



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:51 PM UTC

PDB ID : 7RGA / pdb_00007rga
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

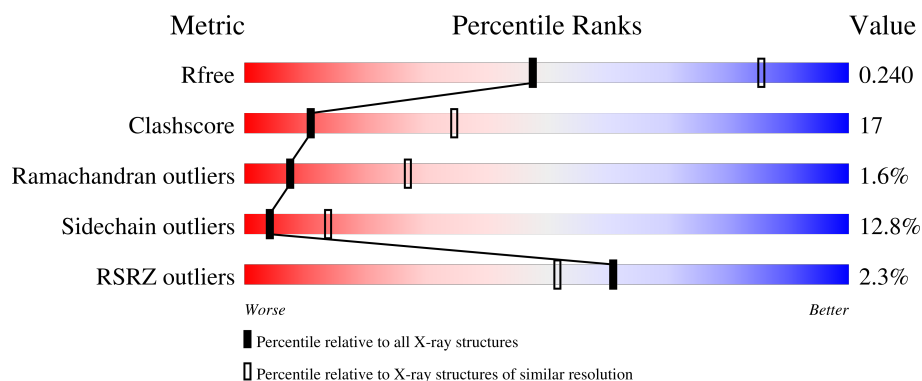
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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	2% 60% 21% . . 13%
1	B	306	2% 54% 27% 5% 13%
1	C	306	3% 57% 24% 6% 13%
1	D	306	57% 26% . 13%
1	E	306	3% 57% 25% 6% . 12%

Continued on next page...

Continued from previous page...

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	-
3	NA	F	303	-	-	-	X

2 Entry composition [i](#)

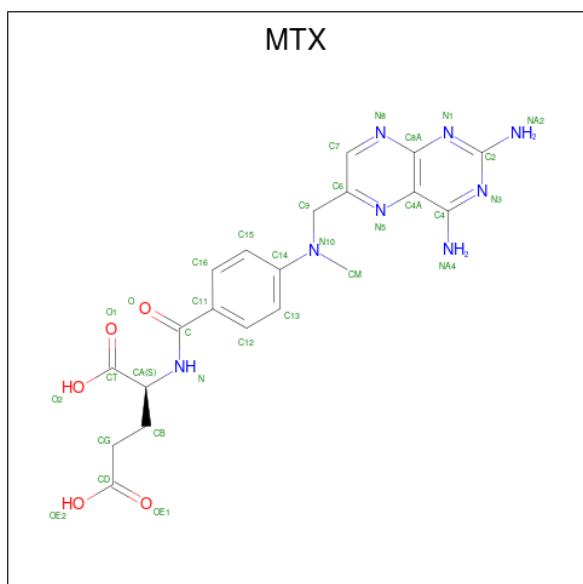
There are 4 unique types of molecules in this entry. The entry contains 14664 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: MTX) (formula: $C_{20}H_{22}N_8O_5$) (labeled as "Ligand of Interest" by depositor).



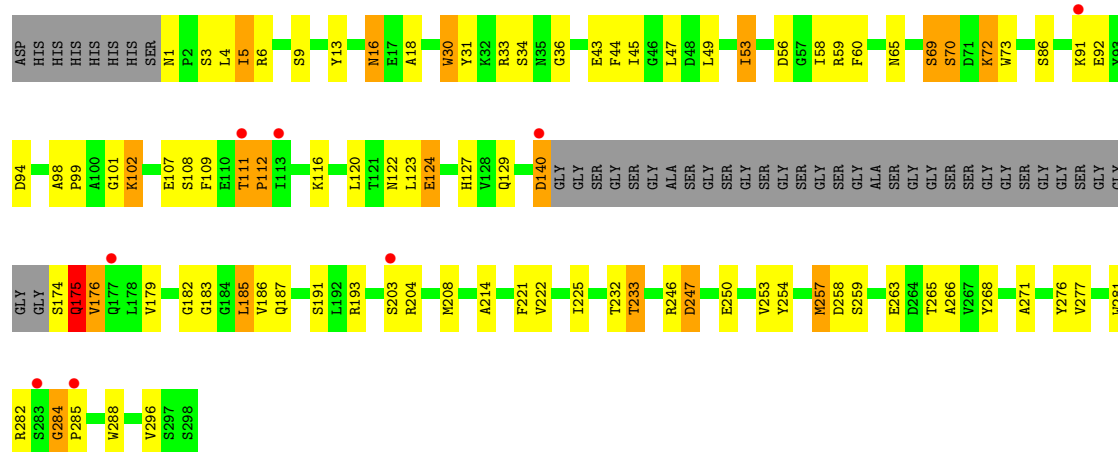
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	20	8	5		
2	B	1	Total	C	N	O	0	0
			33	20	8	5		
2	C	1	Total	C	N	O	0	0
			33	20	8	5		
2	D	1	Total	C	N	O	0	0
			33	20	8	5		
2	E	1	Total	C	N	O	0	0
			33	20	8	5		
2	F	1	Total	C	N	O	0	0
			33	20	8	5		
2	G	1	Total	C	N	O	0	0
			33	20	8	5		

- Molecule 3 is SODIUM ION (CCD ID: 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		

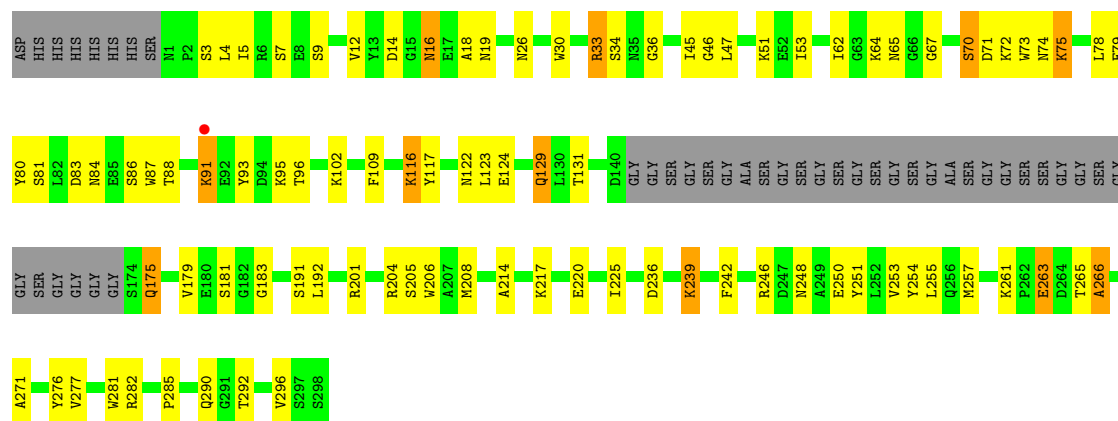
- Molecule 4 is water.

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



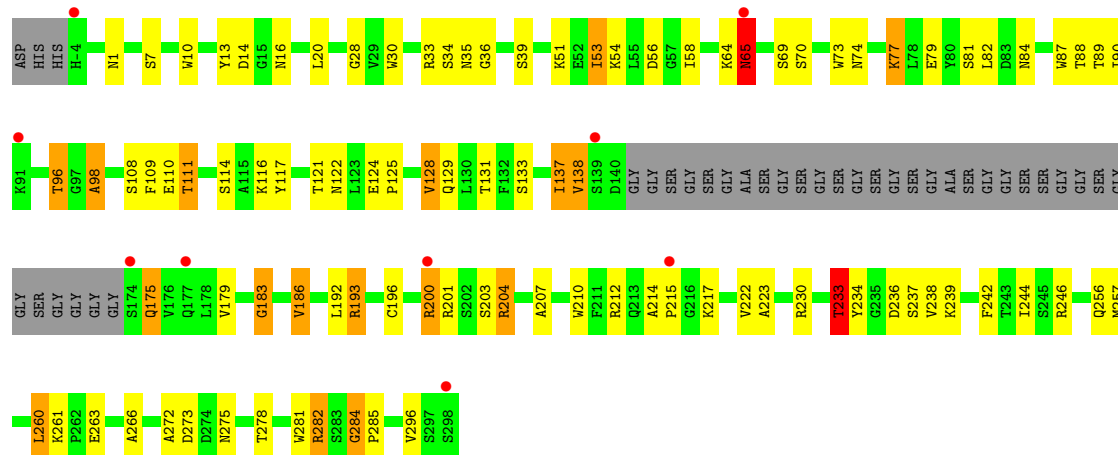
• Molecule 1: nano CLostridial Antibody Mimetic Protein 3 VHH

