



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:49 PM UTC

PDB ID : 1KQO / pdb_00001kqo
Title : Crystal structure of NMN/NaMN adenylyltransferase complexed with deamido-NAD
Authors : Zhou, T.; Kurnasov, O.; Tomchick, D.R.; Binns, D.D.; Grishin, N.V.; Marquez, V.E.; Osterman, A.L.; Zhang, H.
Deposited on : 2002-01-07
Resolution : 2.50 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

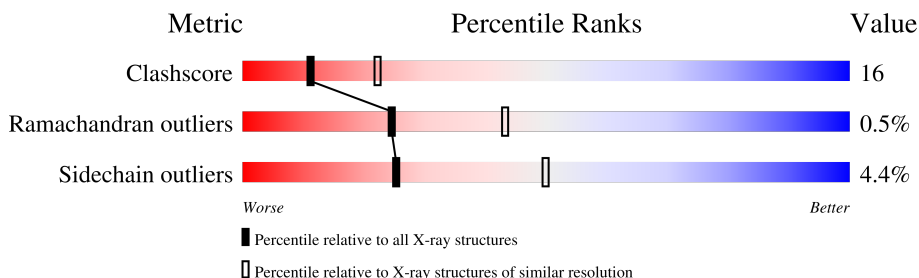
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	279	
1	B	279	
1	C	279	
1	D	279	
1	E	279	
1	F	279	

2 Entry composition i

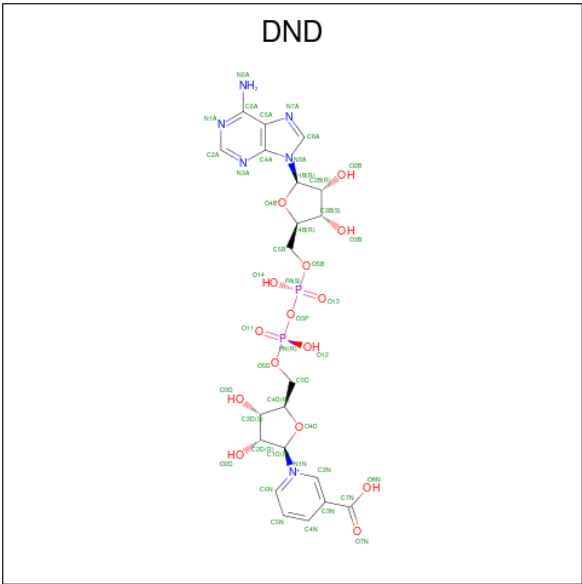
There are 3 unique types of molecules in this entry. The entry contains 11921 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1875	1195	331	343	6			
1	B	233	Total	C	N	O	S	0	0	0
			1875	1195	331	343	6			
1	C	233	Total	C	N	O	S	0	0	0
			1875	1195	331	343	6			
1	D	233	Total	C	N	O	S	0	0	0
			1875	1195	331	343	6			
1	E	233	Total	C	N	O	S	0	0	0
			1875	1195	331	343	6			
1	F	233	Total	C	N	O	S	0	0	0
			1875	1195	331	343	6			

- Molecule 2 is NICOTINIC ACID ADENINE DINUCLEOTIDE (CCD ID: DND) (formula: C₂₁H₂₇N₆O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	6	15	2		

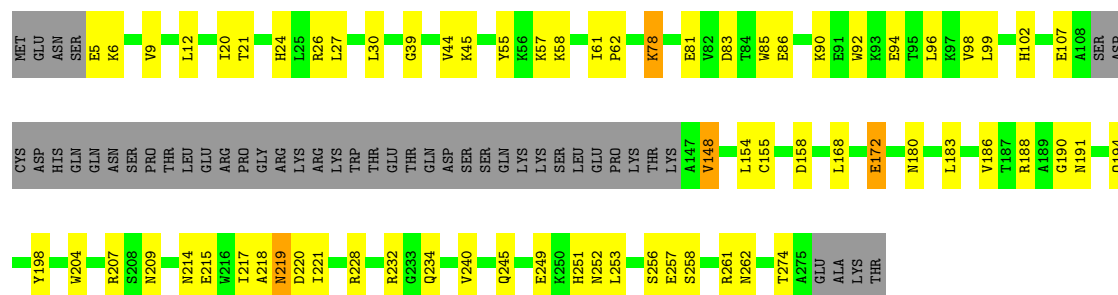
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	68	Total	O	0	0
			68	68		
3	C	80	Total	O	0	0
			80	80		
3	D	65	Total	O	0	0
			65	65		
3	E	57	Total	O	0	0
			57	57		
3	F	47	Total	O	0	0
			47	47		



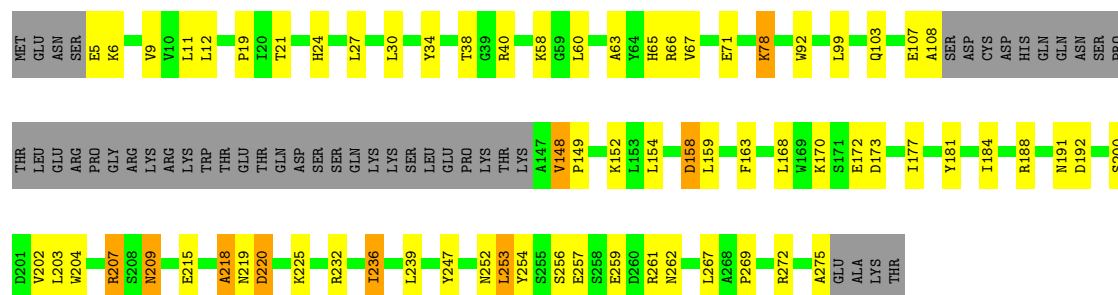
• Molecule 1: NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE

Chain D: 58% 24% 16%



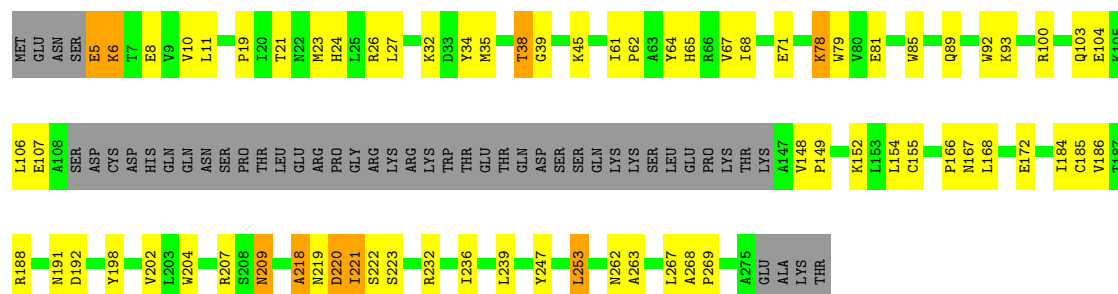
• Molecule 1: NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE

Chain E: 58% 22% 16%



• Molecule 1: NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE

Chain F: 58% 23% 16%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.25Å 90.39Å 137.67Å 90.00° 117.17° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11921	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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: DND

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	0.75	0/1912	1.05	5/2588 (0.2%)
1	B	0.73	1/1912 (0.1%)	1.01	4/2588 (0.2%)
1	C	0.79	1/1912 (0.1%)	1.06	7/2588 (0.3%)
1	D	0.71	0/1912	1.06	7/2588 (0.3%)
1	E	0.62	0/1912	1.04	7/2588 (0.3%)
1	F	0.63	0/1912	1.05	7/2588 (0.3%)
All	All	0.71	2/11472 (0.0%)	1.04	37/15528 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	VAL	CA-CB	5.69	1.61	1.54
1	C	244	VAL	CA-CB	5.22	1.60	1.54

