



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:14 AM UTC

PDB ID : 2C20 / pdb_00002c20
Title : CRYSTAL STRUCTURE OF UDP-GLUCOSE 4-EPIMERASE
Authors : Lebedev, A.A.; Moroz, O.V.; Blagova, E.V.; Levnikov, V.M.; Fogg, M.J.;
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Deposited on : 2005-09-22
Resolution : 2.70 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

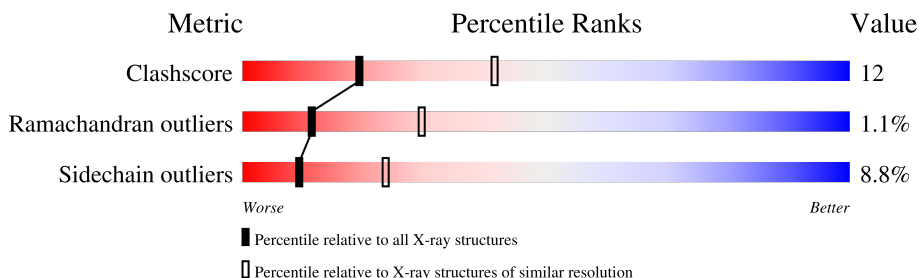
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	330	
1	B	330	
1	C	330	
1	D	330	
1	E	330	
1	F	330	

2 Entry composition [i](#)

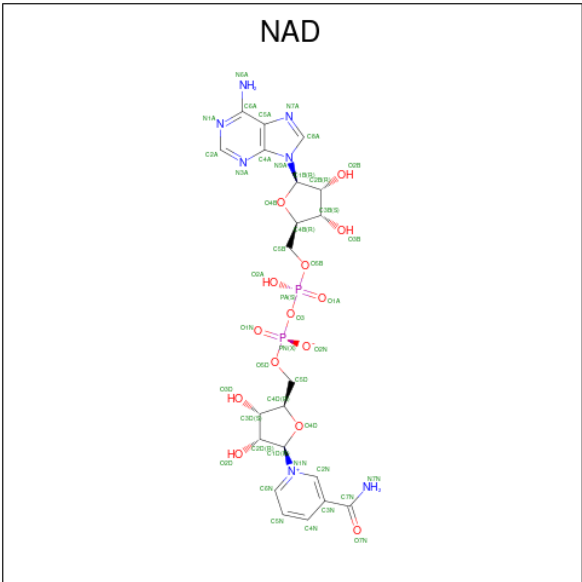
There are 4 unique types of molecules in this entry. The entry contains 16074 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called UDP-GLUCOSE 4-EPIMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	1	0
			2595	1645	440	499	11			
1	B	329	Total	C	N	O	S	0	1	0
			2595	1645	440	499	11			
1	C	329	Total	C	N	O	S	0	1	0
			2595	1645	440	499	11			
1	D	329	Total	C	N	O	S	0	1	0
			2595	1645	440	499	11			
1	E	329	Total	C	N	O	S	0	1	0
			2595	1645	440	499	11			
1	F	329	Total	C	N	O	S	0	1	0
			2595	1645	440	499	11			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

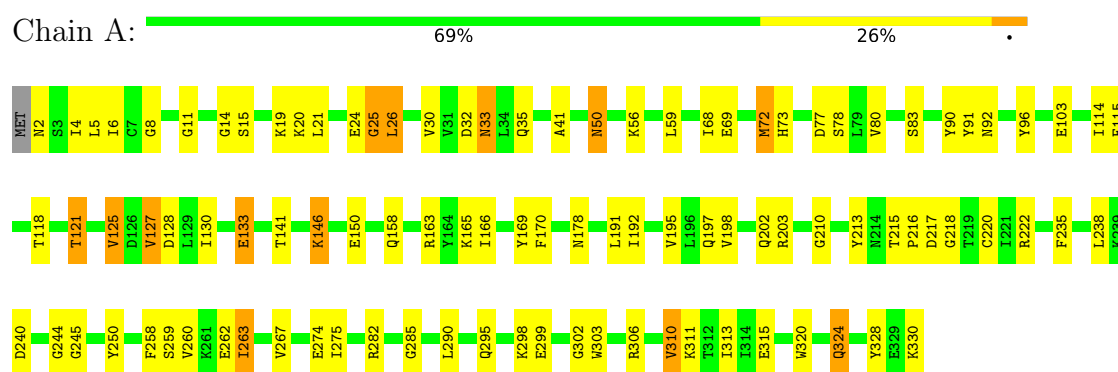
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	41	Total	O	0	0
			41	41		
4	C	38	Total	O	0	0
			38	38		
4	D	36	Total	O	0	0
			36	36		
4	E	36	Total	O	0	0
			36	36		
4	F	42	Total	O	0	0
			42	42		

