



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 08:53 am BST

PDB ID : 6OIW  
Title : Structure of Escherichia coli dGTPase bound to dGTP-1-thiol  
Authors : Barnes, C.O.; Wu, Y.; Calero, G.  
Deposited on : 2019-04-09  
Resolution : 3.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

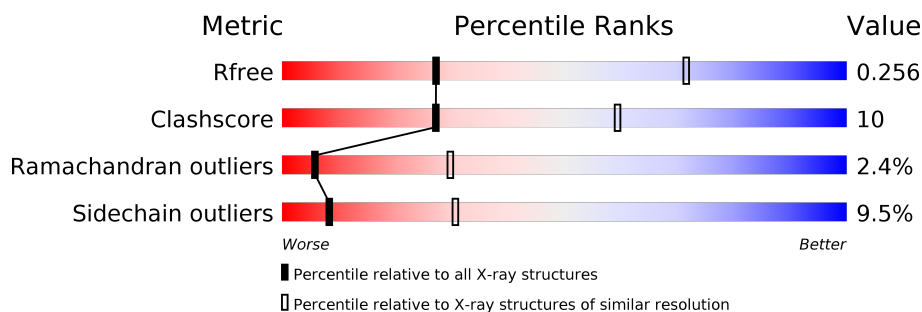
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	505	
1	B	505	
1	C	505	
1	D	505	
1	E	505	
1	F	505	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25272 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 Deoxyguanosinetriphosphate triphosphohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			4179	2663	747	753	16			
1	B	503	Total	C	N	O	S	0	0	0
			4174	2661	746	751	16			
1	C	503	Total	C	N	O	S	0	0	0
			4174	2661	746	751	16			
1	D	504	Total	C	N	O	S	0	0	0
			4179	2663	747	753	16			
1	E	503	Total	C	N	O	S	0	0	0
			4174	2661	746	751	16			
1	F	503	Total	C	N	O	S	0	0	0
			4174	2661	746	751	16			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

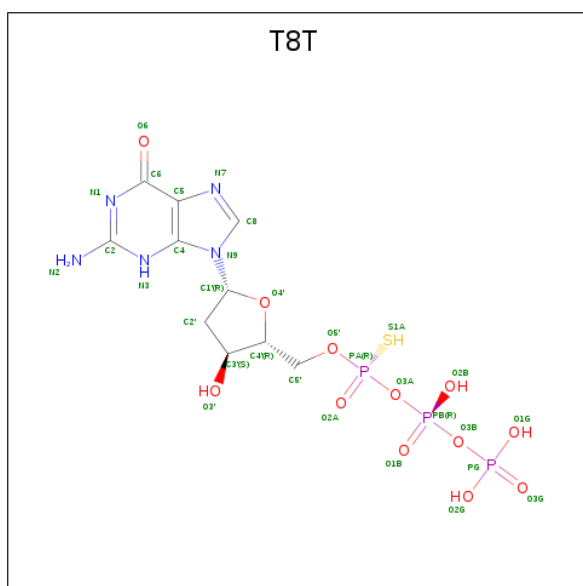
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	F	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 2'-deoxyguanosine-5'-O-(1-thiotriphosphate) (three-letter code: T8T) (formula:  $C_{10}H_{16}N_5O_{12}P_3S$ ).