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	253	LEU	N-CA-C	10.34	122.13	111.07
1	D	253	LEU	N-CA-C	10.04	122.23	111.28
1	B	148	VAL	N-CA-C	8.29	115.76	108.63
1	C	253	LEU	N-CA-C	8.25	121.20	111.71
1	F	6	LYS	N-CA-C	7.54	121.83	110.14
1	F	253	LEU	N-CA-C	7.00	118.91	111.28
1	F	192	ASP	N-CA-C	-6.95	103.82	112.72
1	A	236	ILE	N-CA-C	-6.79	104.69	111.88
1	F	38	THR	N-CA-C	-6.75	104.86	113.23
1	C	239	LEU	N-CA-C	-6.65	105.45	113.97
1	B	236	ILE	N-CA-C	-6.49	106.00	112.17
1	E	256	SER	N-CA-C	-6.46	104.28	111.71
1	E	163	PHE	N-CA-C	-6.32	104.83	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	220	ASP	N-CA-C	6.13	119.18	108.52
1	C	191	ASN	N-CA-C	-5.98	105.47	112.89
1	D	214	ASN	N-CA-C	5.92	118.83	109.96
1	D	256	SER	N-CA-C	-5.83	104.83	111.07
1	F	202	VAL	CB-CA-C	-5.81	104.41	112.02
1	C	38	THR	N-CA-C	-5.78	106.07	113.23
1	A	239	LEU	N-CA-C	-5.77	106.58	113.97
1	D	90	LYS	N-CA-C	-5.73	105.01	112.23
1	A	253	LEU	N-CA-C	5.70	119.04	111.75
1	F	236	ILE	N-CA-C	-5.65	107.23	112.43
1	E	236	ILE	N-CA-C	-5.61	107.27	112.43
1	B	187	THR	N-CA-C	5.57	117.00	108.42
1	C	218	ALA	N-CA-C	5.57	117.53	108.63
1	E	254	TYR	N-CA-C	5.53	118.25	109.24
1	A	180	ASN	N-CA-C	5.50	120.06	113.23
1	B	148	VAL	CB-CA-C	-5.45	105.87	110.94
1	A	84	THR	N-CA-C	5.33	119.63	113.18
1	C	62	PRO	N-CA-C	5.31	119.53	111.15
1	D	219	ASN	N-CA-C	-5.23	100.17	109.06
1	E	103	GLN	N-CA-C	-5.19	105.53	111.14
1	D	85	TRP	N-CA-C	5.19	117.35	111.02
1	C	256	SER	N-CA-C	-5.05	105.77	111.28
1	F	239	LEU	N-CA-C	-5.03	107.53	113.97
1	D	180	ASN	N-CA-C	5.03	119.56	113.38

There are no chirality outliers.

There are no planarity outliers.

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	1875	0	1903	80	0
1	B	1875	0	1903	61	0
1	C	1875	0	1903	86	0
1	D	1875	0	1903	57	0
1	E	1875	0	1903	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1875	0	1903	59	0
2	A	44	0	25	5	0
2	B	44	0	25	2	0
2	C	44	0	25	7	0
2	D	44	0	25	1	0
2	E	44	0	25	0	0
2	F	44	0	25	1	0
3	A	90	0	0	12	0
3	B	68	0	0	16	0
3	C	80	0	0	14	0
3	D	65	0	0	7	0
3	E	57	0	0	10	0
3	F	47	0	0	6	0
All	All	11921	0	11568	376	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 16.

