



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 10:45 PM UTC

PDB ID : 8JR0 / pdb_00008jr0
EMDB ID : EMD-36589
Title : Cryo-EM structure of Mycobacterium tuberculosis ATP synthase in complex with TBAJ-587
Authors : Zhang, Y.; Lai, Y.; Liu, F.; Rao, Z.; Gong, H.
Deposited on : 2023-06-15
Resolution : 2.80 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

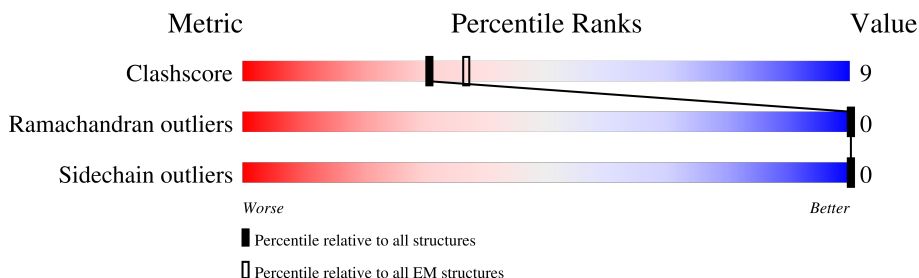
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	549	75% 19% 6%
1	B	549	74% 15% 11%
1	C	549	80% 17% .
2	D	486	81% 15% .
2	E	486	82% 15% .
2	F	486	81% 16% .
3	G	305	77% 17% 6%
4	H	121	71% 27% .
5	1	81	75% 25%

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Mol	Chain	Length	Quality of chain
5	2	81	 74%26%
5	3	81	 75%25%
5	4	81	 77%23%
5	5	81	 84%16%
5	6	81	 78%22%
5	7	81	 74%26%
5	8	81	 75%25%
5	9	81	 74%26%
6	a	250	 57%31%12%
7	b	171	 56%28%16%
8	d	446	 67%33%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 37460 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	517	Total	C	N	O	S	0	0
			3916	2449	684	772	11		
1	B	491	Total	C	N	O	S	0	0
			3740	2341	654	734	11		
1	C	530	Total	C	N	O	S	0	0
			4033	2529	701	792	11		

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	469	Total	C	N	O	S	0	0
			3614	2279	622	701	12		
2	E	469	Total	C	N	O	S	0	0
			3614	2279	622	701	12		
2	F	469	Total	C	N	O	S	0	0
			3614	2279	622	701	12		

- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	287	Total	C	N	O	S	0	0
			2251	1415	398	430	8		

- Molecule 4 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	119	Total	C	N	O	S	0	0
			906	562	162	181	1		

- Molecule 5 is a protein called ATP synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1	81	Total	C	N	O	S	0	0
			567	373	92	99	3		
5	2	81	Total	C	N	O	S	0	0
			567	373	92	99	3		
5	3	81	Total	C	N	O	S	0	0
			567	373	92	99	3		
5	4	81	Total	C	N	O	S	0	0
			567	373	92	99	3		
5	5	81	Total	C	N	O	S	0	0
			567	373	92	99	3		
5	6	81	Total	C	N	O	S	0	0
			567	373	92	99	3		
5	7	81	Total	C	N	O	S	0	0
			567	373	92	99	3		
5	8	81	Total	C	N	O	S	0	0
			567	373	92	99	3		
5	9	81	Total	C	N	O	S	0	0
			567	373	92	99	3		

- Molecule 6 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	a	220	Total	C	N	O	S	0	0
			1706	1145	269	286	6		

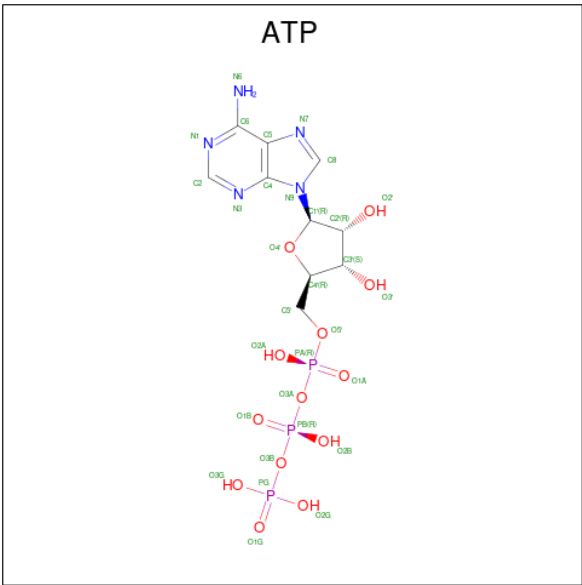
- Molecule 7 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	b	144	Total	C	N	O	S	0	0
			1107	691	201	212	3		

- Molecule 8 is a protein called Multifunctional fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	445	Total	C	N	O	S	0	0
			3424	2131	637	649	7		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

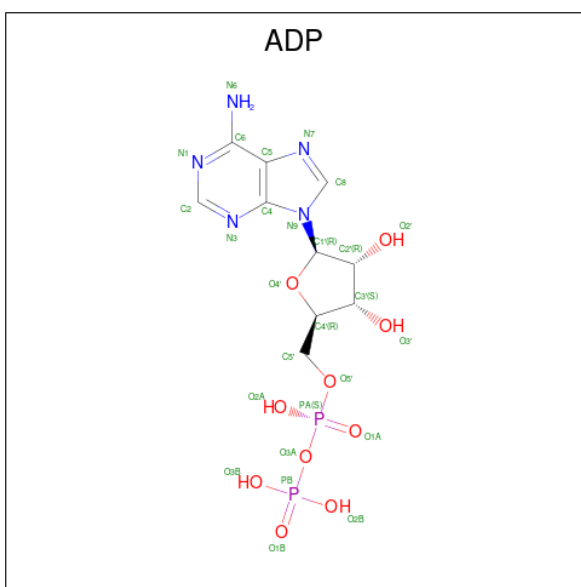


Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

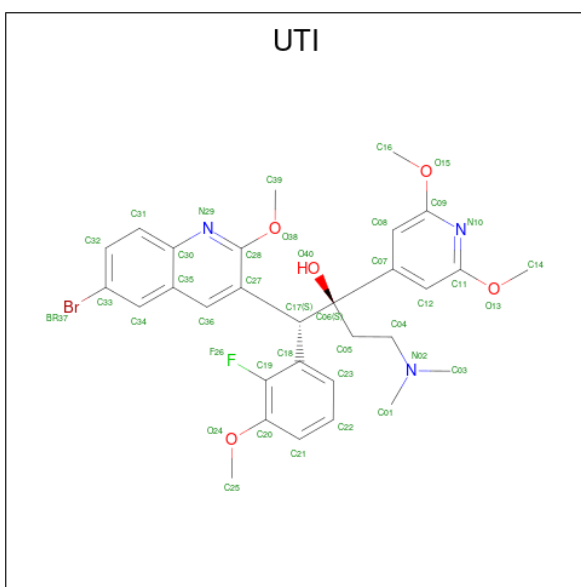
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	
10	B	1	Total	Mg	0
			1	1	
10	C	1	Total	Mg	0
			1	1	
10	D	1	Total	Mg	0
			1	1	
10	F	1	Total	Mg	0
			1	1	

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
11	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 12 is (1 {S},2 {S})-1-(6-bromanyl-2-methoxy-quinolin-3-yl)-2-(2,6-dimethoxypyridin-4-yl)-4-(dimethylamino)-1-(2-fluoranyl-3-methoxy-phenyl)butan-2-ol (CCD ID: UTI) (formula: $C_{30}H_{33}BrFN_3O_5$).

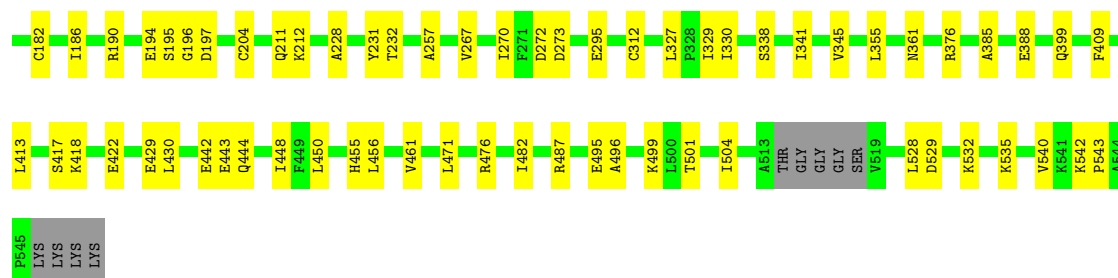


Mol	Chain	Residues	Atoms						AltConf
12	1	1	Total	Br	C	F	N	O	0
			40	1	30	1	3	5	

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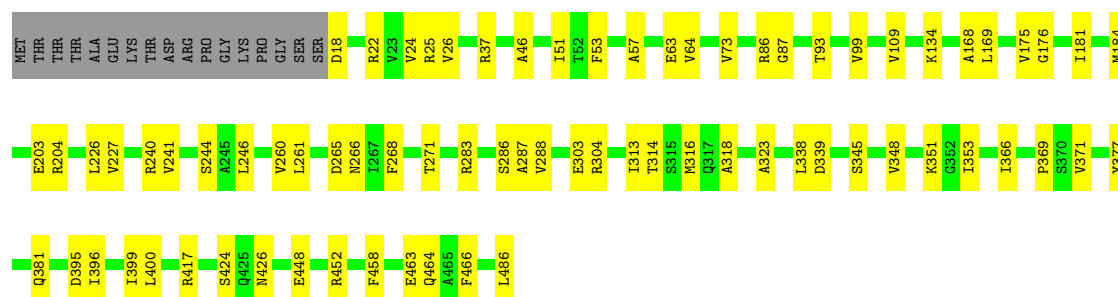
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Mol	Chain	Residues	Atoms						AltConf
12	4	1	Total 40	Br 1	C 30	F 1	N 3	O 5	0
12	5	1	Total 40	Br 1	C 30	F 1	N 3	O 5	0
12	6	1	Total 40	Br 1	C 30	F 1	N 3	O 5	0
12	7	1	Total 40	Br 1	C 30	F 1	N 3	O 5	0
12	8	1	Total 40	Br 1	C 30	F 1	N 3	O 5	0
12	9	1	Total 40	Br 1	C 30	F 1	N 3	O 5	0



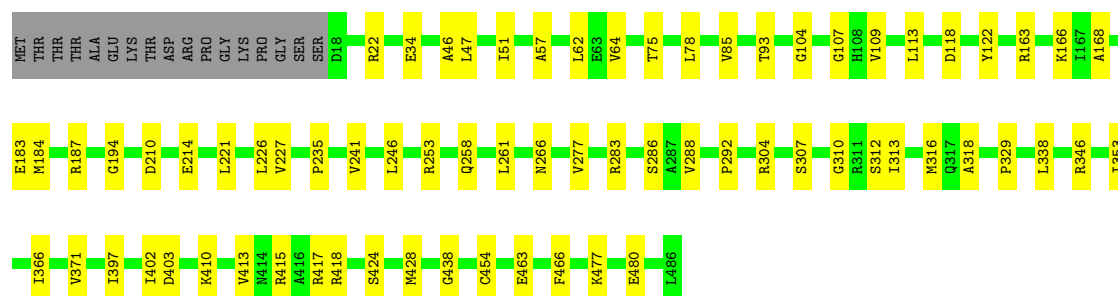
- Molecule 2: ATP synthase subunit beta

Chain D: 81% 15% .



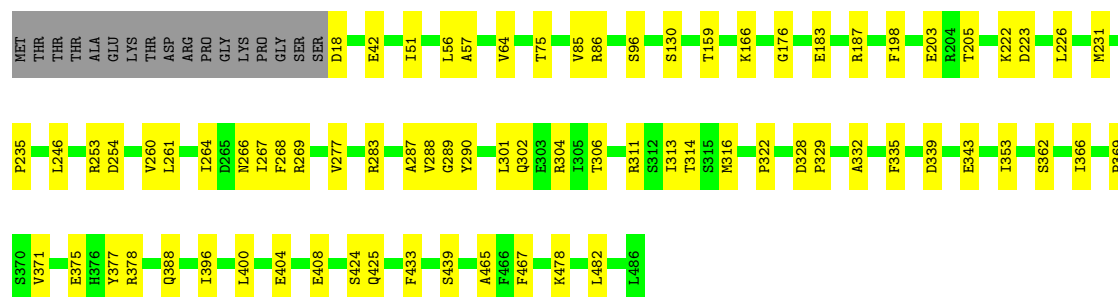
- Molecule 2: ATP synthase subunit beta

Chain E: 82% 15% .



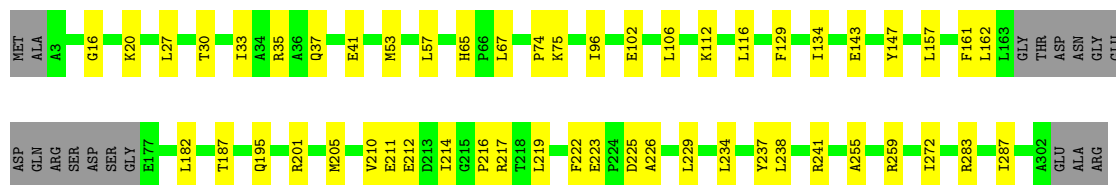
- Molecule 2: ATP synthase subunit beta

Chain F: 81% 16% .



- Molecule 3: ATP synthase gamma chain

Chain G:  77% 17% 6%



- Molecule 4: ATP synthase epsilon chain

Chain H:  71% 27% .



- Molecule 5: ATP synthase subunit c

Chain 1:  75% 25%



- Molecule 5: ATP synthase subunit c

Chain 2:  74% 26%



- Molecule 5: ATP synthase subunit c

Chain 3:  75% 25%



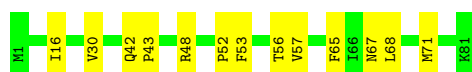
- Molecule 5: ATP synthase subunit c

Chain 4:  77% 23%



- Molecule 5: ATP synthase subunit c

Chain 5:  84% 16%



- Molecule 5: ATP synthase subunit c

Chain 6:  78% 22%



- Molecule 5: ATP synthase subunit c

Chain 7:  74% 26%



- Molecule 5: ATP synthase subunit c

Chain 8:  75% 25%



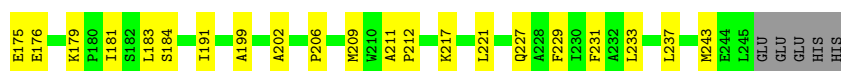
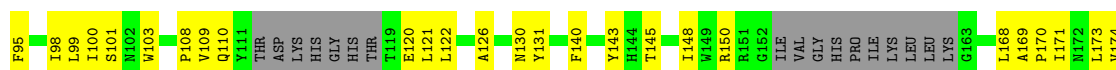
- Molecule 5: ATP synthase subunit c

Chain 9:  74% 26%



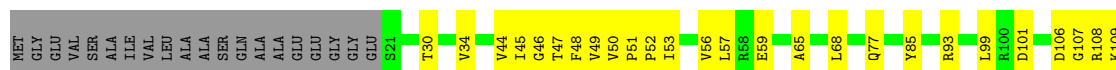
- Molecule 6: ATP synthase subunit a

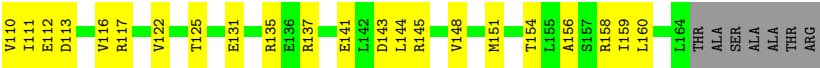
Chain a:  57% 31% 12%



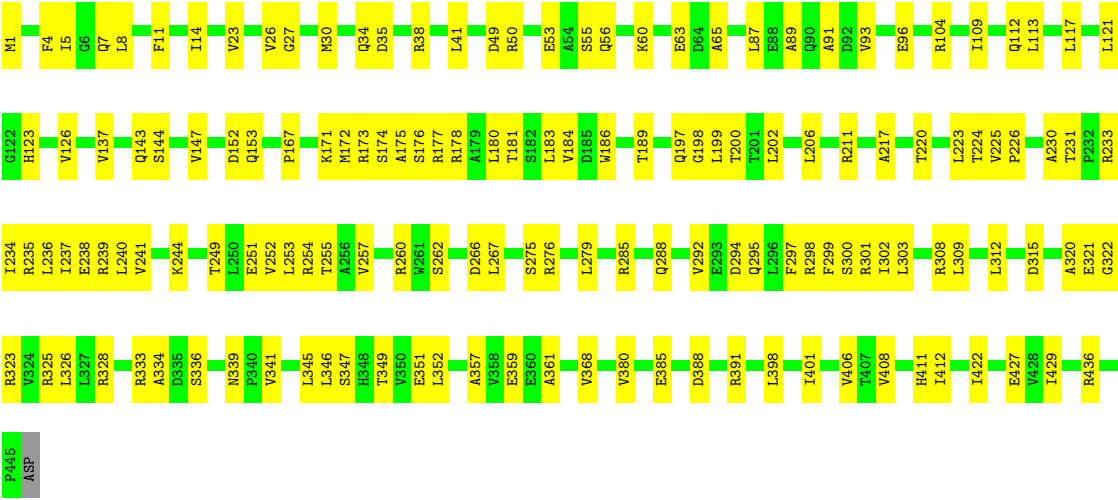
- Molecule 7: ATP synthase subunit b

Chain b:  56% 28% 16%





● Molecule 8: Multifunctional fusion protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81528	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, ADP, UTI

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	0.24	0/3976	0.38	0/5387
1	B	0.24	0/3795	0.38	0/5137
1	C	0.22	0/4094	0.36	0/5543
2	D	0.23	0/3680	0.36	0/4990
2	E	0.21	0/3680	0.34	0/4990
2	F	0.24	0/3680	0.36	0/4990
3	G	0.24	0/2286	0.40	0/3092
4	H	0.33	0/915	0.54	0/1237
5	1	0.25	0/578	0.44	0/784
5	2	0.26	0/578	0.46	0/784
5	3	0.28	0/578	0.47	0/784
5	4	0.29	0/578	0.44	0/784
5	5	0.28	0/578	0.44	0/784
5	6	0.26	0/578	0.44	0/784
5	7	0.25	0/578	0.43	0/784
5	8	0.27	0/578	0.49	0/784
5	9	0.24	0/578	0.41	0/784
6	a	0.24	0/1748	0.46	0/2390
7	b	0.24	0/1118	0.52	0/1512
8	d	0.27	0/3462	0.51	0/4697
All	All	0.24	0/37636	0.41	0/51021

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3916	0	3916	73	0
1	B	3740	0	3744	56	0
1	C	4033	0	4043	65	0
2	D	3614	0	3590	50	0
2	E	3614	0	3591	41	0
2	F	3614	0	3590	53	0
3	G	2251	0	2265	43	0
4	H	906	0	906	24	0
5	1	567	0	585	20	0
5	2	567	0	585	21	0
5	3	567	0	585	18	0
5	4	567	0	585	15	0
5	5	567	0	585	11	0
5	6	567	0	585	15	0
5	7	567	0	585	15	0
5	8	567	0	585	14	0
5	9	567	0	585	17	0
6	a	1706	0	1772	63	0
7	b	1107	0	1132	46	0
8	d	3424	0	3510	115	0
9	A	31	0	12	0	0
9	B	31	0	12	0	0
9	C	31	0	12	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
10	F	1	0	0	0	0
11	D	27	0	12	1	0
11	F	27	0	12	4	0
12	1	40	0	0	6	0
12	4	40	0	0	0	0
12	5	40	0	0	0	0
12	6	40	0	0	1	0
12	7	40	0	0	0	0
12	8	40	0	0	0	0
12	9	40	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	37460	0	37384	666	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 9.