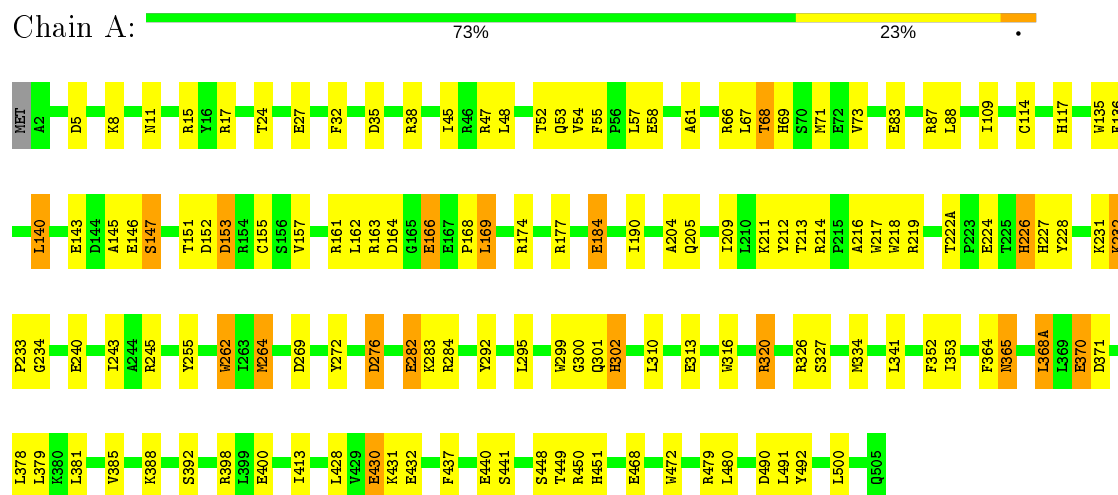


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total 5	O 5	0	0
5	B	4	Total 4	O 4	0	0
5	C	2	Total 2	O 2	0	0
5	D	5	Total 5	O 5	0	0
5	E	4	Total 4	O 4	0	0
5	F	3	Total 3	O 3	0	0

