



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:11 am BST

PDB ID : 1KAQ  
Title : Structure of Bacillus subtilis Nicotinic Acid Mononucleotide Adenylyl Transferase  
Authors : Olland, A.M.; Underwood, K.W.; Czerwinski, R.M.; Lo, M.C.; Aulabaugh, A.; Bard, J.; Stahl, M.L.; Somers, W.S.; Sullivan, F.X.; Chopra, R.  
Deposited on : 2001-11-02  
Resolution : 3.20 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

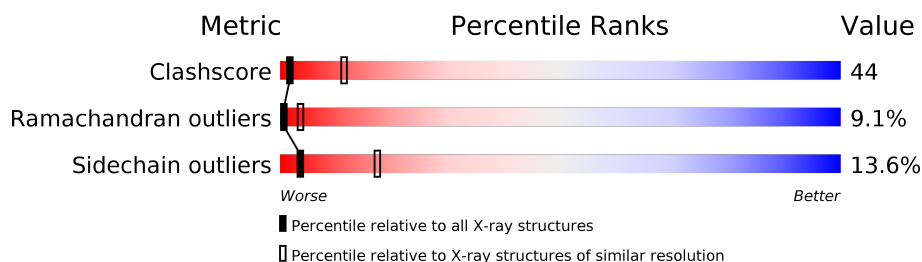
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	194	
1	B	194	
1	C	194	
1	D	194	
1	E	194	
1	F	194	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DND	A	601	X	-	-	-
2	DND	B	501	X	-	-	-
2	DND	C	401	X	-	-	-
2	DND	D	301	X	-	-	-
2	DND	E	201	X	-	-	-
2	DND	F	190	X	-	-	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9268 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 NICOTINATE-NUCLEOTIDE ADENYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1542	1010	246	280	6			
1	B	186	Total	C	N	O	S	0	0	0
			1542	1010	246	280	6			
1	C	186	Total	C	N	O	S	0	0	0
			1542	1010	246	280	6			
1	D	186	Total	C	N	O	S	0	0	0
			1542	1010	246	280	6			
1	E	176	Total	C	N	O	S	0	0	0
			1456	957	231	262	6			
1	F	167	Total	C	N	O	S	0	0	0
			1380	906	216	252	6			

There are 36 discrepancies between the modelled and reference sequences:

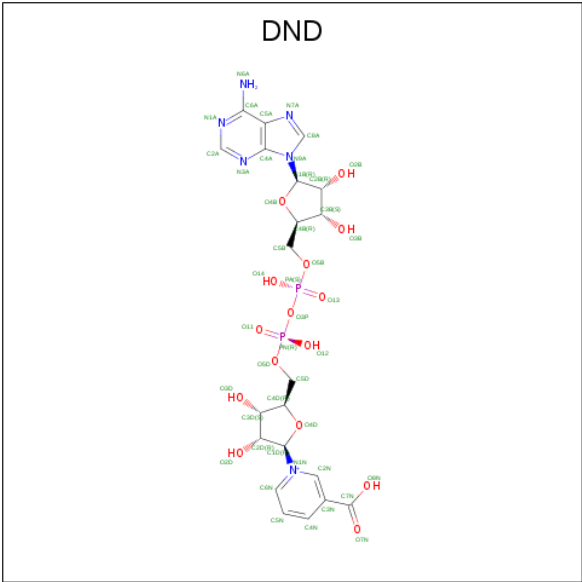
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP P54455
A	-3	MET	-	EXPRESSION TAG	UNP P54455
A	-2	PRO	-	EXPRESSION TAG	UNP P54455
A	-1	GLY	-	EXPRESSION TAG	UNP P54455
A	0	GLY	-	EXPRESSION TAG	UNP P54455
A	1	SER	MET	CLONING ARTIFACT	UNP P54455
B	-4	HIS	-	EXPRESSION TAG	UNP P54455
B	-3	MET	-	EXPRESSION TAG	UNP P54455
B	-2	PRO	-	EXPRESSION TAG	UNP P54455
B	-1	GLY	-	EXPRESSION TAG	UNP P54455
B	0	GLY	-	EXPRESSION TAG	UNP P54455
B	1	SER	MET	CLONING ARTIFACT	UNP P54455
C	-4	HIS	-	EXPRESSION TAG	UNP P54455
C	-3	MET	-	EXPRESSION TAG	UNP P54455
C	-2	PRO	-	EXPRESSION TAG	UNP P54455
C	-1	GLY	-	EXPRESSION TAG	UNP P54455
C	0	GLY	-	EXPRESSION TAG	UNP P54455

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	SER	MET	CLONING ARTIFACT	UNP P54455
D	-4	HIS	-	EXPRESSION TAG	UNP P54455
D	-3	MET	-	EXPRESSION TAG	UNP P54455
D	-2	PRO	-	EXPRESSION TAG	UNP P54455
D	-1	GLY	-	EXPRESSION TAG	UNP P54455
D	0	GLY	-	EXPRESSION TAG	UNP P54455
D	1	SER	MET	CLONING ARTIFACT	UNP P54455
E	-4	HIS	-	EXPRESSION TAG	UNP P54455
E	-3	MET	-	EXPRESSION TAG	UNP P54455
E	-2	PRO	-	EXPRESSION TAG	UNP P54455
E	-1	GLY	-	EXPRESSION TAG	UNP P54455
E	0	GLY	-	EXPRESSION TAG	UNP P54455
E	1	SER	MET	CLONING ARTIFACT	UNP P54455
F	-4	HIS	-	EXPRESSION TAG	UNP P54455
F	-3	MET	-	EXPRESSION TAG	UNP P54455
F	-2	PRO	-	EXPRESSION TAG	UNP P54455
F	-1	GLY	-	EXPRESSION TAG	UNP P54455
F	0	GLY	-	EXPRESSION TAG	UNP P54455
F	1	SER	MET	CLONING ARTIFACT	UNP P54455

- Molecule 2 is NICOTINIC ACID ADENINE DINUCLEOTIDE (three-letter code: DND) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>6</sub>O<sub>15</sub>P<sub>2</sub>).



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

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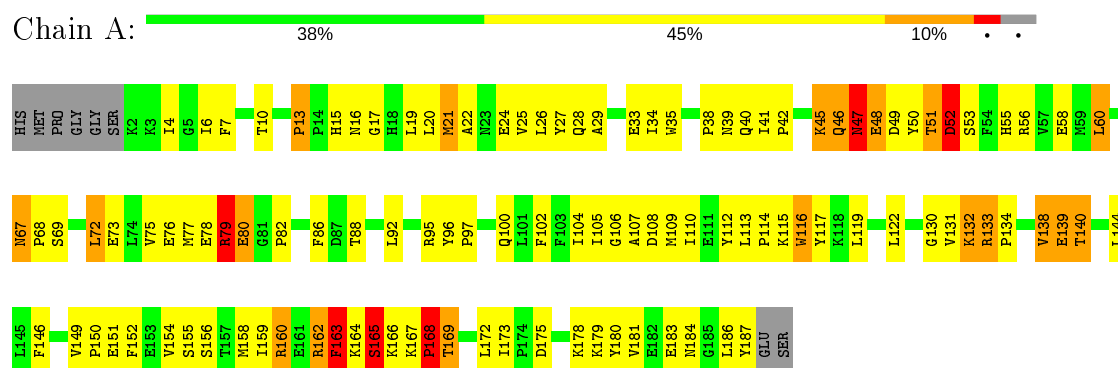
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	6	15	2		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: NICOTINATE-NUCLEOTIDE ADENYLYLTRANSFERASE





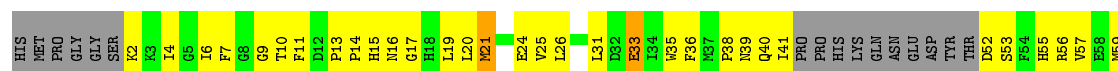
• Molecule 1: NICOTINATE-NUCLEOTIDE ADENYLYLTRANSFERASE

Chain D: 36% 48% 8% . .



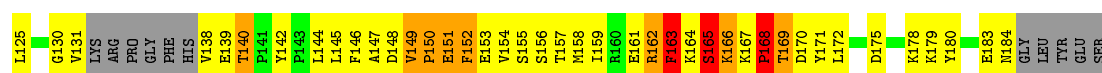
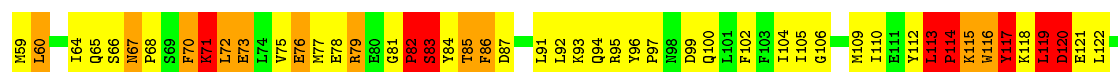
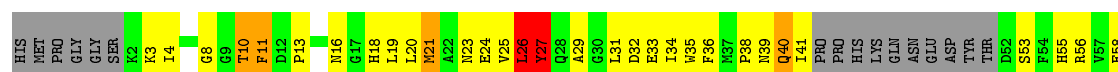
• Molecule 1: NICOTINATE-NUCLEOTIDE ADENYLYLTRANSFERASE

Chain E: 30% 50% 10% 9%



• Molecule 1: NICOTINATE-NUCLEOTIDE ADENYLYLTRANSFERASE

Chain F: 24% 44% 12% 7% 14%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.31 Å   108.78 Å   177.56 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	15.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.279 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9268	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.55	0/1588	0.83	3/2151 (0.1%)
1	B	0.68	4/1588 (0.3%)	0.99	12/2151 (0.6%)
1	C	0.52	0/1588	0.80	1/2151 (0.0%)
1	D	0.57	0/1588	0.81	2/2151 (0.1%)
1	E	0.38	0/1497	0.69	2/2024 (0.1%)
1	F	0.45	0/1416	0.98	8/1914 (0.4%)
All	All	0.53	4/9265 (0.0%)	0.86	28/12542 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	46	GLN	CB-CG	-7.89	1.31	1.52
1	B	45	LYS	C-O	7.04	1.36	1.23
1	B	46	GLN	C-O	5.13	1.33	1.23
1	B	45	LYS	CA-CB	-5.04	1.42	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	149	VAL	C-N-CD	-17.77	81.50	120.60
1	F	113	LEU	C-N-CD	-11.90	94.42	120.60
1	B	49	ASP	CB-CG-OD2	-11.83	107.65	118.30
1	F	81	GLY	N-CA-C	-9.92	88.31	113.10
1	B	55	HIS	N-CA-C	-8.17	88.94	111.00
1	F	149	VAL	C-N-CA	7.73	154.47	122.00
1	B	45	LYS	CA-C-N	-7.01	101.77	117.20
1	A	48	GLU	N-CA-C	-6.94	92.27	111.00
1	B	48	GLU	N-CA-C	6.47	128.46	111.00
1	F	26	LEU	CA-CB-CG	6.21	129.59	115.30
1	B	45	LYS	CA-C-O	6.08	132.87	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	GLN	O-C-N	-6.03	113.06	122.70
1	B	54	PHE	N-CA-C	-5.84	95.23	111.00
1	D	165	SER	N-CA-C	-5.67	95.70	111.00
1	F	165	SER	N-CA-C	-5.62	95.83	111.00
1	B	52	ASP	N-CA-C	5.62	126.16	111.00
1	C	48	GLU	N-CA-C	-5.48	96.20	111.00
1	A	165	SER	N-CA-C	-5.42	96.35	111.00
1	B	53	SER	N-CA-C	-5.34	96.57	111.00
1	F	114	PRO	CA-N-CD	-5.32	104.06	111.50
1	A	52	ASP	N-CA-C	5.28	125.27	111.00
1	B	165	SER	N-CA-C	-5.27	96.77	111.00
1	B	46	GLN	CA-C-O	5.16	130.94	120.10
1	D	52	ASP	N-CA-C	5.13	124.86	111.00
1	E	62	LEU	N-CA-C	-5.12	97.18	111.00
1	B	46	GLN	N-CA-CB	-5.07	101.48	110.60
1	E	165	SER	N-CA-C	-5.04	97.39	111.00
1	F	82	PRO	N-CA-C	-5.03	99.02	112.10

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	1542	0	1523	135	0
1	B	1542	0	1523	155	0
1	C	1542	0	1523	123	0
1	D	1542	0	1523	120	0
1	E	1456	0	1448	137	0
1	F	1380	0	1372	158	0
2	A	44	0	25	8	0
2	B	44	0	25	4	0
2	C	44	0	25	4	0
2	D	44	0	25	8	0
2	E	44	0	25	9	0
2	F	44	0	25	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9268	0	9062	802	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 44.