All (376) 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:158:ASP:HB2	3:E:442:HOH:O	1.57	1.02
1:E:78:LYS:H	1:E:78:LYS:HD2	1.21	1.01
1:B:97:LYS:HD2	3:B:459:HOH:O	1.60	1.01
1:B:78:LYS:H	1:B:78:LYS:HD2	1.24	1.00
1:D:21:THR:H	1:D:24:HIS:HD2	1.05	0.99
1:F:21:THR:H	1:F:24:HIS:HD2	1.08	0.99
1:D:234:GLN:HG2	3:D:449:HOH:O	1.63	0.98
1:E:5:GLU:HG3	1:E:6:LYS:H	1.24	0.98
1:A:194:GLN:HE21	1:A:194:GLN:HA	1.32	0.93
1:E:78:LYS:H	1:E:78:LYS:CD	1.80	0.91
1:C:219:ASN:OD1	1:D:219:ASN:HB2	1.70	0.90
1:A:12:LEU:HG	3:A:465:HOH:O	1.70	0.89
1:F:204:TRP:NE1	1:F:207:ARG:HH21	1.71	0.89
1:D:78:LYS:H	1:D:78:LYS:HD2	1.37	0.89
1:C:254:TYR:HE1	3:C:451:HOH:O	1.58	0.87
1:A:78:LYS:CD	1:A:78:LYS:H	1.86	0.85
1:E:220:ASP:HB2	3:E:441:HOH:O	1.76	0.85
1:B:78:LYS:H	1:B:78:LYS:CD	1.90	0.84
1:E:58:LYS:HE2	1:E:259:GLU:O	1.77	0.83
1:F:65:HIS:HD2	1:F:247:TYR:OH	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:ASP:OD1	1:F:218:ALA:HB3	1.78	0.83
1:E:202:VAL:HG23	3:E:437:HOH:O	1.78	0.83
1:D:158:ASP:HB2	3:D:406:HOH:O	1.79	0.81
1:E:225:LYS:HG3	3:E:447:HOH:O	1.79	0.80
1:A:21:THR:H	1:A:24:HIS:HD2	1.28	0.79
1:D:21:THR:N	1:D:24:HIS:HD2	1.79	0.79
1:A:204:TRP:NE1	1:A:207:ARG:HH21	1.80	0.79
1:D:78:LYS:H	1:D:78:LYS:CD	1.92	0.79
1:F:21:THR:H	1:F:24:HIS:CD2	1.99	0.78
1:F:78:LYS:CD	1:F:78:LYS:H	1.94	0.78
1:E:78:LYS:HD2	1:E:78:LYS:N	1.98	0.77
1:A:158:ASP:HB2	3:A:413:HOH:O	1.83	0.77
1:D:21:THR:H	1:D:24:HIS:CD2	1.96	0.77
1:A:194:GLN:HA	1:A:194:GLN:NE2	2.00	0.77
1:F:78:LYS:H	1:F:78:LYS:HD2	1.50	0.76
1:A:176:GLN:HB2	3:A:484:HOH:O	1.86	0.76
1:B:158:ASP:HB2	3:B:455:HOH:O	1.83	0.76
1:C:78:LYS:CD	1:C:78:LYS:H	1.97	0.76
1:A:194:GLN:HE21	1:A:194:GLN:CA	1.98	0.76
1:C:158:ASP:HB2	3:C:456:HOH:O	1.86	0.75
1:C:21:THR:H	1:C:24:HIS:HD2	1.34	0.75
1:A:92:TRP:CH2	1:A:269:PRO:HG3	2.21	0.75
1:E:152:LYS:HD3	1:E:181:TYR:O	1.86	0.74
1:B:97:LYS:HB2	3:B:459:HOH:O	1.87	0.74
1:E:188:ARG:CZ	1:E:218:ALA:HB1	2.17	0.74
1:B:21:THR:H	1:B:24:HIS:HD2	1.34	0.74
1:C:27:LEU:HD11	2:C:301:DND:C2A	2.18	0.74
1:D:245:GLN:O	1:D:249:GLU:HG2	1.88	0.73
1:A:78:LYS:H	1:A:78:LYS:HD2	1.52	0.73
1:E:5:GLU:HG3	1:E:6:LYS:N	2.02	0.73
1:E:65:HIS:HD2	1:E:247:TYR:OH	1.71	0.73
1:B:167:ASN:O	1:B:270:LEU:HD23	1.88	0.73
1:D:6:LYS:HE2	1:D:39:GLY:O	1.89	0.72
1:A:65:HIS:HD2	1:A:247:TYR:OH	1.73	0.71
1:C:92:TRP:CH2	1:C:269:PRO:HG3	2.25	0.71
1:C:69:MET:SD	3:C:451:HOH:O	2.48	0.71
1:C:245:GLN:O	1:C:249:GLU:HG2	1.90	0.70
1:A:21:THR:H	1:A:24:HIS:CD2	2.10	0.70
1:F:5:GLU:HB3	3:F:441:HOH:O	1.90	0.69
1:F:21:THR:N	1:F:24:HIS:HD2	1.86	0.69
1:F:93:LYS:HB2	3:F:434:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:GLN:NE2	1:C:249:GLU:HG3	2.07	0.68
1:C:194:GLN:HA	1:C:194:GLN:HE21	1.57	0.68
1:E:92:TRP:CH2	1:E:269:PRO:HG3	2.28	0.68
1:E:192:ASP:HB2	3:E:440:HOH:O	1.94	0.68
1:A:173:ASP:HA	3:A:484:HOH:O	1.93	0.68
1:B:204:TRP:CD1	1:F:232:ARG:HD3	2.30	0.67
1:A:172:GLU:O	3:A:484:HOH:O	2.13	0.67
1:A:245:GLN:O	1:A:249:GLU:HG2	1.95	0.66
1:A:219:ASN:HA	1:B:219:ASN:ND2	2.10	0.66
1:C:100:ARG:O	1:C:104:GLU:HG3	1.95	0.66
1:A:183:LEU:C	1:A:183:LEU:HD23	2.21	0.66
1:B:65:HIS:HE1	3:B:446:HOH:O	1.78	0.66
1:E:204:TRP:O	1:E:207:ARG:HB3	1.96	0.65
1:C:77:SER:HA	1:C:78:LYS:HE3	1.78	0.65
1:C:78:LYS:HE2	3:C:457:HOH:O	1.95	0.65
1:C:220:ASP:OD2	1:D:218:ALA:HB3	1.97	0.65
1:C:65:HIS:HD2	1:C:247:TYR:OH	1.78	0.64
1:E:219:ASN:HB3	3:E:449:HOH:O	1.96	0.64
1:D:204:TRP:CZ3	1:E:232:ARG:HB3	2.33	0.64
1:C:257:GLU:HB2	3:C:436:HOH:O	1.96	0.64
1:F:92:TRP:CH2	1:F:269:PRO:HG3	2.32	0.64
1:B:232:ARG:HD3	1:C:204:TRP:CD1	2.33	0.63
1:F:11:LEU:HD22	1:F:184:ILE:HD12	1.81	0.63
1:B:75:LYS:HD2	3:B:418:HOH:O	1.98	0.63
1:B:258:SER:O	1:B:261:ARG:HG3	1.99	0.62
1:C:152:LYS:HD3	1:C:182:GLY:HA3	1.79	0.62
1:F:65:HIS:CD2	1:F:247:TYR:OH	2.49	0.62
1:E:275:ALA:HB2	3:E:453:HOH:O	1.99	0.62
1:E:67:VAL:O	1:E:71:GLU:HG3	1.99	0.62
1:A:60:LEU:HD11	1:A:66:ARG:CZ	2.30	0.62
1:A:220:ASP:CG	1:A:220:ASP:O	2.43	0.61
1:C:194:GLN:HA	1:C:194:GLN:NE2	2.15	0.61
1:C:245:GLN:HE21	1:C:249:GLU:HG3	1.64	0.61
1:E:92:TRP:CZ2	1:E:269:PRO:HG3	2.35	0.61
1:F:6:LYS:HE2	1:F:39:GLY:O	1.99	0.61
1:B:50:PRO:CG	3:B:456:HOH:O	2.49	0.61
1:B:50:PRO:HG2	3:B:456:HOH:O	2.01	0.61
1:C:194:GLN:HE21	1:C:194:GLN:CA	2.13	0.61
1:C:219:ASN:OD1	1:D:219:ASN:CB	2.46	0.60
1:B:57:LYS:NZ	2:B:301:DND:O11	2.33	0.60
1:C:5:GLU:HG3	1:C:6:LYS:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LEU:HD11	1:C:66:ARG:CZ	2.31	0.60
1:E:200:SER:HB3	1:E:203:LEU:HB2	1.83	0.60
1:F:11:LEU:CD2	1:F:184:ILE:HD12	2.32	0.60
1:F:64:TYR:CE2	1:F:68:ILE:HD12	2.36	0.60
1:A:219:ASN:HD22	1:A:220:ASP:N	2.00	0.59
1:B:66:ARG:C	3:B:456:HOH:O	2.45	0.59
1:B:12:LEU:HD23	1:B:99:LEU:HD23	1.84	0.59
1:C:21:THR:H	1:C:24:HIS:CD2	2.18	0.59
1:C:95:THR:OG1	2:C:301:DND:H13	2.02	0.59
1:F:89:GLN:HG3	3:F:434:HOH:O	2.01	0.59
1:C:63:ALA:O	1:C:67:VAL:HG23	2.03	0.59
1:C:5:GLU:HG3	1:C:6:LYS:N	2.18	0.59
1:A:67:VAL:O	1:A:71:GLU:HG3	2.03	0.59
1:C:274:THR:O	1:C:274:THR:HG22	2.03	0.59
1:E:219:ASN:OD1	1:F:219:ASN:HA	2.03	0.59
1:A:218:ALA:HB2	3:A:486:HOH:O	2.03	0.58
1:E:21:THR:H	1:E:24:HIS:HD2	1.50	0.58
1:A:77:SER:HA	1:A:78:LYS:HE3	1.84	0.58
1:F:93:LYS:HD3	3:F:434:HOH:O	2.02	0.58
1:A:204:TRP:CD1	1:D:232:ARG:HD3	2.38	0.58
1:B:93:LYS:HG3	3:B:459:HOH:O	2.03	0.58
1:B:90:LYS:N	3:B:452:HOH:O	2.35	0.58
1:E:11:LEU:HD22	1:E:184:ILE:HD12	1.86	0.58
1:F:34:TYR:O	1:F:38:THR:HG23	2.03	0.58
1:A:13:ALA:C	3:A:465:HOH:O	2.46	0.57
1:D:155:CYS:SG	1:D:183:LEU:HD21	2.44	0.57
1:A:5:GLU:HG3	1:A:6:LYS:H	1.69	0.57
1:B:78:LYS:HD2	1:B:78:LYS:N	2.05	0.57
1:D:83:ASP:OD1	1:D:102:HIS:HE1	1.86	0.57
1:A:14:CYS:N	3:A:465:HOH:O	2.37	0.57
1:A:95:THR:OG1	2:A:301:DND:H13	2.04	0.57
1:D:204:TRP:CE3	1:E:232:ARG:HD3	2.40	0.57
1:E:272:ARG:NH2	3:E:457:HOH:O	2.37	0.57
1:C:268:ALA:HB3	1:C:269:PRO:HD3	1.87	0.57
1:D:215:GLU:HG3	3:D:431:HOH:O	2.05	0.56
1:B:67:VAL:HA	3:B:456:HOH:O	2.04	0.56
1:A:21:THR:N	1:A:24:HIS:HD2	2.02	0.56
1:C:92:TRP:CZ2	1:C:269:PRO:HG3	2.40	0.56
1:B:220:ASP:O	1:B:220:ASP:CG	2.47	0.56
1:C:21:THR:N	1:C:24:HIS:HD2	2.01	0.56
1:A:78:LYS:HD2	1:A:78:LYS:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:ARG:HD3	3:D:424:HOH:O	2.06	0.56
1:C:219:ASN:HD21	1:D:221:ILE:HD11	1.70	0.55
1:C:28:PHE:HB3	1:C:79:TRP:CH2	2.41	0.55
1:C:172:GLU:O	1:C:176:GLN:HG3	2.06	0.55
1:D:258:SER:O	1:D:261:ARG:HG3	2.07	0.55
1:F:78:LYS:HD2	1:F:78:LYS:N	2.18	0.55
1:B:155:CYS:SG	1:B:183:LEU:HD21	2.47	0.55
1:B:162:SER:HB2	1:B:168:LEU:HD23	1.89	0.55
1:B:27:LEU:HD11	1:B:186:VAL:HB	1.88	0.55
1:C:78:LYS:H	1:C:78:LYS:HD2	1.70	0.55
1:D:188:ARG:HG3	3:D:435:HOH:O	2.07	0.55
1:A:5:GLU:HG3	1:A:6:LYS:N	2.22	0.54
1:C:27:LEU:HD11	2:C:301:DND:H24	1.88	0.54
1:D:45:LYS:HD3	1:D:81:GLU:OE1	2.07	0.54
1:A:24:HIS:HE1	3:A:482:HOH:O	1.91	0.54
1:D:61:ILE:HB	1:D:62:PRO:HD2	1.89	0.54
1:D:83:ASP:CG	1:D:102:HIS:HE1	2.16	0.54
1:B:100:ARG:O	1:B:104:GLU:HG3	2.08	0.53
1:E:204:TRP:NE1	1:E:207:ARG:HH21	2.06	0.53
1:D:61:ILE:HB	1:D:62:PRO:CD	2.38	0.53
1:C:158:ASP:CB	3:C:456:HOH:O	2.52	0.53
1:D:55:TYR:CD2	1:D:57:LYS:HB2	2.43	0.53
1:C:85:TRP:O	1:C:89:GLN:HG2	2.08	0.53
1:E:11:LEU:CD2	1:E:184:ILE:HD12	2.38	0.53
1:F:92:TRP:CZ2	1:F:269:PRO:HG3	2.44	0.53
1:A:76:ASN:HB2	3:B:460:HOH:O	2.08	0.53
1:E:188:ARG:NE	1:E:218:ALA:HB1	2.23	0.53
1:D:78:LYS:HD2	1:D:78:LYS:N	2.15	0.53
1:E:21:THR:H	1:E:24:HIS:CD2	2.26	0.53
1:B:27:LEU:CD1	1:B:186:VAL:HB	2.39	0.52
1:B:161:GLU:HG2	1:B:196:PHE:CD1	2.44	0.52
1:C:107:GLU:HG2	1:C:148:VAL:HG11	1.91	0.52
1:C:6:LYS:HE2	1:C:39:GLY:O	2.10	0.52
1:D:5:GLU:HG3	1:D:6:LYS:N	2.25	0.52
1:E:63:ALA:O	1:E:67:VAL:HG23	2.09	0.52
1:A:65:HIS:CD2	1:A:247:TYR:OH	2.60	0.52
1:F:267:LEU:HG	1:F:269:PRO:HD2	1.92	0.51
1:B:21:THR:N	1:B:24:HIS:HD2	2.06	0.51
1:D:83:ASP:CG	1:D:102:HIS:CE1	2.88	0.51
1:C:23:MET:CG	3:C:403:HOH:O	2.58	0.51
1:D:191:ASN:HB2	1:F:191:ASN:HD22	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:TRP:CZ3	1:D:94:GLU:HG3	2.46	0.51
1:B:78:LYS:CD	1:B:78:LYS:N	2.65	0.51
1:D:107:GLU:HG2	1:D:148:VAL:HG11	1.92	0.51
1:B:162:SER:HB2	1:B:168:LEU:CD2	2.41	0.51
1:C:152:LYS:HD3	1:C:181:TYR:O	2.11	0.51
1:F:204:TRP:HE1	1:F:207:ARG:HH21	1.54	0.51
1:A:23:MET:HG2	3:A:480:HOH:O	2.11	0.50
1:A:27:LEU:HD11	2:A:301:DND:H24	1.92	0.50
1:C:245:GLN:HE21	1:C:249:GLU:CG	2.24	0.50
1:A:92:TRP:CZ3	1:A:269:PRO:HG3	2.46	0.50