3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

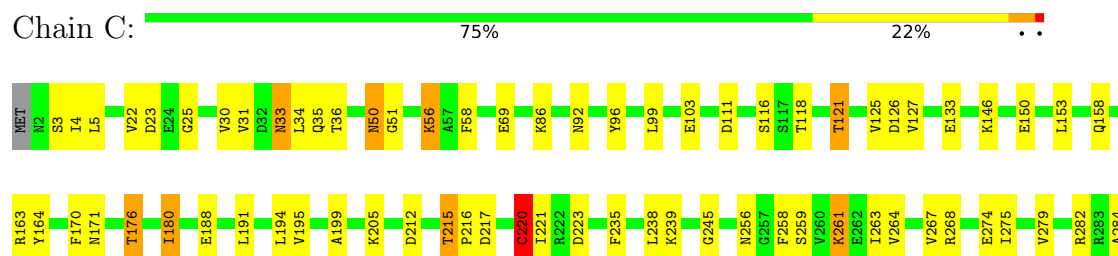
• Molecule 1: UDP-GLUCOSE 4-EPIMERASE



• Molecule 1: UDP-GLUCOSE 4-EPIMERASE



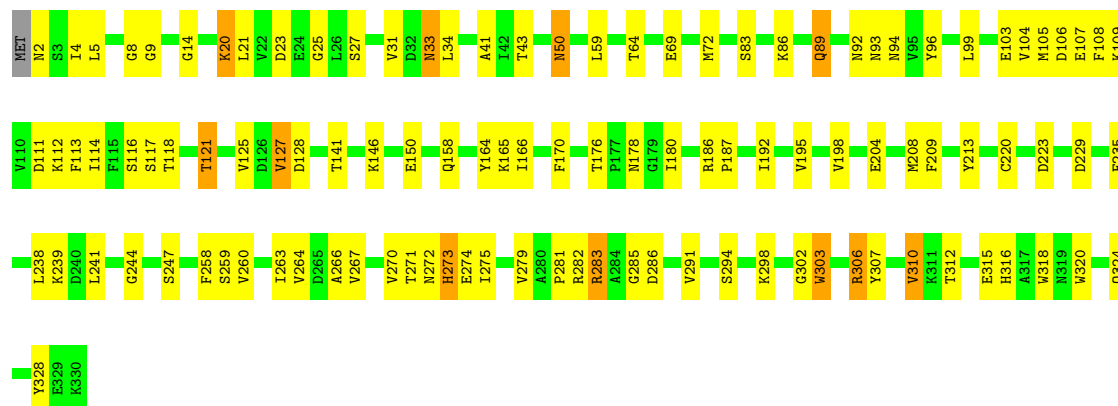
• Molecule 1: UDP-GLUCOSE 4-EPIMERASE





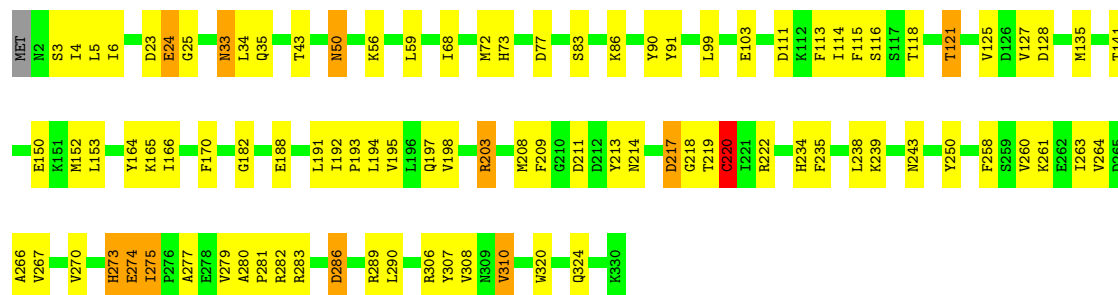
• Molecule 1: UDP-GLUCOSE 4-EPIMERASE

Chain D: 66% 30%



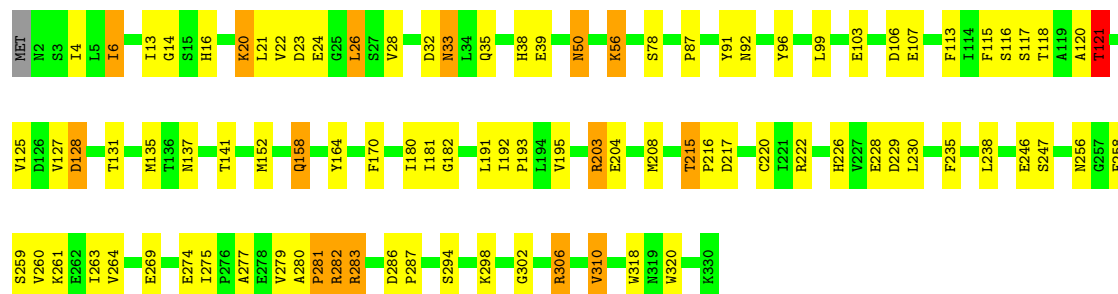
• Molecule 1: UDP-GLUCOSE 4-EPIMERASE

Chain E: 71% 25%



• Molecule 1: UDP-GLUCOSE 4-EPIMERASE

Chain F: 71% 24% 5%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	136.16 Å 136.16 Å 248.65 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.02 – 2.70	Depositor
% Data completeness (in resolution range)	73.1 (25.02-2.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.205 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16074	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.81	0/2656	1.05	8/3600 (0.2%)
1	B	0.87	1/2656 (0.0%)	1.04	6/3600 (0.2%)
1	C	0.84	0/2656	1.04	5/3600 (0.1%)
1	D	0.78	0/2656	1.00	4/3600 (0.1%)
1	E	0.99	5/2656 (0.2%)	0.99	4/3600 (0.1%)
1	F	0.82	0/2656	0.99	4/3600 (0.1%)
All	All	0.86	6/15936 (0.0%)	1.02	31/21600 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	274	GLU	CD-OE2	21.05	1.65	1.25
1	E	274	GLU	CD-OE1	17.71	1.59	1.25
1	E	273	HIS	CE1-NE2	9.17	1.41	1.32
1	B	149	ILE	CA-CB	-6.85	1.46	1.54
1	E	273	HIS	CG-CD2	5.67	1.42	1.35
1	E	273	HIS	CG-ND1	5.65	1.44	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	274	GLU	N-CA-C	7.66	119.71	111.36
1	D	285	GLY	N-CA-C	-7.55	100.91	112.84
1	A	274	GLU	N-CA-C	6.81	118.36	111.07
1	A	127	VAL	N-CA-C	6.40	117.38	108.23
1	C	220	CYS	N-CA-C	6.13	118.72	108.73
1	B	191	LEU	N-CA-C	6.03	117.85	111.28
1	B	220	CYS	N-CA-C	5.99	118.39	109.59
1	F	120	ALA	CA-C-N	5.96	128.55	120.38
1	F	120	ALA	C-N-CA	5.96	128.55	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	286	ASP	CA-C-N	5.93	125.90	120.03
1	E	286	ASP	C-N-CA	5.93	125.90	120.03
1	B	94	ASN	N-CA-C	5.74	117.40	111.03
1	B	3	SER	N-CA-C	5.67	118.79	109.72
1	A	244	GLY	N-CA-C	5.58	123.06	115.30
1	A	324	GLN	CA-C-N	5.58	125.19	119.56
1	A	324	GLN	C-N-CA	5.58	125.19	119.56
1	E	220	CYS	N-CA-C	5.42	117.47	108.20
1	B	14	GLY	N-CA-C	-5.41	105.95	112.49
1	C	286	ASP	CA-C-N	5.36	125.57	120.31
1	C	286	ASP	C-N-CA	5.36	125.57	120.31
1	D	244	GLY	N-CA-C	5.36	121.13	114.37
1	F	121	THR	N-CA-CB	-5.30	102.10	110.06
1	E	3	SER	N-CA-C	5.28	117.42	109.23
1	A	80	VAL	N-CA-C	5.26	115.70	110.23
1	A	125	VAL	N-CA-C	5.19	115.44	108.17
1	D	176	THR	CA-C-N	5.13	126.25	119.84
1	D	176	THR	C-N-CA	5.13	126.25	119.84
1	C	30	VAL	N-CA-C	5.11	115.22	107.75
1	A	30	VAL	N-CA-C	5.05	115.18	108.11
1	B	26	LEU	N-CA-C	5.05	116.62	110.41
1	F	26	LEU	N-CA-C	5.01	116.75	110.24

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	2595	0	2513	65	0
1	B	2595	0	2513	60	0
1	C	2595	0	2513	53	0
1	D	2595	0	2513	64	0
1	E	2595	0	2513	58	0
1	F	2595	0	2513	62	0
2	A	44	0	26	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	26	1	0
2	C	44	0	26	2	0
2	D	44	0	26	1	0
2	E	44	0	26	2	0
2	F	44	0	26	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	41	0	0	0	0
4	B	41	0	0	0	0
4	C	38	0	0	1	0
4	D	36	0	0	0	0
4	E	36	0	0	1	0
4	F	42	0	0	1	0
All	All	16074	0	15234	362	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 12.

