HE2	1:D:116:MET:CE	2.28	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:C:116:MET:CE	1:D:116:MET:HE2	2.28	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:229:MET:HE2	1:A:233:SER:HB3	1.83	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:98:GLU:CD	1:A:98:GLU:H	2.09	0.60
1:A:264:LYS:HE2	1:D:201:ASP:HB3	1.84	0.60
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:272:HIS:O	1:B:273:LYS:C	2.47	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: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:B:16:ASN:ND2	1:B:16:ASN:C	2.61	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
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:16:ASN:C	1:D:16:ASN:ND2	2.61	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ASP:CG	1:C:154:HIS:HE2	2.14	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:D:98:GLU:CD	1:D:98:GLU:H	2.14	0.54
1:D:229:MET:HE2	1:D:233:SER:HB3	1.89	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:C:16:ASN:C	1:C:16:ASN:ND2	2.65	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:D:191:ILE:N	2:D:4780:NAD:O7N	2.38	0.53
1:A:36:ALA:HB2	1:A:82:LEU:HD11	1.91	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:98:GLU:H	1:B:98:GLU:CD	2.18	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
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:B:36:ALA:HB2	1:B:82:LEU:HD11	1.93	0.51
1:B:154:HIS:HE2	1:C:262:ASP:CG	2.19	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:98:GLU:CD	1:C:98:GLU:H	2.18	0.51
1:C:131:LYS:HB3	1:C:132:PRO:HD3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:LEU:HD13	4:C:4423:HOH:O	2.11	0.51
1:C:269:TRP:O	1:C:274:GLU:HB3	2.10	0.50
1:D:207:LYS:HG2	1:D:273:LYS:HE3	1.94	0.50
1:A:103:SER:HB2	1:B:175:ASP:CG	2.36	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:B:229:MET:HE2	1:B:233:SER:HB3	1.93	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:175:ASP:CG	1:D:103:SER:HB2	2.37	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:272:HIS:O	1:A:273:LYS:C	2.56	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:A:175:ASP:CG	1:B:103:SER:HB2	2.38	0.48
1:B:262:ASP:CG	1:C:154:HIS:NE2	2.72	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
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:A:262:ASP:CG	1:D:154:HIS:HE2	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:155:TYR:O	1:C:156:ASN:C	2.58	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: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:A:16:ASN:ND2	1:A:16:ASN:C	2.66	0.46
1:A:86:ASP:O	1:A:138:ALA:HA	2.15	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:B:154:HIS:NE2	1:C:262:ASP:CG	2.74	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: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:A:154:HIS:HE2	1:D:262:ASP:CG	2.24	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:A:230:TYR:CD1	1:A:231:LEU:HD13	2.51	0.45
1:A:262:ASP:O	1:A:263:ASN:C	2.58	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:145:TYR:OH	1:A:152:MET:HE3	2.18	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:46:LYS:HD3	1:C:46:LYS:C	2.43	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: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: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
1:B:266:THR:HG23	4:B:3428:HOH:O	2.17	0.43
1:D:16:ASN:ND2	4:D:5419:HOH:O	2.51	0.43
1:A:46:LYS:HD3	1:A:46:LYS:C	2.44	0.43
1:A:262:ASP:CG	1:D:154:HIS:NE2	2.77	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:272:HIS:O	1:C:273:LYS:C	2.61	0.42
1:D:264:LYS:HE3	1:D:264:LYS:CA	2.49	0.42
1:D:272:HIS:O	1:D:273:LYS:C	2.61	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:46:LYS:HD3	1:B:46:LYS:C	2.43	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:262:ASP:O	1:D:263:ASN:C	2.63	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: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:229:MET:HE2	1:B:229:MET:O	2.20	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
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:B:262:ASP:O	1:B:263:ASN:C	2.63	0.41
1:B:271:LEU:O	1:B:275:GLN:OE1	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:87:PHE:HB2	1:B:232:LEU:HD22	2.02	0.41
1:B:193:THR:N	1:B:196:SER:OG	2.46	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:229:MET:HE2	1:D:229:MET:O	2.21	0.41
1:D:242:GLU:HG3	1:D:243:VAL:N	2.35	0.41
1:A:63:LEU:C	1:A:63:LEU:HD22	2.46	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:D:274:GLU:C	1:D:275:GLN:HG3	2.46	0.40
1:A:150:LYS:HA	1:A:150:LYS:HD3	1.94	0.40
1:B:155:TYR:O	1:B:156:ASN:C	2.64	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:C:262:ASP:O	1:C:263:ASN:C	2.63	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:46:LYS:HD3	1:D:46:LYS:C	2.47	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%)	6	6
1	B	272/275 (99%)	254 (93%)	14 (5%)	4 (2%)	8	8
1	C	272/275 (99%)	252 (93%)	16 (6%)	4 (2%)	8	8
1	D	272/275 (99%)	253 (93%)	15 (6%)	4 (2%)	8	8
All	All	1088/1100 (99%)	1011 (93%)	60 (6%)	17 (2%)	7	7

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%)	208 (92%)	18 (8%)	11	15
1	B	226/227 (100%)	211 (93%)	15 (7%)	15	21
1	C	226/227 (100%)	210 (93%)	16 (7%)	13	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	226/227 (100%)	211 (93%)	15 (7%)	15	21
All	All	904/908 (100%)	840 (93%)	64 (7%)	13	19

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	46	LYS
1	A	63	LEU
1	A	85	LEU
1	A	104	LEU
1	A	133	LEU
1	A	146	LEU
1	A	208	TRP
1	A	209	ASN
1	A	229	MET
1	A	231	LEU
1	A	235	LEU
1	A	242	GLU
1	A	260	GLU
1	A	262	ASP
1	A	264	LYS
1	A	274	GLU
1	A	275	GLN
1	B	16	ASN
1	B	46	LYS
1	B	63	LEU
1	B	85	LEU
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	242	GLU
1	B	262	ASP
1	B	264	LYS
1	B	275	GLN
1	C	16	ASN
1	C	46	LYS
1	C	63	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	85	LEU
1	C	104	LEU
1	C	133	LEU
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	260	GLU
1	C	264	LYS
1	C	274	GLU
1	C	275	GLN
1	D	16	ASN
1	D	46	LYS
1	D	63	LEU
1	D	85	LEU
1	D	104	LEU
1	D	133	LEU
1	D	146	LEU
1	D	208	TRP
1	D	229	MET
1	D	231	LEU
1	D	235	LEU
1	D	242	GLU
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 (41) 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	272	HIS
1	A	275	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	16	ASN
1	B	30	ASN
1	B	53	GLN
1	B	56	ASN
1	B	76	ASN
1	B	156	ASN
1	B	184	ASN
1	B	226	ASN
1	B	272	HIS
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	272	HIS
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	135	ASN
1	D	156	ASN
1	D	184	ASN
1	D	226	ASN
1	D	272	HIS
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 oligosaccharides 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
3	DCN	A	2414	-	17,17,17	3.19	13 (76%)	23,23,23	1.02	1 (4%)
3	DCN	C	4414	-	17,17,17	3.25	13 (76%)	23,23,23	1.00	1 (4%)
3	DCN	B	3414	-	17,17,17	3.22	14 (82%)	23,23,23	1.00	1 (4%)
2	NAD	B	2780	-	46,48,48	1.69	4 (8%)	64,73,73	1.71	12 (18%)
3	DCN	D	5414	-	17,17,17	3.21	13 (76%)	23,23,23	1.00	1 (4%)
2	NAD	D	4780	-	46,48,48	1.70	3 (6%)	64,73,73	1.68	13 (20%)
2	NAD	C	3780	-	46,48,48	1.72	4 (8%)	64,73,73	1.82	12 (18%)
2	NAD	A	1780	-	46,48,48	1.65	4 (8%)	64,73,73	1.81	12 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DCN	A	2414	-	-	0/4/4/4	0/2/2/2
3	DCN	C	4414	-	-	0/4/4/4	0/2/2/2
3	DCN	B	3414	-	-	0/4/4/4	0/2/2/2
2	NAD	B	2780	-	-	2/30/62/62	0/5/5/5
3	DCN	D	5414	-	-	0/4/4/4	0/2/2/2
2	NAD	D	4780	-	1/1/11/11	15/30/62/62	0/5/5/5
2	NAD	C	3780	-	-	4/30/62/62	0/5/5/5
2	NAD	A	1780	-	-	7/30/62/62	0/5/5/5