All (802) 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:F:149:VAL:CG1	1:F:150:PRO:HD3	1.68	1.23
1:B:10:THR:HG22	1:B:39:ASN:HD22	0.99	1.16
1:B:10:THR:HG22	1:B:39:ASN:ND2	1.68	1.08
1:F:113:LEU:HB3	1:F:114:PRO:HD2	1.32	1.08
1:F:149:VAL:HG12	1:F:150:PRO:CD	1.82	1.08
1:E:62:LEU:HD11	1:E:177:VAL:HG23	1.26	1.06
1:A:10:THR:HG22	1:A:39:ASN:ND2	1.71	1.06
1:F:149:VAL:HG12	1:F:150:PRO:HD3	1.09	1.04
1:E:134:PRO:HG3	1:E:151:GLU:HB3	1.40	1.03
1:B:48:GLU:O	1:B:49:ASP:HB2	1.28	1.02
1:A:10:THR:HG22	1:A:39:ASN:HD22	1.21	0.99
1:F:113:LEU:HB3	1:F:114:PRO:CD	1.91	0.99
1:A:134:PRO:HG3	1:A:151:GLU:HB3	1.46	0.97
1:F:116:TRP:HB3	1:F:119:LEU:CD2	1.95	0.96
1:D:78:GLU:O	1:D:78:GLU:HG2	1.64	0.96
1:B:53:SER:O	1:B:54:PHE:O	1.83	0.96
1:A:167:LYS:HE2	1:D:27:TYR:HE2	1.32	0.92
1:D:78:GLU:O	1:D:79:ARG:HB3	1.70	0.92
1:F:149:VAL:CB	1:F:150:PRO:HD3	1.91	0.92
1:E:19:LEU:HB3	1:F:171:TYR:CE2	2.05	0.91
1:F:38:PRO:HG3	1:F:60:LEU:HD12	1.53	0.90
1:A:40:GLN:HA	1:A:77:MET:CE	2.00	0.90
1:F:131:VAL:HG13	1:F:149:VAL:HB	1.54	0.90
1:F:82:PRO:O	1:F:83:SER:HB2	1.72	0.89
1:D:49:ASP:O	1:D:50:TYR:O	1.90	0.88
1:C:45:LYS:HG3	1:C:45:LYS:O	1.75	0.87
1:E:109:MET:HA	1:E:109:MET:HE2	1.56	0.86
1:D:10:THR:HG22	1:D:39:ASN:ND2	1.91	0.85
1:D:38:PRO:HG3	1:D:60:LEU:HD12	1.58	0.85
1:C:44:HIS:O	1:C:45:LYS:HB3	1.76	0.85
1:C:40:GLN:HE21	1:C:40:GLN:HA	1.38	0.85
1:B:4:ILE:HD13	1:B:35:TRP:CZ2	2.13	0.84
1:A:38:PRO:HG3	1:A:60:LEU:HD12	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:PRO:HG3	1:B:151:GLU:HB3	1.61	0.83
1:A:167:LYS:HE2	1:D:27:TYR:CE2	2.13	0.83
1:C:10:THR:HG22	1:C:39:ASN:ND2	1.93	0.83
1:B:168:PRO:O	1:B:169:THR:HG23	1.78	0.82
1:B:54:PHE:O	1:B:55:HIS:HB2	1.78	0.82
1:A:131:VAL:HG13	1:A:149:VAL:HB	1.62	0.82
1:F:168:PRO:O	1:F:169:THR:HG23	1.79	0.82
1:B:2:LYS:HE2	1:B:33:GLU:OE2	1.80	0.81
1:B:48:GLU:O	1:B:49:ASP:CB	2.18	0.81
1:E:40:GLN:HA	1:E:77:MET:CE	2.10	0.81
1:D:134:PRO:HG3	1:D:151:GLU:HB3	1.63	0.80
1:C:38:PRO:HG3	1:C:60:LEU:HD12	1.64	0.80
1:E:10:THR:HG22	1:E:39:ASN:HD22	1.45	0.79
1:A:40:GLN:HA	1:A:77:MET:HE1	1.62	0.79
1:A:78:GLU:O	1:A:79:ARG:HB2	1.81	0.79
1:A:168:PRO:O	1:A:169:THR:HG23	1.83	0.79
1:E:65:GLN:HG3	1:E:66:SER:N	1.97	0.79
1:B:55:HIS:O	1:B:57:VAL:N	2.16	0.78
1:B:44:HIS:O	1:B:45:LYS:HB3	1.82	0.78
1:C:11:PHE:HB3	1:C:14:PRO:HG3	1.64	0.78
1:E:64:ILE:HB	1:E:70:PHE:HB3	1.66	0.78
1:F:27:TYR:N	1:F:27:TYR:CD1	2.49	0.78
1:F:25:VAL:HG11	1:F:104:ILE:HD13	1.64	0.78
1:F:93:LYS:CD	1:F:125:LEU:HB3	2.14	0.78
1:E:89:VAL:HG21	1:E:122:LEU:HD11	1.67	0.77
1:F:36:PHE:O	1:F:38:PRO:HD3	1.84	0.77
1:B:45:LYS:HB2	1:B:48:GLU:HB2	1.67	0.77
1:E:10:THR:HG22	1:E:39:ASN:ND2	2.00	0.77
1:D:51:THR:O	1:D:53:SER:N	2.16	0.76
1:B:53:SER:C	1:B:54:PHE:O	2.17	0.76
1:E:13:PRO:HD2	1:E:156:SER:HB2	1.67	0.76
1:F:113:LEU:CB	1:F:114:PRO:CD	2.57	0.76
1:C:131:VAL:HG13	1:C:149:VAL:HB	1.67	0.76
1:C:45:LYS:CG	1:C:45:LYS:O	2.34	0.76
1:B:72:LEU:HD23	1:B:73:GLU:H	1.51	0.75
1:D:86:PHE:HA	1:D:122:LEU:HD13	1.68	0.75
1:F:163:PHE:CE1	1:F:169:THR:HG21	2.21	0.75
1:C:134:PRO:HB3	1:C:151:GLU:OE2	1.86	0.75
1:E:107:ALA:HB2	1:E:132:LYS:HA	1.67	0.74
1:B:84:TYR:O	1:B:86:PHE:N	2.20	0.74
1:C:168:PRO:O	1:C:169:THR:HG23	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:MET:HG3	1:B:131:VAL:HG11	1.68	0.74
1:A:138:VAL:HG21	1:A:146:PHE:CE1	2.23	0.73
1:A:10:THR:HG23	2:A:601:DND:O11	1.87	0.73
1:B:79:ARG:O	1:B:80:GLU:O	2.07	0.73
1:F:16:ASN:O	1:F:20:LEU:HD12	1.88	0.73
1:F:164:LYS:O	1:F:165:SER:HB2	1.89	0.73
1:B:10:THR:HG23	2:B:501:DND:O11	1.89	0.73
1:E:86:PHE:HA	1:E:122:LEU:HD13	1.69	0.73
1:E:55:HIS:ND1	1:E:186:LEU:HD21	2.04	0.72
1:E:21:MET:HG3	1:E:131:VAL:HG11	1.71	0.72
1:D:21:MET:HG2	2:D:301:DND:H24	1.71	0.72
1:D:41:ILE:HG23	1:D:82:PRO:HA	1.69	0.72
1:F:154:VAL:HA	1:F:158:MET:CE	2.19	0.72
1:D:61:LYS:O	1:D:65:GLN:HG3	1.90	0.72
1:A:154:VAL:HA	1:A:158:MET:CE	2.20	0.72
1:B:40:GLN:OE1	1:B:77:MET:HA	1.90	0.71
1:F:149:VAL:HG12	1:F:150:PRO:CG	2.21	0.71
1:F:4:ILE:HD13	1:F:35:TRP:CZ2	2.26	0.71
1:B:54:PHE:C	1:B:55:HIS:O	2.17	0.71
1:A:40:GLN:HA	1:A:77:MET:HE3	1.70	0.71
1:E:62:LEU:O	1:E:63:ALA:HB3	1.91	0.71
1:D:178:LYS:O	1:D:182:GLU:HG3	1.90	0.71
1:F:85:THR:O	1:F:87:ASP:N	2.24	0.71
1:E:52:ASP:O	1:E:53:SER:HB3	1.89	0.71
1:C:67:ASN:ND2	1:C:69:SER:H	1.89	0.70
1:F:116:TRP:CD1	1:F:116:TRP:O	2.44	0.70
1:A:78:GLU:OE1	1:A:95:ARG:NH2	2.24	0.70
1:B:164:LYS:O	1:B:165:SER:HB2	1.90	0.70
1:E:62:LEU:CD1	1:E:177:VAL:HG23	2.16	0.70
1:B:107:ALA:HB2	1:B:133:ARG:H	1.55	0.70
1:E:11:PHE:HB3	1:E:14:PRO:HG3	1.73	0.70
1:A:41:ILE:HG23	1:A:82:PRO:HA	1.72	0.69
1:E:40:GLN:HA	1:E:77:MET:HE2	1.74	0.69
1:A:4:ILE:HD13	1:A:35:TRP:CZ2	2.27	0.69
1:C:52:ASP:O	1:C:53:SER:HB3	1.91	0.69
1:E:59:MET:O	1:E:62:LEU:HG	1.91	0.69
1:B:41:ILE:HG23	1:B:82:PRO:HA	1.73	0.69
1:C:107:ALA:CB	1:C:133:ARG:H	2.05	0.69
1:F:152:PHE:HD2	1:F:153:GLU:H	1.38	0.69
1:F:152:PHE:HD2	1:F:153:GLU:N	1.91	0.69
1:B:92:LEU:O	1:B:94:GLN:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ASN:C	1:C:67:ASN:HD22	1.96	0.69
1:F:38:PRO:HG3	1:F:60:LEU:CD1	2.22	0.68
1:B:138:VAL:HG21	1:B:146:PHE:CE1	2.29	0.68
1:F:25:VAL:HG11	1:F:104:ILE:CD1	2.23	0.68
1:B:56:ARG:O	1:B:60:LEU:HB2	1.94	0.68
1:F:96:TYR:HB3	1:F:99:ASP:OD2	1.93	0.68
1:D:25:VAL:HG11	1:D:104:ILE:HD13	1.75	0.68
1:E:170:ASP:HB2	1:F:23:ASN:OD1	1.93	0.68
1:A:107:ALA:HB2	1:A:133:ARG:H	1.58	0.68
1:C:89:VAL:HG21	1:C:122:LEU:HD11	1.76	0.68
1:E:62:LEU:HA	1:E:65:GLN:HB3	1.74	0.68
1:A:28:GLN:NE2	1:B:144:LEU:H	1.93	0.67
1:E:21:MET:HG2	2:E:201:DND:H24	1.75	0.67
1:D:10:THR:HG23	2:D:301:DND:O11	1.93	0.67
1:D:11:PHE:HB3	1:D:14:PRO:HG3	1.74	0.67
1:E:40:GLN:HA	1:E:77:MET:HE3	1.74	0.67
1:F:117:TYR:N	1:F:117:TYR:CD2	2.62	0.67
1:B:40:GLN:HA	1:B:77:MET:HE3	1.74	0.67
1:C:44:HIS:H	1:C:44:HIS:CD2	2.13	0.67
1:B:133:ARG:HD3	2:B:501:DND:C6A	2.25	0.67
1:A:134:PRO:CG	1:A:151:GLU:HB3	2.24	0.67
1:A:52:ASP:O	1:A:53:SER:HB3	1.95	0.67
1:C:44:HIS:H	1:C:44:HIS:HD2	1.42	0.67
1:D:10:THR:HG22	1:D:39:ASN:HD22	1.60	0.66
1:C:100:GLN:HG2	1:C:102:PHE:CE1	2.31	0.66
1:A:46:GLN:O	1:A:47:ASN:HB3	1.95	0.66
1:D:67:ASN:ND2	1:D:69:SER:H	1.92	0.66
1:F:179:LYS:O	1:F:183:GLU:HG3	1.96	0.66
1:A:163:PHE:CD2	1:A:181:VAL:HG11	2.31	0.66
1:D:52:ASP:O	1:D:53:SER:HB3	1.95	0.66
1:B:134:PRO:CG	1:B:151:GLU:HB3	2.25	0.66
1:F:153:GLU:HG2	1:F:153:GLU:O	1.95	0.66
1:B:40:GLN:HG3	1:B:77:MET:CE	2.26	0.65
1:D:2:LYS:HB3	1:D:99:ASP:OD1	1.97	0.65
1:E:10:THR:HG23	2:E:201:DND:O11	1.96	0.65
1:B:107:ALA:CB	1:B:133:ARG:H	2.08	0.65
1:D:38:PRO:HG3	1:D:60:LEU:CD1	2.27	0.65
1:F:64:ILE:HB	1:F:70:PHE:HB2	1.77	0.65
1:F:82:PRO:HG2	1:F:83:SER:H	1.61	0.65
1:E:61:LYS:O	1:E:65:GLN:HB3	1.96	0.65
1:C:164:LYS:O	1:C:165:SER:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:ASP:O	1:D:50:TYR:C	2.34	0.65
1:D:6:ILE:CD1	1:D:92:LEU:HD13	2.26	0.65
1:F:114:PRO:HB3	1:F:142:TYR:OH	1.97	0.65
1:B:138:VAL:HG21	1:B:146:PHE:CZ	2.31	0.65
1:C:134:PRO:HG3	1:C:151:GLU:HB2	1.78	0.65
1:A:55:HIS:ND1	1:A:186:LEU:HD21	2.12	0.65
1:A:21:MET:HG2	2:A:601:DND:H24	1.77	0.64
1:E:60:LEU:O	1:E:61:LYS:HB2	1.97	0.64
1:C:131:VAL:O	1:C:132:LYS:HB2	1.97	0.64
1:E:168:PRO:O	1:E:169:THR:HG23	1.97	0.64
1:F:84:TYR:O	1:F:85:THR:O	2.14	0.64
1:B:162:ARG:HG3	1:B:167:LYS:CB	2.28	0.64
1:B:162:ARG:HG3	1:B:167:LYS:HB2	1.77	0.64
1:B:27:TYR:HE2	1:C:167:LYS:HE2	1.62	0.64
1:E:134:PRO:CG	1:E:151:GLU:HB3	2.23	0.64
1:F:116:TRP:HB3	1:F:119:LEU:HD21	1.80	0.64
1:E:171:TYR:CE2	1:F:19:LEU:HB3	2.33	0.64
1:F:154:VAL:HA	1:F:158:MET:HE1	1.77	0.64
1:B:52:ASP:C	1:B:53:SER:O	2.31	0.64
1:A:38:PRO:HG3	1:A:60:LEU:CD1	2.27	0.64
1:C:101:LEU:O	1:C:126:ILE:HG13	1.98	0.64
1:C:44:HIS:O	1:C:45:LYS:CB	2.46	0.64
1:A:163:PHE:CE1	1:A:169:THR:HG21	2.33	0.64
1:B:40:GLN:HG3	1:B:77:MET:HE2	1.80	0.63
1:C:51:THR:O	1:C:53:SER:N	2.32	0.63
1:A:138:VAL:HG21	1:A:146:PHE:CZ	2.34	0.63
1:B:27:TYR:CE2	1:C:167:LYS:HE2	2.33	0.63
1:C:86:PHE:HA	1:C:122:LEU:HD13	1.79	0.63
1:E:163:PHE:CD2	1:E:181:VAL:HG11	2.34	0.63
1:B:164:LYS:HE2	1:B:187:TYR:O	1.98	0.63
1:B:79:ARG:HH12	1:B:83:SER:HA	1.63	0.63
1:A:50:TYR:O	1:A:51:THR:O	2.17	0.63
1:A:75:VAL:O	1:A:78:GLU:HB2	1.99	0.63
1:F:114:PRO:C	1:F:116:TRP:H	2.02	0.63
1:F:153:GLU:CG	1:F:153:GLU:O	2.46	0.63
1:A:78:GLU:CD	1:A:95:ARG:HH22	2.02	0.62
1:E:155:SER:H	1:E:158:MET:HE3	1.63	0.62
1:F:82:PRO:HG2	1:F:83:SER:N	2.13	0.62
1:C:67:ASN:HD22	1:C:68:PRO:N	1.97	0.62
1:D:131:VAL:O	1:D:132:LYS:HB3	1.98	0.62
1:A:109:MET:SD	1:A:116:TRP:HZ3	2.21	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:GLU:OE1	1:D:95:ARG:NH2	2.31	0.62
1:B:141:PRO:HA	1:D:167:LYS:HE3	1.80	0.62
1:C:78:GLU:OE1	1:C:95:ARG:NH2	2.32	0.62
1:F:131:VAL:CG1	1:F:149:VAL:HB	2.28	0.62
1:A:25:VAL:HG11	1:A:104:ILE:HD13	1.81	0.62