All (666) 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)
3:G:214:ILE:HB	3:G:217:ARG:HB2	1.62	0.81
2:F:176:GLY:HA2	11:F:600:ADP:O1A	1.81	0.81
6:a:171:ILE:HD12	6:a:171:ILE:H	1.45	0.80
3:G:214:ILE:HD12	3:G:217:ARG:HG2	1.64	0.79
2:D:184:MET:HG3	2:D:316:MET:HE1	1.66	0.78
6:a:17:THR:HG22	6:a:26:ASN:HA	1.65	0.78
1:C:376:ARG:HA	11:D:600:ADP:O3'	1.84	0.77
1:C:535:LYS:HD2	3:G:201:ARG:HH11	1.49	0.77
5:7:17:MET:HG2	5:7:71:MET:HG3	1.67	0.76
6:a:89:PRO:HB3	7:b:50:VAL:HG21	1.66	0.76
5:2:17:MET:HG2	5:2:71:MET:HG3	1.67	0.75
7:b:50:VAL:HB	7:b:51:PRO:HD3	1.70	0.74
5:4:2:ASP:OD1	5:4:81:LYS:HE3	1.88	0.73
5:4:16:ILE:HG23	5:4:67:ASN:HD22	1.53	0.73
8:d:241:VAL:HA	8:d:244:LYS:HD3	1.69	0.73
5:1:17:MET:HG2	5:1:71:MET:HG3	1.69	0.72
5:8:17:MET:HG2	5:8:71:MET:HG3	1.72	0.72
1:A:167:ARG:HD3	1:A:309:LEU:O	1.88	0.72
1:A:257:ALA:HB1	1:A:267:VAL:HG11	1.70	0.72
1:B:450:LEU:HD21	1:B:471:LEU:HD23	1.71	0.71
2:F:176:GLY:CA	11:F:600:ADP:O1A	2.39	0.71
5:8:16:ILE:HG23	5:8:67:ASN:HD22	1.56	0.71
7:b:111:ILE:HG22	8:d:91:ALA:HB2	1.72	0.70
1:C:450:LEU:HD11	1:C:471:LEU:HD23	1.72	0.70
8:d:171:LYS:O	8:d:173:ARG:NH2	2.25	0.70
1:A:440:PRO:HG2	1:A:443:GLU:HG3	1.71	0.70
2:D:353:ILE:HG23	2:D:424:SER:HB3	1.74	0.69
3:G:195:GLN:OE1	3:G:259:ARG:NH2	2.26	0.69
6:a:183:LEU:HB3	6:a:231:PHE:HE1	1.57	0.69
7:b:137:ARG:HG3	8:d:113:LEU:HD21	1.75	0.69
8:d:225:VAL:HG22	8:d:233:ARG:HD3	1.74	0.68
5:4:17:MET:HG2	5:4:71:MET:HG3	1.74	0.68
1:B:479:GLU:HG3	1:B:503:VAL:HG21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:LYS:NZ	2:F:339:ASP:OD1	2.26	0.68
5:3:1:MET:HE3	5:3:2:ASP:H	1.59	0.68
2:E:168:ALA:HB2	2:E:338:LEU:HD13	1.75	0.68
8:d:294:ASP:OD1	8:d:298:ARG:NH1	2.27	0.68
2:F:267:ILE:HD11	2:F:301:LEU:HD21	1.74	0.67
2:E:353:ILE:HG23	2:E:424:SER:HB3	1.77	0.67
2:F:266:ASN:HB3	2:F:269:ARG:HG2	1.77	0.67
2:E:266:ASN:H	2:E:318:ALA:HB3	1.58	0.66
12:1:600:UTI:F26	6:a:170:PRO:HG2	1.85	0.66
6:a:57:PRO:O	8:d:34:GLN:NE2	2.25	0.66
2:F:203:GLU:OE2	2:F:266:ASN:ND2	2.27	0.66
1:B:117:PRO:HG3	1:B:124:VAL:HG23	1.77	0.66
1:B:294:ARG:NH2	2:F:328:ASP:OD1	2.29	0.66
2:F:400:LEU:HB3	2:F:404:GLU:HG3	1.78	0.66
1:A:24:ALA:O	8:d:436:ARG:NH2	2.29	0.66
1:C:442:GLU:OE1	1:C:487:ARG:NH1	2.29	0.65
2:F:235:PRO:HB2	2:F:277:VAL:HG23	1.78	0.65
8:d:197:GLN:HA	8:d:200:THR:HG22	1.78	0.65
1:B:104:ASP:OD1	1:B:203:ARG:NH1	2.29	0.65
2:F:166:LYS:NZ	2:F:302:GLN:O	2.29	0.65
4:H:52:ARG:NH2	4:H:54:GLU:OE2	2.29	0.64
1:C:540:VAL:HG12	1:C:542:LYS:H	1.62	0.64
1:C:173:ASP:O	1:C:178:LYS:NZ	2.31	0.64
5:3:24:ALA:HB2	5:3:64:TYR:HB2	1.79	0.64
2:E:402:ILE:O	2:E:410:LYS:NZ	2.30	0.64
7:b:137:ARG:HE	8:d:117:LEU:HD21	1.62	0.64
2:E:246:LEU:HD21	2:E:304:ARG:HB2	1.80	0.64
1:A:39:ASP:OD1	2:D:283:ARG:NH2	2.31	0.63
5:9:16:ILE:HG23	5:9:67:ASN:HD22	1.63	0.63
1:A:404:GLU:OE2	3:G:20:LYS:NZ	2.32	0.63
2:F:159:THR:HG21	2:F:362:SER:HB3	1.81	0.63
5:5:16:ILE:HG23	5:5:67:ASN:HD22	1.64	0.63
1:C:471:LEU:HD21	1:C:504:ILE:HG12	1.81	0.62
4:H:103:ASP:HB3	4:H:106:ILE:HG22	1.80	0.62
2:E:415:ARG:NH1	2:E:454:CYS:O	2.31	0.62
5:3:17:MET:HG2	5:3:71:MET:HG3	1.80	0.62
5:2:64:TYR:O	5:2:67:ASN:HB2	2.00	0.62
5:6:32:GLY:HA3	5:7:56:THR:HG21	1.82	0.62
2:D:266:ASN:H	2:D:318:ALA:HB3	1.63	0.61
2:E:210:ASP:O	2:E:214:GLU:HG3	2.00	0.61
5:6:43:PRO:HB3	5:7:48:ARG:NE	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:b:113:ASP:O	7:b:117:ARG:HG2	2.00	0.61
2:E:51:ILE:O	2:E:57:ALA:HA	2.01	0.61
1:A:412:ASP:OD1	3:G:35:ARG:NH2	2.33	0.61
5:1:48:ARG:CZ	5:9:43:PRO:HB3	2.31	0.61
3:G:223:GLU:HB3	4:H:29:VAL:HG11	1.82	0.61
6:a:110:GLN:HA	6:a:120:GLU:HB3	1.83	0.61
2:D:246:LEU:HD21	2:D:304:ARG:HB2	1.83	0.61
3:G:65:HIS:HE1	3:G:67:LEU:HD12	1.66	0.61
12:1:600:UTI:O38	6:a:171:ILE:HD11	2.00	0.60
1:B:211:GLN:HG3	1:B:272:ASP:OD2	2.00	0.60
1:A:7:PRO:HB2	1:A:10:ASP:HB3	1.83	0.60
3:G:216:PRO:HA	5:6:44:GLU:OE2	2.01	0.60
7:b:49:VAL:HG23	7:b:50:VAL:H	1.66	0.59
8:d:325:ARG:HA	8:d:328:ARG:HE	1.68	0.59
1:A:186:ILE:HD11	1:A:270:ILE:HD13	1.85	0.59
1:C:50:VAL:HG21	1:C:74:VAL:HG21	1.85	0.59
8:d:288:GLN:OE1	8:d:339:ASN:ND2	2.36	0.59
8:d:388:ASP:HA	8:d:391:ARG:HG3	1.83	0.59
8:d:325:ARG:HA	8:d:328:ARG:NE	2.18	0.59
1:A:142:ARG:NH2	1:A:310:GLU:O	2.34	0.58
6:a:169:ALA:O	6:a:173:LEU:N	2.35	0.58
8:d:391:ARG:HH11	8:d:408:VAL:HG23	1.69	0.58
1:B:396:ASP:OD2	1:B:423:ARG:NH1	2.36	0.58
5:1:63:ALA:O	5:1:67:ASN:ND2	2.35	0.58
5:9:17:MET:HG2	5:9:71:MET:HG3	1.84	0.58
1:C:429:GLU:HG3	1:C:461:VAL:HG13	1.83	0.58
1:B:5:THR:OG1	1:B:6:ILE:N	2.34	0.58
5:1:32:GLY:HA3	5:2:56:THR:HG21	1.84	0.58
6:a:33:THR:HG21	7:b:34:VAL:HG22	1.86	0.58
1:C:174:ARG:NH2	2:F:343:GLU:OE2	2.37	0.57
8:d:35:ASP:OD1	8:d:38:ARG:NH1	2.36	0.57
8:d:315:ASP:O	8:d:323:ARG:NH2	2.37	0.57
1:C:186:ILE:HD11	1:C:270:ILE:HD13	1.85	0.57
3:G:57:LEU:HD21	3:G:229:LEU:HB3	1.85	0.57
1:A:59:PRO:HG2	1:A:89:GLN:HB3	1.86	0.57
1:B:310:GLU:OE2	2:F:205:THR:OG1	2.20	0.57
2:F:246:LEU:HD21	2:F:304:ARG:HB2	1.86	0.57
8:d:152:ASP:OD1	8:d:153:GLN:N	2.37	0.57
2:F:353:ILE:HG23	2:F:424:SER:HB2	1.85	0.57
1:B:186:ILE:HD11	1:B:270:ILE:HD13	1.86	0.57
8:d:181:THR:HA	8:d:184:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:51:ILE:O	2:F:57:ALA:HA	2.05	0.56
6:a:145:THR:HA	6:a:148:ILE:HG12	1.87	0.56
1:A:451:GLY:HA2	1:A:456:LEU:HD12	1.87	0.56
1:B:13:SER:O	1:B:16:GLU:HG2	2.05	0.56
1:B:39:ASP:OD1	2:E:283:ARG:NH1	2.39	0.56
1:C:178:LYS:HG2	1:C:355:LEU:HD12	1.85	0.56
4:H:37:ARG:NH1	5:4:44:GLU:OE2	2.32	0.56
8:d:23:VAL:HA	8:d:26:VAL:HG12	1.87	0.56
2:E:163:ARG:NH2	2:E:310:GLY:O	2.34	0.56
5:9:61:GLU:OE2	12:9:600:UTI:N02	2.39	0.56
6:a:70:GLN:OE1	6:a:74:GLN:NE2	2.39	0.56
8:d:137:VAL:HG22	8:d:143:GLN:HG2	1.88	0.56
4:H:109:ARG:O	4:H:113:ARG:HG2	2.06	0.56
6:a:170:PRO:O	6:a:173:LEU:HB3	2.05	0.56
6:a:131:TYR:HD2	7:b:34:VAL:HG11	1.71	0.56
8:d:223:LEU:O	8:d:233:ARG:NH2	2.39	0.55
1:B:228:ALA:O	1:B:232:THR:OG1	2.20	0.55
4:H:23:LEU:HD13	4:H:53:VAL:HG22	1.87	0.55
8:d:186:TRP:O	8:d:189:THR:OG1	2.20	0.55
1:A:57:GLU:HG3	1:A:92:LYS:HB2	1.87	0.55
1:C:443:GLU:OE1	1:C:476:ARG:NH2	2.37	0.55
6:a:168:LEU:HB3	6:a:171:ILE:HD13	1.88	0.55
1:C:13:SER:O	1:C:16:GLU:HB3	2.06	0.55
5:8:40:ALA:HB2	5:9:49:LEU:HD21	1.89	0.55
7:b:49:VAL:HG23	7:b:50:VAL:N	2.21	0.55
2:D:261:LEU:HD23	2:D:314:THR:HB	1.88	0.55
5:2:40:ALA:HB2	5:3:49:LEU:HD21	1.88	0.55
3:G:161:PHE:HD2	3:G:162:LEU:HD12	1.72	0.55
8:d:231:THR:O	8:d:234:ILE:HG12	2.07	0.55
5:4:33:ASN:ND2	5:5:30:VAL:O	2.40	0.54
1:A:169:LEU:HD11	1:A:330:ILE:CG1	2.37	0.54
5:6:17:MET:HG2	5:6:71:MET:HG3	1.88	0.54
6:a:131:TYR:CD2	7:b:34:VAL:HG11	2.42	0.54
8:d:49:ASP:OD1	8:d:50:ARG:N	2.41	0.54
1:A:23:THR:OG1	7:b:158:ARG:NH1	2.40	0.54
1:A:481:GLU:O	1:A:485:GLU:HG3	2.07	0.54
1:B:426:ARG:NH2	1:B:459:VAL:O	2.40	0.54
2:D:51:ILE:O	2:D:57:ALA:HA	2.07	0.54
1:B:292:PRO:HB2	1:B:296:ALA:HA	1.88	0.54
8:d:144:SER:HA	8:d:147:VAL:HG22	1.89	0.54
4:H:40:PRO:HA	4:H:72:VAL:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:102:ASP:OD1	4:H:102:ASP:N	2.40	0.54
5:3:48:ARG:O	5:3:51:THR:HG22	2.07	0.54
5:3:64:TYR:O	5:3:67:ASN:HB2	2.08	0.54
5:4:48:ARG:O	5:4:51:THR:HG22	2.08	0.54
8:d:4:PHE:HA	8:d:7:GLN:HG2	1.89	0.54
2:E:286:SER:OG	2:E:292:PRO:HA	2.08	0.54
5:1:30:VAL:O	5:9:33:ASN:ND2	2.36	0.54
1:C:47:LEU:HB3	1:C:50:VAL:HG13	1.90	0.53
2:D:175:VAL:HG23	2:D:176:GLY:H	1.72	0.53
6:a:93:THR:HB	7:b:45:ILE:HD13	1.90	0.53
1:C:15:ILE:HD13	8:d:326:LEU:HD11	1.89	0.53
2:E:253:ARG:HD3	2:E:313:ILE:HG13	1.89	0.53
5:1:50:PHE:HD2	5:1:54:PHE:HE2	1.56	0.53
6:a:126:ALA:HB3	6:a:191:ILE:HG21	1.90	0.53
2:E:417:ARG:NE	2:E:463:GLU:OE2	2.33	0.53
4:H:23:LEU:HD11	4:H:51:VAL:HG13	1.90	0.53
1:B:47:LEU:HB3	1:B:50:VAL:HG13	1.90	0.53
1:B:173:ASP:O	1:B:178:LYS:NZ	2.40	0.53
6:a:130:ASN:ND2	7:b:30:THR:HB	2.24	0.53
5:2:54:PHE:CE2	6:a:237:LEU:HD13	2.43	0.53
8:d:226:PRO:HB2	8:d:260:ARG:HH21	1.74	0.53
5:2:1:MET:HG3	5:2:2:ASP:H	1.73	0.53
1:A:442:GLU:HG3	1:A:483:LEU:HB3	1.90	0.53
4:H:98:ASP:OD2	4:H:106:ILE:HG12	2.09	0.53
12:1:600:UTI:C23	12:1:600:UTI:C12	2.88	0.52
5:7:48:ARG:O	5:7:51:THR:HG22	2.09	0.52
1:A:190:ARG:NH1	1:A:194:GLU:OE2	2.41	0.52
1:A:193:TRP:HA	1:A:201:GLN:HG2	1.91	0.52
6:a:229:PHE:CZ	6:a:233:LEU:HD11	2.44	0.52
2:F:18:ASP:OD1	2:F:18:ASP:N	2.42	0.52
1:A:400:TYR:HB2	1:A:424:GLY:HA3	1.91	0.52
2:D:18:ASP:N	2:D:18:ASP:OD1	2.42	0.52
6:a:109:VAL:HG21	6:a:122:LEU:HG	1.91	0.52
1:A:257:ALA:CB	1:A:267:VAL:HG11	2.39	0.52
1:B:397:LEU:HD22	1:B:401:ARG:HH22	1.75	0.52
1:C:166:GLN:NE2	1:C:168:GLN:OE1	2.43	0.52
1:B:272:ASP:HA	1:B:329:ILE:HD12	1.92	0.52
2:D:203:GLU:HG3	2:D:265:ASP:CG	2.35	0.52
2:D:395:ASP:OD1	2:D:396:ILE:N	2.43	0.52
5:8:1:MET:O	5:8:4:THR:HG22	2.10	0.52
8:d:234:ILE:O	8:d:237:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:VAL:HG21	1:A:257:ALA:HB2	1.92	0.52
1:A:212:LYS:NZ	2:D:339:ASP:OD1	2.43	0.52
7:b:77:GLN:HE22	8:d:55:SER:HA	1.74	0.52
8:d:422:ILE:HD11	8:d:429:ILE:HD12	1.90	0.52
8:d:385:GLU:HG3	8:d:412:ILE:HD11	1.92	0.51
2:E:109:VAL:HG22	2:E:226:LEU:HD12	1.92	0.51
1:B:52:THR:HG22	1:B:53:GLN:HG2	1.93	0.51
2:F:183:GLU:OE2	2:F:187:ARG:NE	2.39	0.51
6:a:62:LEU:HA	6:a:65:GLU:HG2	1.91	0.51
2:F:222:LYS:NZ	2:F:223:ASP:OD2	2.43	0.51
7:b:107:GLY:HA3	8:d:87:LEU:HD23	1.93	0.51
8:d:211:ARG:HG3	8:d:352:LEU:HD21	1.93	0.51
1:C:543:PRO:HG3	3:G:212:GLU:HG2	1.93	0.51
2:F:260:VAL:HB	2:F:313:ILE:HG12	1.93	0.51
6:a:75:VAL:O	6:a:79:ILE:N	2.32	0.51
7:b:45:ILE:HG13	7:b:46:GLY:N	2.26	0.51
6:a:206:PRO:HA	6:a:209:MET:HG2	1.91	0.51
3:G:225:ASP:N	3:G:225:ASP:OD1	2.42	0.51
1:C:211:GLN:NE2	1:C:272:ASP:OD2	2.44	0.51
2:D:109:VAL:HG22	2:D:226:LEU:HD12	1.91	0.51
6:a:199:ALA:O	6:a:202:ALA:HB3	2.11	0.51
8:d:27:GLY:HA2	8:d:30:MET:HE2	1.91	0.51
1:A:410:ALA:HA	1:A:413:LEU:HD12	1.92	0.51
1:C:528:LEU:O	3:G:106:LEU:HD12	2.11	0.51
3:G:214:ILE:HB	3:G:217:ARG:CB	2.36	0.51
8:d:299:PHE:HA	8:d:302:ILE:HG12	1.93	0.51
4:H:38:HIS:HD2	4:H:39:ILE:O	1.93	0.50
6:a:169:ALA:HB3	6:a:170:PRO:HD3	1.92	0.50
1:B:113:PRO:O	1:B:252:THR:OG1	2.26	0.50
1:C:9:ASP:HB3	1:C:11:ILE:HG13	1.93	0.50
1:C:55:LEU:O	1:C:94:THR:OG1	2.20	0.50
5:2:74:PHE:O	5:2:78:THR:HG22	2.11	0.50
1:C:413:LEU:HD23	1:C:417:SER:HB3	1.92	0.50
7:b:107:GLY:O	7:b:111:ILE:HG23	2.12	0.50
2:E:64:VAL:HA	2:E:75:THR:HG22	1.93	0.50
3:G:205:MET:HE1	3:G:234:LEU:HD22	1.94	0.50
1:C:39:ASP:OD1	2:F:283:ARG:NH2	2.44	0.50
2:D:366:ILE:HB	2:D:371:VAL:HG11	1.92	0.50
5:1:49:LEU:HD21	5:9:40:ALA:HB2	1.94	0.50
5:2:71:MET:O	5:2:75:VAL:HG23	2.11	0.50
6:a:140:PHE:HA	6:a:143:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1:600:UTI:C16	6:a:174:VAL:HG21	2.41	0.50
1:B:100:VAL:HG13	1:B:132:LEU:HD21	1.93	0.50
5:5:71:MET:HE1	5:6:70:PHE:CE1	2.47	0.50
2:F:465:ALA:HB2	2:F:482:LEU:HD22	1.93	0.49
5:2:17:MET:HB2	5:3:16:ILE:HG12	1.93	0.49
6:a:72:ARG:HA	6:a:75:VAL:HG22	1.94	0.49
7:b:49:VAL:O	7:b:53:ILE:HD12	2.12	0.49
1:A:144:GLY:O	1:A:146:LYS:NZ	2.45	0.49
5:1:54:PHE:HE1	6:a:168:LEU:HD11	1.77	0.49
5:2:68:LEU:HD11	5:3:70:PHE:CE2	2.48	0.49
2:E:194:GLY:HA2	2:E:258:GLN:HG2	1.95	0.49
2:E:288:VAL:HG21	2:E:329:PRO:CD	2.42	0.49
7:b:56:VAL:O	7:b:59:GLU:HG3	2.13	0.49
6:a:16:HIS:O	6:a:27:THR:N	2.33	0.49
8:d:175:ALA:HB3	8:d:262:SER:OG	2.12	0.49
7:b:144:LEU:HD13	8:d:121:LEU:HD12	1.94	0.49
8:d:236:LEU:O	8:d:240:LEU:HG	2.13	0.49
2:F:261:LEU:HD23	2:F:314:THR:HB	1.94	0.49
6:a:70:GLN:O	6:a:74:GLN:HG2	2.12	0.49
8:d:303:LEU:HA	8:d:309:LEU:HD11	1.95	0.49
1:A:512:ALA:HA	7:b:93:ARG:HH11	1.78	0.48
2:D:288:VAL:HG12	2:D:288:VAL:O	2.12	0.48
5:6:3:PRO:HB3	5:7:5:ILE:HD11	1.95	0.48
6:a:28:ASP:C	6:a:30:VAL:H	2.21	0.48
8:d:230:ALA:HB1	8:d:233:ARG:HE	1.78	0.48
1:A:178:LYS:HE3	1:A:331:GLU:HG2	1.94	0.48
1:B:335:ASN:HD21	1:B:357:THR:HG22	1.78	0.48
1:B:403:LEU:HB3	1:B:421:LEU:HD12	1.94	0.48
6:a:12:VAL:HG22	6:a:13:GLY:H	1.78	0.48
1:A:273:ASP:H	1:A:329:ILE:HB	1.77	0.48
2:D:24:VAL:HG12	2:D:25:ARG:HG3	1.94	0.48
6:a:175:GLU:HG3	6:a:179:LYS:HE3	1.95	0.48
2:D:99:VAL:HG11	2:D:244:SER:HB3	1.95	0.48
5:6:61:GLU:OE1	12:6:600:UTI:N02	2.46	0.48
3:G:53:MET:HE2	4:H:71:SER:HB2	1.96	0.48
5:6:15:LEU:HG	5:7:15:LEU:HD13	1.96	0.48
6:a:72:ARG:HG2	6:a:76:GLU:OE1	2.13	0.48
8:d:53:GLU:O	8:d:56:GLN:HG3	2.14	0.48
8:d:391:ARG:HH11	8:d:408:VAL:CG2	2.25	0.48
1:C:482:ILE:HD11	1:C:499:LYS:HG2	1.94	0.48
5:1:67:ASN:HD21	5:9:21:ALA:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:d:297:PHE:O	8:d:300:SER:OG	2.22	0.48
1:C:361:ASN:HD22	2:F:388:GLN:NE2	2.11	0.48
2:D:22:ARG:HG2	2:D:87:GLY:HA2	1.95	0.48
1:A:365:ARG:NH2	2:D:381:GLN:OE1	2.46	0.48
1:C:190:ARG:NE	1:C:194:GLU:OE2	2.47	0.48
7:b:109:LYS:O	7:b:112:GLU:HG3	2.14	0.48
8:d:252:VAL:HA	8:d:255:THR:HG22	1.96	0.48
8:d:398:LEU:HB3	8:d:406:VAL:HG21	1.95	0.48
1:B:193:TRP:HA	1:B:201:GLN:HG2	1.96	0.48
1:C:270:ILE:HG13	1:C:327:LEU:HB2	1.96	0.48
5:8:3:PRO:O	5:8:6:ALA:HB3	2.14	0.48
6:a:38:LEU:HA	6:a:41:ILE:HG12	1.96	0.48
5:7:40:ALA:HB2	5:8:49:LEU:HD21	1.96	0.48
7:b:159:ILE:HG23	7:b:160:LEU:HD12	1.96	0.47
1:B:18:TYR:HB2	8:d:236:LEU:HD12	1.95	0.47
11:F:600:ADP:H5'1	11:F:600:ADP:H8	1.79	0.47
5:3:59:LEU:O	5:3:62:ALA:HB3	2.13	0.47
7:b:148:VAL:HA	7:b:151:MET:HG2	1.96	0.47
8:d:235:ARG:O	8:d:239:ARG:HG3	2.14	0.47
1:B:400:TYR:OH	1:B:404:GLU:OE1	2.26	0.47
2:F:264:ILE:HG21	2:F:267:ILE:HD13	1.94	0.47
5:5:43:PRO:HB3	5:6:48:ARG:NE	2.29	0.47
8:d:233:ARG:O	8:d:236:LEU:HB3	2.13	0.47
8:d:391:ARG:NH1	8:d:408:VAL:HG23	2.27	0.47
4:H:23:LEU:HD23	4:H:77:VAL:HG21	1.96	0.47
2:D:369:PRO:HG3	2:D:377:TYR:CD2	2.49	0.47
5:1:53:PHE:HA	5:9:36:ILE:HD11	1.95	0.47
5:7:46:GLN:HE21	5:7:50:PHE:HE1	1.63	0.47
8:d:167:PRO:HG2	8:d:368:VAL:HG23	1.97	0.47
1:A:518:SER:OG	7:b:93:ARG:NH2	2.48	0.47
1:A:28:ARG:NH2	8:d:427:GLU:OE2	2.48	0.47
5:4:49:LEU:O	5:4:52:PRO:HD2	2.15	0.47
5:6:2:ASP:OD1	5:6:81:LYS:NZ	2.47	0.47
5:7:1:MET:HG2	5:7:2:ASP:H	1.79	0.47
5:7:26:ILE:O	5:7:30:VAL:HG23	2.15	0.47
5:8:56:THR:OG1	5:8:57:VAL:N	2.48	0.47
5:8:72:ALA:HA	5:8:75:VAL:HG12	1.96	0.47
1:C:409:PHE:CZ	2:F:396:ILE:HD13	2.50	0.47
2:E:235:PRO:HB2	2:E:277:VAL:HG23	1.97	0.47
8:d:186:TRP:CD1	8:d:255:THR:HG21	2.50	0.47
1:A:463:ASP:OD1	1:A:466:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:9:46:GLN:HE21	5:9:50:PHE:HE2	1.62	0.47
8:d:202:LEU:HD13	8:d:249:THR:HG22	1.97	0.47
1:A:52:THR:HG22	1:A:53:GLN:HG2	1.96	0.47
1:A:256:ILE:O	1:A:257:ALA:HB3	2.15	0.47
1:B:272:ASP:O	1:B:329:ILE:HB	2.14	0.47
1:B:399:GLN:OE1	1:B:420:GLN:NE2	2.48	0.47
1:C:338:SER:HB3	2:D:323:ALA:HB1	1.96	0.47
2:D:63:GLU:OE1	2:D:240:ARG:NE	2.45	0.47
8:d:320:ALA:HA	8:d:323:ARG:HB2	1.96	0.47
8:d:422:ILE:HG12	8:d:429:ILE:HB	1.97	0.47
8:d:50:ARG:O	8:d:53:GLU:HG3	2.15	0.46
1:C:58:PHE:HB2	1:C:62:ILE:HB	1.96	0.46
2:F:198:PHE:HB3	2:F:226:LEU:HD23	1.96	0.46
4:H:66:ASP:HB3	4:H:83:SER:OG	2.15	0.46
5:8:43:PRO:HB3	5:9:48:ARG:NE	2.30	0.46
6:a:95:PHE:HE1	6:a:99:LEU:HD22	1.80	0.46
8:d:312:LEU:HD13	8:d:326:LEU:HD21	1.96	0.46
1:A:51:MET:HB3	2:E:85:VAL:HG22	1.97	0.46
5:1:74:PHE:O	5:1:78:THR:HG22	2.16	0.46
5:4:36:ILE:HD11	5:5:53:PHE:HA	1.98	0.46
5:5:52:PRO:O	5:5:56:THR:HG23	2.16	0.46
8:d:380:VAL:HG12	8:d:422:ILE:HG22	1.96	0.46
1:A:169:LEU:HD11	1:A:330:ILE:HG12	1.98	0.46
5:4:71:MET:HE3	5:4:71:MET:HB3	1.77	0.46
6:a:54:THR:O	8:d:41:LEU:HD22	2.16	0.46
7:b:48:PHE:O	7:b:52:PRO:HG2	2.14	0.46
4:H:27:THR:CG2	4:H:43:ALA:HB1	2.45	0.46
4:H:85:GLU:OE1	4:H:113:ARG:NE	2.49	0.46
8:d:321:GLU:HG2	8:d:322:GLY:N	2.30	0.46
1:B:182:CYS:SG	1:B:329:ILE:HD11	2.56	0.46
2:D:64:VAL:HG13	2:D:73:VAL:HG13	1.98	0.46
8:d:4:PHE:HD1	8:d:8:LEU:HD23	1.81	0.46
8:d:123:HIS:O	8:d:126:VAL:HG12	2.16	0.46
8:d:206:LEU:HD23	8:d:275:SER:HB3	1.98	0.46
1:C:273:ASP:H	1:C:329:ILE:HB	1.81	0.46
1:A:406:PHE:HZ	3:G:27:LEU:HD12	1.81	0.46
3:G:74:PRO:HB2	3:G:112:LYS:HD3	1.98	0.46
7:b:131:GLU:O	7:b:135:ARG:HG2	2.16	0.46
1:A:140:VAL:HG11	2:E:118:ASP:HA	1.97	0.45
1:C:5:THR:HG22	8:d:336:SER:HB2	1.98	0.45
2:D:286:SER:OG	2:D:287:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:56:THR:OG1	5:5:57:VAL:N	2.47	0.45
8:d:339:ASN:OD1	8:d:341:VAL:HG12	2.16	0.45
1:B:12:GLN:HG2	1:B:13:SER:N	2.30	0.45
1:B:444:GLN:O	1:B:448:ILE:HG12	2.15	0.45
1:C:182:CYS:SG	1:C:329:ILE:HD11	2.56	0.45
2:D:400:LEU:HD23	2:F:400:LEU:HD11	1.97	0.45
5:9:51:THR:HB	5:9:52:PRO:HD3	1.98	0.45
8:d:93:VAL:O	8:d:96:GLU:HG3	2.16	0.45
1:A:258:GLN:NE2	1:A:311:ARG:HB3	2.31	0.45
1:A:430:LEU:HD22	1:A:451:GLY:HA3	1.99	0.45
2:F:253:ARG:NH1	2:F:306:THR:O	2.49	0.45
5:2:49:LEU:HD23	5:2:49:LEU:HA	1.83	0.45
5:8:30:VAL:O	5:8:33:ASN:HB3	2.17	0.45
6:a:28:ASP:OD2	6:a:121:LEU:HB3	2.17	0.45
7:b:85:TYR:HD1	8:d:65:ALA:HB2	1.81	0.45
2:E:227:VAL:HG12	2:E:241:VAL:HG23	1.99	0.45
6:a:65:GLU:HA	6:a:68:THR:HG22	1.98	0.45
1:B:12:GLN:HA	1:B:15:ILE:HG12	1.98	0.45
1:B:51:MET:HG2	2:F:85:VAL:HG22	1.98	0.45
1:B:464:VAL:O	1:B:467:PHE:HB3	2.17	0.45
1:C:430:LEU:HD13	1:C:456:LEU:HD11	1.98	0.45
2:D:417:ARG:HE	2:D:463:GLU:CD	2.21	0.45
7:b:99:LEU:C	7:b:101:ASP:H	2.25	0.45
1:A:172:GLY:O	1:A:331:GLU:HA	2.16	0.45
1:A:258:GLN:HE22	1:A:311:ARG:HD3	1.81	0.45
5:7:18:ALA:O	5:7:22:ILE:HG13	2.17	0.45
5:4:5:ILE:HD11	5:4:81:LYS:HG3	1.99	0.45
7:b:151:MET:HA	7:b:154:THR:HG22	1.98	0.45
1:C:167:ARG:HH22	2:D:204:ARG:HG2	1.82	0.45
1:C:361:ASN:HD22	2:F:388:GLN:HE21	1.65	0.45
2:F:64:VAL:HA	2:F:75:THR:HG22	1.99	0.45
6:a:108:PRO:HD3	8:d:11:PHE:CD1	2.52	0.45
1:A:159:MET:O	1:A:394:ARG:NH2	2.50	0.44
1:C:529:ASP:HB3	1:C:532:LYS:HG3	1.99	0.44
2:E:107:GLY:HA2	2:E:221:LEU:HG	1.99	0.44
2:E:316:MET:HE2	2:E:316:MET:HB3	1.81	0.44
5:1:71:MET:O	5:1:75:VAL:HG23	2.17	0.44
8:d:220:THR:O	8:d:224:THR:OG1	2.26	0.44
1:C:160:THR:OG1	1:C:160:THR:O	2.33	0.44
2:D:37:ARG:HE	8:d:359:GLU:CD	2.25	0.44
2:D:169:LEU:HD11	2:D:316:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:96:ILE:HD11	3:G:187:THR:OG1	2.16	0.44
5:7:43:PRO:HB3	5:8:48:ARG:CZ	2.47	0.44
6:a:173:LEU:HA	6:a:176:GLU:CD	2.43	0.44
8:d:320:ALA:HB2	8:d:323:ARG:HH11	1.81	0.44
2:E:183:GLU:O	2:E:187:ARG:HG3	2.17	0.44
5:5:42:GLN:NE2	5:5:48:ARG:HH12	2.15	0.44
7:b:51:PRO:HB2	7:b:52:PRO:HD3	1.99	0.44
1:C:69:LEU:HD23	2:D:86:ARG:HG3	1.99	0.44
5:4:26:ILE:O	5:4:30:VAL:HG23	2.17	0.44
6:a:41:ILE:HG22	7:b:44:VAL:HG11	1.99	0.44
7:b:143:ASP:OD1	7:b:144:LEU:N	2.51	0.44
1:A:159:MET:HE1	1:A:394:ARG:HA	1.99	0.44
1:A:450:LEU:HD11	1:A:471:LEU:HD23	1.99	0.44
2:E:78:LEU:HD13	2:E:113:LEU:HD21	1.98	0.44
2:E:183:GLU:OE1	2:E:187:ARG:NE	2.51	0.44
2:F:366:ILE:HB	2:F:371:VAL:HG11	2.00	0.44
5:3:55:ILE:HD11	6:a:233:LEU:HD13	2.00	0.44
7:b:65:ALA:O	7:b:68:LEU:HG	2.18	0.44
8:d:89:ALA:O	8:d:93:VAL:HG13	2.18	0.44
8:d:199:LEU:HD11	8:d:285:ARG:CZ	2.48	0.44
1:A:240:SER:HB3	2:D:303:GLU:HG3	2.00	0.44
1:A:258:GLN:HE21	1:A:311:ARG:HB3	1.82	0.44
1:A:387:LYS:HB2	1:A:387:LYS:HE3	1.78	0.44
1:B:430:LEU:HD13	1:B:456:LEU:HD11	1.99	0.44
1:C:444:GLN:O	1:C:448:ILE:HG12	2.17	0.44
2:D:458:PHE:CE1	2:D:486:LEU:HD12	2.52	0.44
2:F:369:PRO:HG3	2:F:377:TYR:CD2	2.52	0.44
6:a:211:ALA:HB3	6:a:212:PRO:HD3	2.00	0.44
8:d:266:ASP:OD1	8:d:267:LEU:N	2.50	0.44
1:C:535:LYS:HD2	3:G:201:ARG:NH1	2.23	0.44
2:D:266:ASN:OD1	2:D:268:PHE:HB3	2.17	0.44
2:E:418:ARG:HG2	2:E:466:PHE:CE2	2.53	0.44
5:1:56:THR:OG1	5:1:57:VAL:N	2.50	0.44
5:1:48:ARG:O	5:1:51:THR:HG22	2.16	0.44
1:C:9:ASP:HB2	8:d:333:ARG:HH21	1.83	0.44
1:C:257:ALA:HB1	1:C:267:VAL:HG11	2.00	0.44
2:E:47:LEU:HB2	2:E:62:LEU:HB2	1.99	0.44
2:E:307:SER:HA	2:E:312:SER:HA	2.00	0.44
2:E:428:MET:HG2	2:E:438:GLY:HA3	2.00	0.44
3:G:75:LYS:HE2	3:G:75:LYS:HB3	1.69	0.44
3:G:237:TYR:O	3:G:241:ARG:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:59:LYS:HE2	4:H:59:LYS:HB3	1.73	0.44
7:b:47:THR:HG23	7:b:48:PHE:CD1	2.53	0.44
8:d:346:LEU:HD12	8:d:347:SER:N	2.32	0.44
1:B:451:GLY:HA2	1:B:456:LEU:HD12	2.00	0.43
5:3:49:LEU:O	5:3:52:PRO:HD2	2.18	0.43
7:b:113:ASP:O	7:b:116:VAL:HG22	2.18	0.43
1:C:228:ALA:O	1:C:232:THR:OG1	2.22	0.43
2:D:448:GLU:O	2:D:452:ARG:HG3	2.18	0.43
2:F:375:GLU:OE2	2:F:378:ARG:NH2	2.34	0.43
7:b:77:GLN:NE2	8:d:55:SER:HA	2.33	0.43
1:A:41:ILE:HG13	1:A:287:LEU:HB3	2.00	0.43
1:A:228:ALA:O	1:A:232:THR:OG1	2.29	0.43
1:C:107:LEU:HD22	1:C:231:TYR:HA	2.01	0.43
3:G:147:TYR:CE1	4:H:11:VAL:HG21	2.53	0.43
4:H:3:GLU:HB3	4:H:20:ALA:O	2.17	0.43
5:6:52:PRO:O	5:6:56:THR:HG23	2.18	0.43
6:a:81:MET:HE3	6:a:81:MET:HB3	1.92	0.43
7:b:122:VAL:HA	7:b:125:THR:HG22	1.99	0.43
7:b:57:LEU:HD23	7:b:57:LEU:HA	1.84	0.43
8:d:5:ILE:O	8:d:8:LEU:HG	2.19	0.43
8:d:237:ILE:HG13	8:d:238:GLU:N	2.34	0.43
8:d:301:ARG:HG2	8:d:411:HIS:CE1	2.53	0.43
1:A:187:LEU:HD23	1:A:228:ALA:HB2	2.01	0.43
1:A:199:LYS:HA	1:A:199:LYS:HD2	1.81	0.43
1:B:442:GLU:HG2	1:B:443:GLU:N	2.33	0.43
1:C:204:CYS:O	1:C:232:THR:HA	2.19	0.43
1:C:495:GLU:HG3	1:C:496:ALA:N	2.34	0.43
5:8:36:ILE:HD11	5:9:53:PHE:HA	2.00	0.43
7:b:156:ALA:HA	7:b:159:ILE:HG22	2.00	0.43
8:d:357:ALA:O	8:d:361:ALA:N	2.47	0.43
1:A:121:ARG:HH21	8:d:104:ARG:HD3	1.84	0.43
1:A:399:GLN:HA	1:A:402:GLU:HG2	2.01	0.43
1:C:399:GLN:NE2	2:D:351:LYS:O	2.40	0.43
2:D:426:ASN:OD1	2:D:426:ASN:N	2.51	0.43
5:7:16:ILE:HG23	5:7:67:ASN:HD22	1.84	0.43
5:8:17:MET:CG	5:8:71:MET:HG3	2.44	0.43
8:d:87:LEU:HD12	8:d:87:LEU:HA	1.79	0.43
8:d:251:GLU:HA	8:d:254:ARG:HE	1.83	0.43
1:B:294:ARG:HG2	1:B:295:GLU:HG3	2.00	0.43
2:D:168:ALA:HB2	2:D:338:LEU:HD22	2.00	0.43
2:D:345:SER:HB2	2:D:348:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:477:LYS:HA	2:E:480:GLU:HG2	2.00	0.43
4:H:99:SER:OG	4:H:100:GLU:OE1	2.36	0.43
8:d:177:ARG:O	8:d:180:LEU:N	2.52	0.43
1:A:166:GLN:NE2	1:A:168:GLN:OE1	2.50	0.43
2:D:227:VAL:HG12	2:D:241:VAL:HG23	2.00	0.43
2:D:268:PHE:O	2:D:271:THR:N	2.52	0.43
3:G:37:GLN:O	3:G:41:GLU:HG2	2.18	0.43
3:G:283:ARG:O	3:G:287:ILE:HG13	2.19	0.43
6:a:171:ILE:HD12	6:a:171:ILE:N	2.23	0.43
7:b:106:ASP:O	7:b:110:VAL:HG23	2.19	0.43
7:b:109:LYS:HA	7:b:112:GLU:HG3	2.01	0.43
7:b:141:GLU:HG3	7:b:145:ARG:HH11	1.83	0.43
3:G:212:GLU:O	3:G:214:ILE:N	2.51	0.43
8:d:198:GLY:O	8:d:202:LEU:HD23	2.19	0.43
8:d:226:PRO:HB2	8:d:260:ARG:NH2	2.34	0.43
8:d:249:THR:O	8:d:253:LEU:HG	2.19	0.43
1:A:267:VAL:HB	1:A:324:LEU:HD13	2.01	0.42
1:B:149:LEU:HD22	1:B:325:THR:HG21	2.00	0.42
8:d:292:VAL:HA	8:d:295:GLN:HG2	2.01	0.42
1:A:330:ILE:HD11	1:A:345:VAL:HG21	2.01	0.42
3:G:157:LEU:HB3	3:G:182:LEU:HD13	2.00	0.42
12:1:600:UTI:C39	6:a:171:ILE:HD11	2.48	0.42
8:d:235:ARG:O	8:d:238:GLU:HG2	2.19	0.42
1:C:455:HIS:NE2	1:C:501:THR:HG23	2.33	0.42
1:C:528:LEU:HB2	3:G:102:GLU:HB3	2.00	0.42
5:1:40:ALA:HB2	5:2:49:LEU:HD21	2.01	0.42
1:C:47:LEU:HD22	1:C:93:ARG:HG3	2.02	0.42
2:E:166:LYS:HB3	2:E:338:LEU:HD23	2.02	0.42
2:F:408:GLU:HG3	3:G:129:PHE:CE1	2.54	0.42
3:G:30:THR:O	3:G:33:ILE:HG22	2.19	0.42
3:G:205:MET:HE2	3:G:238:LEU:HD21	2.01	0.42
5:3:26:ILE:O	5:3:30:VAL:HG23	2.19	0.42
5:4:52:PRO:O	5:4:56:THR:HG23	2.18	0.42
8:d:217:ALA:O	8:d:220:THR:OG1	2.29	0.42
1:A:410:ALA:HB1	1:A:418:LYS:HD2	2.01	0.42
2:F:254:ASP:O	2:F:311:ARG:NH1	2.53	0.42
5:1:10:LEU:HA	5:1:10:LEU:HD23	1.80	0.42
5:1:71:MET:HE1	5:2:70:PHE:CE1	2.54	0.42
6:a:98:ILE:O	6:a:101:SER:HB2	2.20	0.42
8:d:1:MET:HE3	8:d:1:MET:HB3	1.91	0.42
8:d:398:LEU:HA	8:d:398:LEU:HD23	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ARG:HB2	2:F:433:PHE:HE1	1.83	0.42
1:C:330:ILE:HD11	1:C:345:VAL:HG21	2.01	0.42
2:F:176:GLY:N	11:F:600:ADP:O1A	2.53	0.42
12:1:600:UTI:O15	6:a:174:VAL:HG21	2.19	0.42
5:3:1:MET:HB3	5:3:2:ASP:H	1.71	0.42
5:3:74:PHE:O	5:3:78:THR:HG22	2.18	0.42
1:A:501:THR:O	1:A:505:LYS:HG2	2.19	0.42
1:A:520:VAL:HA	1:A:521:PRO:HD3	1.92	0.42
2:F:425:GLN:NE2	2:F:439:SER:O	2.52	0.42
8:d:292:VAL:HA	8:d:295:GLN:NE2	2.34	0.42
1:B:70:ASP:OD1	1:B:71:GLU:HG2	2.19	0.42
2:E:403:ASP:OD1	2:E:403:ASP:N	2.52	0.42
5:6:56:THR:OG1	5:6:57:VAL:N	2.52	0.42
6:a:171:ILE:O	6:a:175:GLU:N	2.42	0.42
8:d:27:GLY:HA2	8:d:30:MET:HG2	2.01	0.42
8:d:276:ARG:HE	8:d:349:THR:HG22	1.85	0.42
8:d:309:LEU:HA	8:d:312:LEU:HG	2.02	0.42
8:d:351:GLU:C	8:d:352:LEU:HD22	2.44	0.42
3:G:16:GLY:HA2	3:G:272:ILE:HD11	2.02	0.42
5:3:71:MET:HE1	5:4:70:PHE:CE1	2.55	0.42
6:a:150:ARG:NH2	6:a:243:MET:HG2	2.35	0.42
1:A:384:LYS:HD3	1:A:491:LYS:HE2	2.02	0.42
1:B:11:ILE:HD12	1:B:11:ILE:H	1.84	0.42
1:B:113:PRO:HG3	1:B:249:ALA:HB2	2.02	0.42
3:G:222:PHE:CD2	3:G:226:ALA:HB2	2.54	0.42
5:2:50:PHE:HD2	5:2:54:PHE:HE2	1.66	0.42
5:2:66:ILE:O	5:2:69:ALA:HB3	2.19	0.42
1:A:182:CYS:SG	1:A:329:ILE:HD11	2.59	0.41
1:C:14:ALA:HA	1:C:17:GLU:HG3	2.01	0.41
2:E:47:LEU:HD12	2:E:75:THR:HG21	2.02	0.41
2:F:268:PHE:CZ	2:F:322:PRO:HG3	2.55	0.41
3:G:147:TYR:CD1	4:H:11:VAL:HG21	2.55	0.41
3:G:219:LEU:HD11	5:6:42:GLN:HB2	2.02	0.41
4:H:27:THR:HG22	4:H:28:THR:N	2.35	0.41
5:2:46:GLN:HG3	5:2:50:PHE:HE1	1.85	0.41
8:d:177:ARG:O	8:d:178:ARG:C	2.63	0.41
1:B:63:LEU:HD12	1:B:114:LEU:HD13	2.01	0.41
1:C:9:ASP:OD2	8:d:334:ALA:HB2	2.20	0.41
1:C:197:ASP:OD1	1:C:197:ASP:N	2.53	0.41
2:D:37:ARG:NE	8:d:359:GLU:OE2	2.47	0.41
2:E:184:MET:HB3	2:E:261:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:116:LEU:HD23	3:G:134:ILE:HG12	2.02	0.41
5:4:43:PRO:HG3	5:5:48:ARG:NH1	2.35	0.41
6:a:103:TRP:CE2	6:a:221:LEU:HD12	2.55	0.41
6:a:181:ILE:O	6:a:184:SER:OG	2.29	0.41
8:d:279:LEU:HB3	8:d:345:LEU:HD11	2.02	0.41
1:B:314:LYS:NZ	1:B:321:GLY:O	2.52	0.41
1:B:479:GLU:HB3	1:B:482:ILE:HD12	2.02	0.41
1:C:418:LYS:O	1:C:422:GLU:HG2	2.19	0.41
2:F:287:ALA:O	2:F:288:VAL:HB	2.21	0.41
5:9:24:ALA:HB2	5:9:64:TYR:HB2	2.02	0.41
6:a:16:HIS:HB2	6:a:27:THR:HB	2.02	0.41
1:A:169:LEU:HD11	1:A:330:ILE:HG13	2.02	0.41
1:C:15:ILE:O	1:C:19:VAL:HG23	2.20	0.41
1:C:52:THR:HG21	2:D:26:VAL:HG11	2.03	0.41
1:C:385:ALA:O	1:C:388:GLU:HG2	2.20	0.41
2:D:169:LEU:HD12	2:D:181:ILE:HG13	2.02	0.41
2:D:464:GLN:C	2:D:466:PHE:H	2.29	0.41
2:F:96:SER:OG	2:F:130:SER:OG	2.27	0.41
2:F:316:MET:HE3	2:F:316:MET:HB2	1.85	0.41
5:2:49:LEU:O	5:2:52:PRO:HD2	2.20	0.41
5:5:43:PRO:HD3	5:6:48:ARG:NH1	2.36	0.41
5:5:65:PHE:O	5:5:68:LEU:HB3	2.20	0.41
6:a:100:ILE:H	6:a:100:ILE:HD12	1.85	0.41
8:d:308:ARG:NE	8:d:312:LEU:HD23	2.35	0.41
8:d:401:ILE:HD13	8:d:401:ILE:HA	1.93	0.41
1:A:166:GLN:HG3	1:A:350:ASP:HB2	2.02	0.41
1:B:348:ILE:HG23	2:F:231:MET:HE1	2.01	0.41
8:d:172:MET:O	8:d:177:ARG:NE	2.51	0.41
1:A:346:ILE:HG12	1:A:352:GLN:HG2	2.02	0.41
2:D:46:ALA:O	2:D:93:THR:OG1	2.33	0.41
2:D:53:PHE:O	2:D:57:ALA:N	2.53	0.41
2:D:134:LYS:HA	2:D:134:LYS:HD2	1.87	0.41
4:H:90:ILE:HD13	4:H:113:ARG:HA	2.02	0.41
8:d:109:ILE:O	8:d:112:GLN:HG3	2.21	0.41
8:d:174:SER:C	8:d:176:SER:H	2.29	0.41
8:d:183:LEU:HD23	8:d:183:LEU:HA	1.90	0.41
1:A:506:ASN:O	1:A:509:LYS:HG2	2.21	0.41
1:C:295:GLU:O	2:F:287:ALA:HB2	2.20	0.41
3:G:57:LEU:HD11	4:H:42:VAL:HG11	2.02	0.41
1:A:11:ILE:HD13	1:A:11:ILE:HA	1.92	0.41
1:B:430:LEU:HD22	1:B:451:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:LYS:HB2	1:B:508:LYS:HE3	1.88	0.41
1:C:167:ARG:HG2	1:C:312:CYS:HB2	2.01	0.41
2:F:290:TYR:CD2	2:F:329:PRO:HB2	2.56	0.41
2:F:467:PHE:O	2:F:478:LYS:NZ	2.53	0.41
5:1:36:ILE:HD11	5:2:53:PHE:HA	2.02	0.41
5:2:71:MET:HE3	5:2:71:MET:HB3	1.80	0.41
1:A:275:THR:HG23	1:A:330:ILE:HD13	2.02	0.41
1:A:394:ARG:HD3	2:E:346:ARG:HH22	1.85	0.41
1:B:116:GLN:HA	1:B:117:PRO:HD3	1.95	0.41
1:B:187:LEU:HD23	1:B:228:ALA:HB2	2.03	0.41
1:C:341:ILE:O	1:C:345:VAL:HG23	2.21	0.41
2:F:287:ALA:C	2:F:289:GLY:H	2.28	0.41
5:2:52:PRO:O	5:2:56:THR:HG23	2.21	0.41
6:a:31:LEU:O	6:a:35:ILE:HG13	2.20	0.41
7:b:49:VAL:O	7:b:50:VAL:C	2.64	0.41
7:b:108:ARG:O	7:b:111:ILE:HG12	2.21	0.41
8:d:11:PHE:HA	8:d:14:ILE:HG12	2.03	0.41
1:A:393:LEU:HD12	1:A:427:LEU:HD13	2.02	0.41
1:B:13:SER:HA	1:B:16:GLU:CD	2.45	0.41
1:B:97:VAL:HG11	2:F:56:LEU:HD11	2.02	0.41
2:D:377:TYR:O	2:D:381:GLN:HG2	2.21	0.41
2:D:399:ILE:HD13	2:D:399:ILE:HA	1.94	0.41
5:1:56:THR:HG21	5:9:32:GLY:HA3	2.03	0.41
5:1:71:MET:HE3	5:1:71:MET:HB3	1.87	0.41
5:6:65:PHE:O	5:6:68:LEU:HB3	2.21	0.41
5:8:10:LEU:HD13	5:9:9:ALA:HB2	2.03	0.41
3:G:33:ILE:HD12	3:G:255:ALA:HB2	2.02	0.40
5:3:17:MET:HG3	5:3:71:MET:HE2	2.04	0.40
5:7:10:LEU:HD23	5:7:10:LEU:HA	1.93	0.40
6:a:227:GLN:O	6:a:227:GLN:NE2	2.53	0.40
8:d:60:LYS:O	8:d:63:GLU:HG3	2.21	0.40
1:A:131:ALA:HB3	1:A:134:LEU:HG	2.02	0.40
1:B:182:CYS:HB3	1:B:270:ILE:HG12	2.04	0.40
2:E:104:GLY:O	2:E:122:TYR:OH	2.33	0.40
2:F:42:GLU:OE1	2:F:42:GLU:N	2.41	0.40
3:G:143:GLU:N	3:G:143:GLU:OE2	2.54	0.40
3:G:210:VAL:HG23	3:G:211:GLU:N	2.36	0.40
5:9:49:LEU:HA	5:9:49:LEU:HD23	1.76	0.40
1:A:216:ILE:HD13	1:A:236:ALA:HB1	2.03	0.40
6:a:47:LEU:HD11	6:a:61:GLN:HA	2.03	0.40
6:a:65:GLU:O	6:a:69:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:d:233:ARG:NH1	8:d:257:VAL:O	2.54	0.40
8:d:299:PHE:CZ	8:d:303:LEU:HD12	2.57	0.40
1:B:70:ASP:O	2:F:86:ARG:NH1	2.42	0.40
1:C:195:SER:OG	1:C:196:GLY:N	2.55	0.40
2:E:22:ARG:NH1	2:E:34:GLU:OE1	2.54	0.40
2:E:366:ILE:HB	2:E:371:VAL:HG11	2.04	0.40
5:2:71:MET:HE1	5:3:70:PHE:CD1	2.56	0.40
5:3:71:MET:HE1	5:4:70:PHE:CD1	2.55	0.40
5:7:48:ARG:O	5:7:52:PRO:HD3	2.21	0.40
8:d:292:VAL:O	8:d:295:GLN:HG2	2.22	0.40
1:A:113:PRO:HB3	1:A:249:ALA:HA	2.03	0.40
2:D:260:VAL:HB	2:D:313:ILE:HG12	2.04	0.40
2:E:46:ALA:O	2:E:93:THR:OG1	2.32	0.40
2:E:397:ILE:HD11	2:E:413:VAL:HG21	2.03	0.40
2:F:332:ALA:HA	2:F:335:PHE:HD2	1.86	0.40
3:G:20:LYS:HE2	3:G:20:LYS:HB3	1.84	0.40
3:G:96:ILE:HD13	3:G:96:ILE:HA	1.94	0.40
6:a:217:LYS:HD3	6:a:217:LYS:HA	1.89	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 PDB entries followed by that with respect to all EM entries.