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3780	NAD	O7N-C7N	8.85	1.40	1.24
2	D	4780	NAD	O7N-C7N	8.61	1.40	1.24
2	B	2780	NAD	O7N-C7N	8.52	1.40	1.24
2	A	1780	NAD	O7N-C7N	8.37	1.39	1.24
3	D	5414	DCN	C9-C8	6.11	1.50	1.38
3	B	3414	DCN	C9-C8	5.95	1.49	1.38
3	A	2414	DCN	C9-C8	5.89	1.49	1.38
3	C	4414	DCN	C9-C8	5.86	1.49	1.38
3	A	2414	DCN	C6-C5	5.15	1.49	1.40
3	C	4414	DCN	C10-C11	4.93	1.47	1.38
3	D	5414	DCN	C6-C5	4.80	1.48	1.40
3	B	3414	DCN	C3-C2	4.75	1.46	1.38
3	C	4414	DCN	C6-C5	4.59	1.48	1.40
3	C	4414	DCN	C3-C2	4.59	1.46	1.38
3	D	5414	DCN	C10-C11	4.55	1.46	1.38
3	D	5414	DCN	C3-C2	4.53	1.46	1.38
3	A	2414	DCN	C10-C11	4.53	1.46	1.38
3	B	3414	DCN	C10-C11	4.52	1.46	1.38
3	B	3414	DCN	C6-C5	4.41	1.48	1.40
3	A	2414	DCN	C3-C2	4.36	1.46	1.38
3	B	3414	DCN	C1-C6	3.77	1.44	1.38
3	C	4414	DCN	C9-C10	3.73	1.44	1.38
3	D	5414	DCN	C13-C12	3.53	1.44	1.38
3	A	2414	DCN	C9-C10	3.43	1.44	1.38
3	B	3414	DCN	C9-C10	3.41	1.44	1.38
3	C	4414	DCN	C1-C6	3.28	1.43	1.38
3	D	5414	DCN	C9-C10	3.27	1.44	1.38
3	C	4414	DCN	C13-C12	3.27	1.44	1.38
3	A	2414	DCN	C13-C12	3.17	1.43	1.38
3	B	3414	DCN	C13-C12	3.16	1.43	1.38
3	D	5414	DCN	C1-C6	3.05	1.43	1.38
3	C	4414	DCN	C12-C11	2.97	1.43	1.38
3	A	2414	DCN	C12-C11	2.93	1.43	1.38
3	B	3414	DCN	C12-C11	2.80	1.43	1.38
3	D	5414	DCN	C12-C11	2.78	1.43	1.38
3	A	2414	DCN	C3-C4	2.69	1.43	1.38
3	A	2414	DCN	C1-C6	2.68	1.42	1.38
2	B	2780	NAD	C5A-N7A	-2.63	1.34	1.39
3	B	3414	DCN	C3-C4	2.56	1.43	1.38
3	C	4414	DCN	C3-C4	2.54	1.42	1.38
3	B	3414	DCN	O17-C6	-2.52	1.31	1.36
3	A	2414	DCN	C4-C5	2.51	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3780	NAD	C5A-N7A	-2.49	1.34	1.39
3	D	5414	DCN	C3-C4	2.48	1.42	1.38
2	D	4780	NAD	C5A-N7A	-2.47	1.34	1.39
2	A	1780	NAD	C5A-N7A	-2.45	1.34	1.39
3	C	4414	DCN	C4-C5	2.41	1.44	1.39
2	C	3780	NAD	PN-O2N	-2.39	1.44	1.55
3	C	4414	DCN	O17-C6	-2.38	1.31	1.36
2	A	1780	NAD	PN-O2N	-2.37	1.44	1.55
3	C	4414	DCN	C13-C8	2.34	1.43	1.38
3	D	5414	DCN	C4-C5	2.34	1.44	1.39
3	D	5414	DCN	O17-C6	-2.33	1.31	1.36
3	D	5414	DCN	C13-C8	2.32	1.43	1.38
2	B	2780	NAD	PN-O2N	-2.30	1.44	1.55
3	A	2414	DCN	O17-C6	-2.30	1.31	1.36
2	D	4780	NAD	PN-O2N	-2.26	1.44	1.55
3	A	2414	DCN	C13-C8	2.25	1.43	1.38
3	A	2414	DCN	C1-C2	2.23	1.41	1.38
3	B	3414	DCN	C4-C5	2.22	1.44	1.39
3	B	3414	DCN	C13-C8	2.22	1.42	1.38
3	D	5414	DCN	C1-C2	2.19	1.41	1.38
3	C	4414	DCN	C1-C2	2.14	1.41	1.38
2	B	2780	NAD	O4B-C4B	-2.13	1.40	1.45
3	B	3414	DCN	C1-C2	2.11	1.41	1.38
2	A	1780	NAD	PA-O1A	-2.07	1.43	1.50
3	B	3414	DCN	O7-C8	2.05	1.44	1.39
2	C	3780	NAD	C2A-N3A	2.05	1.37	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2780	NAD	N3A-C2A-N1A	-5.60	120.10	128.58
2	D	4780	NAD	N3A-C2A-N1A	-5.47	120.31	128.58
2	C	3780	NAD	O4B-C1B-N9A	5.29	118.24	108.09
2	A	1780	NAD	N3A-C2A-N1A	-5.06	120.93	128.58
2	C	3780	NAD	N3A-C2A-N1A	-4.55	121.69	128.58
2	A	1780	NAD	N9A-C8A-N7A	-4.55	107.48	113.94
2	C	3780	NAD	N9A-C8A-N7A	-4.52	107.52	113.94
2	C	3780	NAD	C5A-C4A-N3A	-4.44	120.61	126.72
2	B	2780	NAD	O4B-C1B-N9A	4.41	116.57	108.09
2	A	1780	NAD	O4B-C1B-N9A	4.35	116.44	108.09
2	A	1780	NAD	C5A-C4A-N3A	-4.23	120.90	126.72
2	D	4780	NAD	N9A-C8A-N7A	-4.20	107.98	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3780	NAD	C5A-N7A-C8A	4.13	109.94	103.45
2	B	2780	NAD	N9A-C8A-N7A	-4.00	108.26	113.94
2	A	1780	NAD	C5A-N7A-C8A	3.95	109.66	103.45
2	A	1780	NAD	C6N-N1N-C2N	-3.57	118.84	121.88
2	B	2780	NAD	C5A-C4A-N3A	-3.56	121.81	126.72
2	A	1780	NAD	O2A-PA-O3	3.53	116.80	107.27
2	C	3780	NAD	C4A-C5A-N7A	-3.45	106.64	110.58
2	D	4780	NAD	C5A-N7A-C8A	3.28	108.60	103.45
2	D	4780	NAD	O4B-C1B-N9A	3.26	114.35	108.09
2	B	2780	NAD	C2A-N3A-C4A	3.17	119.58	111.83
2	D	4780	NAD	C5A-C4A-N3A	-3.16	122.36	126.72
2	A	1780	NAD	C2A-N3A-C4A	3.14	119.51	111.83
2	B	2780	NAD	C5A-N7A-C8A	3.08	108.29	103.45
2	C	3780	NAD	C2A-N3A-C4A	3.07	119.33	111.83
2	A	1780	NAD	C4A-C5A-N7A	-3.05	107.10	110.58
2	B	2780	NAD	C5D-C4D-C3D	-3.04	104.28	115.21
2	D	4780	NAD	C2A-N3A-C4A	3.03	119.22	111.83
2	C	3780	NAD	C6N-N1N-C2N	-2.79	119.50	121.88
2	C	3780	NAD	N3A-C4A-N9A	2.78	131.90	127.17
3	B	3414	DCN	C5-O7-C8	2.78	124.67	117.95
3	C	4414	DCN	C5-O7-C8	2.76	124.64	117.95
3	D	5414	DCN	C5-O7-C8	2.76	124.64	117.95
2	A	1780	NAD	N3A-C4A-N9A	2.76	131.86	127.17
3	A	2414	DCN	C5-O7-C8	2.75	124.61	117.95
2	A	1780	NAD	C4A-N9A-C8A	2.64	108.51	105.74
2	B	2780	NAD	C4A-N9A-C8A	2.61	108.47	105.74
2	D	4780	NAD	O4B-C4B-C5B	2.60	117.67	109.33
2	D	4780	NAD	C4A-C5A-N7A	-2.60	107.61	110.58
2	C	3780	NAD	C4A-N9A-C8A	2.52	108.39	105.74
2	B	2780	NAD	N3A-C4A-N9A	2.46	131.35	127.17
2	D	4780	NAD	C4A-N9A-C8A	2.46	108.32	105.74
2	C	3780	NAD	C5D-C4D-C3D	-2.34	106.78	115.21
2	D	4780	NAD	C6N-N1N-C2N	-2.32	119.90	121.88
2	D	4780	NAD	C4A-N9A-C1B	-2.30	121.26	126.63
2	B	2780	NAD	O2N-PN-O1N	2.28	123.06	112.44
2	A	1780	NAD	C5N-C4N-C3N	-2.23	118.17	120.36
2	D	4780	NAD	O2A-PA-O3	2.23	113.29	107.27
2	B	2780	NAD	C4A-C5A-N7A	-2.14	108.14	110.58
2	C	3780	NAD	C3N-C7N-N7N	2.07	120.28	117.74
2	D	4780	NAD	C2B-C1B-N9A	-2.04	108.23	113.30
2	B	2780	NAD	O4B-C4B-C3B	2.02	109.17	105.15