1:A:164:LYS:O	1:A:165:SER:HB2	2.00	0.62
1:F:93:LYS:HD3	1:F:125:LEU:HB3	1.82	0.62
1:B:40:GLN:HA	1:B:77:MET:CE	2.28	0.62
1:D:67:ASN:HD22	1:D:67:ASN:C	2.02	0.62
1:B:107:ALA:HB3	1:B:133:ARG:HB3	1.81	0.62
1:D:21:MET:HG2	2:D:301:DND:C2A	2.28	0.62
1:E:55:HIS:O	1:E:59:MET:HG3	1.98	0.62
1:A:162:ARG:HG3	1:A:167:LYS:HB3	1.80	0.62
1:B:45:LYS:O	1:B:48:GLU:HB3	2.00	0.62
1:C:13:PRO:HD2	1:C:156:SER:HB2	1.82	0.62
1:D:138:VAL:HG21	1:D:146:PHE:CE1	2.34	0.62
1:D:21:MET:HG3	1:D:131:VAL:HG11	1.81	0.62
1:E:164:LYS:HE2	1:E:187:TYR:O	1.99	0.62
1:E:4:ILE:HD13	1:E:35:TRP:CZ2	2.35	0.61
1:F:100:GLN:HE21	1:F:102:PHE:HZ	1.48	0.61
1:F:26:LEU:HB3	1:F:27:TYR:CD1	2.35	0.61
1:A:78:GLU:O	1:A:79:ARG:CB	2.49	0.61
1:F:119:LEU:O	1:F:121:GLU:N	2.33	0.61
1:A:67:ASN:HD22	1:A:67:ASN:C	2.04	0.61
1:A:21:MET:HG3	1:A:131:VAL:HG11	1.81	0.61
1:B:72:LEU:CD2	1:B:73:GLU:H	2.13	0.61
1:C:44:HIS:N	1:C:44:HIS:CD2	2.67	0.61
1:C:10:THR:HG22	1:C:39:ASN:HD22	1.65	0.61
1:C:10:THR:HG23	2:C:401:DND:O11	2.01	0.61
1:C:155:SER:O	1:C:158:MET:HB3	2.01	0.61
1:D:80:GLU:CD	1:D:80:GLU:H	2.04	0.61
1:D:6:ILE:HD13	1:D:92:LEU:HD13	1.82	0.60
1:E:138:VAL:HG21	1:E:146:PHE:CE1	2.35	0.60
1:A:21:MET:CG	1:A:131:VAL:HG11	2.32	0.60
1:C:131:VAL:O	1:C:132:LYS:CB	2.50	0.60
1:E:179:LYS:O	1:E:183:GLU:HG3	2.02	0.60
1:F:153:GLU:O	1:F:158:MET:HE1	2.01	0.60
1:A:134:PRO:HG3	1:A:151:GLU:CB	2.27	0.60
1:A:109:MET:SD	1:A:116:TRP:CZ3	2.95	0.60
1:F:106:GLY:O	1:F:110:ILE:HG13	2.01	0.60
1:A:50:TYR:O	1:A:50:TYR:CD2	2.55	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:MET:HG3	2:F:190:DND:H2	1.83	0.60
1:B:40:GLN:NE2	1:B:80:GLU:HA	2.17	0.60
1:B:54:PHE:O	1:B:55:HIS:CB	2.42	0.60
1:D:131:VAL:HG13	1:D:149:VAL:HB	1.83	0.60
1:F:163:PHE:CD1	1:F:169:THR:HG21	2.37	0.59
1:C:134:PRO:HG3	1:C:151:GLU:CB	2.33	0.59
1:A:28:GLN:HE21	1:B:144:LEU:H	1.48	0.59
1:C:133:ARG:HG3	1:C:134:PRO:CD	2.33	0.59
1:C:49:ASP:O	1:C:50:TYR:O	2.20	0.59
1:F:116:TRP:O	1:F:117:TYR:C	2.40	0.59
1:B:91:LEU:C	1:B:92:LEU:O	2.39	0.59
1:C:107:ALA:HB2	1:C:132:LYS:HA	1.84	0.59
1:F:27:TYR:H	1:F:27:TYR:HD1	1.40	0.59
1:F:149:VAL:HG12	1:F:150:PRO:HG3	1.85	0.59
1:E:40:GLN:NE2	1:E:80:GLU:HA	2.16	0.59
1:C:107:ALA:HB2	1:C:133:ARG:H	1.66	0.59
1:C:38:PRO:HG3	1:C:60:LEU:CD1	2.32	0.59
1:A:73:GLU:HG3	1:A:75:VAL:HG12	1.84	0.59
1:A:40:GLN:HE22	1:A:80:GLU:N	2.01	0.58
1:B:92:LEU:C	1:B:94:GLN:H	2.07	0.58
1:F:116:TRP:HD1	1:F:116:TRP:O	1.83	0.58
1:B:164:LYS:O	1:B:165:SER:CB	2.50	0.58
1:E:109:MET:HA	1:E:109:MET:CE	2.33	0.58
1:F:110:ILE:HG22	1:F:140:THR:HG23	1.85	0.58
1:A:179:LYS:O	1:A:183:GLU:HG3	2.02	0.58
1:C:168:PRO:C	1:C:169:THR:HG23	2.23	0.58
1:E:157:THR:O	1:E:157:THR:HG22	2.02	0.58
1:A:163:PHE:CD1	1:A:169:THR:HG21	2.39	0.58
1:D:107:ALA:HB2	1:D:132:LYS:HA	1.85	0.58
1:E:19:LEU:HD21	1:E:63:ALA:HB1	1.86	0.58
1:F:8:GLY:O	2:F:190:DND:H16	2.02	0.58
1:A:154:VAL:HA	1:A:158:MET:HE3	1.86	0.58
1:C:41:ILE:HG23	1:C:82:PRO:HA	1.85	0.58
1:A:107:ALA:CB	1:A:133:ARG:H	2.16	0.58
1:D:12:ASP:OD1	1:D:51:THR:HG23	2.03	0.58
1:A:154:VAL:HA	1:A:158:MET:HE1	1.85	0.57
1:B:10:THR:CG2	1:B:39:ASN:HD22	1.94	0.57
1:C:75:VAL:O	1:C:78:GLU:HB2	2.03	0.57
1:A:46:GLN:O	1:A:47:ASN:CB	2.52	0.57
1:D:21:MET:SD	1:D:149:VAL:HG11	2.44	0.57
1:E:133:ARG:HG3	1:E:134:PRO:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:LYS:HD2	1:F:125:LEU:HB3	1.85	0.57
1:B:52:ASP:O	1:B:53:SER:HB3	2.04	0.57
1:E:6:ILE:CD1	1:E:92:LEU:HD13	2.34	0.57
1:C:179:LYS:O	1:C:183:GLU:HG3	2.05	0.57
1:E:167:LYS:HB3	1:E:168:PRO:HD2	1.87	0.57
1:E:21:MET:HG2	2:E:201:DND:C2A	2.35	0.57
1:D:45:LYS:HB2	1:D:48:GLU:HG3	1.87	0.57
1:E:107:ALA:HB3	1:E:133:ARG:H	1.68	0.57
1:F:67:ASN:HD22	1:F:68:PRO:CD	2.17	0.57
1:A:86:PHE:HA	1:A:122:LEU:HD13	1.87	0.57
1:B:44:HIS:N	1:B:44:HIS:ND1	2.37	0.57
1:F:24:GLU:HG3	1:F:149:VAL:HG13	1.87	0.57
1:B:46:GLN:OE1	1:B:82:PRO:CG	2.52	0.57
1:D:119:LEU:CD1	1:D:123:LEU:HG	2.34	0.57
1:A:167:LYS:O	1:A:169:THR:HG22	2.05	0.56
1:E:167:LYS:O	1:E:169:THR:HG22	2.05	0.56
1:B:131:VAL:HG13	1:B:149:VAL:HB	1.87	0.56
1:B:163:PHE:CE1	1:B:169:THR:HG21	2.41	0.56
1:D:134:PRO:CG	1:D:151:GLU:HB3	2.34	0.56
1:E:154:VAL:HA	1:E:158:MET:CE	2.36	0.56
1:B:92:LEU:C	1:B:94:GLN:N	2.57	0.56
1:F:138:VAL:HG21	1:F:146:PHE:CE1	2.40	0.56
1:E:131:VAL:O	1:E:132:LYS:CB	2.52	0.56
1:F:70:PHE:CG	1:F:71:LYS:N	2.67	0.56
1:D:131:VAL:O	1:D:132:LYS:CB	2.54	0.56
1:F:130:GLY:N	1:F:144:LEU:HD21	2.20	0.56
1:F:24:GLU:CB	1:F:149:VAL:HG13	2.36	0.56
1:B:163:PHE:HE2	1:B:181:VAL:HG21	1.70	0.56
1:D:110:ILE:HA	1:D:113:LEU:HD13	1.86	0.56
1:E:155:SER:O	1:E:158:MET:HB3	2.04	0.56
1:F:110:ILE:HG22	1:F:140:THR:CG2	2.36	0.56
1:D:160:ARG:HD3	1:D:187:TYR:CE1	2.41	0.56
1:D:164:LYS:O	1:D:165:SER:HB3	2.05	0.56
1:D:25:VAL:HG11	1:D:104:ILE:CD1	2.35	0.56
1:E:62:LEU:O	1:E:63:ALA:CB	2.54	0.56
1:A:38:PRO:CG	1:A:60:LEU:HD12	2.33	0.55
1:C:4:ILE:HD13	1:C:35:TRP:CZ2	2.41	0.55
1:C:133:ARG:HG3	1:C:134:PRO:HD2	1.88	0.55
1:A:112:TYR:CD1	1:A:115:LYS:O	2.60	0.55
1:D:134:PRO:HG3	1:D:151:GLU:CB	2.34	0.55
1:E:133:ARG:HD3	2:E:201:DND:C6A	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:VAL:O	1:A:132:LYS:CB	2.54	0.55
1:A:21:MET:SD	1:A:149:VAL:HG11	2.46	0.55
1:B:107:ALA:HB2	1:B:132:LYS:HA	1.88	0.55
1:B:163:PHE:CD2	1:B:181:VAL:HG11	2.42	0.55
1:B:167:LYS:O	1:B:169:THR:HG22	2.07	0.55
1:B:41:ILE:HG13	1:B:50:TYR:CZ	2.42	0.55
1:C:181:VAL:HG13	1:C:186:LEU:HB2	1.88	0.55
1:C:110:ILE:HA	1:C:113:LEU:HD13	1.88	0.55
1:C:160:ARG:HD3	1:C:187:TYR:CE1	2.41	0.55
1:C:40:GLN:NE2	1:C:77:MET:SD	2.80	0.55
1:D:67:ASN:HD22	1:D:68:PRO:N	2.05	0.55
1:D:78:GLU:O	1:D:79:ARG:CB	2.51	0.55
1:F:155:SER:O	1:F:158:MET:HB3	2.06	0.55
1:A:27:TYR:HE2	1:D:167:LYS:HE2	1.71	0.54
1:C:85:THR:O	1:C:89:VAL:HG23	2.07	0.54
1:E:59:MET:HB3	1:E:177:VAL:HG22	1.88	0.54
1:F:119:LEU:O	1:F:120:ASP:C	2.45	0.54
1:A:21:MET:SD	1:A:149:VAL:CG1	2.96	0.54
1:B:134:PRO:HG3	1:B:151:GLU:CB	2.36	0.54
1:C:133:ARG:HG3	1:C:134:PRO:N	2.21	0.54
1:C:43:PRO:HD2	1:C:44:HIS:CD2	2.42	0.54
1:F:21:MET:HE3	1:F:131:VAL:HB	1.89	0.54
1:E:134:PRO:HG3	1:E:151:GLU:CB	2.28	0.54
1:F:154:VAL:HA	1:F:158:MET:HE3	1.89	0.54
1:F:25:VAL:O	1:F:26:LEU:O	2.26	0.54
1:A:113:LEU:HD22	1:A:140:THR:HG21	1.88	0.54
1:B:178:LYS:O	1:B:182:GLU:HG3	2.08	0.54
1:E:131:VAL:HG13	1:E:149:VAL:HB	1.90	0.54
1:F:164:LYS:O	1:F:165:SER:CB	2.55	0.54
1:D:93:LYS:HD3	1:D:125:LEU:HD22	1.89	0.54
1:E:163:PHE:HZ	1:E:178:LYS:HG3	1.73	0.54
1:B:147:ALA:O	1:B:149:VAL:HG23	2.08	0.53
1:B:65:GLN:HG3	1:B:66:SER:N	2.23	0.53
1:C:131:VAL:CG1	1:C:149:VAL:HB	2.36	0.53
1:E:133:ARG:NH1	2:E:201:DND:N7A	2.56	0.53
1:E:153:GLU:OE2	1:F:151:GLU:HB2	2.08	0.53
1:B:168:PRO:C	1:B:169:THR:HG23	2.29	0.53
1:B:38:PRO:HG3	1:B:60:LEU:HD12	1.90	0.53
1:A:27:TYR:CE2	1:D:167:LYS:HE2	2.43	0.53
1:F:16:ASN:HA	1:F:19:LEU:HD12	1.90	0.53
1:F:55:HIS:O	1:F:59:MET:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LEU:O	1:B:91:LEU:HD12	2.09	0.53
1:B:157:THR:HG22	1:B:157:THR:O	2.08	0.53
1:C:10:THR:HG22	1:C:39:ASN:HD21	1.70	0.53
1:D:113:LEU:O	1:D:116:TRP:HB3	2.09	0.53
1:E:57:VAL:O	1:E:60:LEU:O	2.26	0.53
1:F:116:TRP:HB3	1:F:119:LEU:HD22	1.87	0.53
1:E:163:PHE:HE2	1:E:181:VAL:HG21	1.73	0.53
1:B:15:HIS:HB3	1:B:173:ILE:HG22	1.90	0.53
1:B:11:PHE:HB3	1:B:14:PRO:HG3	1.91	0.52
1:C:110:ILE:HG22	1:C:140:THR:HG23	1.91	0.52
1:E:19:LEU:HB3	1:F:171:TYR:CZ	2.44	0.52
1:A:164:LYS:O	1:A:165:SER:CB	2.57	0.52
1:A:67:ASN:ND2	1:A:69:SER:H	2.07	0.52
1:B:113:LEU:HD22	1:B:140:THR:HG21	1.90	0.52
1:A:168:PRO:C	1:A:169:THR:HG23	2.30	0.52
1:B:162:ARG:NH2	1:C:24:GLU:OE1	2.42	0.52
1:E:41:ILE:HG23	1:E:82:PRO:HA	1.90	0.52
1:D:12:ASP:OD1	1:D:51:THR:CG2	2.57	0.52
1:F:168:PRO:C	1:F:169:THR:CG2	2.77	0.52
1:F:167:LYS:HB3	1:F:168:PRO:HD2	1.92	0.52
1:B:155:SER:H	1:B:158:MET:HE3	1.74	0.52
1:C:16:ASN:ND2	1:C:172:LEU:C	2.63	0.52
1:E:109:MET:O	1:E:112:TYR:N	2.42	0.52
1:E:163:PHE:CZ	1:E:178:LYS:HG3	2.45	0.52
1:A:21:MET:HG2	2:A:601:DND:C2A	2.40	0.52
1:A:26:LEU:HD13	1:A:34:ILE:HG12	1.90	0.52
1:E:65:GLN:HG3	1:E:66:SER:H	1.71	0.52
1:F:82:PRO:CG	1:F:83:SER:N	2.70	0.52
1:C:162:ARG:HG3	1:C:167:LYS:HB2	1.92	0.52
1:B:67:ASN:HD22	1:B:68:PRO:N	2.08	0.52
1:C:164:LYS:O	1:C:165:SER:CB	2.58	0.52
1:E:131:VAL:CG1	1:E:149:VAL:HB	2.40	0.52
1:D:155:SER:O	1:D:158:MET:HB3	2.10	0.52
1:A:160:ARG:HD3	1:A:187:TYR:CE1	2.45	0.51
1:E:7:PHE:CE1	2:E:201:DND:H18	2.45	0.51
1:B:46:GLN:OE1	1:B:82:PRO:HG3	2.10	0.51
1:E:130:GLY:N	1:E:144:LEU:HD21	2.25	0.51
1:F:23:ASN:O	1:F:27:TYR:CD1	2.63	0.51
1:A:40:GLN:NE2	1:A:80:GLU:HA	2.25	0.51
1:B:67:ASN:HD22	1:B:68:PRO:CD	2.23	0.51
1:C:167:LYS:O	1:C:169:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:PRO:C	1:D:169:THR:HG23	2.30	0.51
1:D:75:VAL:HG13	1:D:76:GLU:N	2.24	0.51