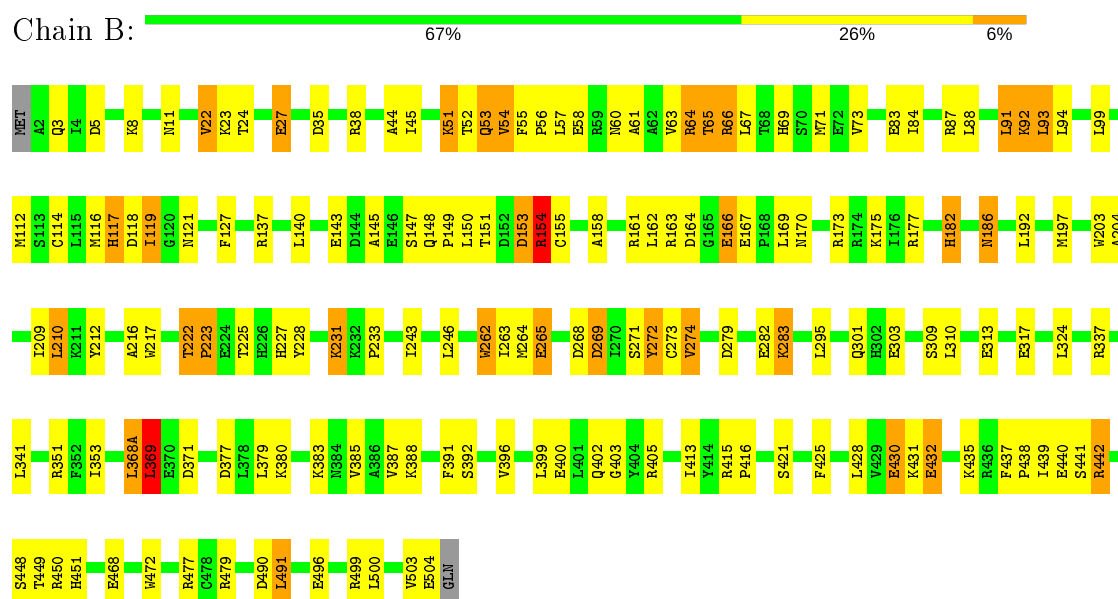
### 3 Residue-property plots

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

- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

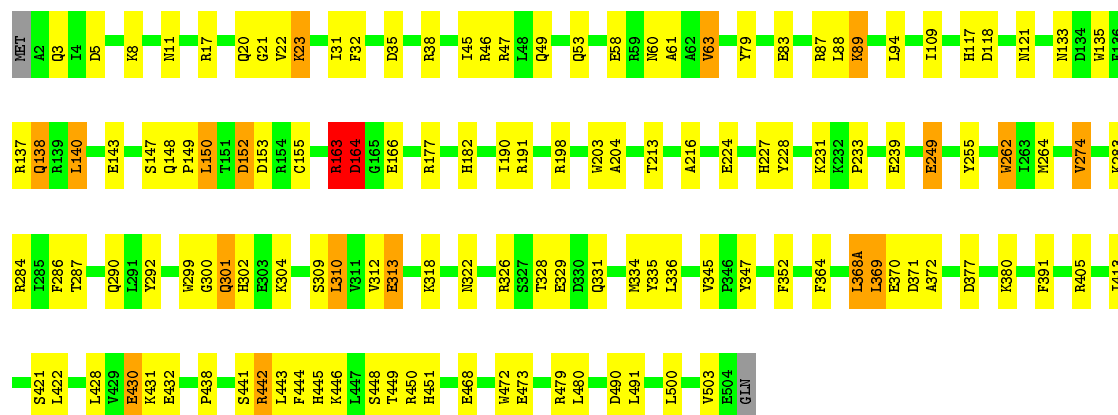


- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase



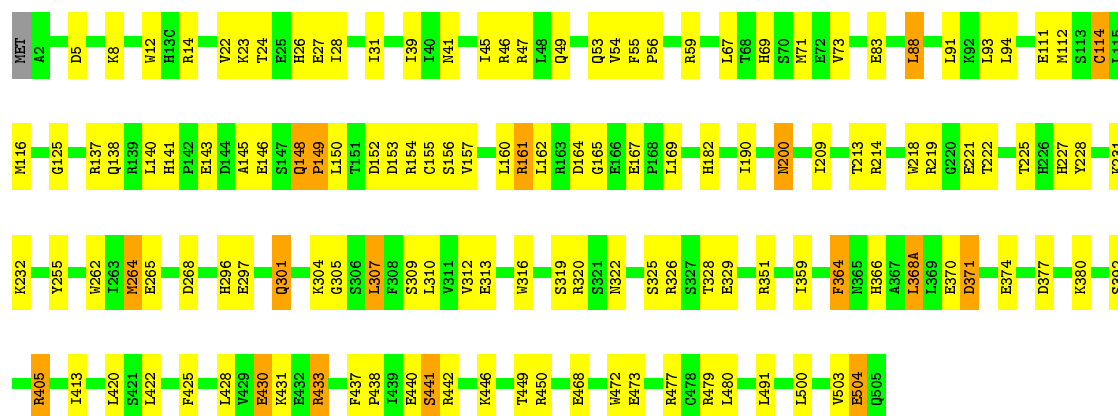
- Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase





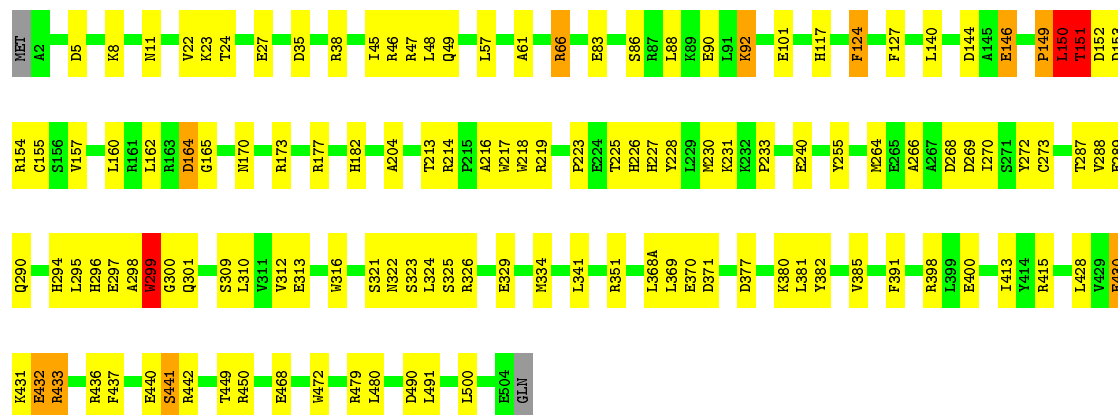
• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

Chain D: 73% 23% .



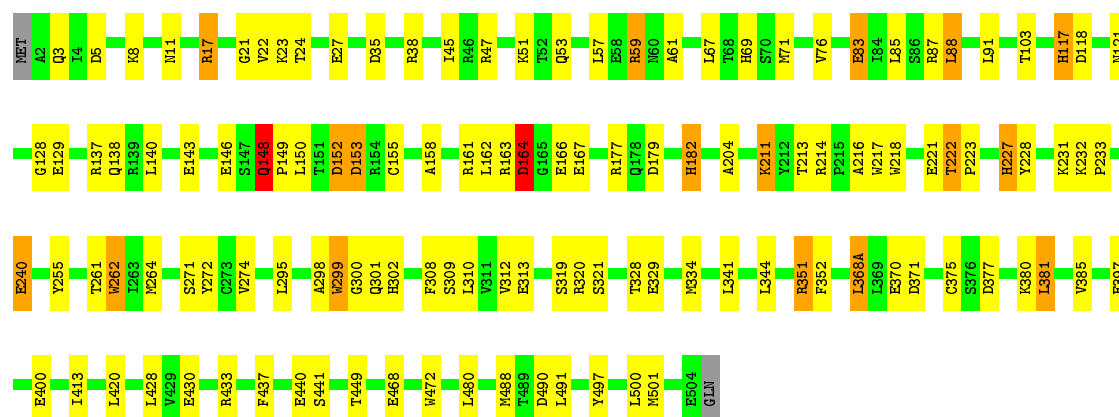
• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

Chain E: 74% 23% .



