



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 29, 2022 – 12:05 PM EDT

PDB ID : 7RGA
Title : Crystal structure of nanoCLAMP3:VHH in complex with MTX
Authors : Guo, Z.; Alexandrov, K.
Deposited on : 2021-07-14
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

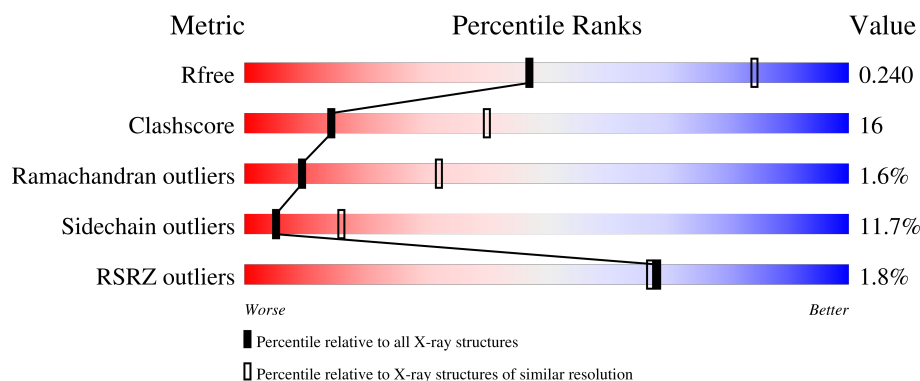
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	306	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>18%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	306	<div> <div></div> <div>58%</div> <div>25%</div> <div>• •</div> <div>13%</div> </div>
1	C	306	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>20%</div> <div>5%</div> <div>13%</div> </div> </div>
1	D	306	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>23%</div> <div>•</div> <div>13%</div> </div> </div>
1	E	306	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>25%</div> <div>•</div> <div>12%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	306	
1	G	306	

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	MTX	A	301	-	-	X	-

2 Entry composition [i](#)

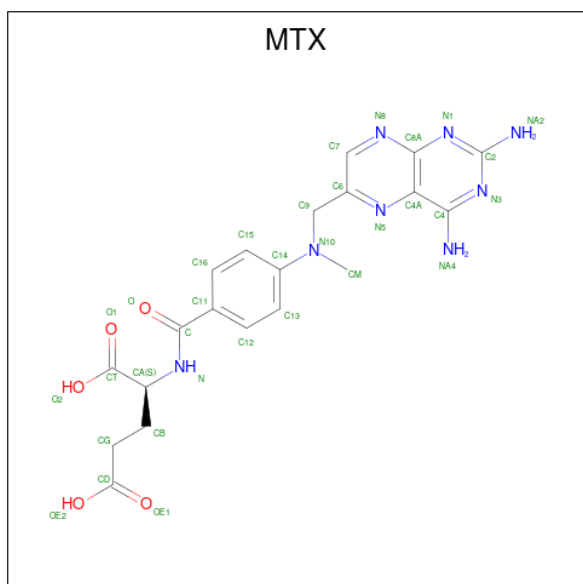
There are 4 unique types of molecules in this entry. The entry contains 14664 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 nano CLostridial Antibody Mimetic Protein 3 VHH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2011	1262	345	401	3			
1	B	265	Total	C	N	O	S	0	0	0
			2064	1293	356	411	4			
1	C	265	Total	C	N	O	S	0	0	0
			2062	1293	353	412	4			
1	D	265	Total	C	N	O	S	0	0	0
			2050	1283	352	411	4			
1	E	270	Total	C	N	O	S	0	0	0
			2104	1316	367	417	4			
1	F	265	Total	C	N	O	S	0	0	0
			2065	1295	356	411	3			
1	G	265	Total	C	N	O	S	0	0	0
			2060	1289	355	412	4			

- Molecule 2 is METHOTREXATE (three-letter code: MTX) (formula: $C_{20}H_{22}N_8O_5$) (labeled as "Ligand of Interest" by depositor).



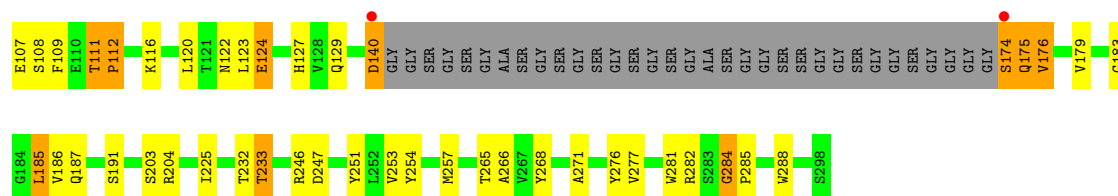
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	20	8	5		
2	B	1	Total	C	N	O	0	0
			33	20	8	5		
2	C	1	Total	C	N	O	0	0
			33	20	8	5		
2	D	1	Total	C	N	O	0	0
			33	20	8	5		
2	E	1	Total	C	N	O	0	0
			33	20	8	5		
2	F	1	Total	C	N	O	0	0
			33	20	8	5		
2	G	1	Total	C	N	O	0	0
			33	20	8	5		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

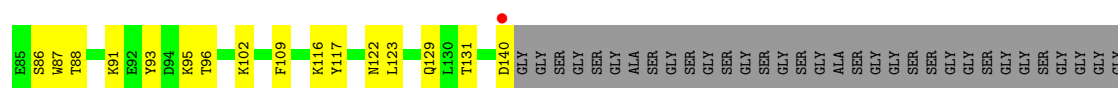
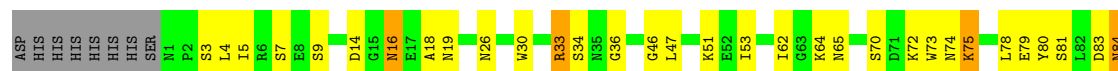
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		
3	B	2	Total	Na	0	0
			2	2		
3	C	2	Total	Na	0	0
			2	2		
3	D	2	Total	Na	0	0
			2	2		
3	E	2	Total	Na	0	0
			2	2		
3	F	2	Total	Na	0	0
			2	2		
3	G	2	Total	Na	0	0
			2	2		

- Molecule 4 is water.

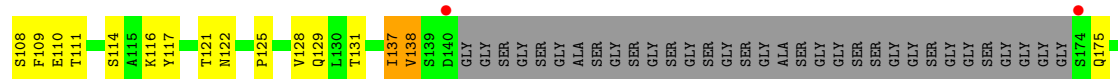
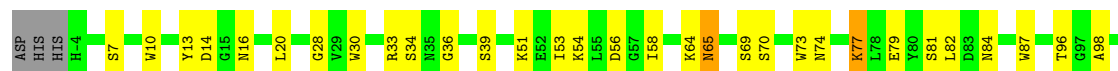
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		



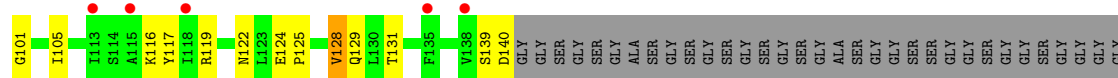
• Molecule 1: nano CLostridial Antibody Mimetic Protein 3 VHH



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4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.20Å 143.97Å 181.81Å 90.00° 94.34° 90.00°	Depositor
Resolution (Å)	48.38 – 2.90 48.38 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.38-2.90) 100.0 (48.38-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.195 , 0.242 0.199 , 0.240	Depositor DCC
R_{free} test set	4949 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	74.1	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14664	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.01	0/2053	1.02	0/2781
1	B	1.05	0/2108	0.98	0/2850
1	C	1.05	0/2106	0.99	0/2849
1	D	0.96	0/2092	0.97	0/2829
1	E	0.93	0/2151	0.98	0/2909
1	F	0.90	0/2109	0.93	0/2852
1	G	0.88	0/2104	0.95	0/2845
All	All	0.97	0/14723	0.98	0/19915