Chain D: 57% 26% 13%

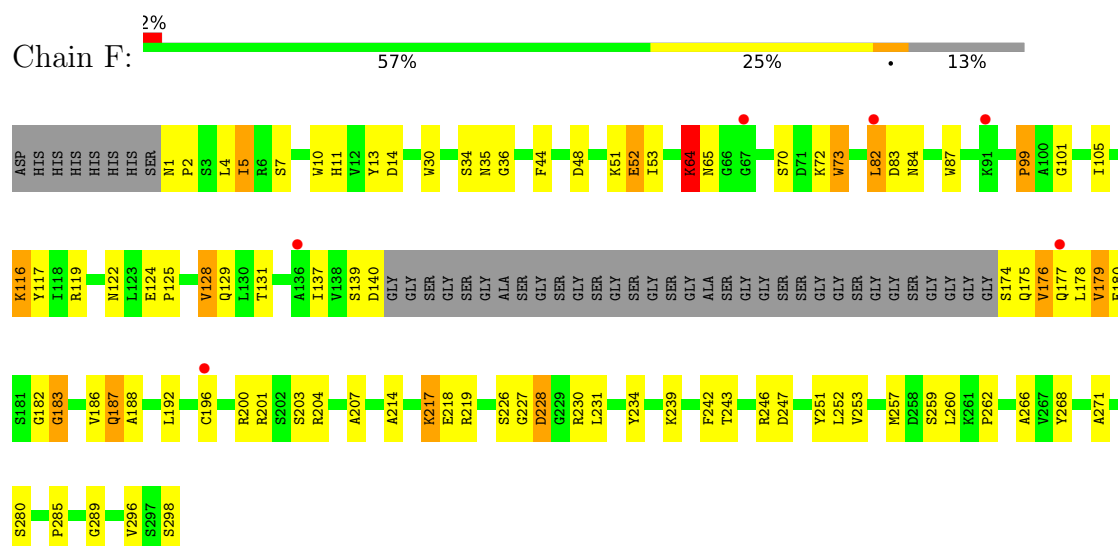


• Molecule 1: nano CLostridial Antibody Mimetic Protein 3 VHH

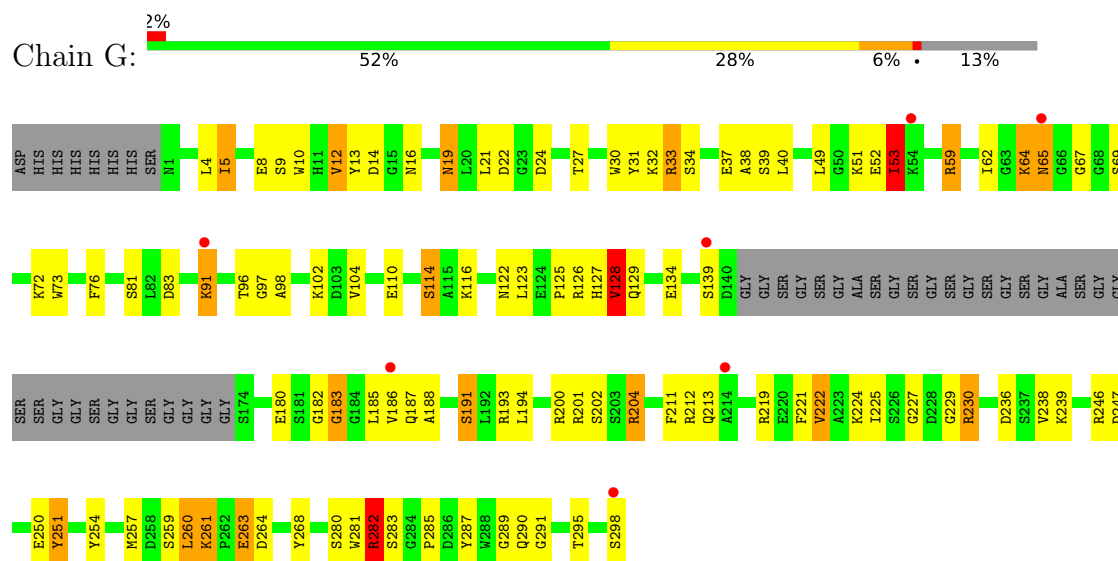
Chain E: 3% 57% 25% 6% 12%



• Molecule 1: nano CLostridial Antibody Mimetic Protein 3 VHH



- Molecule 1: nano CLostridial Antibody Mimetic Protein 3 VHH



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)	0.35 , 64.8	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	1.29	6/2053 (0.3%)	1.36	10/2781 (0.4%)
1	B	1.25	3/2108 (0.1%)	1.31	8/2850 (0.3%)
1	C	1.25	4/2106 (0.2%)	1.34	11/2849 (0.4%)
1	D	1.16	3/2092 (0.1%)	1.31	10/2829 (0.4%)
1	E	1.14	1/2151 (0.0%)	1.30	17/2909 (0.6%)
1	F	1.07	1/2109 (0.0%)	1.22	7/2852 (0.2%)
1	G	1.07	2/2104 (0.1%)	1.23	7/2845 (0.2%)
All	All	1.18	20/14723 (0.1%)	1.30	70/19915 (0.4%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	91	LYS	CA-C	-6.63	1.44	1.52
1	A	90	ILE	C-O	-6.36	1.18	1.24
1	B	100	ALA	CA-CB	-6.30	1.43	1.53
1	G	222	VAL	CA-CB	-6.26	1.49	1.55
1	D	91	LYS	CA-C	-5.93	1.44	1.52
1	A	91	LYS	CA-C	-5.76	1.45	1.52
1	B	91	LYS	CA-C	-5.76	1.45	1.52
1	D	12	VAL	CA-CB	-5.57	1.47	1.54
1	A	12	VAL	C-O	-5.50	1.17	1.24
1	C	175	GLN	CA-C	5.43	1.60	1.52
1	A	198	ALA	CA-CB	-5.32	1.43	1.54
1	C	91	LYS	CA-C	-5.30	1.45	1.52
1	A	41	ALA	CA-CB	-5.24	1.45	1.53
1	B	197	ALA	CA-CB	-5.22	1.45	1.53
1	A	271	ALA	CA-C	-5.17	1.46	1.52
1	C	30	TRP	N-CA	-5.14	1.39	1.46
1	F	207	ALA	CA-CB	-5.10	1.44	1.53
1	C	247	ASP	N-CA	-5.10	1.40	1.46
1	E	88	THR	CA-CB	5.05	1.61	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	12	VAL	C-O	-5.02	1.18	1.24

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	VAL	N-CA-C	9.35	121.92	109.21
1	A	284	GLY	CA-C-N	8.02	128.07	119.89
1	A	284	GLY	C-N-CA	8.02	128.07	119.89
1	B	12	VAL	CB-CA-C	-7.71	102.06	111.08
1	F	82	LEU	N-CA-C	-7.16	103.15	112.68
1	C	34	SER	N-CA-C	7.15	122.39	112.45
1	G	53	ILE	N-CA-C	7.13	118.99	108.65
1	C	221	PHE	CA-C-N	-7.03	115.71	123.16
1	C	221	PHE	C-N-CA	-7.03	115.71	123.16
1	E	1	ASN	CA-C-N	-6.96	113.53	120.21
1	E	1	ASN	C-N-CA	-6.96	113.53	120.21
1	C	182	GLY	N-CA-C	-6.76	102.81	112.81
1	F	179	VAL	N-CA-C	6.69	117.76	108.12
1	E	284	GLY	CA-C-N	6.62	126.38	119.76
1	E	284	GLY	C-N-CA	6.62	126.38	119.76
1	A	248	ASN	N-CA-C	6.50	119.19	111.71
1	F	53	ILE	N-CA-C	6.48	117.50	108.23
1	C	193	ARG	N-CA-C	6.40	119.33	108.90
1	B	284	GLY	CA-C-N	6.34	127.77	119.84
1	B	284	GLY	C-N-CA	6.34	127.77	119.84
1	C	214	ALA	N-CA-C	-6.33	102.11	110.40
1	A	175	GLN	N-CA-C	6.31	124.25	110.80
1	B	214	ALA	CA-C-N	-6.27	113.49	119.76
1	B	214	ALA	C-N-CA	-6.27	113.49	119.76
1	A	27	THR	N-CA-C	-6.25	98.21	108.76
1	D	206	TRP	N-CA-C	6.16	119.96	110.42
1	D	124	GLU	CA-C-N	-6.11	113.39	119.93
1	D	124	GLU	C-N-CA	-6.11	113.39	119.93
1	F	116	LYS	N-CA-C	-6.03	106.08	113.50
1	A	241	ARG	N-CA-C	-6.01	106.59	114.04
1	E	35	ASN	N-CA-C	5.99	120.13	111.56
1	A	53	ILE	N-CA-C	5.99	116.14	107.88
1	E	133	SER	N-CA-C	5.92	123.41	110.80
1	F	243	THR	N-CA-C	5.89	118.02	108.41
1	E	207	ALA	N-CA-C	-5.88	100.97	110.32
1	B	48	ASP	N-CA-C	-5.79	99.74	109.07
1	G	238	VAL	N-CA-C	5.79	119.20	113.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	116	LYS	N-CA-C	-5.78	106.77	113.88
1	B	138	VAL	N-CA-C	5.75	116.76	108.48
1	F	64	LYS	N-CA-C	-5.71	100.61	109.24
1	E	238	VAL	N-CA-C	5.69	118.67	113.20
1	E	175	GLN	N-CA-C	5.67	117.86	110.43
1	E	233	THR	N-CA-C	5.64	117.97	109.23
1	C	31	TYR	N-CA-C	5.63	117.70	108.52
1	G	19	ASN	N-CA-C	-5.60	106.40	113.18
1	G	116	LYS	N-CA-C	-5.59	106.62	113.50
1	C	47	LEU	N-CA-C	5.59	118.56	109.06
1	C	222	VAL	CB-CA-C	-5.58	106.09	111.05
1	E	89	THR	CB-CA-C	-5.52	101.97	110.26
1	E	238	VAL	CB-CA-C	-5.50	105.25	110.70
1	C	53	ILE	N-CA-C	5.50	115.24	108.53
1	A	179	VAL	N-CA-C	5.49	115.96	107.78
1	G	12	VAL	CB-CA-C	-5.40	103.26	111.69
1	D	179	VAL	N-CA-C	5.40	115.67	108.11
1	D	71	ASP	N-CA-C	5.33	117.28	110.61
1	D	214	ALA	CA-C-N	-5.32	114.76	120.03
1	D	214	ALA	C-N-CA	-5.32	114.76	120.03
1	G	67	GLY	N-CA-C	-5.29	100.63	113.18
1	E	111	THR	CB-CA-C	-5.29	103.83	109.85
1	G	128	VAL	N-CA-CB	-5.27	106.26	112.32
1	D	67	GLY	N-CA-C	-5.26	100.71	113.18
1	A	222	VAL	CB-CA-C	-5.22	106.40	111.05
1	E	90	ILE	N-CA-C	5.15	115.82	110.82
1	A	5	ILE	CB-CA-C	-5.12	103.00	110.62
1	F	182	GLY	N-CA-C	-5.11	106.15	112.33
1	C	296	VAL	CB-CA-C	-5.09	104.37	110.99
1	E	98	ALA	CA-C-N	5.09	125.08	119.89
1	E	98	ALA	C-N-CA	5.09	125.08	119.89
1	E	246	ARG	N-CA-C	5.05	116.92	108.99
1	D	129	GLN	N-CA-C	-5.03	99.91	108.26

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2011	0	1886	67	0
1	B	2064	0	1970	73	0
1	C	2062	0	1965	61	0
1	D	2050	0	1956	53	0
1	E	2104	0	1996	76	0
1	F	2065	0	1974	52	0
1	G	2060	0	1957	80	0
2	A	33	0	20	14	0
2	B	33	0	20	4	0
2	C	33	0	20	7	0
2	D	33	0	20	4	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	471	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 17.

