



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:37 AM UTC

PDB ID : 3DMT / pdb_00003dmt
Title : Structure of Glycosomal Glyceraldehyde-3-Phosphate Dehydrogenase from Trypanosoma cruzi in complex with the irreversible iodoacetate inhibitor
Authors : Guido, R.V.C.; Balliano, T.L.; Andricopulo, A.D.; Oliva, G.
Deposited on : 2008-07-01
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)
Xtriage (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

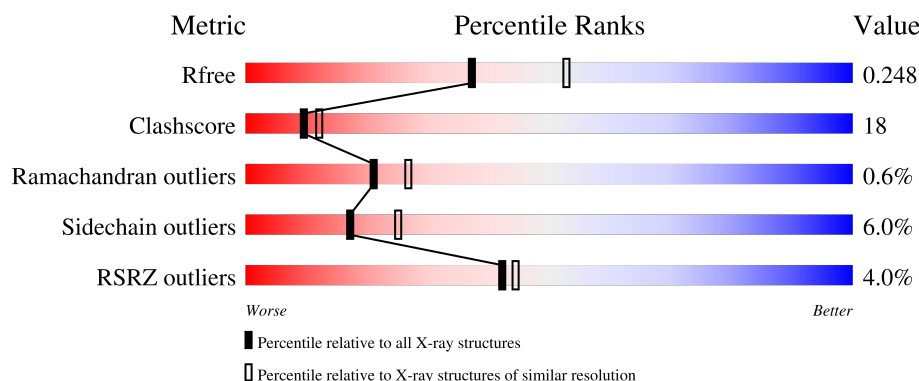
1 Overall quality at a glance

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	359	7% 67% 30% .
1	B	359	3% 68% 29% .
1	D	359	5% 71% 26% .
2	C	359	% 66% 29% 5%

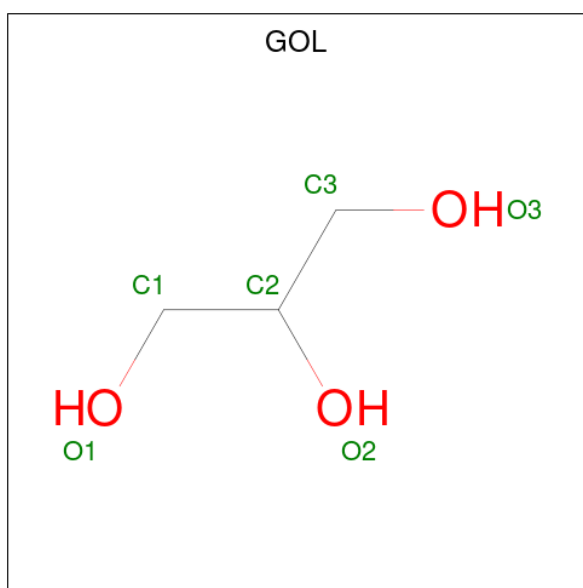
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

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
4	GOL	C	361	-	-	X	X

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		

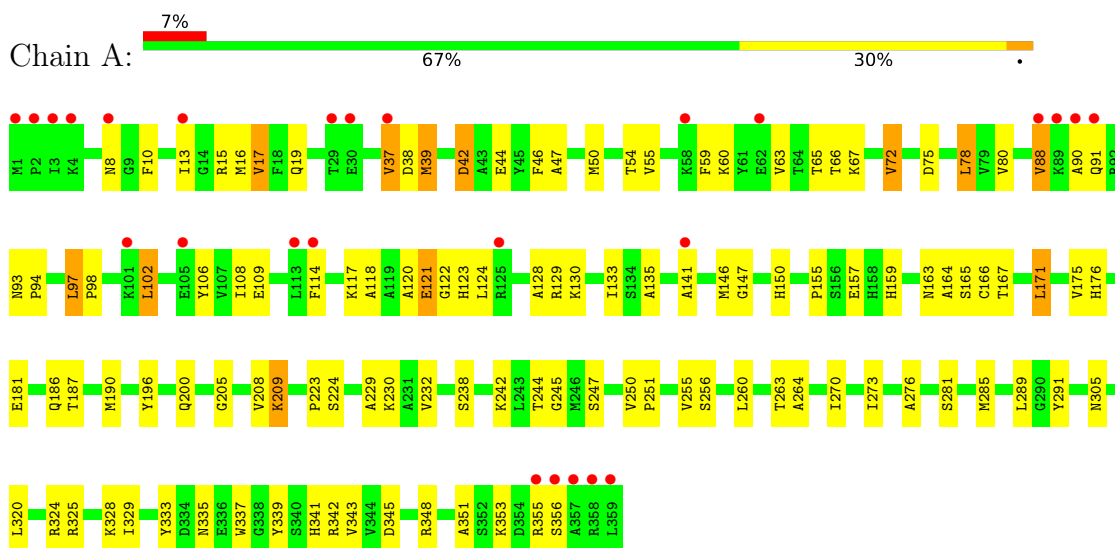
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	195	Total	O	0	0
			195	195		
5	B	294	Total	O	0	0
			294	294		
5	C	297	Total	O	0	0
			297	297		
5	D	219	Total	O	0	0
			219	219		

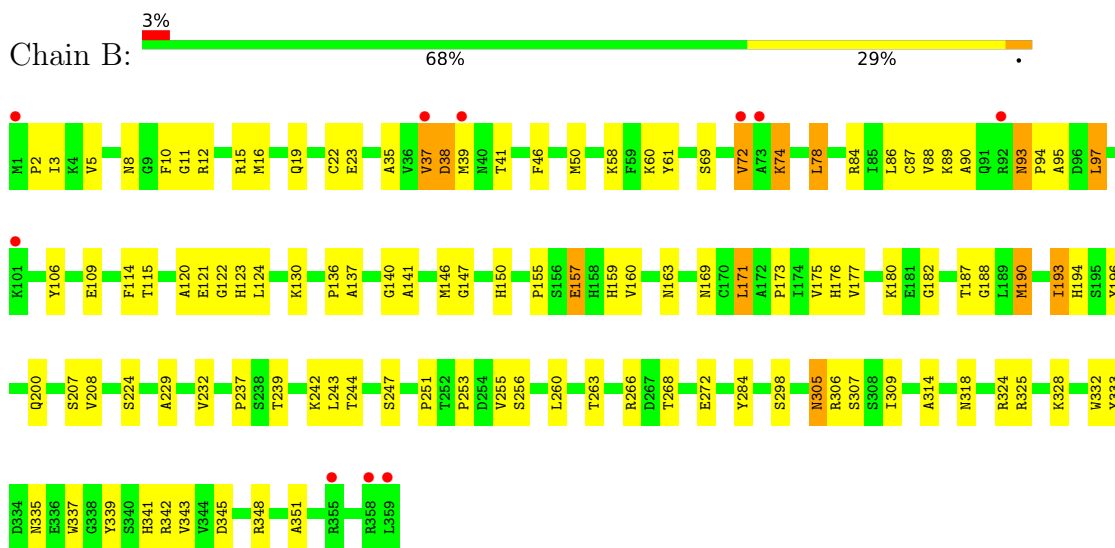
3 Residue-property plots [i](#)

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: Glyceraldehyde-3-phosphate dehydrogenase, glycosomal

