



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 12:50 PM EDT

PDB ID : 1P33  
Title : Pteridine reductase from *Leishmania tarentolae* complex with NADPH and MTX  
Authors : Zhao, H.; Bray, T.; Ouellette, M.; Zhao, M.; Ferre, R.A.; Matthews, D.; Whiteley, J.M.; Varughese, K.I.  
Deposited on : 2003-04-16  
Resolution : 2.86 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

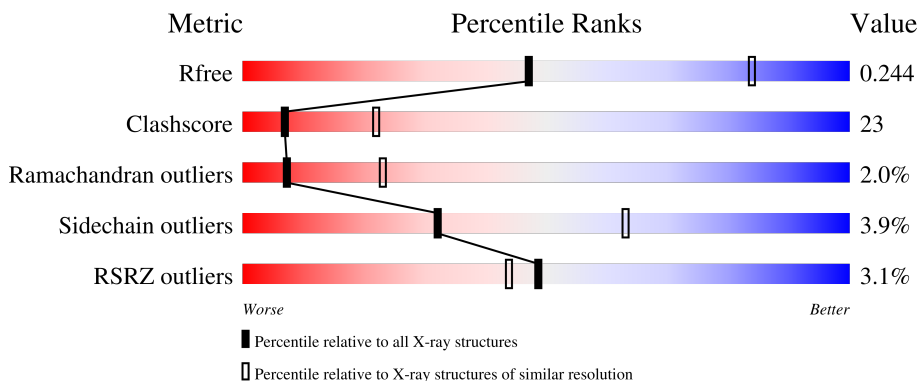
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


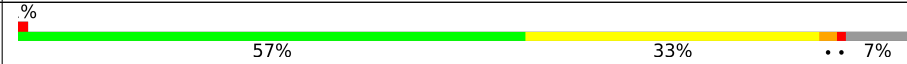
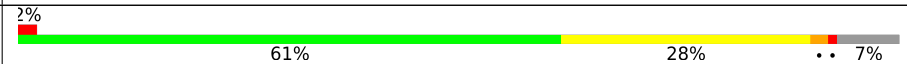

The reported resolution of this entry is 2.86 Å.

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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	289	
1	B	289	
1	C	289	
1	D	289	

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	NDP	A	300	X	-	-	-
2	NDP	B	301	X	-	-	-
2	NDP	D	303	X	-	-	-
3	MTX	A	351	-	X	-	X
3	MTX	B	352	-	X	X	X
3	MTX	C	353	-	X	X	X
3	MTX	D	354	-	X	-	X

## 2 Entry composition [i](#)

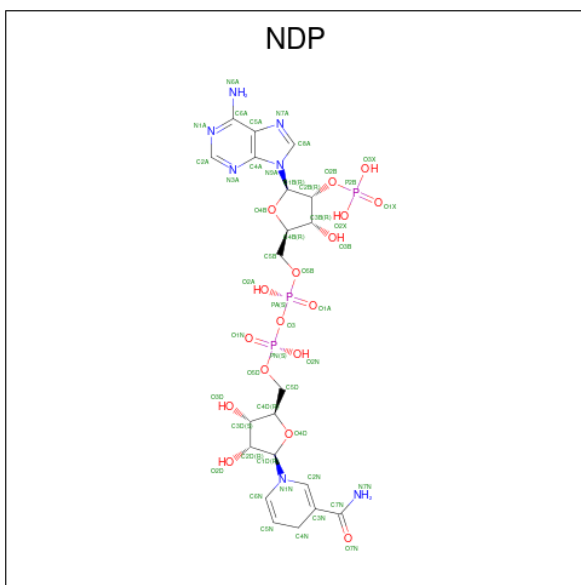
There are 4 unique types of molecules in this entry. The entry contains 8564 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pteridine reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	Total 2009	C 1260	N 348	O 389	S 12	0	0	0
1	B	269	Total 2023	C 1270	N 351	O 390	S 12	0	0	0
1	C	268	Total 2017	C 1267	N 350	O 388	S 12	0	0	0
1	D	268	Total 2018	C 1266	N 350	O 390	S 12	0	0	0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



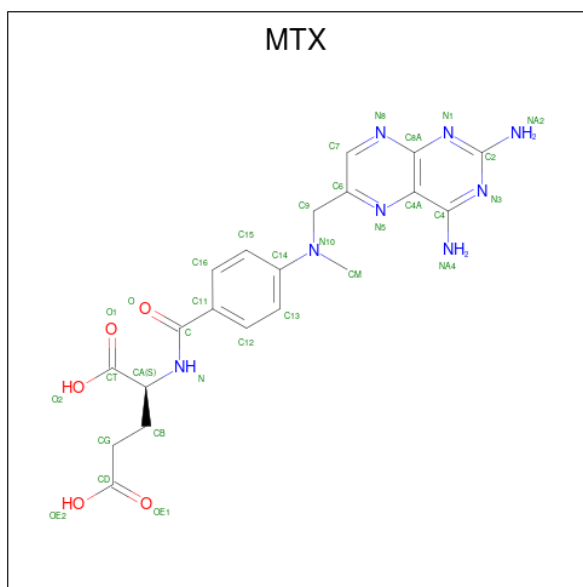
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is METHOTREXATE (three-letter code: MTX) (formula: C<sub>20</sub>H<sub>22</sub>N<sub>8</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	20	8	5		
3	B	1	Total	C	N	O	0	0
			33	20	8	5		
3	C	1	Total	C	N	O	0	0
			33	20	8	5		
3	D	1	Total	C	N	O	0	0
			33	20	8	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	53	Total	O	0	0
			53	53		
4	C	42	Total	O	0	0
			42	42		

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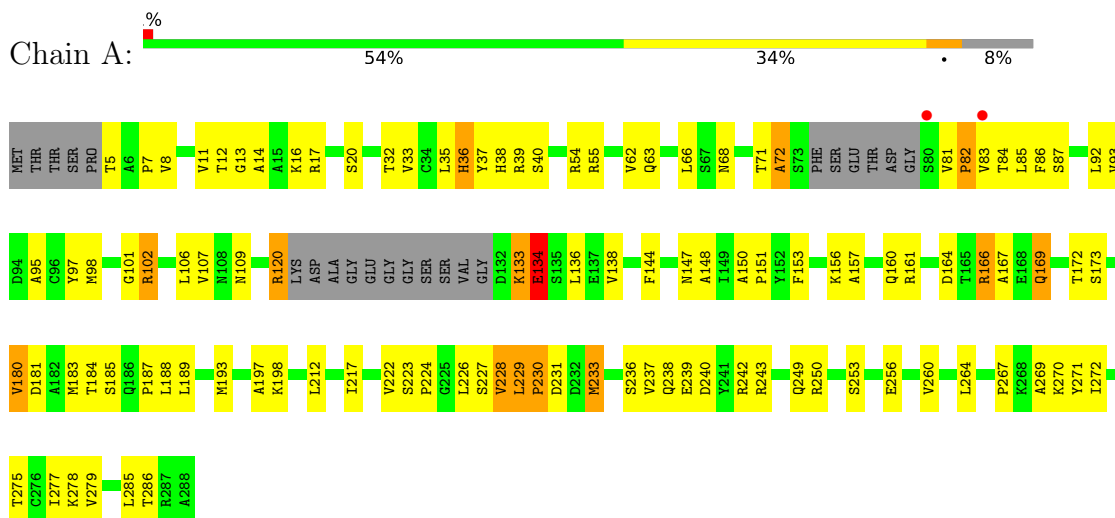
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	D	26	Total	O	0	0
			26	26		

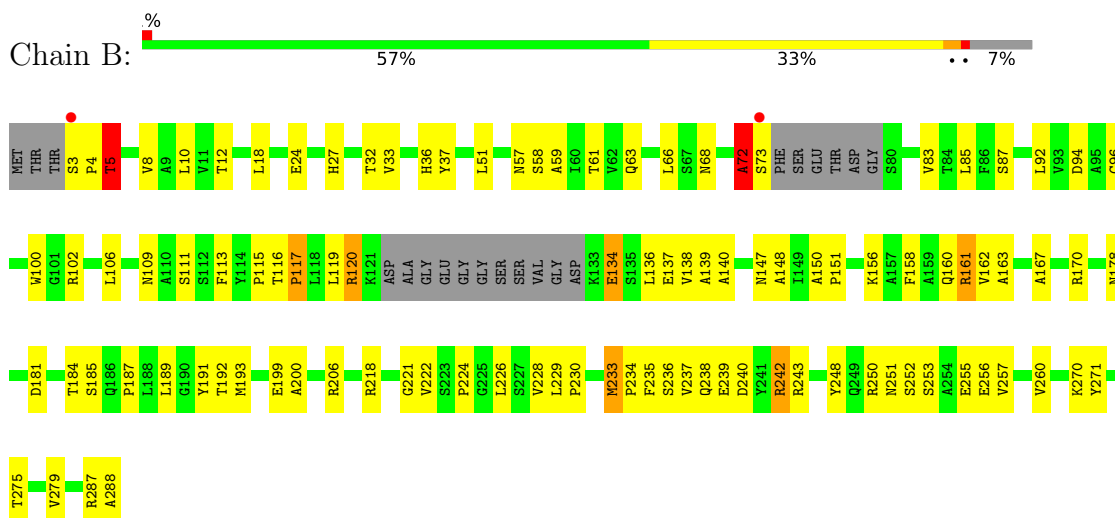
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Pteridine reductase 1

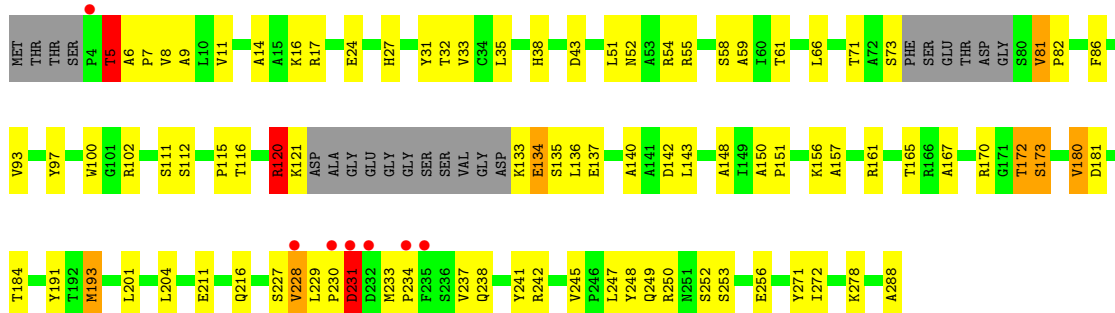


- Molecule 1: Pteridine reductase 1

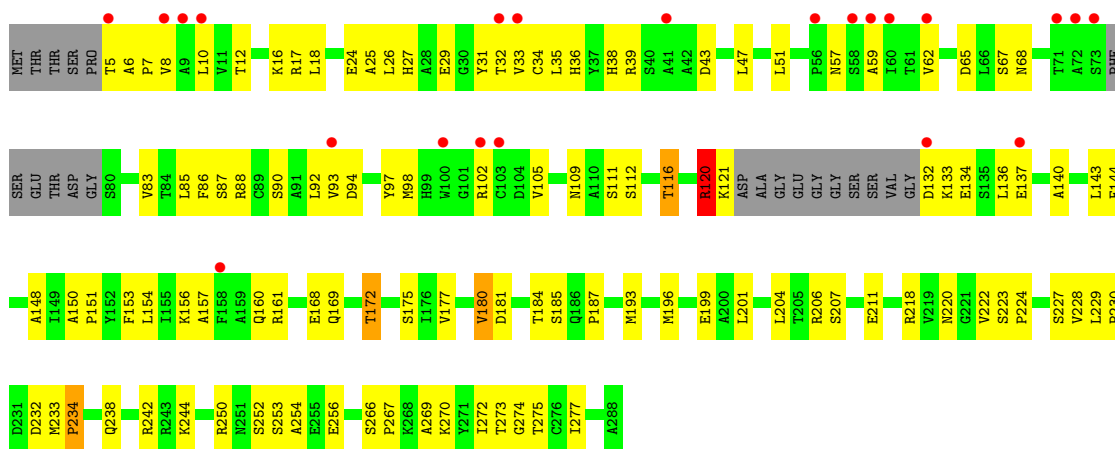


- Molecule 1: Pteridine reductase 1





- Molecule 1: Pteridine reductase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.30Å 96.10Å 195.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.86 82.73 – 2.79	Depositor EDS
% Data completeness (in resolution range)	94.6 (19.98-2.86) 93.8 (82.73-2.79)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 2.77Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.213 , 0.251 0.210 , 0.244	Depositor DCC
$R_{free}$ test set	4105 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtrriage
Anisotropy	0.723	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.026 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8564	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.41	0/2043	0.71	4/2777 (0.1%)
1	B	0.48	1/2058 (0.0%)	0.73	3/2797 (0.1%)
1	C	0.40	0/2052	0.66	2/2788 (0.1%)
1	D	0.37	0/2052	0.64	1/2788 (0.0%)
All	All	0.42	1/8205 (0.0%)	0.69	10/11150 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	72	ALA	C-N	-8.48	1.14	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	ALA	O-C-N	-13.81	100.60	122.70
1	A	134	GLU	N-CA-C	-8.85	87.10	111.00
1	A	72	ALA	N-CA-C	6.61	128.83	111.00
1	C	5	THR	N-CA-C	6.13	127.56	111.00
1	B	134	GLU	N-CA-C	-5.97	94.88	111.00
1	C	120	ARG	N-CA-C	5.82	126.71	111.00
1	B	72	ALA	CA-C-N	5.74	129.83	117.20
1	A	120	ARG	NE-CZ-NH1	-5.49	117.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	120	ARG	N-CA-C	5.34	125.41	111.00
1	A	229	LEU	CA-CB-CG	-5.14	103.47	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	72	ALA	Mainchain

## 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	2009	0	2007	98	0
1	B	2023	0	2027	115	0
1	C	2017	0	2024	105	0
1	D	2018	0	2020	104	0
2	A	48	0	25	2	0
2	B	48	0	25	3	0
2	C	48	0	25	8	0
2	D	48	0	25	3	0
3	A	33	0	20	6	0
3	B	33	0	20	11	0
3	C	33	0	20	11	0
3	D	33	0	20	6	0
4	A	52	0	0	1	0
4	B	53	0	0	4	0
4	C	42	0	0	0	0
4	D	26	0	0	1	0
All	All	8564	0	8258	383	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 23.