All (471) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:111:THR:HG1	1:E:281:TRP:CD1	1.93	0.86
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
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	0.76
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:B:64:LYS:O	1:B:65:ASN:C	2.31	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:282:ARG:HH11	1:B:282:ARG:CG	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:E:128:VAL:HG12	1:E:129:GLN:N	2.08	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:E:51:LYS:C	1:E:116:LYS:HG3	2.22	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:187:GLN:HE22	1:F:298:SER:C	2.05	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:G:4:LEU:HG	1:G:5:ILE:N	2.13	0.62
1:G:263:GLU:H	1:G:263:GLU:CD	2.08	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:C:257:MET:HE3	1:C:268:TYR:CE2	2.36	0.61
1:B:77:LYS:HD2	1:B:123:LEU:HD21	1.82	0.60
2:A:301:MTX:CG	1:B:98:ALA:HA	2.31	0.60
1:A:111:THR:HG1	1:E:281:TRP:HD1	1.43	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:287:TYR:OH	2:G:301:MTX:HB1	2.02	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:B:204:ARG:HG2	1:B:205:SER:N	2.16	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
2:A:301:MTX:O1	2:A:301:MTX:CG	2.45	0.58
1:F:257:MET:HE2	1:F:268:TYR:CE2	2.39	0.57
1:B:281:TRP:O	1:B:282:ARG:C	2.46	0.57
1:E:13:TYR:CD2	1:E:14:ASP:HB2	2.39	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:B:192:LEU:HB3	1:B:257:MET:HE3	1.85	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:D:263:GLU:CD	1:D:263:GLU:H	2.13	0.56
1:G:128:VAL:HG13	1:G:129:GLN:N	2.20	0.56
1:G:187:GLN:HE21	1:G:298:SER:C	2.14	0.56
1:B:263:GLU:H	1:B:263:GLU:CD	2.13	0.55
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:64:LYS:C	1:G:65:ASN:O	2.49	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:48:ASP:C	1:A:48:ASP:OD1	2.50	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: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:C:208:MET:HE2	2:C:301:MTX:C4A	2.38	0.53
1:C:281:TRP:O	1:C:282:ARG:C	2.52	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
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:B:241:ARG:C	1:B:242:PHE:HD1	2.16	0.53
1:A:99:PRO:HB3	1:B:201:ARG:O	2.08	0.53
1:B:275:ASN:OD1	1:B:275:ASN:C	2.52	0.53
1:D:33:ARG:HG3	1:D:34:SER:N	2.24	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:109:PHE:O	1:E:110:GLU:C	2.53	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:83:ASP:O	1:D:84:ASN:CB	2.57	0.51
1:D:208:MET:HE2	2:D:301:MTX:C4A	2.40	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:6:ARG:HD2	1:C:6:ARG:C	2.36	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
2:A:301:MTX:HG2	1:B:97:GLY:C	2.37	0.50
1:D:271:ALA:HB1	1:D:285:PRO:CB	2.40	0.50
1:F:34:SER:O	1:F:35:ASN:HB2	2.11	0.50
1:B:224:LYS:HG3	1:B:276:TYR:CE1	2.46	0.50
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:E:273:ASP:OD2	1:E:284:GLY:C	2.55	0.50
1:A:33:ARG:NH1	1:A:36:GLY:O	2.44	0.50
1:A:30:TRP:NE1	1:A:129:GLN:HE21	2.02	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:C:247:ASP:C	1:C:247:ASP:OD1	2.54	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:C:186:VAL:HG22	1:C:187:GLN:N	2.26	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:GLY:HA2	1:F:246:ARG:NH1	2.27	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:A:208:MET:HE2	2:A:301:MTX:C4A	2.43	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: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:C:58:ILE:C	1:C:58:ILE:HD12	2.38	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:30:TRP:CD1	1:B:30:TRP:C	2.92	0.48
1:C:225:ILE:HD13	1:C:246:ARG:HD2	1.95	0.48
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:MET:CE	1:C:268:TYR:CE2	2.97	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:B:175:GLN:HE21	1:B:175:GLN:C	2.23	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
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
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
1:D:70:SER:OG	1:D:250:GLU:OE1	2.30	0.46
1:A:225:ILE:HB	1:A:244:ILE:HD13	1.98	0.46
1:C:70:SER:OG	1:C:250:GLU:OE1	2.27	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:D:95:LYS:O	1:D:96:THR:C	2.58	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:PHE:CD1	1:F:44:PHE:C	2.94	0.45
1:G:263:GLU:CD	1:G:263:GLU:N	2.74	0.45
1:C:16:ASN:ND2	1:C:18:ALA:H	2.14	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:C:69:SER:O	1:C:70:SER:C	2.56	0.45
1:D:26:ASN:OD1	1:D:102:LYS:HE2	2.17	0.45
1:G:13:TYR:CD1	1:G:13:TYR:C	2.95	0.45
1:A:109:PHE:O	1:A:110:GLU:C	2.59	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:B:95:LYS:O	1:B:96:THR:C	2.56	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:A:109:PHE:C	1:A:111:THR:N	2.74	0.45
1:C:44:PHE:CD1	1:C:44:PHE:C	2.95	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: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:A:52:GLU:C	1:A:53:ILE:CG2	2.90	0.44
1:B:261:LYS:HG3	1:B:263:GLU:HG2	1.99	0.44
1:E:64:LYS:O	1:E:65:ASN:C	2.60	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: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: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:30:TRP:CD1	1:F:30:TRP:C	2.93	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:ASP:OD1	1:F:228:ASP:N	2.36	0.43
1:G:30:TRP:CD1	1:G:30:TRP:C	2.93	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: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
1:A:247:ASP:OD1	1:A:247:ASP:C	2.62	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: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
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:A:134:GLU:C	1:A:135:PHE:CD1	2.97	0.43
1:D:33:ARG:HG3	1:D:34:SER:H	1.83	0.43
1:F:72:LYS:NZ	1:F:99:PRO:O	2.49	0.43
1:F:72:LYS:NZ	1:F:101:GLY:O	2.50	0.43
1:B:49:LEU:HD12	1:B:116:LYS:C	2.43	0.43
1:A:52:GLU:C	1:A:53:ILE:HG22	2.44	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:D:261:LYS:C	1:D:296:VAL:HG11	2.43	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
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:F:257:MET:CE	1:F:268:TYR:CE2	3.01	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:94:ASP:OD1	1:C:94:ASP:C	2.63	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:E:10:TRP:CD1	1:E:10:TRP:H	2.39	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:G:281:TRP:O	1:G:282:ARG:C	2.63	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:D:276:TYR:O	1:D:277:VAL:C	2.63	0.41
1:E:53:ILE:O	1:E:114:SER:CA	2.58	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:255:LEU:HD12	1:D:255:LEU:HA	1.90	0.41
1:D:281:TRP:O	1:D:282:ARG:C	2.64	0.41
1:E:242:PHE:N	1:E:242:PHE:CD1	2.88	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:B:224:LYS:HD3	1:B:280:SER:HB3	2.02	0.40
1:C:258:ASP:O	1:C:259:SER:C	2.63	0.40
1:A:109:PHE:N	1:A:109:PHE:CD1	2.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:212:ARG:HG2	1:G:222:VAL:CG2	2.51	0.40
1:A:24:ASP:OD1	1:A:24:ASP:C	2.64	0.40
1:A:84:ASN:CG	1:A:84:ASN:O	2.65	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
1:B:16:ASN:C	1:B:18:ALA:H	2.30	0.40
1:G:8:GLU:C	1:G:10:TRP:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	261/306 (85%)	244 (94%)	14 (5%)	3 (1%)	11	36
1	B	261/306 (85%)	243 (93%)	14 (5%)	4 (2%)	8	28
1	C	261/306 (85%)	248 (95%)	10 (4%)	3 (1%)	11	36
1	D	261/306 (85%)	242 (93%)	16 (6%)	3 (1%)	11	36
1	E	266/306 (87%)	238 (90%)	25 (9%)	3 (1%)	11	36
1	F	261/306 (85%)	236 (90%)	18 (7%)	7 (3%)	4	16
1	G	261/306 (85%)	228 (87%)	27 (10%)	6 (2%)	5	19
All	All	1832/2142 (86%)	1679 (92%)	124 (7%)	29 (2%)	7	27

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%)	183 (90%)	21 (10%)	7	23
1	B	217/239 (91%)	189 (87%)	28 (13%)	4	13
1	C	217/239 (91%)	190 (88%)	27 (12%)	4	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	216/239 (90%)	190 (88%)	26 (12%)	5	16
1	E	221/239 (92%)	193 (87%)	28 (13%)	4	14
1	F	217/239 (91%)	188 (87%)	29 (13%)	4	12
1	G	216/239 (90%)	182 (84%)	34 (16%)	2	9
All	All	1508/1673 (90%)	1315 (87%)	193 (13%)	4	14

All (193) 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	110	GLU
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	40	LEU
1	B	48	ASP
1	B	49	LEU
1	B	51	LYS
1	B	53	ILE
1	B	69	SER
1	B	72	LYS
1	B	77	LYS
1	B	84	ASN
1	B	88	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	220	GLU
1	B	237	SER
1	B	239	LYS
1	B	243	THR
1	B	250	GLU
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	45	ILE
1	C	53	ILE
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	102	LYS
1	C	108	SER
1	C	111	THR
1	C	124	GLU
1	C	140	ASP
1	C	176	VAL
1	C	185	LEU
1	C	203	SER
1	C	204	ARG
1	C	233	THR
1	C	257	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	263	GLU
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	45	ILE
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	86	SER
1	D	116	LYS
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	239	LYS
1	D	251	TYR
1	D	263	GLU
1	D	290	GLN
1	D	292	THR
1	E	7	SER
1	E	16	ASN
1	E	34	SER
1	E	53	ILE
1	E	54	LYS
1	E	65	ASN
1	E	69	SER
1	E	77	LYS
1	E	82	LEU
1	E	96	THR
1	E	108	SER
1	E	111	THR
1	E	124	GLU
1	E	128	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	137	ILE
1	E	138	VAL
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	217	LYS
1	E	233	THR
1	E	236	ASP
1	E	237	SER
1	E	239	LYS
1	E	260	LEU
1	F	5	ILE
1	F	7	SER
1	F	51	LYS
1	F	52	GLU
1	F	64	LYS
1	F	82	LEU
1	F	99	PRO
1	F	116	LYS
1	F	128	VAL
1	F	137	ILE
1	F	139	SER
1	F	140	ASP
1	F	176	VAL
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	253	VAL
1	F	259	SER
1	F	260	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	280	SER
1	G	5	ILE
1	G	12	VAL
1	G	21	LEU
1	G	33	ARG
1	G	34	SER
1	G	49	LEU
1	G	52	GLU
1	G	53	ILE
1	G	59	ARG
1	G	64	LYS
1	G	91	LYS
1	G	96	THR
1	G	102	LYS
1	G	104	VAL
1	G	114	SER
1	G	128	VAL
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	230	ARG
1	G	236	ASP
1	G	239	LYS
1	G	251	TYR
1	G	259	SER
1	G	260	LEU
1	G	261	LYS
1	G	263	GLU
1	G	282	ARG
1	G	285	PRO
1	G	290	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	A	175	GLN
1	B	11	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	11	HIS
1	C	16	ASN
1	C	129	GLN
1	C	175	GLN
1	C	213	GLN
1	C	293	GLN
1	D	11	HIS
1	D	16	ASN
1	D	129	GLN
1	D	175	GLN
1	D	213	GLN
1	E	11	HIS
1	E	35	ASN
1	E	84	ASN
1	E	129	GLN
1	E	213	GLN
1	F	11	HIS
1	F	35	ASN
1	F	84	ASN
1	F	129	GLN
1	F	187	GLN
1	F	293	GLN
1	G	19	ASN
1	G	65	ASN
1	G	84	ASN
1	G	129	GLN
1	G	187	GLN
1	G	290	GLN
1	G	293	GLN