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	515/549 (94%)	496 (96%)	19 (4%)	0	100	100
1	B	485/549 (88%)	471 (97%)	14 (3%)	0	100	100
1	C	524/549 (95%)	503 (96%)	21 (4%)	0	100	100
2	D	467/486 (96%)	448 (96%)	19 (4%)	0	100	100
2	E	467/486 (96%)	450 (96%)	17 (4%)	0	100	100
2	F	467/486 (96%)	455 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	283/305 (93%)	275 (97%)	8 (3%)	0	100	100
4	H	117/121 (97%)	108 (92%)	9 (8%)	0	100	100
5	1	79/81 (98%)	72 (91%)	7 (9%)	0	100	100
5	2	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
5	3	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
5	4	79/81 (98%)	74 (94%)	5 (6%)	0	100	100
5	5	79/81 (98%)	74 (94%)	5 (6%)	0	100	100
5	6	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
5	7	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
5	8	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
5	9	79/81 (98%)	73 (92%)	6 (8%)	0	100	100
6	a	214/250 (86%)	203 (95%)	11 (5%)	0	100	100
7	b	142/171 (83%)	139 (98%)	3 (2%)	0	100	100
8	d	443/446 (99%)	426 (96%)	17 (4%)	0	100	100
All	All	4835/5127 (94%)	4641 (96%)	194 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	417/444 (94%)	417 (100%)	0	100	100
1	B	400/444 (90%)	400 (100%)	0	100	100
1	C	430/444 (97%)	430 (100%)	0	100	100
2	D	389/403 (96%)	389 (100%)	0	100	100
2	E	389/403 (96%)	389 (100%)	0	100	100
2	F	389/403 (96%)	389 (100%)	0	100	100
3	G	235/248 (95%)	235 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	94/96 (98%)	94 (100%)	0	100	100
5	1	52/52 (100%)	52 (100%)	0	100	100
5	2	52/52 (100%)	52 (100%)	0	100	100
5	3	52/52 (100%)	52 (100%)	0	100	100
5	4	52/52 (100%)	52 (100%)	0	100	100
5	5	52/52 (100%)	52 (100%)	0	100	100
5	6	52/52 (100%)	52 (100%)	0	100	100
5	7	52/52 (100%)	52 (100%)	0	100	100
5	8	52/52 (100%)	52 (100%)	0	100	100
5	9	52/52 (100%)	52 (100%)	0	100	100
6	a	178/204 (87%)	178 (100%)	0	100	100
7	b	117/133 (88%)	117 (100%)	0	100	100
8	d	356/357 (100%)	356 (100%)	0	100	100
All	All	3862/4047 (95%)	3862 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	84	ASN
1	A	141	HIS
1	A	143	GLN
1	A	211	GLN
1	B	141	HIS
1	B	335	ASN
1	B	382	GLN
1	B	420	GLN
1	C	191	GLN
2	D	388	GLN
2	D	394	GLN
2	E	337	HIS
2	F	256	GLN
2	F	388	GLN
3	G	200	HIS
3	G	284	GLN
4	H	38	HIS