All (383) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:THR:HG22	1:B:102:ARG:HH11	1.18	1.06
1:B:239:GLU:HA	1:B:242:ARG:HG3	1.39	1.03
1:B:5:THR:HG22	1:B:102:ARG:NH1	1.77	0.99
1:B:5:THR:CG2	1:B:102:ARG:HH11	1.80	0.94
1:D:242:ARG:HB2	1:D:250:ARG:HA	1.51	0.92
1:D:5:THR:HG23	1:D:102:ARG:HH11	1.34	0.92
1:A:136:LEU:HD11	1:C:156:LYS:NZ	1.87	0.89
3:B:352:MTX:O	3:B:352:MTX:HG2	1.74	0.86
3:C:353:MTX:HG2	3:C:353:MTX:O	1.76	0.86
3:D:354:MTX:O	3:D:354:MTX:HG2	1.76	0.84
1:B:181:ASP:HB3	1:B:184:THR:HG23	1.57	0.84
1:C:230:PRO:HG3	3:C:353:MTX:H13	1.58	0.83
1:B:275:THR:HG21	1:C:278:LYS:HB2	1.59	0.83
3:A:351:MTX:O	3:A:351:MTX:HG2	1.78	0.82
1:A:180:VAL:HG23	1:A:223:SER:HB3	1.63	0.80
1:A:278:LYS:HB2	1:D:275:THR:HG21	1.64	0.80
1:A:160:GLN:HE22	1:C:120:ARG:HG2	1.48	0.79
1:B:68:ASN:HA	1:B:85:LEU:HD22	1.64	0.78
1:B:226:LEU:CD2	3:B:352:MTX:HM1	2.14	0.78
1:B:32:THR:HG23	1:B:58:SER:HA	1.66	0.78
1:C:230:PRO:HD3	3:C:353:MTX:C9	2.14	0.78
1:B:185:SER:O	1:B:187:PRO:HD3	1.83	0.77
1:A:226:LEU:HD23	3:A:351:MTX:HM1	1.67	0.76
1:C:16:LYS:HB2	1:C:16:LYS:NZ	2.03	0.74
1:B:239:GLU:HA	1:B:242:ARG:CG	2.17	0.74
1:A:150:ALA:HB3	1:A:151:PRO:HD3	1.70	0.74
1:C:5:THR:CG2	1:C:102:ARG:HH11	2.01	0.73
1:B:230:PRO:HG2	3:B:352:MTX:H13	1.69	0.73
1:D:8:VAL:HG22	1:D:32:THR:OG1	1.88	0.72
1:C:17:ARG:HG2	1:C:17:ARG:HH11	1.52	0.72
1:A:160:GLN:NE2	1:C:120:ARG:H	1.86	0.72
1:D:229:LEU:HB2	1:D:238:GLN:HE21	1.55	0.72
1:D:222:VAL:O	1:D:224:PRO:HD3	1.89	0.72
1:C:230:PRO:HD3	3:C:353:MTX:H92	1.71	0.72
1:B:226:LEU:HD22	3:B:352:MTX:HM1	1.69	0.71
1:C:238:GLN:O	1:C:242:ARG:HG3	1.89	0.71
1:A:95:ALA:HA	1:A:98:MET:HE3	1.72	0.71
1:B:150:ALA:HB3	1:B:151:PRO:HD3	1.72	0.71
1:D:150:ALA:HB3	1:D:151:PRO:HD3	1.71	0.71
1:A:144:PHE:CE2	1:A:193:MET:HG2	2.26	0.71
1:A:71:THR:O	1:A:82:PRO:HA	1.91	0.70
1:A:136:LEU:HD11	1:C:156:LYS:HZ3	1.53	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:PRO:O	1:A:270:LYS:HG2	1.93	0.68
1:D:12:THR:O	1:D:109:ASN:HB3	1.93	0.68
1:D:26:LEU:O	1:D:31:TYR:HB2	1.93	0.68
1:D:83:VAL:HG12	1:D:87:SER:HB2	1.76	0.68
1:D:230:PRO:HG3	3:D:354:MTX:H7	1.74	0.68
1:C:5:THR:HG23	1:C:102:ARG:HH11	1.57	0.68
1:A:144:PHE:HE2	1:A:193:MET:HG2	1.59	0.67
1:D:5:THR:HG23	1:D:102:ARG:NH1	2.06	0.67
1:A:227:SER:O	1:A:228:VAL:C	2.32	0.67
1:B:218:ARG:HD3	1:B:270:LYS:O	1.94	0.67
1:C:32:THR:HG23	1:C:58:SER:HA	1.76	0.67
1:B:32:THR:CG2	1:B:58:SER:HA	2.24	0.67
1:B:253:SER:OG	1:B:256:GLU:HG3	1.94	0.67
1:A:54:ARG:O	1:A:55:ARG:HG3	1.95	0.67
1:B:72:ALA:O	1:B:73:SER:C	2.33	0.67
1:D:12:THR:HA	1:D:36:HIS:HB3	1.76	0.66
1:C:227:SER:O	1:C:228:VAL:C	2.34	0.66
1:B:156:LYS:NZ	1:D:136:LEU:HD13	2.11	0.66
1:A:8:VAL:HG22	1:A:32:THR:CG2	2.26	0.66
1:B:12:THR:O	1:B:109:ASN:HB3	1.94	0.65
1:D:230:PRO:HG3	3:D:354:MTX:C7	2.26	0.65
1:B:37:TYR:CZ	1:B:63:GLN:HB2	2.32	0.65
1:A:136:LEU:HD11	1:C:156:LYS:HZ2	1.62	0.65
1:B:230:PRO:CG	3:B:352:MTX:H13	2.27	0.64
1:D:35:LEU:HD11	1:D:51:LEU:HD12	1.79	0.64
1:A:226:LEU:CD2	3:A:351:MTX:HM1	2.26	0.64
1:A:278:LYS:HB2	1:D:275:THR:CG2	2.26	0.64
1:B:181:ASP:HB3	1:B:184:THR:CG2	2.25	0.64
1:D:38:HIS:CD2	1:D:39:ARG:HG2	2.33	0.64
1:A:17:ARG:HG2	1:A:17:ARG:HH11	1.63	0.64
1:B:120:ARG:HH11	1:B:120:ARG:HB2	1.61	0.64
1:C:33:VAL:O	1:C:59:ALA:HA	1.98	0.63
1:D:140:ALA:O	1:D:144:PHE:HB2	1.99	0.63
1:A:84:THR:HG21	1:C:137:GLU:OE1	1.99	0.63
1:A:160:GLN:HE22	1:C:120:ARG:CG	2.10	0.63
1:A:238:GLN:O	1:A:242:ARG:HG2	1.98	0.63
1:D:88:ARG:HH11	1:D:88:ARG:HG3	1.63	0.62
1:C:230:PRO:HD3	3:C:353:MTX:H91	1.80	0.62
1:C:242:ARG:HB3	1:C:250:ARG:HA	1.81	0.62
1:D:168:GLU:HG3	1:D:169:GLN:HG3	1.82	0.61
1:A:160:GLN:HE21	1:C:120:ARG:H	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LYS:HZ3	1:D:136:LEU:HD13	1.66	0.61
1:C:229:LEU:HB3	1:C:230:PRO:HD2	1.83	0.61
1:C:234:PRO:HB2	1:C:237:VAL:HG23	1.82	0.61
1:A:228:VAL:HG23	1:A:228:VAL:O	2.01	0.61
1:C:150:ALA:HB3	1:C:151:PRO:HD3	1.82	0.60
1:C:120:ARG:HG3	1:C:121:LYS:H	1.67	0.60
1:A:156:LYS:NZ	1:C:136:LEU:HD11	2.17	0.60
1:B:116:THR:HG21	1:B:193:MET:CE	2.32	0.60
1:B:233:MET:HG3	1:B:238:GLN:HG3	1.84	0.60
1:A:66:LEU:H	2:A:300:NDP:C2A	2.15	0.59
1:D:62:VAL:HG11	1:D:92:LEU:HD23	1.84	0.59
1:A:271:TYR:CE2	1:D:252:SER:HB3	2.37	0.59
1:B:163:ALA:HA	1:B:170:ARG:NH2	2.18	0.59
1:B:12:THR:HA	1:B:36:HIS:HB3	1.85	0.59
1:B:230:PRO:HG3	3:B:352:MTX:C7	2.32	0.59
1:D:185:SER:O	1:D:187:PRO:HD3	2.03	0.59
1:A:253:SER:OG	1:A:256:GLU:HG3	2.03	0.58
1:C:17:ARG:HG2	1:C:17:ARG:NH1	2.14	0.58
1:C:230:PRO:HB3	3:C:353:MTX:H7	1.85	0.58
1:B:158:PHE:O	1:B:162:VAL:HG23	2.03	0.58
1:B:242:ARG:HB3	1:B:250:ARG:HA	1.86	0.58
1:B:239:GLU:O	1:B:243:ARG:HG3	2.03	0.58
1:B:136:LEU:HD11	1:D:156:LYS:NZ	2.18	0.58
1:A:37:TYR:CZ	1:A:63:GLN:HB2	2.39	0.57
1:A:256:GLU:OE2	1:D:270:LYS:HE2	2.04	0.57
1:B:136:LEU:HD11	1:D:156:LYS:HZ1	1.69	0.57
1:B:230:PRO:HG3	3:B:352:MTX:H7	1.87	0.57
1:A:12:THR:O	1:A:109:ASN:HB3	2.03	0.57
1:A:133:LYS:HG3	1:C:86:PHE:CD2	2.40	0.57
1:D:230:PRO:C	1:D:232:ASP:H	2.06	0.57
1:A:286:THR:HB	1:B:288:ALA:HB2	1.86	0.57
1:B:116:THR:HG21	1:B:193:MET:HE2	1.87	0.57
1:A:285:LEU:HD11	1:D:274:GLY:HA3	1.87	0.57
1:D:269:ALA:HB1	1:D:272:ILE:HD12	1.87	0.56
1:B:115:PRO:HG3	1:B:191:TYR:CZ	2.41	0.56
1:B:189:LEU:HD11	1:D:211:GLU:HG3	1.88	0.56
1:C:8:VAL:HG23	1:C:102:ARG:HG3	1.88	0.56
1:C:253:SER:OG	1:C:256:GLU:HG3	2.05	0.56
1:D:220:ASN:OD1	1:D:273:THR:HA	2.06	0.56
1:D:35:LEU:HD13	1:D:47:LEU:HD23	1.88	0.56
1:D:68:ASN:HA	1:D:85:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:GLU:HA	1:D:137:GLU:HG3	1.88	0.56
1:B:222:VAL:O	1:B:224:PRO:HD3	2.05	0.55
1:D:238:GLN:O	1:D:242:ARG:HG2	2.06	0.55
1:C:115:PRO:HG3	1:C:191:TYR:CZ	2.42	0.55
1:A:97:TYR:O	1:A:101:GLY:HA2	2.07	0.55
1:B:94:ASP:OD1	1:B:161:ARG:NH1	2.29	0.55
1:A:239:GLU:HA	1:A:242:ARG:CG	2.36	0.55
1:B:37:TYR:CE1	1:B:63:GLN:HB2	2.42	0.55
1:A:106:LEU:HD12	1:A:107:VAL:N	2.22	0.54
1:B:148:ALA:C	1:B:151:PRO:HD2	2.27	0.54
1:B:238:GLN:O	1:B:242:ARG:HG2	2.06	0.54
1:C:17:ARG:HD3	2:C:302:NDP:O2A	2.07	0.54
1:B:271:TYR:CE2	1:C:252:SER:HB3	2.42	0.54
1:C:54:ARG:O	1:C:55:ARG:HG3	2.08	0.54
1:A:83:VAL:HG12	1:A:87:SER:HB2	1.90	0.54
1:D:94:ASP:HA	1:D:161:ARG:HH12	1.73	0.54
1:C:230:PRO:HB3	3:C:353:MTX:C7	2.38	0.53
1:B:235:PHE:HB3	4:B:436:HOH:O	2.08	0.53
1:D:112:SER:OG	1:D:143:LEU:HA	2.08	0.53
1:B:120:ARG:N	1:D:160:GLN:HE22	2.05	0.53
1:D:230:PRO:C	1:D:232:ASP:N	2.62	0.53
1:A:233:MET:HB3	1:A:238:GLN:HG2	1.90	0.53
1:B:271:TYR:CD2	1:C:252:SER:HB3	2.43	0.53
1:C:81:VAL:HG23	1:C:82:PRO:HD2	1.91	0.53
1:B:234:PRO:HG2	1:B:237:VAL:HG23	1.90	0.53
1:D:88:ARG:HG3	1:D:88:ARG:NH1	2.23	0.53
1:D:97:TYR:HB2	1:D:161:ARG:NH2	2.23	0.53
1:A:133:LYS:HD2	1:A:133:LYS:O	2.09	0.53
1:A:147:ASN:OD1	1:A:198:LYS:HE2	2.09	0.53
1:B:163:ALA:HA	1:B:170:ARG:HH21	1.72	0.53
1:A:134:GLU:O	1:A:138:VAL:HG23	2.08	0.53
1:D:266:SER:HB2	1:D:267:PRO:HD2	1.91	0.53
1:A:97:TYR:CB	1:A:161:ARG:HH21	2.22	0.53
1:D:6:ALA:O	1:D:102:ARG:HD3	2.09	0.53
1:B:27:HIS:CD2	1:B:51:LEU:HD22	2.45	0.52
1:D:116:THR:HG21	1:D:193:MET:CG	2.40	0.52
1:A:16:LYS:HA	1:A:20:SER:HB2	1.90	0.52
1:B:32:THR:HG22	1:B:100:TRP:CZ2	2.44	0.52
1:B:18:LEU:HD13	1:B:257:VAL:HG11	1.90	0.52
1:C:7:PRO:HB2	1:C:31:TYR:CD2	2.45	0.52
1:A:17:ARG:HG2	1:A:17:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:THR:HG21	1:B:100:TRP:CE2	2.44	0.52
1:A:277:ILE:HG12	1:D:277:ILE:HG12	1.91	0.52
1:B:226:LEU:HD23	3:B:352:MTX:HM1	1.92	0.52
1:D:172:THR:O	1:D:172:THR:OG1	2.28	0.52
1:B:275:THR:CG2	1:C:278:LYS:HB2	2.33	0.52
1:A:269:ALA:HB1	1:A:272:ILE:HD12	1.93	0.51
1:A:8:VAL:HA	1:A:32:THR:HG22	1.93	0.51
1:D:227:SER:HA	1:D:252:SER:OG	2.09	0.51
1:C:227:SER:O	1:C:229:LEU:N	2.43	0.51
1:C:27:HIS:CG	1:C:51:LEU:HD22	2.46	0.51
1:D:201:LEU:O	1:D:204:LEU:HB3	2.11	0.51
1:A:212:LEU:HB3	1:A:217:ILE:HB	1.92	0.51
1:D:177:VAL:HA	1:D:220:ASN:O	2.11	0.51
1:D:116:THR:HG21	1:D:193:MET:HG3	1.93	0.51
1:B:233:MET:SD	1:B:238:GLN:HG2	2.51	0.51
1:C:120:ARG:O	1:C:121:LYS:C	2.49	0.50
1:A:93:VAL:HG21	1:A:157:ALA:HB3	1.92	0.50
1:B:167:ALA:HA	1:B:170:ARG:HD2	1.93	0.50
1:C:16:LYS:HB2	1:C:16:LYS:HZ2	1.73	0.50
1:A:17:ARG:NH1	1:A:230:PRO:O	2.45	0.50
1:B:178:ASN:O	1:B:221:GLY:HA2	2.11	0.50
1:C:66:LEU:H	2:C:302:NDP:C2A	2.24	0.50
1:A:13:GLY:HA2	4:A:400:HOH:O	2.12	0.50
1:A:181:ASP:O	1:A:184:THR:HG23	2.12	0.50
1:D:253:SER:OG	1:D:256:GLU:HG3	2.12	0.50
1:B:192:THR:HG23	1:D:207:SER:HB3	1.94	0.50
1:C:16:LYS:HB2	1:C:16:LYS:HZ3	1.74	0.50
1:D:230:PRO:HD2	1:D:233:MET:HG2	1.94	0.50
1:A:133:LYS:HG3	1:C:86:PHE:HD2	1.77	0.50