All (362) 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:E:274:GLU:CD	1:E:274:GLU:OE2	1.65	1.40
1:C:212:ASP:C	1:C:282:ARG:HH22	1.59	1.07
1:F:158:GLN:HE21	1:F:158:GLN:HA	1.35	0.92
1:A:146:LYS:NZ	2:A:401:NAD:O2D	2.02	0.91
1:F:208:MET:HE3	1:F:277:ALA:HB1	1.51	0.91
1:E:280:ALA:HB1	1:E:281:PRO:HD2	1.53	0.91
1:F:158:GLN:HE21	1:F:158:GLN:CA	1.84	0.90
1:E:33:ASN:ND2	1:E:35:GLN:H	1.73	0.87
1:F:191:LEU:O	1:F:195:VAL:HG23	1.76	0.85
1:A:215:THR:HB	1:A:216:PRO:HD2	1.58	0.85
1:A:33:ASN:HD21	1:A:35:GLN:HG2	1.43	0.83
1:F:4:ILE:HD13	1:F:238:LEU:HD21	1.64	0.80
1:F:215:THR:HB	1:F:216:PRO:CD	2.13	0.79
1:A:33:ASN:ND2	1:A:35:GLN:HG2	1.98	0.79
1:C:212:ASP:C	1:C:282:ARG:NH2	2.40	0.79
1:A:311:LYS:O	1:A:315:GLU:HG3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:LYS:O	1:B:243:ASN:ND2	2.15	0.79
1:F:158:GLN:HA	1:F:158:GLN:NE2	1.96	0.79
1:F:217:ASP:OD2	1:F:261:LYS:HB3	1.84	0.77
1:F:215:THR:HB	1:F:216:PRO:HD2	1.65	0.76
1:B:170:PHE:O	2:B:401:NAD:H4N	1.86	0.76
1:B:215:THR:HB	1:B:216:PRO:CD	2.14	0.76
1:F:170:PHE:O	2:F:401:NAD:H4N	1.87	0.75
1:A:118:THR:O	1:A:121:THR:HB	1.88	0.73
1:C:212:ASP:OD1	1:C:282:ARG:NH2	2.21	0.73
1:D:118:THR:O	1:D:121:THR:HB	1.88	0.73
1:F:118:THR:O	1:F:121:THR:HB	1.89	0.73
1:E:208:MET:HE3	1:E:277:ALA:HB1	1.71	0.73
1:B:209:PHE:CD1	1:B:283:ARG:NH1	2.58	0.72
1:C:125:VAL:HG12	1:C:126:ASP:N	2.05	0.71
1:A:191:LEU:HD21	1:A:260:VAL:HG13	1.73	0.71
1:C:33:ASN:ND2	1:C:35:GLN:H	1.88	0.70
1:F:275:ILE:HG22	1:F:275:ILE:O	1.91	0.70
1:F:135[B]:MET:HG3	4:F:2024:HOH:O	1.91	0.70
1:B:275:ILE:O	1:B:275:ILE:HG22	1.90	0.70
1:C:217:ASP:HB2	1:C:261:LYS:HE3	1.71	0.70
1:F:260:VAL:O	1:F:264:VAL:HG23	1.92	0.69
1:E:99:LEU:O	1:E:103:GLU:HG3	1.92	0.69
1:F:226:HIS:HD1	1:F:228:GLU:H	1.42	0.68
1:E:263:ILE:O	1:E:267:VAL:HG23	1.93	0.68
1:B:118:THR:O	1:B:121:THR:HB	1.94	0.68
1:F:220:CYS:O	1:F:259:SER:HA	1.94	0.67
1:E:208:MET:HE2	1:E:264:VAL:HG21	1.75	0.67
1:A:127:VAL:HG22	1:A:128:ASP:N	2.10	0.67
1:B:81:GLY:O	1:B:84:MET:HB2	1.96	0.66
1:A:146:LYS:NZ	2:A:401:NAD:HO2N	1.94	0.66
1:C:4:ILE:HD13	1:C:238:LEU:HD21	1.78	0.65
1:F:4:ILE:CD1	1:F:238:LEU:HD21	2.26	0.65
1:E:165:LYS:HD2	1:E:250:TYR:HE2	1.62	0.65
1:A:263:ILE:O	1:A:267:VAL:HG23	1.97	0.64
1:B:33:ASN:HD22	1:B:33:ASN:C	2.04	0.64
1:D:263:ILE:O	1:D:267:VAL:HG23	1.97	0.64
1:C:125:VAL:HG12	1:C:126:ASP:H	1.63	0.64
1:A:127:VAL:HG22	1:A:128:ASP:H	1.64	0.63
1:C:188:GLU:O	1:C:194:LEU:HD21	1.99	0.62
1:C:5:LEU:HD11	1:C:31:VAL:HG23	1.82	0.62
1:D:208:MET:HE3	1:D:264:VAL:HG21	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ASN:ND2	1:B:35:GLN:H	1.98	0.61
1:A:163:ARG:NH1	1:A:245:GLY:O	2.33	0.61
1:B:220:CYS:O	1:B:259:SER:HA	2.01	0.60
1:E:4:ILE:HD13	1:E:238:LEU:HD21	1.82	0.60
1:E:72:MET:HG2	1:E:114:ILE:HB	1.83	0.60
2:C:401:NAD:N7N	2:C:401:NAD:O1N	2.34	0.60
1:A:125:VAL:HG12	1:A:127:VAL:H	1.66	0.60
1:F:158:GLN:HE21	1:F:158:GLN:N	1.97	0.60
1:C:99:LEU:O	1:C:103:GLU:HG3	2.01	0.60
1:D:117:SER:HA	1:D:146:LYS:HE3	1.84	0.60
1:E:191:LEU:O	1:E:195:VAL:HG23	2.02	0.60
1:A:215:THR:HB	1:A:216:PRO:CD	2.28	0.60
1:B:235:PHE:CE1	1:B:239:LYS:HD2	2.37	0.59
1:C:275:ILE:HG22	1:C:275:ILE:O	2.01	0.59
1:F:4:ILE:HD13	1:F:238:LEU:CD2	2.30	0.59
1:F:24:GLU:OE1	1:F:235:PHE:CZ	2.55	0.59
1:C:284:ALA:O	1:C:286:ASP:N	2.33	0.58
1:B:259:SER:O	1:B:263:ILE:HD13	2.03	0.58
1:D:72:MET:HG2	1:D:114:ILE:HB	1.84	0.58
1:D:99:LEU:O	1:D:103:GLU:HG3	2.03	0.58
1:C:311:LYS:O	1:C:315:GLU:HG3	2.04	0.58
1:A:5:LEU:HB2	1:A:68:ILE:HD12	1.86	0.58
1:D:21:LEU:CD2	1:D:235:PHE:HD1	2.16	0.57
1:E:222:ARG:HD3	1:E:290:LEU:HB2	1.87	0.57
1:D:50:ASN:HD22	1:D:50:ASN:C	2.13	0.57
1:D:320:TRP:CZ3	1:D:324:GLN:HG3	2.40	0.57
1:A:56:LYS:HE3	1:A:103:GLU:OE1	2.05	0.57
1:D:4:ILE:HD13	1:D:238:LEU:HD21	1.87	0.56
1:D:33:ASN:C	1:D:33:ASN:HD22	2.12	0.56
1:F:33:ASN:ND2	1:F:35:GLN:H	2.02	0.56
1:B:263:ILE:O	1:B:267:VAL:HG23	2.04	0.56
1:E:280:ALA:HB1	1:E:281:PRO:CD	2.32	0.56
1:B:215:THR:HB	1:B:216:PRO:HD3	1.86	0.56
1:D:302:GLY:O	1:D:303:TRP:C	2.48	0.56
1:B:24:GLU:OE2	1:B:235:PHE:HE2	1.87	0.55
1:E:118:THR:O	1:E:121:THR:HB	2.05	0.55
1:B:23:ASP:C	1:B:25:GLY:H	2.14	0.55
1:B:79:LEU:HB2	1:B:90:TYR:OH	2.05	0.55
1:F:282:ARG:HG2	1:F:283:ARG:H	1.72	0.55
1:B:6:ILE:HD11	1:B:21:LEU:HD12	1.89	0.55
1:E:320:TRP:CZ3	1:E:324:GLN:HG3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6:ILE:HD11	1:F:21:LEU:CD1	2.36	0.55
1:E:77:ASP:HB3	1:E:90:TYR:CZ	2.42	0.55
1:D:21:LEU:CD2	1:D:235:PHE:CD1	2.89	0.55
1:D:83:SER:HB2	1:D:141:THR:HB	1.88	0.54
1:D:23:ASP:C	1:D:25:GLY:H	2.15	0.54
1:B:121:THR:HG23	1:B:136:THR:HG22	1.89	0.54
1:D:271:THR:HG22	1:D:318:TRP:CE2	2.43	0.54
1:D:9:GLY:HA2	1:D:14:GLY:HA3	1.89	0.54
1:C:125:VAL:CG1	1:C:126:ASP:N	2.71	0.54
1:B:188:GLU:HG2	1:B:193:PRO:HB2	1.90	0.53
1:E:50:ASN:C	1:E:50:ASN:HD22	2.16	0.53
1:E:209:PHE:CD1	1:E:283:ARG:NH2	2.76	0.53
2:A:401:NAD:N7N	2:A:401:NAD:O1N	2.41	0.53
1:A:170:PHE:O	2:A:401:NAD:H4N	2.09	0.53
1:A:41:ALA:HB2	1:A:328:TYR:CE1	2.44	0.53
1:F:246:GLU:HG3	1:F:247:SER:O	2.07	0.53
1:A:197:GLN:OE1	1:A:203:ARG:HD3	2.09	0.53
1:D:306:ARG:HG3	1:D:307:TYR:CE1	2.43	0.53
1:B:215:THR:CB	1:B:216:PRO:CD	2.86	0.52
1:A:259:SER:OG	1:A:262:GLU:HG3	2.09	0.52
1:B:171:ASN:HB2	1:B:223:ASP:O	2.09	0.52
1:A:210:GLY:HA3	1:A:282:ARG:HG2	1.89	0.52
1:C:33:ASN:C	1:C:33:ASN:HD22	2.18	0.52
1:B:178:ASN:OD1	1:B:180:ILE:HB	2.08	0.52
1:E:208:MET:HE3	1:E:277:ALA:CB	2.38	0.52
1:D:164:TYR:O	1:D:247:SER:HA	2.10	0.52
1:B:280:ALA:HB1	1:B:281:PRO:HD2	1.92	0.52
1:A:6:ILE:HD11	1:A:21:LEU:HD12	1.92	0.51
1:F:208:MET:HE3	1:F:277:ALA:CB	2.32	0.51
1:D:266:ALA:O	1:D:270:VAL:HG23	2.10	0.51
1:B:33:ASN:C	1:B:33:ASN:ND2	2.69	0.51
1:C:176:THR:HG21	1:C:180:ILE:HG22	1.91	0.51
1:C:258:PHE:CE2	1:C:310:VAL:HG22	2.45	0.51
1:D:21:LEU:HD22	1:D:235:PHE:CD1	2.46	0.51
1:B:191:LEU:O	1:B:195:VAL:HG23	2.11	0.51
1:A:191:LEU:O	1:A:195:VAL:HG23	2.10	0.51
1:B:173:ALA:O	1:B:226:HIS:HA	2.10	0.51
1:E:33:ASN:HD22	1:E:34:LEU:N	2.08	0.51
1:C:125:VAL:CG1	1:C:126:ASP:H	2.23	0.51
1:C:220:CYS:O	1:C:259:SER:HA	2.11	0.51
1:D:229:ASP:OD1	1:D:306:ARG:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:SER:O	1:D:298:LYS:HG3	2.11	0.50
1:D:271:THR:OG1	1:D:273:HIS:HB2	2.10	0.50
1:F:258:PHE:CE1	1:F:310:VAL:HG13	2.45	0.50
1:F:259:SER:O	1:F:263:ILE:HD13	2.11	0.50
1:D:21:LEU:HD22	1:D:235:PHE:CE1	2.46	0.50
1:E:150:GLU:HG2	1:E:166:ILE:HD13	1.92	0.50
1:B:33:ASN:HD22	1:B:34:LEU:N	2.10	0.50
1:B:50:ASN:C	1:B:50:ASN:HD22	2.19	0.50
1:B:294:SER:HB3	1:B:298:LYS:HE3	1.93	0.50
1:A:197:GLN:HB3	1:A:203:ARG:HG3	1.93	0.50
1:F:215:THR:CB	1:F:216:PRO:CD	2.85	0.50
1:D:213:TYR:CZ	1:D:282:ARG:HG3	2.46	0.50
1:C:50:ASN:C	1:C:50:ASN:HD22	2.19	0.50
1:C:191:LEU:O	1:C:195:VAL:HG23	2.11	0.50
1:F:92:ASN:O	1:F:96:TYR:HB3	2.12	0.50
1:A:125:VAL:HG11	1:A:130:ILE:HG12	1.94	0.49
1:C:212:ASP:H	1:C:282:ARG:HH21	1.60	0.49
1:D:108:PHE:O	1:D:109:LYS:HB2	2.10	0.49
1:C:4:ILE:CD1	1:C:238:LEU:HD21	2.41	0.49
1:B:247:SER:O	1:B:248:ASP:HB2	2.11	0.49
1:C:263:ILE:O	1:C:267:VAL:HG23	2.12	0.49
1:E:170:PHE:O	2:E:401:NAD:H4N	2.12	0.49
1:F:135[B]:MET:HE3	1:F:137:ASN:ND2	2.27	0.49
1:D:170:PHE:O	2:D:401:NAD:H4N	2.12	0.49
1:E:72:MET:HE3	1:E:234:HIS:HB3	1.94	0.49
1:F:16:HIS:CE1	1:F:181:ILE:HD12	2.48	0.49
1:A:165:LYS:HD2	1:A:250:TYR:HE2	1.78	0.49
1:F:33:ASN:C	1:F:33:ASN:HD22	2.19	0.49
1:B:50:ASN:HD22	1:B:51:GLY:N	2.11	0.49
1:E:211:ASP:OD2	1:E:279:VAL:HG11	2.12	0.49
1:C:256:ASN:HA	1:C:291:VAL:HG11	1.93	0.48
1:C:33:ASN:HD22	1:C:34:LEU:N	2.11	0.48
1:B:215:THR:HB	1:B:216:PRO:HD2	1.92	0.48
1:D:213:TYR:HE1	1:D:220:CYS:SG	2.35	0.48
1:E:239:LYS:O	1:E:243:ASN:ND2	2.45	0.48
1:F:50:ASN:C	1:F:50:ASN:HD22	2.21	0.48
1:A:302:GLY:O	1:A:303:TRP:C	2.56	0.48
1:B:20:LYS:HB2	1:B:20:LYS:NZ	2.29	0.48
1:C:35:GLN:HG3	1:C:36:THR:HG23	1.95	0.48
1:A:202:GLN:O	1:A:203:ARG:HG2	2.14	0.48
1:F:99:LEU:O	1:F:103:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:LEU:HD11	1:B:31:VAL:HG23	1.95	0.48
1:B:259:SER:O	1:B:260:VAL:C	2.57	0.48
1:D:2:ASN:HD22	1:D:69:GLU:HB2	1.79	0.48
1:F:229:ASP:OD1	1:F:306:ARG:HG2	2.14	0.48
1:F:117:SER:O	2:F:401:NAD:H6N	2.14	0.47