• Molecule 1: Deoxyguanosinetriphosphate triphosphohydrolase

Chain F: 74% 21% .





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	191.24Å 191.24Å 298.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.48 – 3.35 48.48 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.48-3.35) 99.8 (48.48-3.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.29	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.178 , 0.212 0.233 , 0.256	Depositor DCC
$R_{free}$ test set	2451 reflections (3.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	112.4	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 121.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	25272	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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: MG, T8T, MN

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	0.71	2/4282 (0.0%)	0.80	1/5792 (0.0%)
1	B	0.58	0/4277	0.82	8/5784 (0.1%)
1	C	0.58	0/4277	0.77	3/5784 (0.1%)
1	D	0.51	0/4282	0.73	2/5792 (0.0%)
1	E	0.57	0/4277	0.75	3/5784 (0.1%)
1	F	0.61	0/4277	0.78	1/5784 (0.0%)
All	All	0.60	2/25672 (0.0%)	0.77	18/34720 (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
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	THR	C-O	-7.03	1.09	1.23
1	A	184	GLU	CD-OE1	-5.59	1.19	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	ARG	N-CA-CB	-11.85	89.28	110.60
1	B	153	ASP	C-N-CA	-7.48	103.01	121.70
1	B	265	GLU	CB-CA-C	-7.27	95.86	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	ILE	C-N-CA	6.47	137.88	121.70
1	B	92	LYS	C-N-CA	6.36	137.59	121.70
1	E	150	LEU	C-N-CA	6.27	137.38	121.70
1	B	263	ILE	O-C-N	-6.04	113.03	122.70
1	E	124	PHE	C-N-CA	5.66	134.18	122.30
1	B	51	LYS	N-CA-C	-5.64	95.77	111.00
1	F	370	GLU	C-N-CA	5.54	135.56	121.70
1	D	268	ASP	CB-CG-OD1	5.50	123.25	118.30
1	C	322	ASN	C-N-CA	5.47	135.39	121.70
1	C	163	ARG	C-N-CA	5.25	134.81	121.70
1	D	149	PRO	C-N-CA	5.21	134.72	121.70
1	E	149	PRO	C-N-CA	5.10	134.45	121.70
1	B	166	GLU	C-N-CA	5.06	134.34	121.70
1	A	276	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	140	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	64	ARG	Sidechain
1	C	442	ARG	Sidechain

## 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	4179	0	4129	87	0
1	B	4174	0	4129	153	0
1	C	4174	0	4132	71	0
1	D	4179	0	4129	82	0
1	E	4174	0	4132	76	0
1	F	4174	0	4132	70	0
2	A	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	31	0	13	7	0
4	B	31	0	13	1	0
4	C	31	0	13	4	0
4	D	31	0	13	1	0
4	E	31	0	13	3	0
4	F	31	0	13	4	0
5	A	5	0	0	1	0
5	B	4	0	0	0	0
5	C	2	0	0	0	0
5	D	5	0	0	0	0
5	E	4	0	0	0	0
5	F	3	0	0	0	0
All	All	25272	0	24861	505	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 10.