1:B:83:ASP:CG	1:B:102:HIS:HE1	2.20	0.50
1:C:193:ALA:O	1:C:197:ILE:HG13	2.11	0.50
1:D:20:ILE:HA	1:D:24:HIS:CD2	2.46	0.50
1:E:9:VAL:HG21	1:E:152:LYS:HG3	1.94	0.50
1:F:247:TYR:CE2	1:F:253:LEU:HD11	2.47	0.50
1:C:9:VAL:CG2	1:C:152:LYS:HG3	2.42	0.49
1:A:267:LEU:HG	1:A:269:PRO:HD2	1.94	0.49
1:F:27:LEU:HD11	1:F:186:VAL:HB	1.94	0.49
1:F:268:ALA:HB3	1:F:269:PRO:HD3	1.95	0.49
1:B:35:MET:HE2	1:B:184:ILE:HD11	1.95	0.49
1:C:54:ALA:O	1:C:56:LYS:HG2	2.12	0.49
1:E:30:LEU:HD11	1:E:215:GLU:HA	1.94	0.49
1:D:274:THR:HG22	1:D:274:THR:O	2.12	0.49
1:D:240:VAL:HG23	1:D:245:GLN:HB2	1.94	0.49
1:C:9:VAL:HG21	1:C:152:LYS:HG3	1.95	0.48
1:F:85:TRP:O	1:F:89:GLN:HG2	2.14	0.48
1:A:89:GLN:HA	3:A:419:HOH:O	2.13	0.48
1:B:107:GLU:O	1:B:108:ALA:HB2	2.13	0.48
1:D:86:GLU:CD	1:D:98:VAL:HG21	2.38	0.48
1:A:11:LEU:CD2	1:A:184:ILE:HD12	2.44	0.48
1:E:170:LYS:HE3	1:E:173:ASP:OD2	2.13	0.48
1:C:195:LYS:O	1:C:199:GLU:HG3	2.14	0.48
1:E:12:LEU:HD23	1:E:99:LEU:HD23	1.95	0.48
1:F:188:ARG:CZ	1:F:218:ALA:HB1	2.44	0.48
1:F:220:ASP:O	1:F:222:SER:N	2.47	0.48
1:D:30:LEU:HD11	3:D:431:HOH:O	2.12	0.48
1:B:189:ALA:HB1	1:B:192:ASP:OD2	2.14	0.47
1:C:166:PRO:O	1:C:167:ASN:HB2	2.14	0.47
1:C:92:TRP:CH2	1:C:94:GLU:HG3	2.50	0.47
1:A:231:ARG:HG2	1:A:255:SER:HA	1.95	0.47
1:A:232:ARG:HD3	1:E:204:TRP:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:HIS:CD2	1:C:247:TYR:OH	2.65	0.47
1:F:34:TYR:CD2	1:F:34:TYR:C	2.93	0.47
1:A:52:GLY:HA2	1:A:87:SER:HA	1.97	0.47
1:B:155:CYS:HA	2:B:301:DND:O3B	2.15	0.47
1:E:173:ASP:O	1:E:177:ILE:HG13	2.14	0.46
1:F:223:SER:HB2	3:F:433:HOH:O	2.15	0.46
1:A:9:VAL:HG23	1:A:152:LYS:HG2	1.97	0.46
1:B:155:CYS:O	1:B:185:CYS:HA	2.16	0.46
1:A:107:GLU:O	1:A:108:ALA:HB2	2.16	0.46
1:E:247:TYR:HE2	1:E:253:LEU:HD11	1.80	0.46
1:C:272:ARG:HB3	3:C:479:HOH:O	2.15	0.46
1:E:107:GLU:O	1:E:108:ALA:HB2	2.16	0.46
1:A:204:TRP:CE2	1:A:207:ARG:NH2	2.84	0.46
1:C:26:ARG:HG2	3:C:449:HOH:O	2.16	0.46
1:A:92:TRP:CZ2	1:A:269:PRO:HG3	2.49	0.46
1:B:55:TYR:CD1	1:B:92:TRP:NE1	2.85	0.46
1:C:5:GLU:CG	1:C:6:LYS:H	2.23	0.46
1:F:10:VAL:HG13	1:F:45:LYS:HB3	1.96	0.46
1:A:266:ILE:HD12	1:A:271:GLN:OE1	2.15	0.45
1:E:188:ARG:HD2	3:E:439:HOH:O	2.16	0.45
1:D:220:ASP:HB2	3:D:414:HOH:O	2.15	0.45
1:C:78:LYS:H	1:C:78:LYS:CE	2.29	0.45
1:E:159:LEU:C	1:E:159:LEU:HD23	2.41	0.45
1:F:152:LYS:NZ	1:F:209:ASN:HD21	2.15	0.45
1:A:55:TYR:O	1:A:56:LYS:HB2	2.16	0.45
1:A:23:MET:HE3	1:A:221:ILE:O	2.16	0.45
1:B:237:ARG:O	1:B:238:TYR:HB2	2.16	0.45
1:A:20:ILE:HA	1:A:24:HIS:CD2	2.52	0.45
1:F:262:ASN:O	1:F:263:ALA:C	2.58	0.45
1:A:152:LYS:HD2	1:A:182:GLY:HA3	1.99	0.45
1:B:219:ASN:HD22	1:B:219:ASN:HA	1.54	0.45
1:E:218:ALA:O	1:F:220:ASP:HB3	2.16	0.45
1:F:168:LEU:HD11	2:F:301:DND:H11	1.98	0.45
1:B:23:MET:HE3	1:B:221:ILE:O	2.17	0.45
1:D:228:ARG:HD2	1:D:232:ARG:NH2	2.32	0.45
1:E:34:TYR:O	1:E:38:THR:HG23	2.17	0.45
1:F:100:ARG:O	1:F:104:GLU:HG3	2.17	0.44
1:B:92:TRP:CZ3	1:B:94:GLU:HG3	2.52	0.44
1:B:170:LYS:HE3	1:B:173:ASP:OD1	2.17	0.44
1:C:219:ASN:OD1	1:D:219:ASN:HA	2.17	0.44
1:D:12:LEU:HD23	1:D:99:LEU:HD23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:ARG:O	1:E:262:ASN:HB2	2.18	0.44
1:B:57:LYS:NZ	3:B:463:HOH:O	2.51	0.44
1:C:45:LYS:HG2	1:C:46:GLY:N	2.32	0.44
1:F:219:ASN:O	1:F:220:ASP:HB2	2.17	0.44
1:A:34:TYR:O	1:A:38:THR:HG23	2.17	0.44
1:B:27:LEU:HD12	1:B:186:VAL:HG11	2.00	0.44
1:E:209:ASN:HD22	1:E:209:ASN:HA	1.61	0.44
1:D:96:LEU:HD12	1:D:96:LEU:O	2.18	0.44
1:E:236:ILE:O	1:E:239:LEU:HB2	2.17	0.44
1:A:78:LYS:H	1:A:78:LYS:CE	2.30	0.44
1:C:26:ARG:HA	1:C:26:ARG:HD2	1.64	0.44
1:D:5:GLU:CG	1:D:6:LYS:H	2.31	0.44
1:E:60:LEU:HD11	1:E:66:ARG:CZ	2.48	0.44
1:A:237:ARG:NH1	1:B:78:LYS:HE3	2.32	0.44
1:A:26:ARG:HA	1:A:26:ARG:HD2	1.85	0.44
1:D:172:GLU:CD	1:D:172:GLU:H	2.24	0.43
1:A:219:ASN:C	1:A:219:ASN:ND2	2.75	0.43
1:E:192:ASP:CB	3:E:440:HOH:O	2.58	0.43
1:F:8:GLU:O	1:F:149:PRO:HA	2.18	0.43
1:A:6:LYS:HE2	1:A:39:GLY:O	2.18	0.43
1:A:261:ARG:NH2	3:A:411:HOH:O	2.50	0.43
1:F:27:LEU:CD1	1:F:186:VAL:HB	2.48	0.43
1:A:45:LYS:HG2	1:A:46:GLY:N	2.33	0.43
1:A:209:ASN:HD22	1:A:209:ASN:HA	1.48	0.43
1:B:65:HIS:HD2	1:B:247:TYR:OH	2.01	0.43
1:C:34:TYR:O	1:C:38:THR:HG23	2.18	0.43
1:D:5:GLU:HG3	1:D:6:LYS:H	1.83	0.43
1:D:251:HIS:O	1:D:252:ASN:C	2.62	0.43
1:F:26:ARG:HD2	1:F:26:ARG:HA	1.79	0.43
1:C:255:SER:H	1:C:258:SER:HG	1.67	0.43
1:A:27:LEU:HD11	2:A:301:DND:C2A	2.49	0.43
1:B:58:LYS:NZ	3:B:461:HOH:O	2.45	0.43
1:E:267:LEU:HG	1:E:269:PRO:HD2	2.00	0.43
1:F:61:ILE:HB	1:F:62:PRO:CD	2.49	0.43
1:A:64:TYR:CE2	1:A:68:ILE:HD11	2.54	0.43
1:B:83:ASP:CG	1:B:102:HIS:CE1	2.97	0.43
1:B:170:LYS:HB3	1:B:172:GLU:OE2	2.18	0.43
1:F:64:TYR:CE2	1:F:68:ILE:CD1	3.01	0.43
1:F:198:TYR:HA	1:F:204:TRP:HE3	1.83	0.43
1:C:35:MET:HE2	1:C:184:ILE:HD11	2.01	0.42
1:F:155:CYS:O	1:F:185:CYS:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:221:ILE:O	1:F:221:ILE:HG22	2.18	0.42
1:A:5:GLU:CG	1:A:6:LYS:H	2.28	0.42
1:B:61:ILE:HB	1:B:62:PRO:CD	2.50	0.42
1:C:14:CYS:HB3	2:C:301:DND:O3D	2.19	0.42
1:B:228:ARG:HD2	1:B:232:ARG:NH2	2.35	0.42
1:C:103:GLN:O	1:C:107:GLU:HG3	2.18	0.42
1:A:95:THR:N	2:A:301:DND:O7N	2.51	0.42
1:C:260:ASP:O	1:C:261:ARG:C	2.63	0.42
1:F:45:LYS:HD3	1:F:81:GLU:OE1	2.19	0.42
1:A:237:ARG:O	1:A:238:TYR:HB2	2.20	0.42
1:E:168:LEU:HD12	1:E:168:LEU:HA	1.89	0.42
1:F:23:MET:HE3	1:F:221:ILE:O	2.19	0.42
1:A:232:ARG:HD3	1:E:204:TRP:NE1	2.35	0.42
1:B:260:ASP:O	1:B:261:ARG:C	2.62	0.42
1:C:23:MET:SD	2:C:301:DND:C6A	3.08	0.42
1:C:204:TRP:NE1	1:C:207:ARG:HH21	2.17	0.42
1:C:239:LEU:HD11	1:D:26:ARG:CZ	2.50	0.42
1:E:9:VAL:CG2	1:E:152:LYS:HG3	2.50	0.42
1:D:198:TYR:OH	1:E:225:LYS:HG2	2.20	0.42
1:F:67:VAL:O	1:F:71:GLU:HG3	2.19	0.42
1:B:152:LYS:HD3	1:B:181:TYR:O	2.20	0.42
1:F:61:ILE:HB	1:F:62:PRO:HD2	2.02	0.42
1:C:23:MET:HG2	3:C:403:HOH:O	2.18	0.41
1:C:57:LYS:NZ	2:C:301:DND:O11	2.46	0.41
1:D:168:LEU:O	2:D:301:DND:H12	2.20	0.41
1:F:26:ARG:CG	3:F:402:HOH:O	2.68	0.41
1:C:150:LYS:NZ	3:C:458:HOH:O	2.53	0.41
1:C:190:GLY:O	1:C:194:GLN:HG2	2.20	0.41
1:C:243:LEU:HG	3:C:409:HOH:O	2.20	0.41
1:A:16:SER:HA	1:A:51:VAL:HG12	2.02	0.41
1:A:55:TYR:CE2	1:A:267:LEU:HD11	2.55	0.41
1:F:103:GLN:O	1:F:106:LEU:HB2	2.21	0.41
1:C:27:LEU:HD11	2:C:301:DND:N3A	2.35	0.41
1:C:248:ILE:HG12	3:C:451:HOH:O	2.19	0.41
1:A:168:LEU:HD11	2:A:301:DND:H11	2.03	0.41
1:A:219:ASN:ND2	1:A:220:ASP:N	2.67	0.41
1:D:217:ILE:O	1:D:217:ILE:HG22	2.20	0.41
1:C:159:LEU:HD23	1:C:159:LEU:C	2.45	0.41
1:D:44:VAL:O	1:D:45:LYS:HB2	2.21	0.41
1:D:58:LYS:HA	1:D:262:ASN:HB2	2.03	0.41
1:D:27:LEU:HD12	1:D:186:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:PHE:O	1:A:19:PRO:HA	2.21	0.41
1:A:27:LEU:HD12	1:A:27:LEU:HA	1.82	0.41
1:A:219:ASN:HA	1:B:219:ASN:HD22	1.81	0.41
1:B:64:TYR:HD2	3:B:428:HOH:O	2.04	0.41
1:B:226:ILE:HG23	1:B:236:ILE:HG21	2.03	0.41
1:B:246:GLU:HB3	3:B:434:HOH:O	2.21	0.41
1:C:254:TYR:CE1	3:C:451:HOH:O	2.47	0.41
1:E:27:LEU:HA	1:E:27:LEU:HD12	1.69	0.41
1:E:148:VAL:HA	1:E:149:PRO:HD3	1.85	0.41
1:F:107:GLU:CG	1:F:148:VAL:HG11	2.51	0.41
1:C:152:LYS:NZ	1:C:209:ASN:HD21	2.19	0.41
1:A:23:MET:HB2	1:A:221:ILE:HB	2.03	0.40
1:A:219:ASN:HD22	1:A:219:ASN:C	2.29	0.40
1:C:60:LEU:HD11	1:C:66:ARG:NE	2.36	0.40
1:C:225:LYS:HB3	1:D:217:ILE:HG12	2.03	0.40
1:F:35:MET:HE2	1:F:184:ILE:HD11	2.03	0.40
1:A:170:LYS:HE3	1:A:173:ASP:OD2	2.21	0.40
1:B:225:LYS:HD3	1:C:198:TYR:OH	2.21	0.40
1:C:55:TYR:O	1:C:56:LYS:HB2	2.21	0.40
1:F:166:PRO:O	1:F:167:ASN:HB2	2.21	0.40
1:A:190:GLY:O	1:A:194:GLN:HG2	2.22	0.40
1:B:237:ARG:HG3	1:B:238:TYR:CD1	2.55	0.40
1:C:239:LEU:HD21	1:D:26:ARG:HD3	2.03	0.40
1:F:32:LYS:HB2	1:F:79:TRP:CH2	2.57	0.40
1:D:190:GLY:O	1:D:194:GLN:CG	2.70	0.40
1:A:170:LYS:O	1:A:173:ASP:N	2.47	0.40
1:C:16:SER:O	1:C:17:PHE:C	2.64	0.40
1:C:227:ARG:HD2	1:C:254:TYR:CD2	2.57	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	229/279 (82%)	221 (96%)	8 (4%)	0	100	100
1	B	229/279 (82%)	219 (96%)	8 (4%)	2 (1%)	14	27
1	C	229/279 (82%)	223 (97%)	6 (3%)	0	100	100
1	D	229/279 (82%)	216 (94%)	12 (5%)	1 (0%)	30	49
1	E	229/279 (82%)	221 (96%)	7 (3%)	1 (0%)	30	49
1	F	229/279 (82%)	217 (95%)	9 (4%)	3 (1%)	9	18
All	All	1374/1674 (82%)	1317 (96%)	50 (4%)	7 (0%)	24	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	220	ASP
1	B	218	ALA
1	E	218	ALA
1	F	218	ALA
1	B	254	TYR
1	D	148	VAL
1	F	221	ILE