1:B:228:VAL:O	1:B:228:VAL:HG23	2.12	0.50
1:C:38:HIS:HB2	2:C:302:NDP:N3A	2.27	0.49
1:A:157:ALA:O	1:A:161:ARG:HG2	2.12	0.49
1:A:181:ASP:HB3	1:A:184:THR:CG2	2.43	0.49
1:D:16:LYS:NZ	1:D:16:LYS:HB2	2.27	0.49
1:B:134:GLU:HA	1:B:137:GLU:HG2	1.94	0.49
1:B:206:ARG:NH2	1:D:199:GLU:OE1	2.44	0.49
1:D:27:HIS:CD2	1:D:51:LEU:HD22	2.48	0.49
1:C:134:GLU:O	1:C:134:GLU:HG2	2.12	0.49
1:A:260:VAL:HG21	1:A:279:VAL:HG21	1.94	0.49
1:C:248:TYR:HB2	1:C:250:ARG:HG2	1.95	0.49
1:A:242:ARG:HB2	1:A:250:ARG:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:VAL:CG2	1:A:35:LEU:HD21	2.43	0.49
1:B:252:SER:HB3	1:C:271:TYR:CE2	2.48	0.49
1:C:9:ALA:HB3	1:C:33:VAL:HG12	1.95	0.49
1:C:81:VAL:HG23	1:C:82:PRO:CD	2.43	0.49
1:A:237:VAL:O	1:A:240:ASP:HB2	2.12	0.48
1:B:233:MET:HG2	1:B:238:GLN:HE21	1.78	0.48
1:C:111:SER:HB3	2:C:302:NDP:H3D	1.95	0.48
1:D:25:ALA:O	1:D:29:GLU:HG2	2.14	0.48
1:A:8:VAL:HG22	1:A:32:THR:HG21	1.93	0.48
1:C:5:THR:HG22	1:C:102:ARG:HH11	1.75	0.48
1:D:230:PRO:O	1:D:232:ASP:N	2.46	0.48
1:B:230:PRO:HD3	3:B:352:MTX:H92	1.94	0.48
1:B:120:ARG:HH11	1:B:120:ARG:CB	2.26	0.48
1:B:185:SER:C	1:B:187:PRO:HD3	2.33	0.48
1:B:32:THR:CG2	1:B:100:TRP:CZ2	2.97	0.48
1:B:138:VAL:CG2	1:B:139:ALA:N	2.77	0.48
1:C:16:LYS:HD3	1:C:43:ASP:OD2	2.14	0.48
1:A:164:ASP:OD1	1:C:120:ARG:NH1	2.46	0.48
1:B:120:ARG:H	1:D:160:GLN:HE22	1.62	0.48
1:D:111:SER:HB3	2:D:303:NDP:H3D	1.94	0.48
1:D:120:ARG:HB2	1:D:121:LYS:H	1.44	0.48
1:A:36:HIS:HA	1:A:62:VAL:O	2.14	0.47
1:A:66:LEU:H	2:A:300:NDP:H2A	1.79	0.47
1:C:32:THR:HG21	1:C:100:TRP:CE2	2.48	0.47
1:B:199:GLU:OE1	1:D:206:ARG:NH2	2.47	0.47
1:A:240:ASP:O	1:A:243:ARG:HG2	2.14	0.47
1:C:81:VAL:HG23	1:C:82:PRO:N	2.29	0.47
1:B:140:ALA:HA	1:B:193:MET:SD	2.55	0.47
1:B:248:TYR:CE1	1:C:216:GLN:HG2	2.49	0.47
1:B:248:TYR:HE1	1:C:216:GLN:HG2	1.79	0.47
1:A:120:ARG:HG3	1:A:120:ARG:O	2.14	0.47
1:B:68:ASN:CA	1:B:85:LEU:HD22	2.39	0.47
1:D:201:LEU:HD12	1:D:204:LEU:HD23	1.97	0.47
1:B:230:PRO:HD3	3:B:352:MTX:C9	2.44	0.47
1:C:5:THR:HG21	1:C:102:ARG:HD2	1.96	0.47
1:C:17:ARG:HE	2:C:302:NDP:PA	2.38	0.47
2:C:302:NDP:H2D	3:C:353:MTX:N3	2.30	0.47
1:C:233:MET:HG2	1:C:237:VAL:HB	1.95	0.47
1:B:87:SER:OG	1:D:133:LYS:NZ	2.42	0.47
1:B:27:HIS:CG	1:B:51:LEU:HD22	2.51	0.46
4:B:406:HOH:O	1:D:137:GLU:HG2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LEU:H	2:C:302:NDP:H2A	1.80	0.46
1:A:183:MET:HB3	1:B:287:ARG:NH2	2.31	0.46
1:D:33:VAL:O	1:D:59:ALA:HA	2.15	0.46
1:D:90:SER:O	1:D:94:ASP:HB2	2.15	0.46
1:A:7:PRO:O	1:A:32:THR:HG22	2.14	0.46
1:B:33:VAL:O	1:B:59:ALA:HA	2.14	0.46
1:B:260:VAL:HG21	1:B:279:VAL:HG22	1.97	0.46
1:B:234:PRO:HG2	1:B:237:VAL:CG2	2.45	0.46
1:C:172:THR:O	1:C:172:THR:OG1	2.33	0.46
1:A:188:LEU:HD21	3:A:351:MTX:H16	1.97	0.46
1:B:111:SER:HB2	1:B:147:ASN:OD1	2.16	0.46
1:C:181:ASP:O	1:C:184:THR:HG23	2.16	0.46
1:B:134:GLU:O	1:B:138:VAL:HG13	2.16	0.46
1:B:191:TYR:N	1:B:191:TYR:CD1	2.84	0.46
1:B:161:ARG:N	1:B:161:ARG:HD2	2.31	0.46
1:D:18:LEU:HB2	2:D:303:NDP:O2N	2.16	0.46
1:D:97:TYR:CE2	1:D:161:ARG:HB3	2.51	0.45
1:C:133:LYS:O	1:C:135:SER:N	2.50	0.45
1:D:218:ARG:HD3	1:D:270:LYS:O	2.17	0.45
1:A:242:ARG:O	1:A:249:GLN:C	2.55	0.45
1:B:113:PHE:HB2	3:B:352:MTX:C2	2.46	0.45
1:C:5:THR:HG22	1:C:102:ARG:NH1	2.31	0.45
1:D:233:MET:HA	1:D:234:PRO:HD3	1.89	0.45
1:A:81:VAL:HG23	1:A:82:PRO:O	2.16	0.45
1:C:5:THR:CG2	1:C:102:ARG:HD2	2.46	0.45
1:A:156:LYS:CE	1:C:136:LEU:HD11	2.47	0.45
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.87	0.45
1:C:52:ASN:HA	1:C:55:ARG:O	2.17	0.45
1:D:92:LEU:HD12	1:D:154:LEU:HD21	1.97	0.45
1:C:143:LEU:CD1	1:C:193:MET:HB3	2.47	0.45
1:A:68:ASN:HA	1:A:85:LEU:HD22	1.99	0.45
1:B:8:VAL:HG11	1:B:96:CYS:HB3	1.98	0.45
1:C:148:ALA:C	1:C:151:PRO:HD2	2.38	0.45
1:D:144:PHE:HD2	1:D:193:MET:HE1	1.83	0.44
1:D:148:ALA:C	1:D:151:PRO:HD2	2.37	0.44
2:B:301:NDP:O5D	2:B:301:NDP:H2N	2.17	0.44
1:C:93:VAL:HG21	1:C:157:ALA:HB3	2.00	0.44
1:D:97:TYR:CZ	1:D:161:ARG:HB3	2.51	0.44
1:A:260:VAL:HG21	1:A:279:VAL:CG2	2.48	0.44
1:C:115:PRO:HG3	1:C:191:TYR:CE1	2.52	0.44
1:C:230:PRO:CB	3:C:353:MTX:H7	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:PRO:HB2	1:D:31:TYR:CD2	2.53	0.44
1:D:228:VAL:HG23	1:D:228:VAL:O	2.18	0.44
1:A:38:HIS:CD2	1:A:39:ARG:HG3	2.52	0.44
1:B:260:VAL:HG21	1:B:279:VAL:CG2	2.47	0.44
1:B:3:SER:N	1:B:4:PRO:HD3	2.32	0.44
1:B:120:ARG:N	1:D:160:GLN:NE2	2.66	0.44
3:C:353:MTX:H13	3:C:353:MTX:H91	1.39	0.44
1:D:67:SER:O	1:D:85:LEU:HD13	2.17	0.44
1:A:230:PRO:HD3	3:A:351:MTX:C9	2.48	0.44
1:A:185:SER:O	1:A:187:PRO:HD3	2.18	0.43
1:C:231:ASP:C	1:C:233:MET:H	2.22	0.43
1:D:144:PHE:CD2	1:D:193:MET:HE1	2.52	0.43
1:C:16:LYS:NZ	1:C:16:LYS:CB	2.80	0.43
1:D:86:PHE:HD1	1:D:153:PHE:CD1	2.36	0.43
1:B:116:THR:HG21	1:B:193:MET:HE3	1.99	0.43
1:B:116:THR:N	1:B:117:PRO:HD3	2.33	0.43
1:A:36:HIS:CG	1:A:37:TYR:N	2.86	0.43
1:A:166:ARG:HG3	1:A:169:GLN:HG3	1.99	0.43
1:C:97:TYR:CE1	1:C:161:ARG:HG3	2.53	0.43
1:A:16:LYS:CA	1:A:20:SER:HB2	2.49	0.43
1:A:233:MET:HB3	1:A:238:GLN:CG	2.48	0.43
1:D:10:LEU:HD13	1:D:34:CYS:SG	2.59	0.43
1:D:24:GLU:O	1:D:27:HIS:HB3	2.19	0.43
1:D:93:VAL:HG21	1:D:157:ALA:HB3	2.01	0.43
1:D:181:ASP:HB3	1:D:184:THR:HG23	2.00	0.43
1:A:33:VAL:HG21	1:A:35:LEU:HD21	2.01	0.43
1:C:8:VAL:HA	1:C:32:THR:O	2.19	0.43
1:B:37:TYR:HE2	1:B:61:THR:HB	1.83	0.42
1:C:140:ALA:HA	1:C:193:MET:SD	2.59	0.42
1:C:172:THR:O	1:C:173:SER:HB3	2.18	0.42
1:C:230:PRO:CD	3:C:353:MTX:H7	2.49	0.42
1:B:119:LEU:HA	1:D:160:GLN:NE2	2.35	0.42
1:B:250:ARG:HG3	1:B:251:ASN:O	2.20	0.42
1:A:136:LEU:HD21	1:C:156:LYS:HZ2	1.85	0.42
1:B:57:ASN:HA	4:B:459:HOH:O	2.20	0.42
1:C:288:ALA:OXT	1:D:244:LYS:HE2	2.19	0.42
1:D:105:VAL:HG22	1:D:175:SER:HB3	2.02	0.42
1:A:229:LEU:H	1:A:229:LEU:HG	1.62	0.42
1:D:132:ASP:O	1:D:133:LYS:C	2.57	0.42
1:A:229:LEU:HA	1:A:229:LEU:HD23	1.74	0.42
1:A:229:LEU:O	1:A:230:PRO:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:VAL:HB	1:C:181:ASP:H	1.64	0.42
1:D:83:VAL:CG1	1:D:87:SER:HB2	2.48	0.42
1:D:94:ASP:O	1:D:98:MET:HB2	2.19	0.42
1:D:230:PRO:HD3	3:D:354:MTX:H92	2.02	0.42
1:B:158:PHE:CD1	1:B:158:PHE:C	2.93	0.42
1:D:180:VAL:HG23	1:D:223:SER:OG	2.20	0.42
1:B:229:LEU:HD13	1:B:238:GLN:HG2	2.01	0.42
1:C:71:THR:O	1:C:82:PRO:HA	2.19	0.42
1:C:201:LEU:HD12	1:C:204:LEU:HD23	2.01	0.42
1:A:95:ALA:CA	1:A:98:MET:HE3	2.47	0.42
1:B:10:LEU:HD23	1:B:106:LEU:HD13	2.01	0.41
1:D:18:LEU:CD2	1:D:254:ALA:HA	2.50	0.41
1:B:134:GLU:OE1	1:B:137:GLU:OE2	2.38	0.41
1:B:233:MET:CG	1:B:238:GLN:HE21	2.32	0.41
1:C:245:VAL:O	1:C:249:GLN:HA	2.20	0.41
1:D:232:ASP:HB2	4:D:516:HOH:O	2.20	0.41
1:C:231:ASP:C	1:C:233:MET:N	2.73	0.41
1:A:189:LEU:HD11	1:C:211:GLU:HG3	2.03	0.41
1:A:264:LEU:HD21	1:A:277:ILE:HD12	2.01	0.41
1:B:111:SER:HB3	2:B:301:NDP:H3D	2.01	0.41
1:C:247:LEU:HG	1:C:248:TYR:CE2	2.54	0.41
1:C:6:ALA:HA	1:C:7:PRO:HD3	1.90	0.41
1:A:8:VAL:HG23	1:A:102:ARG:HG3	2.01	0.41
1:A:86:PHE:HD1	1:A:153:PHE:CD1	2.38	0.41
1:B:200:ALA:O	1:D:196:MET:HG2	2.21	0.41
1:C:81:VAL:CG2	1:C:82:PRO:N	2.83	0.41
1:A:230:PRO:HD3	3:A:351:MTX:H91	2.02	0.41
1:D:230:PRO:HD3	3:D:354:MTX:C9	2.50	0.41
1:B:83:VAL:CG1	1:B:87:SER:HB2	2.51	0.41
1:B:242:ARG:HG2	1:B:242:ARG:H	1.60	0.41
1:B:260:VAL:HG22	1:C:272:ILE:HD11	2.03	0.41
1:C:181:ASP:HB3	1:C:184:THR:CG2	2.51	0.41
1:D:230:PRO:CG	3:D:354:MTX:H7	2.46	0.41
1:A:222:VAL:O	1:A:224:PRO:HD3	2.21	0.41
2:D:303:NDP:H8A	2:D:303:NDP:H3B	2.03	0.41
1:A:148:ALA:C	1:A:151:PRO:HD2	2.41	0.41
1:B:160:GLN:OE1	1:D:120:ARG:HG2	2.20	0.41
1:C:35:LEU:O	1:C:61:THR:HA	2.21	0.41
1:C:237:VAL:O	1:C:241:TYR:HD1	2.04	0.41
1:A:147:ASN:HB2	1:A:197:ALA:HB1	2.03	0.40
1:B:24:GLU:HB3	4:B:427:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LEU:H	2:B:301:NDP:C2A	2.32	0.40
1:C:32:THR:HG22	1:C:100:TRP:CZ2	2.56	0.40
1:D:94:ASP:HA	1:D:161:ARG:NH1	2.37	0.40
1:A:120:ARG:O	1:A:120:ARG:CG	2.68	0.40
1:D:38:HIS:ND1	1:D:65:ASP:HA	2.37	0.40
1:A:11:VAL:CG1	1:A:14:ALA:HB2	2.51	0.40
1:B:138:VAL:HG23	1:B:139:ALA:N	2.36	0.40
1:B:233:MET:CG	1:B:238:GLN:HG3	2.50	0.40
1:C:11:VAL:HG12	1:C:14:ALA:HB2	2.03	0.40
1:C:142:ASP:OD1	2:C:302:NDP:N6A	2.54	0.40
1:D:229:LEU:HD13	1:D:238:GLN:HA	2.04	0.40
1:C:112:SER:OG	1:C:143:LEU:HD23	2.21	0.40
1:C:165:THR:HG22	1:C:170:ARG:HG3	2.03	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	261/289 (90%)	236 (90%)	17 (6%)	8 (3%)	4	14
1	B	263/289 (91%)	235 (89%)	26 (10%)	2 (1%)	19	46
1	C	262/289 (91%)	237 (90%)	18 (7%)	7 (3%)	5	16
1	D	262/289 (91%)	217 (83%)	41 (16%)	4 (2%)	10	30
All	All	1048/1156 (91%)	925 (88%)	102 (10%)	21 (2%)	7	23