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-O2N
2	A	1780	NAD	O4D-C4D-C5D-O5D
2	C	3780	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	A	1780	NAD	C3D-C4D-C5D-O5D
2	D	4780	NAD	O4B-C4B-C5B-O5B
2	C	3780	NAD	C3D-C4D-C5D-O5D
2	C	3780	NAD	O4D-C4D-C5D-O5D
2	D	4780	NAD	C3B-C4B-C5B-O5B
2	A	1780	NAD	PN-O3-PA-O1A
2	D	4780	NAD	PA-O3-PN-O1N
2	A	1780	NAD	C5D-O5D-PN-O3
2	A	1780	NAD	C5D-O5D-PN-O1N
2	D	4780	NAD	C5B-O5B-PA-O1A
2	D	4780	NAD	C5B-O5B-PA-O2A
2	D	4780	NAD	C5B-O5B-PA-O3
2	D	4780	NAD	C5D-O5D-PN-O3
2	D	4780	NAD	PN-O3-PA-O2A
2	B	2780	NAD	O4B-C4B-C5B-O5B
2	D	4780	NAD	O4D-C1D-N1N-C6N
2	A	1780	NAD	PN-O3-PA-O2A
2	B	2780	NAD	C3D-C4D-C5D-O5D
2	D	4780	NAD	PN-O3-PA-O1A
2	C	3780	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

8 monomers are involved in 30 short contacts:

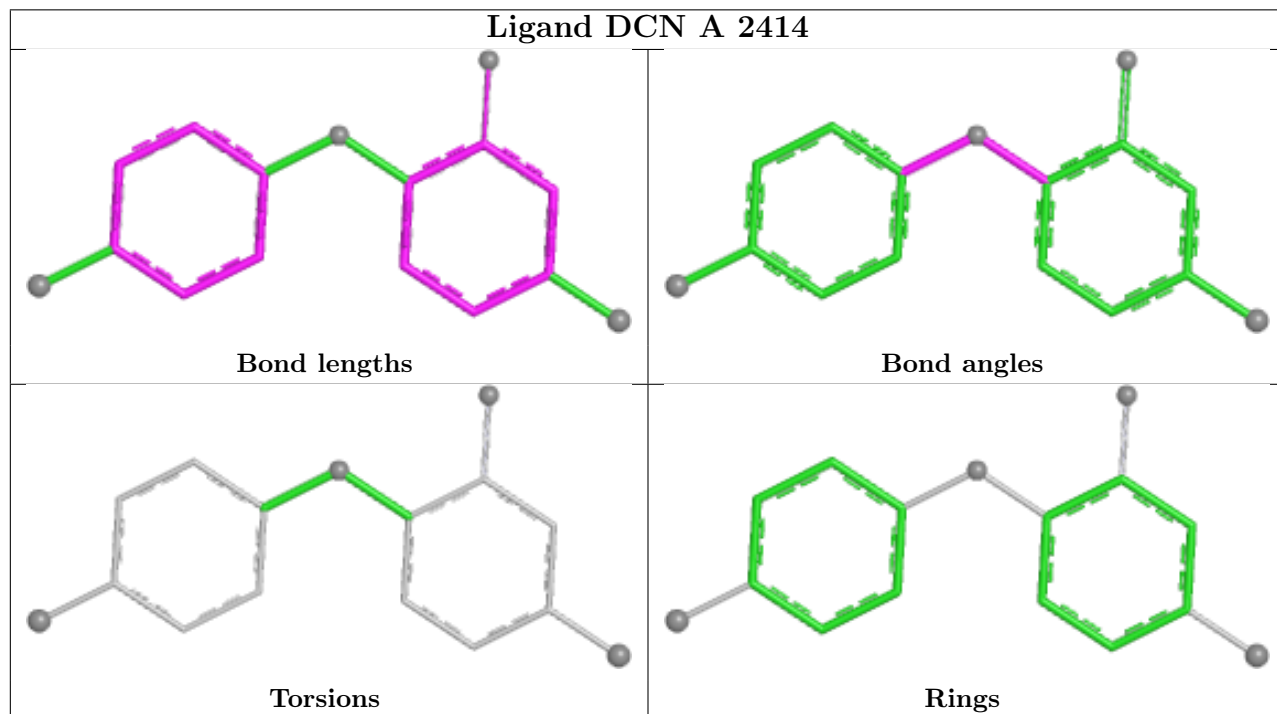
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2414	DCN	5	0
3	C	4414	DCN	4	0
3	B	3414	DCN	4	0
2	B	2780	NAD	1	0
3	D	5414	DCN	5	0