1:A:155:SER:H	1:A:158:MET:HE3	1.76	0.51
1:D:132:LYS:HG3	1:D:132:LYS:O	2.11	0.51
1:F:168:PRO:C	1:F:169:THR:HG23	2.30	0.51
1:B:67:ASN:HD22	1:B:67:ASN:C	2.13	0.51
1:D:26:LEU:HD12	1:D:31:LEU:HB2	1.91	0.51
1:E:60:LEU:O	1:E:61:LYS:CB	2.58	0.51
1:D:105:ILE:HB	1:D:109:MET:HB2	1.93	0.51
1:C:109:MET:SD	1:C:116:TRP:HZ3	2.33	0.51
1:C:44:HIS:ND1	2:C:401:DND:H11	2.26	0.51
1:E:13:PRO:CD	1:E:156:SER:HB2	2.40	0.51
1:A:40:GLN:CA	1:A:77:MET:HE3	2.41	0.51
1:B:160:ARG:HD3	1:B:187:TYR:CE1	2.46	0.51
1:C:21:MET:O	1:C:25:VAL:HG23	2.10	0.51
1:E:168:PRO:C	1:E:169:THR:HG23	2.31	0.51
1:F:114:PRO:HD3	1:F:142:TYR:CE2	2.46	0.51
1:F:67:ASN:HD22	1:F:68:PRO:HD2	1.75	0.51
1:E:171:TYR:CZ	1:F:19:LEU:HB3	2.46	0.51
1:B:72:LEU:HD23	1:B:73:GLU:N	2.24	0.50
1:A:42:PRO:HB2	1:A:45:LYS:HG3	1.93	0.50
1:B:75:VAL:HG11	1:B:92:LEU:HD21	1.94	0.50
1:F:65:GLN:HG3	1:F:66:SER:N	2.25	0.50
1:B:33:GLU:OE1	1:B:71:LYS:HD2	2.11	0.50
1:D:13:PRO:HD2	1:D:156:SER:HB2	1.92	0.50
1:A:76:GLU:HG2	1:A:88:THR:OG1	2.12	0.50
1:B:113:LEU:N	1:B:114:PRO:HD2	2.27	0.50
1:E:86:PHE:CE1	1:E:125:LEU:HD11	2.46	0.50
1:B:72:LEU:CD2	1:B:73:GLU:N	2.74	0.50
1:F:114:PRO:HD3	1:F:142:TYR:CZ	2.46	0.50
1:B:19:LEU:HB3	1:C:171:TYR:CE2	2.45	0.50
1:D:10:THR:HG22	1:D:39:ASN:HD21	1.72	0.50
1:D:110:ILE:HG22	1:D:140:THR:HG23	1.92	0.50
1:A:106:GLY:O	1:A:107:ALA:C	2.48	0.50
1:A:168:PRO:C	1:A:169:THR:CG2	2.80	0.50
1:C:67:ASN:C	1:C:67:ASN:ND2	2.64	0.50
1:D:109:MET:CE	1:D:109:MET:HA	2.41	0.50
1:E:59:MET:O	1:E:62:LEU:CG	2.57	0.50
1:A:6:ILE:N	1:A:102:PHE:O	2.42	0.50
1:B:167:LYS:HE2	1:C:27:TYR:CE2	2.46	0.50
1:B:80:GLU:O	1:B:80:GLU:HG2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LYS:HG2	1:D:27:TYR:CE2	2.46	0.50
1:A:95:ARG:C	1:A:97:PRO:HD3	2.32	0.49
1:B:26:LEU:HD13	1:B:34:ILE:HG12	1.93	0.49
1:F:82:PRO:CG	1:F:83:SER:H	2.22	0.49
1:A:133:ARG:HH12	1:A:155:SER:CB	2.25	0.49
1:E:163:PHE:CE1	1:E:169:THR:HG21	2.47	0.49
1:F:23:ASN:O	1:F:27:TYR:CE1	2.65	0.49
1:B:67:ASN:HD22	1:B:68:PRO:HD2	1.77	0.49
1:C:25:VAL:HG11	1:C:104:ILE:HD13	1.94	0.49
1:C:44:HIS:CG	1:C:44:HIS:O	2.58	0.49
1:D:73:GLU:HG3	1:D:75:VAL:HG12	1.94	0.49
1:E:36:PHE:O	1:E:38:PRO:HD3	2.12	0.49
1:A:163:PHE:CE2	1:A:181:VAL:HG11	2.48	0.49
1:C:134:PRO:HG3	1:C:151:GLU:CG	2.42	0.49
1:F:175:ASP:O	1:F:179:LYS:HG3	2.12	0.49
1:B:117:TYR:OH	1:B:118:LYS:HE3	2.11	0.49
1:B:154:VAL:HA	1:B:158:MET:CE	2.43	0.49
1:B:168:PRO:C	1:B:169:THR:CG2	2.80	0.49
1:B:36:PHE:O	1:B:38:PRO:HD3	2.11	0.49
1:D:138:VAL:HG21	1:D:146:PHE:CZ	2.47	0.49
1:F:113:LEU:HD23	1:F:142:TYR:CD2	2.47	0.49
1:F:73:GLU:HG3	1:F:75:VAL:HG12	1.94	0.49
1:B:25:VAL:HG11	1:B:104:ILE:CD1	2.43	0.49
1:C:113:LEU:O	1:C:116:TRP:HB3	2.13	0.49
1:E:163:PHE:CD1	1:E:169:THR:HG21	2.48	0.49
1:E:2:LYS:HE2	1:E:33:GLU:CD	2.33	0.49
1:E:95:ARG:C	1:E:97:PRO:HD3	2.33	0.49
1:C:157:THR:O	1:C:157:THR:HG22	2.12	0.49
1:F:163:PHE:HE1	1:F:169:THR:HG21	1.75	0.49
1:A:25:VAL:HG11	1:A:104:ILE:CD1	2.43	0.49
1:B:105:ILE:CD1	1:B:110:ILE:HG12	2.43	0.49
1:E:164:LYS:O	1:E:165:SER:CB	2.61	0.49
1:F:115:LYS:O	1:F:115:LYS:HG3	2.13	0.49
1:C:131:VAL:HG12	1:C:132:LYS:N	2.28	0.48
1:C:163:PHE:CE1	1:C:169:THR:HG21	2.48	0.48
1:F:92:LEU:HA	1:F:95:ARG:HB2	1.93	0.48
1:A:19:LEU:HB3	1:D:171:TYR:CE2	2.48	0.48
1:D:101:LEU:O	1:D:126:ILE:HG13	2.13	0.48
1:E:168:PRO:HG3	1:F:27:TYR:CG	2.49	0.48
1:E:139:GLU:O	1:E:140:THR:O	2.32	0.48
1:F:92:LEU:C	1:F:94:GLN:N	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:GLU:HB3	1:B:180:TYR:CE1	2.48	0.48
1:C:162:ARG:HG3	1:C:167:LYS:CB	2.43	0.48
1:D:86:PHE:CD2	1:D:118:LYS:HD2	2.49	0.48
1:E:6:ILE:HD13	1:E:92:LEU:HD13	1.96	0.48
1:F:119:LEU:O	1:F:122:LEU:N	2.46	0.48
1:B:25:VAL:HG11	1:B:104:ILE:HD13	1.94	0.48
1:B:10:THR:CG2	1:B:39:ASN:ND2	2.59	0.48
1:E:15:HIS:HB3	1:E:173:ILE:HG22	1.94	0.48
1:F:167:LYS:O	1:F:169:THR:HG22	2.14	0.48
1:A:172:LEU:HD21	1:D:20:LEU:HD11	1.95	0.48
1:D:16:ASN:ND2	1:D:172:LEU:C	2.67	0.48
1:E:53:SER:HA	1:E:56:ARG:HD3	1.95	0.48
1:F:67:ASN:HD22	1:F:68:PRO:N	2.12	0.48
1:F:85:THR:O	1:F:86:PHE:C	2.52	0.48
1:B:131:VAL:O	1:B:132:LYS:CB	2.61	0.48
1:C:67:ASN:HD22	1:C:69:SER:H	1.62	0.48
1:E:109:MET:HG3	2:E:201:DND:H2	1.95	0.48
1:F:38:PRO:CG	1:F:60:LEU:HD12	2.35	0.48
1:A:133:ARG:HD3	2:A:601:DND:C6A	2.44	0.48
1:C:168:PRO:C	1:C:169:THR:CG2	2.82	0.48
1:B:38:PRO:HG3	1:B:60:LEU:CD1	2.43	0.47
1:D:21:MET:CG	1:D:131:VAL:HG11	2.42	0.47
1:F:113:LEU:HB3	1:F:114:PRO:HD3	1.87	0.47
1:F:21:MET:SD	2:F:190:DND:N3A	2.86	0.47
1:A:53:SER:HA	1:A:56:ARG:NH1	2.29	0.47
1:E:167:LYS:O	1:E:169:THR:CG2	2.62	0.47
1:B:91:LEU:O	1:B:92:LEU:O	2.32	0.47
1:C:162:ARG:C	1:C:164:LYS:H	2.18	0.47
1:C:181:VAL:HG13	1:C:186:LEU:CB	2.43	0.47
1:C:41:ILE:HG13	1:C:50:TYR:CZ	2.49	0.47
1:F:117:TYR:N	1:F:117:TYR:HD2	2.09	0.47
1:A:106:GLY:O	1:A:110:ILE:HG13	2.15	0.47
1:B:133:ARG:HH12	1:B:155:SER:CB	2.26	0.47
1:F:73:GLU:OE2	1:F:75:VAL:HB	2.14	0.47
1:B:115:LYS:O	1:B:116:TRP:HB2	2.14	0.47
1:A:138:VAL:CG2	1:A:139:GLU:N	2.77	0.47
1:A:72:LEU:HD23	1:A:73:GLU:H	1.80	0.47
1:F:13:PRO:HD2	1:F:156:SER:HB2	1.96	0.47
1:C:21:MET:HG3	1:C:131:VAL:HG21	1.96	0.47
1:D:162:ARG:HG3	1:D:167:LYS:CB	2.45	0.47
1:C:107:ALA:HB3	1:C:133:ARG:H	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:THR:O	1:D:161:GLU:HG3	2.14	0.47
2:D:301:DND:N3A	2:D:301:DND:H21	2.30	0.47
1:E:130:GLY:N	1:E:144:LEU:CD2	2.78	0.47
1:F:27:TYR:N	1:F:27:TYR:HD1	2.05	0.47
1:A:13:PRO:HD2	1:A:156:SER:HB2	1.97	0.47
1:A:162:ARG:HG3	1:A:167:LYS:CB	2.43	0.47
1:A:40:GLN:HG3	1:A:77:MET:CE	2.44	0.47
1:B:45:LYS:O	1:B:48:GLU:CB	2.62	0.47
1:E:131:VAL:O	1:E:132:LYS:HB3	2.15	0.46
1:A:163:PHE:HZ	1:A:178:LYS:HG3	1.79	0.46
1:F:64:ILE:HD12	1:F:70:PHE:HB2	1.97	0.46
1:B:136:PHE:CD1	1:B:136:PHE:N	2.82	0.46
1:B:91:LEU:O	1:B:94:GLN:HB2	2.15	0.46
1:C:164:LYS:HD3	1:C:164:LYS:C	2.36	0.46
1:C:55:HIS:ND1	1:C:186:LEU:HD21	2.31	0.46
1:A:105:ILE:HD12	1:A:110:ILE:HG12	1.96	0.46
1:A:163:PHE:CZ	1:A:178:LYS:HG3	2.50	0.46
1:C:117:TYR:OH	1:C:118:LYS:HE3	2.16	0.46
1:E:67:ASN:HD22	1:E:68:PRO:N	2.14	0.46
1:A:67:ASN:HD22	1:A:68:PRO:N	2.14	0.46
1:A:67:ASN:HD22	1:A:69:SER:H	1.64	0.46
1:B:2:LYS:CE	1:B:33:GLU:OE2	2.58	0.46
1:A:115:LYS:O	1:A:116:TRP:HB2	2.15	0.46
1:B:133:ARG:HG2	1:B:136:PHE:CD1	2.51	0.46
1:B:39:ASN:O	1:B:56:ARG:NH2	2.49	0.46
1:C:2:LYS:HE2	1:C:33:GLU:CD	2.35	0.46
1:D:7:PHE:CE1	2:D:301:DND:H18	2.51	0.46
1:D:38:PRO:CG	1:D:60:LEU:HD12	2.36	0.46
1:F:4:ILE:HD13	1:F:35:TRP:CH2	2.50	0.46
1:B:179:LYS:O	1:B:183:GLU:HG3	2.15	0.46
1:C:40:GLN:NE2	1:C:40:GLN:HA	2.20	0.46
1:D:36:PHE:O	1:D:38:PRO:HD3	2.16	0.46
1:D:79:ARG:HD2	1:D:79:ARG:O	2.16	0.46
1:E:162:ARG:HG3	1:E:167:LYS:CB	2.46	0.46
1:E:72:LEU:CD2	1:E:73:GLU:H	2.29	0.46
1:F:72:LEU:O	1:F:73:GLU:HB2	2.16	0.46
1:F:79:ARG:NH1	1:F:83:SER:OG	2.49	0.46
1:E:9:GLY:O	1:E:38:PRO:HA	2.16	0.46
1:F:114:PRO:C	1:F:116:TRP:N	2.67	0.46
1:A:20:LEU:O	1:A:24:GLU:HG2	2.15	0.46
1:A:67:ASN:HA	1:A:68:PRO:HD3	1.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LEU:HD22	1:B:146:PHE:CE1	2.51	0.46
1:B:52:ASP:O	1:B:53:SER:CB	2.64	0.46
1:A:15:HIS:HB3	1:A:173:ILE:HG22	1.97	0.46
1:A:50:TYR:O	1:A:51:THR:C	2.55	0.46
1:A:6:ILE:HD13	1:A:92:LEU:HD13	1.97	0.46
1:D:21:MET:SD	1:D:149:VAL:CG1	3.04	0.46
1:D:154:VAL:HA	1:D:158:MET:CE	2.45	0.46
1:D:163:PHE:O	1:D:164:LYS:HB2	2.16	0.46
1:A:73:GLU:OE2	1:A:75:VAL:N	2.47	0.45
1:E:2:LYS:HB3	1:E:99:ASP:OD1	2.17	0.45
1:A:7:PHE:CE1	2:A:601:DND:H18	2.52	0.45
1:A:117:TYR:N	2:A:601:DND:O8N	2.43	0.45
1:F:144:LEU:HD23	1:F:145:LEU:O	2.16	0.45
1:A:113:LEU:N	1:A:114:PRO:HD2	2.31	0.45
1:D:21:MET:HE3	1:D:149:VAL:CG1	2.46	0.45
1:B:171:TYR:CE2	1:C:19:LEU:HB3	2.51	0.45
1:D:144:LEU:HD22	1:D:146:PHE:CE1	2.52	0.45
1:A:133:ARG:HH12	1:A:155:SER:HB3	1.80	0.45
1:A:164:LYS:HE2	1:A:187:TYR:O	2.16	0.45
1:C:95:ARG:C	1:C:97:PRO:HD3	2.36	0.45
1:D:87:ASP:O	1:D:90:SER:HB2	2.16	0.45
1:A:133:ARG:NH1	1:A:155:SER:HB3	2.32	0.45
1:A:6:ILE:CD1	1:A:92:LEU:HD13	2.46	0.45
1:C:43:PRO:HG3	1:C:83:SER:O	2.17	0.45
1:D:56:ARG:O	1:D:60:LEU:HB2	2.17	0.45
1:D:170:ASP:O	1:D:171:TYR:HB2	2.16	0.45
1:D:21:MET:CE	1:D:131:VAL:HG11	2.47	0.45
1:D:54:PHE:O	1:D:58:GLU:HG2	2.17	0.45
1:D:133:ARG:HG2	1:D:136:PHE:CD1	2.51	0.45
1:D:162:ARG:HG3	1:D:167:LYS:HB2	1.99	0.45
1:E:62:LEU:HD13	1:E:176:LYS:HB2	1.99	0.45
1:E:72:LEU:HD23	1:E:73:GLU:H	1.81	0.45
1:F:86:PHE:CE2	1:F:118:LYS:HD2	2.52	0.45
1:E:6:ILE:HD11	1:E:92:LEU:HD13	1.99	0.45
1:B:65:GLN:HG3	1:B:66:SER:H	1.82	0.44
1:E:138:VAL:HG21	1:E:146:PHE:CZ	2.53	0.44
1:C:115:LYS:O	1:C:116:TRP:HB2	2.17	0.44
1:C:2:LYS:HE2	1:C:33:GLU:OE2	2.17	0.44
1:D:40:GLN:OE1	1:D:77:MET:HA	2.16	0.44
1:F:21:MET:O	1:F:25:VAL:HG23	2.18	0.44
1:A:21:MET:CE	1:A:131:VAL:HG11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:PHE:CE1	2:B:501:DND:H18	2.52	0.44