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	ALA
1	A	228	VAL

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Mol	Chain	Res	Type
1	A	230	PRO
1	A	231	ASP
1	C	120	ARG
1	C	228	VAL
1	D	234	PRO
1	A	134	GLU
1	C	167	ALA
1	C	231	ASP
1	A	40	SER
1	B	5	THR
1	C	173	SER
1	D	17	ARG
1	C	134	GLU
1	C	180	VAL
1	D	57	ASN
1	D	180	VAL
1	A	167	ALA
1	A	180	VAL
1	B	117	PRO

### 5.3.2 Protein sidechains [i](#)

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	216/232 (93%)	202 (94%)	14 (6%)	17	41
1	B	218/232 (94%)	210 (96%)	8 (4%)	34	65
1	C	217/232 (94%)	209 (96%)	8 (4%)	34	65
1	D	217/232 (94%)	213 (98%)	4 (2%)	59	82
All	All	868/928 (94%)	834 (96%)	34 (4%)	32	63

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	36	HIS

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Mol	Chain	Res	Type
1	A	82	PRO
1	A	92	LEU
1	A	102	ARG
1	A	133	LYS
1	A	134	GLU
1	A	166	ARG
1	A	169	GLN
1	A	172	THR
1	A	173	SER
1	A	233	MET
1	A	236	SER
1	A	275	THR
1	B	5	THR
1	B	120	ARG
1	B	161	ARG
1	B	233	MET
1	B	236	SER
1	B	240	ASP
1	B	242	ARG
1	B	255	GLU
1	C	5	THR
1	C	24	GLU
1	C	73	SER
1	C	81	VAL
1	C	116	THR
1	C	172	THR
1	C	193	MET
1	C	231	ASP
1	D	43	ASP
1	D	116	THR
1	D	120	ARG
1	D	172	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	160	GLN
1	A	249	GLN
1	B	38	HIS
1	B	57	ASN
1	B	169	GLN

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Mol	Chain	Res	Type
1	B	238	GLN
1	C	38	HIS
1	C	57	ASN
1	C	186	GLN
1	D	160	GLN
1	D	238	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NDP	C	302	-	45,52,52	1.78	8 (17%)	53,80,80	2.14	13 (24%)
3	MTX	A	351	-	35,35,35	3.95	19 (54%)	46,49,49	5.92	25 (54%)
3	MTX	D	354	-	35,35,35	4.23	24 (68%)	46,49,49	5.76	24 (52%)
3	MTX	B	352	-	35,35,35	4.19	24 (68%)	46,49,49	5.74	26 (56%)
3	MTX	C	353	-	35,35,35	4.14	22 (62%)	46,49,49	5.74	23 (50%)
2	NDP	D	303	-	45,52,52	1.71	7 (15%)	53,80,80	2.17	13 (24%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NDP	A	300	-	45,52,52	1.75	6 (13%)	53,80,80	2.88	17 (32%)
2	NDP	B	301	-	45,52,52	1.74	7 (15%)	53,80,80	2.52	16 (30%)

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	NDP	C	302	-	-	6/30/77/77	0/5/5/5
3	MTX	A	351	-	-	7/25/25/25	0/3/3/3
3	MTX	D	354	-	-	8/25/25/25	0/3/3/3
3	MTX	B	352	-	-	7/25/25/25	0/3/3/3
3	MTX	C	353	-	-	6/25/25/25	0/3/3/3
2	NDP	D	303	-	1/1/14/17	6/30/77/77	0/5/5/5
2	NDP	A	300	-	1/1/14/17	7/30/77/77	0/5/5/5
2	NDP	B	301	-	1/1/14/17	6/30/77/77	0/5/5/5

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	354	MTX	C7-N8	12.49	1.52	1.31
3	B	352	MTX	C7-N8	12.47	1.52	1.31
3	A	351	MTX	C7-N8	11.44	1.50	1.31
3	C	353	MTX	C7-N8	11.40	1.50	1.31
3	B	352	MTX	C7-C6	8.47	1.54	1.39
3	B	352	MTX	C9-N10	8.00	1.62	1.46
3	D	354	MTX	C7-C6	7.94	1.53	1.39
3	C	353	MTX	C9-N10	7.88	1.62	1.46
3	C	353	MTX	C7-C6	7.47	1.52	1.39
3	D	354	MTX	C9-N10	7.21	1.60	1.46
3	A	351	MTX	C7-C6	7.15	1.52	1.39
3	B	352	MTX	OE1-CD	6.86	1.44	1.22
3	D	354	MTX	OE1-CD	6.84	1.44	1.22
3	C	353	MTX	OE1-CD	6.80	1.44	1.22
3	A	351	MTX	OE1-CD	6.75	1.44	1.22
3	A	351	MTX	C13-C14	6.66	1.52	1.39
3	C	353	MTX	C13-C14	6.45	1.52	1.39
3	A	351	MTX	C9-N10	6.39	1.59	1.46
3	D	354	MTX	C4-N3	5.90	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	354	MTX	C13-C14	5.83	1.50	1.39
3	A	351	MTX	C6-N5	5.80	1.43	1.32
3	C	353	MTX	C16-C11	5.72	1.49	1.39
3	D	354	MTX	C16-C11	5.58	1.48	1.39
3	A	351	MTX	C16-C11	5.36	1.48	1.39
3	B	352	MTX	C16-C11	5.36	1.48	1.39
3	B	352	MTX	C13-C14	5.16	1.49	1.39
3	C	353	MTX	C4-N3	5.09	1.43	1.33
3	D	354	MTX	C6-N5	5.06	1.41	1.32
2	D	303	NDP	C4N-C3N	-5.05	1.40	1.49
2	B	301	NDP	P2B-O2B	-4.99	1.49	1.59
3	C	353	MTX	C16-C15	4.91	1.47	1.38
2	A	300	NDP	C4N-C3N	-4.87	1.40	1.49
3	B	352	MTX	C4-N3	4.79	1.42	1.33
3	B	352	MTX	C13-C12	4.78	1.47	1.38
3	A	351	MTX	C13-C12	4.75	1.47	1.38
3	D	354	MTX	C13-C12	4.72	1.47	1.38
2	D	303	NDP	C4N-C5N	-4.71	1.36	1.48
3	A	351	MTX	C4-N3	4.68	1.42	1.33
3	C	353	MTX	C13-C12	4.66	1.47	1.38
3	A	351	MTX	C16-C15	4.65	1.47	1.38
2	A	300	NDP	C4N-C5N	-4.62	1.36	1.48
2	B	301	NDP	C4N-C3N	-4.60	1.40	1.49
2	A	300	NDP	P2B-O2B	-4.59	1.50	1.59
3	B	352	MTX	C6-N5	4.58	1.40	1.32
3	C	353	MTX	C6-N5	4.53	1.40	1.32
3	B	352	MTX	C16-C15	4.52	1.47	1.38
2	C	302	NDP	C4N-C5N	-4.46	1.37	1.48
2	C	302	NDP	C4N-C3N	-4.46	1.41	1.49
3	D	354	MTX	C16-C15	4.46	1.46	1.38
2	B	301	NDP	C4N-C5N	-4.44	1.37	1.48
3	C	353	MTX	CA-N	4.40	1.55	1.45
3	B	352	MTX	CA-N	4.37	1.55	1.45
3	D	354	MTX	CA-N	4.28	1.54	1.45
2	D	303	NDP	P2B-O2B	-4.21	1.51	1.59
2	C	302	NDP	P2B-O2B	-4.14	1.51	1.59
3	C	353	MTX	C14-N10	4.10	1.50	1.39
3	B	352	MTX	C14-N10	4.05	1.50	1.39
3	C	353	MTX	C4A-C8A	3.99	1.47	1.40
3	B	352	MTX	CG-CD	3.97	1.59	1.50
3	A	351	MTX	CA-N	3.88	1.54	1.45
2	D	303	NDP	C2N-C3N	3.84	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	351	MTX	CG-CD	3.81	1.59	1.50
3	D	354	MTX	C14-N10	3.79	1.50	1.39
2	A	300	NDP	C2N-C3N	3.78	1.45	1.34
3	D	354	MTX	C4A-C8A	3.68	1.47	1.40
3	C	353	MTX	CG-CD	3.66	1.59	1.50
3	D	354	MTX	CG-CD	3.65	1.59	1.50
2	C	302	NDP	C2N-C3N	3.61	1.45	1.34
2	B	301	NDP	C2N-C3N	3.53	1.44	1.34
3	B	352	MTX	C15-C14	3.51	1.46	1.39
2	C	302	NDP	PA-O2A	-3.48	1.39	1.55
3	A	351	MTX	C14-N10	3.35	1.48	1.39
3	C	353	MTX	C-N	3.27	1.41	1.34
3	B	352	MTX	C-N	3.23	1.41	1.34
3	D	354	MTX	C15-C14	3.18	1.45	1.39
3	D	354	MTX	C-N	3.16	1.41	1.34
3	D	354	MTX	C2-N3	2.98	1.40	1.35
2	C	302	NDP	C6N-C5N	2.98	1.38	1.33
3	C	353	MTX	CM-N10	2.96	1.51	1.46
3	A	351	MTX	CM-N10	2.81	1.50	1.46
2	A	300	NDP	C6N-C5N	2.76	1.38	1.33
2	A	300	NDP	C3B-C4B	-2.66	1.46	1.53
3	A	351	MTX	C-N	2.66	1.40	1.34
3	D	354	MTX	CM-N10	2.65	1.50	1.46
2	B	301	NDP	C3B-C4B	-2.62	1.46	1.53
3	B	352	MTX	C4A-C8A	2.60	1.45	1.40
3	C	353	MTX	C2-N3	2.52	1.39	1.35
2	B	301	NDP	C6N-C5N	2.50	1.37	1.33
2	C	302	NDP	O4B-C1B	2.46	1.44	1.41
2	D	303	NDP	C6N-C5N	2.45	1.37	1.33
3	C	353	MTX	C15-C14	2.45	1.44	1.39
2	D	303	NDP	O4B-C1B	2.44	1.44	1.41
3	D	354	MTX	C2-NA2	2.42	1.38	1.33
3	C	353	MTX	CA-CT	2.42	1.58	1.52
3	A	351	MTX	C4A-C8A	2.39	1.44	1.40
3	B	352	MTX	O1-CT	2.35	1.29	1.22
2	C	302	NDP	C3B-C4B	-2.32	1.47	1.53
3	D	354	MTX	O1-CT	2.29	1.29	1.22
2	D	303	NDP	C3B-C4B	-2.29	1.47	1.53
3	B	352	MTX	C2-NA2	2.27	1.38	1.33
3	B	352	MTX	CA-CT	2.25	1.58	1.52
3	D	354	MTX	CA-CT	2.24	1.58	1.52
3	B	352	MTX	O-C	-2.23	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	351	MTX	O1-CT	2.19	1.28	1.22
3	D	354	MTX	C4A-N5	2.19	1.41	1.37
3	A	351	MTX	C15-C14	2.18	1.43	1.39
3	C	353	MTX	C9-C6	2.18	1.54	1.51
2	B	301	NDP	O4B-C1B	2.16	1.44	1.41
3	B	352	MTX	C9-C6	2.15	1.54	1.51
3	B	352	MTX	CM-N10	2.13	1.49	1.46
3	B	352	MTX	CB-CG	2.11	1.59	1.52
3	A	351	MTX	C9-C6	2.09	1.54	1.51
3	C	353	MTX	O1-CT	2.09	1.28	1.22
3	B	352	MTX	C2-N3	2.06	1.39	1.35
3	D	354	MTX	CB-CG	2.05	1.59	1.52
3	D	354	MTX	O-C	-2.03	1.19	1.23
3	C	353	MTX	O-C	-2.00	1.19	1.23