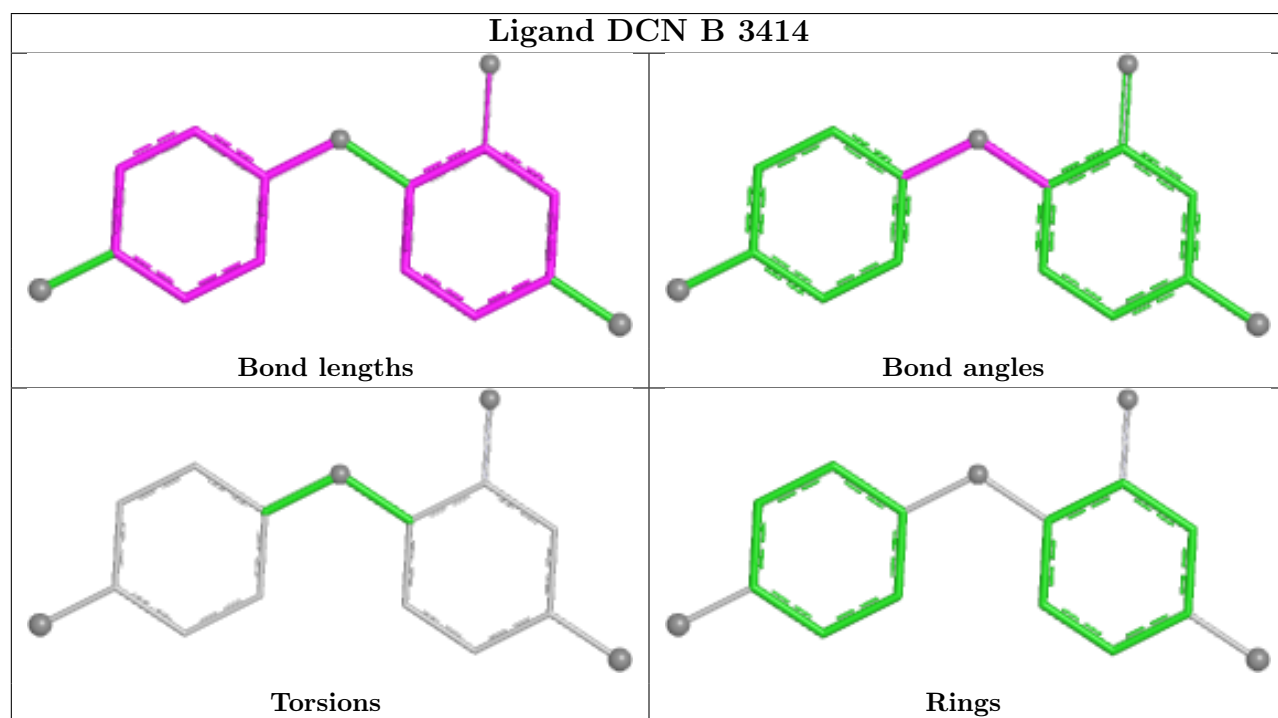
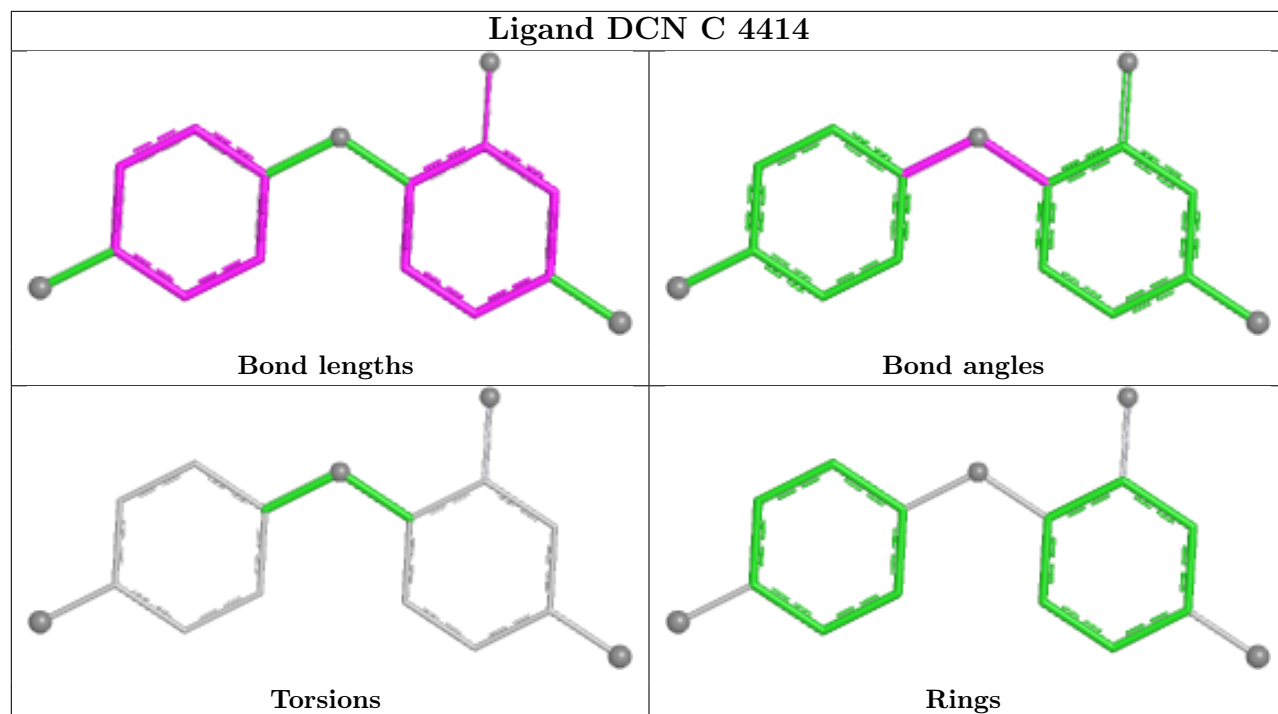
Continued on next page...