1:A:220:CYS:H	1:A:260:VAL:HG23	1.78	0.47
1:D:111:ASP:OD1	1:D:112:LYS:HG3	2.14	0.47
1:A:127:VAL:CG2	1:A:128:ASP:H	2.25	0.47
2:E:401:NAD:N7N	2:E:401:NAD:O1N	2.48	0.47
1:A:91:TYR:CD1	1:B:152:MET:HE2	2.49	0.47
1:E:213:TYR:HB2	1:E:218:GLY:O	2.14	0.47
1:B:275:ILE:O	1:B:275:ILE:CG2	2.60	0.47
1:E:113:PHE:HE2	1:E:115:PHE:HB2	1.79	0.47
1:F:32:ASP:OD1	2:F:401:NAD:H1B	2.14	0.47
1:A:77:ASP:HB3	1:A:90:TYR:CE2	2.49	0.47
1:B:4:ILE:HD13	1:B:238:LEU:HD21	1.97	0.47
1:C:111:ASP:C	1:C:111:ASP:OD1	2.56	0.47
1:D:258:PHE:CD1	1:D:310:VAL:HG13	2.49	0.47
1:E:91:TYR:CD1	1:F:152:MET:HE2	2.49	0.47
1:A:213:TYR:CZ	1:A:282:ARG:NE	2.83	0.47
1:C:297:ALA:O	1:C:301:LEU:HB2	2.15	0.47
1:A:33:ASN:CG	1:A:35:GLN:HG2	2.39	0.47
1:E:113:PHE:O	1:E:164:TYR:HA	2.15	0.47
1:A:127:VAL:CG2	1:A:128:ASP:N	2.76	0.46
1:B:274:GLU:HG3	1:B:275:ILE:H	1.80	0.46
1:C:264:VAL:HG12	1:C:268:ARG:NH1	2.29	0.46
1:C:164:TYR:C	1:C:164:TYR:CD2	2.93	0.46
1:F:164:TYR:O	1:F:247:SER:HA	2.14	0.46
1:C:180:ILE:HG12	4:C:2030:HOH:O	2.15	0.46
1:F:128:ASP:OD2	1:F:128:ASP:N	2.48	0.46
1:D:271:THR:C	1:D:273:HIS:N	2.73	0.46
1:D:312:THR:O	1:D:315:GLU:HB2	2.15	0.46
1:A:240:ASP:OD1	1:A:245:GLY:HA3	2.16	0.46
1:A:178:ASN:C	1:A:178:ASN:OD1	2.58	0.46
1:C:258:PHE:CD2	1:C:310:VAL:HG22	2.51	0.46
1:F:6:ILE:HD11	1:F:21:LEU:HD12	1.96	0.46
1:D:220:CYS:O	1:D:259:SER:HA	2.16	0.46
1:E:113:PHE:CE2	1:E:115:PHE:HB2	2.51	0.46
1:E:266:ALA:O	1:E:270:VAL:HG23	2.15	0.46
1:C:125:VAL:HG12	1:C:127:VAL:H	1.81	0.46
1:E:258:PHE:CD1	1:E:310:VAL:HG13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ASN:O	1:B:96:TYR:HB3	2.16	0.46
1:D:312:THR:HG22	1:D:316:HIS:CE1	2.51	0.46
1:E:152:MET:HE2	1:F:91:TYR:CD1	2.51	0.46
1:F:275:ILE:O	1:F:275:ILE:CG2	2.63	0.46
1:A:72:MET:HG3	1:A:114:ILE:HB	1.97	0.45
1:F:208:MET:HE2	1:F:264:VAL:HG21	1.98	0.45
1:E:219:THR:HB	1:E:260:VAL:HB	1.99	0.45
1:A:24:GLU:O	1:A:26:LEU:N	2.49	0.45
1:E:192:ILE:N	1:E:193:PRO:HD2	2.31	0.45
1:A:50:ASN:C	1:A:50:ASN:HD22	2.24	0.45
1:D:209:PHE:HB3	1:D:283:ARG:HD3	1.98	0.45
1:F:298:LYS:O	1:F:302:GLY:HA2	2.17	0.45
1:D:5:LEU:HD11	1:D:31:VAL:HG23	1.99	0.45
1:E:127:VAL:HG22	1:E:128:ASP:H	1.82	0.45
1:B:320:TRP:CZ3	1:B:324:GLN:HG3	2.51	0.45
1:D:104:VAL:O	1:D:105:MET:C	2.60	0.45
1:A:295:GLN:O	1:A:299:GLU:HG3	2.17	0.45
1:D:165:LYS:HE2	1:D:241:LEU:CD2	2.46	0.45
1:F:113:PHE:O	1:F:164:TYR:HA	2.17	0.45
1:A:198:VAL:HA	1:A:203:ARG:O	2.17	0.45
1:E:33:ASN:ND2	1:E:33:ASN:C	2.74	0.45
1:D:195:VAL:O	1:D:198:VAL:HB	2.17	0.44
1:A:222:ARG:HD3	1:A:290:LEU:HB2	1.98	0.44
1:B:165:LYS:HE2	1:B:241:LEU:CD2	2.47	0.44
1:C:171:ASN:HB2	1:C:223:ASP:O	2.18	0.44
1:B:4:ILE:HD13	1:B:238:LEU:CD2	2.48	0.44
1:C:215:THR:HG21	1:C:221:ILE:HG12	1.99	0.44
1:D:235:PHE:HE2	1:D:239:LYS:CE	2.30	0.44
1:A:310:VAL:HA	1:A:313:ILE:HD12	2.00	0.44
1:B:198:VAL:HG22	1:B:203:ARG:HG2	1.99	0.44
1:A:258:PHE:CD1	1:A:310:VAL:HG13	2.52	0.44
1:B:258:PHE:HB3	1:B:263:ILE:HD11	1.98	0.44
1:F:38:HIS:O	1:F:39:GLU:C	2.61	0.44
1:B:87:PRO:HA	1:B:141:THR:HG21	1.99	0.44
1:C:92:ASN:O	1:C:96:TYR:HB3	2.17	0.44
1:C:163:ARG:NH1	1:C:245:GLY:O	2.50	0.44
1:C:170:PHE:O	2:C:401:NAD:H4N	2.17	0.44
1:F:113:PHE:HE2	1:F:115:PHE:HB2	1.82	0.44
1:A:4:ILE:HD13	1:A:238:LEU:CD2	2.48	0.44
1:A:20:LYS:HE2	1:A:235:PHE:CD2	2.53	0.44
1:A:24:GLU:O	1:A:25:GLY:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ILE:N	1:B:263:ILE:HD12	2.33	0.44
1:D:223:ASP:HB2	1:D:291:VAL:HA	1.99	0.44
1:F:87:PRO:HA	1:F:141:THR:HG21	2.00	0.44
1:B:111:ASP:OD1	1:B:111:ASP:C	2.61	0.44
1:C:215:THR:HB	1:C:216:PRO:HD2	1.99	0.44
1:D:209:PHE:CD2	1:D:283:ARG:HD2	2.53	0.44
1:F:222:ARG:NH2	1:F:287:PRO:HD2	2.33	0.44
1:F:6:ILE:HD11	1:F:21:LEU:HD11	1.99	0.43
1:A:146:LYS:HD2	1:A:146:LYS:HA	1.64	0.43
1:A:213:TYR:CE2	1:A:282:ARG:NH2	2.86	0.43
1:A:150:GLU:HG2	1:A:166:ILE:HD13	2.00	0.43
1:D:93:ASN:ND2	1:D:94:ASN:OD1	2.51	0.43
1:D:178:ASN:OD1	1:D:178:ASN:C	2.60	0.43
1:D:209:PHE:CG	1:D:283:ARG:HD2	2.53	0.43
1:F:192:ILE:N	1:F:193:PRO:HD2	2.34	0.43
1:A:33:ASN:HD21	1:A:35:GLN:CG	2.24	0.43
1:D:125:VAL:HG12	1:D:127:VAL:H	1.83	0.43
1:B:117:SER:HA	1:B:146:LYS:HE2	2.00	0.43
1:C:153:LEU:HD23	1:C:153:LEU:HA	1.75	0.43
1:E:273:HIS:O	1:E:275:ILE:HD12	2.18	0.43
1:F:280:ALA:HB1	1:F:281:PRO:HD2	2.01	0.43
1:D:106:ASP:O	1:D:107:GLU:C	2.61	0.43
1:E:33:ASN:HD21	1:E:35:GLN:H	1.62	0.43
1:E:217:ASP:OD2	1:E:261:LYS:HB3	2.19	0.43
1:A:92:ASN:O	1:A:96:TYR:HB3	2.18	0.43
1:B:164:TYR:O	1:B:247:SER:HA	2.19	0.43
1:D:165:LYS:HE2	1:D:241:LEU:HD21	2.00	0.43
1:C:286:ASP:HA	1:C:287:PRO:HD3	1.83	0.43
1:B:258:PHE:CD1	1:B:310:VAL:HG13	2.54	0.43
1:D:4:ILE:HD13	1:D:238:LEU:CD2	2.48	0.43
1:B:72:MET:HG2	1:B:114:ILE:HB	2.00	0.42
1:E:33:ASN:HD22	1:E:33:ASN:C	2.26	0.42
1:F:56:LYS:HE3	1:F:103:GLU:OE1	2.19	0.42
1:C:199:ALA:HB2	1:C:275:ILE:HD11	2.02	0.42
1:C:56:LYS:HE2	1:C:103:GLU:OE1	2.19	0.42
1:D:213:TYR:HE1	1:D:220:CYS:HG	1.57	0.42
1:A:11:GLY:O	1:A:15:SER:HB3	2.18	0.42
1:C:150:GLU:O	1:C:153:LEU:HB2	2.19	0.42
1:A:83:SER:HB2	1:A:141:THR:HB	2.01	0.42
1:A:298:LYS:HG2	1:A:303:TRP:O	2.20	0.42
1:C:212:ASP:CA	1:C:282:ARG:NH2	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:TYR:OH	1:D:282:ARG:HG3	2.19	0.42
1:F:20:LYS:NZ	1:F:235:PHE:HD2	2.17	0.42
1:F:226:HIS:HD1	1:F:228:GLU:N	2.14	0.42
1:A:320:TRP:CZ3	1:A:324:GLN:HG3	2.54	0.42
1:D:41:ALA:HB2	1:D:328:TYR:CE1	2.54	0.42
1:D:92:ASN:O	1:D:96:TYR:HB3	2.19	0.42
1:E:258:PHE:CE1	1:E:310:VAL:HG13	2.54	0.42
1:A:202:GLN:C	1:A:203:ARG:HG2	2.45	0.42
1:B:274:GLU:HG3	1:B:275:ILE:N	2.34	0.42
1:C:51:GLY:HA3	1:C:58:PHE:CZ	2.55	0.42
1:C:170:PHE:HB2	1:C:223:ASP:HB3	2.01	0.42
1:B:265:ASP:OD1	1:B:268:ARG:NH1	2.53	0.41
1:C:118:THR:HG22	1:C:146:LYS:HG3	2.02	0.41
1:D:150:GLU:HG2	1:D:166:ILE:HD13	2.01	0.41
1:E:73:HIS:CD2	1:E:73:HIS:C	2.98	0.41
1:E:153:LEU:HD23	1:E:153:LEU:HA	1.86	0.41
1:A:169:TYR:CE2	2:A:401:NAD:C5N	3.03	0.41
1:B:167:PHE:CE1	1:B:234:HIS:HA	2.55	0.41
1:B:223:ASP:HB2	1:B:291:VAL:HA	2.01	0.41
1:C:23:ASP:C	1:C:25:GLY:H	2.27	0.41
1:D:33:ASN:C	1:D:33:ASN:ND2	2.78	0.41
1:D:158:GLN:HE21	1:D:158:GLN:N	2.18	0.41
1:E:23:ASP:C	1:E:25:GLY:H	2.27	0.41
1:E:56:LYS:CE	1:E:103:GLU:OE1	2.68	0.41
1:A:8:GLY:O	1:A:14:GLY:HA3	2.21	0.41
1:C:118:THR:O	1:C:121:THR:HB	2.19	0.41
1:E:111:ASP:C	1:E:111:ASP:OD1	2.62	0.41
1:E:182:GLY:HA3	1:E:320:TRP:CG	2.55	0.41
1:A:73:HIS:HD2	1:A:115:PHE:CE1	2.38	0.41
1:A:213:TYR:CE2	1:A:282:ARG:CZ	3.04	0.41
1:D:275:ILE:O	1:D:275:ILE:HG22	2.19	0.41
1:E:195:VAL:O	1:E:198:VAL:HB	2.20	0.41
1:D:86:LYS:HB3	1:D:89:GLN:HG2	2.03	0.41
1:D:113:PHE:O	1:D:164:TYR:HA	2.20	0.41
1:E:5:LEU:HB2	1:E:68:ILE:HD12	2.01	0.41
1:F:203:ARG:HH11	1:F:203:ARG:CG	2.33	0.41
1:F:286:ASP:HA	1:F:287:PRO:HD3	1.71	0.41
1:E:135[A]:MET:HG2	4:E:2018:HOH:O	2.20	0.41
1:F:203:ARG:HH11	1:F:203:ARG:HG3	1.86	0.41
1:B:20:LYS:HB2	1:B:20:LYS:HZ2	1.84	0.41
1:E:306:ARG:HG3	1:E:307:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ALA:HB2	1:A:328:TYR:CZ	2.56	0.41
1:C:56:LYS:CE	1:C:103:GLU:OE1	2.68	0.41
1:E:56:LYS:HE3	1:E:103:GLU:OE1	2.21	0.41
1:E:83:SER:HB2	1:E:141:THR:HB	2.02	0.41
1:E:188:GLU:O	1:E:194:LEU:HD21	2.21	0.41
1:F:13:ILE:O	1:F:14:GLY:C	2.61	0.41
1:D:8:GLY:O	1:D:14:GLY:HA3	2.21	0.40
1:D:20:LYS:O	1:D:21:LEU:C	2.64	0.40
1:B:170:PHE:O	1:B:171:ASN:ND2	2.54	0.40
1:F:182:GLY:HA3	1:F:320:TRP:CD2	2.56	0.40
1:A:33:ASN:H	1:A:33:ASN:HD22	1.69	0.40
1:D:186:ARG:HA	1:D:187:PRO:HA	1.95	0.40
1:E:219:THR:HB	1:E:220:CYS:H	1.73	0.40
1:F:106:ASP:O	1:F:107:GLU:C	2.65	0.40
1:A:133:GLU:H	1:A:133:GLU:HG2	1.73	0.40
1:B:73:HIS:CD2	1:B:73:HIS:C	2.99	0.40
1:E:114:ILE:HD11	1:E:238:LEU:HA	2.03	0.40
1:E:197:GLN:HB3	1:E:203:ARG:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	328/330 (99%)	297 (90%)	27 (8%)	4 (1%)	10	27
1	B	328/330 (99%)	307 (94%)	19 (6%)	2 (1%)	21	44
1	C	328/330 (99%)	309 (94%)	17 (5%)	2 (1%)	21	44
1	D	328/330 (99%)	302 (92%)	22 (7%)	4 (1%)	10	27
1	E	328/330 (99%)	291 (89%)	33 (10%)	4 (1%)	10	27
1	F	328/330 (99%)	301 (92%)	22 (7%)	5 (2%)	8	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1968/1980 (99%)	1807 (92%)	140 (7%)	21 (1%)	11	29