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Mol	Chain	Res	Type
5	3	33	ASN
5	4	67	ASN
5	5	42	GLN
5	5	46	GLN
5	6	33	ASN
5	6	42	GLN
5	6	46	GLN
5	7	46	GLN
5	7	67	ASN
5	8	33	ASN
5	8	67	ASN
6	a	227	GLN
6	a	241	GLN
7	b	82	GLN
8	d	143	GLN
8	d	295	GLN
8	d	411	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	UTI	4	600	-	43,43,43	1.67	9 (20%)	56,62,62	1.84	15 (26%)
12	UTI	8	600	-	43,43,43	1.68	10 (23%)	56,62,62	1.92	14 (25%)
9	ATP	B	600	10	32,33,33	1.32	5 (15%)	48,52,52	1.74	10 (20%)
9	ATP	A	600	10	32,33,33	1.32	5 (15%)	48,52,52	1.74	10 (20%)
9	ATP	C	600	10	32,33,33	1.32	5 (15%)	48,52,52	1.74	9 (18%)
11	ADP	D	600	10	28,29,29	1.36	5 (17%)	43,45,45	1.87	11 (25%)
12	UTI	6	600	-	43,43,43	1.68	10 (23%)	56,62,62	1.85	13 (23%)
12	UTI	9	600	-	43,43,43	1.67	11 (25%)	56,62,62	1.87	15 (26%)
11	ADP	F	600	10	28,29,29	1.37	4 (14%)	43,45,45	1.87	9 (20%)
12	UTI	5	600	-	43,43,43	1.66	9 (20%)	56,62,62	1.84	14 (25%)
12	UTI	7	600	-	43,43,43	1.67	8 (18%)	56,62,62	1.79	14 (25%)
12	UTI	1	600	-	43,43,43	1.51	9 (20%)	56,62,62	2.34	18 (32%)