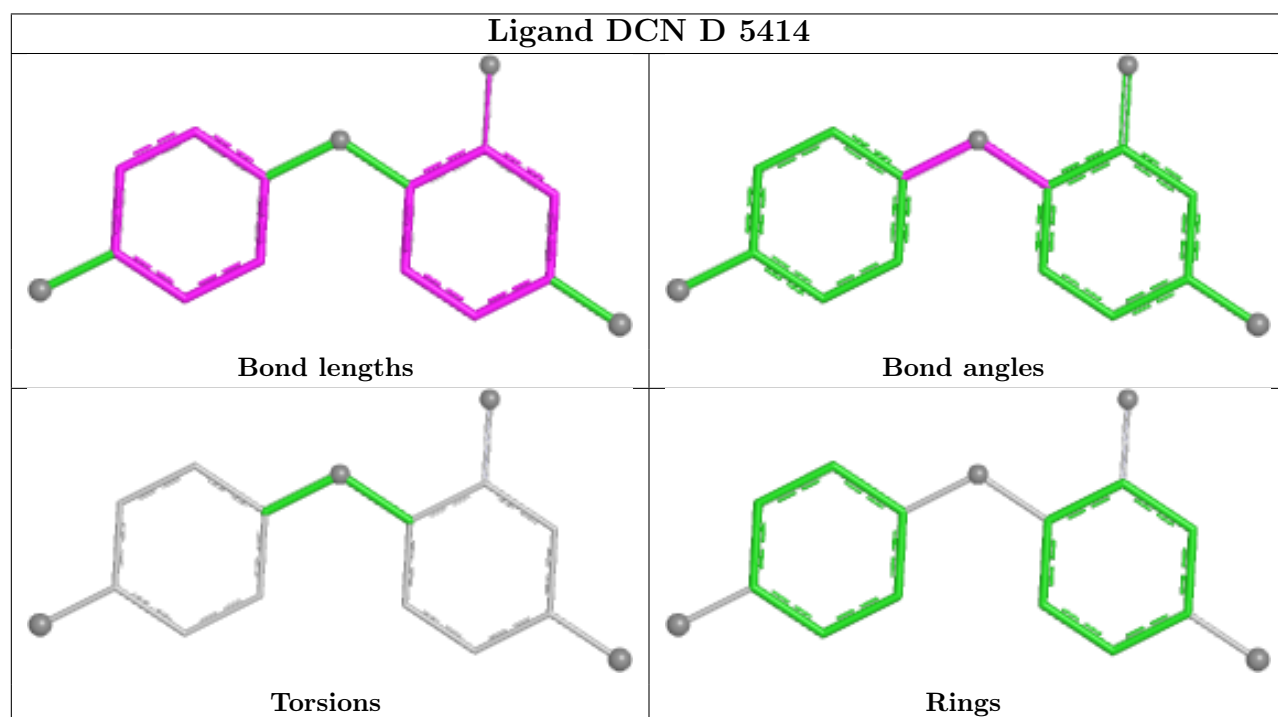
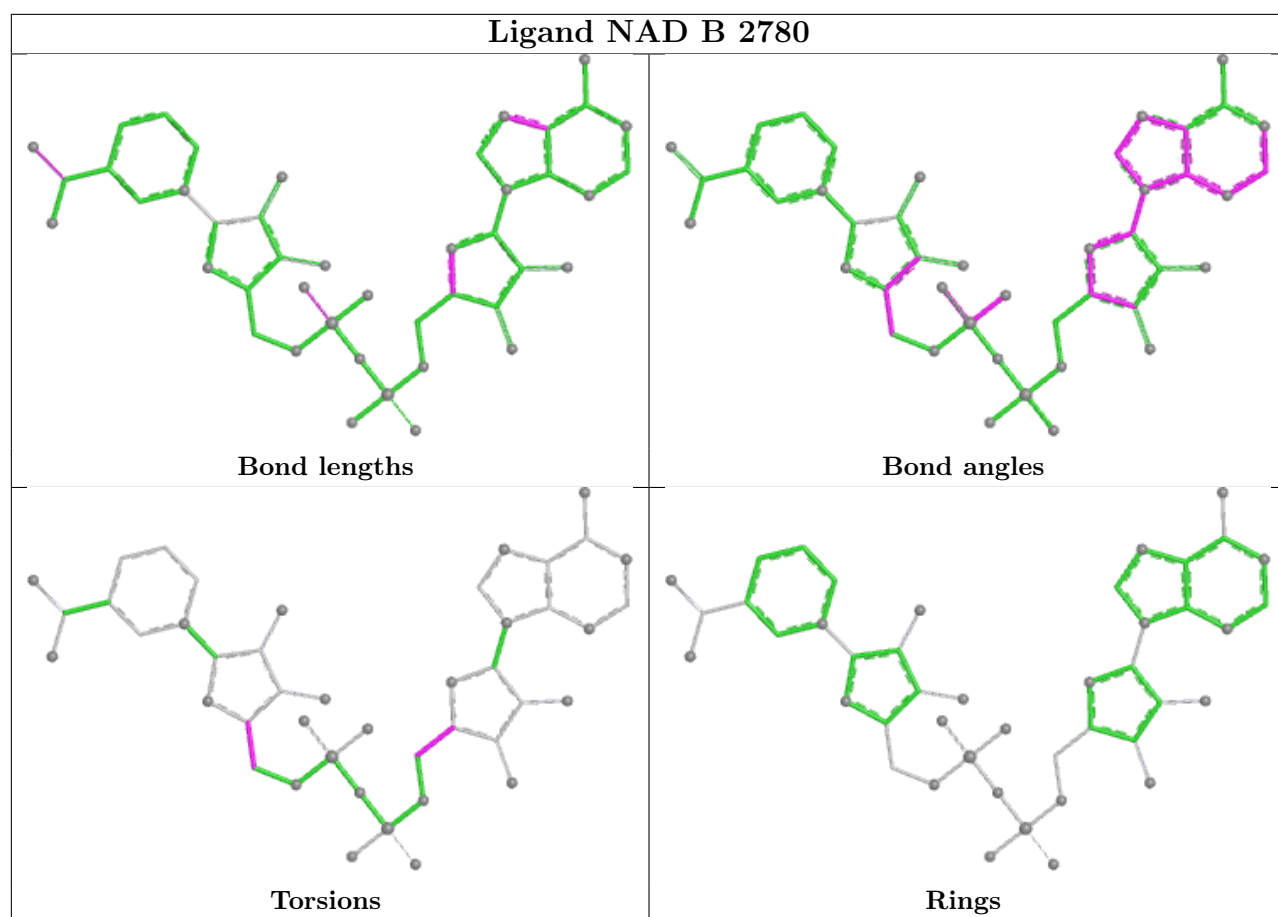
Continued from previous page...

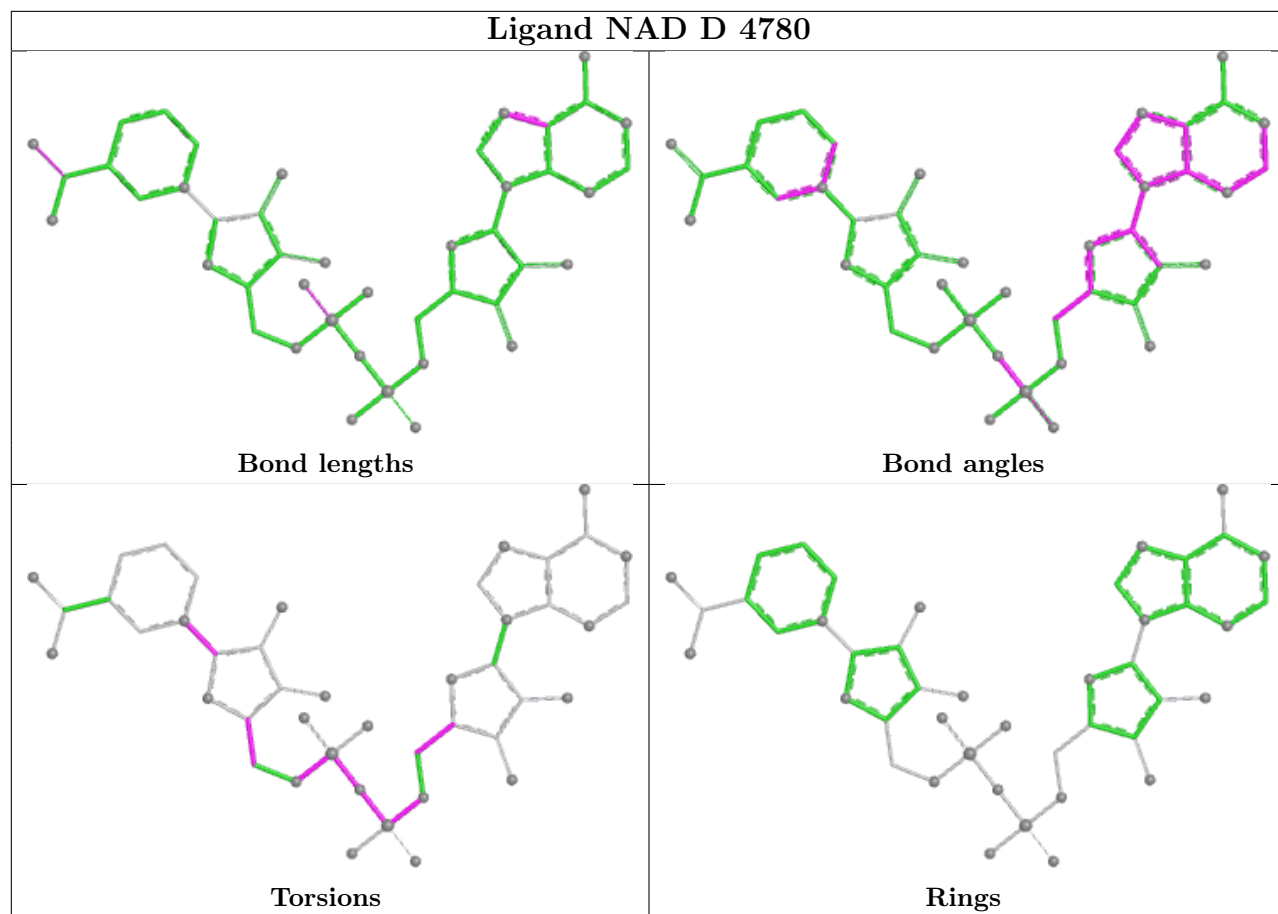
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4780	NAD	3	0
2	C	3780	NAD	3	0
2	A	1780	NAD	5	0