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	204/248 (82%)	196 (96%)	8 (4%)	28	55
1	B	204/248 (82%)	192 (94%)	12 (6%)	18	37
1	C	204/248 (82%)	195 (96%)	9 (4%)	25	50
1	D	204/248 (82%)	197 (97%)	7 (3%)	32	60
1	E	204/248 (82%)	192 (94%)	12 (6%)	18	37
1	F	204/248 (82%)	198 (97%)	6 (3%)	37	65
All	All	1224/1488 (82%)	1170 (96%)	54 (4%)	25	50

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LYS
1	A	154	LEU
1	A	172	GLU
1	A	194	GLN
1	A	200	SER
1	A	209	ASN
1	A	217	ILE
1	A	220	ASP
1	B	9	VAL
1	B	78	LYS
1	B	154	LEU
1	B	172	GLU
1	B	202	VAL
1	B	207	ARG
1	B	219	ASN
1	B	220	ASP
1	B	245	GLN
1	B	246	GLU
1	B	252	ASN
1	B	257	GLU
1	C	23	MET
1	C	27	LEU
1	C	78	LYS
1	C	154	LEU
1	C	172	GLU
1	C	194	GLN
1	C	200	SER
1	C	209	ASN
1	C	260	ASP
1	D	9	VAL
1	D	78	LYS
1	D	154	LEU
1	D	172	GLU
1	D	207	ARG
1	D	209	ASN
1	D	257	GLU
1	E	19	PRO
1	E	40	ARG
1	E	78	LYS
1	E	148	VAL
1	E	154	LEU
1	E	158	ASP
1	E	172	GLU