5.3.3 RNA ⓘ

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 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	A	301	-	35,35,35	2.07	7 (20%)	47,49,49	2.84	24 (51%)
2	MTX	C	301	-	35,35,35	2.22	9 (25%)	47,49,49	2.65	19 (40%)
2	MTX	B	301	-	35,35,35	2.58	10 (28%)	47,49,49	2.46	14 (29%)
2	MTX	G	301	-	35,35,35	1.93	4 (11%)	47,49,49	2.26	18 (38%)
2	MTX	E	301	-	35,35,35	1.93	8 (22%)	47,49,49	2.49	18 (38%)
2	MTX	F	301	-	35,35,35	2.22	8 (22%)	47,49,49	2.82	20 (42%)
2	MTX	D	301	-	35,35,35	1.87	8 (22%)	47,49,49	2.06	12 (25%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MTX	F	301	-	-	11/25/25/25	0/3/3/3
2	MTX	D	301	-	-	9/25/25/25	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	MTX	CG-CD	8.23	1.69	1.50
2	B	301	MTX	C7-N8	7.01	1.43	1.31
2	A	301	MTX	C7-N8	6.51	1.42	1.31
2	A	301	MTX	O-C	6.30	1.38	1.23
2	F	301	MTX	O-C	6.27	1.38	1.23
2	G	301	MTX	O-C	6.20	1.37	1.23
2	C	301	MTX	O-C	6.13	1.37	1.23
2	C	301	MTX	CG-CD	6.01	1.64	1.50
2	D	301	MTX	O-C	5.97	1.37	1.23
2	F	301	MTX	C7-N8	5.91	1.41	1.31
2	E	301	MTX	C7-N8	5.57	1.41	1.31
2	G	301	MTX	C11-C	-5.50	1.38	1.50
2	G	301	MTX	C7-N8	5.04	1.40	1.31
2	E	301	MTX	O-C	5.04	1.35	1.23
2	D	301	MTX	C7-N8	4.91	1.40	1.31
2	C	301	MTX	C11-C	-4.77	1.39	1.50
2	B	301	MTX	O-C	4.73	1.34	1.23
2	E	301	MTX	C11-C	-4.65	1.40	1.50
2	A	301	MTX	C11-C	-4.58	1.40	1.50
2	F	301	MTX	CG-CD	4.47	1.60	1.50
2	B	301	MTX	C11-C	-4.27	1.40	1.50
2	C	301	MTX	C7-N8	4.19	1.38	1.31
2	F	301	MTX	C11-C	-4.14	1.41	1.50
2	D	301	MTX	C11-C	-4.04	1.41	1.50
2	B	301	MTX	CB-CG	3.73	1.64	1.52
2	C	301	MTX	C8A-N8	-3.32	1.32	1.37
2	F	301	MTX	CA-CT	3.25	1.60	1.52
2	E	301	MTX	C4A-N5	-2.89	1.31	1.37
2	F	301	MTX	C-N	2.86	1.40	1.34
2	A	301	MTX	OE1-CD	2.84	1.31	1.22
2	F	301	MTX	CA-N	2.82	1.51	1.45
2	B	301	MTX	C9-C6	2.81	1.56	1.51
2	B	301	MTX	CA-CT	-2.77	1.45	1.52
2	C	301	MTX	C14-N10	-2.77	1.31	1.38
2	D	301	MTX	CA-N	2.63	1.51	1.45
2	A	301	MTX	C13-C12	2.58	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	MTX	CB-CG	2.54	1.60	1.52
2	D	301	MTX	CG-CD	2.50	1.56	1.50
2	E	301	MTX	C9-N10	-2.46	1.41	1.46
2	D	301	MTX	C8A-N8	-2.43	1.33	1.37
2	E	301	MTX	O2-CT	-2.39	1.23	1.30
2	C	301	MTX	O1-CT	2.29	1.28	1.22
2	A	301	MTX	C16-C11	2.26	1.42	1.39
2	B	301	MTX	C6-N5	2.21	1.36	1.32
2	E	301	MTX	CA-N	2.20	1.50	1.45
2	E	301	MTX	OE1-CD	2.20	1.29	1.22
2	D	301	MTX	CB-CG	2.19	1.59	1.52
2	F	301	MTX	C6-N5	2.18	1.36	1.32
2	A	301	MTX	C8A-N8	-2.15	1.34	1.37
2	D	301	MTX	O1-CT	2.09	1.28	1.22
2	B	301	MTX	O1-CT	2.06	1.28	1.22
2	C	301	MTX	CA-CT	-2.05	1.47	1.52
2	B	301	MTX	C2-NA2	2.05	1.38	1.33
2	G	301	MTX	C9-C6	2.01	1.54	1.51

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	MTX	C11-C-N	-7.38	103.35	117.04
2	F	301	MTX	CM-N10-C14	-7.36	107.41	119.59
2	B	301	MTX	CT-CA-N	-7.28	93.67	110.57
2	C	301	MTX	CM-N10-C14	-7.26	107.58	119.59
2	F	301	MTX	N1-C2-N3	-6.38	119.10	127.21
2	E	301	MTX	C2-N1-C8A	6.09	122.05	115.48
2	G	301	MTX	C2-N1-C8A	6.06	122.02	115.48
2	A	301	MTX	N8-C8A-N1	5.85	122.14	115.77
2	C	301	MTX	N1-C2-N3	-5.83	119.80	127.21
2	B	301	MTX	CB-CG-CD	5.68	127.64	112.49
2	F	301	MTX	C2-N1-C8A	5.65	121.58	115.48
2	E	301	MTX	CA-N-C	5.65	135.12	121.56
2	A	301	MTX	CG-CB-CA	-5.52	102.99	113.16
2	C	301	MTX	CT-CA-N	-5.45	97.92	110.57
2	B	301	MTX	N1-C2-N3	-5.16	120.65	127.21
2	F	301	MTX	CA-N-C	5.08	133.74	121.56
2	B	301	MTX	CM-N10-C14	-5.07	111.21	119.59
2	D	301	MTX	CM-N10-C14	-5.04	111.24	119.59
2	G	301	MTX	N8-C8A-N1	5.02	121.24	115.77
2	B	301	MTX	C2-N1-C8A	5.00	120.88	115.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	MTX	CM-N10-C14	-4.93	111.43	119.59
2	D	301	MTX	N1-C2-N3	-4.89	120.99	127.21
2	F	301	MTX	C4-C4A-N5	4.68	123.93	120.33
2	E	301	MTX	N1-C2-N3	-4.67	121.28	127.21
2	E	301	MTX	CM-N10-C9	-4.62	103.07	115.11
2	G	301	MTX	CM-N10-C14	-4.58	112.01	119.59
2	A	301	MTX	O-C-N	4.43	130.89	122.47
2	A	301	MTX	N1-C2-N3	-4.41	121.60	127.21
2	F	301	MTX	C9-C6-N5	4.39	124.22	117.09
2	C	301	MTX	C2-N1-C8A	4.39	120.22	115.48
2	F	301	MTX	C13-C14-N10	-4.38	115.48	121.59
2	A	301	MTX	C13-C12-C11	-4.38	116.12	120.80
2	D	301	MTX	N8-C8A-N1	4.35	120.51	115.77
2	C	301	MTX	C7-C6-N5	-4.34	118.06	120.87
2	F	301	MTX	O-C-N	4.33	130.69	122.47
2	G	301	MTX	C15-C14-N10	-4.32	115.56	121.59
2	C	301	MTX	CB-CA-N	4.20	119.23	110.91
2	A	301	MTX	CM-N10-C14	-4.20	112.64	119.59
2	C	301	MTX	CB-CG-CD	4.20	123.68	112.49
2	D	301	MTX	CA-N-C	4.09	131.37	121.56
2	A	301	MTX	C2-N1-C8A	4.06	119.86	115.48
2	A	301	MTX	C7-C6-N5	-4.03	118.25	120.87
2	D	301	MTX	CM-N10-C9	-4.01	104.65	115.11
2	D	301	MTX	C7-C6-N5	-3.92	118.33	120.87
2	F	301	MTX	C15-C14-N10	3.88	127.00	121.59
2	B	301	MTX	N8-C8A-N1	3.86	119.98	115.77
2	F	301	MTX	N8-C8A-N1	3.85	119.96	115.77
2	C	301	MTX	N8-C8A-N1	3.84	119.95	115.77
2	A	301	MTX	CA-N-C	3.83	130.75	121.56
2	C	301	MTX	C9-N10-C14	-3.80	115.56	120.17
2	D	301	MTX	C2-N1-C8A	3.79	119.57	115.48
2	C	301	MTX	CM-N10-C9	-3.79	105.24	115.11
2	G	301	MTX	N1-C2-N3	-3.66	122.56	127.21
2	B	301	MTX	CB-CA-N	3.56	117.96	110.91
2	E	301	MTX	C11-C-N	-3.56	110.44	117.04
2	A	301	MTX	C4A-C4-NA4	-3.49	115.00	120.31
2	E	301	MTX	C15-C14-N10	-3.49	116.72	121.59
2	E	301	MTX	N8-C8A-N1	3.46	119.54	115.77
2	A	301	MTX	C15-C16-C11	3.40	124.43	120.80
2	F	301	MTX	C7-C6-N5	-3.34	118.70	120.87
2	A	301	MTX	C4-C4A-N5	-3.33	117.76	120.33
2	C	301	MTX	C4A-C4-NA4	-3.22	115.40	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	MTX	C6-C7-N8	-3.21	120.06	123.14
2	B	301	MTX	CM-N10-C9	-3.20	106.76	115.11
2	A	301	MTX	C15-C14-N10	-3.20	117.13	121.59
2	F	301	MTX	C11-C-N	-3.16	111.18	117.04
2	G	301	MTX	C4A-C8A-N1	-3.15	116.86	121.74
2	G	301	MTX	CB-CG-CD	-3.14	104.11	112.49
2	C	301	MTX	C9-C6-N5	3.11	122.14	117.09
2	E	301	MTX	CG-CB-CA	-3.09	107.46	113.16
2	G	301	MTX	C13-C12-C11	-3.08	117.51	120.80
2	C	301	MTX	O2-CT-O1	3.07	131.04	124.08
2	E	301	MTX	NA2-C2-N3	3.05	121.80	117.22
2	E	301	MTX	O-C-N	3.04	128.25	122.47
2	G	301	MTX	O-C-N	3.02	128.21	122.47
2	E	301	MTX	C4A-C8A-N1	-2.98	117.12	121.74
2	A	301	MTX	NA4-C4-N3	2.91	124.94	117.11
2	G	301	MTX	OE1-CD-CG	-2.90	113.90	123.09
2	A	301	MTX	C16-C11-C	-2.84	111.40	120.60
2	B	301	MTX	O2-CT-O1	2.84	130.51	124.08
2	F	301	MTX	NA2-C2-N3	2.82	121.45	117.22
2	A	301	MTX	C12-C11-C	2.82	129.73	120.60
2	E	301	MTX	C6-C7-N8	-2.80	120.45	123.14
2	D	301	MTX	O-C-N	2.78	127.75	122.47
2	C	301	MTX	C6-C9-N10	-2.74	108.26	112.95
2	E	301	MTX	CB-CA-N	2.71	116.26	110.91
2	B	301	MTX	C4A-C4-NA4	-2.70	116.19	120.31
2	B	301	MTX	C7-C6-N5	-2.70	119.12	120.87
2	B	301	MTX	CB-CA-CT	-2.69	103.97	110.35
2	C	301	MTX	NA4-C4-N3	2.66	124.25	117.11
2	B	301	MTX	C6-C7-N8	-2.65	120.60	123.14
2	C	301	MTX	NA2-C2-N3	2.59	121.11	117.22
2	A	301	MTX	OE2-CD-OE1	2.58	129.98	123.33
2	A	301	MTX	C9-N10-C14	-2.53	117.10	120.17
2	D	301	MTX	C9-C6-N5	2.53	121.20	117.09
2	B	301	MTX	C9-C6-N5	2.50	121.16	117.09
2	A	301	MTX	C12-C13-C14	2.48	123.44	120.30
2	G	301	MTX	CM-N10-C9	-2.45	108.73	115.11
2	C	301	MTX	O1-CT-CA	-2.44	114.39	122.26
2	A	301	MTX	O-C-C11	2.43	125.72	120.90
2	G	301	MTX	CB-CA-CT	2.41	116.08	110.35
2	D	301	MTX	C15-C14-N10	-2.41	118.23	121.59
2	G	301	MTX	C7-C6-N5	-2.39	119.32	120.87
2	F	301	MTX	C7-N8-C8A	2.39	120.53	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	MTX	C16-C15-C14	-2.39	117.28	120.30
2	E	301	MTX	NA4-C4-N3	2.38	123.52	117.11
2	F	301	MTX	C9-C6-C7	-2.38	117.05	121.38
2	F	301	MTX	C4A-C4-NA4	-2.34	116.74	120.31
2	A	301	MTX	NA2-C2-N1	2.33	121.42	117.79
2	G	301	MTX	C16-C11-C	-2.28	113.22	120.60
2	E	301	MTX	O1-CT-CA	-2.26	114.96	122.26
2	F	301	MTX	C6-N5-C4A	2.24	121.33	118.17
2	C	301	MTX	OE2-CD-CG	2.22	121.02	114.00
2	E	301	MTX	C4-C4A-N5	-2.20	118.63	120.33
2	G	301	MTX	C11-C-N	-2.20	112.96	117.04
2	A	301	MTX	CB-CA-N	2.18	115.22	110.91
2	F	301	MTX	C6-C9-N10	-2.13	109.30	112.95
2	C	301	MTX	C11-C-N	-2.09	113.17	117.04
2	D	301	MTX	C13-C14-N10	2.09	124.50	121.59
2	F	301	MTX	CB-CA-CT	2.09	115.31	110.35
2	G	301	MTX	CA-N-C	2.09	126.57	121.56
2	G	301	MTX	C4A-C4-NA4	-2.07	117.16	120.31
2	D	301	MTX	NA2-C2-N1	2.05	120.99	117.79
2	G	301	MTX	NA4-C4-N3	2.05	122.61	117.11
2	E	301	MTX	C7-N8-C8A	-2.04	114.36	117.20