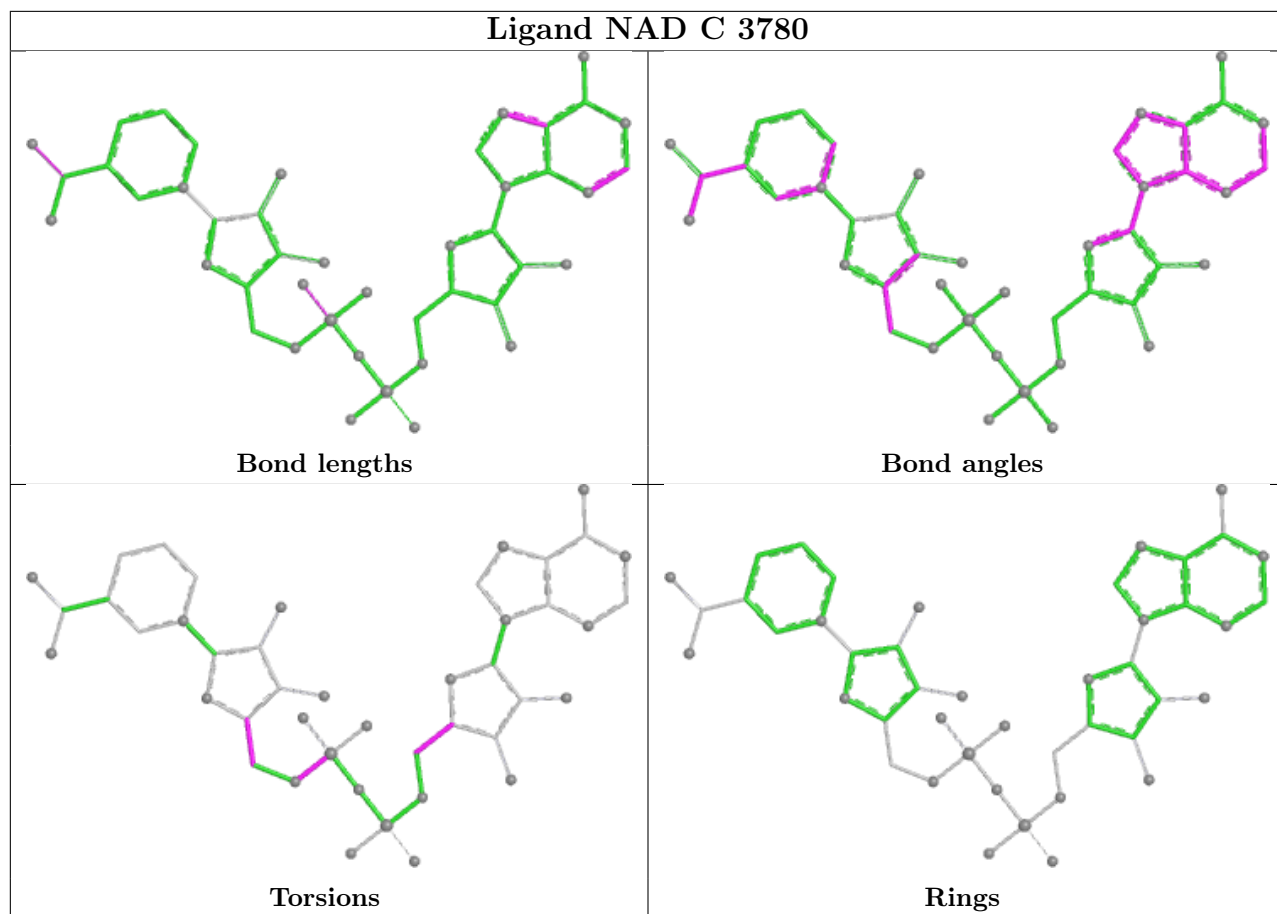
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

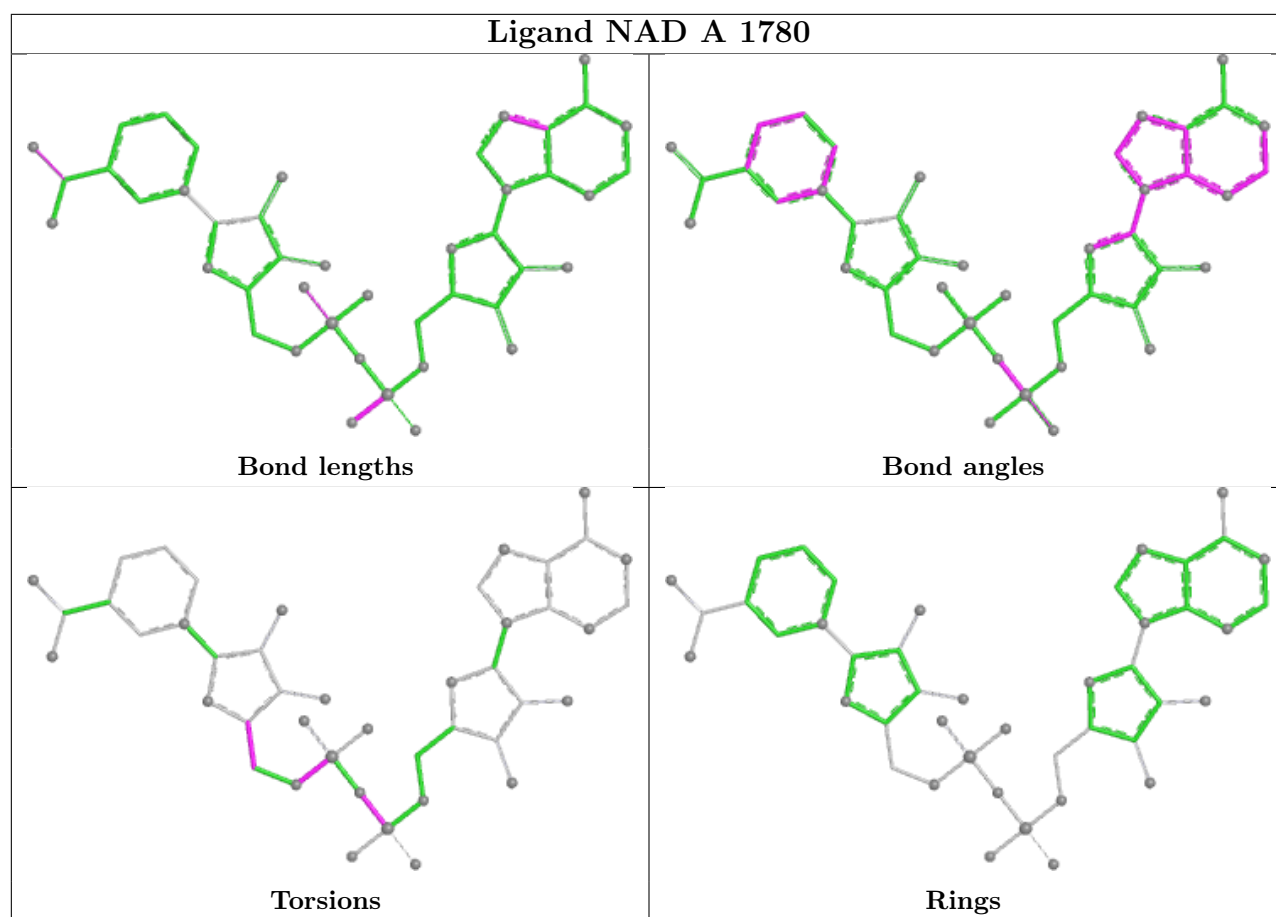












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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