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Mol	Chain	Res	Type
1	E	191	ASN
1	E	207	ARG
1	E	209	ASN
1	E	252	ASN
1	E	257	GLU
1	F	5	GLU
1	F	19	PRO
1	F	78	LYS
1	F	154	LEU
1	F	172	GLU
1	F	209	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	65	HIS
1	A	194	GLN
1	A	206	HIS
1	A	209	ASN
1	A	214	ASN
1	A	219	ASN
1	A	234	GLN
1	B	24	HIS
1	B	65	HIS
1	B	89	GLN
1	B	102	HIS
1	B	191	ASN
1	B	209	ASN
1	B	219	ASN
1	B	251	HIS
1	C	24	HIS
1	C	65	HIS
1	C	102	HIS
1	C	194	GLN
1	C	206	HIS
1	C	209	ASN
1	C	245	GLN
1	D	24	HIS
1	D	65	HIS
1	D	102	HIS
1	D	176	GLN

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Mol	Chain	Res	Type
1	D	209	ASN
1	E	24	HIS
1	E	65	HIS
1	E	102	HIS
1	E	206	HIS
1	E	209	ASN
1	E	273	ASN
1	F	24	HIS
1	F	65	HIS
1	F	76	ASN
1	F	191	ASN
1	F	206	HIS
1	F	209	ASN
1	F	211	HIS
1	F	271	GLN

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 ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DND	B	301	-	46,48,48	2.13	9 (19%)	64,73,73	1.20	5 (7%)
2	DND	F	301	-	46,48,48	2.36	8 (17%)	64,73,73	1.20	5 (7%)
2	DND	E	301	-	46,48,48	2.20	9 (19%)	64,73,73	1.22	6 (9%)
2	DND	C	301	-	46,48,48	2.41	9 (19%)	64,73,73	1.33	8 (12%)
2	DND	A	301	-	46,48,48	2.28	9 (19%)	64,73,73	1.33	10 (15%)
2	DND	D	301	-	46,48,48	2.21	11 (23%)	64,73,73	1.19	6 (9%)

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	DND	B	301	-	-	6/30/62/62	0/5/5/5
2	DND	F	301	-	-	5/30/62/62	0/5/5/5
2	DND	E	301	-	-	4/30/62/62	0/5/5/5
2	DND	C	301	-	-	5/30/62/62	0/5/5/5
2	DND	A	301	-	-	4/30/62/62	0/5/5/5
2	DND	D	301	-	-	5/30/62/62	0/5/5/5

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	DND	C5N-C4N	8.56	1.53	1.38
2	F	301	DND	C5N-C4N	8.48	1.53	1.38
2	E	301	DND	C5N-C4N	7.84	1.52	1.38
2	C	301	DND	C5N-C4N	7.61	1.51	1.38
2	C	301	DND	C4N-C3N	7.48	1.50	1.39
2	D	301	DND	C5N-C4N	7.34	1.51	1.38
2	B	301	DND	C5N-C4N	7.30	1.51	1.38
2	F	301	DND	C4N-C3N	7.13	1.50	1.39
2	A	301	DND	C4N-C3N	6.77	1.49	1.39
2	E	301	DND	C4N-C3N	6.49	1.49	1.39
2	C	301	DND	C2N-C3N	6.31	1.49	1.39
2	B	301	DND	C4N-C3N	6.02	1.48	1.39
2	D	301	DND	C4N-C3N	5.73	1.48	1.39
2	F	301	DND	C2N-C3N	5.41	1.47	1.39
2	C	301	DND	O7N-C7N	5.15	1.37	1.22
2	A	301	DND	C2N-N1N	5.01	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	DND	C2N-N1N	4.96	1.40	1.35
2	F	301	DND	O7N-C7N	4.94	1.37	1.22
2	D	301	DND	O7N-C7N	4.89	1.36	1.22
2	B	301	DND	O7N-C7N	4.80	1.36	1.22
2	E	301	DND	O7N-C7N	4.79	1.36	1.22
2	E	301	DND	C2N-C3N	4.66	1.46	1.39
2	E	301	DND	C2N-N1N	4.45	1.39	1.35
2	B	301	DND	C2N-C3N	4.32	1.45	1.39
2	A	301	DND	O7N-C7N	4.31	1.35	1.22
2	C	301	DND	C2N-N1N	4.30	1.39	1.35
2	C	301	DND	C6N-N1N	4.27	1.45	1.35
2	D	301	DND	C2N-C3N	4.16	1.45	1.39
2	D	301	DND	PN-O3P	4.07	1.63	1.59
2	B	301	DND	C6N-N1N	4.00	1.44	1.35
2	F	301	DND	C6N-N1N	3.95	1.44	1.35
2	B	301	DND	C2N-N1N	3.94	1.39	1.35
2	D	301	DND	PA-O3P	3.84	1.63	1.59
2	E	301	DND	C6N-N1N	3.72	1.43	1.35
2	A	301	DND	C2N-C3N	3.63	1.44	1.39
2	A	301	DND	C6N-N1N	3.61	1.43	1.35
2	D	301	DND	C6N-N1N	3.59	1.43	1.35
2	D	301	DND	C2N-N1N	3.47	1.38	1.35
2	A	301	DND	O4B-C1B	-3.13	1.34	1.42
2	C	301	DND	O8N-C7N	-3.02	1.21	1.30
2	D	301	DND	C6N-C5N	-2.99	1.32	1.38
2	C	301	DND	O4B-C1B	-2.90	1.35	1.42
2	A	301	DND	O8N-C7N	-2.85	1.22	1.30
2	E	301	DND	C2A-N1A	2.75	1.38	1.33
2	B	301	DND	C2A-N1A	2.64	1.38	1.33
2	D	301	DND	O4B-C1B	-2.63	1.35	1.42
2	B	301	DND	C6N-C5N	-2.56	1.33	1.38
2	E	301	DND	O8N-C7N	-2.42	1.23	1.30
2	A	301	DND	C2A-N1A	2.41	1.38	1.33
2	F	301	DND	C2A-N1A	2.38	1.38	1.33
2	C	301	DND	C8A-N7A	2.34	1.36	1.31
2	B	301	DND	O8N-C7N	-2.21	1.23	1.30
2	D	301	DND	C2A-N1A	2.21	1.37	1.33
2	F	301	DND	C6N-C5N	-2.08	1.34	1.38
2	E	301	DND	C6N-C5N	-2.06	1.34	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	DND	C5N-C4N-C3N	-4.92	115.53	120.36
2	C	301	DND	C5N-C4N-C3N	-4.86	115.59	120.36
2	F	301	DND	C5N-C4N-C3N	-4.49	115.95	120.36
2	B	301	DND	C5N-C4N-C3N	-4.45	115.99	120.36
2	E	301	DND	C5N-C4N-C3N	-4.34	116.10	120.36
2	D	301	DND	C5N-C4N-C3N	-4.18	116.25	120.36
2	C	301	DND	C6N-N1N-C2N	-4.06	118.42	121.88
2	F	301	DND	C6N-N1N-C2N	-4.02	118.46	121.88
2	E	301	DND	C6N-N1N-C2N	-3.90	118.56	121.88
2	A	301	DND	C6N-N1N-C2N	-3.77	118.67	121.88
2	B	301	DND	C6N-N1N-C2N	-3.73	118.70	121.88
2	C	301	DND	C5N-C6N-N1N	3.71	125.45	120.38
2	D	301	DND	C6N-N1N-C2N	-3.34	119.04	121.88
2	E	301	DND	O4B-C1B-C2B	-3.25	99.65	106.62
2	B	301	DND	C5N-C6N-N1N	3.06	124.56	120.38
2	D	301	DND	O14-PA-O3P	3.02	115.43	107.27
2	F	301	DND	C5N-C6N-N1N	3.01	124.48	120.38
2	A	301	DND	O4B-C1B-C2B	-3.00	100.20	106.62
2	A	301	DND	C4N-C3N-C7N	2.99	126.30	120.37
2	E	301	DND	C5N-C6N-N1N	2.94	124.39	120.38
2	C	301	DND	O4B-C1B-C2B	-2.94	100.33	106.62
2	B	301	DND	O4B-C1B-C2B	-2.88	100.45	106.62
2	D	301	DND	O4B-C1B-C2B	-2.87	100.48	106.62
2	A	301	DND	C2N-C3N-C7N	-2.76	115.03	119.78
2	D	301	DND	C5N-C6N-N1N	2.73	124.11	120.38
2	C	301	DND	O14-PA-O3P	2.73	114.65	107.27
2	B	301	DND	O14-PA-O3P	2.69	114.54	107.27
2	F	301	DND	O4B-C1B-C2B	-2.43	101.41	106.62
2	F	301	DND	C4N-C3N-C7N	2.39	125.10	120.37
2	A	301	DND	O14-PA-O3P	2.36	113.66	107.27
2	E	301	DND	O14-PA-O3P	2.32	113.53	107.27
2	A	301	DND	C6N-N1N-C1D	2.20	124.04	119.73
2	A	301	DND	C5N-C6N-N1N	2.18	123.36	120.38
2	E	301	DND	C4N-C3N-C7N	2.18	124.68	120.37
2	C	301	DND	O12-PN-O5D	2.16	117.38	107.57
2	D	301	DND	C4N-C3N-C7N	2.16	124.65	120.37
2	C	301	DND	O5D-C5D-C4D	-2.15	101.67	108.99
2	A	301	DND	O3P-PA-O13	-2.11	104.36	110.70
2	A	301	DND	O3P-PN-O11	2.00	116.73	110.70
2	C	301	DND	O3P-PN-O11	2.00	116.73	110.70