All (505) 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:153:ASP:O	1:B:155:CYS:N	1.58	1.32
1:A:53:GLN:NE2	4:A:603:T8T:O3'	1.67	1.25
1:C:53:GLN:NE2	4:C:602:T8T:O3'	1.70	1.24
1:B:147:SER:OG	1:B:148:GLN:OE1	1.55	1.22
1:F:53:GLN:NE2	4:F:603:T8T:O3'	1.74	1.19
1:A:58:GLU:CD	1:A:283:LYS:NZ	1.98	1.17
1:A:58:GLU:OE1	1:A:283:LYS:NZ	1.82	1.11
1:B:116:MET:CE	1:B:209:ILE:HG21	1.82	1.10
1:B:52:THR:HG21	1:B:57:LEU:H	1.17	1.09
1:B:147:SER:CB	1:B:148:GLN:OE1	2.01	1.08
1:B:54:VAL:HG23	1:B:55:PHE:HD1	1.13	1.08
1:C:58:GLU:CD	1:C:283:LYS:NZ	2.05	1.08
1:B:92:LYS:H	1:B:93:LEU:HB2	1.01	1.08
1:B:55:PHE:HE2	1:B:283:LYS:HD3	1.18	1.06
1:B:55:PHE:CE2	1:B:283:LYS:HD3	1.92	1.05
1:A:58:GLU:CD	1:A:283:LYS:HZ1	1.55	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:GLU:OE1	1:C:442:ARG:NH2	1.91	1.02
1:A:232:LYS:NZ	4:A:603:T8T:O1G	1.94	0.98
1:B:92:LYS:N	1:B:93:LEU:HB2	1.78	0.98
1:B:54:VAL:HG23	1:B:55:PHE:CD1	1.98	0.98
1:C:58:GLU:OE1	1:C:283:LYS:NZ	1.98	0.94
1:A:400:GLU:OE1	1:B:442:ARG:NH2	2.02	0.93
1:A:53:GLN:NE2	4:A:603:T8T:HO3'	1.52	0.93
1:B:52:THR:HG21	1:B:57:LEU:N	1.82	0.92
1:B:116:MET:HE2	1:B:209:ILE:HG21	1.51	0.91
4:E:603:T8T:S1A	4:E:603:T8T:O3G	2.29	0.91
1:F:299:TRP:CD1	1:F:308:PHE:HB2	2.06	0.91
1:B:55:PHE:CE2	1:B:283:LYS:CD	2.52	0.91
1:B:55:PHE:HE2	1:B:283:LYS:CD	1.86	0.89
1:C:58:GLU:CD	1:C:283:LYS:HZ2	1.69	0.88
1:B:153:ASP:OD2	1:B:162:LEU:N	2.07	0.87
4:C:602:T8T:O2G	4:C:602:T8T:O2B	1.85	0.87
1:B:148:GLN:N	1:B:148:GLN:OE1	2.07	0.87
1:E:299:TRP:HB3	1:E:300:GLY:CA	2.05	0.87
1:A:58:GLU:OE2	1:A:283:LYS:NZ	2.04	0.85
1:C:198:ARG:HG3	1:E:325:SER:HB3	1.55	0.85
1:E:117:HIS:NE2	1:E:268:ASP:OD1	2.09	0.85
1:F:149:PRO:HA	1:F:150:LEU:HB2	1.58	0.85
1:E:298:ALA:HB3	1:E:381:LEU:HD12	1.58	0.85
1:B:212:TYR:OH	1:B:231:LYS:NZ	2.10	0.84
4:A:603:T8T:H5'	4:A:603:T8T:H8	1.60	0.83
1:B:147:SER:HB2	1:B:148:GLN:OE1	1.77	0.83
1:D:351:ARG:NH2	1:D:370:GLU:HB2	1.93	0.83
1:E:299:TRP:HB3	1:E:300:GLY:HA2	1.58	0.83
1:A:58:GLU:CD	1:A:283:LYS:HZ3	1.72	0.82
1:B:73:VAL:HG22	1:B:271:SER:OG	1.80	0.82
1:B:52:THR:O	1:B:66:ARG:NH1	2.13	0.81
1:A:55:PHE:CE2	1:A:283:LYS:HG3	2.16	0.81
1:B:147:SER:OG	1:B:148:GLN:CD	2.19	0.81
1:B:54:VAL:CG2	1:B:55:PHE:HD1	1.94	0.80
1:C:299:TRP:HE1	1:C:302:HIS:HB2	1.46	0.80
1:D:23:LYS:HB2	1:D:28:ILE:HD11	1.64	0.79
1:D:442:ARG:NE	1:E:400:GLU:OE1	2.15	0.79
1:B:69:HIS:O	1:B:73:VAL:HG23	1.83	0.79
1:B:116:MET:HE3	1:B:209:ILE:HG21	1.64	0.79
1:B:222:THR:HB	1:B:223:PRO:HA	1.64	0.79