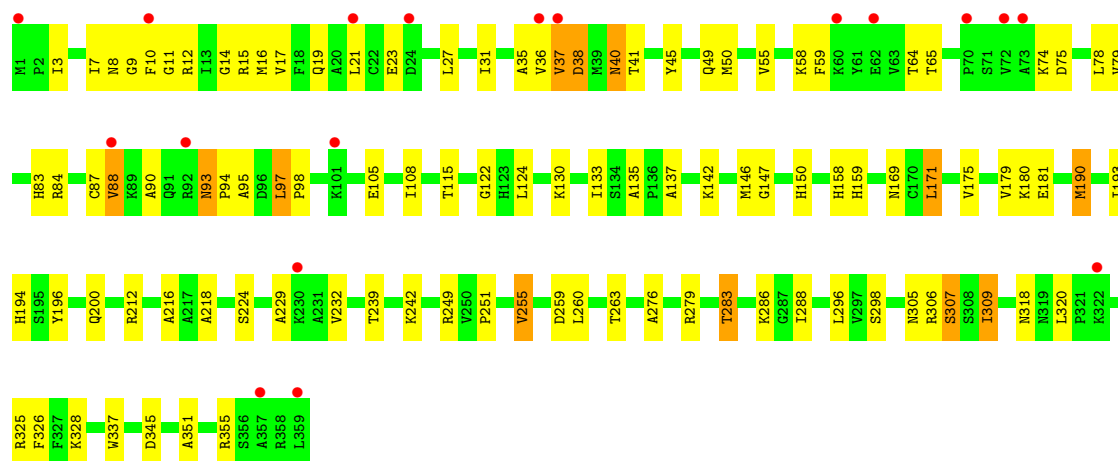


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, glycosomal

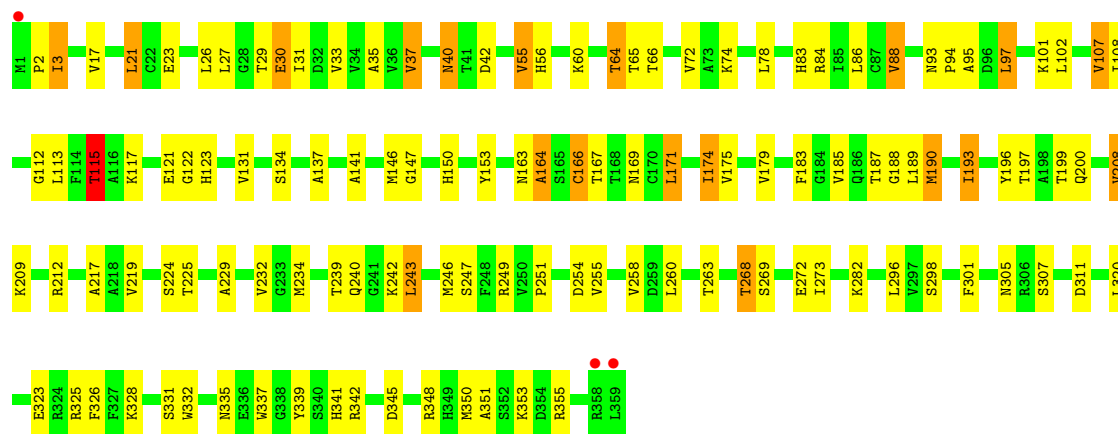


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase, glycosomal





• Molecule 2: Glyceraldehyde-3-phosphate dehydrogenase, glycosomal



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.75Å 83.71Å 105.61Å 90.00° 96.44° 90.00°	Depositor
Resolution (Å)	38.10 – 2.30 38.10 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.5 (38.10-2.30) 96.5 (38.10-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.62 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX (phenix.refine)	Depositor
R, R_{free}	0.186 , 0.252 0.185 , 0.248	Depositor DCC
R_{free} test set	2987 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12123	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CCS, 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	0.71	0/2786	0.94	5/3778 (0.1%)
1	B	0.73	0/2786	0.97	4/3778 (0.1%)
1	D	0.69	0/2786	0.94	4/3778 (0.1%)
2	C	0.75	0/2779	0.97	2/3767 (0.1%)
All	All	0.72	0/11137	0.95	15/15101 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	115	THR	N-CA-C	-7.49	104.29	113.50
1	B	93	ASN	CA-C-N	5.92	127.24	119.84
1	B	93	ASN	C-N-CA	5.92	127.24	119.84
1	D	288	ILE	N-CA-C	-5.52	106.81	111.56
1	A	17	VAL	N-CA-C	-5.48	105.16	110.42
1	A	93	ASN	CA-C-N	5.36	126.54	119.84
1	A	93	ASN	C-N-CA	5.36	126.54	119.84
1	A	250	VAL	CA-C-N	5.34	126.52	119.84
1	A	250	VAL	C-N-CA	5.34	126.52	119.84
1	B	69	SER	CA-C-N	5.17	124.83	119.56
1	B	69	SER	C-N-CA	5.17	124.83	119.56
2	C	225	THR	N-CA-C	-5.17	103.70	110.53
1	D	283	THR	CB-CA-C	-5.11	109.07	116.54
1	D	93	ASN	CA-C-N	5.05	125.33	119.47
1	D	93	ASN	C-N-CA	5.05	125.33	119.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2733	0	2721	89	0
1	B	2733	0	2722	98	0
1	D	2733	0	2722	95	0
2	C	2737	0	2723	120	0
3	A	44	0	26	5	0
3	B	44	0	26	3	0
3	C	44	0	26	7	0
3	D	44	0	26	3	0
4	C	6	0	8	5	0
5	A	195	0	0	13	0
5	B	294	0	0	15	0
5	C	297	0	0	21	0
5	D	219	0	0	10	0
All	All	12123	0	11000	387	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 18.