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	A	301	MTX	CT-CA-N-C
2	F	301	MTX	CT-CA-N-C
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	C	301	MTX	CA-CB-CG-CD
2	F	301	MTX	O-C-C11-C12
2	D	301	MTX	CT-CA-N-C
2	E	301	MTX	N-CA-CB-CG
2	F	301	MTX	N-C-C11-C12
2	B	301	MTX	CT-CA-CB-CG
2	C	301	MTX	CT-CA-CB-CG

Continued on next page...

Continued from previous page...

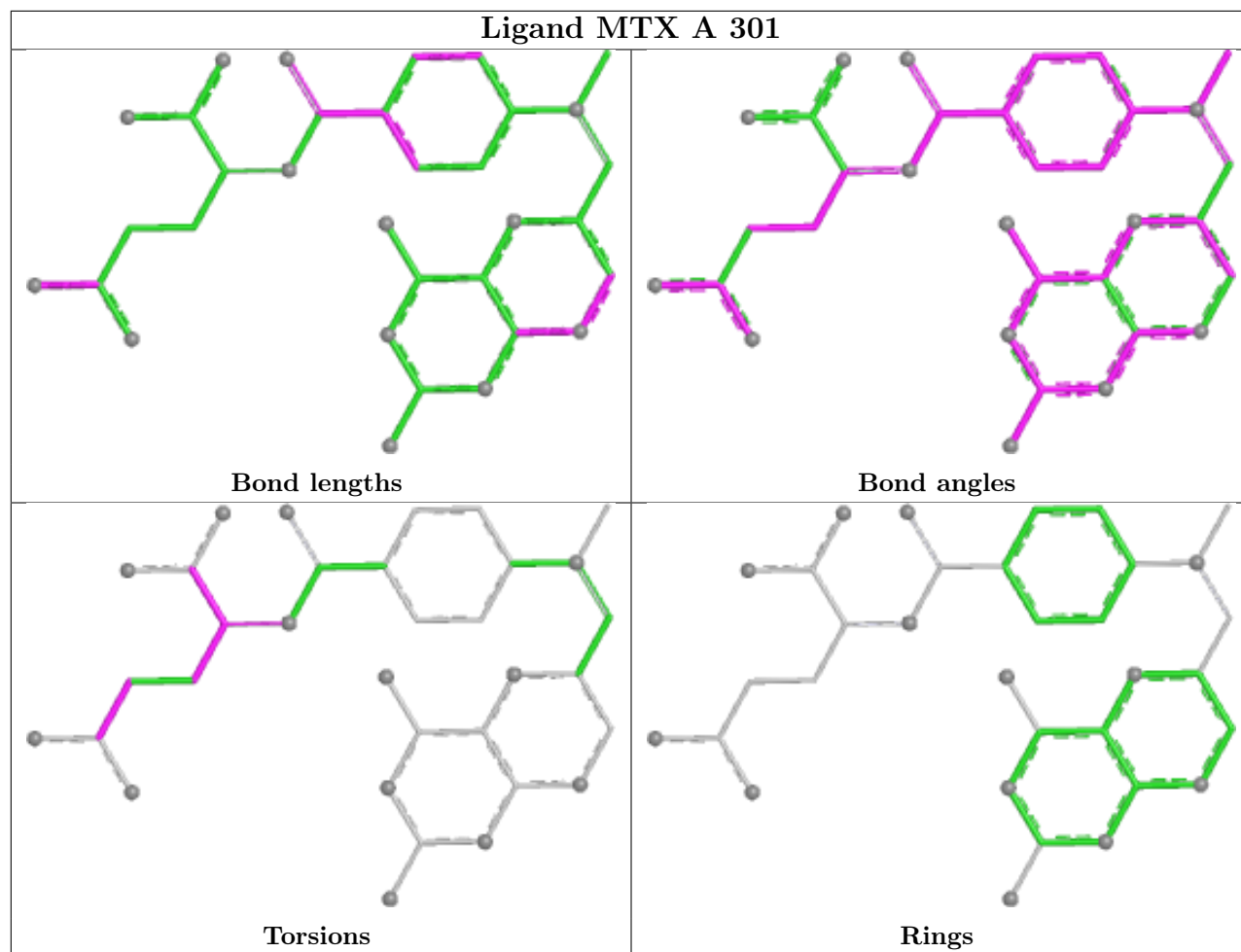
Mol	Chain	Res	Type	Atoms
2	F	301	MTX	CT-CA-CB-CG
2	C	301	MTX	C13-C14-N10-CM
2	C	301	MTX	C15-C14-N10-CM
2	B	301	MTX	N-CA-CB-CG
2	A	301	MTX	N-CA-CT-O1
2	A	301	MTX	N-CA-CT-O2
2	D	301	MTX	CT-CA-CB-CG
2	G	301	MTX	CT-CA-CB-CG
2	D	301	MTX	CB-CA-CT-O1
2	D	301	MTX	CB-CA-CT-O2
2	G	301	MTX	OE1-CD-CG-CB
2	C	301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

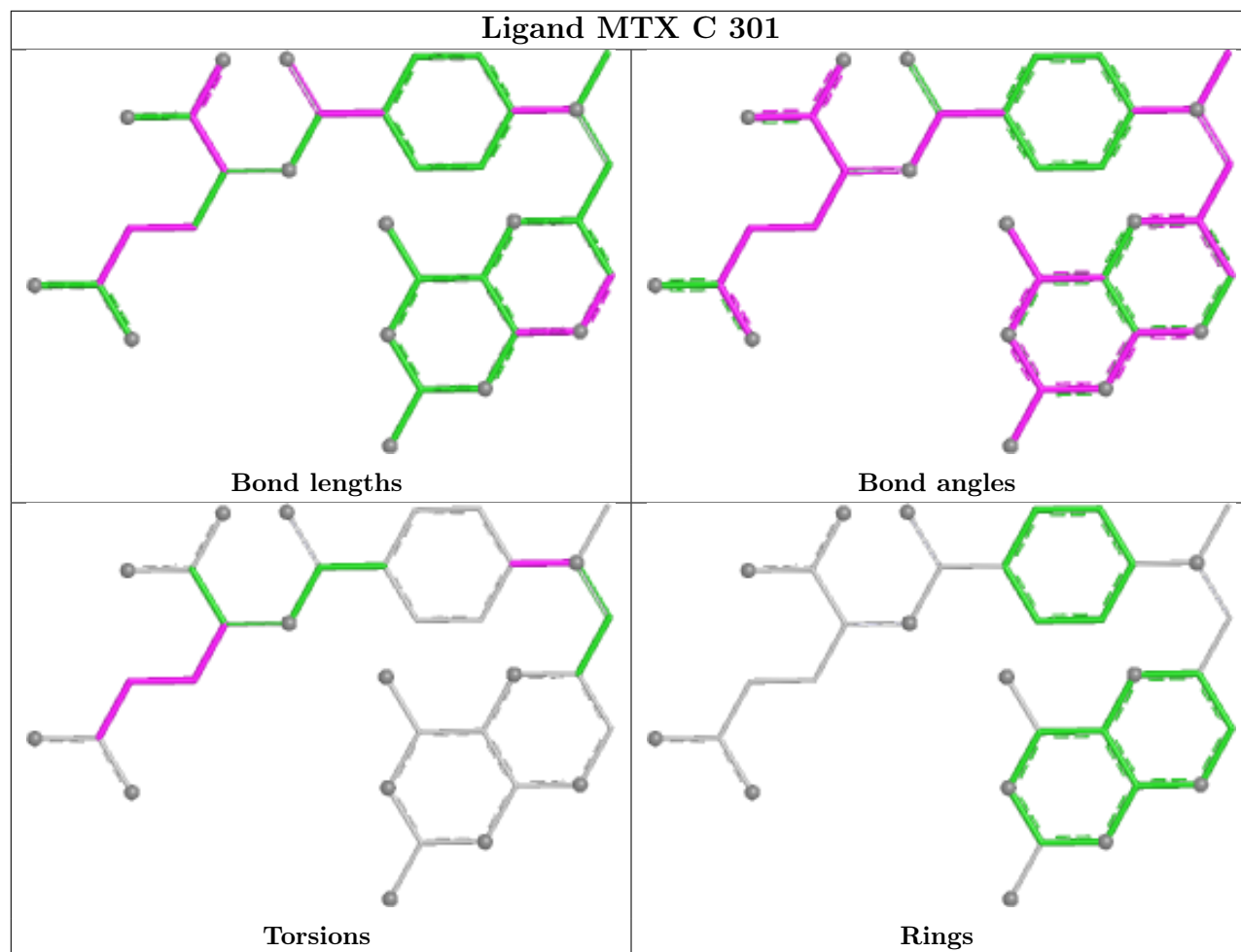
There are no ring outliers.