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	2011	0	1886	57	0
1	B	2064	0	1970	70	0
1	C	2062	0	1965	56	0
1	D	2050	0	1956	49	0
1	E	2104	0	1996	72	0
1	F	2065	0	1974	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2060	0	1957	77	0
2	A	33	0	20	13	0
2	B	33	0	20	4	0
2	C	33	0	20	6	0
2	D	33	0	20	3	0
2	E	33	0	20	7	0
2	F	33	0	20	1	0
2	G	33	0	20	7	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
4	A	3	0	0	0	0
All	All	14664	0	13844	443	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (443) 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)
2:B:301:MTX:CD	2:B:301:MTX:CT	2.36	1.03
1:G:59:ARG:HH21	1:G:59:ARG:HG2	1.20	1.02
1:B:38:ALA:HB2	1:B:127:HIS:HD2	1.26	1.00
1:A:200:ARG:HG3	1:A:200:ARG:HH11	1.20	1.00
1:B:265:THR:HG23	1:B:295:THR:HA	1.44	0.97
1:A:265:THR:HG23	1:A:295:THR:HA	1.47	0.94
2:C:301:MTX:CT	2:C:301:MTX:CD	2.45	0.94
1:A:230:ARG:HD3	1:B:230:ARG:HH21	1.34	0.93
1:D:16:ASN:HD22	1:D:18:ALA:H	0.97	0.92
2:C:301:MTX:CD	2:C:301:MTX:O1	2.18	0.91
1:E:30:TRP:HA	1:E:131:THR:HG22	1.54	0.89
2:A:301:MTX:O1	2:A:301:MTX:HG1	1.73	0.89
1:A:204:ARG:HG3	1:B:97:GLY:HA2	1.55	0.88
1:D:33:ARG:HG2	1:D:33:ARG:HH11	1.37	0.88
1:E:193:ARG:HH21	1:E:193:ARG:HG3	1.40	0.85
1:G:59:ARG:HH21	1:G:59:ARG:CG	1.90	0.85
1:B:38:ALA:HB2	1:B:127:HIS:CD2	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:LYS:O	1:G:65:ASN:O	1.95	0.84
1:E:53:ILE:O	1:E:114:SER:HA	1.76	0.84
1:E:128:VAL:CG1	1:E:129:GLN:H	1.91	0.84
1:C:175:GLN:HG3	1:C:176:VAL:H	1.42	0.84
1:D:16:ASN:ND2	1:D:18:ALA:H	1.75	0.84
1:A:30:TRP:HE1	1:A:129:GLN:HE21	1.25	0.83
1:E:284:GLY:N	1:E:285:PRO:CD	2.42	0.82
1:A:233:THR:HG22	1:A:276:TYR:OH	1.80	0.81
2:E:301:MTX:HG2	1:G:98:ALA:HA	1.60	0.81
1:F:4:LEU:HD12	1:F:5:ILE:N	1.96	0.81
1:C:111:THR:CG2	1:C:111:THR:O	2.27	0.81
1:E:230:ARG:HH21	1:G:230:ARG:HD3	1.47	0.78
1:C:225:ILE:HG13	1:C:232:THR:HG22	1.65	0.78
1:A:204:ARG:HG3	1:B:97:GLY:CA	2.13	0.77
1:C:175:GLN:HG3	1:C:176:VAL:N	1.99	0.77
1:D:183:GLY:HA2	1:D:192:LEU:HD21	1.67	0.76
1:F:176:VAL:HG22	1:F:177:GLN:N	2.00	0.75
1:E:230:ARG:HH21	1:G:230:ARG:CD	2.00	0.75
1:E:128:VAL:HG12	1:E:129:GLN:H	1.52	0.75
1:G:204:ARG:HH11	1:G:204:ARG:CG	2.00	0.75
1:B:38:ALA:CB	1:B:127:HIS:HD2	2.00	0.74
1:E:58:ILE:HG22	1:E:137:ILE:HG22	1.68	0.74
2:E:301:MTX:CG	1:G:98:ALA:HA	2.18	0.73
1:D:33:ARG:NH1	1:D:36:GLY:O	2.21	0.73
1:B:73:TRP:CE2	1:B:122:ASN:HB2	2.24	0.73
1:B:263:GLU:OE2	1:B:263:GLU:N	2.22	0.72
1:E:200:ARG:HG3	1:E:200:ARG:HH11	1.54	0.72
1:D:30:TRP:HE1	1:D:129:GLN:HE21	1.37	0.72
1:C:65:ASN:OD1	1:C:102:LYS:HE3	1.89	0.72
1:A:175:GLN:O	1:A:175:GLN:NE2	2.22	0.72
1:F:228:ASP:OD2	1:F:230:ARG:HD2	1.89	0.71
1:A:20:LEU:O	1:A:21:LEU:HG	1.90	0.71
1:C:30:TRP:HE1	1:C:129:GLN:HE21	1.37	0.71
1:C:175:GLN:CG	1:C:176:VAL:H	2.02	0.71
1:F:4:LEU:HD12	1:F:5:ILE:H	1.54	0.71
2:C:301:MTX:O1	2:C:301:MTX:OE1	2.09	0.71
1:D:16:ASN:HD22	1:D:18:ALA:N	1.82	0.70
1:D:30:TRP:HE1	1:D:129:GLN:NE2	1.88	0.70
1:F:226:SER:O	1:F:246:ARG:NH1	2.24	0.70
1:G:180:GLU:OE2	1:G:289:GLY:HA3	1.91	0.70
1:E:284:GLY:H	1:E:285:PRO:CD	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:301:MTX:O	2:G:301:MTX:O2	2.11	0.69
1:D:271:ALA:HB1	1:D:285:PRO:HB3	1.74	0.69
1:E:204:ARG:HG3	1:G:97:GLY:HA3	1.75	0.69
1:G:128:VAL:CG1	1:G:129:GLN:N	2.55	0.69
1:B:30:TRP:HE1	1:B:129:GLN:HE21	1.40	0.69
2:B:301:MTX:CD	2:B:301:MTX:O2	2.39	0.69
1:E:56:ASP:HB2	1:E:138:VAL:HG12	1.74	0.69
1:A:224:LYS:HE2	1:A:280:SER:HB3	1.74	0.69
1:A:33:ARG:HG2	1:A:33:ARG:HH11	1.57	0.68
1:A:222:VAL:HG13	1:A:238:VAL:HG21	1.75	0.68
1:A:230:ARG:HD3	1:B:230:ARG:NH2	2.06	0.68
1:E:128:VAL:CG1	1:E:129:GLN:N	2.55	0.68
1:F:176:VAL:CG2	1:F:177:GLN:H	2.06	0.68
1:B:84:ASN:O	1:B:84:ASN:ND2	2.25	0.68
2:B:301:MTX:O2	2:B:301:MTX:OE2	2.12	0.68
1:B:64:LYS:O	1:B:65:ASN:C	2.31	0.67
1:B:282:ARG:HH11	1:B:282:ARG:CG	2.08	0.67
1:E:128:VAL:HG12	1:E:129:GLN:N	2.08	0.67
1:F:176:VAL:CG2	1:F:177:GLN:N	2.58	0.67
1:C:60:PHE:HD2	1:C:120:LEU:HD11	1.60	0.67
1:D:201:ARG:NH2	1:D:248:ASN:O	2.27	0.67
2:B:301:MTX:CD	2:B:301:MTX:O1	2.43	0.66
1:A:230:ARG:CD	1:B:230:ARG:HH21	2.06	0.66
1:B:282:ARG:HG3	1:B:282:ARG:O	1.95	0.66
2:D:301:MTX:OE2	2:D:301:MTX:O1	2.14	0.65
1:C:111:THR:O	1:C:111:THR:HG22	1.97	0.65
1:C:285:PRO:HG2	1:C:288:TRP:CZ2	2.32	0.65
1:A:111:THR:OG1	1:E:281:TRP:NE1	2.30	0.65
1:E:193:ARG:HG3	1:E:193:ARG:NH2	2.12	0.65
1:B:193:ARG:HD2	1:B:256:GLN:OE1	1.97	0.65
1:C:30:TRP:HE1	1:C:129:GLN:NE2	1.95	0.65
1:C:271:ALA:HB1	1:C:285:PRO:HB3	1.77	0.65
1:D:33:ARG:HG2	1:D:36:GLY:O	1.97	0.64
2:E:301:MTX:HG2	1:G:98:ALA:CA	2.27	0.64
1:F:84:ASN:HB2	1:F:117:TYR:CE2	2.31	0.64
2:G:301:MTX:OE1	2:G:301:MTX:CT	2.46	0.64
1:A:95:LYS:HE3	1:A:103:ASP:OD1	1.98	0.64
1:B:180:GLU:OE2	1:B:289:GLY:HA3	1.97	0.64
1:E:70:SER:O	1:E:128:VAL:HG13	1.96	0.64
1:E:204:ARG:CG	1:G:97:GLY:HA3	2.28	0.64
1:G:4:LEU:HG	1:G:5:ILE:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:HH11	1:A:200:ARG:CG	2.02	0.64
1:B:13:TYR:HB2	1:B:32:LYS:HG3	1.80	0.63
1:G:212:ARG:NH1	1:G:264:ASP:HA	2.14	0.63
1:F:30:TRP:HE1	1:F:129:GLN:HE21	1.47	0.63
1:D:33:ARG:HG2	1:D:33:ARG:NH1	2.09	0.63
1:E:98:ALA:HA	2:G:301:MTX:OE1	1.98	0.63
1:A:200:ARG:HG3	1:A:200:ARG:NH1	1.98	0.63
1:A:233:THR:CG2	1:A:276:TYR:OH	2.47	0.63
1:D:5:ILE:HG13	1:D:5:ILE:O	1.97	0.63
1:B:281:TRP:O	1:B:283:SER:N	2.32	0.62
1:G:268:TYR:O	1:G:291:GLY:HA2	1.98	0.62
1:B:84:ASN:HB2	1:B:117:TYR:CE1	2.34	0.62
1:C:111:THR:O	1:C:111:THR:HG23	1.99	0.62
1:G:19:ASN:HB3	1:G:27:THR:HB	1.82	0.62
1:A:111:THR:OG1	1:E:281:TRP:CD1	2.52	0.62
1:F:180:GLU:OE2	1:F:289:GLY:HA3	2.00	0.61
1:C:107:GLU:HA	1:C:107:GLU:OE2	2.00	0.61
1:C:175:GLN:HG3	1:C:176:VAL:HG13	1.82	0.61
1:B:262:PRO:HA	1:B:296:VAL:HB	1.81	0.61
1:A:193:ARG:HD2	1:A:256:GLN:OE1	2.01	0.61
1:B:77:LYS:HD2	1:B:123:LEU:HD21	1.82	0.60
1:E:51:LYS:C	1:E:116:LYS:HG3	2.22	0.60
2:A:301:MTX:CG	1:B:98:ALA:HA	2.31	0.60
1:E:284:GLY:H	1:E:285:PRO:HD3	1.66	0.60
1:G:73:TRP:HA	1:G:126:ARG:HG2	1.83	0.60
1:G:4:LEU:O	1:G:5:ILE:HG23	2.02	0.59
1:D:73:TRP:CE2	1:D:122:ASN:HB2	2.37	0.59
1:G:59:ARG:HG2	1:G:59:ARG:NH2	2.02	0.59
1:G:287:TYR:OH	2:G:301:MTX:HB1	2.02	0.59
1:B:204:ARG:HG2	1:B:205:SER:N	2.16	0.59
1:G:128:VAL:HG13	1:G:129:GLN:H	1.66	0.59
1:F:73:TRP:CE2	1:F:122:ASN:HB2	2.38	0.59
1:F:176:VAL:HG22	1:F:177:GLN:H	1.63	0.59
1:F:187:GLN:HE22	1:F:298:SER:C	2.05	0.59
1:C:174:SER:O	1:C:175:GLN:CB	2.51	0.59
1:E:282:ARG:HD2	1:E:282:ARG:O	2.03	0.59
1:A:52:GLU:O	1:A:53:ILE:HG22	2.03	0.58
1:F:271:ALA:HB1	1:F:285:PRO:HB3	1.84	0.58
1:C:129:GLN:HE22	1:C:179:VAL:HG12	1.69	0.58
1:D:225:ILE:HD13	1:D:246:ARG:HG2	1.84	0.58
1:G:37:GLU:OE1	1:G:193:ARG:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:MTX:O1	2:A:301:MTX:CG	2.45	0.58
1:E:13:TYR:CD2	1:E:14:ASP:HB2	2.39	0.57
1:G:263:GLU:H	1:G:263:GLU:CD	2.08	0.57
1:A:30:TRP:HE1	1:A:129:GLN:NE2	2.00	0.57
1:F:179:VAL:O	1:F:196:CYS:HA	2.03	0.57
1:G:32:LYS:HD3	1:G:180:GLU:O	2.04	0.57
1:D:261:LYS:HB3	1:D:263:GLU:OE1	2.04	0.57
1:C:284:GLY:H	1:C:285:PRO:CD	2.18	0.57
1:G:261:LYS:HB3	1:G:263:GLU:HG2	1.87	0.57
1:A:51:LYS:O	1:A:53:ILE:HG23	2.03	0.57
1:E:193:ARG:HG3	1:E:256:GLN:OE1	2.05	0.56
1:E:284:GLY:N	1:E:285:PRO:HD2	2.19	0.56
1:G:204:ARG:HH11	1:G:204:ARG:HG3	1.69	0.56
1:B:30:TRP:HD1	1:B:31:TYR:N	2.03	0.56
1:G:73:TRP:CE2	1:G:122:ASN:HB2	2.40	0.56
1:B:72:LYS:HE2	1:B:101:GLY:O	2.06	0.56
1:G:128:VAL:HG13	1:G:129:GLN:N	2.20	0.56
1:E:36:GLY:H	1:E:183:GLY:H	1.53	0.55
1:G:16:ASN:H	1:G:19:ASN:HD21	1.54	0.55
1:B:49:LEU:HD12	1:B:116:LYS:O	2.07	0.55
1:B:268:TYR:O	1:B:291:GLY:HA2	2.06	0.55
1:E:81:SER:HB2	1:E:87:TRP:CE3	2.41	0.55
1:F:87:TRP:CH2	1:F:119:ARG:HD3	2.42	0.55
1:F:227:GLY:HA2	1:F:246:ARG:HH12	1.71	0.55
1:A:13:TYR:HB2	1:A:32:LYS:HG3	1.87	0.55
1:E:128:VAL:HG13	1:E:129:GLN:H	1.70	0.55
1:E:261:LYS:HB3	1:E:263:GLU:OE1	2.07	0.55
1:C:233:THR:HG23	1:C:276:TYR:OH	2.07	0.54
1:F:183:GLY:HA2	1:F:192:LEU:HD21	1.89	0.54
1:G:227:GLY:HA2	1:G:246:ARG:NH1	2.22	0.54
1:A:110:GLU:OE2	1:E:282:ARG:HB3	2.07	0.54
1:A:284:GLY:N	1:A:285:PRO:HD2	2.23	0.54
1:A:33:ARG:HG2	1:A:36:GLY:O	2.08	0.53
2:A:301:MTX:HG2	1:B:98:ALA:HA	1.90	0.53
1:C:6:ARG:HD2	1:C:6:ARG:O	2.08	0.53
1:C:257:MET:HE3	1:C:268:TYR:CE2	2.43	0.53
1:B:4:LEU:HD22	1:B:20:LEU:HD12	1.90	0.53
1:C:265:THR:O	1:C:266:ALA:HB2	2.07	0.53
1:D:109:PHE:CD1	1:D:109:PHE:N	2.73	0.53
1:E:200:ARG:HG3	1:E:200:ARG:NH1	2.21	0.53
1:F:30:TRP:HA	1:F:131:THR:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:TRP:HE1	1:B:129:GLN:NE2	2.06	0.53
2:G:301:MTX:OE1	2:G:301:MTX:O1	2.26	0.53
1:A:99:PRO:HB3	1:B:201:ARG:O	2.08	0.53
1:D:33:ARG:HG3	1:D:34:SER:N	2.24	0.53
1:B:281:TRP:O	1:B:282:ARG:C	2.46	0.53
2:A:301:MTX:HG2	1:B:98:ALA:N	2.24	0.53
1:B:76:PHE:CD1	1:B:76:PHE:N	2.76	0.53
1:E:214:ALA:HB1	1:E:215:PRO:HD2	1.90	0.52
1:G:30:TRP:HE1	1:G:129:GLN:HE21	1.56	0.52
1:G:211:PHE:HA	1:G:222:VAL:HG23	1.92	0.52
1:A:201:ARG:HA	1:A:251:TYR:CE2	2.44	0.52
1:B:14:ASP:OD1	1:B:15:GLY:N	2.43	0.52
1:C:129:GLN:HE22	1:C:179:VAL:CG1	2.22	0.52
1:C:185:LEU:HD12	1:C:186:VAL:N	2.24	0.52
1:F:234:TYR:CE2	1:F:242:PHE:O	2.62	0.52
1:G:59:ARG:CG	1:G:59:ARG:NH2	2.57	0.52
1:E:260:LEU:HD23	1:E:260:LEU:N	2.25	0.52
1:G:30:TRP:HD1	1:G:31:TYR:N	2.08	0.52
1:F:48:ASP:OD1	1:F:117:TYR:CE1	2.63	0.52
1:G:37:GLU:CG	1:G:193:ARG:HD3	2.40	0.52
1:G:194:LEU:O	1:G:254:TYR:HA	2.10	0.52
2:E:301:MTX:HG1	2:E:301:MTX:O2	2.07	0.51
1:G:204:ARG:CG	1:G:204:ARG:NH1	2.66	0.51
1:F:13:TYR:CD1	1:F:14:ASP:HB2	2.45	0.51
1:F:34:SER:O	1:F:35:ASN:HB2	2.11	0.51
1:D:263:GLU:CD	1:D:263:GLU:H	2.13	0.51
1:G:187:GLN:HE21	1:G:298:SER:C	2.14	0.51
1:B:282:ARG:HH11	1:B:282:ARG:HG2	1.75	0.51
1:C:72:LYS:HE3	1:C:101:GLY:O	2.11	0.51
1:B:263:GLU:H	1:B:263:GLU:CD	2.13	0.51
1:C:186:VAL:HG22	1:C:187:GLN:N	2.26	0.51
1:D:83:ASP:O	1:D:84:ASN:CB	2.57	0.51
1:E:10:TRP:N	1:E:10:TRP:CD1	2.76	0.51
1:E:28:GLY:HA3	1:E:64:LYS:HD2	1.93	0.51
1:E:284:GLY:N	1:E:285:PRO:HD3	2.21	0.51
1:C:284:GLY:H	1:C:285:PRO:HD2	1.76	0.51
1:D:236:ASP:HA	1:D:239:LYS:HD3	1.93	0.51
1:E:203:SER:OG	1:G:97:GLY:HA2	2.11	0.51
1:E:234:TYR:CE1	1:E:244:ILE:HG22	2.45	0.51
1:D:271:ALA:HB1	1:D:285:PRO:CB	2.40	0.50
1:B:224:LYS:HG3	1:B:276:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:PHE:CD1	1:C:109:PHE:N	2.75	0.50
1:A:73:TRP:CE2	1:A:122:ASN:HB2	2.47	0.50
1:F:1:ASN:N	1:F:2:PRO:HD2	2.26	0.50
1:F:13:TYR:CE1	1:F:14:ASP:HB2	2.47	0.50
1:G:213:GLN:HB3	1:G:219:ARG:HA	1.93	0.50
1:G:247:ASP:OD2	1:G:250:GLU:HG3	2.10	0.50
1:A:208:MET:HG3	1:A:253:VAL:HG21	1.94	0.50
1:A:33:ARG:NH1	1:A:36:GLY:O	2.44	0.50
1:G:64:LYS:C	1:G:65:ASN:O	2.49	0.50
1:E:30:TRP:HE1	1:E:129:GLN:HE21	1.59	0.50
1:A:284:GLY:H	1:A:285:PRO:HD2	1.77	0.49
1:B:38:ALA:CB	1:B:127:HIS:CD2	2.83	0.49
1:G:81:SER:OG	1:G:83:ASP:OD1	2.30	0.49
1:F:105:ILE:HG22	1:F:105:ILE:O	2.12	0.49
1:F:128:VAL:HG23	1:F:252:LEU:HD11	1.93	0.49
1:D:265:THR:O	1:D:266:ALA:HB2	2.12	0.49
1:E:230:ARG:NH2	1:G:230:ARG:HD3	2.23	0.49
1:F:227:GLY:HA2	1:F:246:ARG:NH1	2.27	0.49
1:A:48:ASP:C	1:A:48:ASP:OD1	2.50	0.49
1:G:62:ILE:HD12	1:G:72:LYS:HG2	1.93	0.49
1:A:134:GLU:O	1:A:135:PHE:CD1	2.65	0.49
1:D:242:PHE:CE2	1:D:257:MET:HG2	2.47	0.49
1:E:56:ASP:HB2	1:E:138:VAL:CG1	2.42	0.49
1:A:33:ARG:HG2	1:A:33:ARG:NH1	2.25	0.49
1:F:174:SER:HB3	1:F:200:ARG:HH12	1.78	0.49
1:D:84:ASN:ND2	1:D:117:TYR:CE1	2.81	0.49
1:E:30:TRP:HE1	1:E:129:GLN:HG2	1.77	0.49
2:D:301:MTX:O	2:D:301:MTX:O2	2.31	0.49
1:E:73:TRP:CE2	1:E:122:ASN:HB2	2.47	0.49
1:A:213:GLN:HB2	1:A:219:ARG:HG3	1.94	0.48
1:B:219:ARG:HD2	1:B:282:ARG:HD2	1.95	0.48
1:B:241:ARG:C	1:B:242:PHE:HD1	2.16	0.48
1:C:281:TRP:O	1:C:282:ARG:C	2.52	0.48
1:F:36:GLY:H	1:F:183:GLY:H	1.61	0.48
1:G:65:ASN:HD22	1:G:65:ASN:H	1.60	0.48
1:D:30:TRP:HA	1:D:131:THR:HG22	1.95	0.48
1:E:183:GLY:HA3	1:E:192:LEU:HD21	1.95	0.48
1:G:211:PHE:CD1	1:G:221:PHE:HA	2.49	0.48
1:A:116:LYS:HB3	1:A:117:TYR:CD1	2.48	0.48
1:B:275:ASN:OD1	1:B:275:ASN:C	2.52	0.48
1:C:225:ILE:HD13	1:C:246:ARG:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:76:PHE:HA	1:G:123:LEU:HG	1.94	0.48
1:B:265:THR:O	1:B:266:ALA:HB2	2.14	0.48
1:D:91:LYS:HE2	1:D:93:TYR:CE2	2.49	0.48
1:A:13:TYR:CD2	1:A:14:ASP:HB2	2.49	0.47
1:G:225:ILE:HD11	1:G:229:GLY:HA2	1.95	0.47
1:A:33:ARG:HH11	1:A:33:ARG:CG	2.25	0.47
1:B:139:SER:O	1:B:140:ASP:HB3	2.14	0.47
1:G:281:TRP:O	1:G:283:SER:N	2.46	0.47
1:C:122:ASN:ND2	1:C:124:GLU:O	2.47	0.47
1:E:84:ASN:HB2	1:E:117:TYR:CE2	2.49	0.47
1:B:180:GLU:OE1	1:B:291:GLY:N	2.43	0.47
1:C:127:HIS:N	1:C:127:HIS:CD2	2.82	0.47
1:C:257:MET:CE	1:C:268:TYR:CE2	2.97	0.47
1:B:267:VAL:HG12	1:B:269:TYR:CE2	2.50	0.47
1:G:128:VAL:HG12	1:G:129:GLN:N	2.29	0.47
1:G:182:GLY:O	1:G:183:GLY:O	2.33	0.47
1:B:20:LEU:O	1:B:134:GLU:HA	2.15	0.47
1:E:109:PHE:O	1:E:110:GLU:C	2.53	0.47
1:E:212:ARG:HD3	1:E:222:VAL:HG22	1.97	0.47
1:G:182:GLY:HA3	1:G:194:LEU:CD2	2.45	0.47
1:E:210:TRP:HD1	1:E:244:ILE:HD12	1.79	0.47
1:C:6:ARG:HA	1:C:44:PHE:CE1	2.50	0.47
1:C:49:LEU:HB2	1:C:116:LYS:O	2.15	0.47
1:G:33:ARG:NH2	1:G:40:LEU:HD12	2.30	0.47
1:G:260:LEU:N	1:G:260:LEU:HD23	2.30	0.47
1:C:33:ARG:NH2	1:C:43:GLU:OE1	2.36	0.47
1:C:73:TRP:CE2	1:C:122:ASN:HB2	2.49	0.47
1:G:39:SER:O	1:G:125:PRO:HA	2.14	0.47
2:E:301:MTX:HM1	2:E:301:MTX:H15	1.56	0.46
2:A:301:MTX:CD	2:A:301:MTX:CT	2.92	0.46
1:C:36:GLY:H	1:C:183:GLY:H	1.63	0.46
1:E:179:VAL:O	1:E:196:CYS:HA	2.15	0.46
1:F:214:ALA:HB3	1:F:217:LYS:HG3	1.98	0.46
2:F:301:MTX:HM1	2:F:301:MTX:H13	1.33	0.46
1:D:75:LYS:HA	1:D:93:TYR:O	2.15	0.46
1:D:261:LYS:HD3	1:D:263:GLU:HG2	1.98	0.46
1:C:6:ARG:HD2	1:C:6:ARG:C	2.36	0.46
2:C:301:MTX:H13	2:C:301:MTX:H92	1.70	0.46
1:G:19:ASN:HB3	1:G:27:THR:CB	2.44	0.46
2:A:301:MTX:HG2	1:B:98:ALA:CA	2.45	0.46
1:C:191:SER:HA	1:C:257:MET:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:LEU:HG	1:D:5:ILE:N	2.31	0.46
1:F:262:PRO:HA	1:F:296:VAL:HB	1.98	0.46
1:G:69:SER:OG	1:G:251:TYR:HB3	2.16	0.46
2:G:301:MTX:HM1	2:G:301:MTX:H15	1.48	0.46
1:A:84:ASN:OD1	1:A:87:TRP:HZ2	1.98	0.46
1:A:239:LYS:HB2	1:A:239:LYS:HE3	1.72	0.46
1:D:46:GLY:O	1:D:47:LEU:HD23	2.15	0.46
1:E:230:ARG:HH21	1:G:230:ARG:HD2	1.79	0.46
2:A:301:MTX:HG2	1:B:97:GLY:C	2.37	0.46
1:A:225:ILE:HB	1:A:244:ILE:HD13	1.98	0.46
1:D:196:CYS:HG	1:D:270:CYS:HG	1.63	0.46
1:E:13:TYR:CE2	1:E:14:ASP:HB2	2.51	0.46
1:E:33:ARG:HD3	1:E:36:GLY:O	2.16	0.46
1:G:193:ARG:HG3	1:G:193:ARG:HH21	1.80	0.46
1:A:77:LYS:HE3	1:A:123:LEU:HD21	1.97	0.45
1:A:284:GLY:N	1:A:285:PRO:CD	2.79	0.45
1:C:98:ALA:HA	1:C:99:PRO:HD3	1.80	0.45
1:D:74:ASN:ND2	1:D:96:THR:HG23	2.30	0.45
1:C:16:ASN:ND2	1:C:18:ALA:H	2.14	0.45
1:C:247:ASP:C	1:C:247:ASP:OD1	2.54	0.45
1:F:83:ASP:O	1:F:84:ASN:HB3	2.16	0.45
1:F:226:SER:HB3	1:F:231:LEU:HB2	1.97	0.45
1:D:26:ASN:OD1	1:D:102:LYS:HE2	2.17	0.45
1:B:102:LYS:HE3	1:B:102:LYS:HB2	1.67	0.45
1:G:38:ALA:HB2	1:G:127:HIS:HD1	1.82	0.45
1:E:260:LEU:O	1:E:261:LYS:HG3	2.17	0.45
2:G:301:MTX:O2	2:G:301:MTX:C	2.65	0.45
1:G:13:TYR:CD1	1:G:14:ASP:HB2	2.52	0.45
1:A:30:TRP:HA	1:A:131:THR:HG22	1.98	0.45
1:C:56:ASP:OD1	1:C:112:PRO:HG3	2.17	0.45
1:C:225:ILE:HG13	1:C:232:THR:CG2	2.40	0.45
1:F:257:MET:HE2	1:F:268:TYR:CE2	2.52	0.45
1:B:37:GLU:HG2	1:B:193:ARG:HG2	1.98	0.45
2:D:301:MTX:HM1	2:D:301:MTX:H15	1.57	0.45
1:E:77:LYS:HG3	1:E:121:THR:HB	1.98	0.45
2:A:301:MTX:O1	2:A:301:MTX:OE2	2.34	0.44
1:B:261:LYS:HG3	1:B:263:GLU:HG2	1.99	0.44
1:G:22:ASP:OD2	1:G:24:ASP:HB3	2.18	0.44
2:A:301:MTX:CT	2:A:301:MTX:OE2	2.66	0.44
1:B:71:ASP:OD1	1:B:72:LYS:HE3	2.17	0.44
1:E:273:ASP:OD2	1:E:284:GLY:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:GLU:HG3	1:D:87:TRP:CE3	2.53	0.44
1:D:183:GLY:H	1:D:192:LEU:HD11	1.83	0.44
1:E:81:SER:HB2	1:E:87:TRP:CZ3	2.52	0.44
1:F:5:ILE:O	1:F:5:ILE:HG13	2.17	0.44
1:C:58:ILE:C	1:C:58:ILE:HD12	2.38	0.44
1:E:20:LEU:HD23	1:E:20:LEU:HA	1.49	0.44
1:F:84:ASN:O	1:F:84:ASN:ND2	2.50	0.44
1:G:212:ARG:HG2	1:G:222:VAL:HG22	1.99	0.44
1:A:71:ASP:HB2	1:A:131:THR:OG1	2.17	0.44
1:D:16:ASN:H	1:D:19:ASN:ND2	2.16	0.44
2:A:301:MTX:H15	2:A:301:MTX:HM1	1.55	0.43
1:F:228:ASP:OD1	1:F:228:ASP:N	2.36	0.43
1:B:30:TRP:HA	1:B:131:THR:HG22	2.00	0.43
1:C:175:GLN:CG	1:C:176:VAL:N	2.69	0.43
2:C:301:MTX:H15	2:C:301:MTX:HM1	1.62	0.43
1:F:64:LYS:HB2	1:F:131:THR:HB	2.01	0.43
1:B:30:TRP:CD1	1:B:30:TRP:C	2.92	0.43
1:B:261:LYS:HB3	1:B:261:LYS:HE2	1.67	0.43
1:C:13:TYR:CE2	1:C:179:VAL:HG21	2.54	0.43
1:D:175:GLN:HE21	1:D:175:GLN:HB2	1.67	0.43
2:A:301:MTX:H13	2:A:301:MTX:H92	1.84	0.43
1:D:236:ASP:O	1:D:239:LYS:HB2	2.19	0.43
1:B:95:LYS:O	1:B:96:THR:C	2.56	0.43
1:B:225:ILE:CG1	1:B:229:GLY:HA2	2.48	0.43
1:C:174:SER:O	1:C:175:GLN:HB3	2.18	0.43
1:C:271:ALA:HB1	1:C:285:PRO:CB	2.48	0.43
1:F:70:SER:O	1:F:128:VAL:CG2	2.67	0.43
1:F:257:MET:CE	1:F:268:TYR:CE2	3.01	0.43
2:C:301:MTX:O1	2:C:301:MTX:C	2.64	0.43
1:G:182:GLY:HA3	1:G:194:LEU:HD23	2.01	0.43
1:D:33:ARG:HG3	1:D:34:SER:H	1.83	0.43
1:F:72:LYS:NZ	1:F:101:GLY:O	2.50	0.43
1:F:72:LYS:NZ	1:F:99:PRO:O	2.49	0.43
1:C:69:SER:O	1:C:70:SER:C	2.56	0.42
1:F:83:ASP:O	1:F:84:ASN:CB	2.67	0.42
1:G:53:ILE:O	1:G:114:SER:HA	2.19	0.42
1:E:242:PHE:CE2	1:E:257:MET:HG2	2.53	0.42
1:C:186:VAL:CG2	1:C:187:GLN:N	2.83	0.42
1:E:77:LYS:HD2	1:E:79:GLU:OE2	2.19	0.42
1:C:123:LEU:HD23	1:C:123:LEU:HA	1.87	0.42
1:D:80:TYR:CE1	1:D:88:THR:HB	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:SER:HA	1:G:257:MET:O	2.20	0.42
1:C:5:ILE:HG12	1:C:5:ILE:O	2.18	0.42
1:B:55:LEU:HD23	1:B:55:LEU:HA	1.85	0.42
1:F:10:TRP:O	1:F:11:HIS:HB3	2.19	0.42
1:F:183:GLY:CA	1:F:192:LEU:HD21	2.49	0.42
1:B:72:LYS:NZ	1:B:99:PRO:O	2.52	0.42
1:B:192:LEU:HD12	1:B:192:LEU:HA	1.70	0.42
1:D:33:ARG:NH1	1:D:33:ARG:CG	2.73	0.42
1:E:73:TRP:NE1	1:E:122:ASN:HB2	2.35	0.42
1:A:201:ARG:HA	1:A:251:TYR:HE2	1.85	0.42
1:B:175:GLN:HE21	1:B:175:GLN:C	2.23	0.42
1:E:39:SER:O	1:E:125:PRO:HA	2.19	0.42
1:E:212:ARG:HB2	1:E:266:ALA:HB3	2.02	0.42
1:A:33:ARG:NH1	1:A:33:ARG:CG	2.80	0.42
1:A:51:LYS:O	1:A:53:ILE:CG2	2.68	0.42
1:D:62:ILE:HG13	1:D:72:LYS:CD	2.50	0.42
1:B:30:TRP:CD1	1:B:31:TYR:N	2.86	0.41
1:B:37:GLU:CG	1:B:193:ARG:HG2	2.50	0.41
1:D:83:ASP:O	1:D:84:ASN:HB2	2.19	0.41
1:E:74:ASN:OD1	1:E:96:THR:HA	2.21	0.41
1:D:122:ASN:OD1	1:D:123:LEU:N	2.53	0.41
1:A:104:VAL:H	1:A:104:VAL:HG23	1.57	0.41
1:D:81:SER:HB2	1:D:87:TRP:CE3	2.55	0.41
1:G:204:ARG:NH1	1:G:204:ARG:HG2	2.36	0.41
1:G:224:LYS:HE2	1:G:280:SER:HB3	2.02	0.41
1:C:56:ASP:OD2	1:C:140:ASP:HB3	2.20	0.41
1:E:186:VAL:O	1:E:296:VAL:HG13	2.19	0.41
1:E:272:ALA:CB	2:E:301:MTX:HM2	2.50	0.41
1:E:282:ARG:O	1:E:282:ARG:CD	2.68	0.41
1:F:48:ASP:OD1	1:F:117:TYR:HE1	2.02	0.41
1:G:51:LYS:H	1:G:51:LYS:HG2	1.71	0.41
1:E:223:ALA:HA	1:E:233:THR:O	2.21	0.41
1:D:253:VAL:HG12	1:D:254:TYR:N	2.36	0.41
1:E:53:ILE:O	1:E:114:SER:CA	2.58	0.41
1:G:263:GLU:CD	1:G:263:GLU:N	2.74	0.41
1:A:5:ILE:H	1:A:5:ILE:HG13	1.72	0.41
1:B:185:LEU:HD23	1:F:247:ASP:HB2	2.03	0.41
1:C:253:VAL:HG12	1:C:254:TYR:N	2.36	0.41
1:D:95:LYS:O	1:D:96:THR:C	2.58	0.41
1:D:255:LEU:HD12	1:D:255:LEU:HA	1.90	0.41
1:E:242:PHE:N	1:E:242:PHE:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:PHE:CD1	1:F:44:PHE:C	2.94	0.41
1:A:93:TYR:N	1:A:93:TYR:CD1	2.89	0.41
2:E:301:MTX:HG2	1:G:98:ALA:N	2.36	0.41
1:G:134:GLU:OE1	1:G:134:GLU:HA	2.21	0.41
1:A:109:PHE:C	1:A:111:THR:N	2.74	0.40
1:B:224:LYS:HD3	1:B:280:SER:HB3	2.02	0.40
1:G:13:TYR:CD1	1:G:13:TYR:C	2.95	0.40
1:A:109:PHE:N	1:A:109:PHE:CD1	2.87	0.40
2:A:301:MTX:HG1	1:B:98:ALA:HA	2.03	0.40
1:B:204:ARG:CG	1:B:205:SER:N	2.84	0.40
1:F:124:GLU:HA	1:F:125:PRO:HD3	1.94	0.40
1:A:109:PHE:O	1:A:110:GLU:C	2.59	0.40
1:G:212:ARG:HG2	1:G:222:VAL:CG2	2.51	0.40
1:E:275:ASN:HB3	1:E:278:THR:OG1	2.22	0.40
1:F:70:SER:O	1:F:128:VAL:HG22	2.22	0.40
1:G:185:LEU:HA	1:G:295:THR:O	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	261/306 (85%)	244 (94%)	14 (5%)	3 (1%)	14	42
1	B	261/306 (85%)	243 (93%)	14 (5%)	4 (2%)	10	34
1	C	261/306 (85%)	248 (95%)	10 (4%)	3 (1%)	14	42
1	D	261/306 (85%)	242 (93%)	16 (6%)	3 (1%)	14	42
1	E	266/306 (87%)	238 (90%)	25 (9%)	3 (1%)	14	42
1	F	261/306 (85%)	236 (90%)	18 (7%)	7 (3%)	5	19
1	G	261/306 (85%)	228 (87%)	27 (10%)	6 (2%)	6	23
All	All	1832/2142 (86%)	1679 (92%)	124 (7%)	29 (2%)	9	32