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	DND	C5D-O5D-PN-O11
2	B	301	DND	C5B-O5B-PA-O13
2	D	301	DND	C5D-O5D-PN-O11
2	E	301	DND	C5D-O5D-PN-O11
2	C	301	DND	O4D-C4D-C5D-O5D
2	A	301	DND	C3D-C4D-C5D-O5D
2	C	301	DND	C3D-C4D-C5D-O5D
2	A	301	DND	O4D-C4D-C5D-O5D
2	D	301	DND	O4D-C4D-C5D-O5D
2	D	301	DND	C3D-C4D-C5D-O5D
2	A	301	DND	PN-O3P-PA-O13
2	E	301	DND	PN-O3P-PA-O13
2	F	301	DND	PN-O3P-PA-O13
2	B	301	DND	O4B-C4B-C5B-O5B
2	F	301	DND	O4D-C4D-C5D-O5D
2	F	301	DND	C3D-C4D-C5D-O5D
2	B	301	DND	PN-O3P-PA-O14
2	C	301	DND	C5B-O5B-PA-O13
2	D	301	DND	C5B-O5B-PA-O13
2	F	301	DND	C5D-O5D-PN-O11
2	D	301	DND	O4B-C4B-C5B-O5B
2	B	301	DND	O4D-C4D-C5D-O5D
2	B	301	DND	C3B-C4B-C5B-O5B
2	A	301	DND	PN-O3P-PA-O14
2	C	301	DND	PN-O3P-PA-O13
2	C	301	DND	PN-O3P-PA-O14
2	F	301	DND	PN-O3P-PA-O14
2	E	301	DND	O4D-C4D-C5D-O5D
2	E	301	DND	PN-O3P-PA-O14

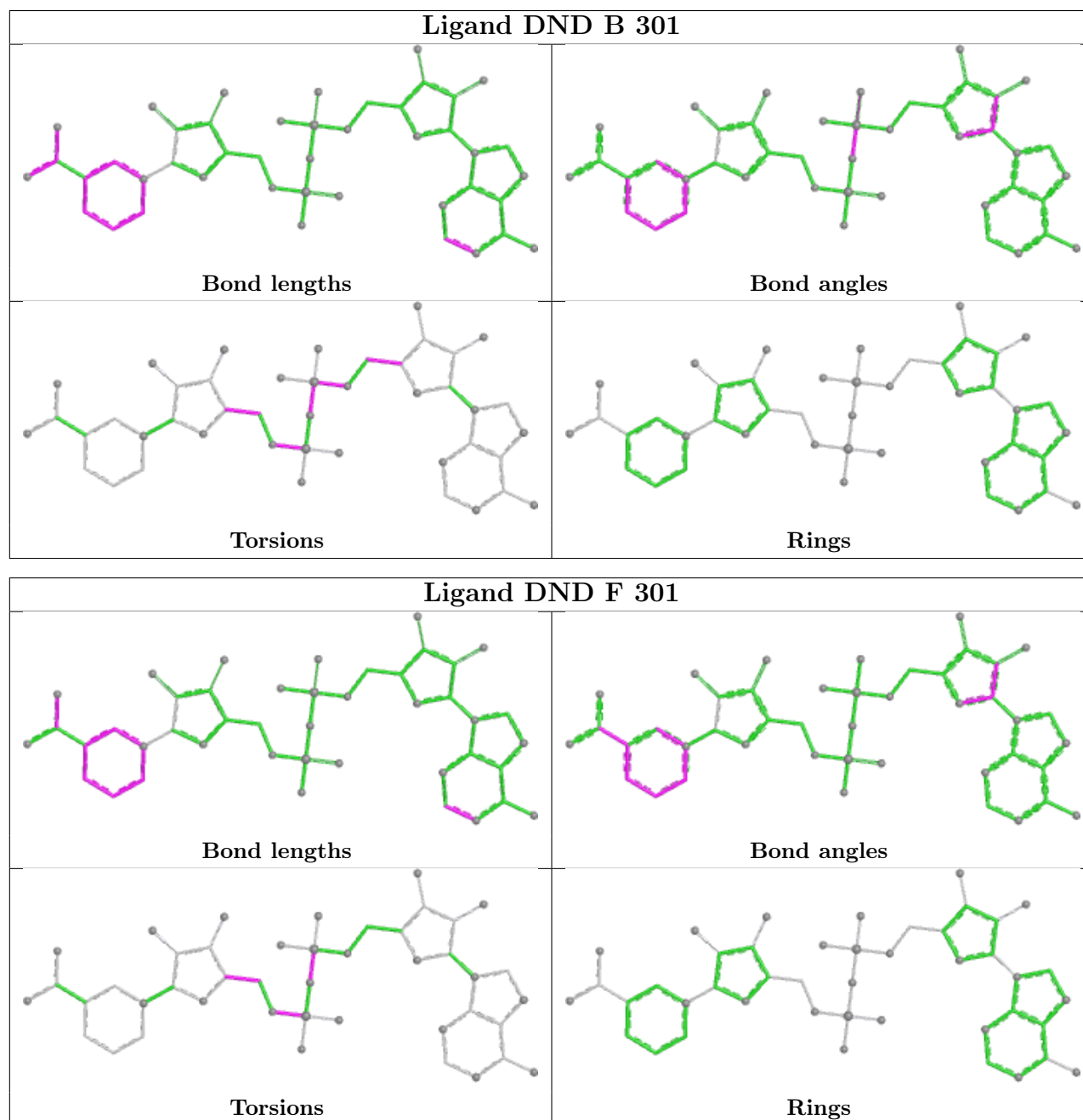
There are no ring outliers.