All (387) 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:A:16:MET:HG2	5:A:435:HOH:O	1.41	1.18
1:B:37:VAL:HG22	3:B:360:NAD:H2A	1.40	0.99
1:A:305:ASN:HB3	5:A:535:HOH:O	1.72	0.88
1:A:47:ALA:HA	1:A:50:MET:HE3	1.58	0.84
1:D:37:VAL:HG22	3:D:360:NAD:H2A	1.57	0.83
1:A:66:THR:HG22	5:A:480:HOH:O	1.80	0.82
2:C:311:ASP:HB2	5:C:445:HOH:O	1.79	0.81
1:A:50:MET:HE1	1:A:78:LEU:HG	1.63	0.81
1:A:147:GLY:H	1:A:150:HIS:HD2	1.29	0.80
1:D:16:MET:HG2	5:D:471:HOH:O	1.80	0.79
1:B:19:GLN:HG3	5:B:375:HOH:O	1.83	0.79
2:C:3:ILE:HG22	2:C:355:ARG:HH21	1.47	0.78
2:C:37:VAL:HG22	3:C:360:NAD:H2A	1.64	0.78
1:D:8:ASN:HA	1:D:37:VAL:HG13	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:PHE:HE2	1:D:50:MET:HE2	1.49	0.77
2:C:147:GLY:H	2:C:150:HIS:HD2	1.31	0.77
2:C:171:LEU:HD13	2:C:232:VAL:HG21	1.67	0.77
1:A:190:MET:HG2	1:A:229:ALA:HB2	1.68	0.76
2:C:190:MET:HG2	2:C:229:ALA:HB2	1.66	0.76
1:B:2:PRO:HB3	5:B:531:HOH:O	1.86	0.76
1:A:186:GLN:HB2	1:A:263:THR:HG23	1.68	0.76
2:C:239:THR:HA	2:C:242:LYS:HE2	1.68	0.75
2:C:147:GLY:H	2:C:150:HIS:CD2	2.04	0.75
1:A:171:LEU:HG	1:A:190:MET:HE2	1.67	0.75
2:C:101:LYS:HG3	5:C:430:HOH:O	1.86	0.75
1:A:176:HIS:HD2	5:A:425:HOH:O	1.68	0.74
1:B:190:MET:HG2	1:B:229:ALA:HB2	1.68	0.74
2:C:26:LEU:HD22	2:C:30:GLU:HG3	1.68	0.74
1:D:147:GLY:H	1:D:150:HIS:CD2	2.06	0.74
1:B:37:VAL:CG2	3:B:360:NAD:H2A	2.17	0.74
1:B:176:HIS:HE1	5:B:411:HOH:O	1.72	0.73
2:C:188:GLY:HA3	2:C:243:LEU:HD13	1.70	0.73
1:A:147:GLY:H	1:A:150:HIS:CD2	2.05	0.73
1:A:238:SER:O	1:A:242:LYS:HE2	1.89	0.72
1:A:171:LEU:HD13	1:A:232:VAL:HG21	1.72	0.71
2:C:37:VAL:HB	2:C:88:VAL:HG22	1.71	0.71
2:C:107:VAL:HG11	2:C:123:HIS:HB3	1.71	0.71
1:B:348:ARG:HD2	5:B:510:HOH:O	1.91	0.71
2:C:199:THR:HG23	4:C:361:GOL:H32	1.71	0.70
2:C:268:THR:HG22	2:C:269:SER:H	1.54	0.70
1:B:115:THR:HG23	1:B:136:PRO:O	1.92	0.70
1:D:50:MET:HE1	1:D:78:LEU:HG	1.74	0.69
1:D:37:VAL:CG2	3:D:360:NAD:H2A	2.23	0.68
2:C:174:ILE:HD11	2:C:331:SER:HB2	1.74	0.68
1:A:190:MET:HG3	1:A:245:GLY:HA3	1.76	0.68
1:A:263:THR:HA	1:A:325:ARG:O	1.95	0.66
2:C:94:PRO:HA	2:C:97:LEU:HD22	1.78	0.66
1:D:21:LEU:HD11	1:D:31:ILE:HD13	1.78	0.65
1:B:50:MET:HE1	1:B:78:LEU:HG	1.78	0.65
2:C:331:SER:HA	5:C:445:HOH:O	1.96	0.65
1:B:10:PHE:HE2	1:B:50:MET:HE2	1.60	0.65
1:D:38:ASP:O	1:D:90:ALA:HB2	1.96	0.65
1:D:171:LEU:HD22	1:D:175:VAL:HG23	1.80	0.64
1:A:42:ASP:O	1:A:46:PHE:HD1	1.80	0.64
1:B:74:LYS:HG3	5:B:410:HOH:O	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLY:O	1:B:266:ARG:HD3	1.97	0.64
1:A:171:LEU:HD22	1:A:175:VAL:HG23	1.80	0.64
1:D:93:ASN:OD1	1:D:95:ALA:HB3	1.98	0.63
1:B:171:LEU:HD22	1:B:175:VAL:HG23	1.81	0.63
2:C:23:GLU:OE1	5:C:650:HOH:O	2.16	0.63
2:C:117:LYS:O	2:C:121:GLU:HG3	1.98	0.63
1:D:10:PHE:CE2	1:D:50:MET:HE2	2.33	0.63
1:B:157:GLU:HG3	5:B:459:HOH:O	1.99	0.63
1:A:8:ASN:HA	1:A:37:VAL:HG13	1.80	0.62
1:B:78:LEU:HD22	1:B:87:CYS:SG	2.38	0.62
1:B:171:LEU:HD13	1:B:232:VAL:HG21	1.81	0.62
1:A:114:PHE:O	1:A:120:ALA:HB2	2.00	0.62
1:A:117:LYS:HG3	1:A:141:ALA:HB2	1.82	0.62
2:C:239:THR:HB	2:C:243:LEU:HD23	1.82	0.61
1:D:169:ASN:O	1:D:307:SER:HB2	1.99	0.61
2:C:196:TYR:HA	2:C:200:GLN:NE2	2.15	0.61
2:C:171:LEU:HD22	2:C:175:VAL:HG23	1.82	0.61
1:A:47:ALA:HA	1:A:50:MET:CE	2.31	0.61
1:D:181:GLU:HG3	1:D:276:ALA:HB1	1.84	0.60
1:B:147:GLY:H	1:B:150:HIS:CD2	2.20	0.60
1:B:23:GLU:OE2	1:B:341:HIS:CE1	2.55	0.59
1:D:19:GLN:HG3	1:D:59:PHE:CE1	2.37	0.59
1:A:285:MET:HB3	1:A:289:LEU:HB3	1.84	0.59
1:D:171:LEU:HD13	1:D:232:VAL:HG21	1.85	0.59
1:A:167:THR:HG22	1:A:190:MET:HE1	1.85	0.59
2:C:341:HIS:HE1	5:C:650:HOH:O	1.85	0.59
2:C:84:ARG:NH2	5:C:498:HOH:O	2.34	0.59
1:D:306:ARG:HB2	1:D:309:ILE:CD1	2.33	0.58
1:B:306:ARG:HB2	1:B:309:ILE:CD1	2.32	0.58
1:D:45:TYR:O	1:D:49:GLN:HG3	2.04	0.58
1:A:38:ASP:O	1:A:90:ALA:HB2	2.03	0.58
1:D:283:THR:O	1:D:286:LYS:HB2	2.04	0.58
2:C:185:VAL:O	2:C:242:LYS:HE3	2.03	0.58
1:B:137:ALA:HB3	1:B:141:ALA:HB3	1.85	0.58
1:A:281:SER:HG	1:A:291:TYR:HD1	1.50	0.57
1:B:46:PHE:C	1:B:50:MET:HE3	2.28	0.57
1:D:224:SER:HB2	1:D:249:ARG:NH2	2.20	0.57
2:C:94:PRO:HA	2:C:97:LEU:CD2	2.35	0.57
1:D:147:GLY:H	1:D:150:HIS:HD2	1.53	0.57
1:D:64:THR:HG22	1:D:65:THR:H	1.69	0.57
1:A:146:MET:HE2	1:A:345:ASP:HB3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:107:VAL:HG11	2:C:123:HIS:CB	2.35	0.57
1:D:190:MET:HG2	1:D:229:ALA:HB2	1.87	0.56
1:B:207:SER:HB2	5:B:542:HOH:O	2.05	0.56
2:C:260:LEU:O	2:C:328:LYS:HA	2.05	0.56
1:B:266:ARG:NH2	1:B:272:GLU:OE1	2.36	0.56
2:C:351:ALA:O	2:C:355:ARG:HG2	2.06	0.56
1:A:39:MET:HE1	3:A:360:NAD:C8A	2.35	0.56
1:B:38:ASP:O	1:B:90:ALA:HB2	2.06	0.56
2:C:196:TYR:HA	2:C:200:GLN:HE22	1.71	0.56
1:A:15:ARG:O	1:A:19:GLN:HG3	2.07	0.55
1:D:64:THR:HG22	1:D:65:THR:N	2.21	0.55
1:D:84:ARG:NH2	5:D:444:HOH:O	2.39	0.55
2:C:332:TRP:CD1	5:C:445:HOH:O	2.59	0.55
2:C:112:GLY:HA2	3:C:360:NAD:O3D	2.07	0.55
1:B:306:ARG:HB2	1:B:309:ILE:HD11	1.88	0.54
1:A:17:VAL:HG11	1:A:108:ILE:HD13	1.90	0.54
1:A:320:LEU:HD13	1:B:187:THR:HG23	1.89	0.54
2:C:197:THR:OG1	4:C:361:GOL:H11	2.07	0.54
1:B:86:LEU:HD23	1:B:88:VAL:HG12	1.89	0.54
1:B:150:HIS:HE1	5:B:471:HOH:O	1.89	0.54
1:A:348:ARG:HD2	5:A:422:HOH:O	2.08	0.54
2:C:21:LEU:HD11	2:C:31:ILE:HD13	1.89	0.54
2:C:171:LEU:HD12	2:C:229:ALA:HA	1.89	0.54
1:A:165:SER:HB2	5:A:511:HOH:O	2.07	0.54
1:A:260:LEU:O	1:A:328:LYS:HA	2.08	0.54
2:C:197:THR:OG1	4:C:361:GOL:H31	2.08	0.54
1:B:94:PRO:HA	1:B:97:LEU:HD22	1.90	0.54
2:C:234:MET:HE2	5:C:403:HOH:O	2.08	0.54
1:A:196:TYR:HA	1:A:200:GLN:NE2	2.22	0.54
1:A:166:CYS:HB3	3:A:360:NAD:H5N	1.90	0.53
2:C:174:ILE:HD11	2:C:331:SER:CB	2.38	0.53
2:C:183:PHE:CD1	2:C:268:THR:HG21	2.44	0.53
2:C:282:LYS:HE2	5:C:580:HOH:O	2.08	0.53
1:A:118:ALA:O	1:A:121:GLU:HB2	2.09	0.53
1:A:124:LEU:HA	1:A:128:ALA:O	2.09	0.53
1:A:251:PRO:HB2	1:B:251:PRO:HB2	1.91	0.53
1:B:239:THR:HA	1:B:242:LYS:HD2	1.91	0.53
2:C:146:MET:HB2	2:C:342:ARG:HD3	1.90	0.53
1:A:130:LYS:NZ	1:A:159:HIS:HD2	2.07	0.52
2:C:35:ALA:HB1	2:C:88:VAL:HG13	1.90	0.52
3:A:360:NAD:O2N	3:A:360:NAD:N7N	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:MET:HA	1:B:39:MET:HE3	1.91	0.52
2:C:55:VAL:HG22	2:C:56:HIS:CD2	2.43	0.52
1:D:196:TYR:HA	1:D:200:GLN:NE2	2.24	0.52
1:B:196:TYR:HA	1:B:200:GLN:NE2	2.25	0.52
2:C:2:PRO:HB3	2:C:29:THR:O	2.10	0.52
2:C:167:THR:HG21	2:C:190:MET:HE1	1.92	0.52
1:A:320:LEU:HG	1:B:244:THR:HG22	1.90	0.52
1:D:159:HIS:HE1	5:D:485:HOH:O	1.91	0.52
1:A:273:ILE:HG21	1:A:329:ILE:HD11	1.92	0.52
2:C:337:TRP:O	2:C:341:HIS:HD2	1.93	0.52
1:B:188:GLY:HA3	1:B:243:LEU:HD23	1.92	0.52
1:A:16:MET:SD	1:A:337:TRP:HZ3	2.33	0.52
1:D:351:ALA:O	1:D:355:ARG:HD3	2.10	0.51
2:C:320:LEU:HB2	2:C:323:GLU:HB2	1.92	0.51
1:B:84:ARG:NH2	5:B:495:HOH:O	2.42	0.51
2:C:72:VAL:HG12	2:C:74:LYS:O	2.11	0.51
1:D:78:LEU:HD22	1:D:87:CYS:SG	2.50	0.51
1:A:229:ALA:HB3	1:A:244:THR:HA	1.92	0.51
1:A:339:TYR:O	1:A:343:VAL:HG23	2.11	0.51
2:C:323:GLU:HG2	2:C:326:PHE:O	2.10	0.51
2:C:17:VAL:HG11	2:C:108:ILE:HD13	1.92	0.51
2:C:166:CCS:HD2	3:C:360:NAD:C4N	2.40	0.51
2:C:208:VAL:HG23	5:C:408:HOH:O	2.10	0.51
1:B:93:ASN:C	1:B:93:ASN:HD22	2.18	0.51
2:C:326:PHE:HE1	1:D:326:PHE:CE1	2.29	0.51
1:B:208:VAL:HG22	5:B:446:HOH:O	2.11	0.51
1:B:260:LEU:O	1:B:328:LYS:HA	2.11	0.51
2:C:263:THR:HA	2:C:325:ARG:O	2.11	0.51
1:B:58:LYS:HG3	5:D:451:HOH:O	2.12	0.50
2:C:40:ASN:C	2:C:40:ASN:HD22	2.20	0.50
3:D:360:NAD:N7N	3:D:360:NAD:O2N	2.44	0.50
2:C:268:THR:HG22	2:C:272:GLU:HB3	1.93	0.50
2:C:193:ILE:HD12	1:D:193:ILE:HG13	1.93	0.50
1:B:50:MET:HE1	1:B:78:LEU:CG	2.41	0.50
2:C:33:VAL:H	2:C:83:HIS:HE1	1.58	0.50
1:B:169:ASN:O	1:B:307:SER:HB3	2.11	0.50
2:C:153:TYR:CE2	2:C:350:MET:HA	2.46	0.50
1:A:230:LYS:HE2	5:A:388:HOH:O	2.11	0.50
1:D:181:GLU:OE2	1:D:279:ARG:NH2	2.45	0.49
1:B:93:ASN:C	1:B:93:ASN:ND2	2.70	0.49
1:B:194:HIS:HA	1:B:256:SER:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:GLN:HG3	1:D:59:PHE:CD1	2.47	0.49
1:D:224:SER:HB2	1:D:249:ARG:CZ	2.43	0.49
1:A:121:GLU:O	1:A:124:LEU:HB2	2.13	0.49
1:D:40:ASN:H	1:D:40:ASN:ND2	2.09	0.49
1:A:91:GLN:HG2	1:A:97:LEU:HD13	1.95	0.49
1:B:314:ALA:O	1:B:318:ASN:ND2	2.41	0.49
2:C:296:LEU:O	1:D:212:ARG:HD3	2.12	0.49
1:D:159:HIS:CE1	5:D:485:HOH:O	2.66	0.49
1:B:146:MET:HB2	1:B:342:ARG:HD3	1.93	0.49
2:C:224:SER:HB3	2:C:247:SER:HB3	1.95	0.49
1:B:266:ARG:NH1	5:B:477:HOH:O	2.46	0.48
3:C:360:NAD:N7N	3:C:360:NAD:O2N	2.44	0.48
1:B:146:MET:HE2	1:B:345:ASP:HB3	1.94	0.48
2:C:326:PHE:CE1	1:D:326:PHE:CE1	3.02	0.48
2:C:240:GLN:NE2	5:C:485:HOH:O	2.47	0.48
1:D:146:MET:HE2	1:D:345:ASP:HB3	1.95	0.48
2:C:301:PHE:CZ	2:C:332:TRP:CD1	3.02	0.48
1:B:193:ILE:HD12	1:B:193:ILE:N	2.28	0.48