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	175	GLN
1	D	65	ASN
1	F	65	ASN
1	G	65	ASN
1	G	183	GLY
1	G	188	ALA
1	G	282	ARG
1	B	51	LYS
1	B	282	ARG
1	G	9	SER
1	A	21	LEU
1	A	112	PRO
1	B	65	ASN
1	B	266	ALA
1	D	217	LYS
1	E	65	ASN
1	F	52	GLU
1	F	175	GLN
1	A	176	VAL
1	D	266	ALA
1	E	282	ARG
1	G	110	GLU
1	C	112	PRO
1	F	73	TRP
1	F	266	ALA
1	F	183	GLY
1	F	188	ALA
1	E	183	GLY
1	C	284	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	204/239 (85%)	184 (90%)	20 (10%)	8 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	217/239 (91%)	189 (87%)	28 (13%)	4	13
1	C	217/239 (91%)	192 (88%)	25 (12%)	5	17
1	D	216/239 (90%)	188 (87%)	28 (13%)	4	12
1	E	221/239 (92%)	199 (90%)	22 (10%)	7	23
1	F	217/239 (91%)	188 (87%)	29 (13%)	4	11
1	G	216/239 (90%)	191 (88%)	25 (12%)	5	16
All	All	1508/1673 (90%)	1331 (88%)	177 (12%)	5	16