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	351	MTX	CM-N10-C14	30.31	171.91	119.57
3	C	353	MTX	CM-N10-C14	29.25	170.08	119.57
3	D	354	MTX	CM-N10-C14	28.02	167.97	119.57
3	B	352	MTX	CM-N10-C14	27.25	166.64	119.57
3	B	352	MTX	CM-N10-C9	-14.88	75.34	114.84
3	D	354	MTX	CM-N10-C9	-14.58	76.13	114.84
3	C	353	MTX	CM-N10-C9	-13.96	77.78	114.84
3	A	351	MTX	CM-N10-C9	-13.71	78.44	114.84
2	A	300	NDP	O2A-PA-O1A	12.63	174.67	112.24
3	C	353	MTX	C6-C9-N10	9.38	129.68	113.60
3	A	351	MTX	C6-C7-N8	-9.32	114.00	123.13
2	B	301	NDP	O2A-PA-O1A	8.98	156.66	112.24
3	B	352	MTX	C6-C7-N8	-8.94	114.37	123.13
3	D	354	MTX	C6-C7-N8	-8.78	114.53	123.13
3	B	352	MTX	C6-C9-N10	8.47	128.12	113.60
3	D	354	MTX	C6-C9-N10	8.02	127.34	113.60
3	B	352	MTX	C13-C14-N10	7.68	132.65	121.62
3	C	353	MTX	C6-C7-N8	-7.20	116.08	123.13
3	A	351	MTX	C6-C9-N10	7.15	125.86	113.60
3	A	351	MTX	N1-C2-N3	-6.93	117.98	127.22
3	B	352	MTX	N1-C2-N3	-6.92	117.99	127.22
3	D	354	MTX	N1-C2-N3	-6.88	118.05	127.22
2	C	302	NDP	O3X-P2B-O1X	-6.86	83.82	110.68
2	A	300	NDP	O3X-P2B-O1X	-6.78	84.12	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NDP	O3X-P2B-O1X	-6.66	84.62	110.68
3	D	354	MTX	C13-C14-N10	6.62	131.12	121.62
3	C	353	MTX	N1-C2-N3	-6.54	118.50	127.22
2	D	303	NDP	O3X-P2B-O1X	-6.34	85.85	110.68
2	D	303	NDP	O3X-P2B-O2X	-6.27	83.68	107.64
3	A	351	MTX	C2-N1-C8A	6.26	122.51	115.36
3	C	353	MTX	C9-C6-N5	6.25	126.98	116.96
3	A	351	MTX	C7-N8-C8A	6.18	122.90	116.69
3	B	352	MTX	C15-C14-N10	-6.10	112.85	121.62
2	C	302	NDP	O3X-P2B-O2X	-6.09	84.36	107.64
3	D	354	MTX	C9-C6-N5	6.03	126.63	116.96
3	B	352	MTX	C9-C6-N5	6.03	126.63	116.96
2	B	301	NDP	O3X-P2B-O2X	-5.98	84.79	107.64
2	A	300	NDP	O2A-PA-O5B	-5.95	80.10	107.75
3	D	354	MTX	C2-N1-C8A	5.88	122.08	115.36
3	A	351	MTX	C9-C6-N5	5.80	126.25	116.96
2	A	300	NDP	O3X-P2B-O2X	-5.68	85.92	107.64
3	D	354	MTX	C7-N8-C8A	5.68	122.40	116.69
3	B	352	MTX	C7-N8-C8A	5.63	122.35	116.69
3	B	352	MTX	C2-N1-C8A	5.53	121.67	115.36
3	D	354	MTX	C15-C14-N10	-5.17	114.19	121.62
2	D	303	NDP	O3X-P2B-O2B	-5.16	82.86	105.99
3	C	353	MTX	C2-N1-C8A	5.09	121.17	115.36
3	A	351	MTX	C4-C4A-N5	5.00	124.18	120.33
2	B	301	NDP	O3X-P2B-O2B	-4.98	83.66	105.99
3	A	351	MTX	C13-C14-N10	4.96	128.74	121.62
3	C	353	MTX	C7-N8-C8A	4.87	121.58	116.69
2	A	300	NDP	O3X-P2B-O2B	-4.86	84.21	105.99
2	D	303	NDP	C3N-C2N-N1N	-4.86	116.17	123.10
3	C	353	MTX	C9-C6-C7	-4.79	113.23	121.60
2	C	302	NDP	O3X-P2B-O2B	-4.78	84.59	105.99
3	C	353	MTX	C13-C14-N10	4.76	128.46	121.62
3	A	351	MTX	C9-C6-C7	-4.53	113.69	121.60
2	A	300	NDP	C3N-C2N-N1N	-4.53	116.64	123.10
3	D	354	MTX	C9-C6-C7	-4.51	113.73	121.60
3	A	351	MTX	CA-N-C	4.40	132.38	121.60
2	B	301	NDP	C3N-C2N-N1N	-4.37	116.86	123.10
3	B	352	MTX	C9-C6-C7	-4.29	114.12	121.60
3	D	354	MTX	CA-N-C	4.28	132.08	121.60
3	C	353	MTX	CA-N-C	4.28	132.07	121.60
2	C	302	NDP	C3N-C2N-N1N	-4.26	117.02	123.10
3	D	354	MTX	C4-C4A-N5	4.26	123.61	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	352	MTX	CA-N-C	4.18	131.82	121.60
3	C	353	MTX	C11-C-N	4.03	124.78	117.06
2	B	301	NDP	O4B-C4B-C3B	4.02	113.07	105.11
3	B	352	MTX	CB-CG-CD	3.96	123.02	112.51
2	A	300	NDP	O4B-C4B-C3B	3.95	112.94	105.11
3	A	351	MTX	CB-CG-CD	3.89	122.83	112.51
3	B	352	MTX	C11-C-N	3.81	124.37	117.06
3	A	351	MTX	C11-C-N	3.81	124.36	117.06
3	D	354	MTX	CB-CG-CD	3.73	122.41	112.51
3	C	353	MTX	CB-CG-CD	3.71	122.36	112.51
3	D	354	MTX	C11-C-N	3.70	124.17	117.06
2	B	301	NDP	O2B-C2B-C3B	3.67	124.97	111.68
3	A	351	MTX	C15-C14-N10	-3.52	116.55	121.62
2	C	302	NDP	C5B-C4B-C3B	3.50	128.29	115.18
2	A	300	NDP	O2X-P2B-O1X	3.40	123.98	110.68
2	D	303	NDP	C5B-C4B-C3B	3.29	127.51	115.18
2	C	302	NDP	O2X-P2B-O1X	3.29	123.54	110.68
2	B	301	NDP	O2X-P2B-O1X	3.28	123.54	110.68
2	C	302	NDP	O4B-C4B-C3B	3.25	111.54	105.11
2	D	303	NDP	O2B-C2B-C3B	3.25	123.45	111.68
2	B	301	NDP	C5B-C4B-C3B	3.24	127.34	115.18
2	A	300	NDP	O2B-C2B-C3B	3.23	123.40	111.68
3	C	353	MTX	C15-C14-N10	-3.22	117.00	121.62
2	D	303	NDP	O2X-P2B-O1X	3.21	123.23	110.68
2	A	300	NDP	C5B-C4B-C3B	3.20	127.17	115.18
3	C	353	MTX	C4-C4A-N5	3.19	122.78	120.33
3	A	351	MTX	C16-C15-C14	3.18	124.50	120.32
2	D	303	NDP	O4B-C4B-C3B	3.12	111.28	105.11
3	C	353	MTX	C16-C15-C14	3.03	124.31	120.32
2	C	302	NDP	O2B-C2B-C3B	3.02	122.63	111.68
2	D	303	NDP	O4B-C4B-C5B	2.96	119.12	109.37
3	B	352	MTX	C4-C4A-N5	2.95	122.60	120.33
2	D	303	NDP	O2A-PA-O5B	2.88	121.12	107.75
2	B	301	NDP	O7N-C7N-N7N	-2.87	116.16	122.88
3	D	354	MTX	C4A-C4-N3	-2.87	119.13	121.01
3	C	353	MTX	CG-CB-CA	2.86	118.50	113.16
2	C	302	NDP	O7N-C7N-N7N	-2.80	116.33	122.88
2	A	300	NDP	O7N-C7N-N7N	-2.79	116.34	122.88
3	D	354	MTX	CG-CB-CA	2.78	118.36	113.16
3	B	352	MTX	CG-CB-CA	2.65	118.10	113.16
2	B	301	NDP	O2X-P2B-O2B	2.62	117.72	105.99
2	D	303	NDP	O7N-C7N-N7N	-2.60	116.79	122.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NDP	O2A-PA-O5B	-2.59	95.73	107.75
2	A	300	NDP	O2X-P2B-O2B	2.58	117.55	105.99
2	D	303	NDP	O2X-P2B-O2B	2.57	117.50	105.99
2	A	300	NDP	O4B-C4B-C5B	2.56	117.80	109.37
2	B	301	NDP	O4B-C4B-C5B	2.54	117.73	109.37
3	C	353	MTX	O-C-C11	-2.49	116.50	120.94
3	B	352	MTX	C7-C6-N5	-2.48	119.23	120.85
3	A	351	MTX	CG-CB-CA	2.48	117.78	113.16
2	B	301	NDP	O4B-C1B-C2B	2.46	110.85	106.59
3	B	352	MTX	C6-N5-C4A	2.44	121.98	118.04
2	C	302	NDP	O2X-P2B-O2B	2.42	116.82	105.99
3	D	354	MTX	C16-C15-C14	2.42	123.50	120.32
2	C	302	NDP	C1D-N1N-C2N	-2.40	117.11	121.11
3	D	354	MTX	NA2-C2-N1	2.38	121.67	117.79
2	B	301	NDP	C1D-N1N-C2N	-2.37	117.16	121.11
2	C	302	NDP	O4B-C4B-C5B	2.36	117.13	109.37
3	B	352	MTX	C16-C15-C14	2.32	123.38	120.32
3	B	352	MTX	C15-C14-C13	-2.30	114.48	119.16
3	B	352	MTX	O-C-N	-2.30	118.22	122.45
3	B	352	MTX	NA2-C2-N1	2.29	121.52	117.79
3	C	353	MTX	C15-C14-C13	-2.27	114.54	119.16
3	D	354	MTX	O-C-N	-2.26	118.28	122.45
2	A	300	NDP	O4B-C1B-C2B	2.26	110.51	106.59
3	A	351	MTX	NA2-C2-N1	2.25	121.47	117.79
2	A	300	NDP	O5D-PN-O1N	2.25	117.87	109.07
3	A	351	MTX	C15-C14-C13	-2.24	114.61	119.16
2	C	302	NDP	O2A-PA-O1A	2.24	123.30	112.24
3	D	354	MTX	C15-C14-C13	-2.20	114.68	119.16
3	B	352	MTX	CB-CA-CT	2.20	115.66	110.35
3	A	351	MTX	C15-C16-C11	-2.19	118.23	120.78
2	A	300	NDP	O3B-C3B-C4B	-2.19	104.72	111.05
3	A	351	MTX	C2-N3-C4	2.18	122.94	116.72
3	A	351	MTX	O-C-N	-2.17	118.45	122.45
3	B	352	MTX	N8-C8A-N1	2.17	118.30	115.82
3	B	352	MTX	C2-N3-C4	2.16	122.89	116.72
3	C	353	MTX	C2-N3-C4	2.15	122.86	116.72
3	D	354	MTX	C2-N3-C4	2.15	122.85	116.72
3	A	351	MTX	O-C-C11	-2.12	117.15	120.94
3	C	353	MTX	C15-C16-C11	-2.09	118.35	120.78
3	A	351	MTX	NA2-C2-N3	2.09	120.50	117.25
2	B	301	NDP	O3B-C3B-C4B	-2.08	105.03	111.05
2	D	303	NDP	O4D-C1D-C2D	-2.08	102.11	106.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	NDP	C1D-N1N-C2N	-2.06	117.67	121.11
3	D	354	MTX	CB-CA-CT	2.04	115.27	110.35
3	C	353	MTX	O-C-N	-2.04	118.70	122.45
3	D	354	MTX	C6-N5-C4A	2.04	121.33	118.04
3	C	353	MTX	NA2-C2-N1	2.03	121.09	117.79
3	A	351	MTX	C4A-C4-N3	-2.01	119.69	121.01
3	B	352	MTX	C4A-C4-N3	-2.00	119.69	121.01

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	300	NDP	C4B
2	B	301	NDP	C4B
2	D	303	NDP	C4B

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	NDP	C5B-O5B-PA-O2A
2	A	300	NDP	O4D-C1D-N1N-C6N
2	B	301	NDP	C3B-C2B-O2B-P2B
2	B	301	NDP	O4D-C1D-N1N-C6N
2	C	302	NDP	O4D-C1D-N1N-C6N
2	A	300	NDP	C3B-C4B-C5B-O5B
2	C	302	NDP	C3B-C4B-C5B-O5B
2	D	303	NDP	C3B-C4B-C5B-O5B
2	A	300	NDP	C3B-C2B-O2B-P2B
2	C	302	NDP	C3B-C2B-O2B-P2B
2	D	303	NDP	C3B-C2B-O2B-P2B
2	D	303	NDP	O4D-C1D-N1N-C6N
3	B	352	MTX	CB-CA-N-C
2	B	301	NDP	C3B-C4B-C5B-O5B
3	D	354	MTX	CB-CA-N-C
3	C	353	MTX	CB-CA-N-C
2	C	302	NDP	C1B-C2B-O2B-P2B
3	A	351	MTX	CT-CA-N-C
2	A	300	NDP	C1B-C2B-O2B-P2B
2	B	301	NDP	C1B-C2B-O2B-P2B
2	D	303	NDP	C1B-C2B-O2B-P2B
3	A	351	MTX	CB-CA-N-C
3	B	352	MTX	N-CA-CT-O2
3	D	354	MTX	N-CA-CT-O2

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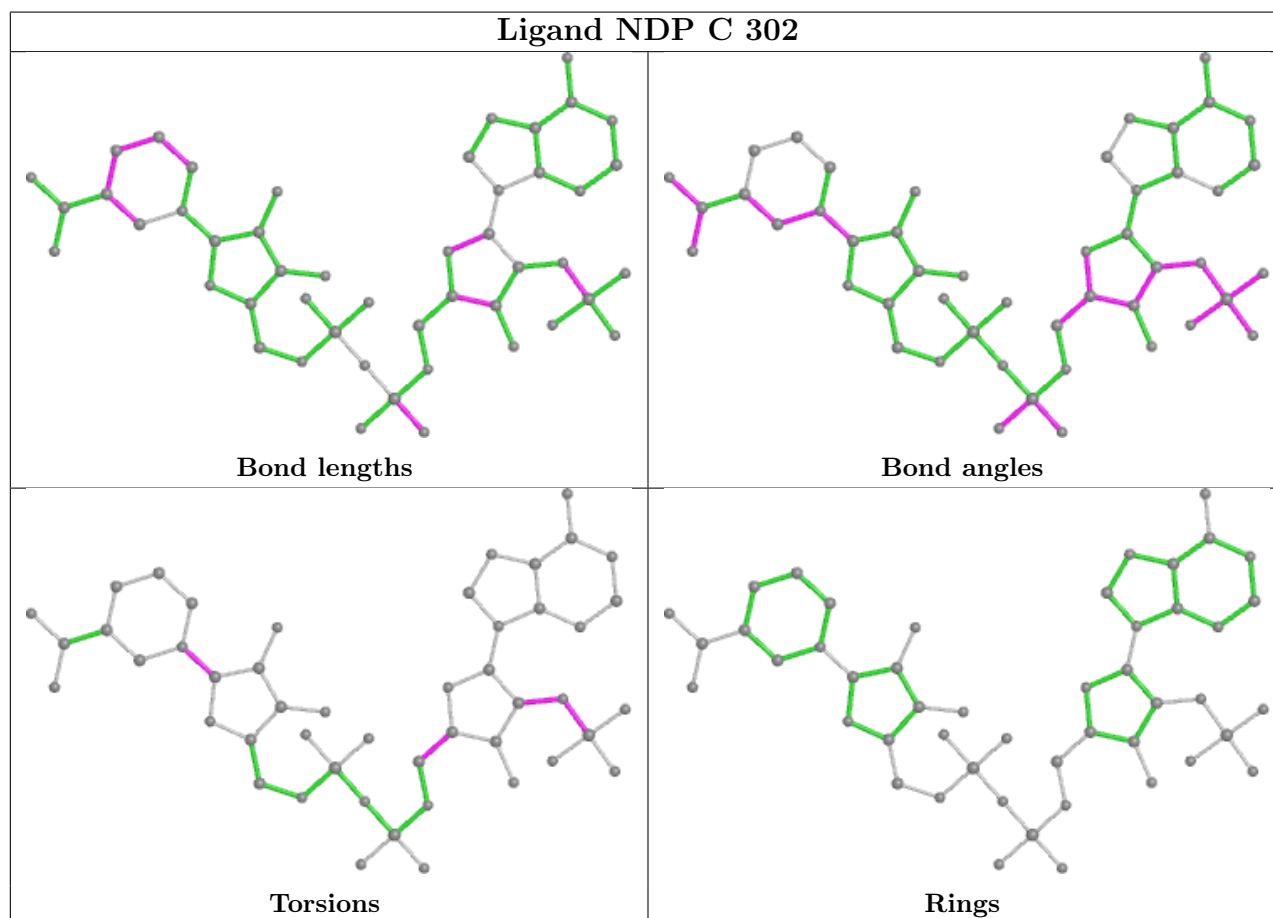
Mol	Chain	Res	Type	Atoms
3	C	353	MTX	CT-CA-N-C
3	D	354	MTX	CT-CA-N-C
2	A	300	NDP	O4B-C4B-C5B-O5B
2	B	301	NDP	O4B-C4B-C5B-O5B
3	B	352	MTX	CT-CA-N-C
3	A	351	MTX	N-CA-CT-O2
3	C	353	MTX	N-CA-CT-O2
3	A	351	MTX	N-CA-CT-O1
3	B	352	MTX	N-CA-CT-O1
3	C	353	MTX	N-CA-CT-O1
3	D	354	MTX	N-CA-CT-O1
3	C	353	MTX	CB-CA-CT-O2
2	C	302	NDP	O4B-C4B-C5B-O5B
2	D	303	NDP	O4B-C4B-C5B-O5B
2	A	300	NDP	C2B-O2B-P2B-O1X
2	B	301	NDP	C2B-O2B-P2B-O1X
3	A	351	MTX	CB-CA-CT-O2
3	B	352	MTX	CB-CA-CT-O2
3	D	354	MTX	CB-CA-CT-O2
3	C	353	MTX	CB-CA-CT-O1
3	A	351	MTX	CB-CA-CT-O1
3	B	352	MTX	CB-CA-CT-O1
3	D	354	MTX	CB-CA-CT-O1
3	A	351	MTX	C6-C9-N10-C14
3	B	352	MTX	C6-C9-N10-C14
3	D	354	MTX	C6-C9-N10-C14
2	C	302	NDP	C2B-O2B-P2B-O3X
2	D	303	NDP	C2N-C3N-C7N-N7N
3	D	354	MTX	OE1-CD-CG-CB