1:B:94:PRO:HB3	1:B:123:HIS:CE1	2.48	0.48
1:B:130:LYS:NZ	1:B:159:HIS:HD2	2.11	0.48
2:C:35:ALA:HB1	2:C:88:VAL:CG1	2.43	0.48
1:A:337:TRP:O	1:A:341:HIS:HD2	1.96	0.48
1:A:106:TYR:OH	1:A:351:ALA:HA	2.14	0.48
1:A:205:GLY:HA2	5:A:515:HOH:O	2.14	0.48
1:A:256:SER:HB2	1:A:333:TYR:CZ	2.49	0.48
1:D:10:PHE:CE1	1:D:36:VAL:HG11	2.49	0.48
1:A:129:ARG:HG3	1:A:130:LYS:HG2	1.96	0.47
1:B:23:GLU:HA	1:B:60:LYS:HD3	1.96	0.47
1:B:8:ASN:HA	1:B:37:VAL:HG13	1.95	0.47
1:A:37:VAL:HB	1:A:88:VAL:HG22	1.96	0.47
1:B:130:LYS:NZ	1:B:155:PRO:O	2.47	0.47
2:C:95:ALA:HA	2:C:122:GLY:O	2.13	0.47
1:A:94:PRO:HB2	1:A:122:GLY:HA3	1.95	0.47
2:C:268:THR:HG23	2:C:272:GLU:OE2	2.15	0.47
2:C:341:HIS:CE1	5:C:650:HOH:O	2.64	0.47
1:A:37:VAL:HG22	3:A:360:NAD:H2A	1.97	0.47
1:B:176:HIS:CD2	5:B:647:HOH:O	2.68	0.47
1:A:263:THR:HG21	5:A:476:HOH:O	2.14	0.47
1:D:298:SER:HB2	5:D:445:HOH:O	2.14	0.47
1:A:130:LYS:HZ1	1:A:159:HIS:HD2	1.61	0.47
1:D:37:VAL:HG22	1:D:37:VAL:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:SER:HB3	1:B:247:SER:HB3	1.97	0.46
2:C:197:THR:HG21	4:C:361:GOL:H11	1.97	0.46
1:A:209:LYS:HE3	1:A:209:LYS:HA	1.95	0.46
1:B:50:MET:HG2	5:B:375:HOH:O	2.15	0.46
1:D:65:THR:HB	1:D:75:ASP:HB3	1.98	0.46
1:A:10:PHE:CE2	1:A:15:ARG:HG2	2.50	0.46
1:B:23:GLU:OE2	1:B:341:HIS:HE1	1.97	0.46
2:C:134:SER:O	3:C:360:NAD:H6N	2.16	0.46
2:C:115:THR:HG22	5:C:461:HOH:O	2.16	0.46
1:B:58:LYS:HE3	5:D:451:HOH:O	2.16	0.46
1:D:11:GLY:O	1:D:15:ARG:HB2	2.16	0.46
1:B:12:ARG:HH11	1:B:15:ARG:NH2	2.13	0.46
2:C:339:TYR:CG	3:C:360:NAD:H5N	2.50	0.46
1:A:155:PRO:HG3	1:A:353:LYS:O	2.16	0.46
1:D:11:GLY:O	1:D:12:ARG:C	2.56	0.46
1:D:94:PRO:HA	1:D:97:LEU:HD23	1.98	0.46
1:D:130:LYS:NZ	1:D:159:HIS:HD2	2.13	0.46
1:B:121:GLU:HG3	1:B:160:VAL:HG21	1.97	0.45
2:C:239:THR:HB	2:C:243:LEU:CD2	2.46	0.45
1:B:16:MET:SD	1:B:337:TRP:HZ3	2.40	0.45
1:B:106:TYR:OH	1:B:351:ALA:HA	2.16	0.45
2:C:187:THR:HG23	1:D:320:LEU:CD1	2.47	0.45
1:D:298:SER:CB	5:D:445:HOH:O	2.64	0.45
1:A:98:PRO:HG2	1:A:102:LEU:HD22	1.98	0.45
1:D:17:VAL:O	1:D:21:LEU:HB2	2.17	0.45
1:B:263:THR:HA	1:B:325:ARG:O	2.17	0.45
1:D:17:VAL:HG11	1:D:108:ILE:HD13	1.99	0.45
1:A:54:THR:HG21	1:D:216:ALA:HB3	1.99	0.45
1:A:223:PRO:CG	1:B:332:TRP:HZ2	2.29	0.45
2:C:200:GLN:CD	2:C:249:ARG:HD2	2.42	0.45
1:D:196:TYR:HA	1:D:200:GLN:HE22	1.81	0.45
1:A:181:GLU:HG3	1:A:276:ALA:HB1	1.98	0.45
2:C:183:PHE:CE1	2:C:268:THR:HG21	2.51	0.45
1:A:50:MET:O	1:A:59:PHE:HB2	2.16	0.45
2:C:348:ARG:HD2	5:C:503:HOH:O	2.17	0.45
1:A:176:HIS:CD2	5:A:425:HOH:O	2.55	0.45
1:B:3:ILE:HG22	1:B:5:VAL:HG23	1.99	0.45
1:A:133:ILE:C	1:A:135:ALA:H	2.25	0.44
2:C:93:ASN:HD22	2:C:94:PRO:HD2	1.82	0.44
2:C:137:ALA:HB3	2:C:141:ALA:HB3	1.99	0.44
2:C:188:GLY:O	2:C:243:LEU:HA	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:LYS:NZ	1:D:159:HIS:CD2	2.86	0.44
1:A:109:GLU:OE2	1:A:123:HIS:NE2	2.48	0.44
1:A:320:LEU:CD1	1:B:187:THR:CG2	2.95	0.44
1:D:21:LEU:HD11	1:D:31:ILE:CD1	2.46	0.44
1:D:181:GLU:CD	1:D:279:ARG:HH21	2.26	0.44
1:B:16:MET:SD	1:B:337:TRP:CZ3	3.11	0.44
2:C:187:THR:HG21	1:D:326:PHE:HB3	2.00	0.44
1:D:21:LEU:CD1	1:D:31:ILE:HD13	2.46	0.44
1:D:50:MET:O	1:D:59:PHE:HB2	2.17	0.44
2:C:187:THR:CG2	1:D:320:LEU:CD1	2.96	0.44
1:D:171:LEU:HD21	1:D:260:LEU:HD13	2.00	0.44
1:B:196:TYR:HA	1:B:200:GLN:HE22	1.82	0.44
1:D:263:THR:HA	1:D:325:ARG:O	2.16	0.44
1:B:12:ARG:HH11	1:B:15:ARG:HH21	1.65	0.44
2:C:115:THR:CG2	5:C:461:HOH:O	2.66	0.44
2:C:200:GLN:HB3	2:C:217:ALA:HB2	1.99	0.44
1:D:23:GLU:OE1	1:D:337:TRP:CZ2	2.70	0.44
1:D:259:ASP:OD1	1:D:328:LYS:HE3	2.18	0.44
1:A:320:LEU:CD1	1:B:187:THR:HG23	2.47	0.44
1:B:256:SER:HB2	1:B:333:TYR:CZ	2.53	0.44
2:C:27:LEU:HB2	5:C:469:HOH:O	2.17	0.44
2:C:146:MET:HE2	2:C:345:ASP:HB3	1.99	0.44
1:A:13:ILE:O	1:A:17:VAL:HG23	2.18	0.44
1:A:130:LYS:NZ	1:A:159:HIS:CD2	2.85	0.44
1:A:196:TYR:HA	1:A:200:GLN:HE22	1.80	0.44
1:D:218:ALA:O	1:D:251:PRO:HB3	2.18	0.44
1:A:167:THR:CG2	1:A:190:MET:HE1	2.46	0.43
1:A:176:HIS:HE1	5:A:451:HOH:O	2.00	0.43
1:B:114:PHE:O	1:B:120:ALA:HB2	2.17	0.43
2:C:40:ASN:ND2	2:C:42:ASP:H	2.16	0.43
2:C:163:ASN:O	2:C:164:ALA:HB3	2.17	0.43
2:C:212:ARG:HD3	1:D:296:LEU:O	2.18	0.43
1:D:255:VAL:HG11	1:D:298:SER:O	2.19	0.43
1:A:63:VAL:HG22	1:A:80:VAL:HG22	2.01	0.43
1:B:93:ASN:HD22	1:B:94:PRO:HD2	1.83	0.43
2:C:30:GLU:OE2	2:C:348:ARG:NH1	2.51	0.43
1:A:335:ASN:O	3:A:360:NAD:H4N	2.18	0.43
1:D:260:LEU:O	1:D:328:LYS:HA	2.18	0.43
2:C:107:VAL:HG13	2:C:131:VAL:HG22	2.00	0.43
1:B:298:SER:HB3	1:B:332:TRP:HZ3	1.84	0.43
1:D:133:ILE:C	1:D:135:ALA:H	2.27	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:LYS:HD2	1:D:180:LYS:N	2.32	0.43
2:C:64:THR:CG2	2:C:65:THR:N	2.81	0.43
1:A:67:LYS:HB3	1:A:72:VAL:HG22	2.01	0.42
1:A:190:MET:O	1:A:245:GLY:HA3	2.19	0.42
1:B:305:ASN:C	1:B:305:ASN:HD22	2.27	0.42
2:C:55:VAL:HG21	2:C:254:ASP:CB	2.49	0.42
2:C:268:THR:CG2	2:C:269:SER:H	2.23	0.42
2:C:305:ASN:HB3	5:C:393:HOH:O	2.19	0.42
2:C:335:ASN:O	3:C:360:NAD:H4N	2.18	0.42
2:C:101:LYS:HE3	5:C:430:HOH:O	2.19	0.42
2:C:298:SER:HB3	2:C:332:TRP:HZ3	1.84	0.42
1:A:44:GLU:HG2	5:A:429:HOH:O	2.19	0.42
1:A:65:THR:HB	1:A:75:ASP:HB3	2.01	0.42
1:B:140:GLY:HA2	5:B:636:HOH:O	2.19	0.42
1:B:237:PRO:HD2	5:B:551:HOH:O	2.19	0.42
2:C:183:PHE:CD1	2:C:273:ILE:HD13	2.54	0.42
2:C:298:SER:HB3	2:C:332:TRP:CZ3	2.54	0.42
1:D:190:MET:O	1:D:190:MET:HG3	2.16	0.42
1:A:171:LEU:CG	1:A:190:MET:HE2	2.43	0.42
1:B:109:GLU:OE2	1:B:123:HIS:NE2	2.37	0.42
1:B:11:GLY:O	1:B:12:ARG:C	2.60	0.42
1:B:337:TRP:O	1:B:341:HIS:HD2	2.02	0.42
2:C:83:HIS:HD2	5:C:433:HOH:O	2.02	0.42
1:D:10:PHE:CE2	1:D:15:ARG:HG3	2.55	0.42
1:B:22:CYS:O	1:B:61:TYR:HE1	2.03	0.42
1:B:41:THR:HG21	1:B:89:LYS:HG2	2.02	0.42
1:B:180:LYS:HE2	1:B:284:TYR:CE2	2.55	0.42
1:D:83:HIS:HB2	5:D:546:HOH:O	2.20	0.42
1:D:239:THR:HA	1:D:242:LYS:HD2	2.01	0.42
1:B:339:TYR:O	1:B:343:VAL:HG23	2.20	0.41
2:C:175:VAL:O	2:C:179:VAL:HG23	2.19	0.41
2:C:209:LYS:HE2	5:C:525:HOH:O	2.20	0.41
1:D:142:LYS:HB2	1:D:158:HIS:CD2	2.55	0.41
1:A:16:MET:SD	1:A:337:TRP:CZ3	3.13	0.41
2:C:174:ILE:CD1	2:C:331:SER:HB2	2.45	0.41
1:D:79:VAL:HA	1:D:83:HIS:O	2.20	0.41
1:A:146:MET:HB2	1:A:342:ARG:HD3	2.01	0.41
2:C:115:THR:HB	5:C:484:HOH:O	2.18	0.41
1:D:35:ALA:HB1	1:D:88:VAL:HG22	2.02	0.41
2:C:200:GLN:NE2	2:C:249:ARG:HD2	2.36	0.41
1:D:175:VAL:O	1:D:179:VAL:HG23	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:94:PRO:HB3	2:C:123:HIS:CE1	2.55	0.41
2:C:169:ASN:O	2:C:307:SER:HB3	2.21	0.41
1:A:224:SER:HB3	1:A:247:SER:HB3	2.02	0.41
1:A:324:ARG:HG2	5:A:492:HOH:O	2.20	0.41
1:B:163:ASN:O	1:B:169:ASN:ND2	2.48	0.41
2:C:33:VAL:H	2:C:83:HIS:CE1	2.37	0.41
2:C:189:LEU:HD13	1:D:328:LYS:HB2	2.02	0.41
2:C:246:MET:HB3	1:D:318:ASN:CG	2.46	0.41
1:D:115:THR:HA	1:D:133:ILE:HG21	2.02	0.41
1:D:306:ARG:HB2	1:D:309:ILE:HD11	2.02	0.41
1:A:270:ILE:HD12	1:A:270:ILE:HA	1.90	0.41
1:B:253:PRO:HG3	2:C:219:VAL:HG11	2.02	0.41
1:B:335:ASN:O	3:B:360:NAD:H4N	2.21	0.41
2:C:35:ALA:HA	2:C:86:LEU:O	2.20	0.41
1:D:21:LEU:CD1	1:D:31:ILE:CD1	2.99	0.41
1:D:124:LEU:HD21	1:D:159:HIS:HB3	2.01	0.41
1:B:35:ALA:HB1	1:B:88:VAL:HG13	2.01	0.41
1:B:46:PHE:O	1:B:50:MET:HE3	2.20	0.41
1:D:23:GLU:OE1	1:D:337:TRP:HZ2	2.02	0.41
1:D:64:THR:HG21	5:D:460:HOH:O	2.21	0.41
1:B:175:VAL:CG1	1:B:239:THR:HG21	2.51	0.41
1:D:7:ILE:HB	1:D:36:VAL:HG12	2.03	0.41
1:D:9:GLY:O	1:D:14:GLY:HA3	2.21	0.41
1:B:268:THR:O	1:B:324:ARG:HA	2.21	0.41
2:C:196:TYR:CD2	2:C:251:PRO:HA	2.56	0.41
1:A:163:ASN:O	1:A:164:ALA:HB3	2.21	0.40
1:B:93:ASN:HD22	1:B:94:PRO:N	2.19	0.40
2:C:342:ARG:NE	2:C:342:ARG:HA	2.36	0.40
1:D:16:MET:SD	1:D:337:TRP:CZ3	3.14	0.40
1:B:86:LEU:CD2	1:B:88:VAL:HG12	2.51	0.40
1:D:200:GLN:NE2	1:D:249:ARG:HD2	2.37	0.40
1:A:186:GLN:HG3	1:A:264:ALA:O	2.21	0.40
1:B:173:PRO:O	1:B:177:VAL:HG23	2.22	0.40
2:C:3:ILE:HD12	2:C:351:ALA:HB2	2.04	0.40
2:C:196:TYR:CE2	2:C:251:PRO:HA	2.55	0.40
1:D:95:ALA:HA	1:D:122:GLY:O	2.21	0.40
1:D:194:HIS:O	1:D:249:ARG:HA	2.22	0.40
1:B:196:TYR:CE2	1:B:251:PRO:HA	2.56	0.40
1:B:95:ALA:HA	1:B:122:GLY:O	2.22	0.40
1:B:196:TYR:CD2	1:B:251:PRO:HA	2.57	0.40
2:C:197:THR:CB	4:C:361:GOL:H31	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:246:MET:HE3	2:C:246:MET:HB2	1.97	0.40
1:D:97:LEU:HA	1:D:98:PRO:HD3	1.92	0.40
1:D:115:THR:O	1:D:137:ALA:HA	2.21	0.40
1:D:130:LYS:HZ1	1:D:159:HIS:CD2	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	357/359 (99%)	337 (94%)	17 (5%)	3 (1%)	16	20
1	B	357/359 (99%)	341 (96%)	14 (4%)	2 (1%)	21	27
1	D	357/359 (99%)	337 (94%)	19 (5%)	1 (0%)	36	46
2	C	356/359 (99%)	337 (95%)	17 (5%)	2 (1%)	21	27
All	All	1427/1436 (99%)	1352 (95%)	67 (5%)	8 (1%)	21	27