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	286	ASP
1	A	25	GLY
1	D	272	ASN
1	F	281	PRO
1	F	282	ARG
1	A	285	GLY
1	B	286	ASP
1	C	285	GLY
1	D	303	TRP
1	E	24	GLU
1	F	23	ASP
1	E	214	ASN
1	E	282	ARG
1	A	218	GLY
1	F	215	THR
1	B	215	THR
1	F	22	VAL
1	D	281	PRO
1	E	275	ILE
1	A	275	ILE
1	D	286	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/277 (100%)	256 (93%)	20 (7%)	13	32
1	B	276/277 (100%)	245 (89%)	31 (11%)	6	15
1	C	276/277 (100%)	251 (91%)	25 (9%)	9	22
1	D	276/277 (100%)	253 (92%)	23 (8%)	10	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	276/277 (100%)	258 (94%)	18 (6%)	15	37
1	F	276/277 (100%)	248 (90%)	28 (10%)	7	18
All	All	1656/1662 (100%)	1511 (91%)	145 (9%)	9	23

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	19	LYS
1	A	26	LEU
1	A	32	ASP
1	A	33	ASN
1	A	50	ASN
1	A	59	LEU
1	A	69	GLU
1	A	72	MET
1	A	78	SER
1	A	121	THR
1	A	133	GLU
1	A	146	LYS
1	A	158	GLN
1	A	192	ILE
1	A	217	ASP
1	A	263	ILE
1	A	306	ARG
1	A	310	VAL
1	A	330	LYS
1	B	3	SER
1	B	19	LYS
1	B	20	LYS
1	B	33	ASN
1	B	67	ASN
1	B	86	LYS
1	B	116	SER
1	B	121	THR
1	B	124	GLU
1	B	125	VAL
1	B	126	ASP
1	B	127	VAL
1	B	133	GLU
1	B	176	THR

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Mol	Chain	Res	Type
1	B	180	ILE
1	B	189	THR
1	B	203	ARG
1	B	208	MET
1	B	231	VAL
1	B	239	LYS
1	B	256	ASN
1	B	269	GLU
1	B	275	ILE
1	B	279	VAL
1	B	283	ARG
1	B	298	LYS
1	B	306	ARG
1	B	308	VAL
1	B	309	ASN
1	B	310	VAL
1	B	319	ASN
1	C	3	SER
1	C	22	VAL
1	C	33	ASN
1	C	50	ASN
1	C	56	LYS
1	C	69	GLU
1	C	86	LYS
1	C	116	SER
1	C	121	THR
1	C	133	GLU
1	C	158	GLN
1	C	176	THR
1	C	180	ILE
1	C	205	LYS
1	C	215	THR
1	C	220	CYS
1	C	235	PHE
1	C	239	LYS
1	C	261	LYS
1	C	279	VAL
1	C	286	ASP
1	C	289	ARG
1	C	308	VAL
1	C	310	VAL
1	C	330	LYS

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Mol	Chain	Res	Type
1	D	20	LYS
1	D	27	SER
1	D	33	ASN
1	D	34	LEU
1	D	43	THR
1	D	50	ASN
1	D	59	LEU
1	D	64	THR
1	D	89	GLN
1	D	116	SER
1	D	121	THR
1	D	127	VAL
1	D	128	ASP
1	D	180	ILE
1	D	192	ILE
1	D	204	GLU
1	D	260	VAL
1	D	273	HIS
1	D	274	GLU
1	D	279	VAL
1	D	283	ARG
1	D	306	ARG
1	D	310	VAL
1	E	6	ILE
1	E	24	GLU
1	E	33	ASN
1	E	43	THR
1	E	50	ASN
1	E	59	LEU
1	E	86	LYS
1	E	116	SER
1	E	121	THR
1	E	125	VAL
1	E	203	ARG
1	E	217	ASP
1	E	220	CYS
1	E	235	PHE
1	E	286	ASP
1	E	289	ARG
1	E	308	VAL
1	E	310	VAL
1	F	6	ILE

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Mol	Chain	Res	Type
1	F	20	LYS
1	F	26	LEU
1	F	28	VAL
1	F	33	ASN
1	F	50	ASN
1	F	56	LYS
1	F	78	SER
1	F	116	SER
1	F	121	THR
1	F	125	VAL
1	F	127	VAL
1	F	128	ASP
1	F	131	THR
1	F	158	GLN
1	F	180	ILE
1	F	203	ARG
1	F	204	GLU
1	F	230	LEU
1	F	256	ASN
1	F	269	GLU
1	F	274	GLU
1	F	279	VAL
1	F	283	ARG
1	F	294	SER
1	F	306	ARG
1	F	310	VAL
1	F	318	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	50	ASN
1	A	65	GLN
1	A	73	HIS
1	A	158	GLN
1	A	161	ASN
1	A	171	ASN
1	B	33	ASN
1	B	50	ASN
1	B	65	GLN
1	B	67	ASN

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Mol	Chain	Res	Type
1	B	89	GLN
1	B	137	ASN
1	B	171	ASN
1	B	316	HIS
1	B	319	ASN
1	C	2	ASN
1	C	33	ASN
1	C	50	ASN
1	C	65	GLN
1	C	158	GLN
1	C	161	ASN
1	C	171	ASN
1	C	197	GLN
1	C	254	ASN
1	C	321	HIS
1	D	2	ASN
1	D	33	ASN
1	D	50	ASN
1	D	65	GLN
1	D	89	GLN
1	D	158	GLN
1	D	171	ASN
1	D	251	ASN
1	E	33	ASN
1	E	50	ASN
1	E	65	GLN
1	E	73	HIS
1	E	254	ASN
1	F	33	ASN
1	F	50	ASN
1	F	89	GLN
1	F	158	GLN
1	F	171	ASN
1	F	251	ASN
1	F	273	HIS
1	F	316	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAD	A	401	-	46,48,48	2.09	8 (17%)	64,73,73	1.59	12 (18%)
2	NAD	B	401	-	46,48,48	2.01	8 (17%)	64,73,73	1.59	10 (15%)
2	NAD	F	401	-	46,48,48	1.96	7 (15%)	64,73,73	1.45	9 (14%)
2	NAD	E	401	-	46,48,48	2.09	7 (15%)	64,73,73	1.65	11 (17%)
2	NAD	D	401	-	46,48,48	2.01	8 (17%)	64,73,73	1.67	8 (12%)
2	NAD	C	401	-	46,48,48	1.96	7 (15%)	64,73,73	1.68	15 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	401	-	-	6/30/62/62	0/5/5/5
2	NAD	B	401	-	-	5/30/62/62	0/5/5/5
2	NAD	F	401	-	-	8/30/62/62	0/5/5/5
2	NAD	E	401	-	-	3/30/62/62	0/5/5/5
2	NAD	D	401	-	-	11/30/62/62	0/5/5/5
2	NAD	C	401	-	-	12/30/62/62	0/5/5/5

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	O7N-C7N	9.95	1.42	1.24
2	D	401	NAD	O7N-C7N	9.89	1.42	1.24
2	F	401	NAD	O7N-C7N	9.56	1.41	1.24
2	C	401	NAD	O7N-C7N	9.56	1.41	1.24
2	B	401	NAD	O7N-C7N	9.55	1.41	1.24
2	E	401	NAD	O7N-C7N	9.44	1.41	1.24
2	E	401	NAD	PN-O3	6.04	1.66	1.59
2	A	401	NAD	PN-O3	5.58	1.65	1.59
2	B	401	NAD	PN-O3	5.51	1.65	1.59
2	F	401	NAD	PN-O3	5.17	1.65	1.59
2	D	401	NAD	PN-O3	4.62	1.64	1.59
2	C	401	NAD	PN-O3	4.38	1.64	1.59
2	E	401	NAD	C2N-N1N	4.37	1.39	1.35
2	C	401	NAD	C2N-N1N	3.19	1.38	1.35
2	A	401	NAD	PA-O3	3.19	1.62	1.59
2	A	401	NAD	C2A-N3A	2.96	1.39	1.33
2	D	401	NAD	C2A-N3A	2.93	1.39	1.33
2	B	401	NAD	C2A-N3A	2.92	1.39	1.33
2	F	401	NAD	PA-O3	2.86	1.62	1.59
2	F	401	NAD	C2N-N1N	2.81	1.38	1.35
2	C	401	NAD	C2A-N3A	2.80	1.38	1.33
2	A	401	NAD	C5A-N7A	-2.76	1.34	1.39
2	A	401	NAD	C2N-N1N	2.74	1.38	1.35
2	E	401	NAD	C2A-N1A	2.70	1.38	1.33
2	D	401	NAD	C5A-N7A	-2.69	1.34	1.39
2	E	401	NAD	C2A-N3A	2.66	1.38	1.33
2	D	401	NAD	C2A-N1A	2.48	1.38	1.33
2	F	401	NAD	C2A-N1A	2.46	1.38	1.33
2	B	401	NAD	C2N-N1N	2.44	1.37	1.35
2	B	401	NAD	PA-O3	2.44	1.62	1.59
2	D	401	NAD	C8A-N7A	2.41	1.36	1.31
2	A	401	NAD	C2A-N1A	2.41	1.38	1.33
2	B	401	NAD	C8A-N7A	2.38	1.36	1.31
2	F	401	NAD	C2A-N3A	2.36	1.38	1.33
2	E	401	NAD	C8A-N7A	2.35	1.36	1.31
2	C	401	NAD	C2A-N1A	2.33	1.38	1.33
2	D	401	NAD	C2N-N1N	2.29	1.37	1.35
2	B	401	NAD	C2A-N1A	2.29	1.38	1.33
2	E	401	NAD	C5A-N7A	-2.28	1.34	1.39
2	C	401	NAD	C8A-N7A	2.22	1.35	1.31
2	F	401	NAD	C5A-N7A	-2.18	1.35	1.39
2	A	401	NAD	C8A-N7A	2.13	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NAD	PA-O3	2.11	1.61	1.59
2	B	401	NAD	C6N-N1N	2.10	1.40	1.35
2	C	401	NAD	C5A-N7A	-2.04	1.35	1.39