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	7	SER
1	A	26	ASN
1	A	52	GLU
1	A	53	ILE
1	A	54	LYS
1	A	77	LYS
1	A	104	VAL
1	A	111	THR
1	A	138	VAL
1	A	175	GLN
1	A	187	GLN
1	A	200	ARG
1	A	201	ARG
1	A	233	THR
1	A	237	SER
1	A	239	LYS
1	A	251	TYR
1	A	252	LEU
1	A	261	LYS
1	B	7	SER
1	B	35	ASN
1	B	48	ASP
1	B	49	LEU
1	B	51	LYS
1	B	53	ILE
1	B	65	ASN
1	B	72	LYS
1	B	77	LYS

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Mol	Chain	Res	Type
1	B	84	ASN
1	B	88	THR
1	B	102	LYS
1	B	114	SER
1	B	124	GLU
1	B	138	VAL
1	B	139	SER
1	B	175	GLN
1	B	186	VAL
1	B	205	SER
1	B	217	LYS
1	B	220	GLU
1	B	237	SER
1	B	239	LYS
1	B	243	THR
1	B	251	TYR
1	B	263	GLU
1	B	282	ARG
1	B	285	PRO
1	C	1	ASN
1	C	3	SER
1	C	4	LEU
1	C	5	ILE
1	C	9	SER
1	C	16	ASN
1	C	47	LEU
1	C	59	ARG
1	C	69	SER
1	C	70	SER
1	C	72	LYS
1	C	86	SER
1	C	92	GLU
1	C	108	SER
1	C	111	THR
1	C	124	GLU
1	C	140	ASP
1	C	174	SER
1	C	176	VAL
1	C	185	LEU
1	C	203	SER
1	C	204	ARG
1	C	233	THR

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Mol	Chain	Res	Type
1	C	251	TYR
1	C	277	VAL
1	D	3	SER
1	D	7	SER
1	D	9	SER
1	D	14	ASP
1	D	16	ASN
1	D	33	ARG
1	D	51	LYS
1	D	53	ILE
1	D	64	LYS
1	D	70	SER
1	D	75	LYS
1	D	78	LEU
1	D	84	ASN
1	D	86	SER
1	D	116	LYS
1	D	140	ASP
1	D	175	GLN
1	D	181	SER
1	D	191	SER
1	D	204	ARG
1	D	205	SER
1	D	220	GLU
1	D	236	ASP
1	D	239	LYS
1	D	251	TYR
1	D	263	GLU
1	D	282	ARG
1	D	292	THR
1	E	7	SER
1	E	16	ASN
1	E	34	SER
1	E	54	LYS
1	E	65	ASN
1	E	69	SER
1	E	77	LYS
1	E	82	LEU
1	E	108	SER
1	E	111	THR
1	E	137	ILE
1	E	138	VAL

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Mol	Chain	Res	Type
1	E	175	GLN
1	E	186	VAL
1	E	193	ARG
1	E	200	ARG
1	E	201	ARG
1	E	204	ARG
1	E	236	ASP
1	E	237	SER
1	E	239	LYS
1	E	251	TYR
1	F	7	SER
1	F	16	ASN
1	F	51	LYS
1	F	52	GLU
1	F	64	LYS
1	F	65	ASN
1	F	77	LYS
1	F	82	LEU
1	F	84	ASN
1	F	99	PRO
1	F	116	LYS
1	F	128	VAL
1	F	139	SER
1	F	140	ASP
1	F	178	LEU
1	F	186	VAL
1	F	187	GLN
1	F	201	ARG
1	F	203	SER
1	F	204	ARG
1	F	217	LYS
1	F	218	GLU
1	F	219	ARG
1	F	228	ASP
1	F	239	LYS
1	F	251	TYR
1	F	260	LEU
1	F	280	SER
1	F	282	ARG
1	G	21	LEU
1	G	33	ARG
1	G	34	SER

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Mol	Chain	Res	Type
1	G	49	LEU
1	G	52	GLU
1	G	53	ILE
1	G	59	ARG
1	G	91	LYS
1	G	96	THR
1	G	114	SER
1	G	139	SER
1	G	186	VAL
1	G	191	SER
1	G	200	ARG
1	G	201	ARG
1	G	202	SER
1	G	204	ARG
1	G	236	ASP
1	G	239	LYS
1	G	251	TYR
1	G	259	SER
1	G	260	LEU
1	G	263	GLU
1	G	282	ARG
1	G	290	GLN

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

Mol	Chain	Res	Type
1	A	129	GLN
1	A	175	GLN
1	B	11	HIS
1	B	16	ASN
1	B	35	ASN
1	B	127	HIS
1	B	129	GLN
1	B	175	GLN
1	B	177	GLN
1	B	213	GLN
1	C	1	ASN
1	C	16	ASN
1	C	129	GLN
1	C	175	GLN
1	D	11	HIS
1	D	16	ASN

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Mol	Chain	Res	Type
1	D	129	GLN
1	D	175	GLN
1	E	11	HIS
1	E	35	ASN
1	E	129	GLN
1	F	16	ASN
1	F	19	ASN
1	F	35	ASN
1	F	84	ASN
1	F	129	GLN
1	F	177	GLN
1	F	187	GLN
1	G	19	ASN
1	G	65	ASN
1	G	84	ASN
1	G	129	GLN
1	G	175	GLN
1	G	187	GLN
1	G	290	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 14 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MTX	B	301	-	35,35,35	2.63	9 (25%)	46,49,49	2.45	16 (34%)
2	MTX	F	301	-	35,35,35	2.31	8 (22%)	46,49,49	2.82	20 (43%)
2	MTX	E	301	-	35,35,35	2.01	8 (22%)	46,49,49	2.48	20 (43%)
2	MTX	A	301	-	35,35,35	2.17	7 (20%)	46,49,49	2.79	24 (52%)
2	MTX	C	301	-	35,35,35	2.31	8 (22%)	46,49,49	2.58	19 (41%)
2	MTX	G	301	-	35,35,35	2.05	4 (11%)	46,49,49	2.23	18 (39%)
2	MTX	D	301	-	35,35,35	1.97	8 (22%)	46,49,49	2.05	12 (26%)

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	MTX	B	301	-	-	5/25/25/25	0/3/3/3
2	MTX	F	301	-	-	11/25/25/25	0/3/3/3
2	MTX	E	301	-	-	8/25/25/25	0/3/3/3
2	MTX	A	301	-	-	7/25/25/25	0/3/3/3
2	MTX	C	301	-	-	6/25/25/25	0/3/3/3
2	MTX	G	301	-	-	8/25/25/25	0/3/3/3
2	MTX	D	301	-	-	9/25/25/25	0/3/3/3

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	MTX	CG-CD	8.20	1.69	1.50
2	B	301	MTX	C7-N8	7.25	1.43	1.31
2	A	301	MTX	O-C	7.24	1.38	1.23
2	F	301	MTX	O-C	7.21	1.38	1.23
2	G	301	MTX	O-C	7.12	1.37	1.23
2	C	301	MTX	O-C	7.05	1.37	1.23
2	D	301	MTX	O-C	6.86	1.37	1.23
2	A	301	MTX	C7-N8	6.74	1.42	1.31
2	F	301	MTX	C7-N8	6.13	1.41	1.31
2	C	301	MTX	CG-CD	5.99	1.64	1.50
2	E	301	MTX	O-C	5.80	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	MTX	C11-C	-5.79	1.38	1.50
2	E	301	MTX	C7-N8	5.78	1.41	1.31
2	B	301	MTX	O-C	5.44	1.34	1.23
2	G	301	MTX	C7-N8	5.24	1.40	1.31
2	D	301	MTX	C7-N8	5.09	1.40	1.31
2	C	301	MTX	C11-C	-5.02	1.39	1.50
2	E	301	MTX	C11-C	-4.89	1.40	1.50
2	A	301	MTX	C11-C	-4.82	1.40	1.50
2	B	301	MTX	C11-C	-4.49	1.40	1.50
2	F	301	MTX	CG-CD	4.45	1.60	1.50
2	F	301	MTX	C11-C	-4.36	1.41	1.50
2	C	301	MTX	C7-N8	4.36	1.38	1.31
2	D	301	MTX	C11-C	-4.25	1.41	1.50
2	B	301	MTX	CB-CG	3.60	1.64	1.52
2	C	301	MTX	C8A-N8	-3.38	1.32	1.37
2	F	301	MTX	CA-CT	3.17	1.60	1.52
2	F	301	MTX	C-N	3.07	1.40	1.34
2	E	301	MTX	C4A-N5	-2.96	1.31	1.37
2	B	301	MTX	C9-C6	2.88	1.56	1.51
2	F	301	MTX	CA-N	2.79	1.51	1.45
2	A	301	MTX	OE1-CD	2.79	1.31	1.22
2	C	301	MTX	C14-N10	-2.64	1.31	1.39
2	B	301	MTX	CA-CT	-2.64	1.45	1.52
2	D	301	MTX	CA-N	2.61	1.51	1.45
2	D	301	MTX	CG-CD	2.49	1.56	1.50
2	E	301	MTX	C9-N10	-2.47	1.41	1.46
2	C	301	MTX	CB-CG	2.45	1.60	1.52
2	D	301	MTX	C8A-N8	-2.45	1.33	1.37
2	A	301	MTX	C13-C12	2.33	1.43	1.38
2	E	301	MTX	O2-CT	-2.30	1.23	1.30
2	C	301	MTX	O1-CT	2.21	1.28	1.22
2	E	301	MTX	CA-N	2.18	1.50	1.45
2	A	301	MTX	C8A-N8	-2.16	1.34	1.37
2	E	301	MTX	OE1-CD	2.15	1.29	1.22
2	D	301	MTX	CB-CG	2.12	1.59	1.52
2	B	301	MTX	C6-N5	2.09	1.36	1.32
2	F	301	MTX	C6-N5	2.07	1.36	1.32
2	A	301	MTX	C16-C11	2.06	1.42	1.39
2	G	301	MTX	C9-C6	2.06	1.54	1.51
2	B	301	MTX	C2-NA2	2.04	1.38	1.33
2	D	301	MTX	O1-CT	2.02	1.28	1.22