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
12	UTI	4	600	-	-	4/34/34/34	0/4/4/4
12	UTI	8	600	-	-	10/34/34/34	0/4/4/4
9	ATP	B	600	10	-	8/22/38/38	0/3/3/3
9	ATP	A	600	10	-	8/22/38/38	0/3/3/3
9	ATP	C	600	10	-	8/22/38/38	0/3/3/3
11	ADP	D	600	10	-	2/16/32/32	0/3/3/3
12	UTI	6	600	-	-	6/34/34/34	0/4/4/4
12	UTI	9	600	-	-	8/34/34/34	0/4/4/4
11	ADP	F	600	10	-	3/16/32/32	0/3/3/3
12	UTI	5	600	-	-	6/34/34/34	0/4/4/4
12	UTI	7	600	-	-	7/34/34/34	0/4/4/4
12	UTI	1	600	-	-	6/34/34/34	0/4/4/4

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	600	ADP	C5-C4	4.43	1.47	1.39
9	B	600	ATP	C5-C4	4.41	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	600	ATP	C5-C4	4.40	1.46	1.39
9	A	600	ATP	C5-C4	4.39	1.46	1.39
11	D	600	ADP	C5-C4	4.26	1.46	1.39
12	6	600	UTI	O13-C11	4.19	1.41	1.35
12	8	600	UTI	O13-C11	4.16	1.41	1.35
12	1	600	UTI	C35-C30	-4.16	1.36	1.42
12	5	600	UTI	O13-C11	4.15	1.41	1.35
12	7	600	UTI	O13-C11	4.13	1.41	1.35
12	9	600	UTI	O13-C11	4.13	1.41	1.35
12	4	600	UTI	O13-C11	4.09	1.41	1.35
12	1	600	UTI	O13-C11	3.83	1.41	1.35
12	6	600	UTI	O40-C06	-3.70	1.37	1.43
12	4	600	UTI	O40-C06	-3.65	1.37	1.43
12	8	600	UTI	O15-C09	3.64	1.41	1.35
12	5	600	UTI	O40-C06	-3.64	1.37	1.43
12	1	600	UTI	O40-C06	-3.63	1.37	1.43
12	7	600	UTI	O15-C09	3.60	1.41	1.35
12	7	600	UTI	O40-C06	-3.59	1.37	1.43
12	5	600	UTI	C35-C30	-3.58	1.36	1.42
12	8	600	UTI	C35-C30	-3.57	1.36	1.42
12	9	600	UTI	O15-C09	3.56	1.40	1.35
12	6	600	UTI	O15-C09	3.56	1.40	1.35
12	9	600	UTI	O40-C06	-3.53	1.37	1.43
12	5	600	UTI	O15-C09	3.52	1.40	1.35
12	7	600	UTI	C35-C30	-3.50	1.37	1.42
12	4	600	UTI	O15-C09	3.49	1.40	1.35
12	9	600	UTI	C35-C30	-3.46	1.37	1.42
12	8	600	UTI	O40-C06	-3.45	1.37	1.43
12	4	600	UTI	C35-C30	-3.42	1.37	1.42
12	6	600	UTI	C35-C30	-3.31	1.37	1.42
12	8	600	UTI	O38-C28	3.24	1.40	1.35
12	7	600	UTI	O38-C28	3.19	1.39	1.35
12	9	600	UTI	O38-C28	3.18	1.39	1.35
12	5	600	UTI	O38-C28	3.18	1.39	1.35
12	4	600	UTI	O38-C28	3.18	1.39	1.35
12	6	600	UTI	O38-C28	3.17	1.39	1.35
12	8	600	UTI	C06-C07	3.02	1.56	1.52
12	6	600	UTI	C06-C07	2.99	1.56	1.52
12	1	600	UTI	C06-C17	-2.99	1.53	1.57
12	7	600	UTI	C06-C07	2.95	1.56	1.52
12	9	600	UTI	C06-C07	2.92	1.56	1.52
12	4	600	UTI	C06-C07	2.86	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	600	UTI	C06-C07	2.73	1.56	1.52
12	9	600	UTI	O24-C20	2.73	1.41	1.37
12	7	600	UTI	O24-C20	2.68	1.41	1.37
12	6	600	UTI	O24-C20	2.65	1.41	1.37
12	5	600	UTI	O24-C20	2.63	1.41	1.37
12	4	600	UTI	O24-C20	2.61	1.41	1.37
12	8	600	UTI	O24-C20	2.60	1.41	1.37
9	C	600	ATP	C5-C6	2.59	1.48	1.41
12	1	600	UTI	O15-C09	2.57	1.39	1.35
9	B	600	ATP	C5-C6	2.57	1.48	1.41
9	A	600	ATP	C5-C6	2.56	1.48	1.41
11	F	600	ADP	C5-C6	2.51	1.48	1.41
11	D	600	ADP	C5-C6	2.49	1.47	1.41
11	F	600	ADP	C5-N7	-2.49	1.34	1.39
11	D	600	ADP	C5-N7	-2.48	1.34	1.39
9	C	600	ATP	C5-N7	-2.42	1.34	1.39
9	B	600	ATP	C5-N7	-2.38	1.34	1.39
9	A	600	ATP	C5-N7	-2.37	1.34	1.39
12	8	600	UTI	C18-C17	2.31	1.55	1.52
12	1	600	UTI	C06-C07	2.28	1.55	1.52
12	6	600	UTI	C18-C17	2.28	1.55	1.52
12	1	600	UTI	O24-C20	2.26	1.40	1.37
9	C	600	ATP	C8-N7	2.21	1.35	1.31
9	B	600	ATP	C8-N7	2.20	1.35	1.31
12	8	600	UTI	C05-C04	2.20	1.57	1.52
12	4	600	UTI	BR37-C33	2.19	1.94	1.90
12	9	600	UTI	C05-C04	2.16	1.57	1.52
9	A	600	ATP	C8-N7	2.16	1.35	1.31
12	9	600	UTI	BR37-C33	2.16	1.94	1.90
12	7	600	UTI	C05-C04	2.15	1.57	1.52
12	6	600	UTI	BR37-C33	2.14	1.94	1.90
12	8	600	UTI	BR37-C33	2.14	1.94	1.90
12	1	600	UTI	C05-C04	2.14	1.57	1.52
12	4	600	UTI	C05-C04	2.13	1.57	1.52
11	F	600	ADP	C8-N7	2.09	1.35	1.31
11	D	600	ADP	C8-N7	2.09	1.35	1.31
9	A	600	ATP	C4-N9	-2.09	1.33	1.37
12	1	600	UTI	O38-C28	2.07	1.38	1.35
12	5	600	UTI	C05-C04	2.07	1.57	1.52
9	B	600	ATP	C4-N9	-2.06	1.33	1.37
9	C	600	ATP	C4-N9	-2.06	1.33	1.37
12	9	600	UTI	C18-C17	2.04	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	9	600	UTI	C34-C33	2.04	1.40	1.36
11	D	600	ADP	C4-N9	-2.03	1.33	1.37
12	6	600	UTI	C05-C04	2.03	1.57	1.52
12	5	600	UTI	BR37-C33	2.01	1.94	1.90