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NAD	N3A-C2A-N1A	-6.81	118.27	128.58
2	B	401	NAD	N3A-C2A-N1A	-6.04	119.44	128.58
2	E	401	NAD	N3A-C2A-N1A	-5.73	119.91	128.58
2	F	401	NAD	N3A-C2A-N1A	-5.58	120.13	128.58
2	A	401	NAD	N3A-C2A-N1A	-5.50	120.26	128.58
2	A	401	NAD	C5A-C4A-N3A	-5.16	119.61	126.72
2	C	401	NAD	N3A-C2A-N1A	-5.03	120.97	128.58
2	D	401	NAD	C5A-C4A-N3A	-4.85	120.04	126.72
2	C	401	NAD	C5A-C4A-N3A	-4.85	120.05	126.72
2	E	401	NAD	C5A-C4A-N3A	-4.52	120.49	126.72
2	B	401	NAD	C5A-C4A-N3A	-4.43	120.61	126.72
2	D	401	NAD	C2A-N3A-C4A	4.01	121.63	111.83
2	B	401	NAD	C2A-N3A-C4A	3.62	120.67	111.83
2	D	401	NAD	N9A-C8A-N7A	-3.59	108.85	113.94
2	C	401	NAD	C3N-C7N-N7N	3.53	122.09	117.74
2	A	401	NAD	C2A-N3A-C4A	3.51	120.40	111.83
2	E	401	NAD	C2A-N3A-C4A	3.40	120.15	111.83
2	B	401	NAD	N9A-C8A-N7A	-3.36	109.17	113.94
2	F	401	NAD	N9A-C8A-N7A	-3.31	109.25	113.94
2	D	401	NAD	N3A-C4A-N9A	3.27	132.72	127.17
2	C	401	NAD	C2A-N3A-C4A	3.26	119.80	111.83
2	F	401	NAD	C5A-C4A-N3A	-3.26	122.23	126.72
2	A	401	NAD	N9A-C8A-N7A	-3.25	109.32	113.94
2	C	401	NAD	O7N-C7N-C3N	-3.22	115.66	119.60
2	A	401	NAD	C5A-N7A-C8A	3.21	108.50	103.45
2	E	401	NAD	C6N-N1N-C2N	-3.17	119.18	121.88
2	B	401	NAD	C6N-N1N-C2N	-3.15	119.20	121.88
2	E	401	NAD	N9A-C8A-N7A	-3.14	109.49	113.94
2	A	401	NAD	N3A-C4A-N9A	3.07	132.39	127.17
2	C	401	NAD	C6N-N1N-C2N	-3.01	119.32	121.88
2	F	401	NAD	C6N-N1N-C2N	-2.99	119.33	121.88
2	C	401	NAD	N3A-C4A-N9A	2.96	132.20	127.17
2	B	401	NAD	C5A-N7A-C8A	2.93	108.05	103.45
2	D	401	NAD	C5A-N7A-C8A	2.90	108.00	103.45
2	E	401	NAD	N3A-C4A-N9A	2.80	131.93	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	NAD	O2N-PN-O3	2.79	114.81	107.27
2	E	401	NAD	C3N-C7N-N7N	2.78	121.17	117.74
2	C	401	NAD	N9A-C8A-N7A	-2.77	110.01	113.94
2	B	401	NAD	N3A-C4A-N9A	2.75	131.84	127.17
2	C	401	NAD	C5A-N7A-C8A	2.74	107.75	103.45
2	D	401	NAD	O2N-PN-O3	2.72	114.63	107.27
2	E	401	NAD	C5A-N7A-C8A	2.71	107.71	103.45
2	F	401	NAD	C5A-N7A-C8A	2.67	107.65	103.45
2	F	401	NAD	C2A-N3A-C4A	2.63	118.27	111.83
2	E	401	NAD	O7N-C7N-N7N	-2.57	118.91	122.62
2	A	401	NAD	O4B-C1B-C2B	-2.56	101.14	106.62
2	D	401	NAD	C6N-N1N-C2N	-2.55	119.71	121.88
2	C	401	NAD	O4B-C1B-N9A	-2.54	103.21	108.09
2	A	401	NAD	C3N-C7N-N7N	2.48	120.79	117.74
2	A	401	NAD	C6A-C5A-C4A	2.46	120.53	117.18
2	C	401	NAD	O4B-C1B-C2B	-2.41	101.45	106.62
2	A	401	NAD	C4A-C5A-N7A	-2.38	107.86	110.58
2	E	401	NAD	O4B-C1B-C2B	-2.37	101.54	106.62
2	B	401	NAD	O5B-C5B-C4B	-2.30	101.15	108.99
2	C	401	NAD	O2B-C2B-C1B	2.29	117.99	110.10
2	C	401	NAD	C6A-C5A-C4A	2.27	120.28	117.18
2	F	401	NAD	O2N-PN-O1N	2.20	122.66	112.44
2	F	401	NAD	O5B-C5B-C4B	-2.15	101.66	108.99
2	C	401	NAD	C4A-C5A-N7A	-2.15	108.12	110.58
2	C	401	NAD	O2N-PN-O3	2.12	113.01	107.27
2	B	401	NAD	C4A-C5A-N7A	-2.09	108.19	110.58
2	B	401	NAD	O2N-PN-O1N	2.09	122.15	112.44
2	F	401	NAD	N3A-C4A-N9A	2.06	130.68	127.17
2	A	401	NAD	O7N-C7N-N7N	-2.02	119.70	122.62
2	A	401	NAD	C5A-C4A-N9A	2.00	108.00	105.81

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5D-O5D-PN-O2N
2	B	401	NAD	C5D-O5D-PN-O3
2	B	401	NAD	C5D-O5D-PN-O2N
2	C	401	NAD	C5B-O5B-PA-O1A
2	C	401	NAD	C5B-O5B-PA-O3
2	C	401	NAD	PN-O3-PA-O5B
2	C	401	NAD	C5D-O5D-PN-O3

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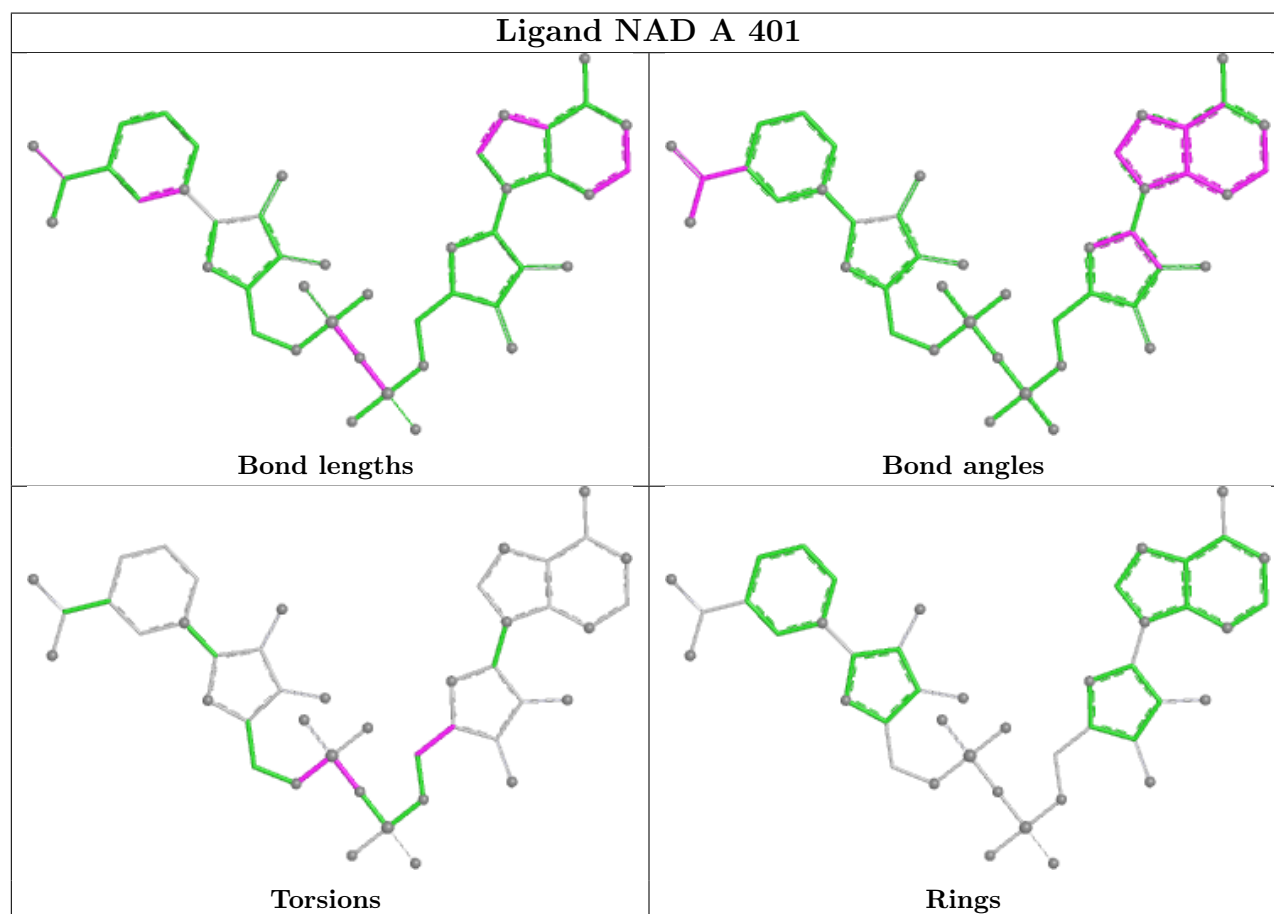
Mol	Chain	Res	Type	Atoms
2	C	401	NAD	C5D-O5D-PN-O2N
2	D	401	NAD	C5B-O5B-PA-O1A
2	D	401	NAD	C5B-O5B-PA-O3
2	D	401	NAD	PN-O3-PA-O5B
2	D	401	NAD	C5D-O5D-PN-O3
2	D	401	NAD	C5D-O5D-PN-O1N
2	D	401	NAD	C5D-O5D-PN-O2N
2	F	401	NAD	C5D-O5D-PN-O3
2	F	401	NAD	C5D-O5D-PN-O1N
2	F	401	NAD	C5D-O5D-PN-O2N
2	D	401	NAD	O4B-C4B-C5B-O5B
2	C	401	NAD	PA-O3-PN-O1N
2	D	401	NAD	PA-O3-PN-O1N
2	D	401	NAD	C3B-C4B-C5B-O5B
2	F	401	NAD	PN-O3-PA-O5B
2	C	401	NAD	C3B-C4B-C5B-O5B
2	C	401	NAD	PA-O3-PN-O2N
2	A	401	NAD	C5D-O5D-PN-O3
2	A	401	NAD	C5D-O5D-PN-O1N
2	B	401	NAD	C5D-O5D-PN-O1N
2	C	401	NAD	C5B-O5B-PA-O2A
2	C	401	NAD	C5D-O5D-PN-O1N
2	D	401	NAD	C5B-O5B-PA-O2A
2	E	401	NAD	C5D-O5D-PN-O3
2	F	401	NAD	C5B-O5B-PA-O1A
2	F	401	NAD	C5B-O5B-PA-O2A
2	F	401	NAD	C5B-O5B-PA-O3
2	C	401	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	PA-O3-PN-O2N
2	D	401	NAD	PA-O3-PN-O2N
2	C	401	NAD	O4D-C4D-C5D-O5D
2	A	401	NAD	O4B-C4B-C5B-O5B
2	B	401	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	PA-O3-PN-O1N
2	B	401	NAD	PA-O3-PN-O2N
2	F	401	NAD	PA-O3-PN-O2N
2	E	401	NAD	PA-O3-PN-O2N
2	E	401	NAD	O4B-C4B-C5B-O5B