1:C:102:PHE:C	1:C:126:ILE:HD11	2.37	0.44
1:D:79:ARG:CD	1:D:79:ARG:O	2.65	0.44
1:E:67:ASN:C	1:E:67:ASN:HD22	2.19	0.44
1:F:34:ILE:O	1:F:70:PHE:O	2.36	0.44
1:A:181:VAL:HG13	1:A:186:LEU:HB2	1.99	0.44
1:B:130:GLY:N	1:B:144:LEU:HD21	2.33	0.44
1:B:92:LEU:O	1:B:93:LYS:C	2.55	0.44
1:E:162:ARG:NH2	1:F:24:GLU:OE1	2.51	0.44
1:F:162:ARG:C	1:F:164:LYS:H	2.21	0.44
1:F:40:GLN:NE2	1:F:82:PRO:O	2.50	0.44
1:C:75:VAL:HG13	1:C:76:GLU:N	2.32	0.44
1:A:16:ASN:O	1:A:17:GLY:C	2.55	0.44
1:A:22:ALA:HB1	1:A:34:ILE:HG21	1.99	0.44
1:D:95:ARG:C	1:D:97:PRO:HD3	2.38	0.44
1:F:26:LEU:HB3	1:F:27:TYR:HD1	1.81	0.44
1:A:149:VAL:O	1:A:150:PRO:C	2.54	0.44
1:A:75:VAL:HG11	1:A:92:LEU:HD21	2.00	0.44
1:C:25:VAL:HG11	1:C:104:ILE:CD1	2.48	0.44
1:E:113:LEU:N	1:E:114:PRO:HD2	2.33	0.44
1:E:170:ASP:O	1:E:171:TYR:HB2	2.18	0.44
1:F:86:PHE:CZ	1:F:118:LYS:HD2	2.53	0.44
1:F:157:THR:O	1:F:161:GLU:HG3	2.18	0.44
1:F:168:PRO:O	1:F:169:THR:CG2	2.60	0.44
1:B:16:ASN:ND2	1:B:172:LEU:C	2.71	0.44
1:C:133:ARG:HG2	1:C:136:PHE:CD1	2.53	0.44
1:D:58:GLU:HB3	1:D:180:TYR:CE1	2.52	0.44
1:F:24:GLU:CG	1:F:149:VAL:HG13	2.47	0.44
1:F:152:PHE:CD2	1:F:153:GLU:N	2.79	0.44
1:C:67:ASN:HA	1:C:68:PRO:HD3	1.81	0.43
1:E:159:ILE:O	1:E:163:PHE:N	2.35	0.43
1:F:119:LEU:HA	1:F:119:LEU:HD13	1.82	0.43
1:B:13:PRO:HD2	1:B:156:SER:HB2	1.99	0.43
1:E:108:ASP:OD1	1:E:109:MET:N	2.42	0.43
1:D:155:SER:H	1:D:158:MET:HE3	1.83	0.43
1:F:147:ALA:O	1:F:149:VAL:HG23	2.18	0.43
1:B:145:LEU:HA	1:B:145:LEU:HD23	1.87	0.43
1:C:6:ILE:N	1:C:102:PHE:O	2.48	0.43
1:D:67:ASN:ND2	1:D:67:ASN:C	2.68	0.43
1:F:159:ILE:HA	1:F:162:ARG:HB2	2.00	0.43
1:A:113:LEU:O	1:A:119:LEU:HD22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ILE:HD13	1:D:92:LEU:CD1	2.48	0.43
1:D:73:GLU:OE2	1:D:75:VAL:N	2.51	0.43
1:D:163:PHE:HE2	1:D:181:VAL:HG21	1.83	0.43
1:E:168:PRO:C	1:E:169:THR:CG2	2.86	0.43
1:C:113:LEU:N	1:C:114:PRO:HD2	2.34	0.43
1:C:166:LYS:HB3	1:C:166:LYS:HE3	1.80	0.43
1:C:93:LYS:HD3	1:C:125:LEU:HD22	2.01	0.43
1:D:92:LEU:C	1:D:94:GLN:H	2.22	0.43
1:E:64:ILE:O	1:E:64:ILE:HG13	2.19	0.43
1:C:76:GLU:HG2	1:C:88:THR:OG1	2.19	0.43
1:F:40:GLN:HE21	1:F:40:GLN:HB2	1.61	0.43
1:A:29:ALA:O	1:B:127:GLN:NE2	2.50	0.43
1:B:55:HIS:ND1	1:B:186:LEU:HD21	2.34	0.43
1:C:85:THR:HG22	1:C:89:VAL:HG23	2.01	0.43
1:D:41:ILE:HG13	1:D:50:TYR:CZ	2.54	0.43
1:E:7:PHE:HE1	2:E:201:DND:H19	1.84	0.43
1:F:120:ASP:N	1:F:120:ASP:OD1	2.51	0.43
1:F:58:GLU:HB3	1:F:180:TYR:CE1	2.54	0.43
1:A:77:MET:C	1:A:79:ARG:H	2.23	0.43
1:F:10:THR:O	1:F:11:PHE:C	2.57	0.43
1:F:114:PRO:CB	1:F:142:TYR:OH	2.67	0.43
1:B:40:GLN:CG	1:B:77:MET:HE2	2.47	0.42
1:C:109:MET:HA	1:C:109:MET:CE	2.49	0.42
1:D:9:GLY:N	2:D:301:DND:O3D	2.52	0.42
1:E:109:MET:CA	1:E:109:MET:HE2	2.38	0.42
1:E:79:ARG:O	1:E:80:GLU:HB2	2.18	0.42
1:A:80:GLU:HG3	1:A:80:GLU:H	1.63	0.42
1:B:112:TYR:CD1	1:B:115:LYS:O	2.72	0.42
1:C:10:THR:CG2	2:C:401:DND:O11	2.66	0.42
1:E:102:PHE:C	1:E:126:ILE:HD11	2.38	0.42
1:A:131:VAL:O	1:A:132:LYS:HB2	2.19	0.42
1:A:53:SER:HA	1:A:56:ARG:HH11	1.84	0.42
2:A:601:DND:N3A	2:A:601:DND:H21	2.35	0.42
1:B:168:PRO:C	1:B:170:ASP:H	2.23	0.42
1:B:66:SER:O	1:B:68:PRO:HD3	2.19	0.42
1:B:167:LYS:HE2	1:C:27:TYR:HE2	1.84	0.42
1:E:2:LYS:HE2	1:E:33:GLU:OE2	2.19	0.42
1:E:20:LEU:HD13	1:F:171:TYR:HB2	2.01	0.42
1:F:92:LEU:C	1:F:94:GLN:H	2.22	0.42
1:A:107:ALA:HB3	1:A:133:ARG:HB3	2.01	0.42
1:B:181:VAL:HG13	1:B:186:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ARG:NH1	2:D:301:DND:N7A	2.68	0.42
1:E:107:ALA:CB	1:E:133:ARG:H	2.32	0.42
1:F:113:LEU:HD12	1:F:116:TRP:CE3	2.55	0.42
1:A:163:PHE:HE2	1:A:181:VAL:HG21	1.85	0.42
1:C:163:PHE:CZ	1:C:178:LYS:HG3	2.54	0.42
1:E:133:ARG:HD3	2:E:201:DND:N6A	2.35	0.42
1:B:144:LEU:HD23	1:B:145:LEU:O	2.20	0.42
1:C:105:ILE:HB	1:C:109:MET:HB2	2.01	0.42
1:C:163:PHE:HZ	1:C:178:LYS:HG3	1.85	0.42
1:D:168:PRO:C	1:D:170:ASP:H	2.22	0.42
1:F:26:LEU:CD1	1:F:31:LEU:HB2	2.49	0.42
1:F:72:LEU:HD23	1:F:72:LEU:HA	1.90	0.42
1:A:58:GLU:HB3	1:A:180:TYR:CE1	2.54	0.42
1:B:168:PRO:O	1:B:169:THR:CG2	2.61	0.42
1:F:116:TRP:O	1:F:117:TYR:O	2.37	0.42
1:F:3:LYS:N	1:F:32:ASP:OD2	2.52	0.42
1:A:130:GLY:N	1:A:144:LEU:HD21	2.35	0.42
1:C:122:LEU:O	1:C:125:LEU:N	2.50	0.42
2:C:401:DND:H17	2:C:401:DND:H3	2.02	0.42
1:D:7:PHE:CE2	1:D:22:ALA:HB2	2.55	0.42
1:E:105:ILE:CD1	1:E:110:ILE:HG12	2.50	0.42
1:E:106:GLY:O	1:E:110:ILE:HG13	2.19	0.42
1:E:154:VAL:HA	1:E:158:MET:HE1	2.01	0.42
1:A:21:MET:SD	1:A:149:VAL:HG12	2.60	0.42
1:B:154:VAL:HA	1:B:158:MET:HE1	2.01	0.42
1:B:167:LYS:HB3	1:B:168:PRO:HD2	2.02	0.42
1:C:138:VAL:HG21	1:C:146:PHE:CZ	2.55	0.42
1:F:105:ILE:HA	2:F:190:DND:H19	2.01	0.42
1:F:26:LEU:O	1:F:29:ALA:N	2.42	0.42
1:B:21:MET:CG	1:B:131:VAL:HG11	2.42	0.42
1:B:149:VAL:O	1:B:150:PRO:C	2.58	0.42
1:B:20:LEU:O	1:B:24:GLU:HG2	2.20	0.42
1:D:44:HIS:CD2	2:D:301:DND:H11	2.55	0.42
1:A:100:GLN:HG3	1:B:100:GLN:HG3	2.02	0.41
1:B:163:PHE:CD1	1:B:169:THR:HG21	2.55	0.41
1:B:96:TYR:N	1:B:97:PRO:HD3	2.35	0.41
1:B:2:LYS:HB3	1:B:99:ASP:OD1	2.20	0.41
1:D:107:ALA:HB3	1:D:133:ARG:H	1.85	0.41
1:D:12:ASP:CG	1:D:51:THR:HG23	2.40	0.41
1:E:102:PHE:CA	1:E:126:ILE:HD11	2.50	0.41
1:A:133:ARG:NH1	2:A:601:DND:N7A	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:TYR:N	1:A:97:PRO:HD3	2.34	0.41
1:D:164:LYS:O	1:D:165:SER:CB	2.66	0.41
1:D:44:HIS:ND1	1:D:44:HIS:N	2.67	0.41
1:F:113:LEU:CB	1:F:114:PRO:HD2	2.01	0.41
1:E:24:GLU:HG3	1:E:149:VAL:HG13	2.01	0.41
1:B:131:VAL:CG1	1:B:149:VAL:HB	2.50	0.41
1:C:138:VAL:HG21	1:C:146:PHE:CE1	2.55	0.41
1:D:21:MET:HE3	1:D:131:VAL:CG1	2.50	0.41
1:F:21:MET:HE2	1:F:131:VAL:HG21	2.02	0.41
2:F:190:DND:H3	2:F:190:DND:H17	2.02	0.41
1:A:79:ARG:HA	1:A:79:ARG:HD2	1.76	0.41
1:B:4:ILE:CG2	1:B:5:GLY:N	2.84	0.41
1:D:133:ARG:HG3	1:D:134:PRO:N	2.35	0.41
1:E:117:TYR:O	1:E:118:LYS:HB2	2.21	0.41
1:B:131:VAL:HG13	1:B:149:VAL:CB	2.51	0.41
1:B:4:ILE:HG22	1:B:5:GLY:N	2.36	0.41
1:B:9:GLY:HA3	2:B:501:DND:H16	2.03	0.41
1:F:16:ASN:ND2	1:F:172:LEU:C	2.74	0.41
1:F:85:THR:HB	1:F:86:PHE:H	1.57	0.41
1:B:51:THR:O	1:B:53:SER:N	2.54	0.41
1:D:173:ILE:O	1:D:174:PRO:C	2.59	0.41
1:E:25:VAL:HG11	1:E:104:ILE:CD1	2.51	0.41
1:F:53:SER:HA	1:F:56:ARG:HD3	2.01	0.41
1:F:91:LEU:O	1:F:95:ARG:N	2.52	0.41
1:C:161:GLU:O	1:C:164:LYS:O	2.38	0.41
1:E:26:LEU:HD12	1:E:31:LEU:HB2	2.03	0.41
1:A:159:ILE:H	1:A:159:ILE:HG12	1.68	0.41
1:A:180:TYR:C	1:A:180:TYR:CD2	2.95	0.41
1:D:181:VAL:HG13	1:D:186:LEU:HB2	2.02	0.41
1:E:21:MET:CG	1:E:131:VAL:HG11	2.47	0.41
1:E:16:ASN:O	1:E:17:GLY:C	2.59	0.41
1:F:26:LEU:HD23	1:F:27:TYR:CE1	2.55	0.41
1:F:65:GLN:HG3	1:F:66:SER:H	1.85	0.41
1:B:40:GLN:HE22	1:B:80:GLU:H	1.67	0.41
1:C:40:GLN:CA	1:C:40:GLN:HE21	2.12	0.41
1:C:78:GLU:CD	1:C:95:ARG:HH22	2.22	0.41
1:D:168:PRO:O	1:D:170:ASP:N	2.54	0.41
1:D:179:LYS:O	1:D:180:TYR:C	2.58	0.41
1:E:138:VAL:O	1:E:139:GLU:CG	2.69	0.41
1:E:41:ILE:CG2	1:E:81:GLY:O	2.69	0.41
1:C:156:SER:C	1:C:158:MET:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:GLU:OE2	1:C:75:VAL:N	2.53	0.41
1:E:162:ARG:HH21	1:F:24:GLU:CD	2.25	0.41
1:F:84:TYR:CE1	1:F:117:TYR:CD1	3.09	0.41
1:F:40:GLN:NE2	1:F:76:GLU:O	2.54	0.41
1:C:39:ASN:O	1:C:56:ARG:NH2	2.51	0.40
1:C:67:ASN:HD22	1:C:68:PRO:CD	2.33	0.40
1:D:154:VAL:HA	1:D:158:MET:HE3	2.03	0.40
1:C:170:ASP:OD2	1:C:178:LYS:NZ	2.53	0.40
1:B:141:PRO:CA	1:D:167:LYS:HE3	2.49	0.40
1:E:102:PHE:N	1:E:126:ILE:HD11	2.36	0.40
1:E:138:VAL:O	1:E:139:GLU:HG3	2.21	0.40
1:E:78:GLU:OE2	1:E:95:ARG:NH2	2.41	0.40
1:F:170:ASP:OD2	1:F:178:LYS:NZ	2.55	0.40
1:B:157:THR:O	1:B:161:GLU:HG3	2.21	0.40
1:B:41:ILE:HA	1:B:42:PRO:HD3	1.91	0.40
1:A:112:TYR:O	1:A:113:LEU:C	2.58	0.40
1:B:113:LEU:O	1:B:116:TRP:HB3	2.22	0.40
1:D:163:PHE:CE1	1:D:169:THR:HG21	2.57	0.40
1:E:25:VAL:HG11	1:E:104:ILE:HD13	2.03	0.40
1:E:79:ARG:NH2	1:E:88:THR:OG1	2.54	0.40
1:F:96:TYR:N	1:F:97:PRO:HD3	2.35	0.40
1:A:4:ILE:HG21	1:A:35:TRP:CD2	2.56	0.40
1:B:107:ALA:O	1:B:110:ILE:HB	2.21	0.40
1:C:112:TYR:O	1:C:113:LEU:C	2.60	0.40
1:C:90:SER:O	1:C:91:LEU:C	2.59	0.40
1:D:41:ILE:HG23	1:D:41:ILE:O	2.22	0.40
1:E:115:LYS:O	1:E:116:TRP:HB2	2.21	0.40
1:E:157:THR:O	1:E:157:THR:CG2	2.69	0.40
1:E:164:LYS:O	1:E:165:SER:HB2	2.21	0.40
1:E:181:VAL:HG13	1:E:186:LEU:HB2	2.04	0.40
1:F:18:HIS:O	1:F:21:MET:HB2	2.21	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	184/194 (95%)	139 (76%)	31 (17%)	14 (8%)	1	7
1	B	184/194 (95%)	145 (79%)	18 (10%)	21 (11%)	0	2
1	C	184/194 (95%)	151 (82%)	19 (10%)	14 (8%)	1	7
1	D	184/194 (95%)	144 (78%)	27 (15%)	13 (7%)	1	8
1	E	172/194 (89%)	142 (83%)	21 (12%)	9 (5%)	2	15
1	F	161/194 (83%)	111 (69%)	24 (15%)	26 (16%)	0	0
All	All	1069/1164 (92%)	832 (78%)	140 (13%)	97 (9%)	1	3