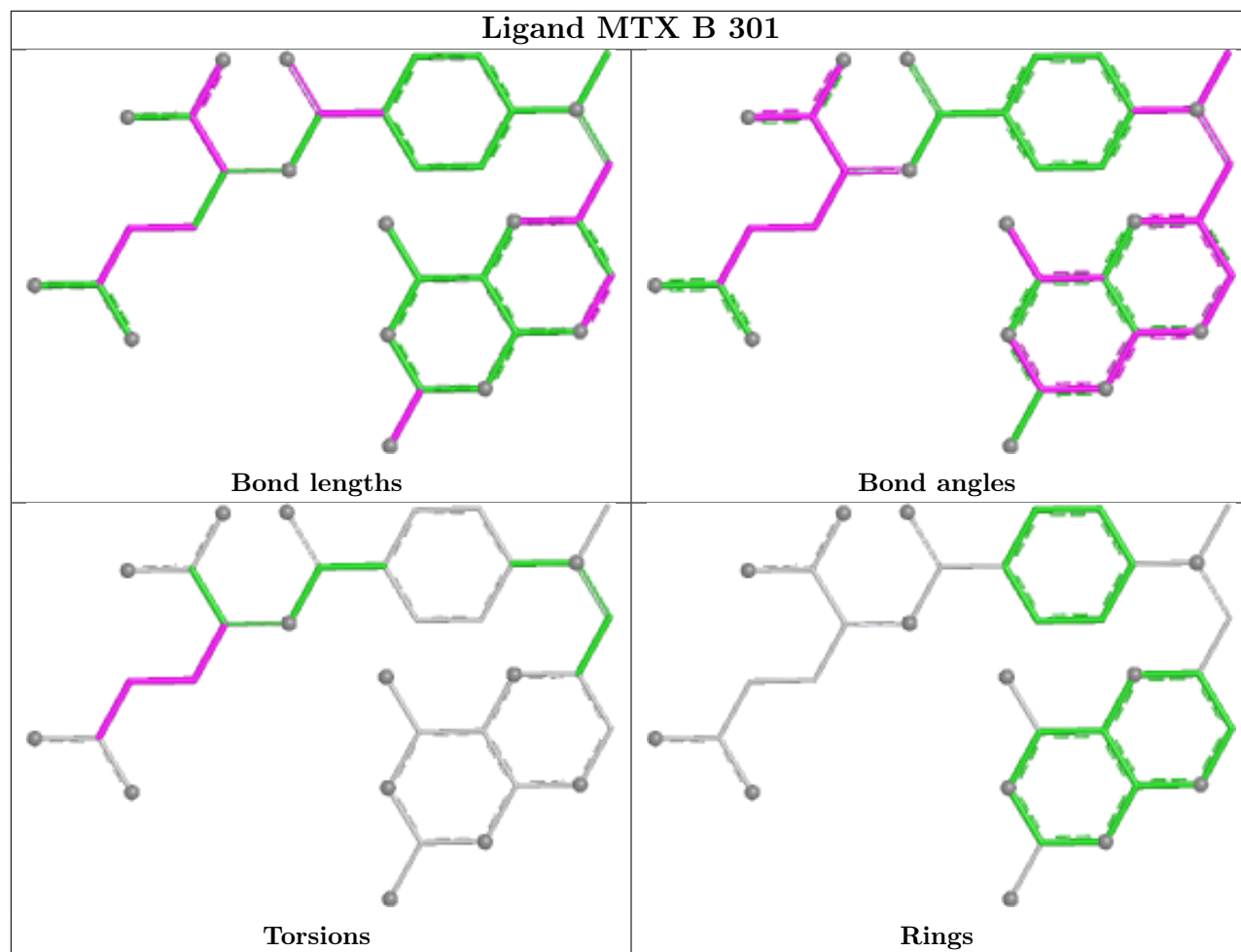
7 monomers are involved in 44 short contacts:

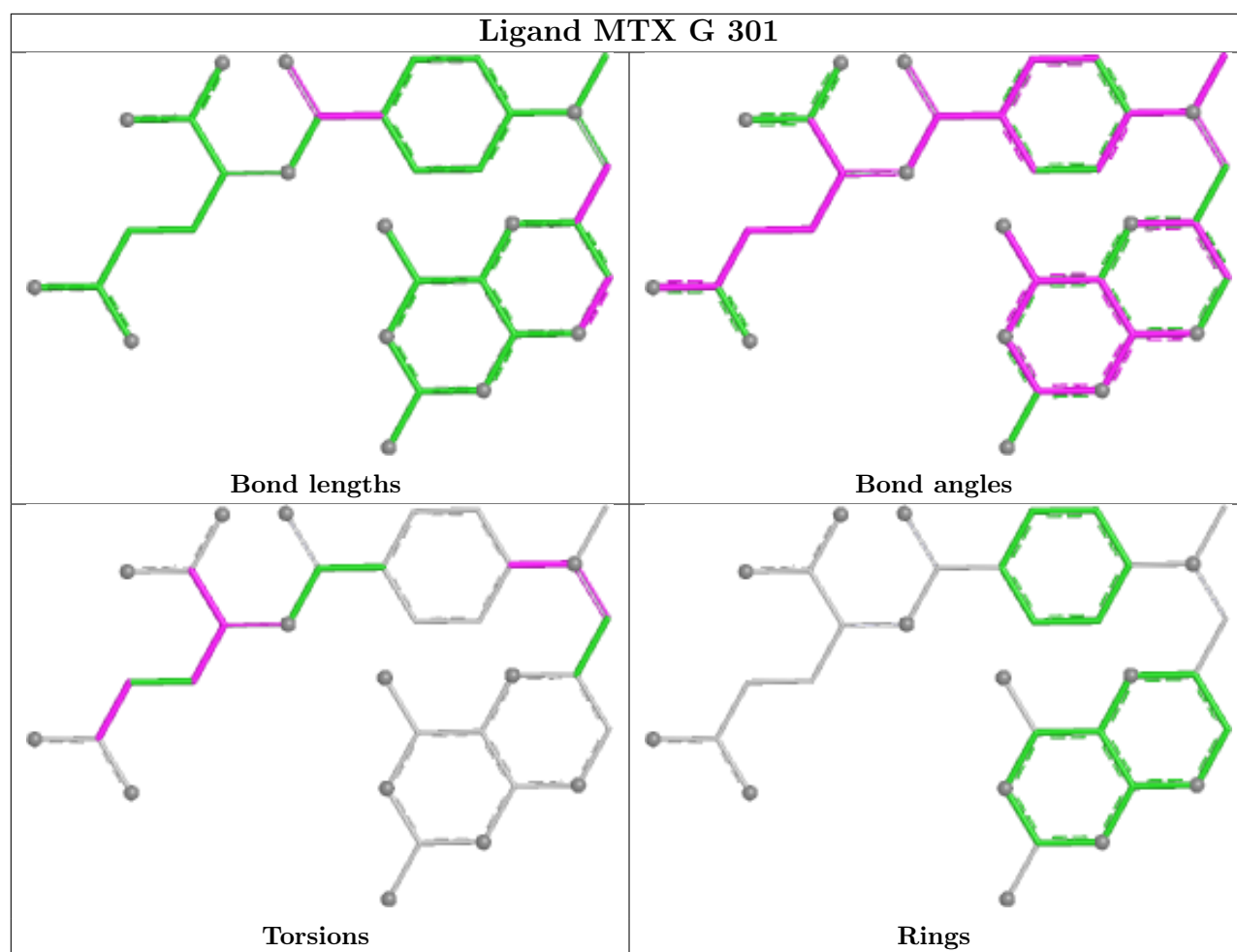
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	MTX	14	0
2	C	301	MTX	7	0
2	B	301	MTX	4	0
2	G	301	MTX	7	0
2	E	301	MTX	7	0
2	F	301	MTX	1	0
2	D	301	MTX	4	0

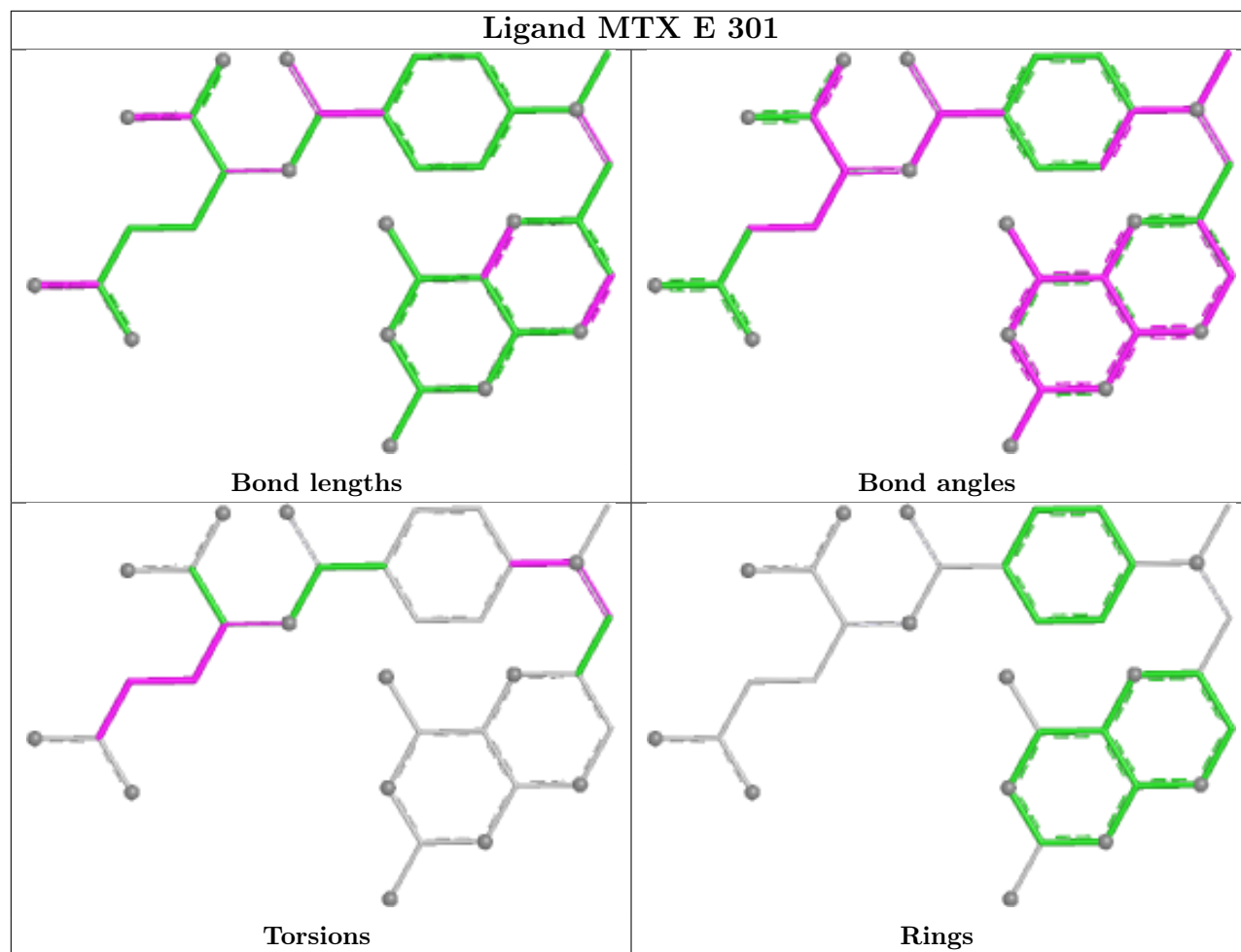
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