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	1	600	UTI	C39-O38-C28	-8.02	109.70	117.20
12	8	600	UTI	C27-C28-N29	-6.19	120.86	125.71
12	9	600	UTI	C27-C28-N29	-5.96	121.04	125.71
11	F	600	ADP	C5-C4-N3	-5.80	118.73	126.72
11	D	600	ADP	C5-C4-N3	-5.78	118.76	126.72
9	A	600	ATP	C5-C4-N3	-5.71	118.86	126.72
12	6	600	UTI	C27-C28-N29	-5.70	121.24	125.71
12	7	600	UTI	C27-C28-N29	-5.68	121.26	125.71
12	1	600	UTI	C09-N10-C11	5.68	121.55	115.69
9	B	600	ATP	C5-C4-N3	-5.67	118.91	126.72
9	C	600	ATP	C5-C4-N3	-5.67	118.91	126.72
12	5	600	UTI	C27-C28-N29	-5.64	121.29	125.71
12	4	600	UTI	C27-C28-N29	-5.61	121.31	125.71
12	6	600	UTI	C09-N10-C11	5.35	121.21	115.69
12	4	600	UTI	C09-N10-C11	5.33	121.19	115.69
12	1	600	UTI	C27-C28-N29	-5.31	121.55	125.71
12	7	600	UTI	C09-N10-C11	5.30	121.16	115.69
12	9	600	UTI	C09-N10-C11	5.28	121.14	115.69
12	1	600	UTI	C16-O15-C09	-5.27	109.48	117.33
12	8	600	UTI	C09-N10-C11	5.24	121.09	115.69
12	5	600	UTI	C09-N10-C11	5.14	120.99	115.69
12	6	600	UTI	O24-C20-C19	4.88	119.98	116.28
12	7	600	UTI	O24-C20-C19	4.80	119.92	116.28
12	8	600	UTI	O24-C20-C19	4.75	119.89	116.28
11	F	600	ADP	N3-C4-N9	4.66	135.09	127.17
11	D	600	ADP	N3-C4-N9	4.62	135.03	127.17
12	4	600	UTI	O24-C20-C19	4.57	119.75	116.28
12	9	600	UTI	O24-C20-C19	4.57	119.75	116.28
12	5	600	UTI	O24-C20-C19	4.51	119.70	116.28
9	A	600	ATP	N3-C4-N9	4.51	134.84	127.17
9	B	600	ATP	N3-C4-N9	4.50	134.82	127.17
9	C	600	ATP	N3-C4-N9	4.48	134.78	127.17
12	1	600	UTI	O38-C28-C27	4.28	120.13	115.05
12	5	600	UTI	C39-O38-C28	-4.08	113.39	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	1	600	UTI	C25-O24-C20	-3.96	111.70	117.51
12	9	600	UTI	O38-C28-C27	3.87	119.64	115.05
12	9	600	UTI	C39-O38-C28	-3.85	113.60	117.20
12	1	600	UTI	C36-C27-C17	-3.78	118.77	123.66
11	D	600	ADP	C2-N3-C4	3.76	121.02	111.83
11	F	600	ADP	C2-N3-C4	3.70	120.87	111.83
9	A	600	ATP	C2-N3-C4	3.63	120.70	111.83
9	C	600	ATP	C2-N3-C4	3.62	120.67	111.83
9	B	600	ATP	C2-N3-C4	3.60	120.62	111.83
12	8	600	UTI	O38-C28-C27	3.52	119.22	115.05
12	8	600	UTI	C39-O38-C28	-3.48	113.95	117.20
12	5	600	UTI	O38-C28-C27	3.46	119.16	115.05
9	A	600	ATP	C4-C5-N7	-3.46	106.63	110.58
9	B	600	ATP	C4-C5-N7	-3.44	106.65	110.58
12	4	600	UTI	O38-C28-C27	3.44	119.13	115.05
9	C	600	ATP	C4-C5-N7	-3.42	106.67	110.58
11	D	600	ADP	N3-C2-N1	-3.42	123.41	128.58
11	D	600	ADP	C4-C5-N7	-3.38	106.72	110.58
12	7	600	UTI	O38-C28-C27	3.36	119.04	115.05
11	F	600	ADP	C4-C5-N7	-3.36	106.74	110.58
12	4	600	UTI	C39-O38-C28	-3.31	114.10	117.20
12	6	600	UTI	C39-O38-C28	-3.31	114.11	117.20
11	F	600	ADP	N3-C2-N1	-3.28	123.62	128.58
12	6	600	UTI	O38-C28-C27	3.19	118.84	115.05
9	A	600	ATP	N3-C2-N1	-3.18	123.77	128.58
9	C	600	ATP	N3-C2-N1	-3.18	123.77	128.58
9	B	600	ATP	N3-C2-N1	-3.15	123.81	128.58
12	7	600	UTI	C39-O38-C28	-3.14	114.26	117.20
12	8	600	UTI	C36-C27-C17	-3.04	119.73	123.66
12	8	600	UTI	C25-O24-C20	-3.00	113.11	117.51
12	1	600	UTI	C12-C11-N10	-3.00	120.66	124.16
12	4	600	UTI	C25-O24-C20	-2.93	113.22	117.51
12	1	600	UTI	O24-C20-C19	2.88	118.46	116.28
12	1	600	UTI	C14-O13-C11	-2.86	113.07	117.33
12	6	600	UTI	C25-O24-C20	-2.82	113.38	117.51
12	6	600	UTI	O40-C06-C17	2.82	112.04	108.41
9	B	600	ATP	C4-N9-C8	2.80	108.67	105.74
11	D	600	ADP	C2'-C1'-N9	-2.78	106.39	113.30
11	D	600	ADP	C4-N9-C8	2.76	108.64	105.74
9	A	600	ATP	C4-N9-C8	2.76	108.64	105.74
12	5	600	UTI	C16-O15-C09	-2.74	113.25	117.33
12	8	600	UTI	O24-C20-C21	-2.74	119.69	124.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	600	UTI	C25-O24-C20	-2.73	113.50	117.51
9	C	600	ATP	C4-N9-C8	2.73	108.61	105.74
12	6	600	UTI	O24-C20-C21	-2.72	119.71	124.30
12	8	600	UTI	C36-C27-C28	2.70	118.72	116.23
12	8	600	UTI	O40-C06-C17	2.69	111.87	108.41
12	7	600	UTI	C14-O13-C11	-2.67	113.35	117.33
12	7	600	UTI	O24-C20-C21	-2.66	119.82	124.30
11	F	600	ADP	C4-N9-C8	2.63	108.50	105.74
12	6	600	UTI	C16-O15-C09	-2.61	113.44	117.33
12	8	600	UTI	C28-N29-C30	2.59	121.80	116.38
12	4	600	UTI	C16-O15-C09	-2.57	113.51	117.33
12	4	600	UTI	O24-C20-C21	-2.57	119.97	124.30
12	9	600	UTI	C28-N29-C30	2.56	121.75	116.38
12	1	600	UTI	C28-N29-C30	2.55	121.73	116.38
12	9	600	UTI	C36-C27-C28	2.55	118.58	116.23
12	6	600	UTI	C36-C27-C28	2.55	118.58	116.23
12	7	600	UTI	C28-N29-C30	2.54	121.71	116.38
12	5	600	UTI	C28-N29-C30	2.53	121.69	116.38
12	1	600	UTI	C28-C27-C17	2.52	123.12	119.77
12	8	600	UTI	C14-O13-C11	-2.51	113.59	117.33
12	6	600	UTI	C28-N29-C30	2.51	121.64	116.38
11	D	600	ADP	C5-N7-C8	2.51	107.39	103.45
9	A	600	ATP	C5-N7-C8	2.50	107.38	103.45
9	B	600	ATP	C5-N7-C8	2.50	107.38	103.45
12	1	600	UTI	C05-C06-C17	2.49	113.43	110.49
11	F	600	ADP	C5-N7-C8	2.49	107.37	103.45
9	C	600	ATP	C5-N7-C8	2.49	107.36	103.45
12	4	600	UTI	C14-O13-C11	-2.49	113.63	117.33
12	9	600	UTI	O24-C20-C21	-2.48	120.12	124.30
12	5	600	UTI	C23-C18-C19	2.47	119.45	116.69
11	F	600	ADP	C3'-C2'-C1'	2.47	106.14	101.46
12	4	600	UTI	C28-N29-C30	2.45	121.52	116.38
12	5	600	UTI	C14-O13-C11	-2.45	113.69	117.33
12	5	600	UTI	O24-C20-C21	-2.44	120.18	124.30
12	7	600	UTI	C25-O24-C20	-2.43	113.95	117.51
12	9	600	UTI	C16-O15-C09	-2.38	113.79	117.33
12	6	600	UTI	C12-C11-N10	-2.37	121.40	124.16
12	9	600	UTI	C12-C11-N10	-2.36	121.41	124.16
12	1	600	UTI	C06-C17-C27	-2.35	107.92	112.41
12	8	600	UTI	C08-C09-N10	-2.34	121.43	124.16
12	7	600	UTI	C08-C09-N10	-2.34	121.43	124.16
12	4	600	UTI	C23-C18-C19	2.33	119.29	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	7	600	UTI	C36-C27-C28	2.32	118.37	116.23
12	9	600	UTI	C25-O24-C20	-2.30	114.14	117.51
11	D	600	ADP	C3'-C2'-C1'	2.30	105.81	101.46
12	4	600	UTI	C12-C11-N10	-2.26	121.52	124.16
12	4	600	UTI	C36-C27-C28	2.26	118.31	116.23
12	7	600	UTI	C12-C11-N10	-2.22	121.57	124.16
12	4	600	UTI	C08-C09-N10	-2.21	121.57	124.16
12	1	600	UTI	O24-C20-C21	-2.20	120.59	124.30
12	5	600	UTI	C12-C11-N10	-2.19	121.60	124.16
12	6	600	UTI	C08-C09-N10	-2.19	121.61	124.16
12	4	600	UTI	O40-C06-C17	2.19	111.22	108.41
12	9	600	UTI	C14-O13-C11	-2.18	114.08	117.33
11	F	600	ADP	C2'-C1'-N9	-2.17	107.91	113.30
12	9	600	UTI	C23-C18-C19	2.17	119.11	116.69
12	8	600	UTI	C12-C11-N10	-2.16	121.64	124.16
12	5	600	UTI	C36-C27-C28	2.15	118.21	116.23
12	9	600	UTI	O40-C06-C17	2.13	111.14	108.41
12	9	600	UTI	C08-C09-N10	-2.12	121.69	124.16
9	A	600	ATP	C6-C5-N7	2.11	136.16	132.09
9	B	600	ATP	C6-C5-N7	2.11	136.16	132.09
12	5	600	UTI	C08-C09-N10	-2.11	121.70	124.16
9	C	600	ATP	C6-C5-N7	2.10	136.15	132.09
12	7	600	UTI	C23-C18-C19	2.07	119.00	116.69
11	D	600	ADP	C6-C5-N7	2.07	136.07	132.09
12	1	600	UTI	C07-C08-C09	-2.07	115.95	117.87
9	B	600	ATP	N9-C8-N7	-2.05	111.03	113.94
11	D	600	ADP	N9-C8-N7	-2.04	111.04	113.94
9	A	600	ATP	N9-C8-N7	-2.03	111.05	113.94
12	1	600	UTI	C36-C27-C28	2.03	118.10	116.23
9	C	600	ATP	N9-C8-N7	-2.03	111.05	113.94
12	1	600	UTI	C07-C06-C17	2.03	113.48	110.54
12	7	600	UTI	O40-C06-C17	2.02	111.01	108.41
9	B	600	ATP	C3'-C2'-C1'	2.01	105.27	101.46
9	A	600	ATP	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	600	ATP	C5'-O5'-PA-O1A
9	B	600	ATP	C5'-O5'-PA-O1A
9	C	600	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
11	F	600	ADP	C5'-O5'-PA-O1A
11	F	600	ADP	C5'-O5'-PA-O3A
12	1	600	UTI	C19-C20-O24-C25
12	1	600	UTI	C27-C28-O38-C39
12	1	600	UTI	N29-C28-O38-C39
12	4	600	UTI	C19-C20-O24-C25
12	4	600	UTI	C27-C28-O38-C39
12	5	600	UTI	C19-C20-O24-C25
12	5	600	UTI	C27-C28-O38-C39
12	6	600	UTI	C19-C20-O24-C25
12	7	600	UTI	C12-C11-O13-C14
12	7	600	UTI	N10-C11-O13-C14
12	7	600	UTI	C19-C20-O24-C25
12	8	600	UTI	C12-C11-O13-C14
12	8	600	UTI	N10-C11-O13-C14
12	8	600	UTI	C06-C17-C18-C19
12	8	600	UTI	C19-C20-O24-C25
12	9	600	UTI	C12-C11-O13-C14
12	9	600	UTI	N10-C11-O13-C14
12	9	600	UTI	C19-C20-O24-C25
12	6	600	UTI	C12-C11-O13-C14
12	7	600	UTI	C08-C09-O15-C16
12	6	600	UTI	N10-C11-O13-C14
12	7	600	UTI	N10-C09-O15-C16
12	8	600	UTI	N10-C09-O15-C16
12	4	600	UTI	N29-C28-O38-C39
12	5	600	UTI	N29-C28-O38-C39
11	D	600	ADP	O4'-C4'-C5'-O5'
12	1	600	UTI	C05-C04-N02-C03
12	8	600	UTI	C08-C09-O15-C16
12	9	600	UTI	C21-C20-O24-C25
12	7	600	UTI	C21-C20-O24-C25
12	8	600	UTI	C21-C20-O24-C25
12	6	600	UTI	C21-C20-O24-C25
12	1	600	UTI	C21-C20-O24-C25
12	1	600	UTI	C05-C04-N02-C01
12	7	600	UTI	C05-C04-N02-C03
12	8	600	UTI	C05-C04-N02-C03
9	A	600	ATP	O4'-C4'-C5'-O5'
9	B	600	ATP	O4'-C4'-C5'-O5'
9	C	600	ATP	O4'-C4'-C5'-O5'
12	5	600	UTI	C21-C20-O24-C25

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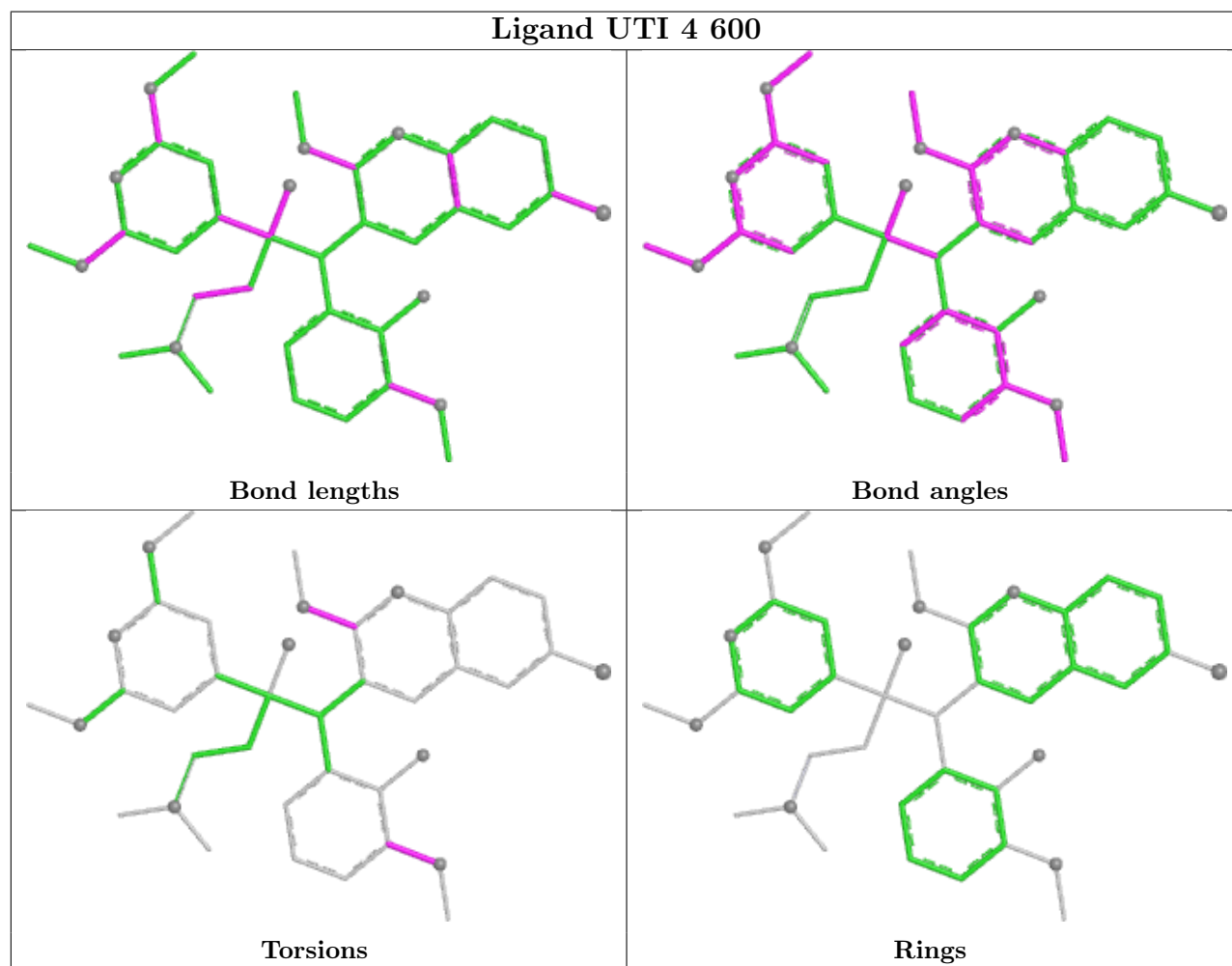
Mol	Chain	Res	Type	Atoms
12	6	600	UTI	N10-C09-O15-C16
12	4	600	UTI	C21-C20-O24-C25
12	8	600	UTI	C05-C04-N02-C01
12	6	600	UTI	C08-C09-O15-C16
11	D	600	ADP	C3'-C4'-C5'-O5'
9	A	600	ATP	PA-O3A-PB-O1B
9	B	600	ATP	PA-O3A-PB-O1B
9	C	600	ATP	PA-O3A-PB-O1B
9	A	600	ATP	C3'-C4'-C5'-O5'
12	8	600	UTI	C06-C17-C18-C23
9	B	600	ATP	C3'-C4'-C5'-O5'
9	C	600	ATP	C3'-C4'-C5'-O5'
9	A	600	ATP	C5'-O5'-PA-O2A
9	A	600	ATP	C5'-O5'-PA-O3A
9	B	600	ATP	C5'-O5'-PA-O2A
9	B	600	ATP	C5'-O5'-PA-O3A
9	C	600	ATP	C5'-O5'-PA-O2A
9	C	600	ATP	C5'-O5'-PA-O3A
11	F	600	ADP	C5'-O5'-PA-O2A
12	9	600	UTI	N29-C28-O38-C39
12	5	600	UTI	C12-C11-O13-C14
12	9	600	UTI	C05-C04-N02-C03
12	5	600	UTI	N10-C11-O13-C14
9	A	600	ATP	PG-O3B-PB-O2B
9	A	600	ATP	PA-O3A-PB-O2B
9	B	600	ATP	PG-O3B-PB-O2B
9	B	600	ATP	PA-O3A-PB-O2B
9	C	600	ATP	PG-O3B-PB-O2B
9	C	600	ATP	PA-O3A-PB-O2B
12	9	600	UTI	C27-C28-O38-C39
12	9	600	UTI	C04-C05-C06-C07

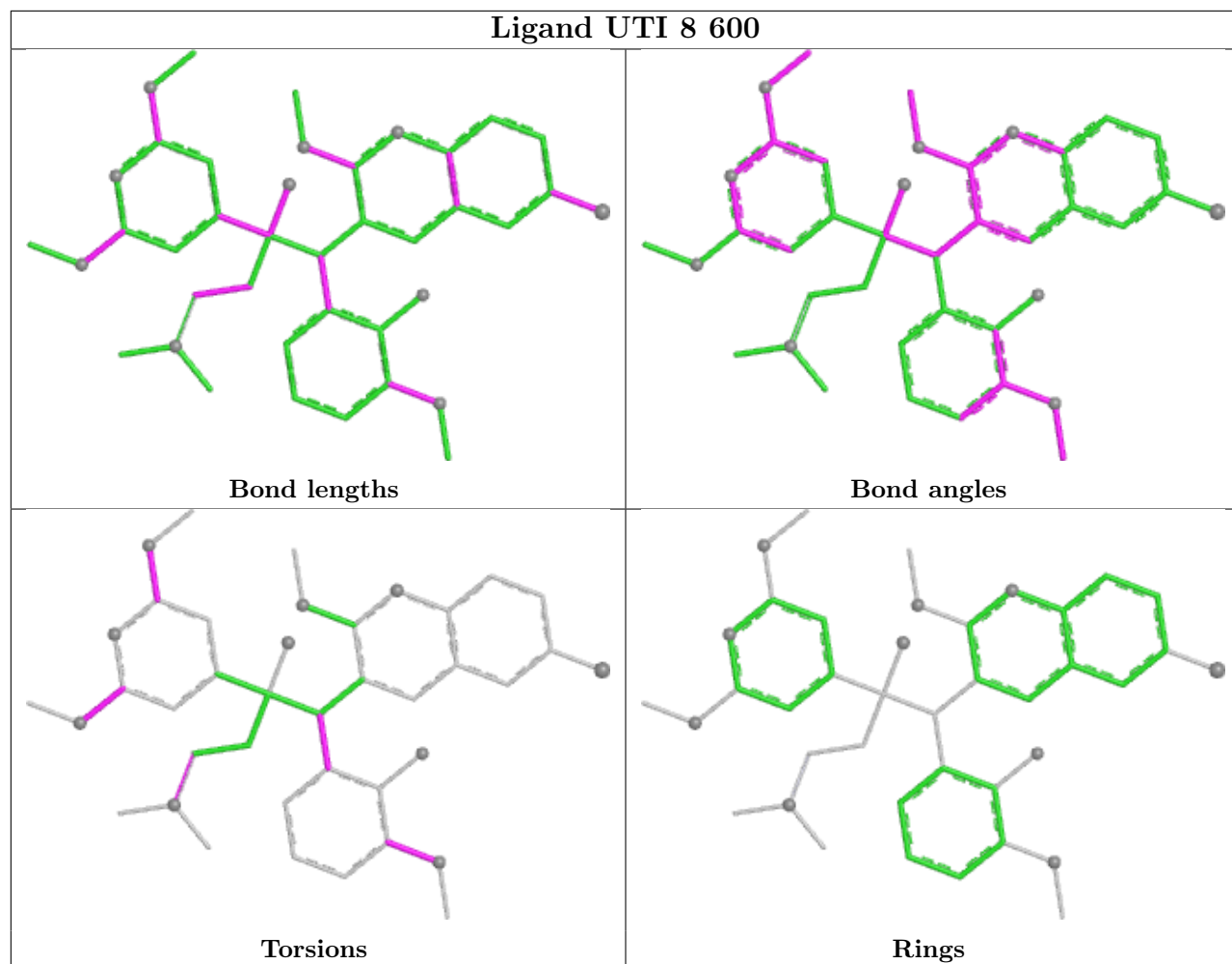
There are no ring outliers.