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, 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	16 (5%) 29 31	16, 31, 51, 90	0
1	B	274/275 (99%)	0.31	14 (5%) 33 35	14, 28, 49, 90	0
1	C	274/275 (99%)	0.38	17 (6%) 26 28	14, 29, 51, 89	0
1	D	274/275 (99%)	0.37	16 (5%) 29 31	17, 30, 49, 89	0
All	All	1096/1100 (99%)	0.37	63 (5%) 29 31	14, 29, 51, 90	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	273	LYS	4.2
1	C	272	HIS	4.1
1	B	273	LYS	4.0
1	D	273	LYS	3.8
1	B	272	HIS	3.8
1	C	261	LYS	3.7
1	A	259	GLU	3.7
1	C	259	GLU	3.7
1	B	208	TRP	3.6
1	B	260	GLU	3.6
1	C	260	GLU	3.6
1	B	261	LYS	3.5
1	D	261	LYS	3.4
1	A	264	LYS	3.4
1	D	274	GLU	3.4
1	A	260	GLU	3.4
1	B	259	GLU	3.4
1	A	272	HIS	3.3
1	B	274	GLU	3.3
1	D	259	GLU	3.3
1	A	56	ASN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	263	ASN	3.2
1	B	275	GLN	3.2
1	B	265	ALA	3.1
1	A	262	ASP	3.1
1	D	275	GLN	3.1
1	A	261	LYS	3.1
1	D	260	GLU	3.0
1	C	208	TRP	2.9
1	B	3	PHE	2.9
1	C	264	LYS	2.8
1	B	263	ASN	2.8
1	C	201	ASP	2.8
1	C	274	GLU	2.7
1	A	273	LYS	2.7
1	A	263	ASN	2.7
1	D	263	ASN	2.7
1	C	3	PHE	2.6
1	D	201	ASP	2.6
1	D	272	HIS	2.6
1	D	208	TRP	2.6
1	D	3	PHE	2.6
1	D	154	HIS	2.6
1	C	192	ARG	2.5
1	A	274	GLU	2.5
1	D	262	ASP	2.5
1	B	154	HIS	2.4
1	C	262	ASP	2.4
1	B	192	ARG	2.3
1	D	192	ARG	2.3
1	C	56	ASN	2.2
1	A	198	GLY	2.2
1	A	207	LYS	2.2
1	C	275	GLN	2.2
1	A	201	ASP	2.2
1	A	44	LEU	2.1
1	C	82	LEU	2.1
1	A	154	HIS	2.1
1	C	68	GLU	2.1
1	D	265	ALA	2.1
1	D	69	GLU	2.1
1	B	207	LYS	2.0
1	A	46	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

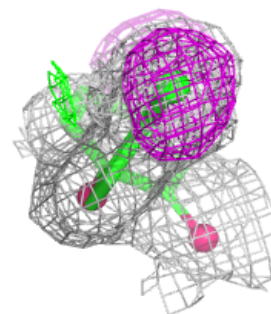
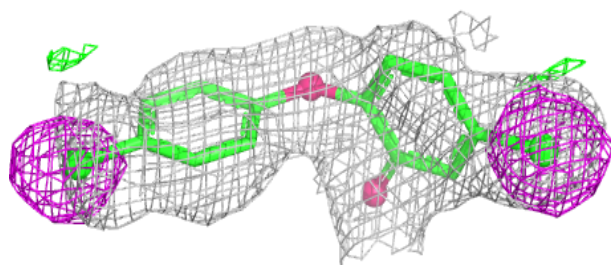
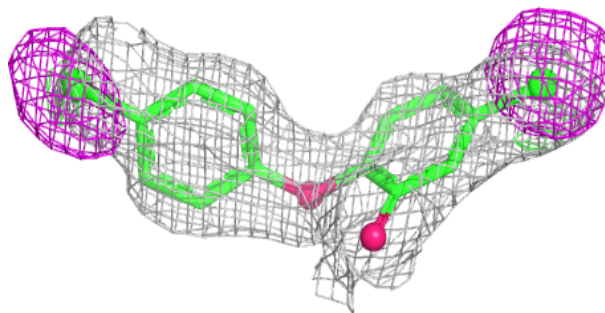
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	DCN	B	3414	16/16	0.80	0.15	6,26,29,30	0
3	DCN	C	4414	16/16	0.81	0.16	11,26,29,30	0
3	DCN	D	5414	16/16	0.83	0.15	6,26,30,32	0
3	DCN	A	2414	16/16	0.85	0.13	11,28,33,33	0
2	NAD	A	1780	44/44	0.92	0.09	20,28,31,34	0
2	NAD	B	2780	44/44	0.92	0.08	16,24,28,30	0
2	NAD	C	3780	44/44	0.93	0.08	18,23,27,28	0
2	NAD	D	4780	44/44	0.93	0.08	18,27,31,32	0

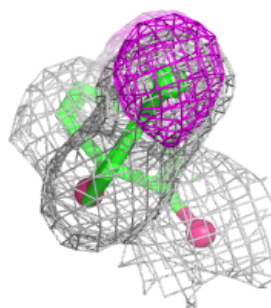
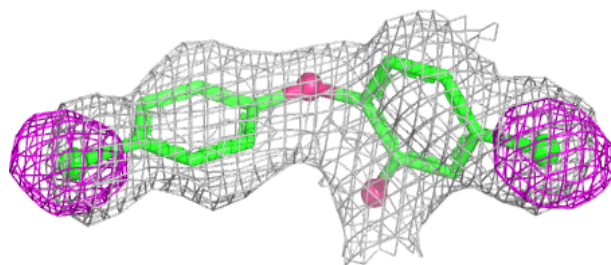
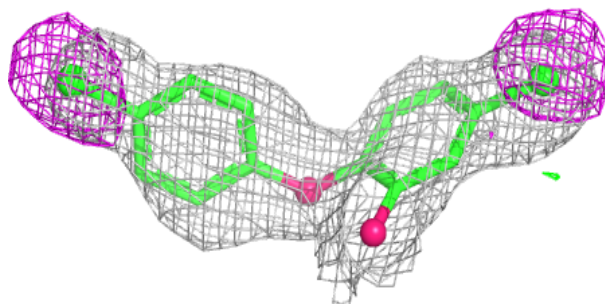
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DCN 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)

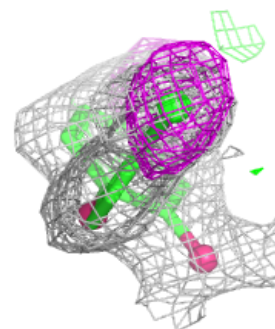
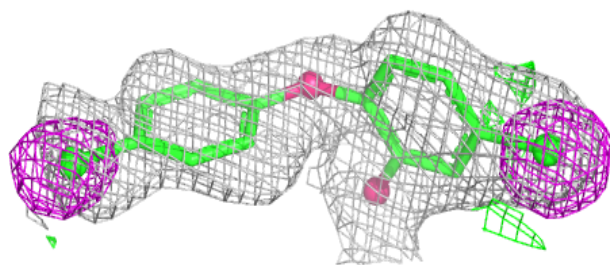
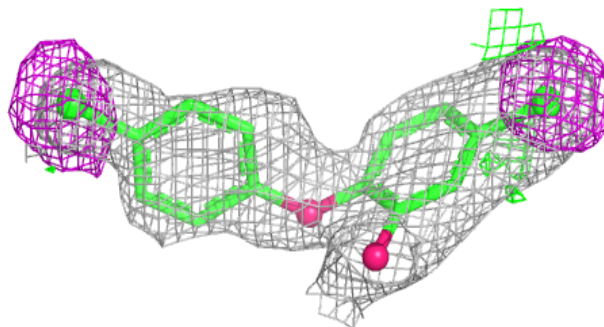
**Electron density around DCN C 4414:**