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	SER
1	A	255	VAL
1	B	255	VAL
2	C	255	VAL
1	D	255	VAL
1	A	42	ASP
1	B	72	VAL
2	C	164	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/296 (99%)	277 (94%)	16 (6%)	19	28
1	B	293/296 (99%)	281 (96%)	12 (4%)	27	41
1	D	293/296 (99%)	276 (94%)	17 (6%)	18	26
2	C	292/295 (99%)	267 (91%)	25 (9%)	10	13
All	All	1171/1183 (99%)	1101 (94%)	70 (6%)	17	25

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	39	MET
1	A	55	VAL
1	A	60	LYS
1	A	72	VAL
1	A	78	LEU
1	A	88	VAL
1	A	97	LEU
1	A	102	LEU
1	A	121	GLU
1	A	157	GLU
1	A	171	LEU
1	A	187	THR
1	A	208	VAL
1	A	209	LYS
1	A	355	ARG
1	B	37	VAL
1	B	38	ASP
1	B	72	VAL
1	B	74	LYS
1	B	78	LEU
1	B	97	LEU
1	B	124	LEU
1	B	157	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	171	LEU
1	B	190	MET
1	B	193	ILE
1	B	305	ASN
2	C	3	ILE
2	C	21	LEU
2	C	30	GLU
2	C	37	VAL
2	C	40	ASN
2	C	55	VAL
2	C	60	LYS
2	C	64	THR
2	C	66	THR
2	C	78	LEU
2	C	88	VAL
2	C	97	LEU
2	C	102	LEU
2	C	107	VAL
2	C	113	LEU
2	C	115	THR
2	C	171	LEU
2	C	174	ILE
2	C	190	MET
2	C	193	ILE
2	C	208	VAL
2	C	243	LEU
2	C	258	VAL
2	C	268	THR
2	C	353	LYS
1	D	3	ILE
1	D	27	LEU
1	D	37	VAL
1	D	38	ASP
1	D	40	ASN
1	D	41	THR
1	D	55	VAL
1	D	58	LYS
1	D	74	LYS
1	D	88	VAL
1	D	97	LEU
1	D	105	GLU
1	D	171	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	190	MET
1	D	305	ASN
1	D	307	SER
1	D	309	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	150	HIS
1	A	159	HIS
1	A	176	HIS
1	A	186	GLN
1	A	200	GLN
1	A	341	HIS
1	B	19	GLN
1	B	83	HIS
1	B	93	ASN
1	B	150	HIS
1	B	159	HIS
1	B	176	HIS
1	B	200	GLN
1	B	305	ASN
1	B	341	HIS
2	C	19	GLN
2	C	40	ASN
2	C	93	ASN
2	C	150	HIS
2	C	176	HIS
2	C	186	GLN
2	C	200	GLN
2	C	240	GLN
2	C	341	HIS
1	D	8	ASN
1	D	49	GLN
1	D	83	HIS
1	D	150	HIS
1	D	151	HIS
1	D	159	HIS
1	D	176	HIS
1	D	200	GLN
1	D	305	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CCS	C	166	2	8,9,10	1.14	1 (12%)	7,10,12	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CCS	C	166	2	-	0/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	166	CCS	CD-SG	-2.17	1.76	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	166	CCS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	NAD	D	360	-	46,48,48	1.26	5 (10%)	64,73,73	1.56	10 (15%)
3	NAD	A	360	-	46,48,48	1.20	3 (6%)	64,73,73	1.46	9 (14%)
3	NAD	C	360	-	46,48,48	1.21	6 (13%)	64,73,73	1.75	11 (17%)
4	GOL	C	361	-	5,5,5	0.31	0	5,5,5	0.28	0
3	NAD	B	360	-	46,48,48	1.26	5 (10%)	64,73,73	1.56	11 (17%)