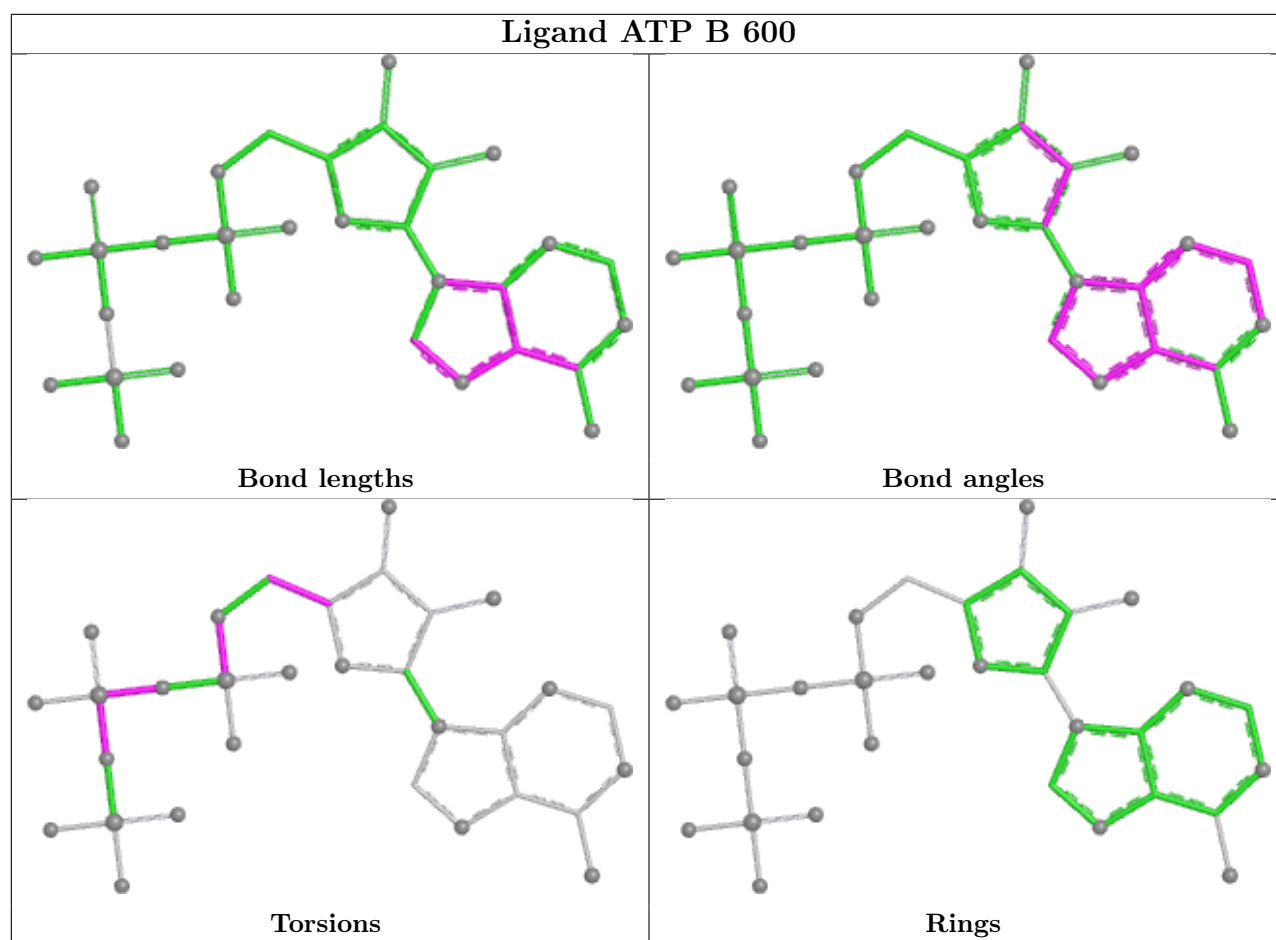
5 monomers are involved in 13 short contacts:

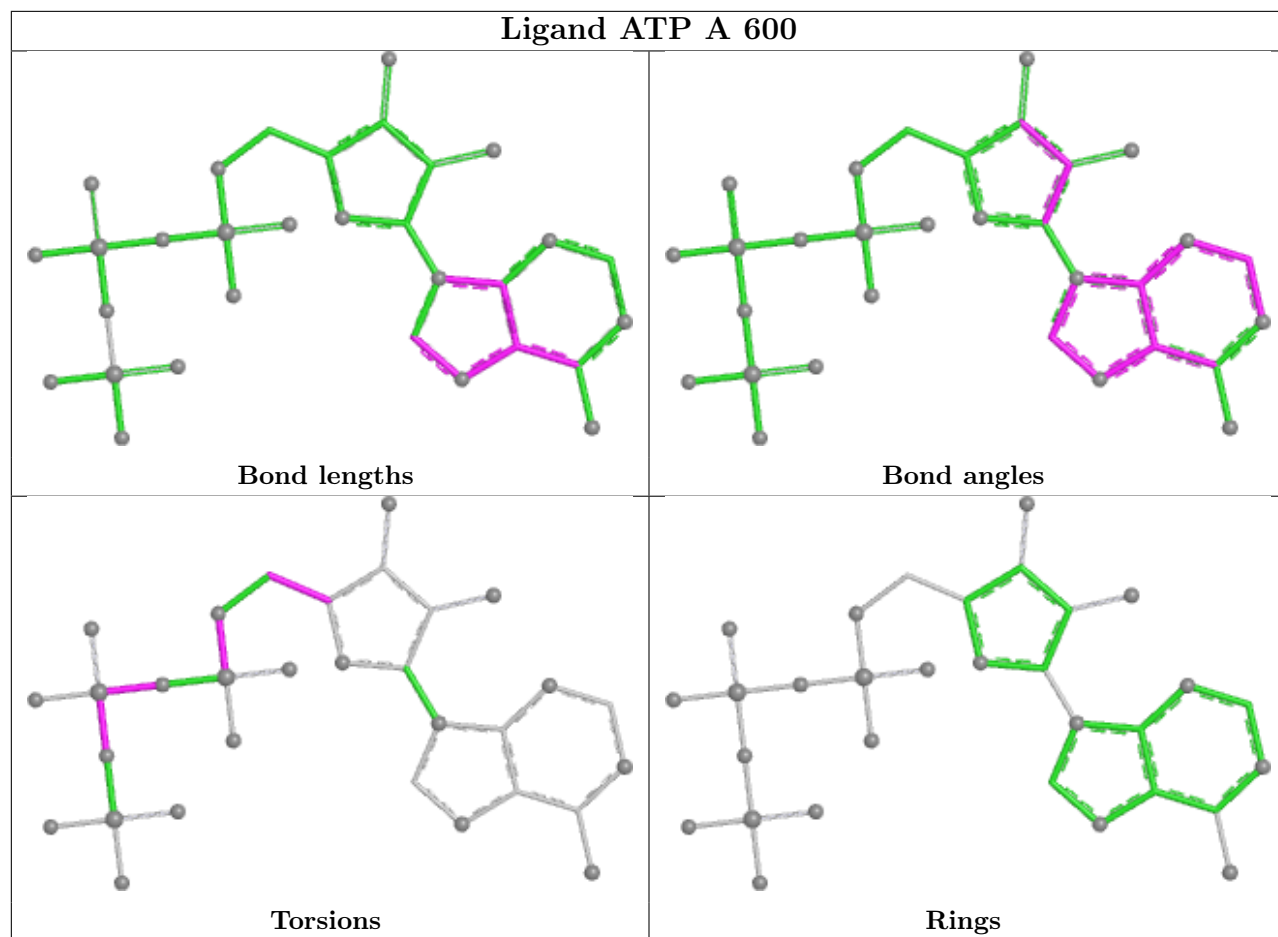
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	600	ADP	1	0
12	6	600	UTI	1	0
12	9	600	UTI	1	0
11	F	600	ADP	4	0
12	1	600	UTI	6	0

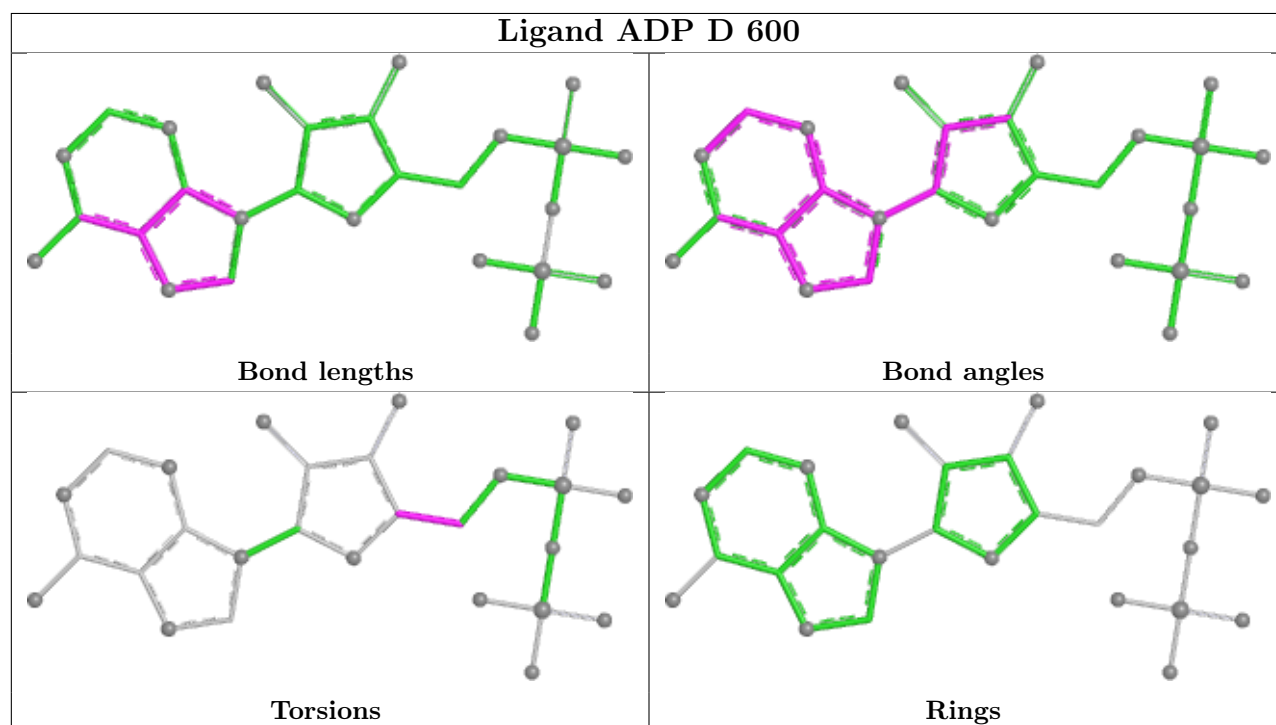
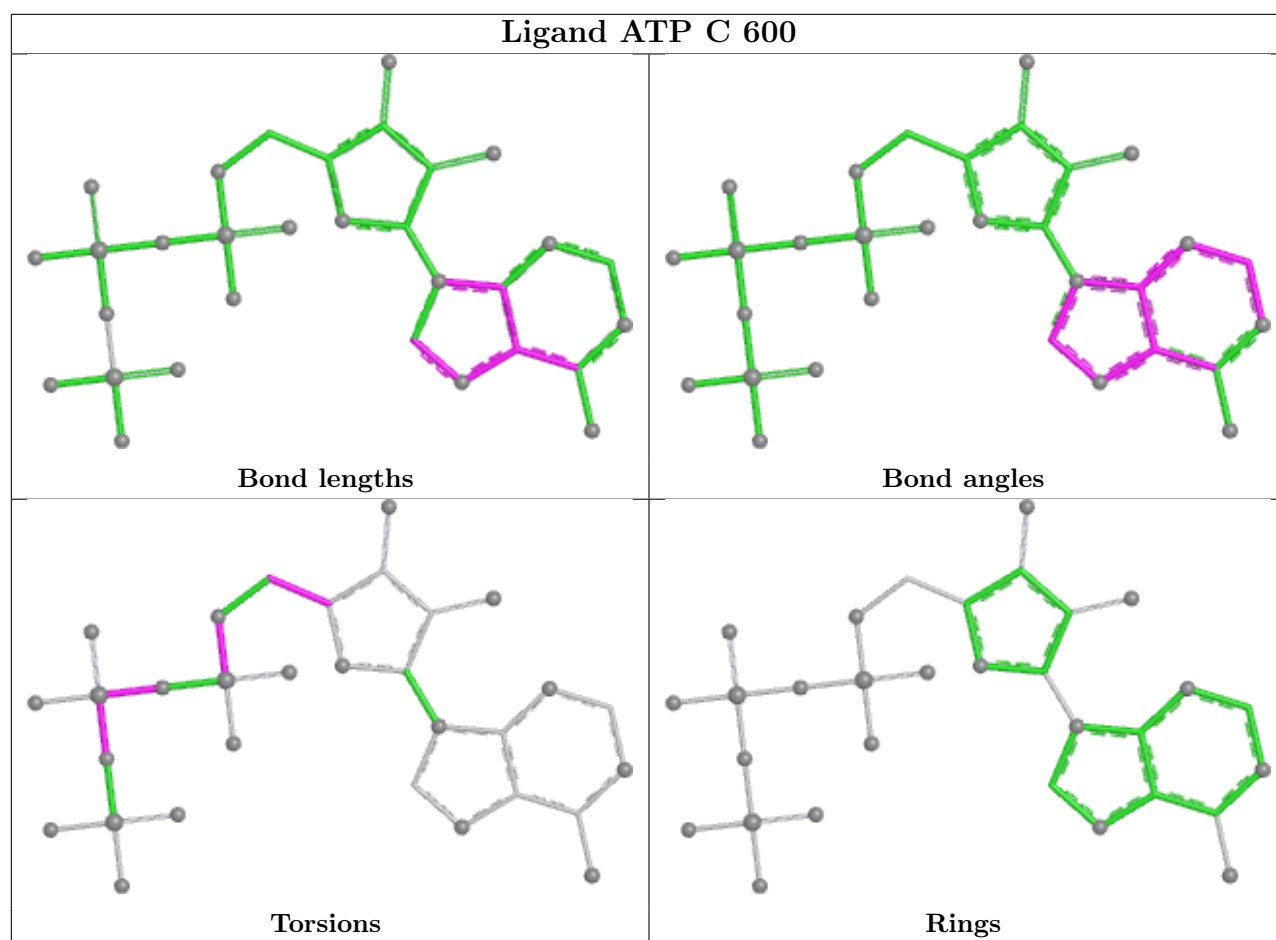
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