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	51	THR
1	A	52	ASP
1	A	79	ARG
1	A	80	GLU
1	A	132	LYS
1	A	139	GLU
1	A	140	THR
1	A	165	SER
1	B	49	ASP
1	B	52	ASP
1	B	54	PHE
1	B	80	GLU
1	B	93	LYS
1	B	140	THR
1	B	164	LYS
1	B	165	SER
1	B	186	LEU
1	C	45	LYS
1	C	50	TYR
1	C	52	ASP
1	C	80	GLU
1	C	132	LYS
1	C	140	THR
1	C	165	SER
1	D	50	TYR
1	D	52	ASP

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Mol	Chain	Res	Type
1	D	79	ARG
1	D	132	LYS
1	D	140	THR
1	D	164	LYS
1	D	165	SER
1	E	132	LYS
1	E	140	THR
1	E	165	SER
1	F	26	LEU
1	F	73	GLU
1	F	82	PRO
1	F	83	SER
1	F	85	THR
1	F	86	PHE
1	F	113	LEU
1	F	114	PRO
1	F	116	TRP
1	F	120	ASP
1	F	140	THR
1	F	165	SER
1	B	56	ARG
1	B	92	LEU
1	B	132	LYS
1	B	139	GLU
1	B	163	PHE
1	C	139	GLU
1	D	139	GLU
1	E	61	LYS
1	E	80	GLU
1	F	117	TYR
1	F	139	GLU
1	F	150	PRO
1	F	163	PHE
1	A	108	ASP
1	B	85	THR
1	C	164	LYS
1	D	80	GLU
1	D	166	LYS
1	E	166	LYS
1	F	27	TYR
1	F	72	LEU
1	F	78	GLU