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	NAD	D	360	-	-	14/30/62/62	0/5/5/5
3	NAD	A	360	-	-	7/30/62/62	0/5/5/5
3	NAD	C	360	-	-	8/30/62/62	0/5/5/5
4	GOL	C	361	-	-	2/4/4/4	-
3	NAD	B	360	-	-	5/30/62/62	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	360	NAD	C2N-N1N	5.05	1.40	1.35
3	A	360	NAD	C2N-N1N	4.67	1.40	1.35
3	B	360	NAD	C2N-N1N	4.35	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	360	NAD	C2N-N1N	3.84	1.39	1.35
3	D	360	NAD	C5A-N7A	-3.18	1.33	1.39
3	B	360	NAD	O4D-C1D	3.07	1.44	1.40
3	D	360	NAD	O4D-C1D	2.93	1.44	1.40
3	B	360	NAD	C5A-N7A	-2.83	1.33	1.39
3	A	360	NAD	O4D-C1D	2.81	1.44	1.40
3	C	360	NAD	C5A-N7A	-2.79	1.34	1.39
3	A	360	NAD	C5A-N7A	-2.72	1.34	1.39
3	B	360	NAD	PA-O3	2.61	1.62	1.59
3	C	360	NAD	C6N-N1N	2.46	1.40	1.35
3	D	360	NAD	C4A-N9A	-2.36	1.32	1.37
3	B	360	NAD	C4A-N9A	-2.18	1.33	1.37
3	C	360	NAD	PA-O3	2.12	1.61	1.59
3	C	360	NAD	C4A-N9A	-2.08	1.33	1.37
3	D	360	NAD	C6N-N1N	2.04	1.40	1.35
3	C	360	NAD	C8A-N9A	-2.02	1.34	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	360	NAD	C5A-C4A-N3A	-5.37	119.32	126.72
3	C	360	NAD	N3A-C2A-N1A	-5.05	120.94	128.58
3	B	360	NAD	C5A-C4A-N3A	-4.88	120.00	126.72
3	D	360	NAD	N3A-C2A-N1A	-4.87	121.21	128.58
3	D	360	NAD	C5A-C4A-N3A	-4.83	120.06	126.72
3	A	360	NAD	C5A-C4A-N3A	-4.77	120.14	126.72
3	A	360	NAD	N3A-C2A-N1A	-4.31	122.06	128.58
3	B	360	NAD	N3A-C2A-N1A	-4.09	122.40	128.58
3	C	360	NAD	N3A-C4A-N9A	4.06	134.06	127.17
3	C	360	NAD	N9A-C8A-N7A	-3.86	108.46	113.94
3	C	360	NAD	C2A-N3A-C4A	3.83	121.18	111.83
3	D	360	NAD	C2A-N3A-C4A	3.62	120.66	111.83
3	B	360	NAD	C4A-C5A-N7A	-3.51	106.57	110.58
3	B	360	NAD	N9A-C8A-N7A	-3.41	109.10	113.94
3	D	360	NAD	C4D-O4D-C1D	-3.39	106.82	109.92
3	A	360	NAD	N3A-C4A-N9A	3.31	132.80	127.17
3	C	360	NAD	C5A-N7A-C8A	3.27	108.59	103.45
3	A	360	NAD	C2A-N3A-C4A	3.25	119.77	111.83
3	B	360	NAD	C2A-N3A-C4A	3.23	119.73	111.83
3	B	360	NAD	C5A-N7A-C8A	3.21	108.50	103.45
3	A	360	NAD	N9A-C8A-N7A	-3.16	109.45	113.94
3	C	360	NAD	C4A-N9A-C8A	3.14	109.04	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	360	NAD	C3N-C7N-N7N	-2.98	114.06	117.74
3	D	360	NAD	N9A-C8A-N7A	-2.95	109.75	113.94
3	D	360	NAD	N3A-C4A-N9A	2.92	132.14	127.17
3	C	360	NAD	C4A-C5A-N7A	-2.89	107.28	110.58
3	B	360	NAD	N3A-C4A-N9A	2.85	132.01	127.17
3	A	360	NAD	C5A-N7A-C8A	2.70	107.70	103.45
3	A	360	NAD	C6N-N1N-C2N	-2.70	119.58	121.88
3	B	360	NAD	C3N-C7N-N7N	-2.68	114.44	117.74
3	D	360	NAD	C4A-C5A-N7A	-2.68	107.52	110.58
3	A	360	NAD	C4A-C5A-N7A	-2.65	107.56	110.58
3	D	360	NAD	C5A-N7A-C8A	2.63	107.58	103.45
3	C	360	NAD	C4D-O4D-C1D	-2.44	107.69	109.92
3	A	360	NAD	C4A-N9A-C8A	2.38	108.24	105.74
3	D	360	NAD	O3-PA-O1A	-2.29	103.81	110.70
3	C	360	NAD	O4D-C4D-C5D	-2.25	102.13	109.33
3	B	360	NAD	C5B-C4B-C3B	-2.24	107.15	115.21
3	B	360	NAD	O3-PA-O1A	-2.18	104.15	110.70
3	B	360	NAD	C4A-N9A-C8A	2.00	107.84	105.74
3	C	360	NAD	O4B-C1B-C2B	-2.00	102.33	106.62

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	360	NAD	C5B-O5B-PA-O1A
3	A	360	NAD	O4D-C1D-N1N-C2N
3	A	360	NAD	O4D-C1D-N1N-C6N
3	A	360	NAD	C2D-C1D-N1N-C6N
3	B	360	NAD	O4D-C1D-N1N-C2N
3	B	360	NAD	O4D-C1D-N1N-C6N
3	B	360	NAD	C2D-C1D-N1N-C2N
3	B	360	NAD	C2D-C1D-N1N-C6N
3	C	360	NAD	C5B-O5B-PA-O1A
3	C	360	NAD	O4D-C1D-N1N-C2N
3	C	360	NAD	O4D-C1D-N1N-C6N
3	C	360	NAD	C2D-C1D-N1N-C2N
3	C	360	NAD	C2D-C1D-N1N-C6N
3	D	360	NAD	C5B-O5B-PA-O1A
3	D	360	NAD	O4D-C1D-N1N-C2N
3	D	360	NAD	O4D-C1D-N1N-C6N
3	D	360	NAD	C2D-C1D-N1N-C2N
3	D	360	NAD	C2D-C1D-N1N-C6N

Continued on next page...

Continued from previous page...

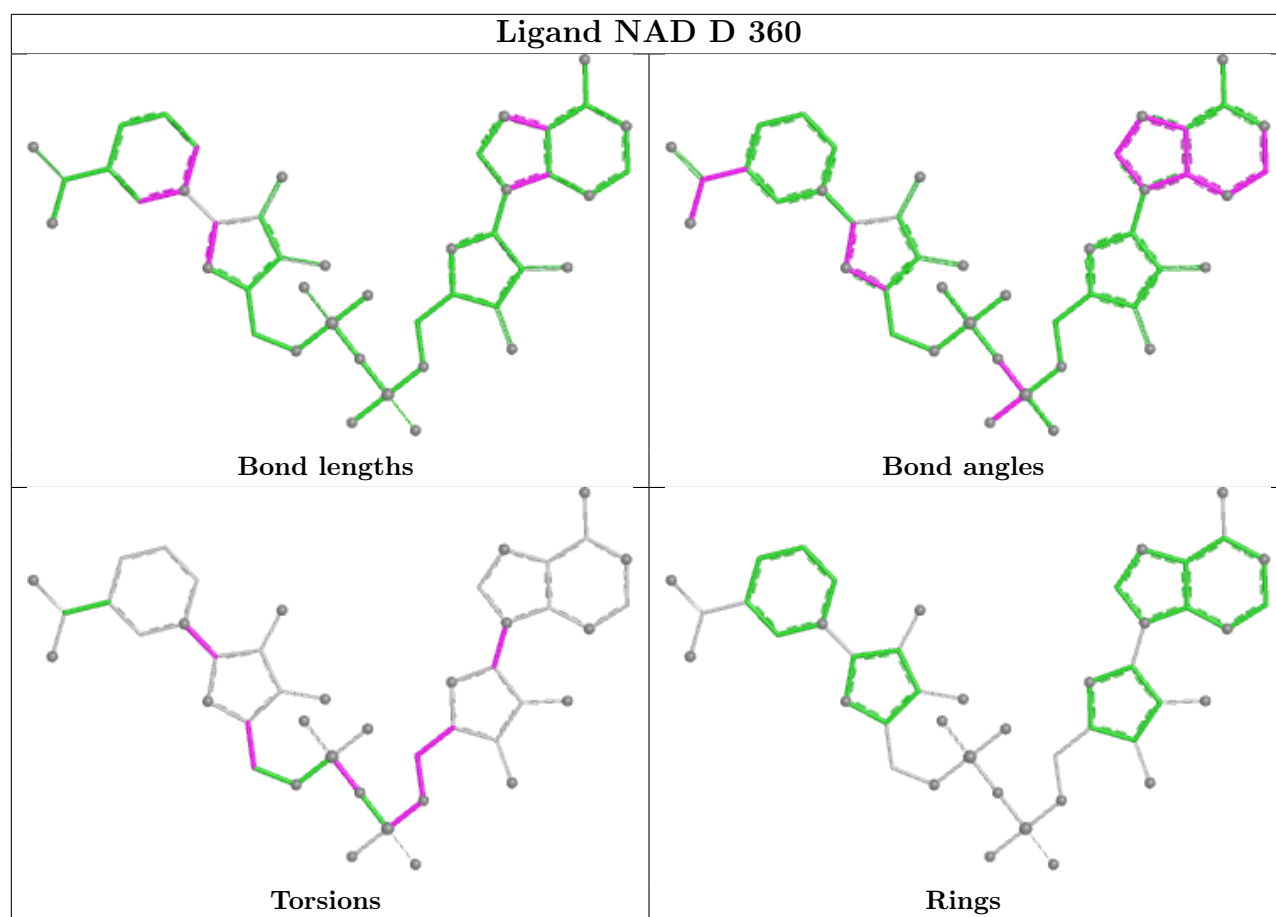
Mol	Chain	Res	Type	Atoms
4	C	361	GOL	C1-C2-C3-O3
4	C	361	GOL	O2-C2-C3-O3
3	D	360	NAD	C2B-C1B-N9A-C8A
3	B	360	NAD	C2B-C1B-N9A-C8A
3	C	360	NAD	C2B-C1B-N9A-C8A
3	D	360	NAD	C5B-O5B-PA-O2A
3	D	360	NAD	C5B-O5B-PA-O3
3	C	360	NAD	C2B-C1B-N9A-C4A
3	D	360	NAD	C2B-C1B-N9A-C4A
3	A	360	NAD	C2D-C1D-N1N-C2N
3	D	360	NAD	C4B-C5B-O5B-PA
3	D	360	NAD	O4B-C1B-N9A-C8A
3	A	360	NAD	C2B-C1B-N9A-C8A
3	A	360	NAD	O4D-C4D-C5D-O5D
3	D	360	NAD	O4D-C4D-C5D-O5D
3	D	360	NAD	PA-O3-PN-O2N
3	D	360	NAD	O4B-C4B-C5B-O5B
3	C	360	NAD	O4B-C1B-N9A-C8A