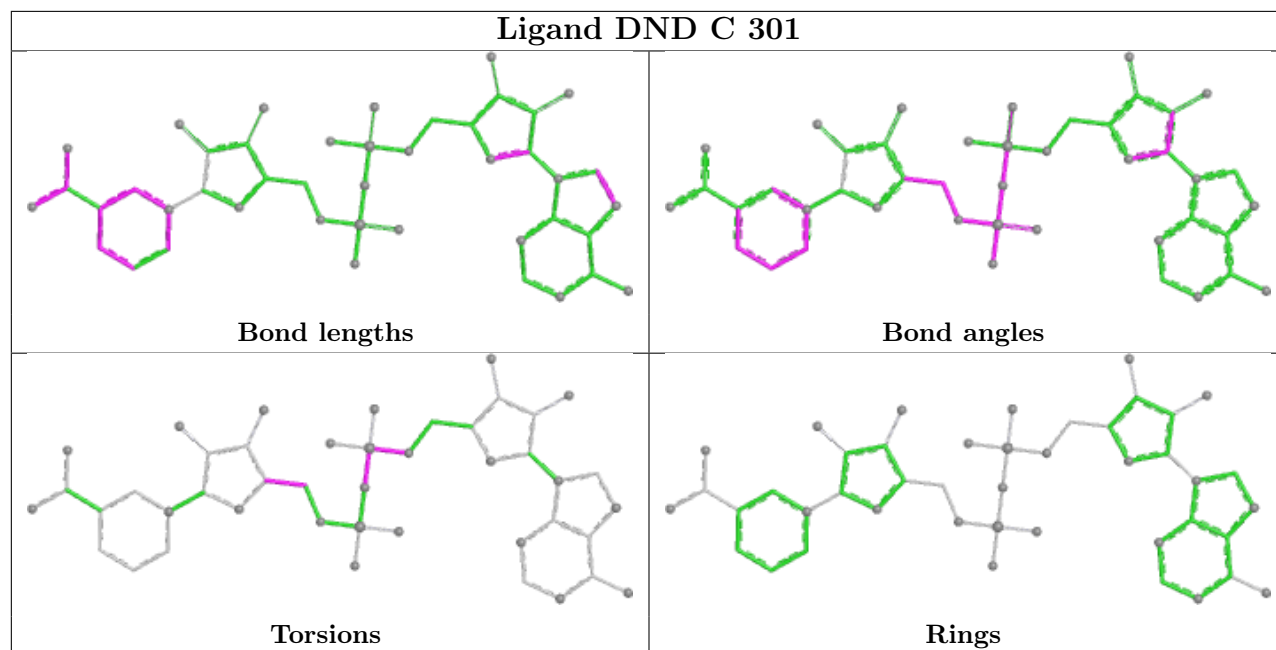
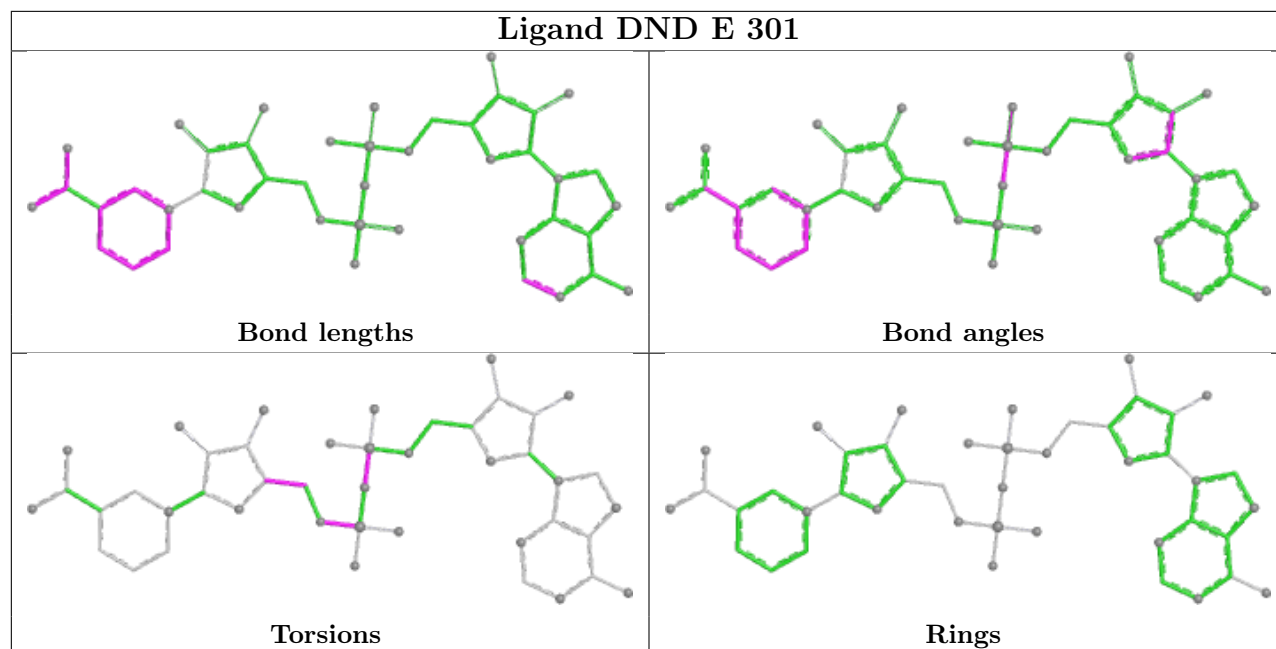
5 monomers are involved in 16 short contacts:

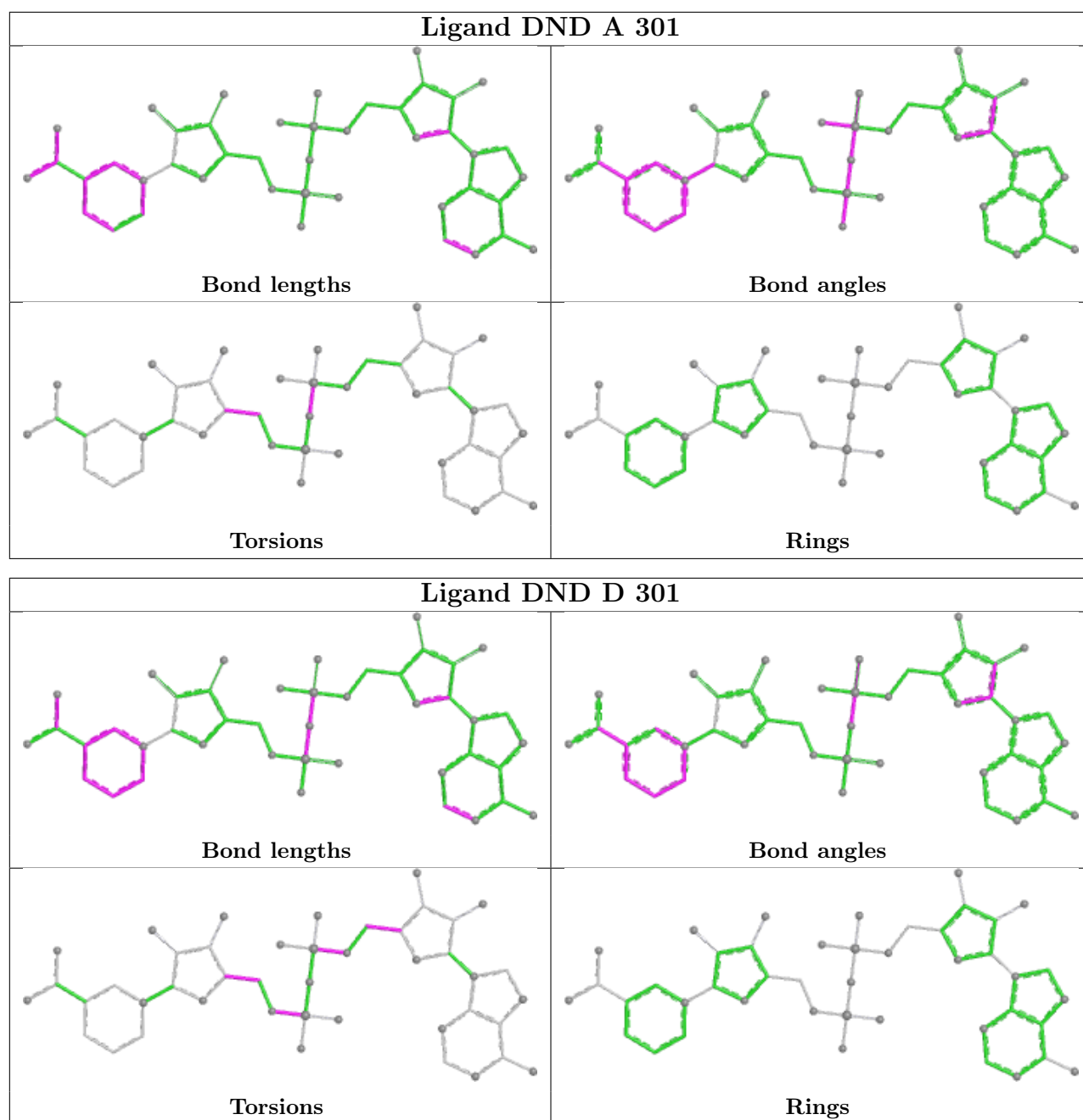
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	DND	2	0
2	F	301	DND	1	0
2	C	301	DND	7	0
2	A	301	DND	5	0
2	D	301	DND	1	0

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.