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	MTX	C11-C-N	-7.15	103.35	117.06
2	B	301	MTX	CT-CA-N	-7.12	93.67	110.55
2	F	301	MTX	CM-N10-C14	-7.04	107.41	119.57
2	C	301	MTX	CM-N10-C14	-6.94	107.58	119.57
2	F	301	MTX	N1-C2-N3	-6.09	119.10	127.22
2	E	301	MTX	C2-N1-C8A	5.86	122.05	115.36
2	G	301	MTX	C2-N1-C8A	5.84	122.02	115.36
2	B	301	MTX	CB-CG-CD	5.70	127.64	112.51
2	C	301	MTX	N1-C2-N3	-5.57	119.80	127.22
2	A	301	MTX	N8-C8A-N1	5.54	122.14	115.82
2	E	301	MTX	CA-N-C	5.53	135.12	121.60
2	F	301	MTX	C2-N1-C8A	5.45	121.58	115.36
2	A	301	MTX	CG-CB-CA	-5.44	102.99	113.16
2	C	301	MTX	CT-CA-N	-5.33	97.92	110.55
2	F	301	MTX	CA-N-C	4.96	133.74	121.60
2	B	301	MTX	N1-C2-N3	-4.93	120.65	127.22
2	B	301	MTX	CM-N10-C14	-4.84	111.21	119.57
2	B	301	MTX	C2-N1-C8A	4.84	120.88	115.36
2	D	301	MTX	CM-N10-C14	-4.82	111.24	119.57
2	G	301	MTX	N8-C8A-N1	4.75	121.24	115.82
2	E	301	MTX	CM-N10-C14	-4.71	111.43	119.57
2	F	301	MTX	C4-C4A-N5	4.68	123.93	120.33
2	D	301	MTX	N1-C2-N3	-4.67	120.99	127.22
2	A	301	MTX	O-C-N	4.59	130.89	122.45
2	F	301	MTX	C9-C6-N5	4.53	124.22	116.96
2	F	301	MTX	O-C-N	4.48	130.69	122.45
2	E	301	MTX	N1-C2-N3	-4.46	121.28	127.22
2	E	301	MTX	CM-N10-C9	-4.43	103.07	114.84
2	G	301	MTX	CM-N10-C14	-4.38	112.01	119.57
2	C	301	MTX	C7-C6-N5	-4.28	118.06	120.85
2	F	301	MTX	C13-C14-N10	-4.27	115.48	121.62
2	C	301	MTX	C2-N1-C8A	4.26	120.22	115.36
2	A	301	MTX	N1-C2-N3	-4.21	121.60	127.22
2	G	301	MTX	C15-C14-N10	-4.21	115.56	121.62
2	C	301	MTX	CB-CG-CD	4.21	123.68	112.51
2	C	301	MTX	CB-CA-N	4.13	119.23	110.88
2	D	301	MTX	N8-C8A-N1	4.11	120.51	115.82
2	A	301	MTX	CM-N10-C14	-4.01	112.64	119.57
2	A	301	MTX	C13-C12-C11	-4.01	116.12	120.78
2	D	301	MTX	CA-N-C	3.99	131.37	121.60
2	A	301	MTX	C7-C6-N5	-3.97	118.25	120.85
2	A	301	MTX	C2-N1-C8A	3.95	119.86	115.36
2	D	301	MTX	C7-C6-N5	-3.86	118.33	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	MTX	CM-N10-C9	-3.84	104.65	114.84
2	F	301	MTX	C7-N8-C8A	3.82	120.53	116.69
2	F	301	MTX	C15-C14-N10	3.75	127.00	121.62
2	A	301	MTX	CA-N-C	3.74	130.75	121.60
2	D	301	MTX	C2-N1-C8A	3.69	119.57	115.36
2	B	301	MTX	N8-C8A-N1	3.64	119.98	115.82
2	F	301	MTX	N8-C8A-N1	3.63	119.96	115.82
2	C	301	MTX	CM-N10-C9	-3.62	105.24	114.84
2	C	301	MTX	N8-C8A-N1	3.62	119.95	115.82
2	A	301	MTX	C4A-C4-NA4	-3.52	115.00	120.35
2	B	301	MTX	CB-CA-N	3.50	117.96	110.88
2	G	301	MTX	N1-C2-N3	-3.50	122.56	127.22
2	E	301	MTX	C11-C-N	-3.46	110.44	117.06
2	E	301	MTX	C15-C14-N10	-3.40	116.72	121.62
2	A	301	MTX	C4-C4A-N5	-3.33	117.76	120.33
2	F	301	MTX	C7-C6-N5	-3.29	118.70	120.85
2	C	301	MTX	C4A-C4-NA4	-3.26	115.40	120.35
2	E	301	MTX	N8-C8A-N1	3.25	119.54	115.82
2	C	301	MTX	C9-C6-N5	3.23	122.14	116.96
2	G	301	MTX	CB-CG-CD	-3.16	104.11	112.51
2	E	301	MTX	O-C-N	3.15	128.25	122.45
2	A	301	MTX	C15-C16-C11	3.14	124.43	120.78
2	G	301	MTX	O-C-N	3.13	128.21	122.45
2	F	301	MTX	C6-C7-N8	-3.13	120.06	123.13
2	A	301	MTX	C15-C14-N10	-3.12	117.13	121.62
2	C	301	MTX	C6-C9-N10	-3.11	108.26	113.60
2	F	301	MTX	C11-C-N	-3.07	111.18	117.06
2	C	301	MTX	O2-CT-O1	3.06	131.04	124.09
2	E	301	MTX	CG-CB-CA	-3.05	107.46	113.16
2	B	301	MTX	CM-N10-C9	-3.04	106.76	114.84
2	G	301	MTX	C4A-C8A-N1	-2.99	116.86	121.71
2	E	301	MTX	NA2-C2-N3	2.92	121.80	117.25
2	A	301	MTX	NA4-C4-N3	2.89	124.94	117.07
2	D	301	MTX	O-C-N	2.88	127.75	122.45
2	E	301	MTX	C4A-C4-N3	-2.88	119.12	121.01
2	G	301	MTX	OE1-CD-CG	-2.86	113.90	123.08
2	A	301	MTX	C16-C11-C	-2.85	111.40	120.62
2	B	301	MTX	O2-CT-O1	2.83	130.51	124.09
2	E	301	MTX	C4A-C8A-N1	-2.83	117.12	121.71
2	A	301	MTX	C12-C11-C	2.81	129.73	120.62
2	G	301	MTX	C13-C12-C11	-2.81	117.51	120.78
2	B	301	MTX	C4A-C4-NA4	-2.74	116.19	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	MTX	C6-C7-N8	-2.73	120.45	123.13
2	F	301	MTX	NA2-C2-N3	2.70	121.45	117.25
2	A	301	MTX	O-C-C11	2.68	125.72	120.94
2	A	301	MTX	OE2-CD-OE1	2.68	129.98	123.30
2	E	301	MTX	CB-CA-N	2.67	116.26	110.88
2	B	301	MTX	C7-C6-N5	-2.65	119.12	120.85
2	D	301	MTX	C9-C6-N5	2.65	121.20	116.96
2	B	301	MTX	CB-CA-CT	-2.65	103.97	110.35
2	C	301	MTX	NA4-C4-N3	2.64	124.25	117.07
2	B	301	MTX	C9-C6-N5	2.62	121.16	116.96
2	F	301	MTX	C9-C6-C7	-2.60	117.05	121.60
2	B	301	MTX	C6-C7-N8	-2.58	120.60	123.13
2	F	301	MTX	C6-C9-N10	-2.51	109.30	113.60
2	C	301	MTX	NA2-C2-N3	2.48	121.11	117.25
2	C	301	MTX	O1-CT-CA	-2.40	114.39	122.26
2	G	301	MTX	CB-CA-CT	2.38	116.08	110.35
2	F	301	MTX	C4A-C4-NA4	-2.37	116.74	120.35
2	E	301	MTX	NA4-C4-N3	2.37	123.52	117.07
2	A	301	MTX	C12-C13-C14	2.37	123.44	120.32
2	D	301	MTX	C15-C14-N10	-2.36	118.23	121.62
2	G	301	MTX	C7-C6-N5	-2.34	119.32	120.85
2	E	301	MTX	C7-N8-C8A	-2.33	114.36	116.69
2	A	301	MTX	C16-C15-C14	-2.31	117.28	120.32
2	G	301	MTX	CM-N10-C9	-2.30	108.73	114.84
2	G	301	MTX	C16-C11-C	-2.28	113.22	120.62
2	A	301	MTX	NA2-C2-N1	2.23	121.42	117.79
2	E	301	MTX	O1-CT-CA	-2.22	114.96	122.26
2	E	301	MTX	C4-C4A-N5	-2.20	118.63	120.33
2	A	301	MTX	C6-C9-N10	-2.19	109.84	113.60
2	C	301	MTX	OE2-CD-CG	2.17	121.02	114.03
2	B	301	MTX	C6-C9-N10	-2.16	109.90	113.60
2	E	301	MTX	C6-C9-N10	-2.15	109.91	113.60
2	A	301	MTX	CB-CA-N	2.15	115.22	110.88
2	G	301	MTX	C11-C-N	-2.14	112.96	117.06
2	G	301	MTX	C4A-C4-NA4	-2.10	117.16	120.35
2	D	301	MTX	C6-C9-N10	-2.08	110.03	113.60
2	C	301	MTX	C7-N8-C8A	2.07	118.78	116.69
2	F	301	MTX	CB-CA-CT	2.05	115.31	110.35
2	B	301	MTX	C4A-C4-N3	2.05	122.36	121.01
2	G	301	MTX	NA4-C4-N3	2.04	122.61	117.07
2	F	301	MTX	C6-N5-C4A	2.04	121.33	118.04
2	C	301	MTX	C11-C-N	-2.03	113.17	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	MTX	CA-N-C	2.03	126.57	121.60
2	D	301	MTX	C13-C14-N10	2.01	124.50	121.62

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	MTX	CT-CA-N-C
2	A	301	MTX	CT-CA-CB-CG
2	B	301	MTX	CA-CB-CG-CD
2	E	301	MTX	CT-CA-N-C
2	E	301	MTX	CT-CA-CB-CG
2	F	301	MTX	CT-CA-N-C
2	F	301	MTX	CT-CA-CB-CG
2	F	301	MTX	O-C-C11-C16
2	F	301	MTX	N-C-C11-C16
2	A	301	MTX	N-CA-CB-CG
2	F	301	MTX	O-C-C11-C12
2	C	301	MTX	CA-CB-CG-CD
2	D	301	MTX	CT-CA-N-C
2	C	301	MTX	C13-C14-N10-CM
2	F	301	MTX	N-C-C11-C12
2	E	301	MTX	N-CA-CB-CG
2	B	301	MTX	CT-CA-CB-CG
2	C	301	MTX	CT-CA-CB-CG
2	C	301	MTX	C15-C14-N10-CM
2	B	301	MTX	N-CA-CB-CG
2	A	301	MTX	N-CA-CT-O1
2	A	301	MTX	N-CA-CT-O2
2	D	301	MTX	CT-CA-CB-CG
2	F	301	MTX	N-CA-CT-O1
2	G	301	MTX	CT-CA-CB-CG
2	D	301	MTX	CB-CA-CT-O1
2	D	301	MTX	CB-CA-CT-O2
2	G	301	MTX	CT-CA-N-C
2	C	301	MTX	OE2-CD-CG-CB
2	D	301	MTX	OE1-CD-CG-CB
2	C	301	MTX	OE1-CD-CG-CB
2	B	301	MTX	OE2-CD-CG-CB
2	F	301	MTX	N-CA-CT-O2
2	B	301	MTX	OE1-CD-CG-CB
2	G	301	MTX	OE1-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
2	A	301	MTX	OE1-CD-CG-CB
2	G	301	MTX	CB-CA-CT-O1
2	G	301	MTX	OE2-CD-CG-CB
2	A	301	MTX	OE2-CD-CG-CB
2	E	301	MTX	CA-CB-CG-CD
2	G	301	MTX	C13-C14-N10-C9
2	D	301	MTX	OE2-CD-CG-CB
2	D	301	MTX	N-CA-CT-O1
2	F	301	MTX	N-CA-CB-CG
2	G	301	MTX	CB-CA-CT-O2
2	F	301	MTX	OE1-CD-CG-CB
2	D	301	MTX	N-CA-CB-CG
2	E	301	MTX	OE1-CD-CG-CB
2	E	301	MTX	OE2-CD-CG-CB
2	F	301	MTX	OE2-CD-CG-CB
2	E	301	MTX	N-CA-CT-O1
2	G	301	MTX	C15-C14-N10-C9
2	E	301	MTX	C6-C9-N10-CM
2	D	301	MTX	C15-C14-N10-CM

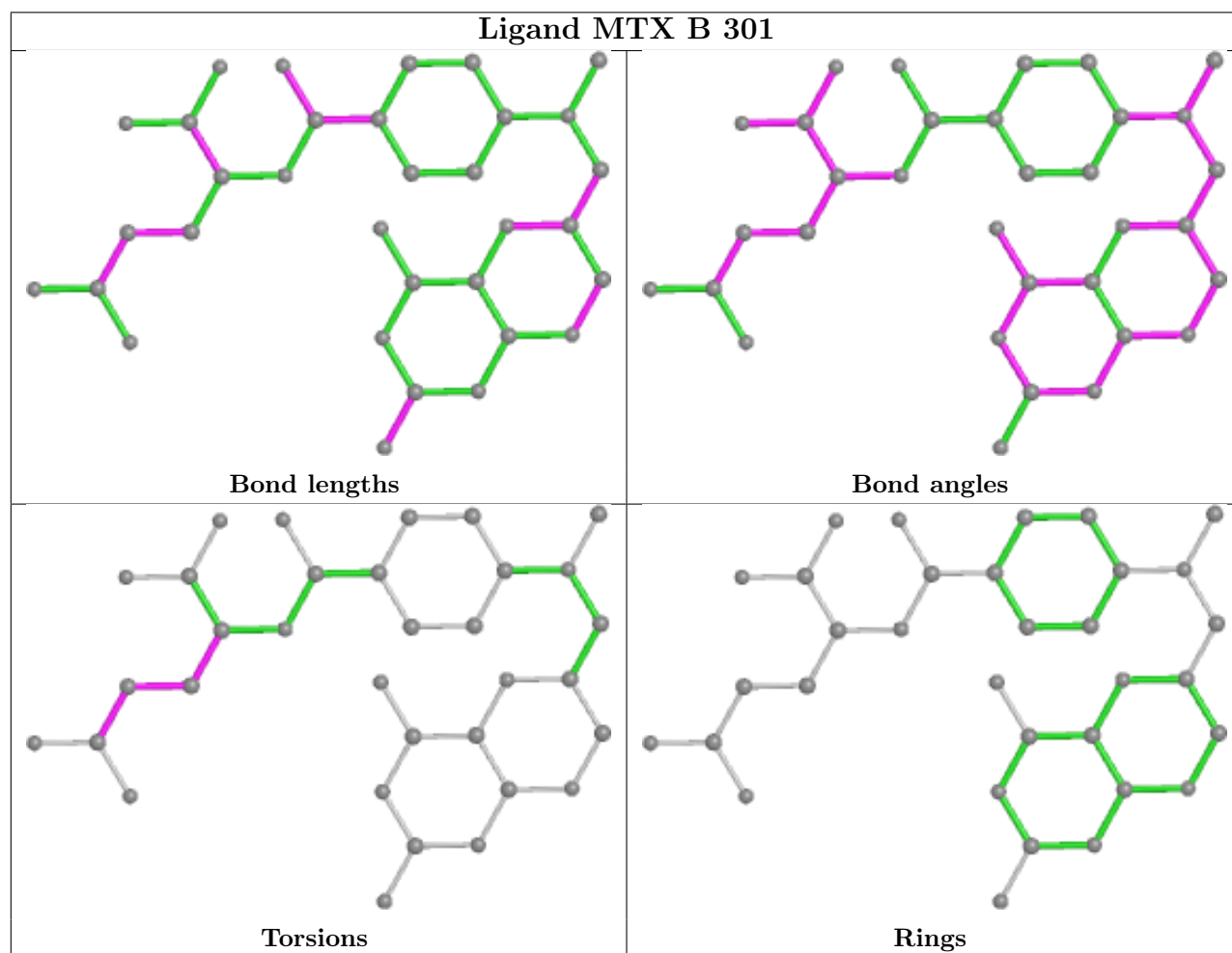
There are no ring outliers.