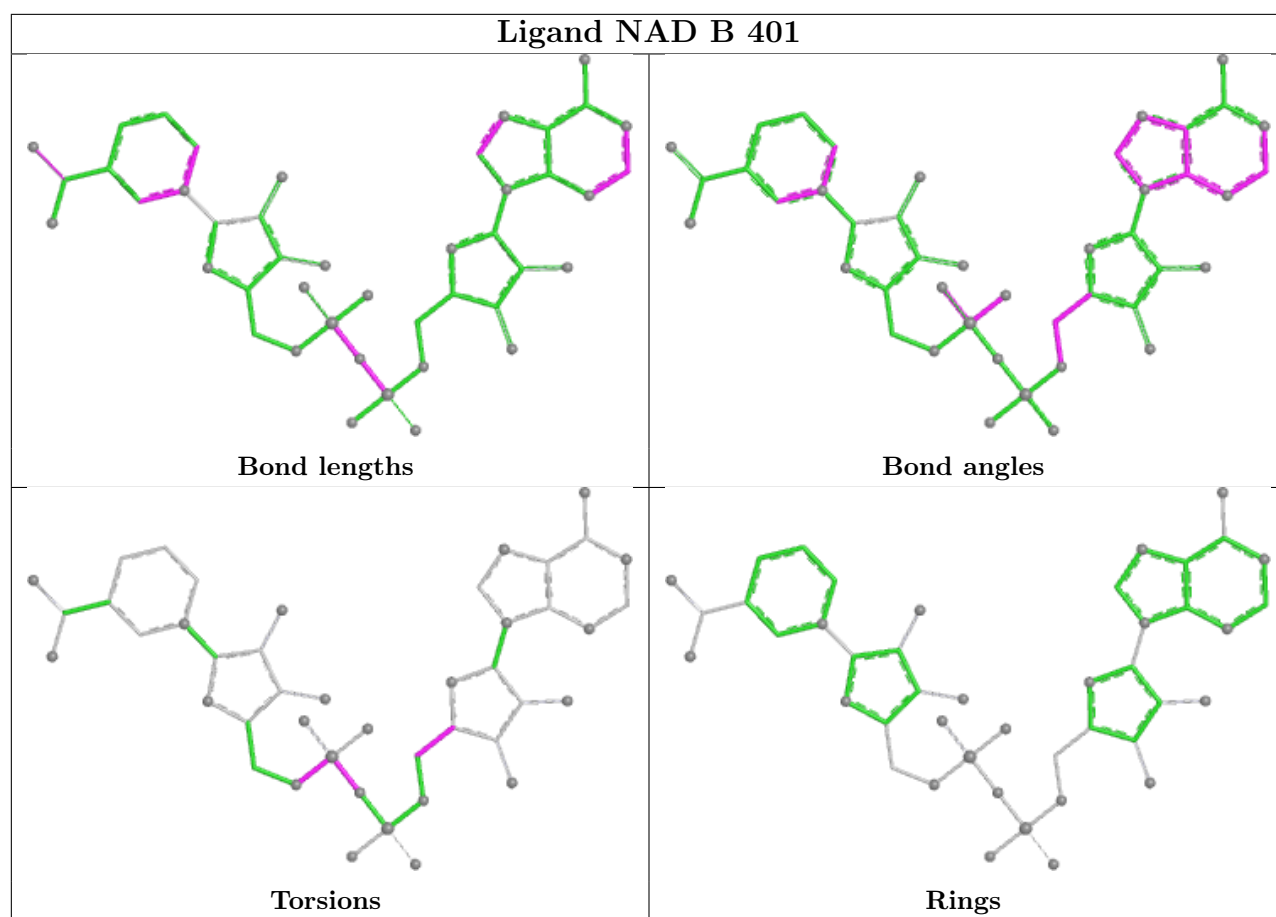
There are no ring outliers.

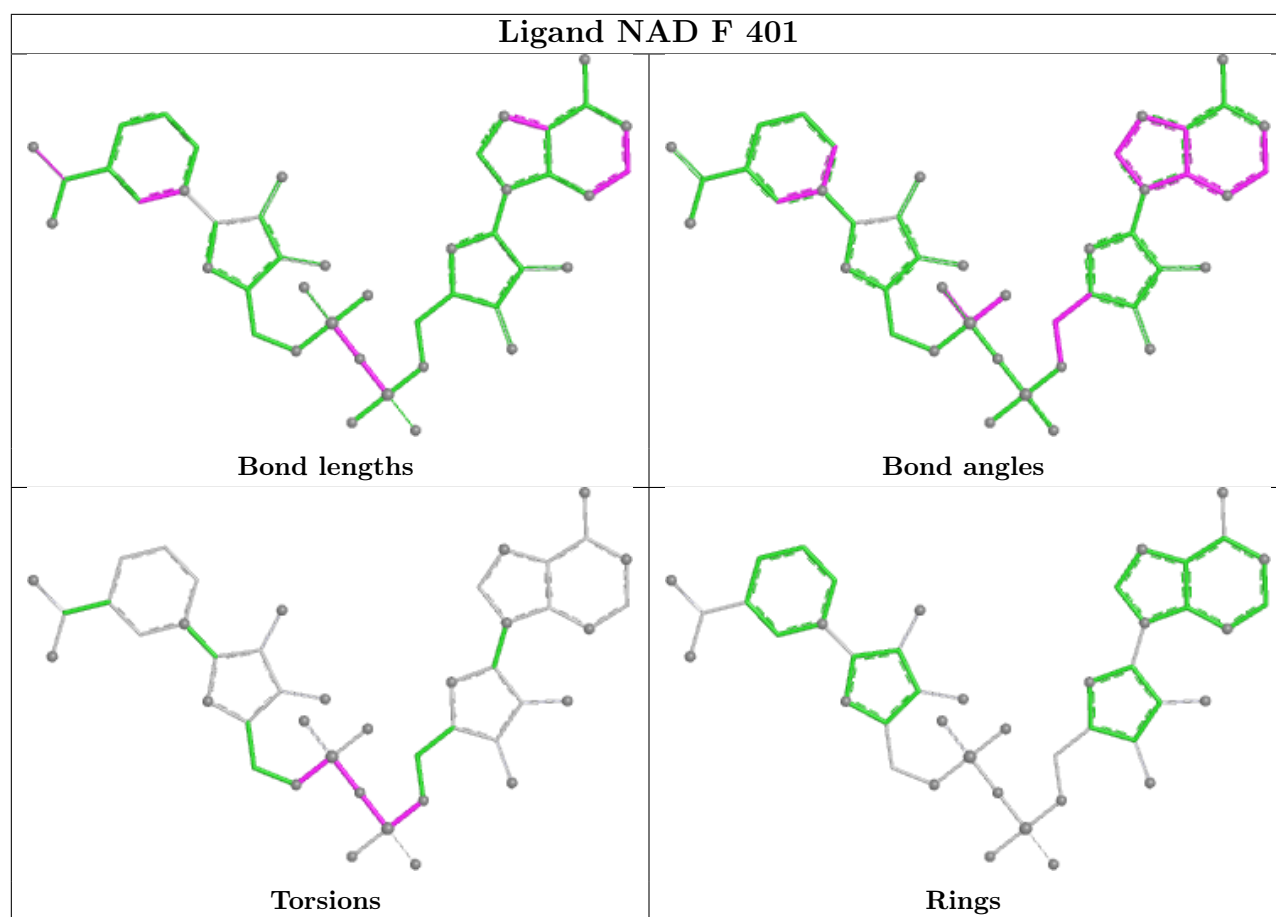
6 monomers are involved in 14 short contacts:

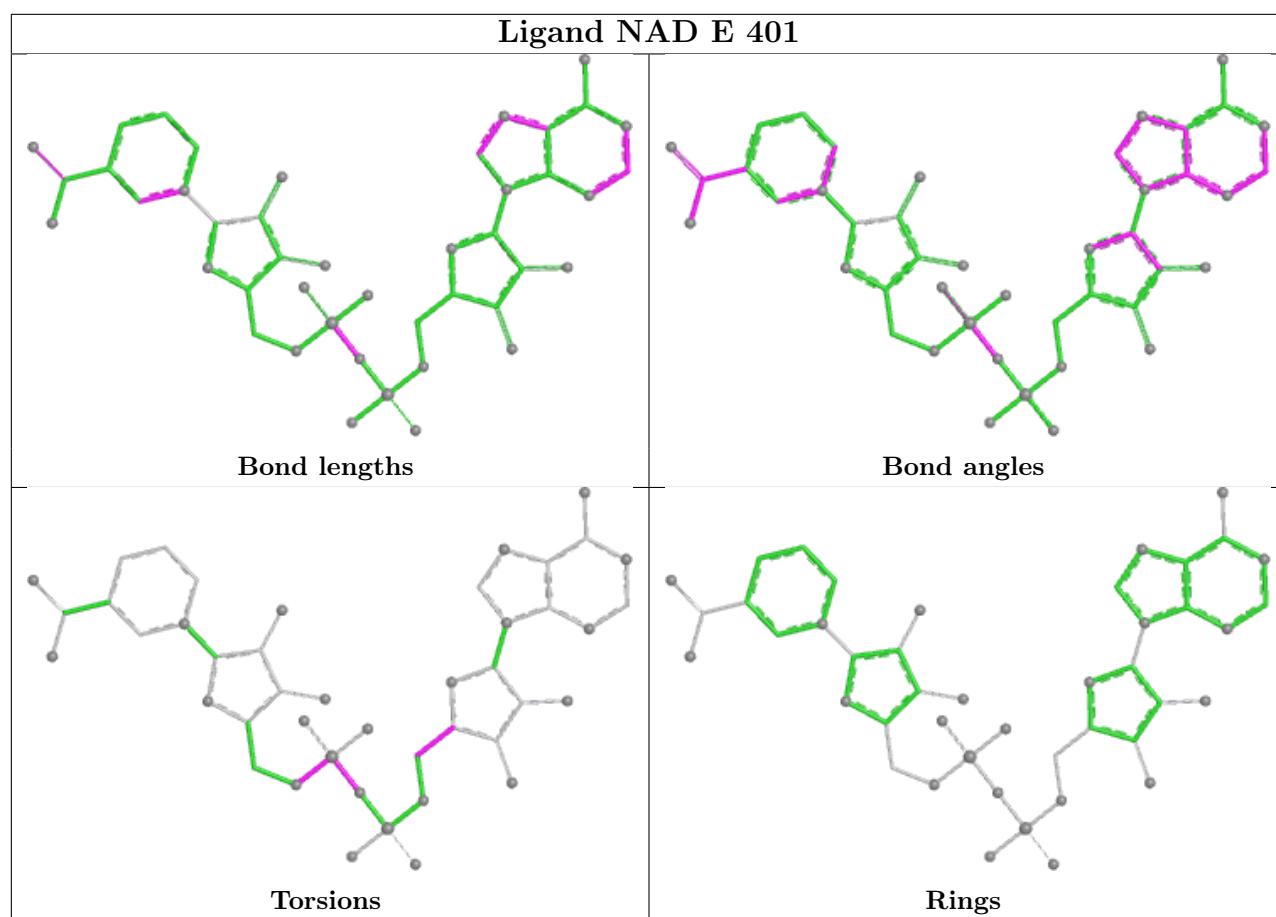
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAD	5	0
2	B	401	NAD	1	0
2	F	401	NAD	3	0
2	E	401	NAD	2	0
2	D	401	NAD	1	0
2	C	401	NAD	2	0

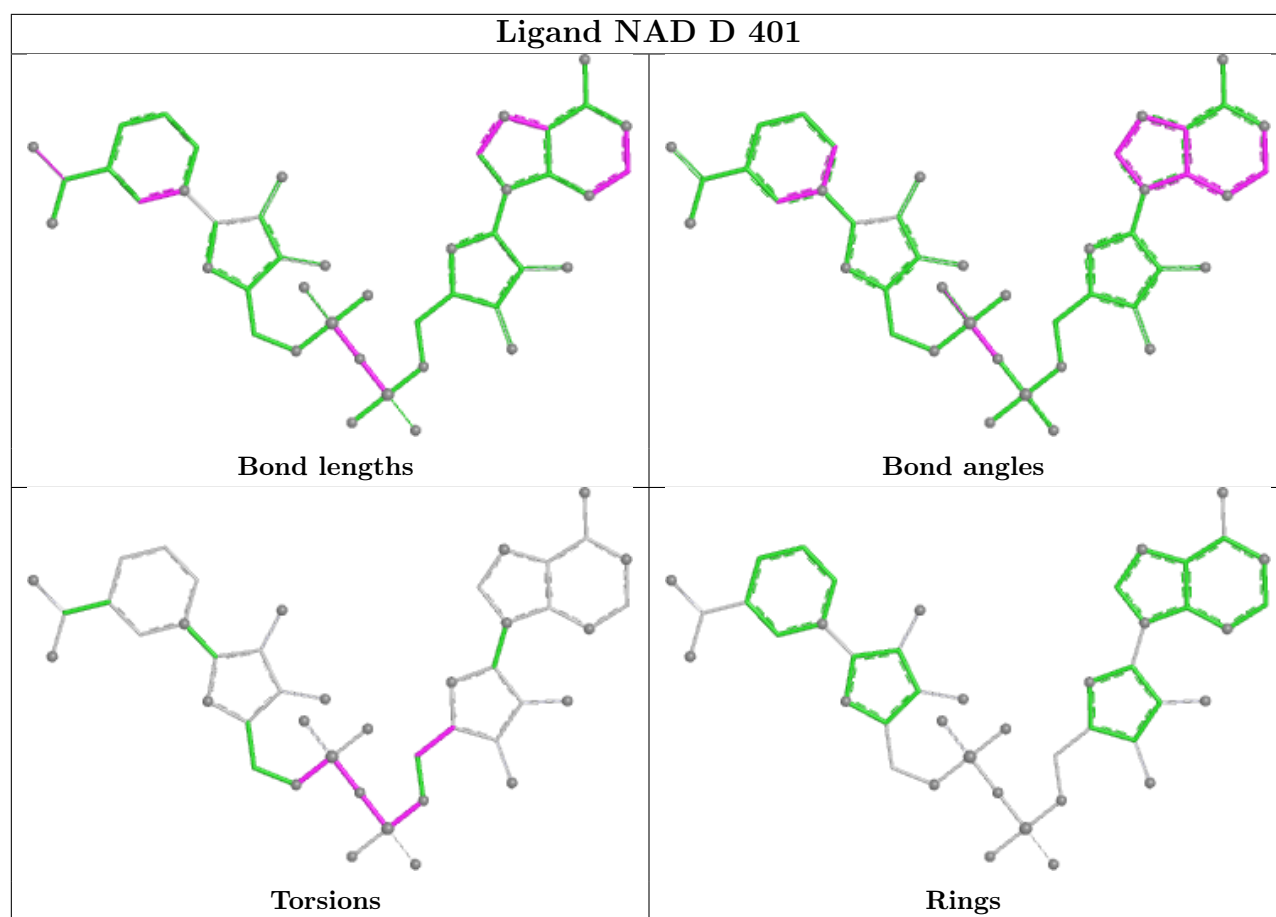
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

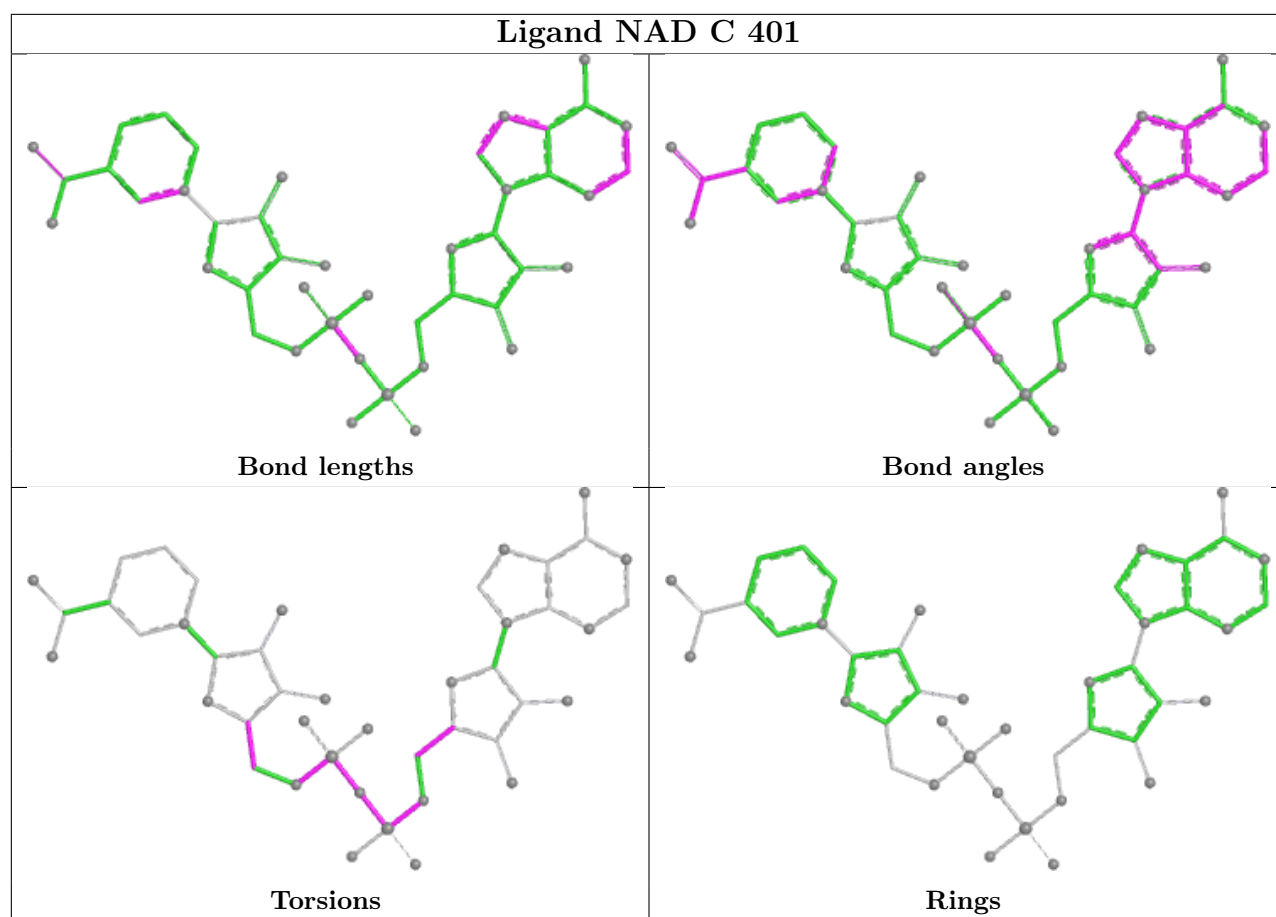












5.7 Other polymers [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.