1:F:309:SER:HA	1:F:313:GLU:HB3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:LYS:NZ	4:F:603:T8T:O2G	2.18	0.76
1:A:53:GLN:OE1	1:A:66:ARG:NH1	2.18	0.76
4:E:603:T8T:O1G	4:E:603:T8T:O2B	2.01	0.76
1:F:217:TRP:CH2	1:F:240:GLU:HG2	2.21	0.75
1:F:117:HIS:O	1:F:118:ASP:HB2	1.84	0.75
1:B:265:GLU:O	1:B:269:ASP:OD1	2.02	0.75
1:A:68:THR:HG22	1:A:71:MET:HE3	1.69	0.75
1:B:116:MET:HE2	1:B:209:ILE:CG2	2.17	0.74
1:F:299:TRP:HD1	1:F:308:PHE:HB2	1.53	0.73
1:A:69:HIS:O	1:A:73:VAL:HG23	1.88	0.73
1:E:150:LEU:HA	1:E:151:THR:HB	1.69	0.73
1:D:364:PHE:HE1	1:D:366:HIS:HB2	1.54	0.73
1:F:299:TRP:HE3	1:F:300:GLY:H	1.35	0.73
1:C:438:PRO:O	1:C:442:ARG:CD	2.37	0.73
1:B:268:ASP:O	1:B:272:TYR:CD2	2.42	0.73
1:A:292:TYR:OH	1:A:313:GLU:HG2	1.88	0.72
1:E:226:HIS:HB2	1:E:230:MET:HE3	1.71	0.72
1:B:153:ASP:O	1:B:154:ARG:C	2.21	0.72
1:B:65:THR:HG21	1:D:49:GLN:OE1	1.88	0.72
1:B:92:LYS:H	1:B:93:LEU:CB	1.93	0.72
1:B:153:ASP:C	1:B:155:CYS:N	2.42	0.71
1:C:53:GLN:NE2	4:C:602:T8T:HO3'	1.89	0.71
1:F:437:PHE:HB3	1:F:440:GLU:HB2	1.73	0.71
1:B:309:SER:HA	1:B:313:GLU:HB3	1.74	0.70
1:C:118:ASP:HA	1:C:121:ASN:HD22	1.56	0.70
1:C:203:TRP:CD1	1:C:249:GLU:HG2	2.26	0.69
1:A:398:ARG:HH11	1:B:499:ARG:HH11	1.40	0.69
1:B:216:ALA:HA	1:B:233:PRO:HB3	1.73	0.69
1:C:428:LEU:HD11	1:C:441:SER:HA	1.75	0.69
1:A:269:ASP:OD2	5:A:701:HOH:O	2.10	0.68
1:B:116:MET:CE	1:B:209:ILE:CG2	2.67	0.68
1:E:226:HIS:CB	1:E:230:MET:HE3	2.24	0.68
1:A:109:ILE:HA	1:A:205:GLN:HE22	1.58	0.68
1:C:224:GLU:HA	1:C:227:HIS:CD2	2.29	0.68
1:D:503:VAL:O	1:D:504:GLU:HB2	1.93	0.67
1:E:299:TRP:CB	1:E:300:GLY:HA2	2.24	0.67
1:C:443:LEU:O	1:C:446:LYS:N	2.28	0.67
1:F:217:TRP:HH2	1:F:240:GLU:HG2	1.60	0.67
1:B:150:LEU:N	1:B:150:LEU:HD12	2.10	0.67
1:E:164:ASP:H	1:E:165:GLY:HA3	1.59	0.66
1:E:309:SER:HA	1:E:313:GLU:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:PHE:CE2	1:B:283:LYS:CG	2.79	0.66
1:A:168:PRO:HD2	1:A:169:LEU:HD23	1.78	0.66
1:D:91:LEU:HB3	1:D:93:LEU:HD13	1.76	0.66
1:F:221:GLU:C	1:F:223:PRO:HD2	2.17	0.66
1:C:287:THR:HG23	1:C:290:GLN:H	1.61	0.65
1:B:400:GLU:CD	1:C:442:ARG:HH21	1.97	0.65
1:D:164:ASP:N	1:D:165:GLY:HA3	2.11	0.65
1:F:309:SER:HA	1:F:313:GLU:CB	2.26	0.65
1:C:438:PRO:O	1:C:442:ARG:HD3	1.96	0.65
1:F:381:LEU:O	1:F:385:VAL:HG23	1.95	0.65
1:B:55:PHE:CD2	1:B:283:LYS:CD	2.80	0.65
1:B:53:GLN:HG3	1:B:54:VAL:HG13	1.80	0.64
1:B:186:ASN:HD22	1:B:186:ASN:H	1.45	0.64
1:B:145:ALA:HA	1:B:162:LEU:HD11	1.78	0.64
1:E:433:ARG:NH2	1:F:397:GLU:OE2	2.30	0.64
1:B:149:PRO:HB3	1:B:162:LEU:O	1.98	0.64
1:B:69:HIS:NE2	1:B:272:TYR:HB3	2.13	0.64