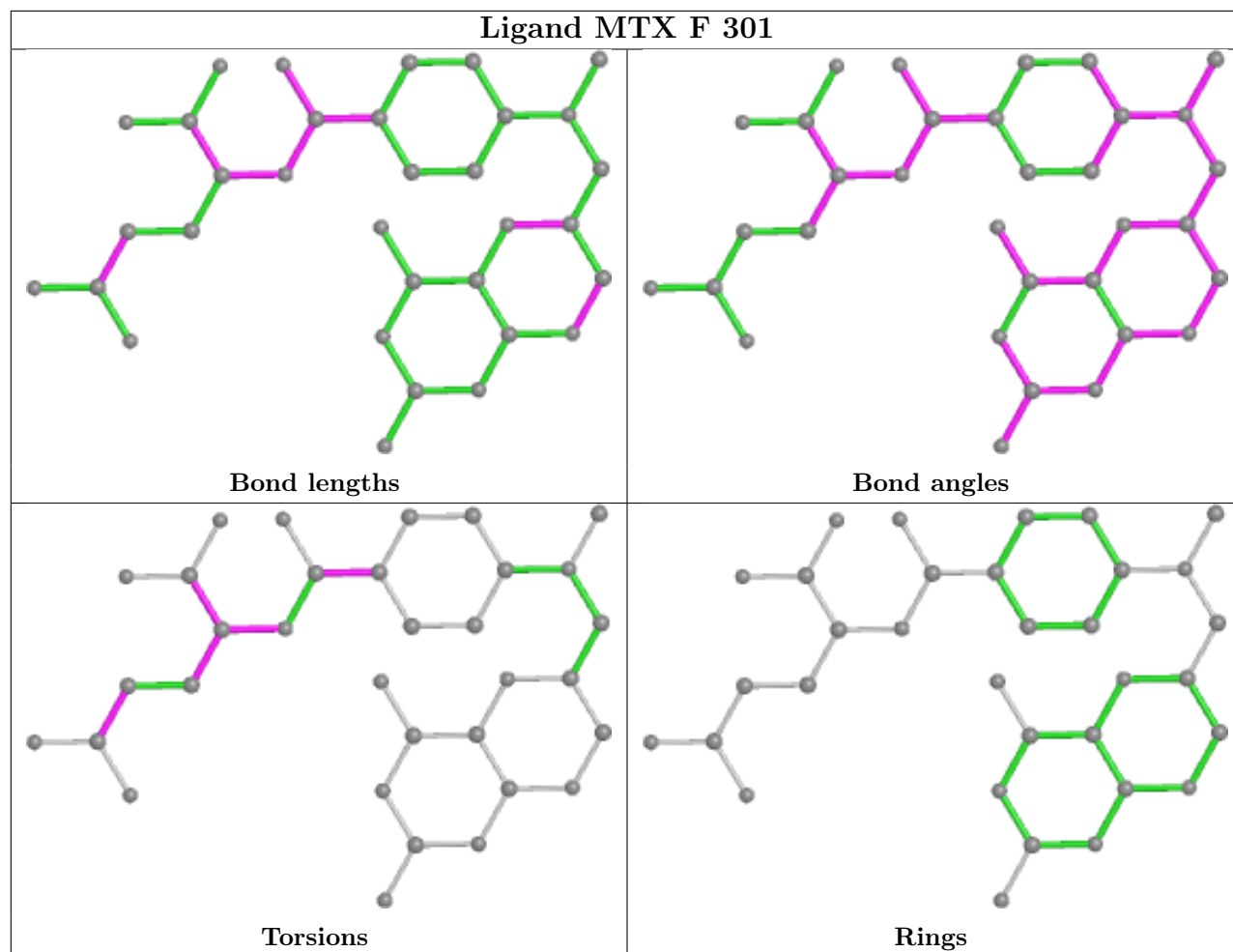
7 monomers are involved in 41 short contacts:

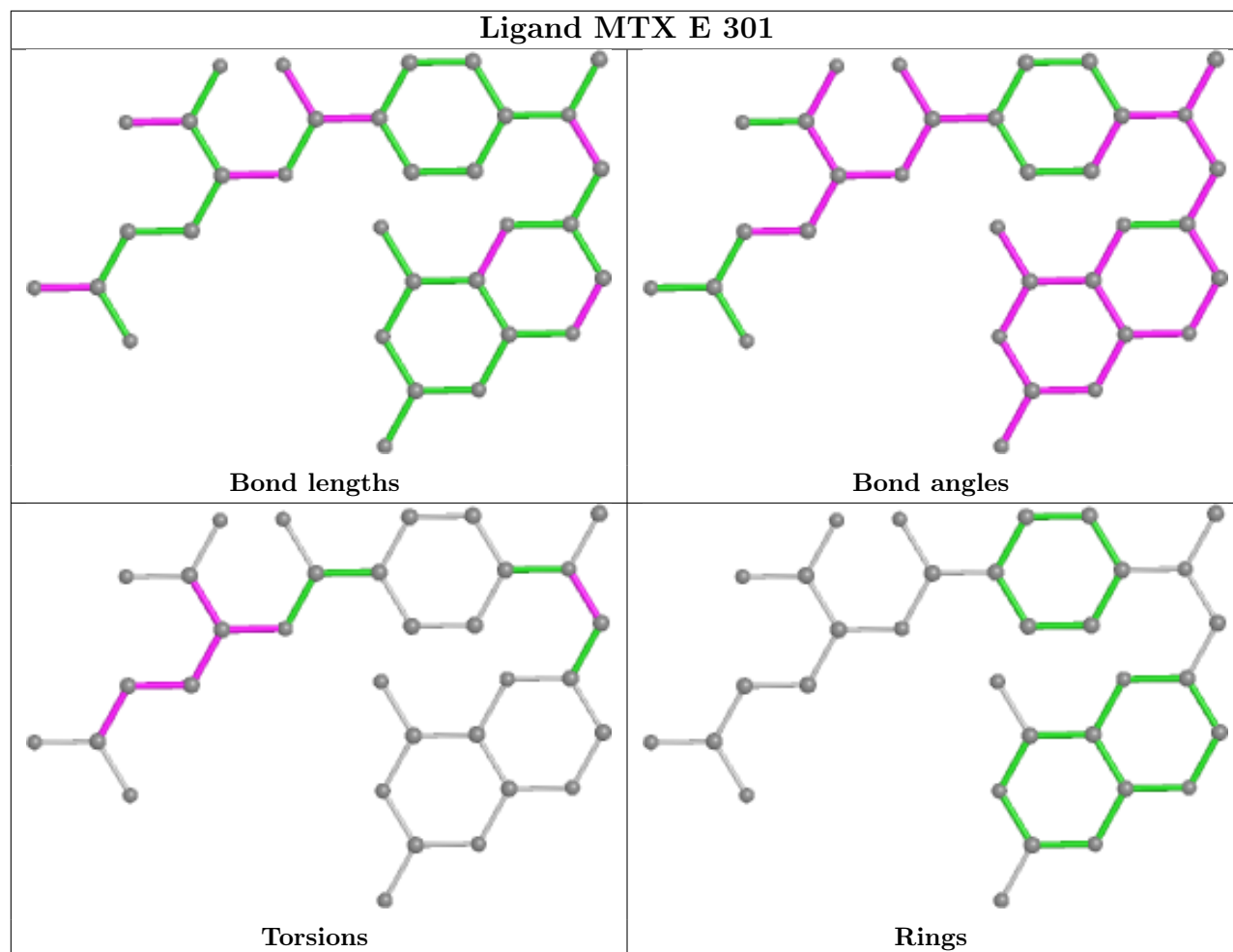
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	MTX	4	0
2	F	301	MTX	1	0
2	E	301	MTX	7	0
2	A	301	MTX	13	0
2	C	301	MTX	6	0
2	G	301	MTX	7	0
2	D	301	MTX	3	0

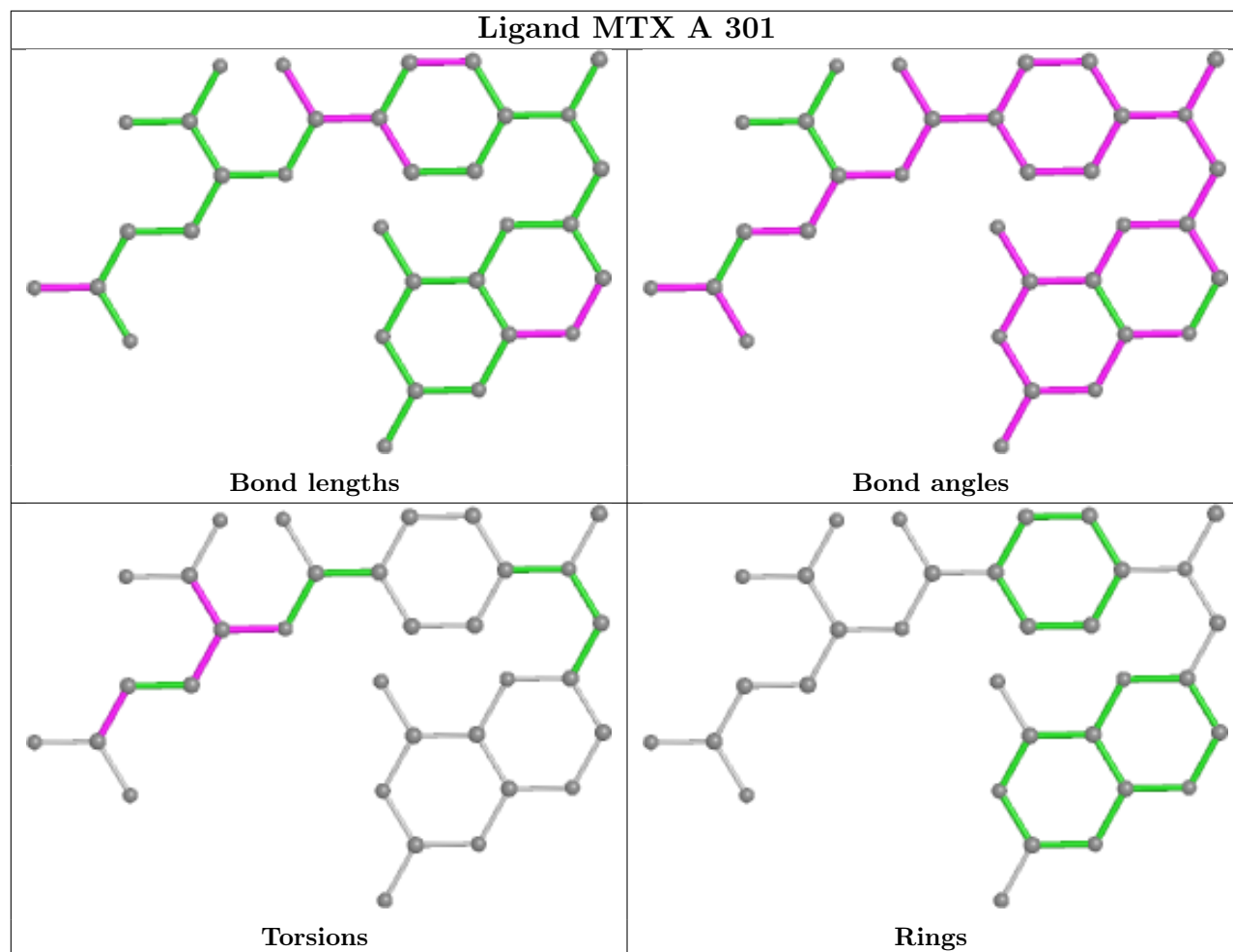
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