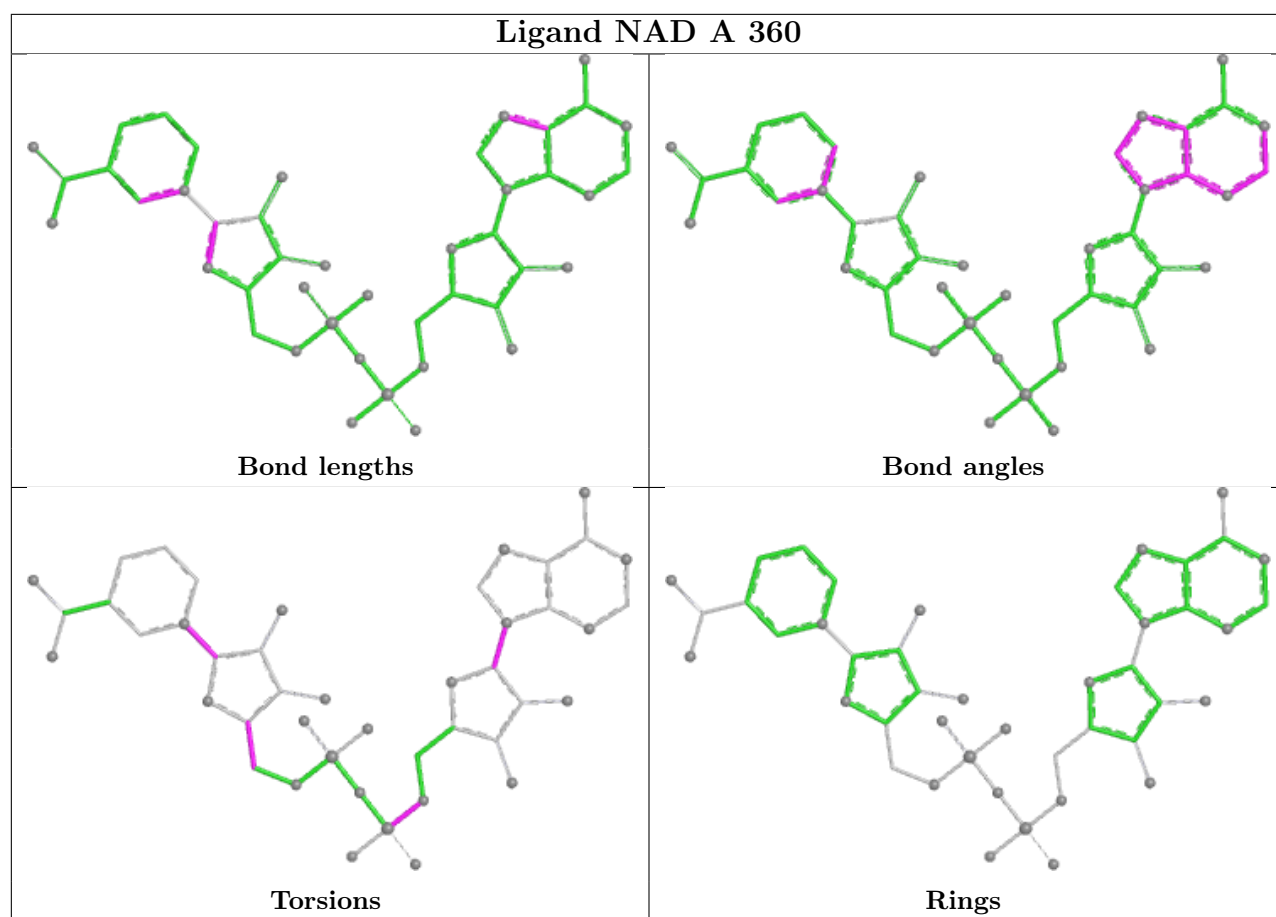
There are no ring outliers.

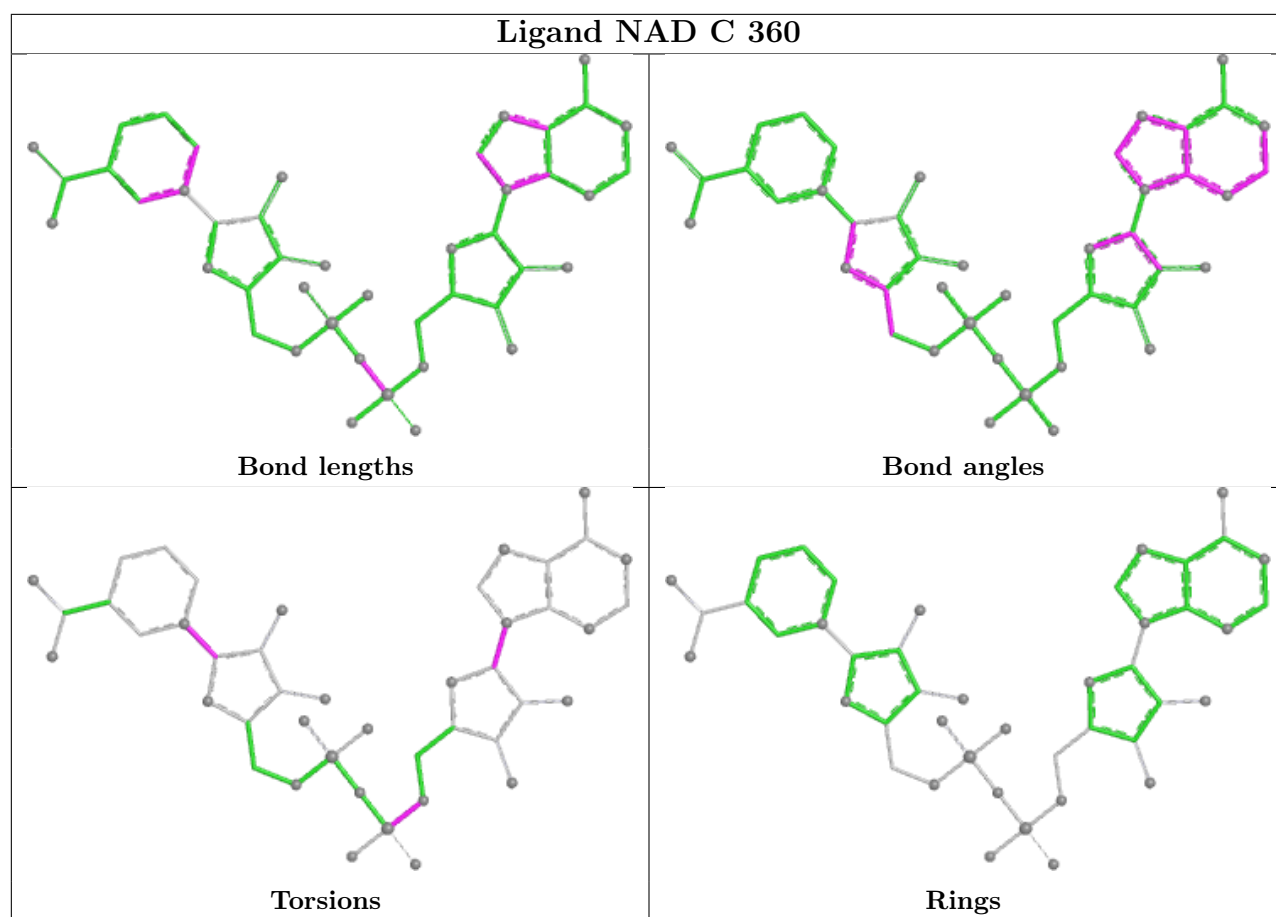
5 monomers are involved in 23 short contacts:

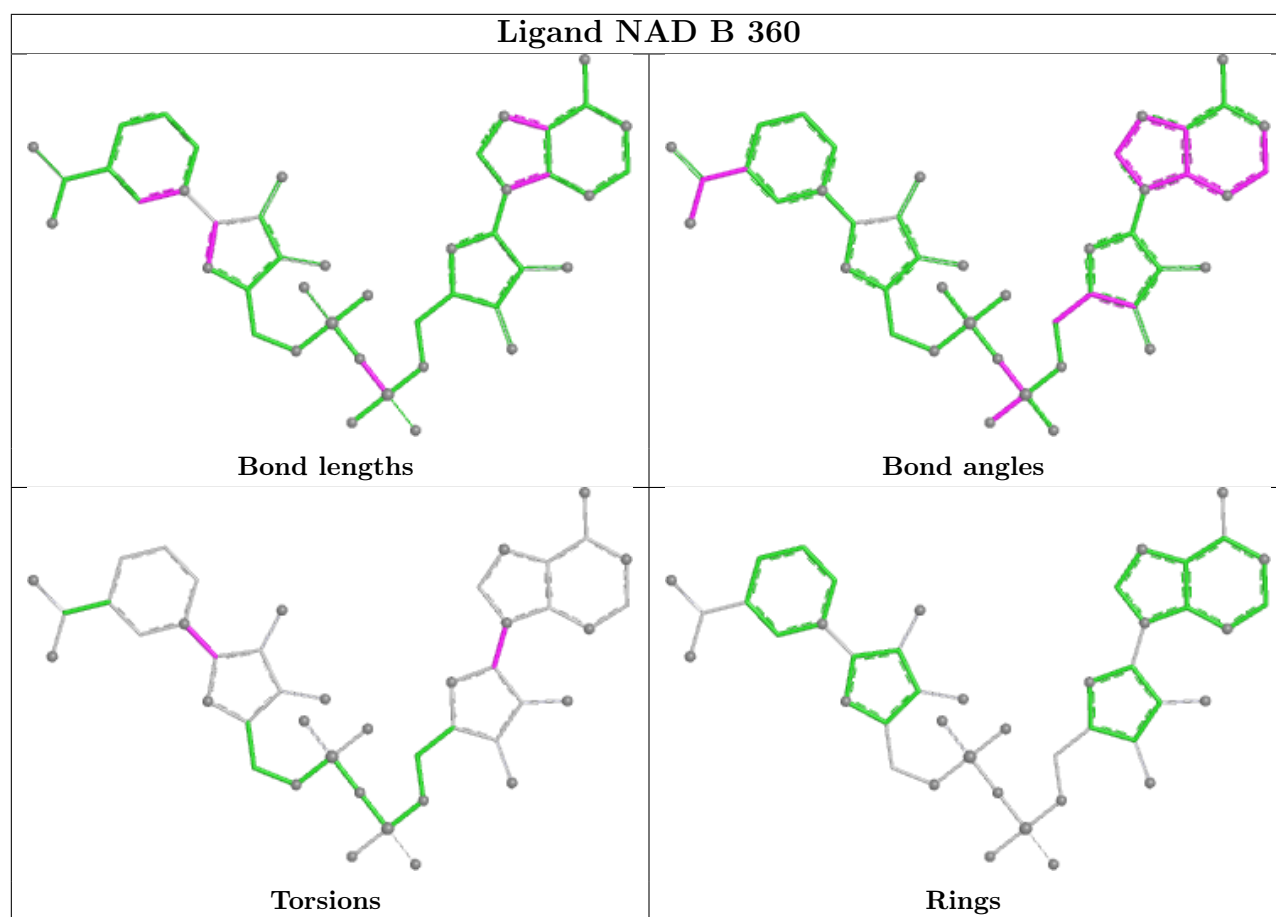
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	360	NAD	3	0
3	A	360	NAD	5	0
3	C	360	NAD	7	0
4	C	361	GOL	5	0
3	B	360	NAD	3	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	359/359 (100%)	0.77	26 (7%) 21 23	0, 18, 38, 43	24 (6%)
1	B	359/359 (100%)	0.01	10 (2%) 55 57	0, 16, 26, 39	7 (1%)
1	D	359/359 (100%)	0.29	18 (5%) 34 35	0, 19, 39, 46	14 (3%)
2	C	358/359 (99%)	-0.23	3 (0%) 82 83	7, 16, 28, 44	3 (0%)
All	All	1435/1436 (99%)	0.21	57 (3%) 42 44	0, 17, 36, 46	48 (3%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	LEU	32.5
1	A	1	MET	30.1
1	D	72	VAL	29.8
1	A	2	PRO	27.8
1	A	356	SER	27.8
1	B	359	LEU	27.4
1	A	357	ALA	26.4
1	A	358	ARG	26.2
1	B	358	ARG	23.4
1	A	355	ARG	15.4
1	D	1	MET	10.4
1	D	92	ARG	9.4
1	A	90	ALA	7.2
1	B	92	ARG	6.5
1	D	101	LYS	6.0
1	A	30	GLU	5.7
1	A	101	LYS	5.2
1	A	4	LYS	5.1
1	D	24	ASP	5.1
1	B	72	VAL	4.8
1	D	62	GLU	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	73	ALA	4.4
1	A	62	GLU	4.2
1	D	230	LYS	4.1
1	D	70	PRO	3.9
1	B	355	ARG	3.8
2	C	359	LEU	3.8
1	A	105	GLU	3.7
1	A	29	THR	3.7
1	B	101	LYS	3.7
1	B	1	MET	3.5
1	A	91	GLN	3.5
1	A	13	ILE	3.2
1	A	58	LYS	3.1
1	A	37	VAL	3.0
2	C	1	MET	3.0
1	A	3	ILE	2.9
1	A	89	LYS	2.9
1	B	39	MET	2.9
1	D	21	LEU	2.8
1	D	37	VAL	2.7
1	A	88	VAL	2.7
1	B	37	VAL	2.7
1	D	60	LYS	2.7
1	A	114	PHE	2.6
1	D	36	VAL	2.6
1	A	141	ALA	2.5
1	D	73	ALA	2.5
1	D	359	LEU	2.5
1	D	10	PHE	2.4
1	D	88	VAL	2.3
1	A	113	LEU	2.2
1	D	357	ALA	2.2
2	C	358	ARG	2.1
1	A	125	ARG	2.1
1	D	322	LYS	2.0
1	A	8	ASN	2.0

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

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($\text{\AA}^2$)	Q<0.9
2	CCS	C	166	10/11	0.97	0.07	12,12,16,18	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

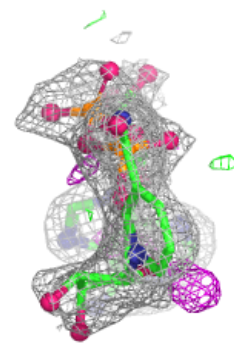
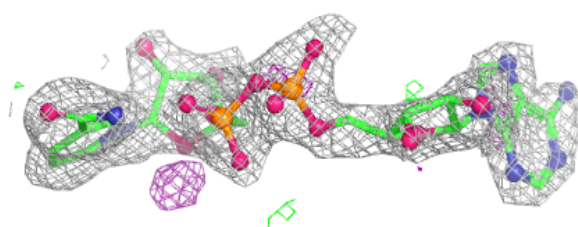
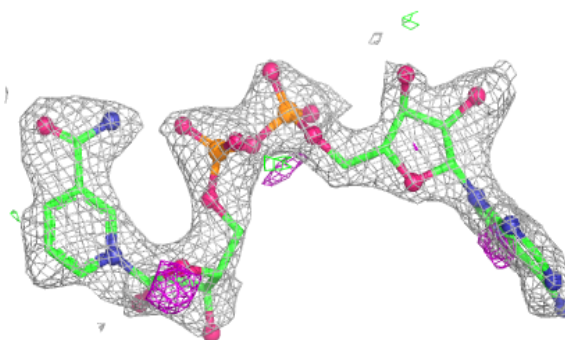
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	C	361	6/6	0.71	0.44	43,47,48,49	6
3	NAD	A	360	44/44	0.90	0.10	20,31,33,33	0
3	NAD	D	360	44/44	0.93	0.09	16,24,31,32	0
3	NAD	B	360	44/44	0.94	0.08	18,23,29,29	0
3	NAD	C	360	44/44	0.97	0.06	10,13,17,20	0

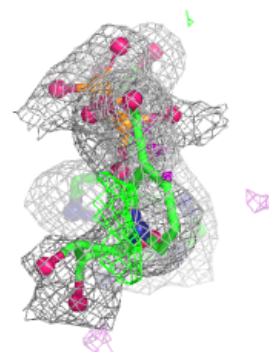
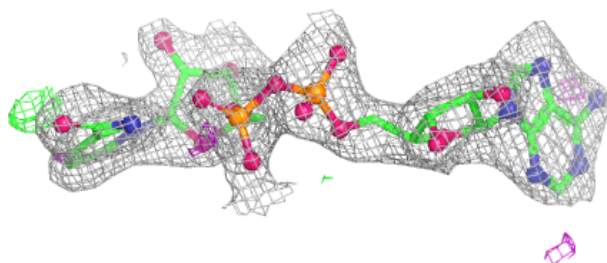
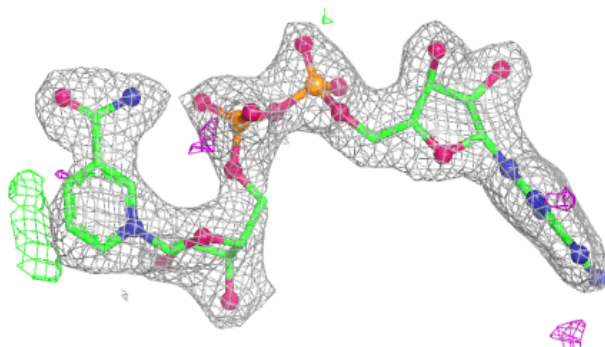
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 360:

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

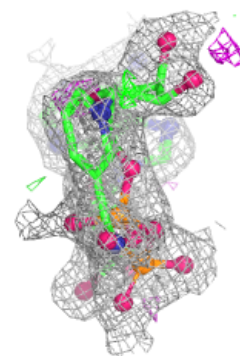
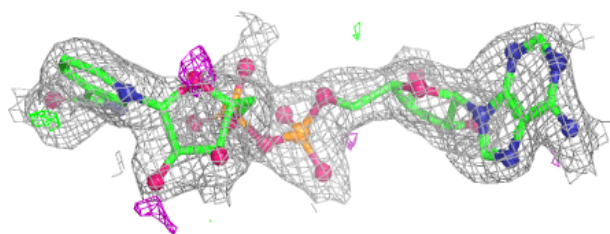
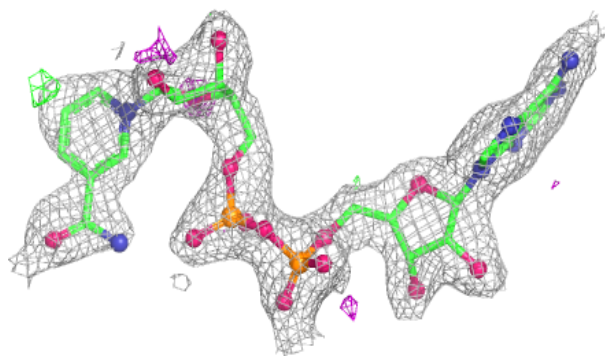
**Electron density around NAD D 360:**

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

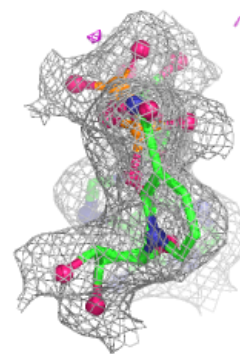
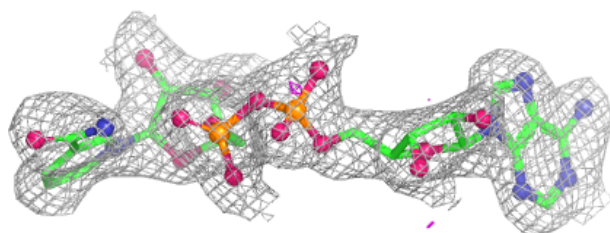
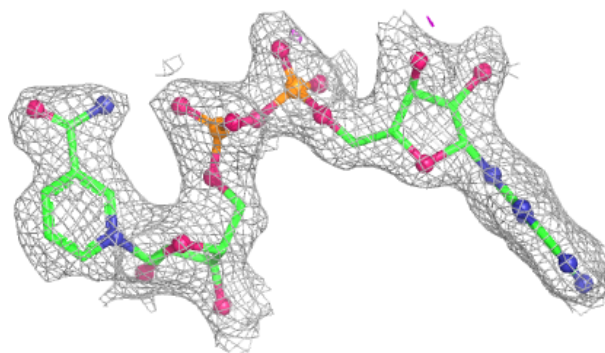


Electron density around NAD B 360:

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

**Electron density around NAD C 360:**

$2mF_o-DF_c$ (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.