1:A:226:HIS:HA	1:A:365:ASN:HD21	1.62	0.64
1:A:71:MET:HE1	1:F:67:LEU:HD21	1.81	0.63
1:B:118:ASP:HA	1:B:121:ASN:HD22	1.63	0.63
1:D:364:PHE:CE1	1:D:366:HIS:HB2	2.34	0.63
1:C:58:GLU:HG2	1:C:63:VAL:HG11	1.81	0.63
1:B:186:ASN:ND2	1:B:186:ASN:H	1.97	0.63
1:B:170:ASN:HB3	1:B:173:ARG:HH11	1.65	0.62
1:B:153:ASP:HB3	1:B:177:ARG:HH22	1.63	0.62
1:C:299:TRP:NE1	1:C:302:HIS:HB2	2.13	0.62
1:B:496:GLU:HG2	1:B:499:ARG:NH2	2.13	0.62
1:C:58:GLU:HG3	1:C:60:ASN:H	1.64	0.62
1:E:127:PHE:CE2	1:E:400:GLU:HG2	2.34	0.62
1:A:370:GLU:HG3	1:A:371:ASP:HB2	1.82	0.62
1:C:331:GLN:HG3	1:C:335:TYR:CE2	2.34	0.61
1:C:117:HIS:O	1:C:118:ASP:HB2	1.99	0.61
1:B:150:LEU:H	1:B:150:LEU:HD12	1.65	0.61
1:B:438:PRO:O	1:B:442:ARG:HD2	2.01	0.61
1:B:368(A):LEU:O	1:B:369:LEU:HB2	2.01	0.61
1:B:150:LEU:H	1:B:150:LEU:CD1	2.14	0.60
1:F:351:ARG:HD2	1:F:368(A):LEU:O	2.01	0.60
1:B:55:PHE:CE2	1:B:283:LYS:HG3	2.36	0.60
1:E:226:HIS:CB	1:E:230:MET:CE	2.79	0.60
1:B:127:PHE:CE2	1:B:400:GLU:HB3	2.37	0.60
1:E:287:THR:HG23	1:E:290:GLN:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:351:ARG:NH2	1:E:370:GLU:HB2	2.16	0.60
1:C:438:PRO:O	1:C:442:ARG:HD2	2.01	0.60
1:E:149:PRO:HB3	1:E:162:LEU:HB3	1.84	0.60
1:D:157:VAL:HG11	1:D:160:LEU:HD23	1.84	0.60
1:B:88:LEU:HD13	1:B:353:ILE:HG12	1.84	0.59
1:C:309:SER:HA	1:C:313:GLU:HB2	1.82	0.59
1:C:287:THR:HG22	1:C:290:GLN:HE21	1.67	0.59
1:E:226:HIS:HB3	1:E:230:MET:CE	2.33	0.59
1:A:428:LEU:HD11	1:A:441:SER:HA	1.84	0.59
1:B:55:PHE:CD2	1:B:283:LYS:HD2	2.38	0.59
1:A:155:CYS:HB2	1:A:177:ARG:NH1	2.17	0.59
1:A:55:PHE:CD2	1:A:283:LYS:HE2	2.38	0.59
1:E:155:CYS:HB2	1:E:177:ARG:NH1	2.18	0.59
1:B:438:PRO:HG2	1:B:439:ILE:HD12	1.83	0.58
1:D:359:ILE:HG13	1:D:364:PHE:HD2	1.67	0.58
1:E:150:LEU:CA	1:E:151:THR:HB	2.33	0.58
1:E:216:ALA:HA	1:E:233:PRO:HB3	1.86	0.58
1:F:295:LEU:HD23	1:F:385:VAL:HG21	1.84	0.58
1:A:67:LEU:HG	1:A:71:MET:HE2	1.85	0.58
1:C:443:LEU:O	1:C:444:PHE:C	2.42	0.58
1:F:223:PRO:HB2	1:F:227:HIS:HA	1.84	0.58
1:A:67:LEU:O	1:A:71:MET:HE2	2.04	0.58
1:D:148:GLN:HE21	1:D:149:PRO:HG3	1.69	0.58
1:C:53:GLN:HE21	4:C:602:T8T:HO3'	1.40	0.57
1:B:60:ASN:O	1:B:63:VAL:HG23	2.03	0.57
1:C:224:GLU:HA	1:C:227:HIS:HD2	1.67	0.57
1:E:428:LEU:HD11	1:E:441:SER:HA	1.86	0.57
1:C:163:ARG:HG2	1:C:164:ASP:HB2	1.87	0.57
1:E:442:ARG:NE	1:F:400:GLU:OE1	2.37	0.57
1:C:155:CYS:HB2	1:C:177:ARG:NH1	2.20	0.57
1:F:158:ALA:HA	1:F:161:ARG:HE	1.70	0.57
1:B:387:VAL:HG13	1:B:388:LYS:HD2	1.86	0.57
1:A:224:GLU:HA	1:A:227:HIS:CD2	2.40	0.56