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Mol	Chain	Res	Type
1	A	168	PRO
1	B	45	LYS
1	B	108	ASP
1	B	166	LYS
1	C	90	SER
1	C	163	PHE
1	C	168	PRO
1	D	169	THR
1	E	168	PRO
1	F	39	ASN
1	F	71	LYS
1	F	119	LEU
1	A	116	TRP
1	A	163	PHE
1	B	11	PHE
1	B	116	TRP
1	B	168	PRO
1	D	163	PHE
1	D	168	PRO
1	F	11	PHE
1	F	70	PHE
1	F	168	PRO
1	A	166	LYS
1	C	116	TRP
1	C	169	THR
1	E	139	GLU
1	F	166	LYS
1	E	141	PRO

### 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	171/177 (97%)	149 (87%)	22 (13%)	4	19
1	B	171/177 (97%)	149 (87%)	22 (13%)	4	19
1	C	171/177 (97%)	148 (86%)	23 (14%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	171/177 (97%)	147 (86%)	24 (14%)	3	16
1	E	161/177 (91%)	143 (89%)	18 (11%)	6	25
1	F	154/177 (87%)	127 (82%)	27 (18%)	2	9
All	All	999/1062 (94%)	863 (86%)	136 (14%)	3	17

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PRO
1	A	21	MET
1	A	33	GLU
1	A	45	LYS
1	A	46	GLN
1	A	47	ASN
1	A	48	GLU
1	A	49	ASP
1	A	60	LEU
1	A	67	ASN
1	A	72	LEU
1	A	79	ARG
1	A	133	ARG
1	A	138	VAL
1	A	152	PHE
1	A	160	ARG
1	A	162	ARG
1	A	163	PHE
1	A	168	PRO
1	A	169	THR
1	A	175	ASP
1	A	184	ASN
1	B	13	PRO
1	B	21	MET
1	B	33	GLU
1	B	44	HIS
1	B	47	ASN
1	B	49	ASP
1	B	60	LEU
1	B	66	SER
1	B	67	ASN
1	B	72	LEU
1	B	77	MET

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Mol	Chain	Res	Type
1	B	80	GLU
1	B	83	SER
1	B	138	VAL
1	B	152	PHE
1	B	160	ARG
1	B	162	ARG
1	B	163	PHE
1	B	166	LYS
1	B	168	PRO
1	B	169	THR
1	B	184	ASN
1	C	10	THR
1	C	33	GLU
1	C	40	GLN
1	C	44	HIS
1	C	46	GLN
1	C	49	ASP
1	C	60	LEU
1	C	67	ASN
1	C	72	LEU
1	C	79	ARG
1	C	133	ARG
1	C	138	VAL
1	C	150	PRO
1	C	151	GLU
1	C	152	PHE
1	C	160	ARG
1	C	162	ARG
1	C	163	PHE
1	C	166	LYS
1	C	168	PRO
1	C	169	THR
1	C	175	ASP
1	C	184	ASN
1	D	10	THR
1	D	21	MET
1	D	33	GLU
1	D	44	HIS
1	D	48	GLU
1	D	49	ASP
1	D	50	TYR
1	D	60	LEU

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Mol	Chain	Res	Type
1	D	67	ASN
1	D	72	LEU
1	D	78	GLU
1	D	79	ARG
1	D	133	ARG
1	D	141	PRO
1	D	148	ASP
1	D	152	PHE
1	D	160	ARG
1	D	162	ARG
1	D	163	PHE
1	D	166	LYS
1	D	168	PRO
1	D	169	THR
1	D	175	ASP
1	D	184	ASN
1	E	21	MET
1	E	33	GLU
1	E	60	LEU
1	E	65	GLN
1	E	67	ASN
1	E	72	LEU
1	E	77	MET
1	E	133	ARG
1	E	138	VAL
1	E	152	PHE
1	E	160	ARG
1	E	162	ARG
1	E	163	PHE
1	E	166	LYS
1	E	168	PRO
1	E	169	THR
1	E	175	ASP
1	E	184	ASN
1	F	10	THR
1	F	21	MET
1	F	27	TYR
1	F	33	GLU
1	F	40	GLN
1	F	41	ILE
1	F	60	LEU
1	F	67	ASN

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Mol	Chain	Res	Type
1	F	71	LYS
1	F	76	GLU
1	F	77	MET
1	F	79	ARG
1	F	83	SER
1	F	112	TYR
1	F	115	LYS
1	F	117	TYR
1	F	119	LEU
1	F	120	ASP
1	F	148	ASP
1	F	151	GLU
1	F	152	PHE
1	F	162	ARG
1	F	163	PHE
1	F	166	LYS
1	F	168	PRO
1	F	169	THR
1	F	184	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	28	GLN
1	A	39	ASN
1	A	46	GLN
1	A	67	ASN
1	A	184	ASN
1	B	16	ASN
1	B	23	ASN
1	B	28	GLN
1	B	39	ASN
1	B	67	ASN
1	B	94	GLN
1	B	184	ASN
1	C	16	ASN
1	C	28	GLN
1	C	39	ASN
1	C	40	GLN
1	C	44	HIS
1	C	46	GLN

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Mol	Chain	Res	Type
1	C	55	HIS
1	C	67	ASN
1	C	100	GLN
1	C	137	HIS
1	D	16	ASN
1	D	39	ASN
1	D	67	ASN
1	E	16	ASN
1	E	39	ASN
1	E	67	ASN
1	E	184	ASN
1	F	16	ASN
1	F	40	GLN
1	F	55	HIS
1	F	67	ASN
1	F	184	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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	501	-	40,48,48	1.13	3 (7%)	47,73,73	1.21	4 (8%)
2	DND	A	601	-	40,48,48	1.11	3 (7%)	47,73,73	1.23	5 (10%)
2	DND	E	201	-	40,48,48	1.09	2 (5%)	47,73,73	1.36	6 (12%)
2	DND	D	301	-	40,48,48	1.11	4 (10%)	47,73,73	1.31	5 (10%)
2	DND	C	401	-	40,48,48	1.14	3 (7%)	47,73,73	1.33	5 (10%)
2	DND	F	190	-	40,48,48	1.00	1 (2%)	47,73,73	1.40	6 (12%)

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	501	-	3/3/11/11	9/22/62/62	0/5/5/5
2	DND	A	601	-	3/3/11/11	10/22/62/62	0/5/5/5
2	DND	E	201	-	3/3/11/11	10/22/62/62	0/5/5/5
2	DND	D	301	-	3/3/11/11	9/22/62/62	0/5/5/5
2	DND	C	401	-	3/3/11/11	8/22/62/62	0/5/5/5
2	DND	F	190	-	3/3/11/11	8/22/62/62	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	DND	C2A-N3A	3.58	1.37	1.32
2	B	501	DND	C2N-N1N	3.47	1.39	1.35
2	E	201	DND	C2N-N1N	3.22	1.38	1.35
2	F	190	DND	C2A-N3A	3.09	1.37	1.32
2	D	301	DND	C2N-N1N	3.07	1.38	1.35
2	A	601	DND	C2A-N3A	2.76	1.36	1.32
2	C	401	DND	C2N-N1N	2.75	1.38	1.35
2	A	601	DND	C2N-N1N	2.64	1.38	1.35
2	D	301	DND	C2A-N3A	2.61	1.36	1.32
2	B	501	DND	C2A-N3A	2.52	1.36	1.32
2	E	201	DND	C2A-N3A	2.41	1.36	1.32
2	D	301	DND	C2A-N1A	2.20	1.38	1.33
2	C	401	DND	C2A-N1A	2.13	1.37	1.33
2	B	501	DND	C6A-C5A	-2.11	1.35	1.43
2	A	601	DND	O4B-C4B	-2.09	1.40	1.45
2	D	301	DND	O4B-C4B	-2.06	1.40	1.45

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	DND	C6N-N1N-C2N	-5.57	116.89	121.97
2	E	201	DND	C6N-N1N-C2N	-5.46	117.00	121.97
2	D	301	DND	C6N-N1N-C2N	-5.08	117.34	121.97
2	F	190	DND	C6N-N1N-C2N	-5.03	117.39	121.97
2	A	601	DND	C6N-N1N-C2N	-4.91	117.50	121.97
2	B	501	DND	C6N-N1N-C2N	-4.41	117.95	121.97
2	E	201	DND	O4B-C1B-C2B	-3.48	101.83	106.93
2	F	190	DND	C3N-C2N-N1N	3.39	123.74	120.43
2	C	401	DND	C3N-C2N-N1N	3.38	123.73	120.43
2	D	301	DND	C3N-C2N-N1N	3.22	123.58	120.43
2	A	601	DND	C3N-C2N-N1N	3.15	123.51	120.43
2	B	501	DND	N3A-C2A-N1A	-2.97	124.03	128.68
2	F	190	DND	O4B-C1B-C2B	-2.96	102.60	106.93
2	B	501	DND	O4B-C1B-C2B	-2.93	102.64	106.93
2	C	401	DND	N3A-C2A-N1A	-2.92	124.12	128.68
2	F	190	DND	N3A-C2A-N1A	-2.89	124.15	128.68
2	D	301	DND	N3A-C2A-N1A	-2.86	124.21	128.68
2	E	201	DND	C3N-C2N-N1N	2.86	123.22	120.43
2	A	601	DND	N3A-C2A-N1A	-2.73	124.41	128.68
2	B	501	DND	C3N-C2N-N1N	2.67	123.03	120.43
2	F	190	DND	C3D-C2D-C1D	2.62	104.92	100.98
2	C	401	DND	O4B-C1B-C2B	-2.56	103.19	106.93
2	E	201	DND	N3A-C2A-N1A	-2.52	124.73	128.68
2	D	301	DND	C3D-C2D-C1D	2.51	104.76	100.98
2	E	201	DND	C3D-C2D-C1D	2.29	104.42	100.98
2	F	190	DND	C3B-C2B-C1B	2.20	104.29	100.98
2	D	301	DND	O4B-C1B-C2B	-2.10	103.86	106.93
2	A	601	DND	C3D-C2D-C1D	2.03	104.04	100.98
2	E	201	DND	C5N-C6N-N1N	2.02	123.31	120.40
2	C	401	DND	C3D-C2D-C1D	2.01	104.00	100.98
2	A	601	DND	O4B-C1B-C2B	-2.01	103.99	106.93

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	501	DND	C1B
2	B	501	DND	C2B
2	B	501	DND	C3B
2	A	601	DND	C1B
2	A	601	DND	C2B
2	A	601	DND	C3B
2	E	201	DND	C1B

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Mol	Chain	Res	Type	Atom
2	E	201	DND	C2B
2	E	201	DND	C3B
2	D	301	DND	C1B
2	D	301	DND	C2B
2	D	301	DND	C3B
2	C	401	DND	C1B
2	C	401	DND	C2B
2	C	401	DND	C3B
2	F	190	DND	C1B
2	F	190	DND	C2B
2	F	190	DND	C3B

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	DND	C5D-O5D-PN-O11
2	B	501	DND	C5D-O5D-PN-O12
2	B	501	DND	C5D-O5D-PN-O3P
2	B	501	DND	C5B-O5B-PA-O3P
2	B	501	DND	C5B-O5B-PA-O14
2	B	501	DND	O4B-C4B-C5B-O5B
2	B	501	DND	C3B-C4B-C5B-O5B
2	A	601	DND	C5D-O5D-PN-O12
2	A	601	DND	C5D-O5D-PN-O3P
2	A	601	DND	C5B-O5B-PA-O3P
2	A	601	DND	C5B-O5B-PA-O13
2	A	601	DND	C5B-O5B-PA-O14
2	A	601	DND	O4B-C4B-C5B-O5B
2	A	601	DND	C3B-C4B-C5B-O5B
2	E	201	DND	C5D-O5D-PN-O11
2	E	201	DND	C5D-O5D-PN-O3P
2	E	201	DND	C5B-O5B-PA-O3P
2	E	201	DND	C5B-O5B-PA-O14
2	E	201	DND	O4B-C4B-C5B-O5B
2	E	201	DND	C3B-C4B-C5B-O5B
2	D	301	DND	C5D-O5D-PN-O11
2	D	301	DND	C5D-O5D-PN-O12
2	D	301	DND	C5D-O5D-PN-O3P
2	D	301	DND	C5B-O5B-PA-O3P
2	D	301	DND	C5B-O5B-PA-O13
2	D	301	DND	C5B-O5B-PA-O14
2	D	301	DND	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	D	301	DND	C3B-C4B-C5B-O5B
2	C	401	DND	C5D-O5D-PN-O11
2	C	401	DND	C5D-O5D-PN-O12
2	C	401	DND	C5D-O5D-PN-O3P
2	C	401	DND	C5B-O5B-PA-O3P
2	C	401	DND	O4B-C4B-C5B-O5B
2	C	401	DND	C3B-C4B-C5B-O5B
2	F	190	DND	C5D-O5D-PN-O11
2	F	190	DND	C5D-O5D-PN-O12
2	F	190	DND	C5D-O5D-PN-O3P
2	F	190	DND	C5B-O5B-PA-O3P
2	F	190	DND	C5B-O5B-PA-O14
2	F	190	DND	O4B-C4B-C5B-O5B
2	F	190	DND	C3B-C4B-C5B-O5B
2	A	601	DND	O4D-C4D-C5D-O5D
2	A	601	DND	C3D-C4D-C5D-O5D
2	B	501	DND	C5B-O5B-PA-O13
2	A	601	DND	C5D-O5D-PN-O11
2	E	201	DND	C5D-O5D-PN-O12
2	E	201	DND	C5B-O5B-PA-O13
2	C	401	DND	C5B-O5B-PA-O14
2	F	190	DND	C5B-O5B-PA-O13
2	E	201	DND	O4D-C4D-C5D-O5D
2	B	501	DND	O4D-C4D-C5D-O5D
2	D	301	DND	O4D-C4D-C5D-O5D
2	E	201	DND	C3D-C4D-C5D-O5D
2	C	401	DND	C5B-O5B-PA-O13