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

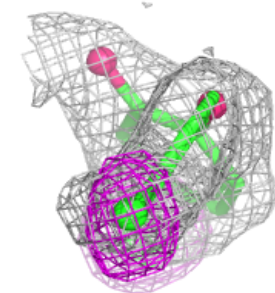
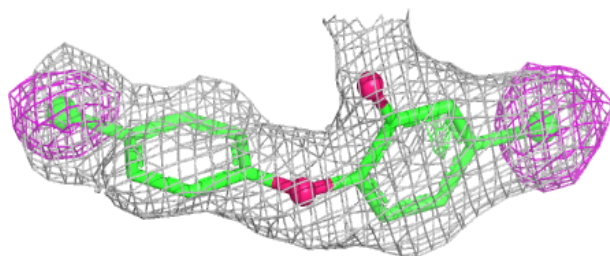
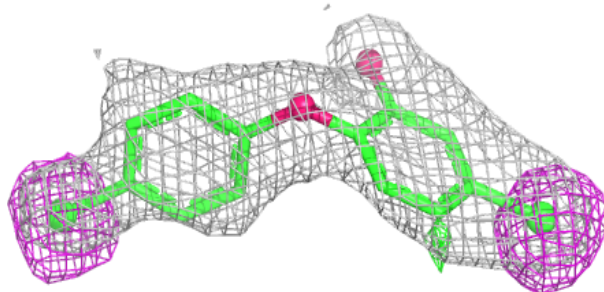


Electron density around DCN D 5414:

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

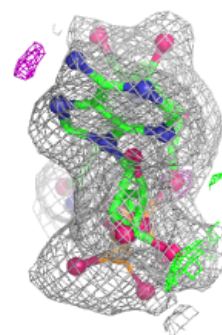
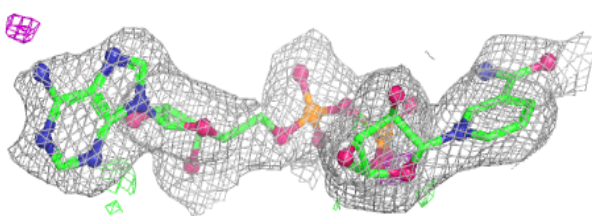
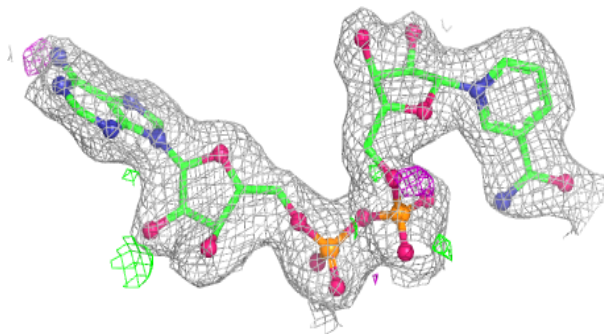
**Electron density around DCN A 2414:**

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

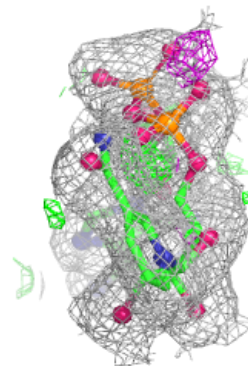
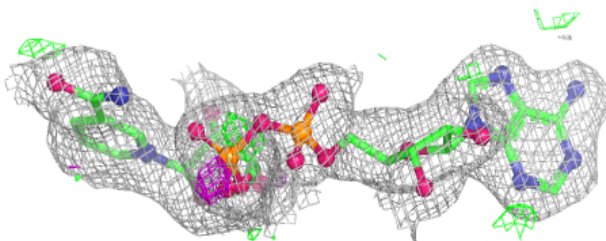
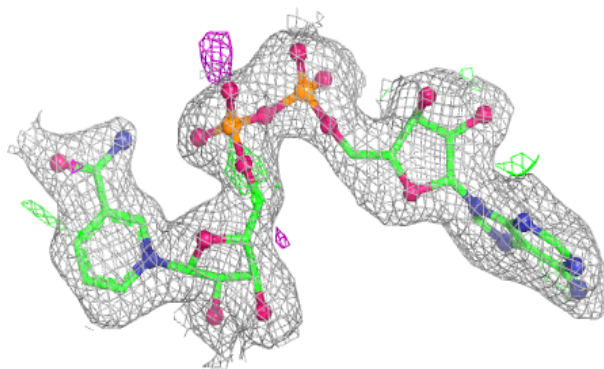


Electron density around NAD A 1780:

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

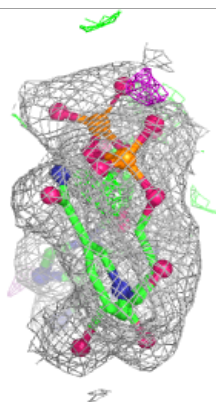
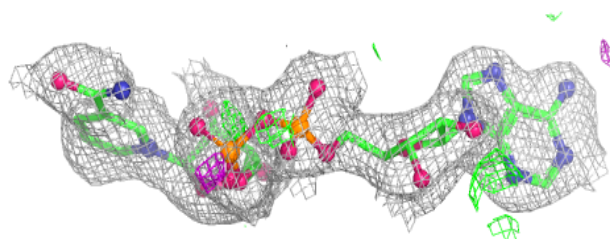
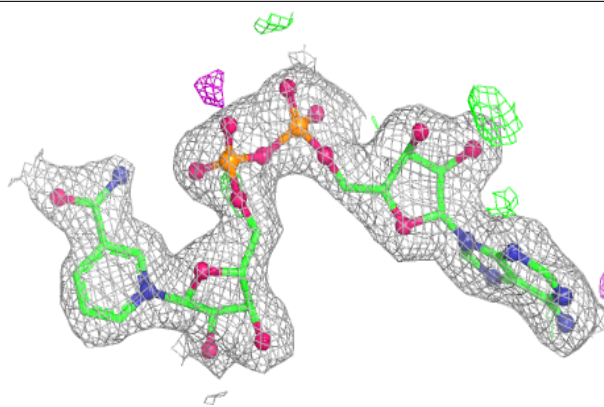
**Electron density around NAD B 2780:**

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

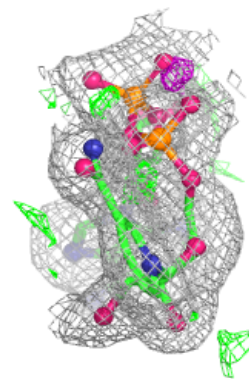
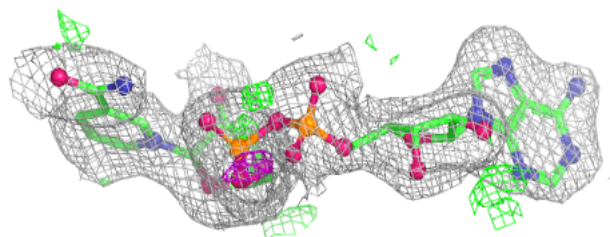
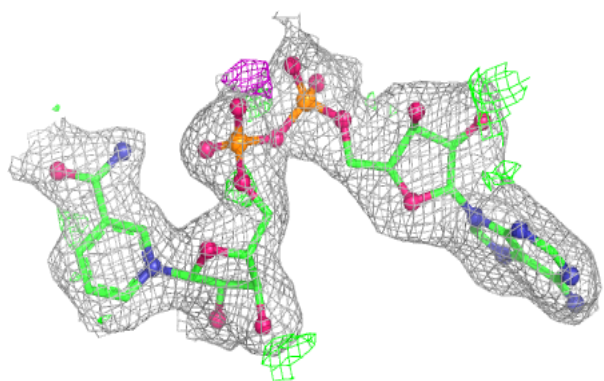


Electron density around NAD C 3780:

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

**Electron density around NAD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.