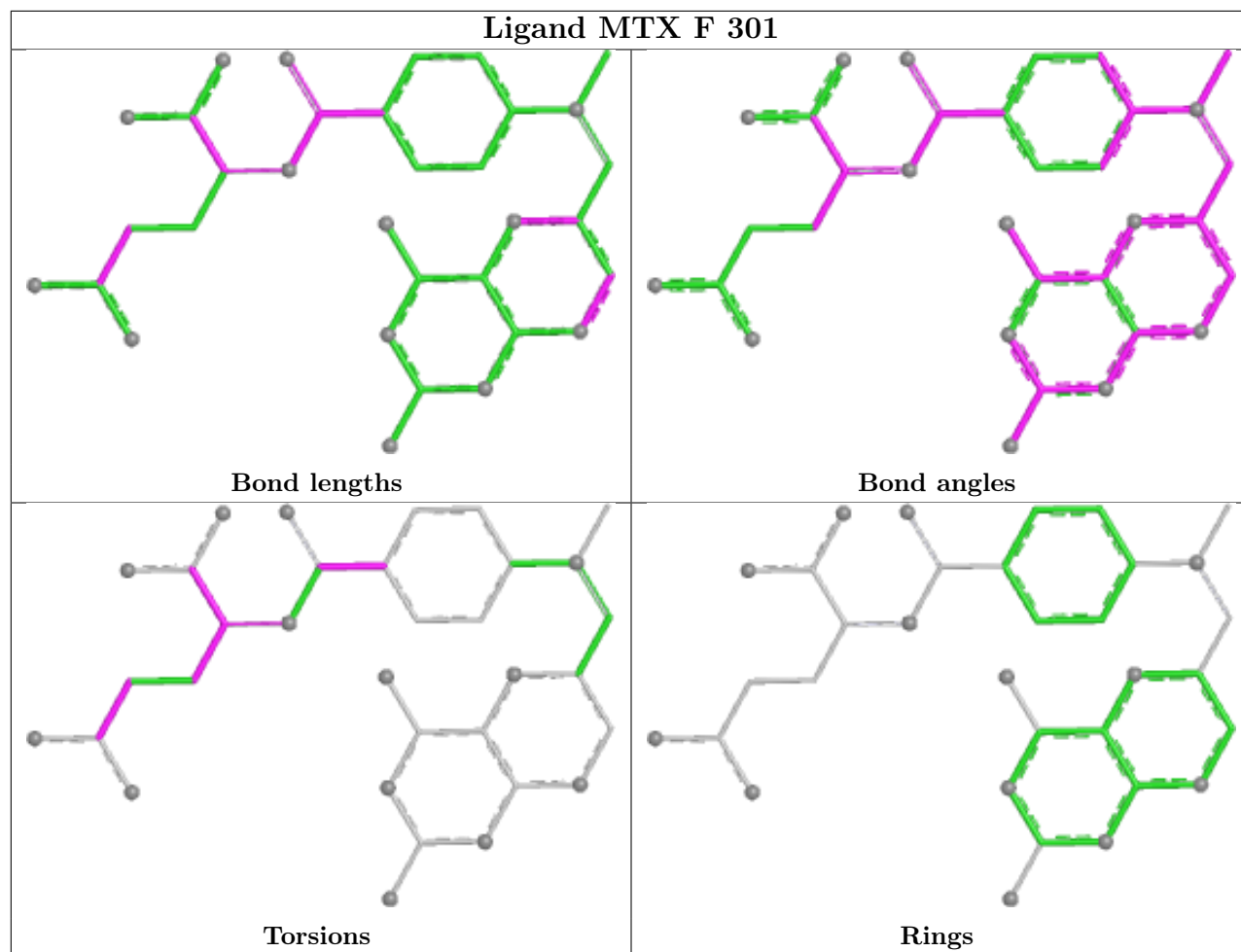


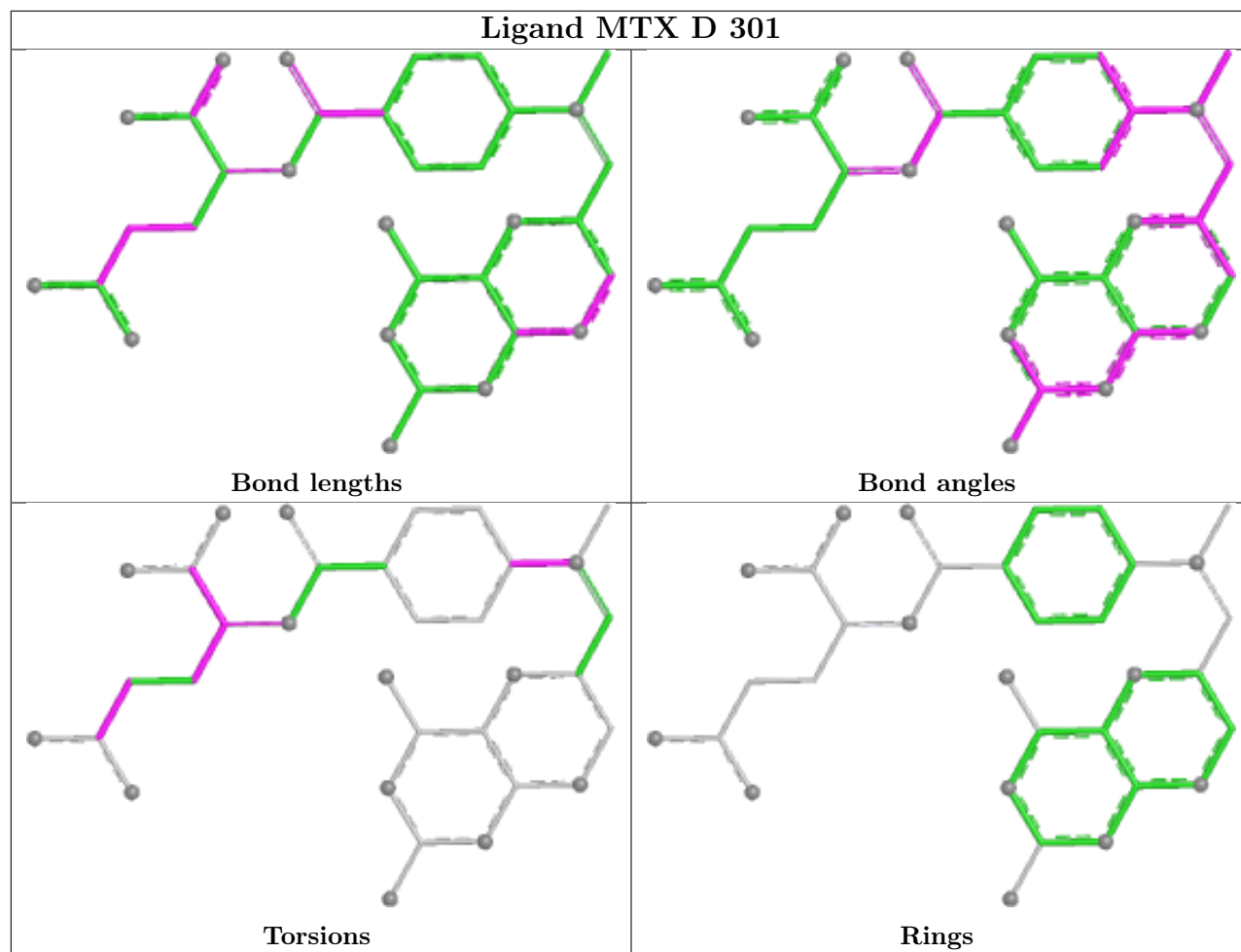












5.7 Other polymers [i](#)

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%)	-0.24	7 (2%) 57 48	26, 59, 84, 107	1 (0%)
1	B	265/306 (86%)	-0.21	5 (1%) 66 58	23, 64, 88, 108	1 (0%)
1	C	265/306 (86%)	-0.26	8 (3%) 52 43	25, 62, 88, 114	1 (0%)
1	D	265/306 (86%)	-0.22	1 (0%) 88 85	25, 68, 87, 105	1 (0%)
1	E	270/306 (88%)	0.10	9 (3%) 49 40	31, 77, 102, 117	1 (0%)
1	F	265/306 (86%)	-0.04	6 (2%) 61 52	36, 77, 107, 120	1 (0%)
1	G	265/306 (86%)	0.07	7 (2%) 57 48	30, 84, 111, 125	1 (0%)
All	All	1860/2142 (86%)	-0.11	43 (2%) 61 52	23, 71, 100, 125	7 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	91	LYS	14.4
1	E	91	LYS	12.6
1	F	91	LYS	10.7
1	A	91	LYS	10.4
1	C	91	LYS	9.4
1	B	91	LYS	9.1
1	D	91	LYS	8.5
1	E	298	SER	4.6
1	G	65	ASN	4.0
1	E	-4	HIS	4.0
1	A	174	SER	3.4
1	A	113	ILE	3.3
1	F	82	LEU	3.2
1	C	140	ASP	3.0
1	G	298	SER	3.0
1	C	111	THR	2.9
1	G	186	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	174	SER	2.9
1	E	139	SER	2.8
1	G	139	SER	2.7
1	C	283	SER	2.7
1	B	282	ARG	2.6
1	A	175	GLN	2.5
1	C	177	GLN	2.5
1	G	214	ALA	2.5
1	B	138	VAL	2.4
1	E	65	ASN	2.3
1	F	136	ALA	2.3
1	C	285	PRO	2.3
1	A	112	PRO	2.2
1	F	177	GLN	2.2
1	E	215	PRO	2.2
1	F	196	CYS	2.2
1	G	54	LYS	2.2
1	A	65	ASN	2.2
1	A	66	GLY	2.2
1	C	203	SER	2.2
1	F	67	GLY	2.2
1	B	65	ASN	2.1
1	E	177	GLN	2.1
1	E	200	ARG	2.0
1	B	66	GLY	2.0
1	C	113	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

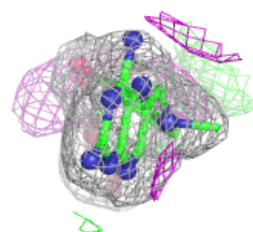
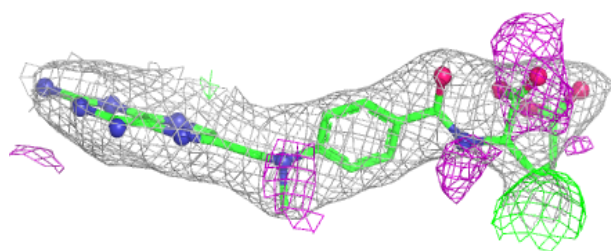
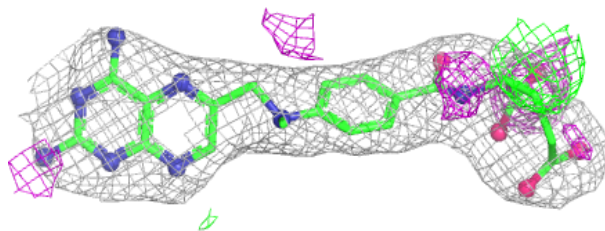
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	F	303	1/1	0.29	0.44	87,87,87,87	0
3	NA	A	303	1/1	0.45	0.23	69,69,69,69	0
3	NA	D	303	1/1	0.61	0.25	74,74,74,74	0
3	NA	G	303	1/1	0.80	0.24	82,82,82,82	0
3	NA	B	303	1/1	0.81	0.15	79,79,79,79	0
3	NA	E	303	1/1	0.86	0.12	76,76,76,76	0
3	NA	C	303	1/1	0.90	0.14	55,55,55,55	0
2	MTX	C	301	33/33	0.93	0.10	59,67,81,83	0
2	MTX	D	301	33/33	0.93	0.12	71,76,95,99	0
2	MTX	B	301	33/33	0.93	0.09	45,56,76,77	0
2	MTX	F	301	33/33	0.95	0.10	48,83,116,117	0
2	MTX	G	301	33/33	0.95	0.10	69,74,92,94	0
2	MTX	A	301	33/33	0.95	0.09	50,55,69,77	0
2	MTX	E	301	33/33	0.96	0.09	60,65,92,95	0
3	NA	A	302	1/1	0.98	0.04	63,63,63,63	0
3	NA	F	302	1/1	0.98	0.03	84,84,84,84	0
3	NA	C	302	1/1	0.99	0.03	63,63,63,63	0
3	NA	E	302	1/1	0.99	0.03	77,77,77,77	0
3	NA	G	302	1/1	0.99	0.04	85,85,85,85	0
3	NA	B	302	1/1	0.99	0.04	87,87,87,87	0
3	NA	D	302	1/1	1.00	0.02	52,52,52,52	0