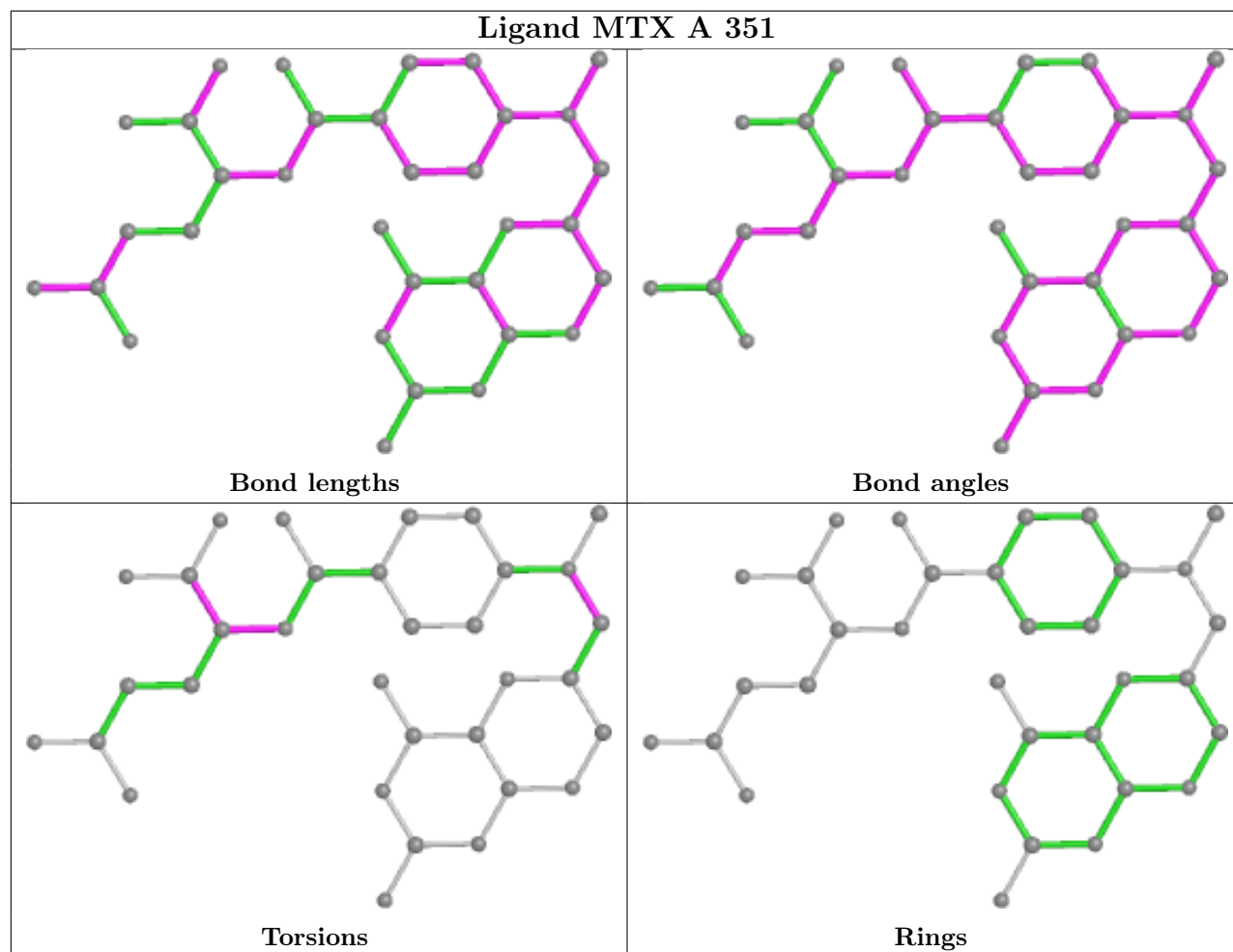
There are no ring outliers.

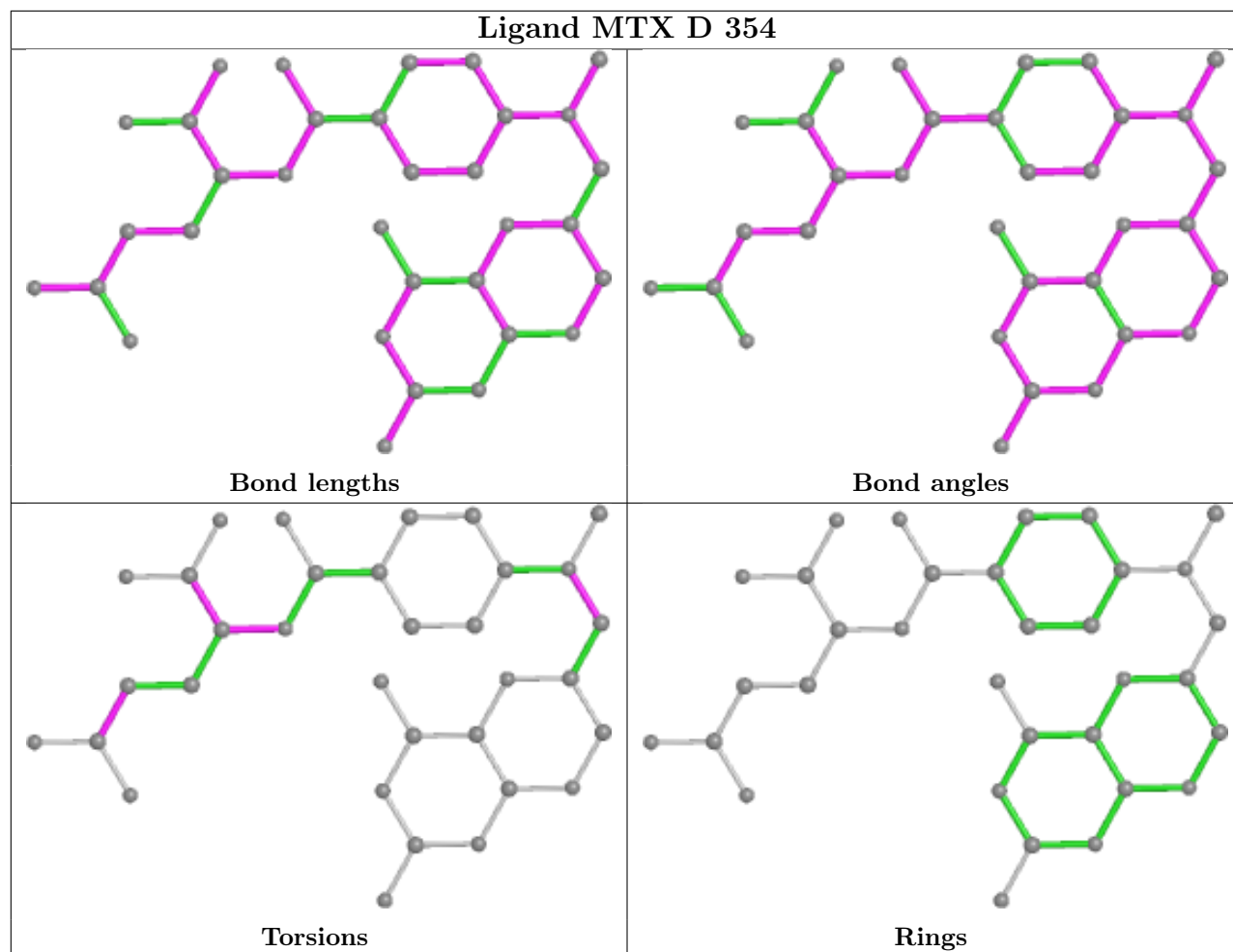
8 monomers are involved in 49 short contacts:

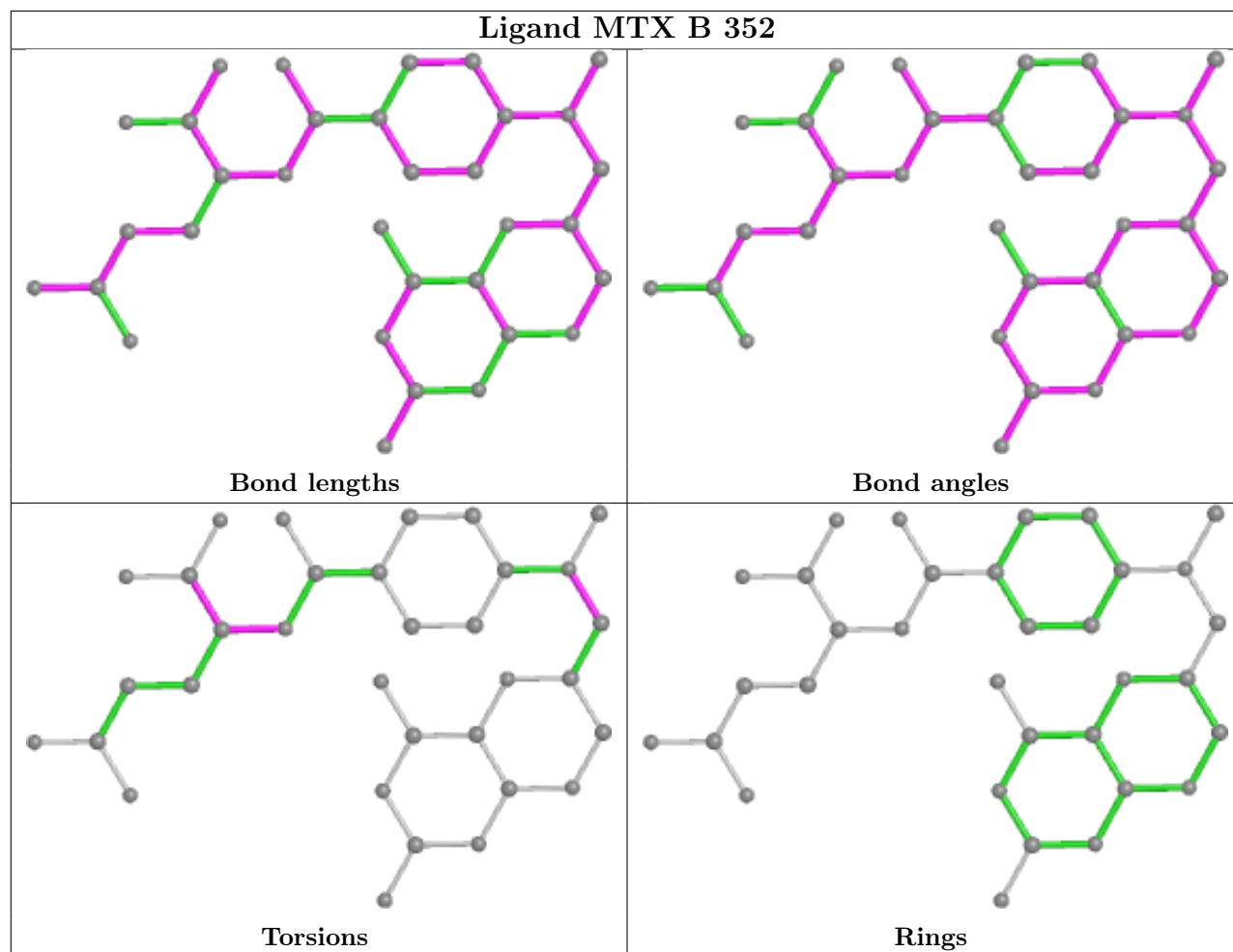
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	302	NDP	8	0
3	A	351	MTX	6	0
3	D	354	MTX	6	0
3	B	352	MTX	11	0
3	C	353	MTX	11	0
2	D	303	NDP	3	0
2	A	300	NDP	2	0
2	B	301	NDP	3	0