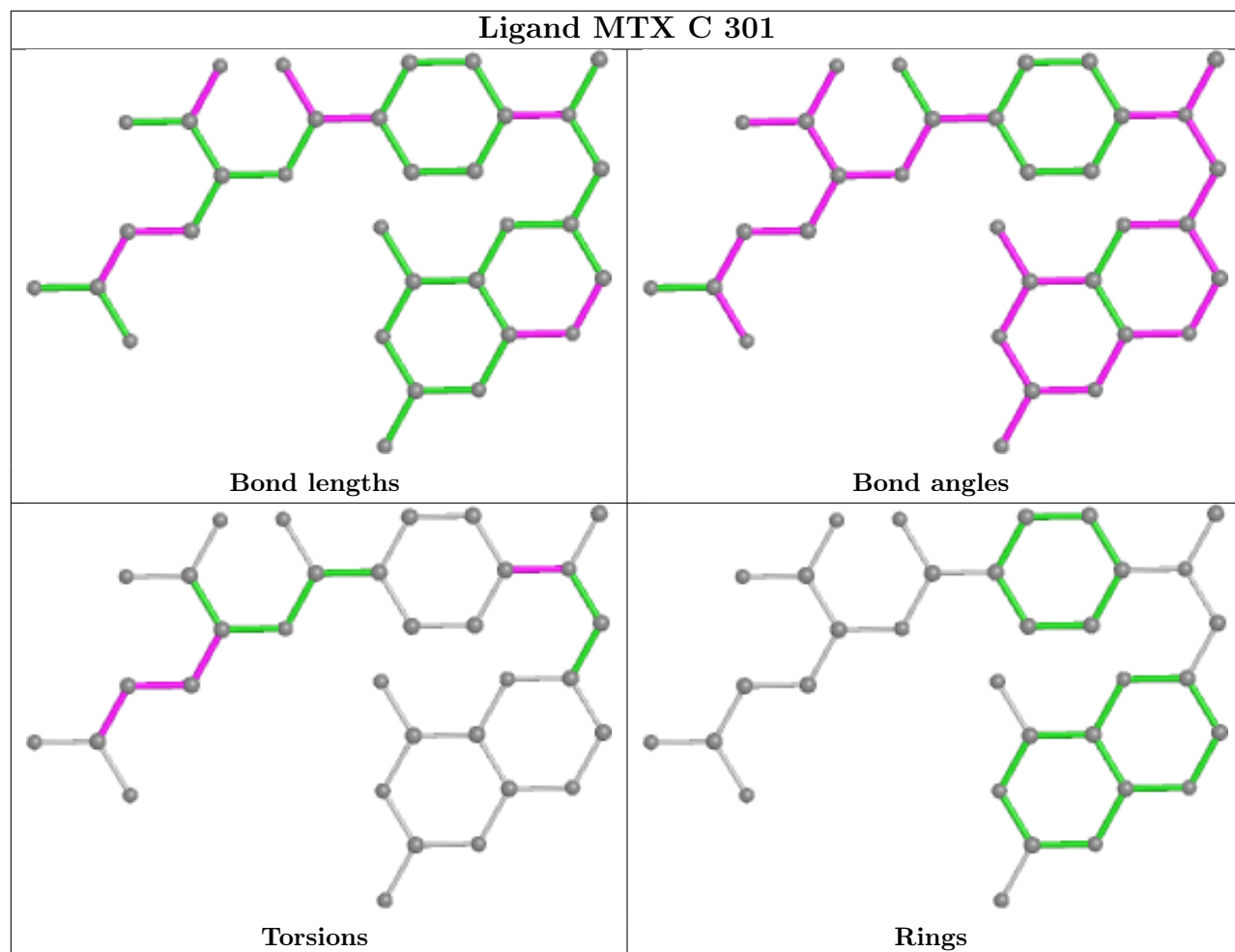
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

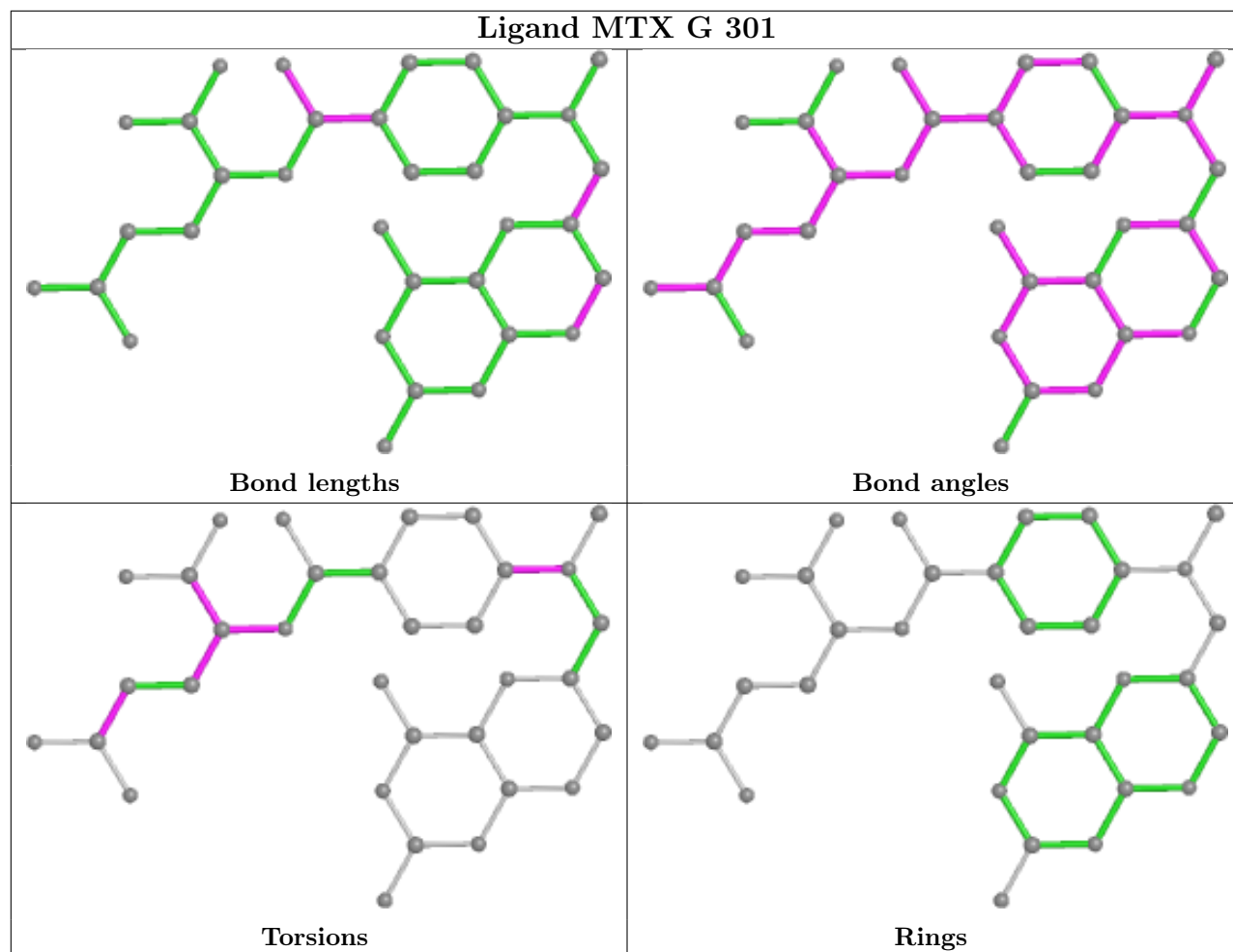


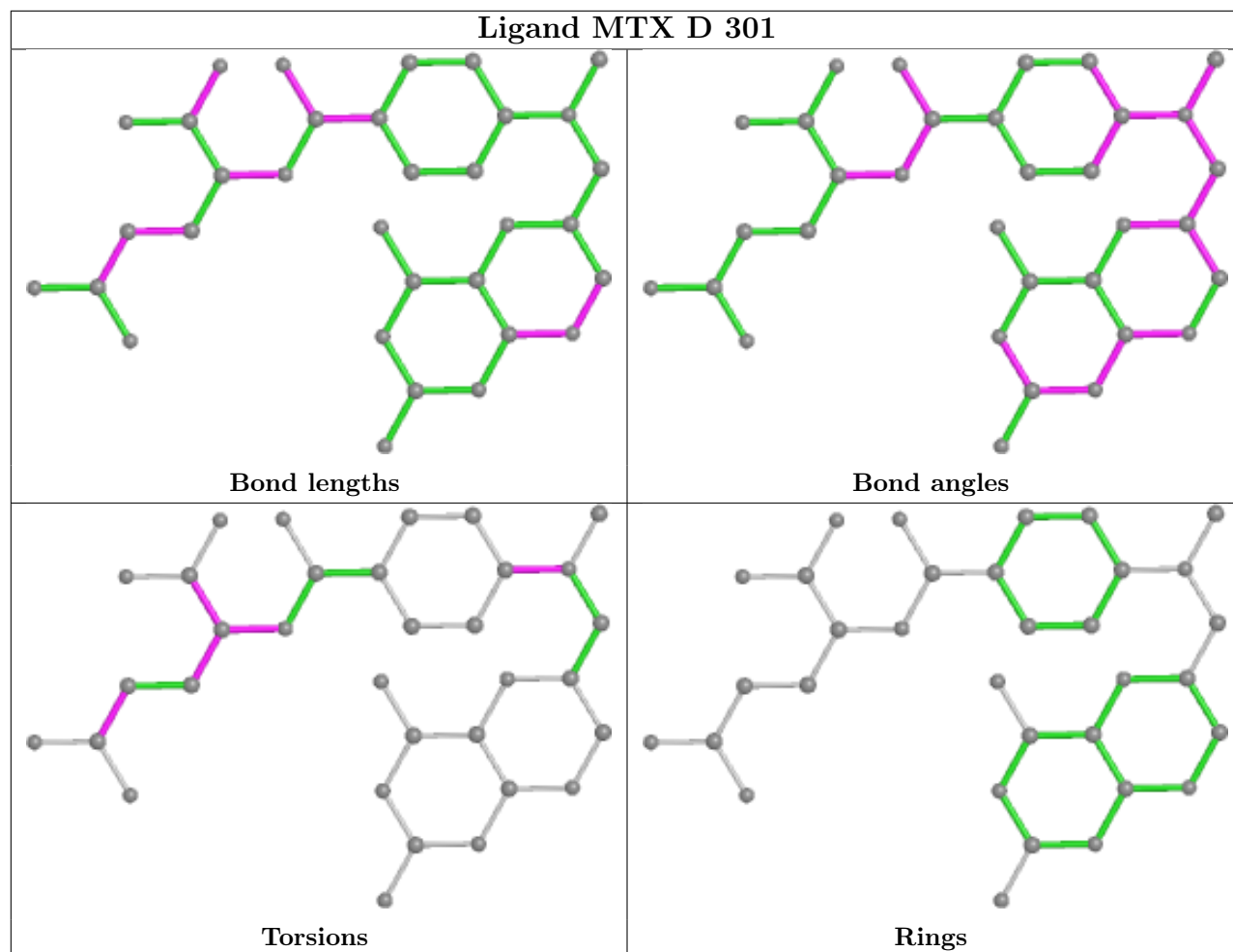












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	265/306 (86%)	0.03	2 (0%)	86 86	45, 59, 84, 107	1 (0%)
1	B	265/306 (86%)	0.10	1 (0%)	92 93	45, 64, 88, 108	1 (0%)
1	C	265/306 (86%)	0.01	2 (0%)	86 86	47, 62, 88, 114	1 (0%)
1	D	265/306 (86%)	0.05	2 (0%)	86 86	50, 68, 87, 105	1 (0%)
1	E	270/306 (88%)	0.18	2 (0%)	87 87	61, 77, 102, 117	1 (0%)
1	F	265/306 (86%)	0.23	12 (4%)	33 29	58, 77, 107, 120	1 (0%)
1	G	265/306 (86%)	0.36	13 (4%)	29 26	60, 84, 111, 125	1 (0%)
All	All	1860/2142 (86%)	0.14	34 (1%)	68 67	45, 71, 100, 125	7 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	174	SER	4.3
1	F	51	LYS	4.1
1	G	260	LEU	3.9
1	F	82	LEU	3.7
1	G	140	ASP	3.5
1	F	115	ALA	3.0
1	G	216	GLY	2.8
1	F	138	VAL	2.8
1	F	57	GLY	2.7
1	A	174	SER	2.7
1	C	140	ASP	2.7
1	E	140	ASP	2.6
1	G	297	SER	2.6
1	F	49	LEU	2.5
1	G	82	LEU	2.5
1	D	298	SER	2.4
1	F	118	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	298	SER	2.4
1	D	140	ASP	2.3
1	F	80	TYR	2.3
1	G	215	PRO	2.3
1	F	50	GLY	2.2
1	G	235	GLY	2.2
1	G	257	MET	2.2
1	G	194	LEU	2.1
1	G	55	LEU	2.1
1	F	113	ILE	2.1
1	G	255	LEU	2.1
1	A	51	LYS	2.1
1	G	54	LYS	2.1
1	B	113	ILE	2.1
1	F	135	PHE	2.0
1	F	177	GLN	2.0
1	C	174	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

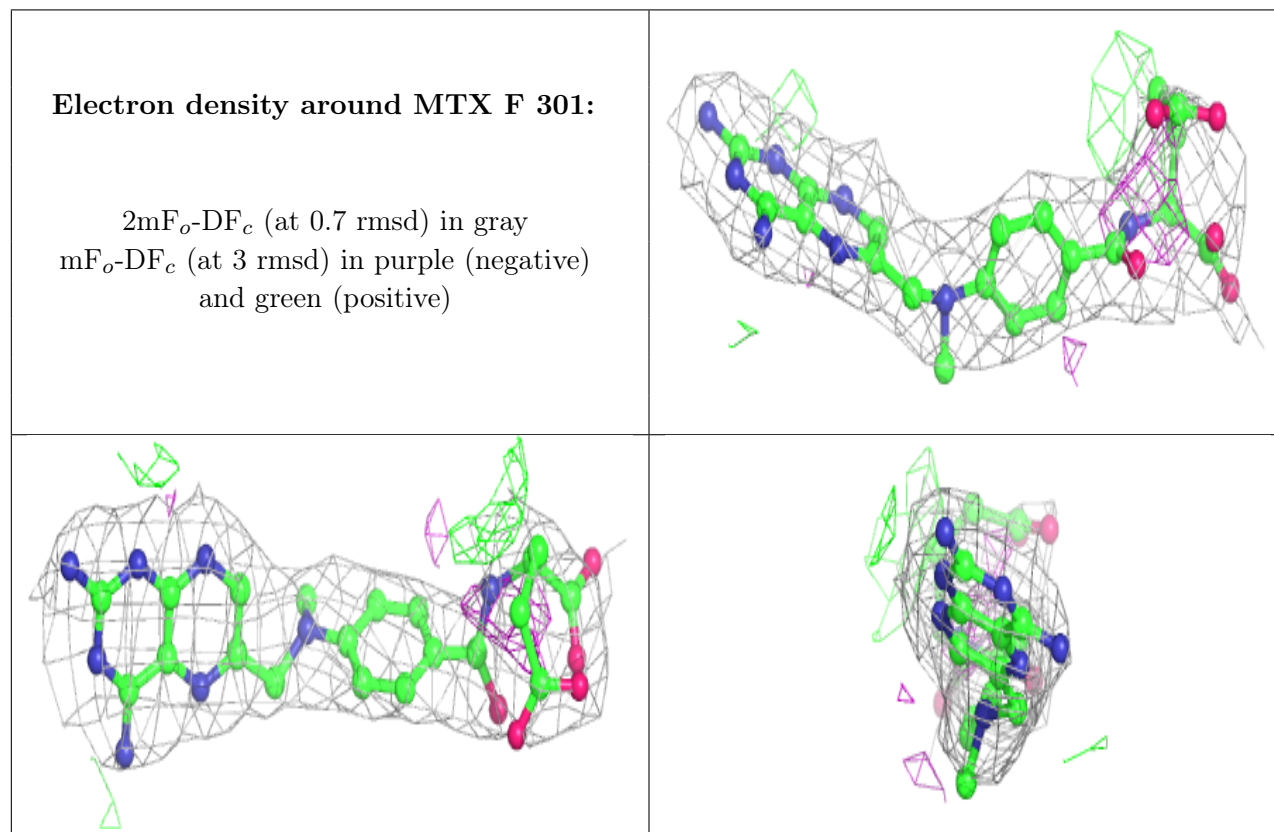
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NA	B	303	1/1	0.63	0.30	79,79,79,79	0
3	NA	F	303	1/1	0.72	0.24	87,87,87,87	0
3	NA	A	303	1/1	0.83	0.12	69,69,69,69	0
3	NA	D	303	1/1	0.85	0.12	74,74,74,74	0
3	NA	G	303	1/1	0.85	0.27	82,82,82,82	0
2	MTX	F	301	33/33	0.93	0.27	48,83,116,117	0