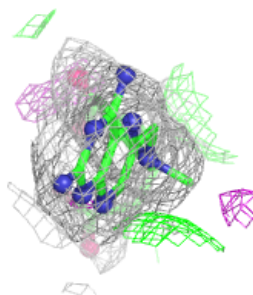
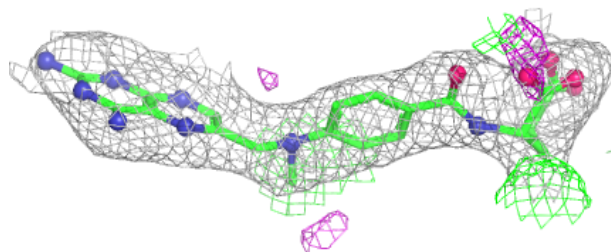
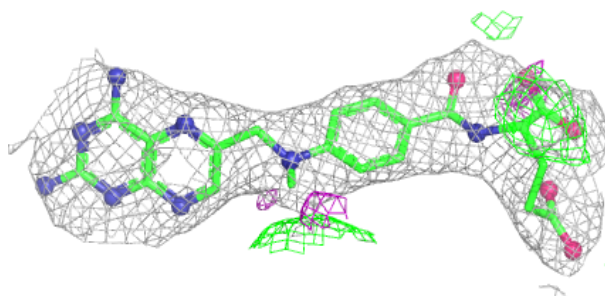
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

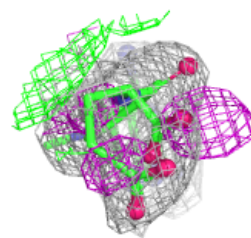
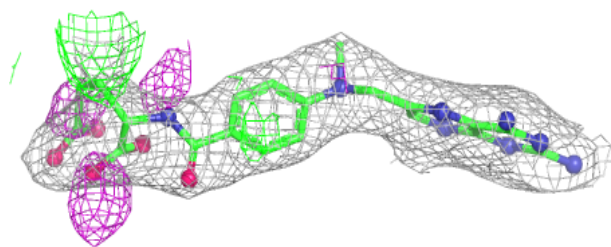
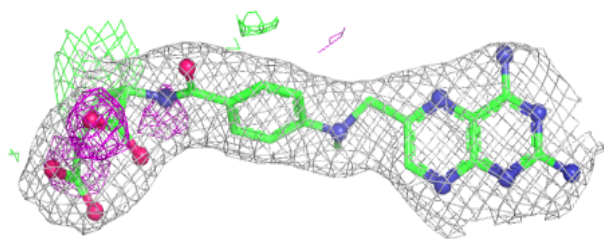
**Electron density around MTX D 301:**

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

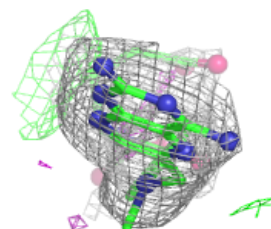
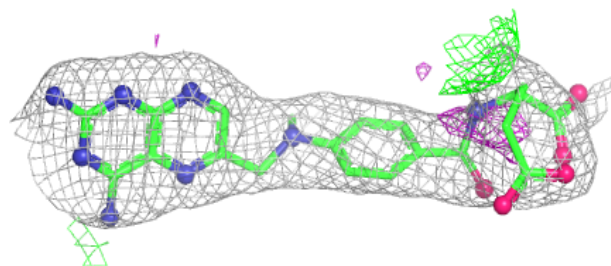
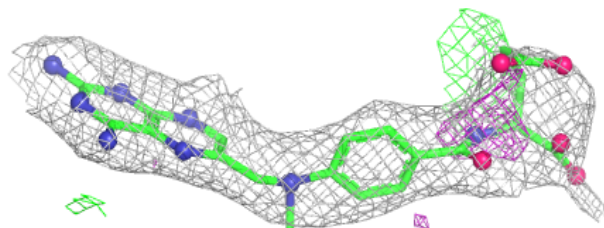


Electron density around MTX B 301:

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

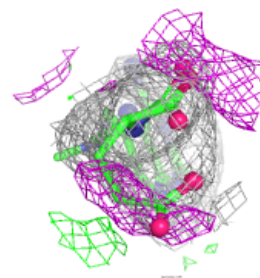
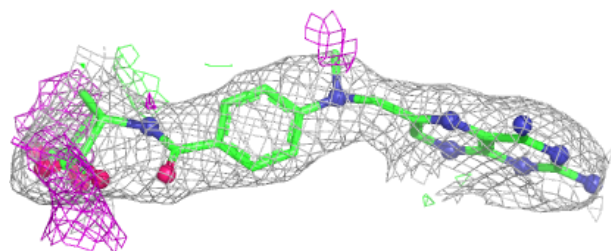
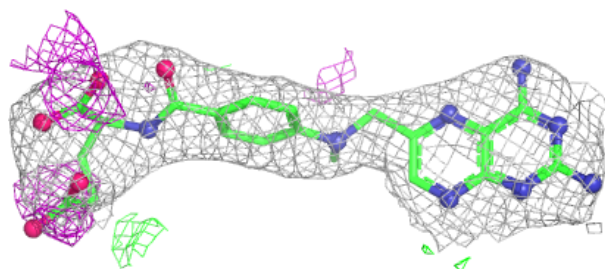
**Electron density around MTX F 301:**

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

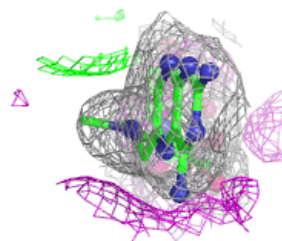
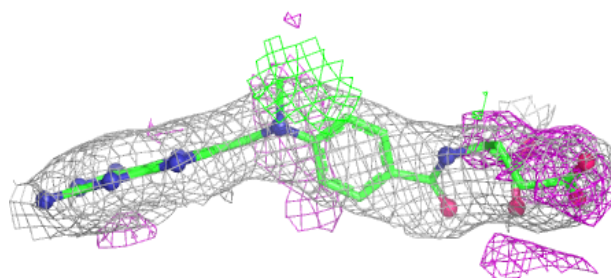
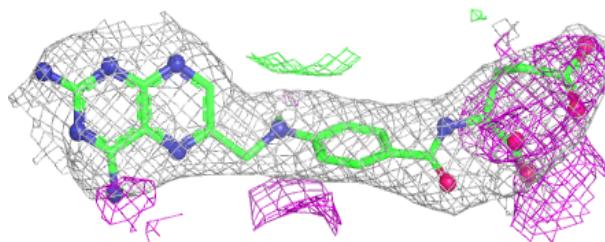


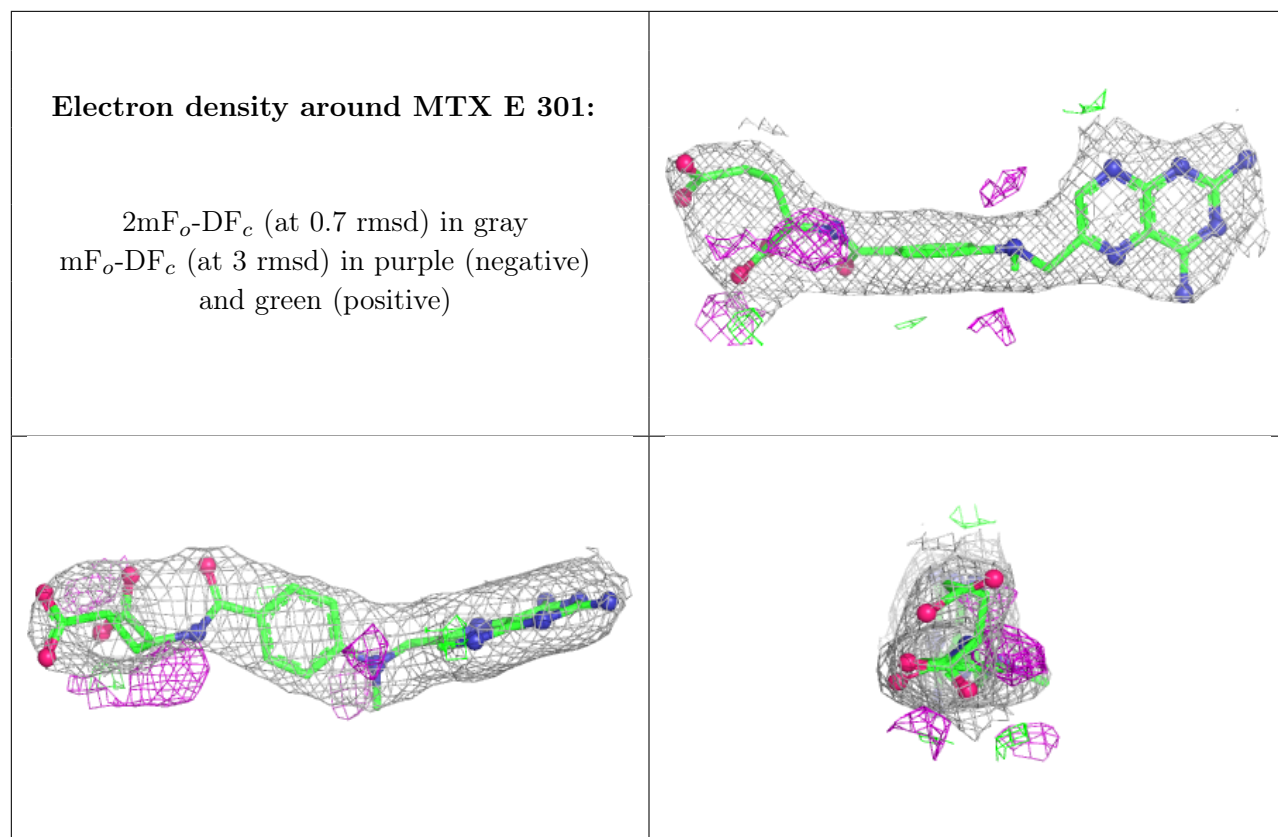
Electron density around MTX G 301:

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

**Electron density around MTX 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.