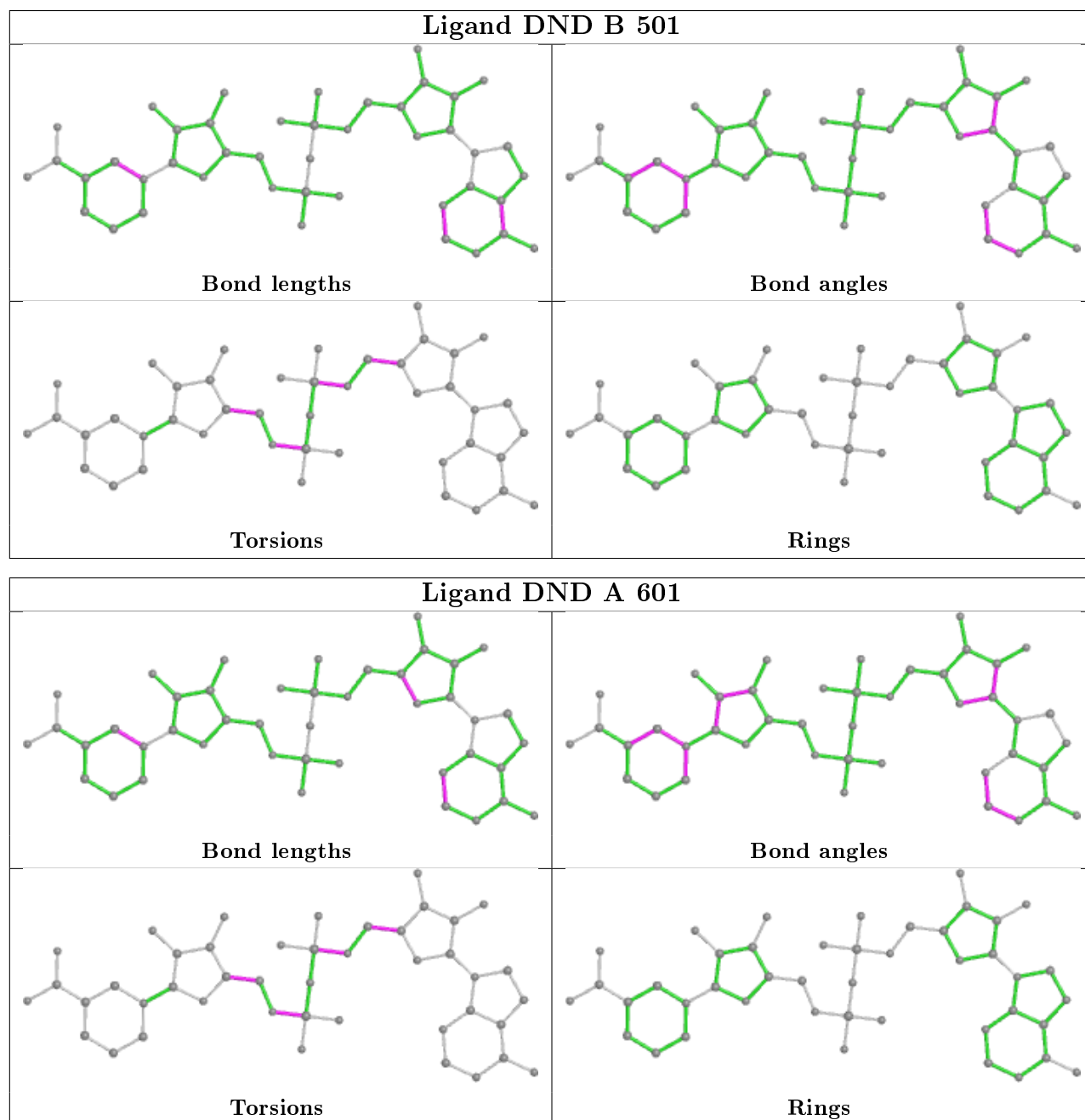
There are no ring outliers.

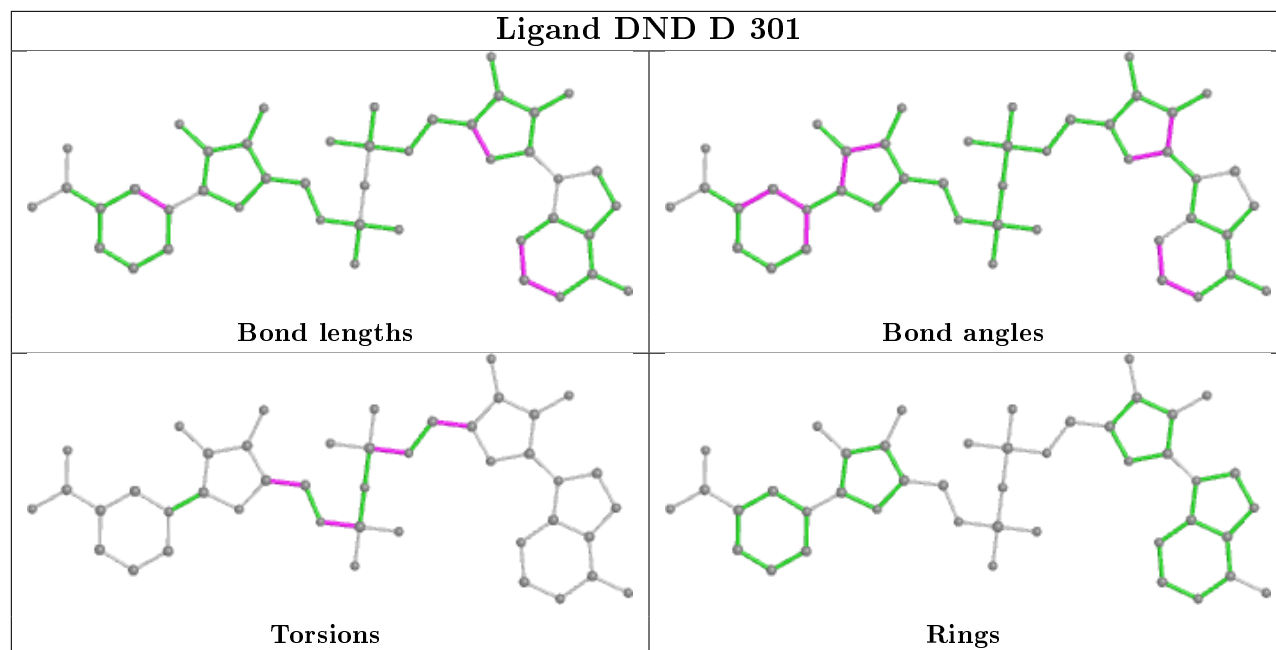
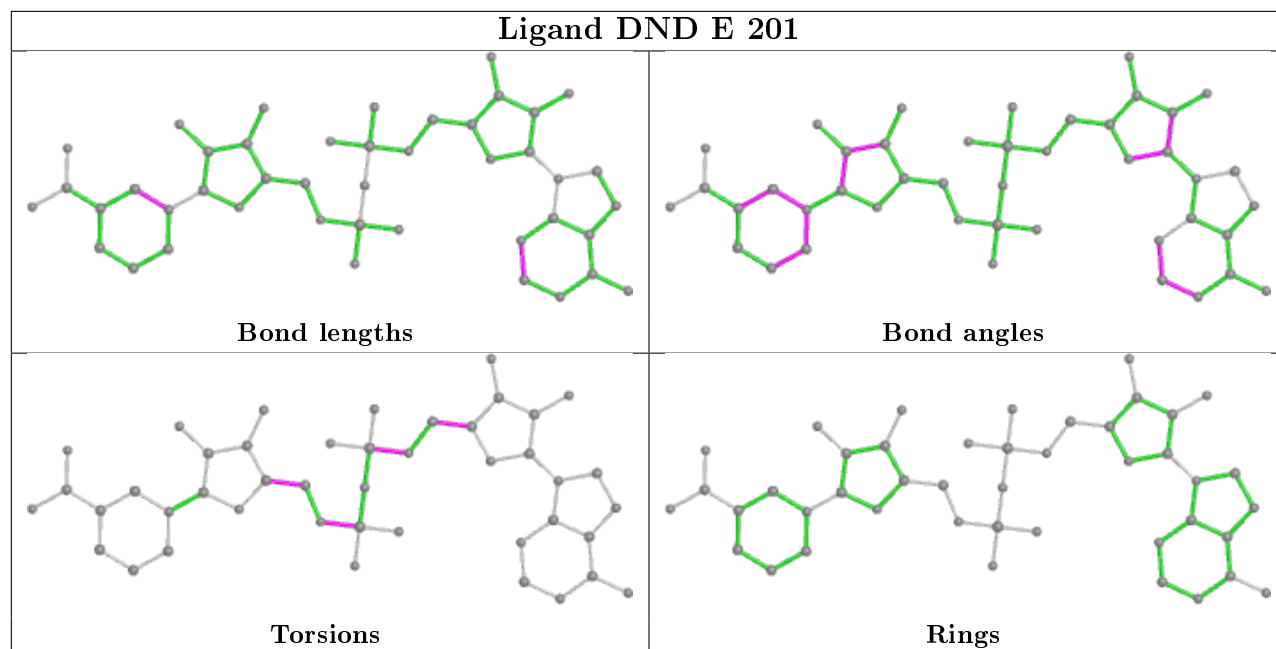
6 monomers are involved in 38 short contacts:

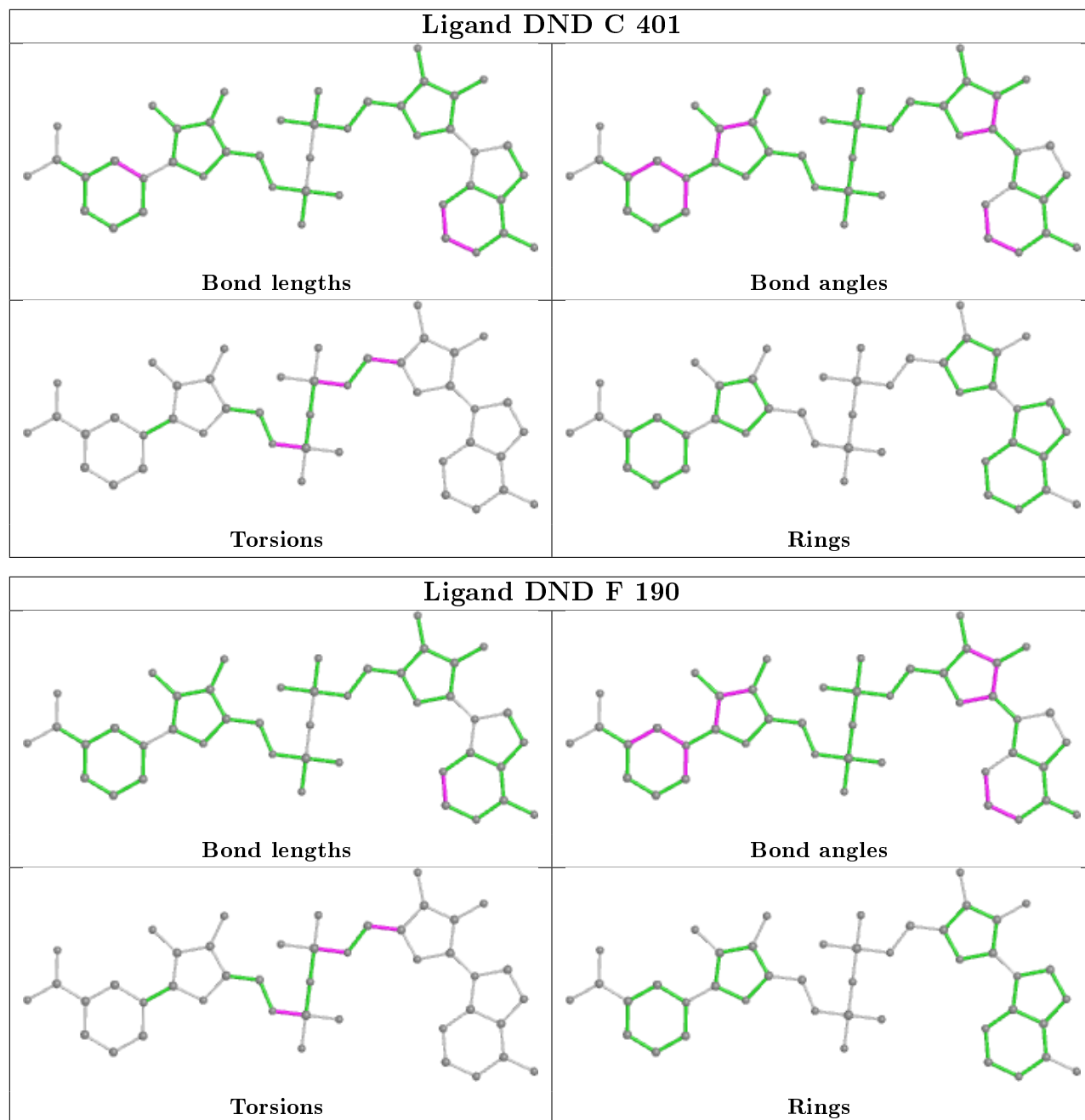
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	DND	4	0
2	A	601	DND	8	0
2	E	201	DND	9	0
2	D	301	DND	8	0
2	C	401	DND	4	0
2	F	190	DND	5	0

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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.