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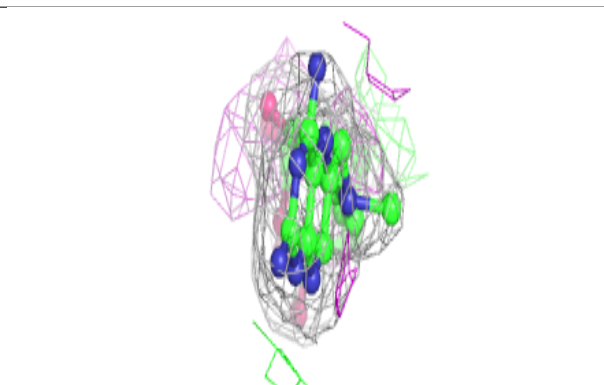
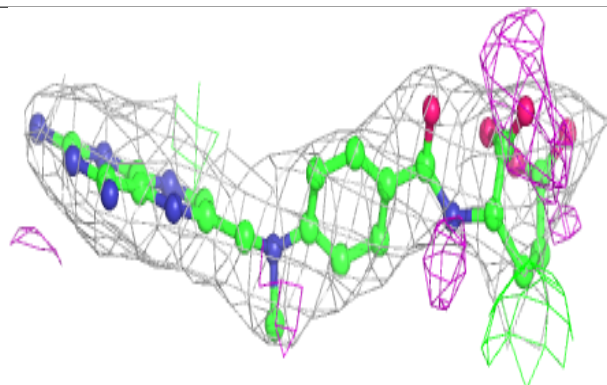
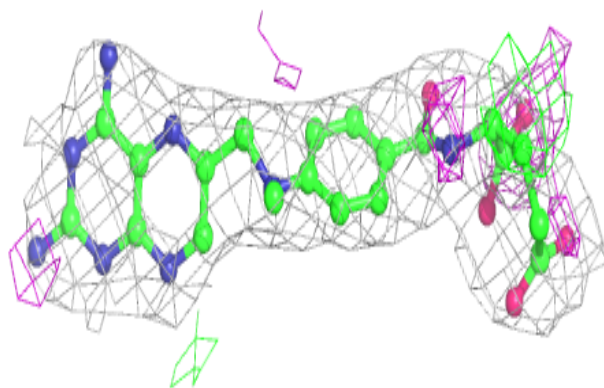
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NA	E	302	1/1	0.93	0.09	77,77,77,77	0
2	MTX	C	301	33/33	0.95	0.23	59,67,81,83	0
3	NA	C	303	1/1	0.95	0.24	55,55,55,55	0
2	MTX	D	301	33/33	0.95	0.25	71,76,95,99	0
3	NA	A	302	1/1	0.96	0.04	63,63,63,63	0
2	MTX	E	301	33/33	0.96	0.24	60,65,92,95	0
3	NA	F	302	1/1	0.96	0.07	84,84,84,84	0
2	MTX	A	301	33/33	0.96	0.22	50,55,69,77	0
2	MTX	G	301	33/33	0.96	0.24	69,74,92,94	0
3	NA	C	302	1/1	0.97	0.05	63,63,63,63	0
2	MTX	B	301	33/33	0.97	0.22	45,56,76,77	0
3	NA	G	302	1/1	0.97	0.07	85,85,85,85	0
3	NA	E	303	1/1	0.97	0.20	76,76,76,76	0
3	NA	B	302	1/1	0.98	0.08	87,87,87,87	0
3	NA	D	302	1/1	0.99	0.07	52,52,52,52	0

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

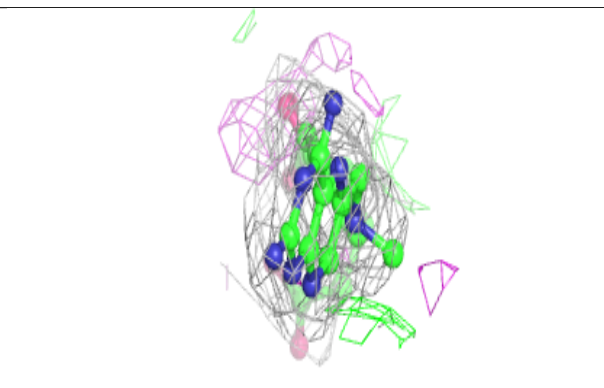
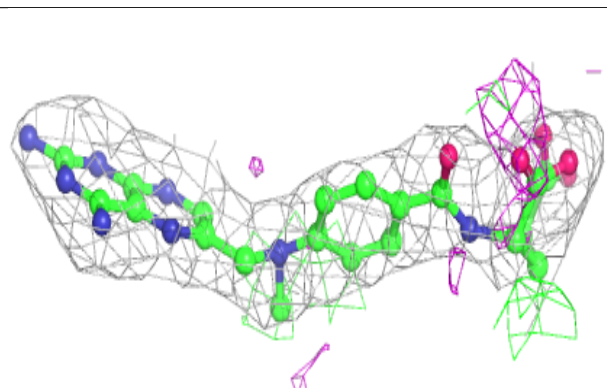
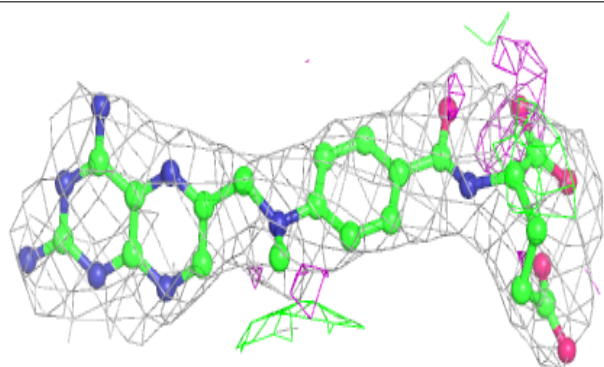


Electron density around MTX C 301:

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

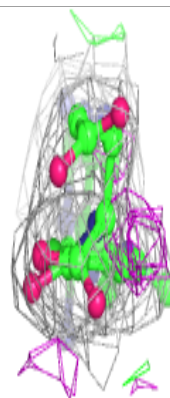
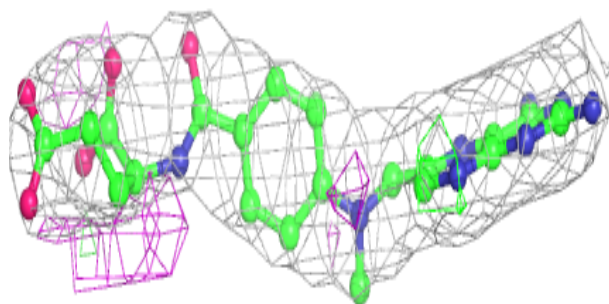
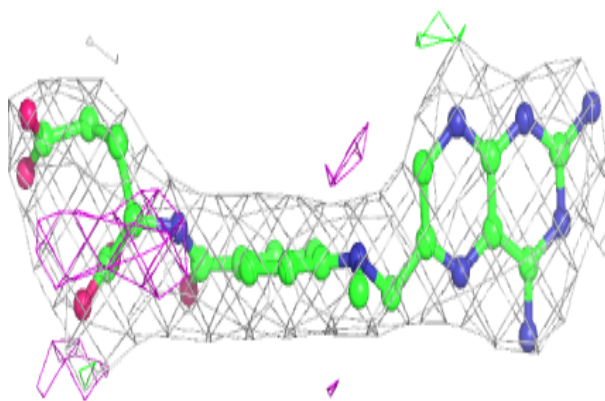
**Electron density around MTX D 301:**

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

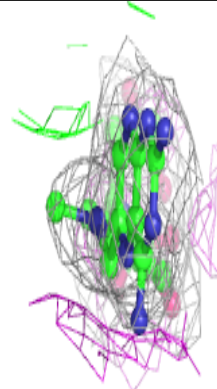
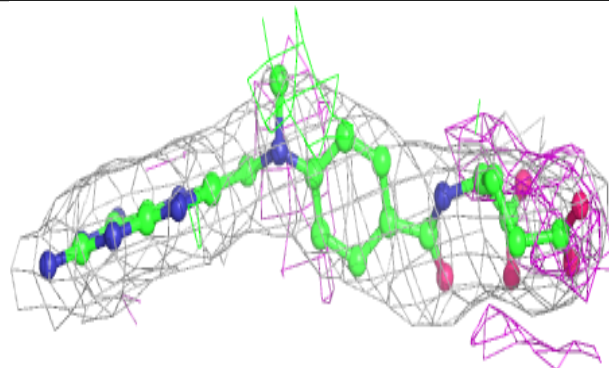
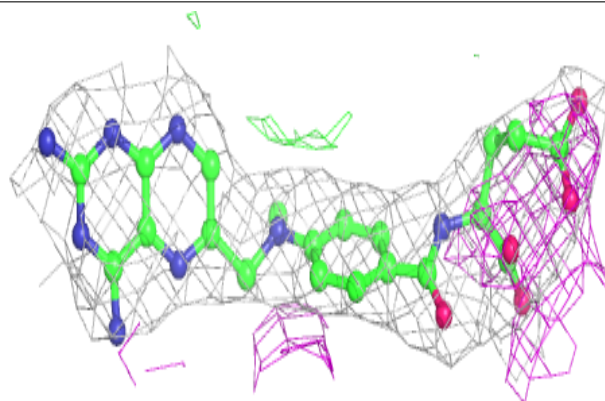


Electron density around MTX E 301:

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

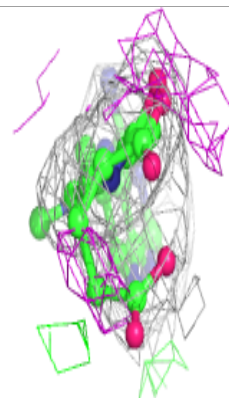
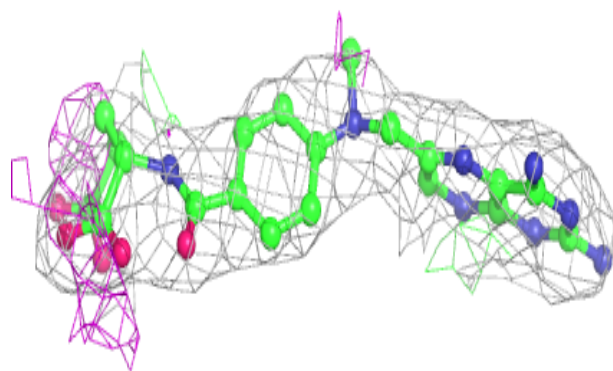
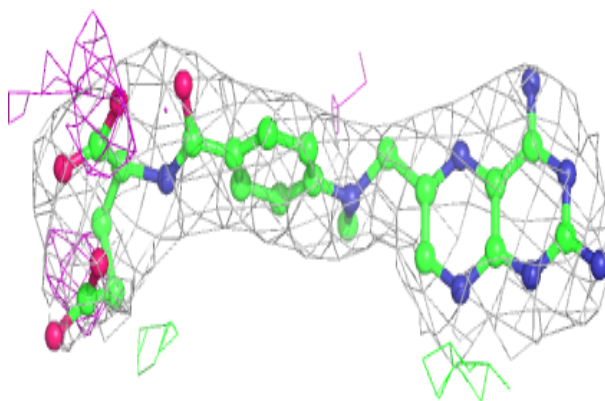
**Electron density around MTX A 301:**

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

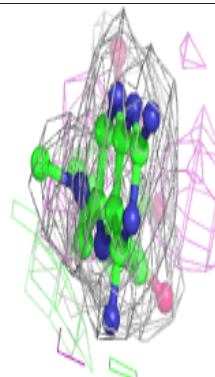
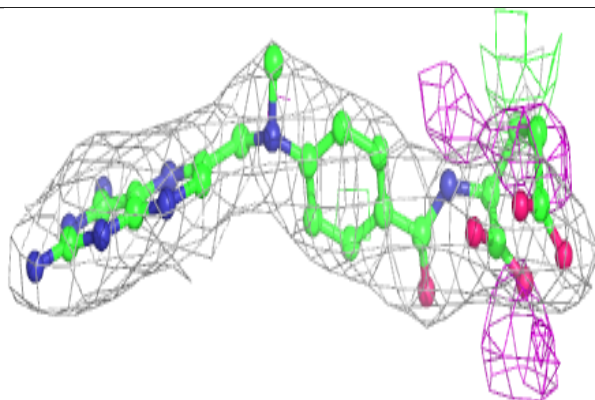
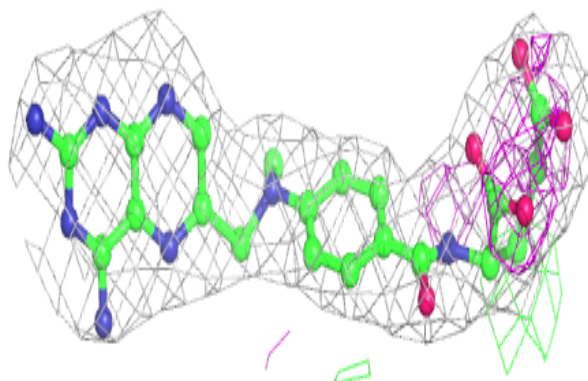


Electron density around MTX G 301:

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

**Electron density around MTX B 301:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.