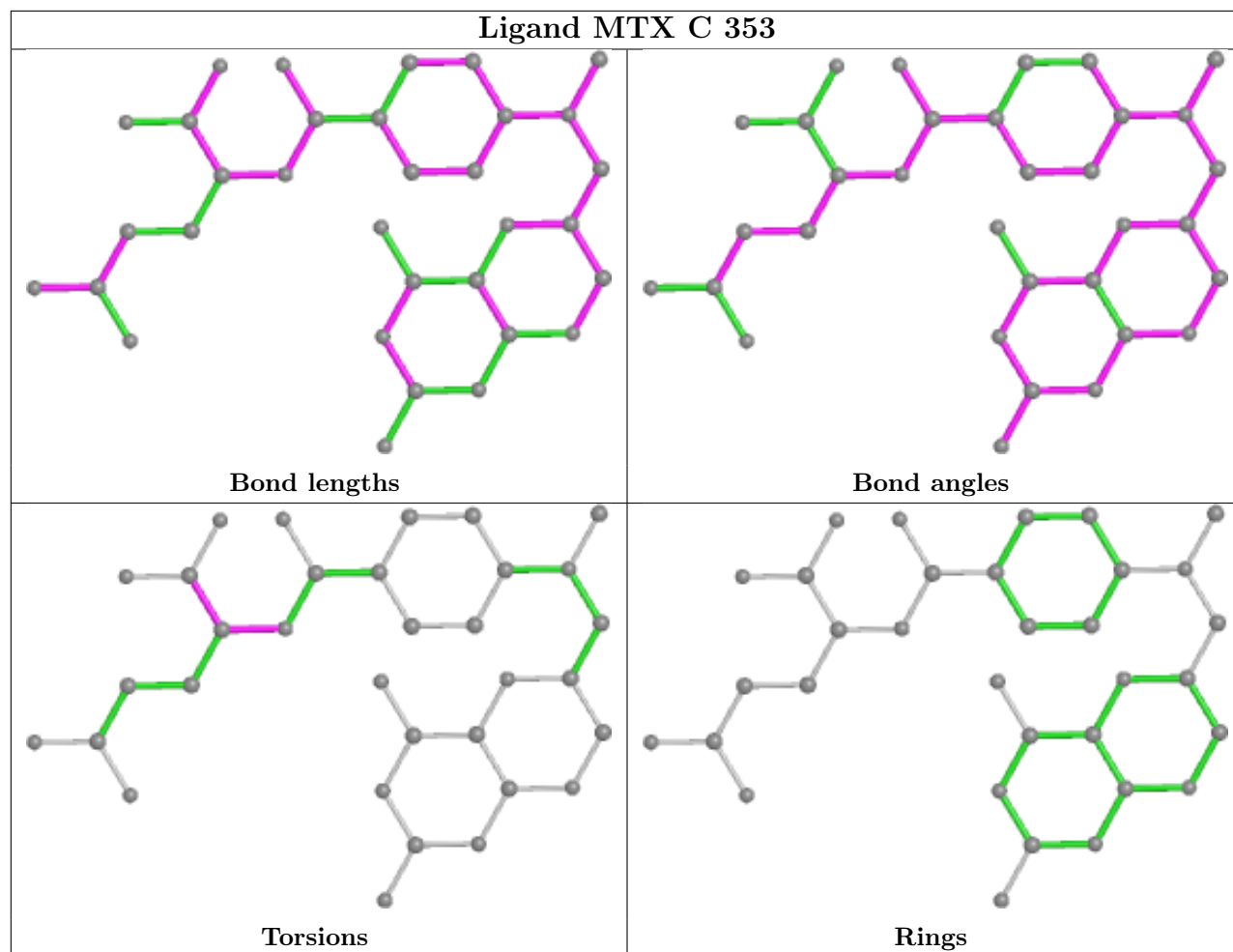
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

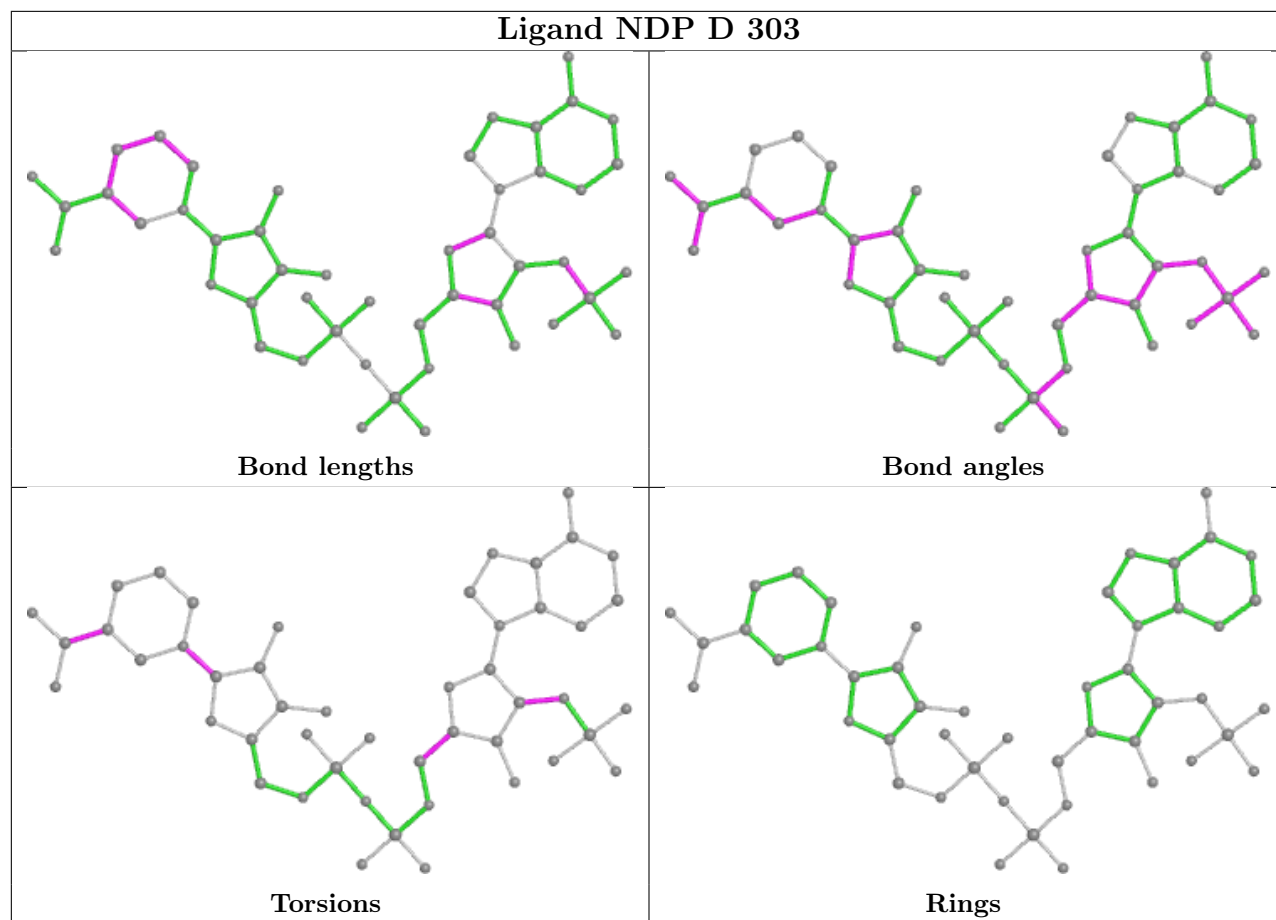


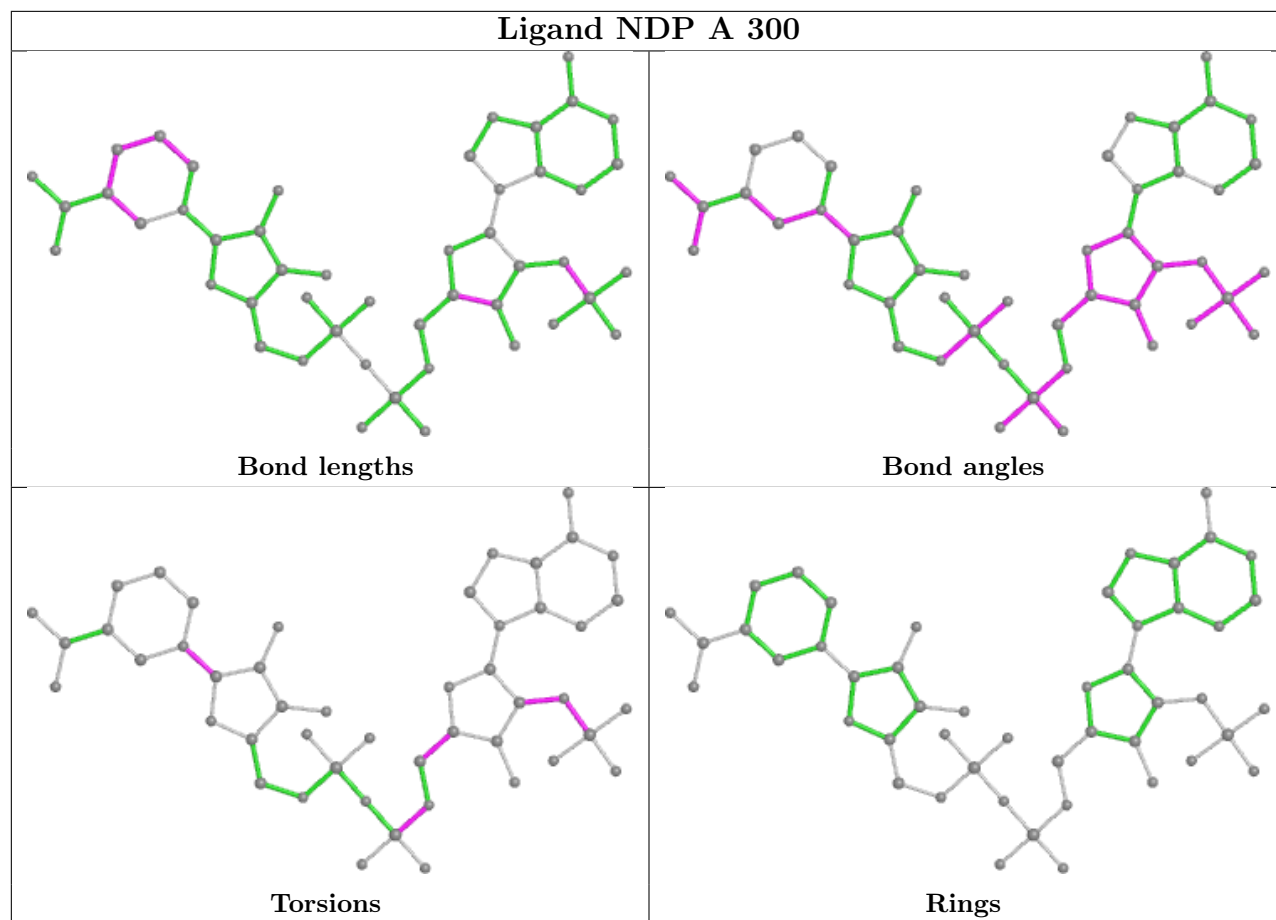




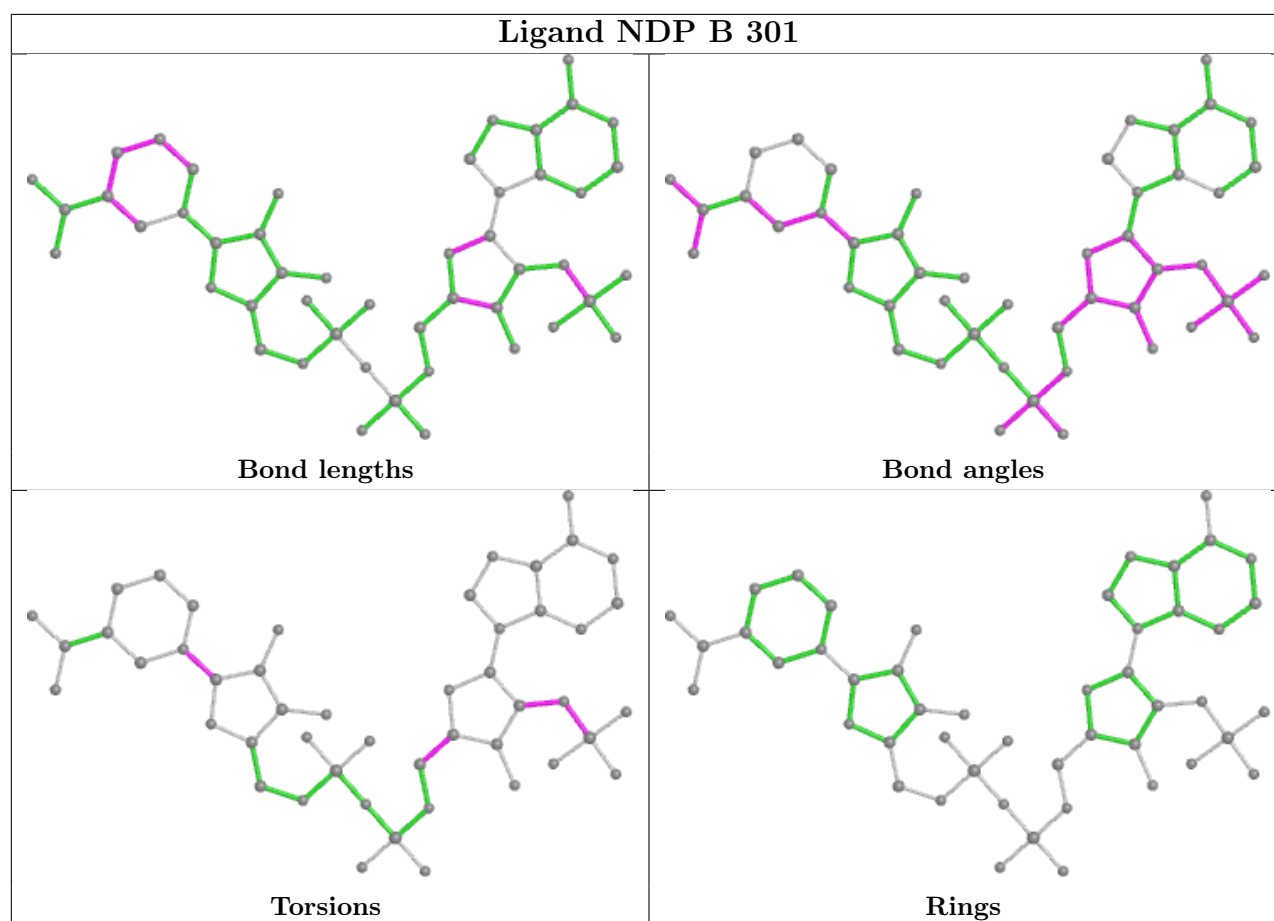












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	72:ALA	C	73:SER	N	1.14

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	267/289 (92%)	-0.04	2 (0%) 87 87	25, 39, 68, 93	0
1	B	269/289 (93%)	-0.17	2 (0%) 87 87	21, 37, 66, 94	0
1	C	268/289 (92%)	0.21	7 (2%) 56 52	19, 40, 76, 95	0
1	D	268/289 (92%)	0.40	22 (8%) 11 8	28, 52, 85, 99	0
All	All	1072/1156 (92%)	0.10	33 (3%) 49 44	19, 41, 79, 99	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	8	VAL	4.2
1	B	3	SER	4.1
1	D	72	ALA	4.0
1	D	32	THR	3.9
1	D	73	SER	3.9
1	C	228	VAL	3.7
1	D	33	VAL	3.5
1	D	59	ALA	3.5
1	C	235	PHE	3.3
1	D	60	ILE	3.3
1	D	100	TRP	3.2
1	D	132	ASP	3.1
1	C	230	PRO	3.0
1	D	9	ALA	2.8
1	B	73	SER	2.8
1	A	80	SER	2.8
1	D	103	CYS	2.8
1	D	93	VAL	2.7
1	D	71	THR	2.7
1	D	102	ARG	2.7
1	D	56	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	232	ASP	2.4
1	C	231	ASP	2.3
1	D	5	THR	2.3
1	D	58	SER	2.3
1	C	4	PRO	2.3
1	C	234	PRO	2.2
1	D	137	GLU	2.2
1	D	10	LEU	2.1
1	A	83	VAL	2.1
1	D	41	ALA	2.1
1	D	158	PHE	2.1
1	D	62	VAL	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.