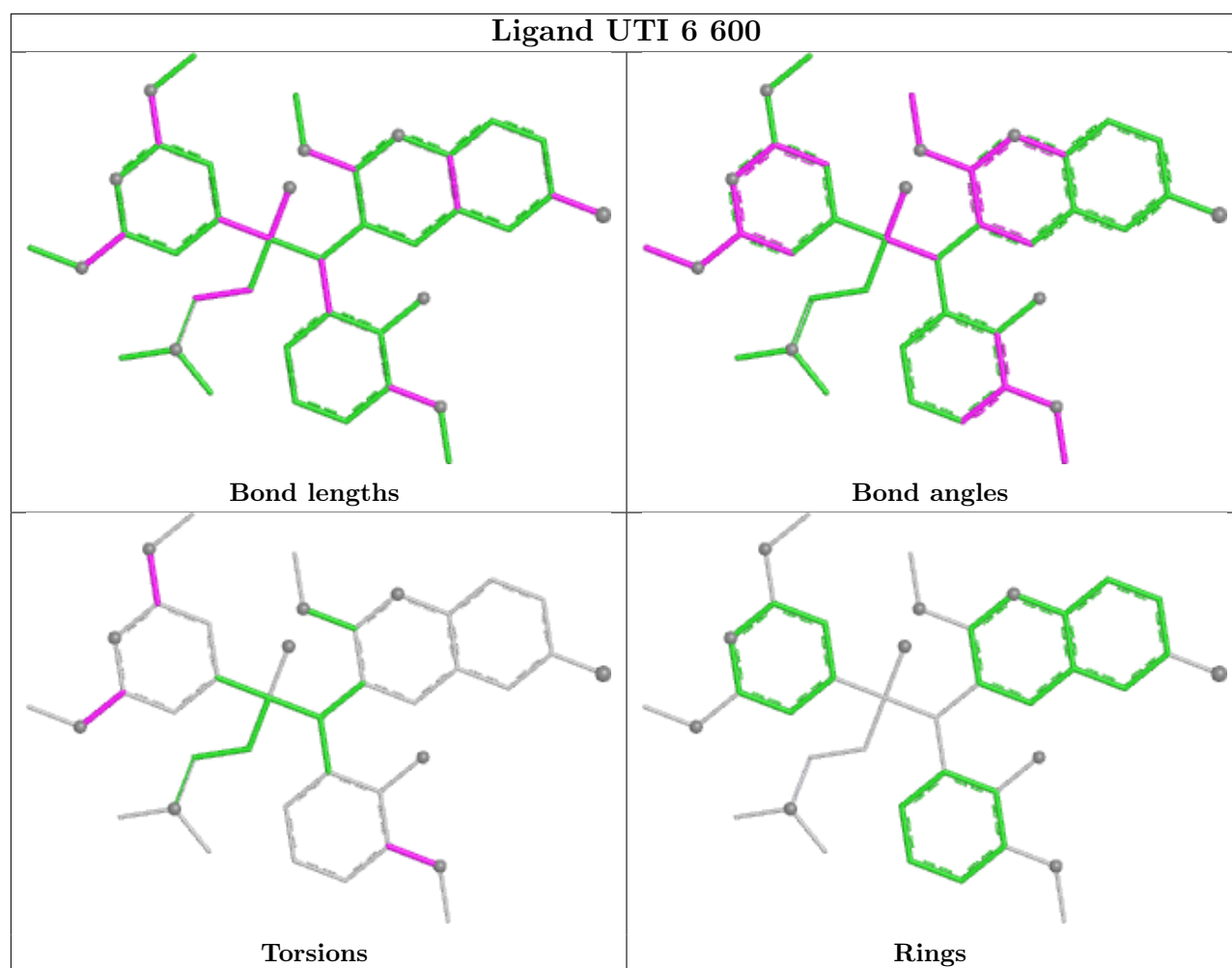




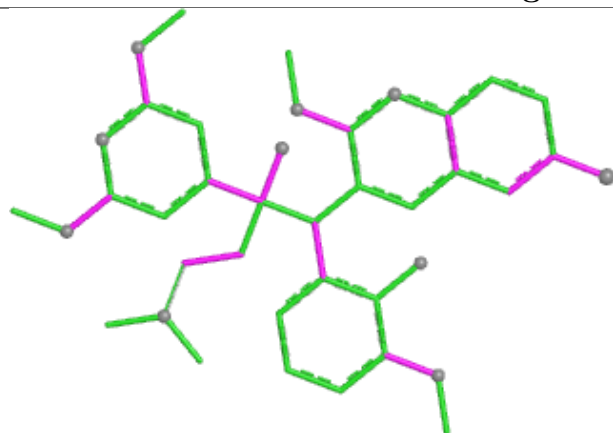




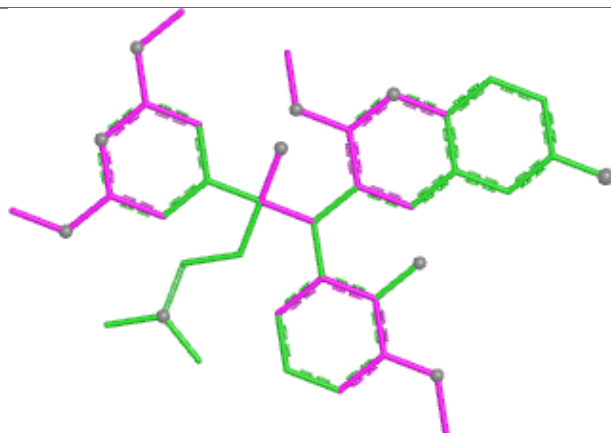




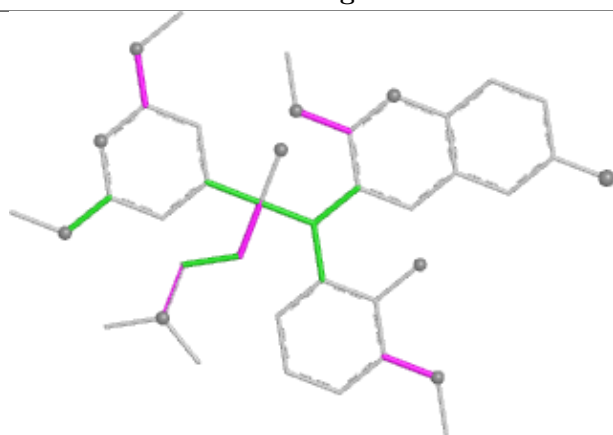
Ligand UTI 9 600



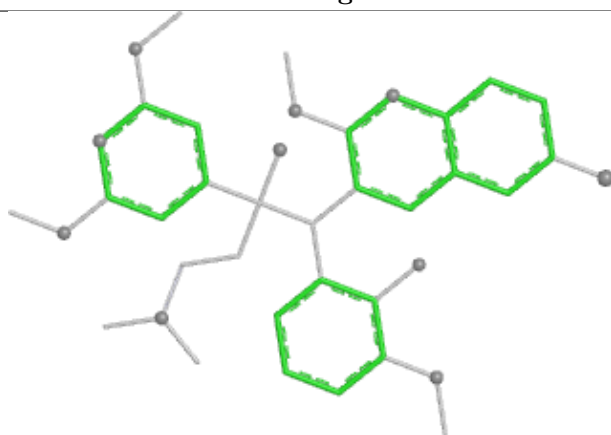
Bond lengths



Bond angles

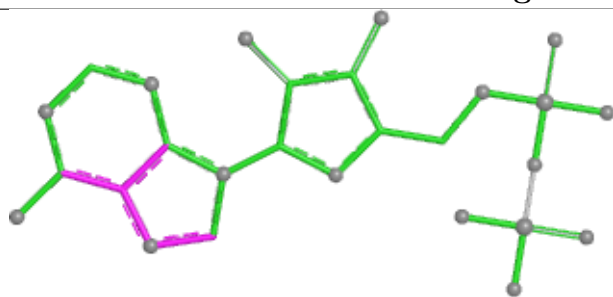


Torsions

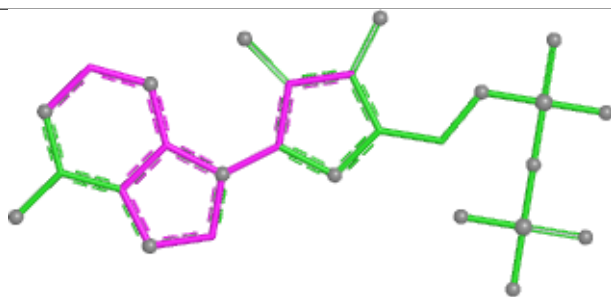


Rings

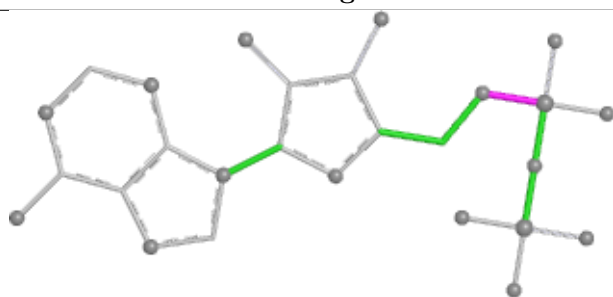
Ligand ADP F 600



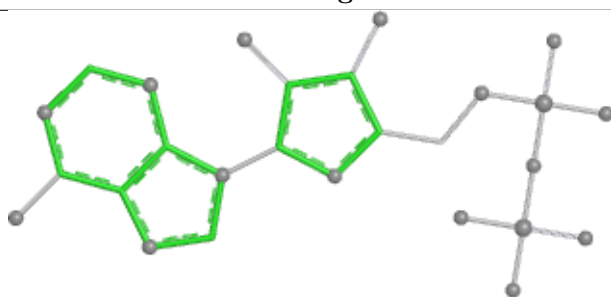
Bond lengths



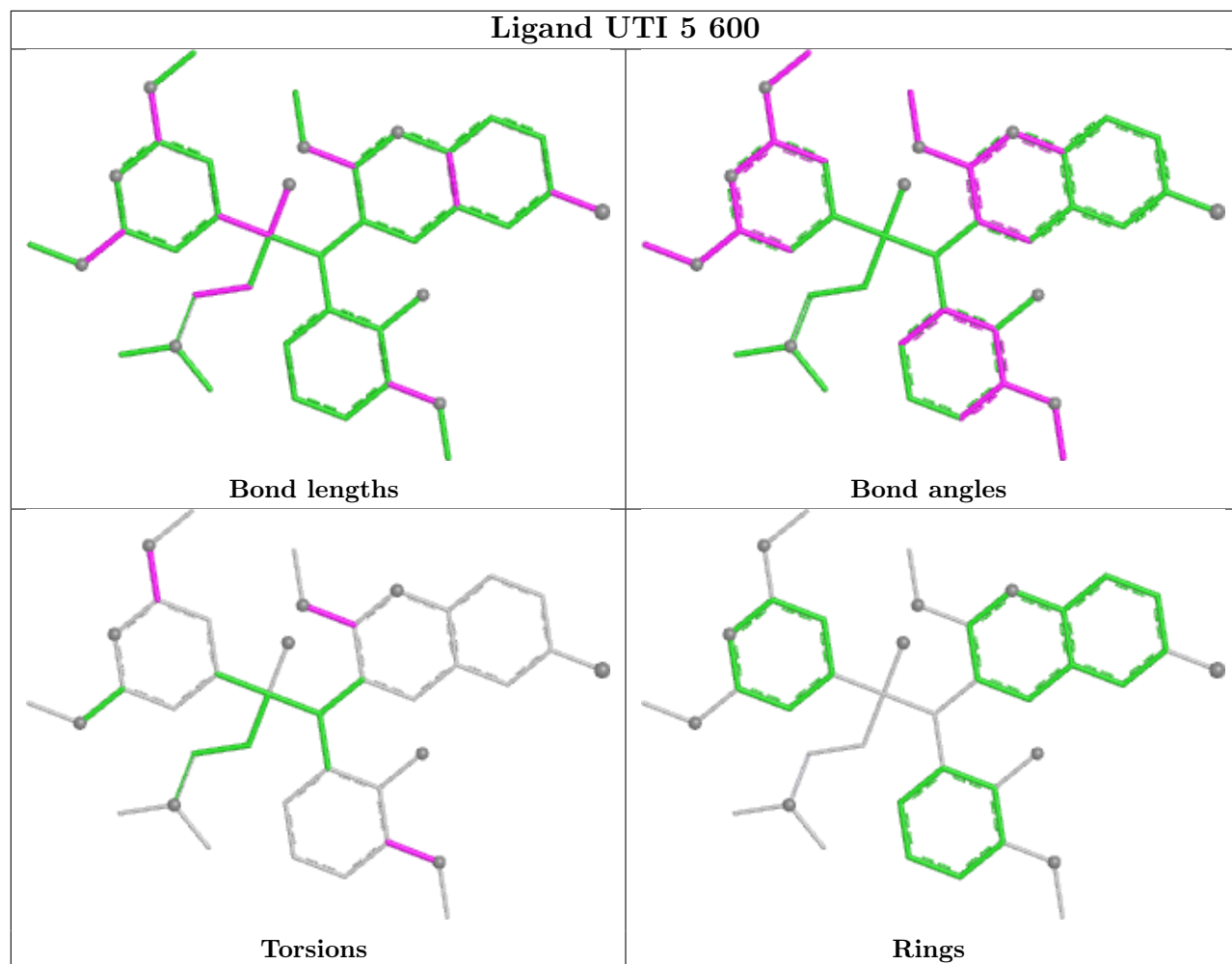
Bond angles

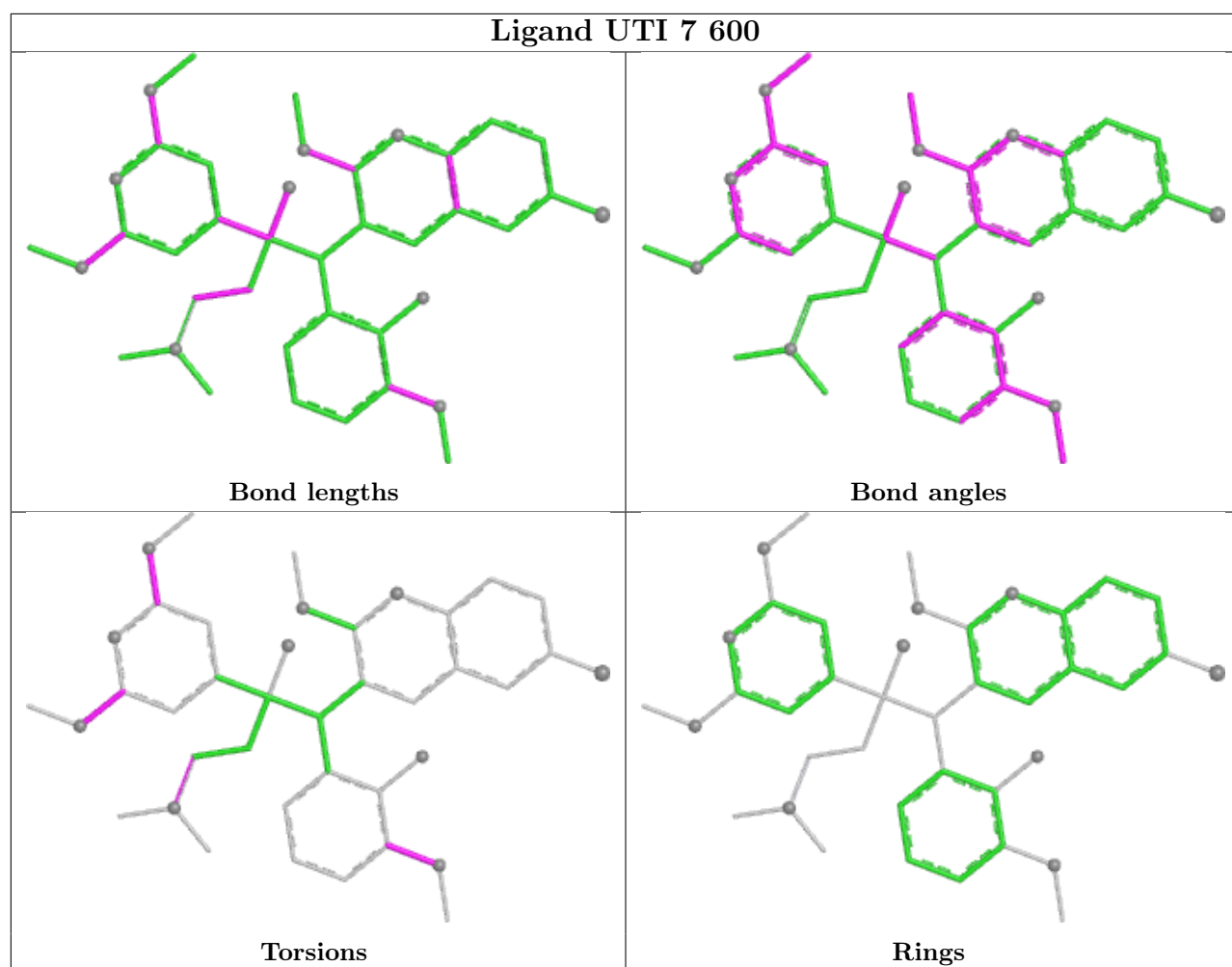


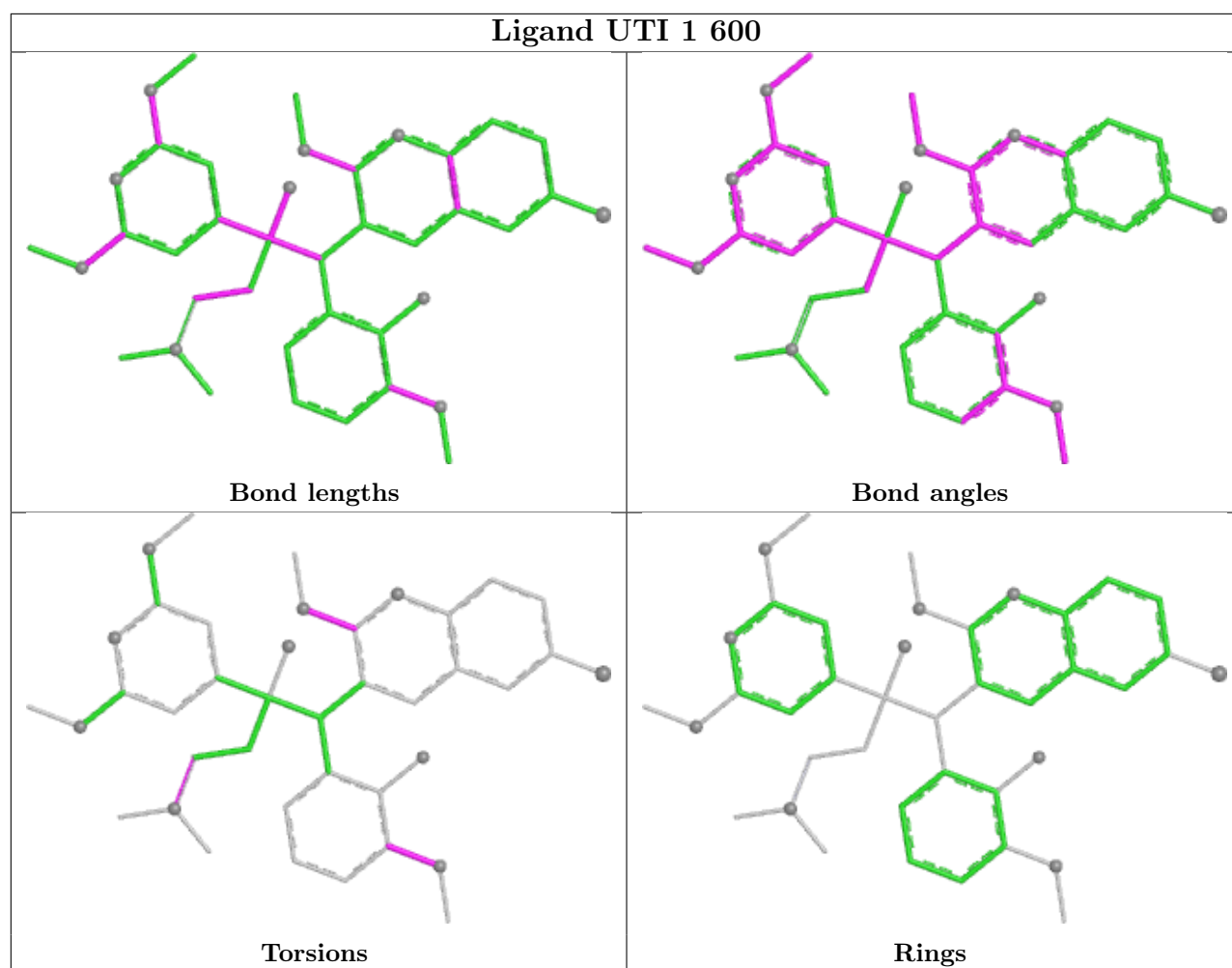
Torsions



Rings







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 Map visualisation

This section contains visualisations of the EMDB entry EMD-36589. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.