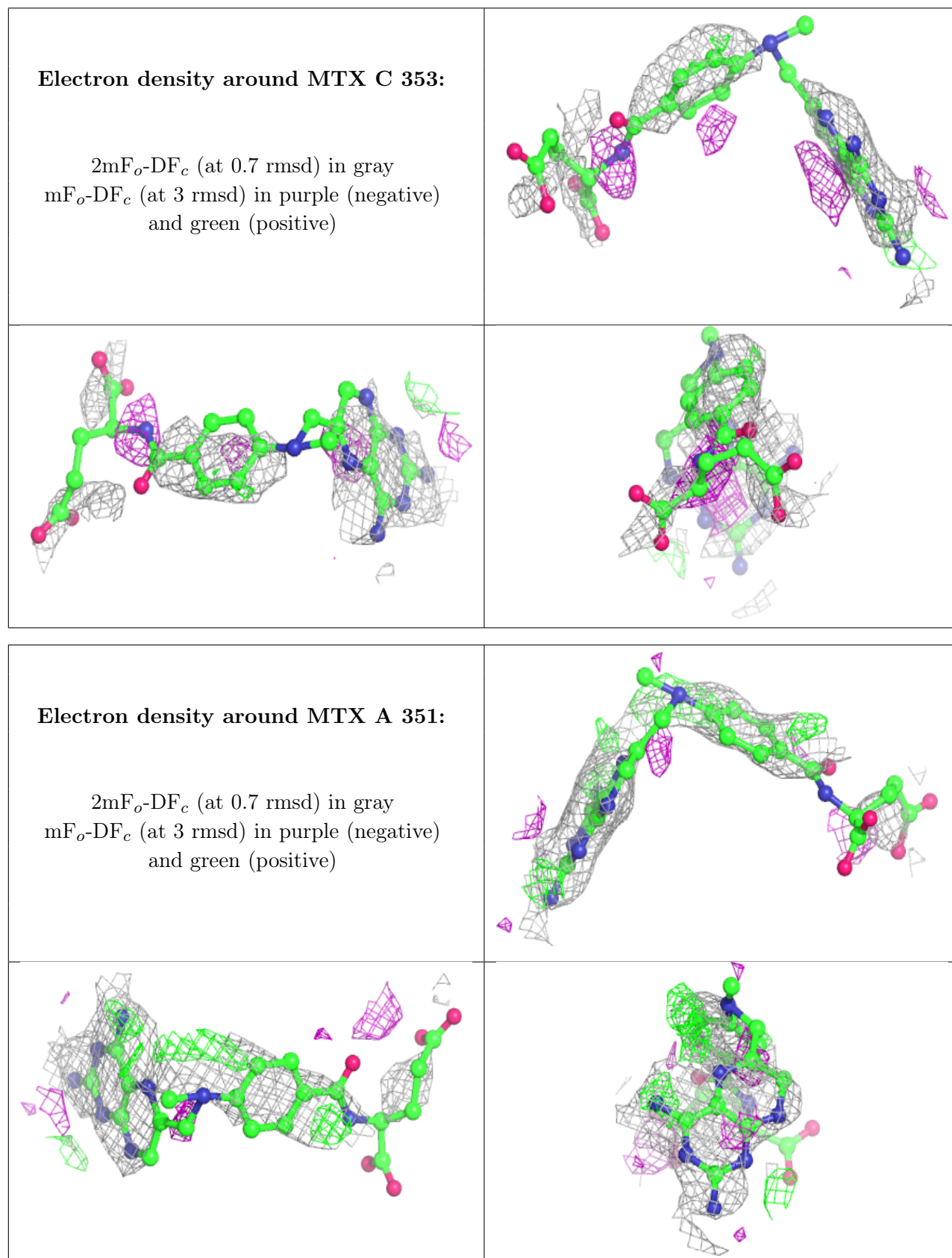
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	MTX	C	353	33/33	0.61	0.73	103,114,119,119	0
3	MTX	A	351	33/33	0.67	0.60	93,113,124,124	0
3	MTX	D	354	33/33	0.67	0.55	127,135,140,140	0
3	MTX	B	352	33/33	0.68	0.72	135,141,144,145	0
2	NDP	D	303	48/48	0.91	0.22	36,56,63,66	0
2	NDP	C	302	48/48	0.93	0.25	41,49,58,63	0
2	NDP	A	300	48/48	0.93	0.23	32,35,49,53	0
2	NDP	B	301	48/48	0.93	0.21	29,40,46,51	0

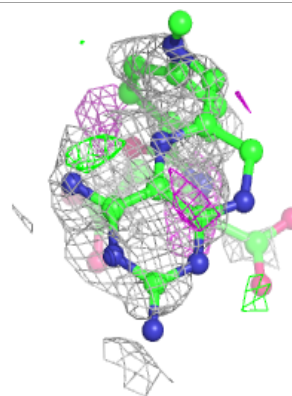
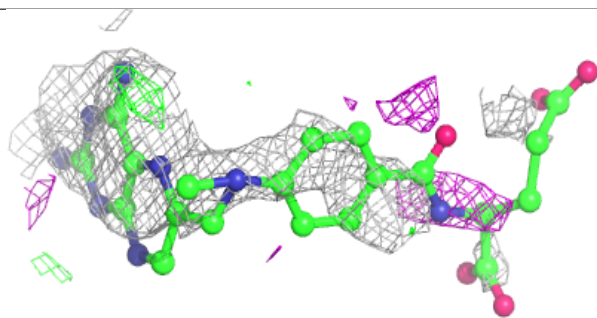
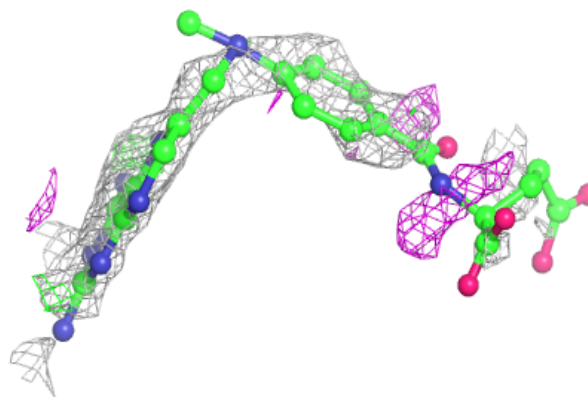
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

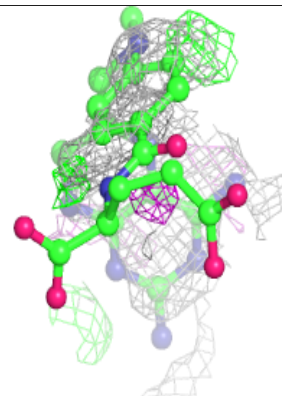
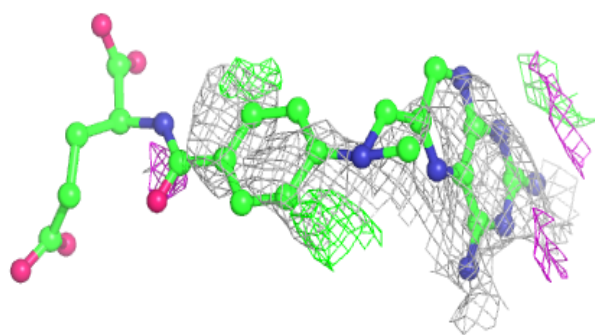
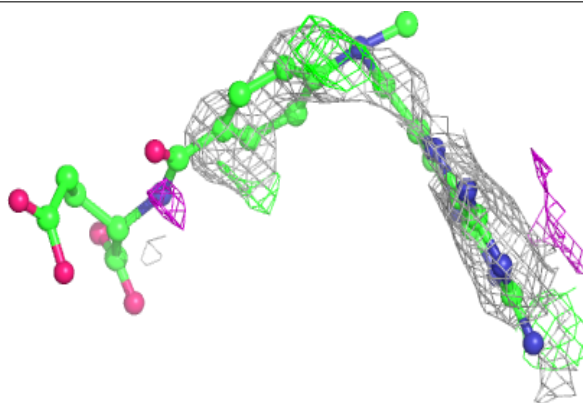


**Electron density around MTX D 354:**

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

**Electron density around MTX B 352:**

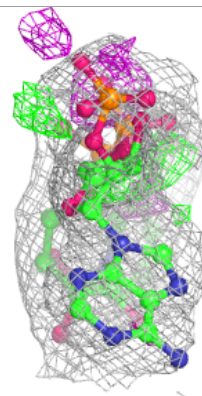
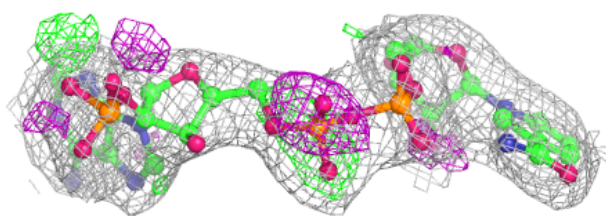
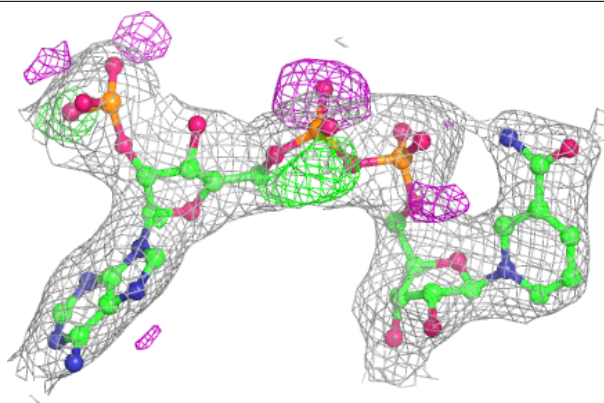
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



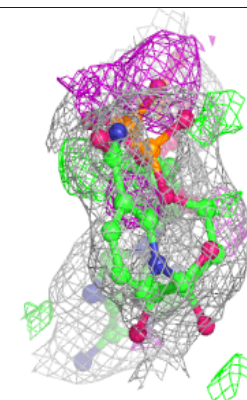
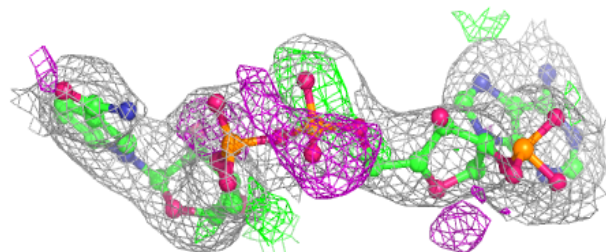
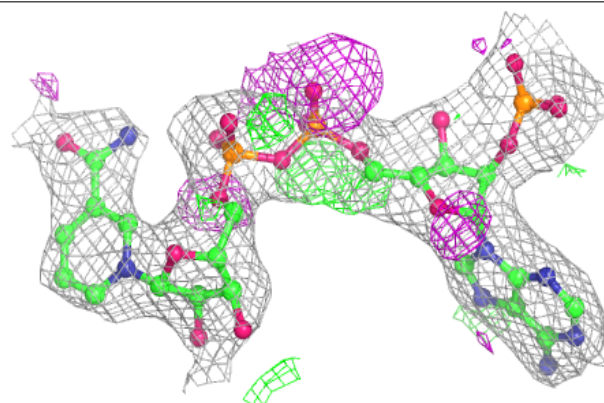


**Electron density around NDP D 303:**

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

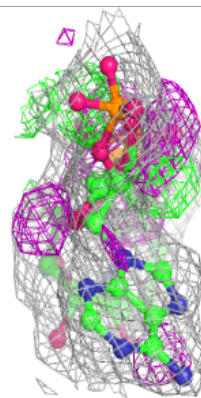
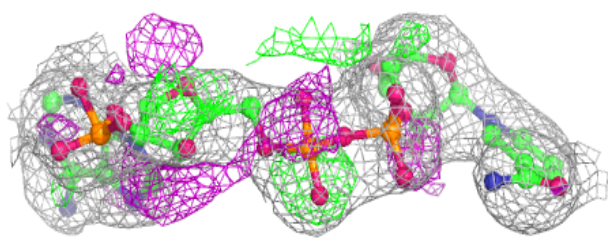
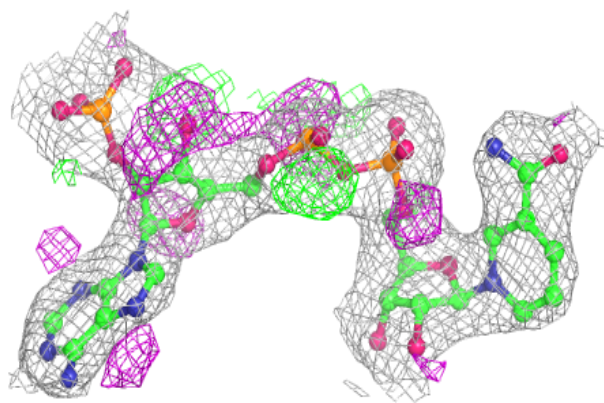
**Electron density around NDP C 302:**

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

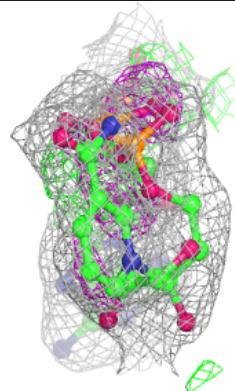
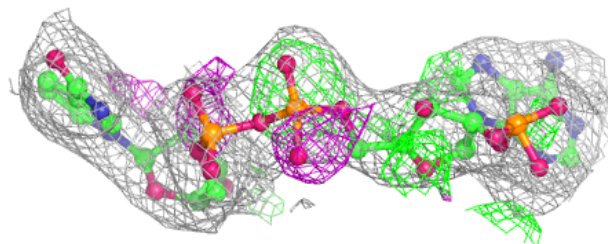
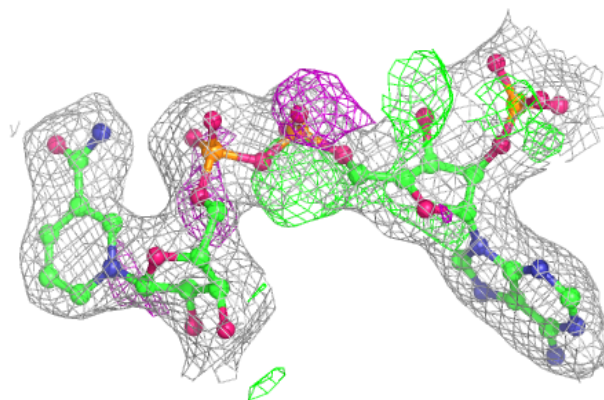


**Electron density around NDP A 300:**

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

**Electron density around NDP 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.