1:A:398:ARG:NH1	1:B:499:ARG:HH11	2.03	0.56
1:B:351:ARG:NH1	1:B:371:ASP:HB2	2.20	0.56
1:D:433:ARG:NH2	1:D:442:ARG:HH22	2.03	0.56
1:B:273:CYS:SG	1:B:379:LEU:HD22	2.46	0.56
1:D:167:GLU:HG3	1:D:169:LEU:HB2	1.87	0.56
1:A:48:LEU:HD22	1:A:66:ARG:HB3	1.87	0.55
4:B:602:T8T:O1G	4:B:602:T8T:S1A	2.64	0.55
1:F:428:LEU:HD11	1:F:441:SER:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ALA:HA	1:C:233:PRO:HB3	1.88	0.55
1:C:292:TYR:OH	1:C:313:GLU:HG2	2.06	0.55
1:B:55:PHE:HE2	1:B:283:LYS:CG	2.17	0.55
1:A:212:TYR:O	1:A:234:GLY:HA3	2.06	0.55
1:B:379:LEU:O	1:B:383:LYS:HG3	2.06	0.55
1:B:337:ARG:NE	1:D:41:ASN:OD1	2.40	0.55
1:A:295:LEU:HD23	1:A:385:VAL:HG21	1.89	0.55
1:B:491:LEU:HD21	1:D:59:ARG:NE	2.21	0.55
1:E:164:ASP:N	1:E:165:GLY:HA3	2.21	0.55
1:F:216:ALA:HA	1:F:233:PRO:HB3	1.87	0.55
1:A:352:PHE:HB2	1:A:368(A):LEU:HD21	1.89	0.55
1:B:222:THR:HB	1:B:223:PRO:CA	2.33	0.54
1:C:352:PHE:HB2	1:C:368(A):LEU:HD21	1.87	0.54
1:D:214:ARG:HH11	1:D:218:TRP:HB3	1.72	0.54
1:A:276:ASP:OD2	4:A:603:T8T:H2'A	2.07	0.54
1:B:388:LYS:O	1:B:392:SER:OG	2.12	0.54
1:B:391:PHE:N	1:B:391:PHE:CD1	2.72	0.54
1:D:442:ARG:NH2	1:E:400:GLU:OE1	2.40	0.54
1:A:492:TYR:HD1	1:F:59:ARG:HH12	1.55	0.54
1:E:287:THR:HG22	1:E:290:GLN:HE21	1.73	0.54
1:D:304:LYS:N	1:D:305:GLY:HA2	2.22	0.54
1:B:61:ALA:HB1	1:D:47:ARG:HA	1.89	0.54
1:A:153:ASP:HB3	1:A:161:ARG:HG2	1.91	0.53
1:B:67:LEU:HD21	1:D:71:MET:HE1	1.88	0.53
1:A:299:TRP:O	1:A:301:GLN:HA	2.07	0.53
1:E:226:HIS:HB3	1:E:230:MET:HE2	1.91	0.53
1:D:145:ALA:HA	1:D:162:LEU:HD11	1.89	0.53
1:B:210:LEU:HD11	1:B:243:ILE:HD12	1.89	0.53
1:B:54:VAL:CG2	1:B:55:PHE:CD1	2.78	0.53
1:A:146:GLU:HB2	1:A:219:ARG:NH1	2.23	0.53
1:A:213:THR:HB	1:A:255:TYR:HA	1.91	0.53
1:F:155:CYS:HB2	1:F:177:ARG:NH1	2.22	0.53
4:F:603:T8T:H5'A	4:F:603:T8T:O1B	2.08	0.53
1:A:67:LEU:HD21	1:F:71:MET:CE	2.39	0.53
1:A:87:ARG:HG2	1:A:353:ILE:HD13	1.91	0.52
1:B:203:TRP:HE3	1:B:246:LEU:HD12	1.73	0.52
1:A:53:GLN:HG3	1:A:54:VAL:HG23	1.90	0.52
1:D:262:TRP:HB3	1:D:368(A):LEU:HD13	1.90	0.52
1:A:381:LEU:O	1:A:381:LEU:HD12	2.10	0.52
1:A:400:GLU:OE2	4:A:603:T8T:N2	2.35	0.52
1:D:155:CYS:HB3	1:D:161:ARG:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:THR:HB	1:C:255:TYR:HA	1.91	0.52
1:D:28:ILE:HA	1:D:31:ILE:HD12	1.92	0.52
1:A:135:TRP:O	1:A:136:PHE:HB2	2.10	0.52
1:B:64:ARG:NH2	1:D:46:ARG:CZ	2.72	0.52
1:C:135:TRP:O	1:C:138:GLN:HG3	2.10	0.51
1:B:405:ARG:HD2	1:C:500:LEU:O	2.10	0.51
4:A:603:T8T:C5'	4:A:603:T8T:H8	2.35	0.51
1:D:24:THR:HB	1:D:27:GLU:HB2	1.93	0.51
1:D:446:LYS:NZ	1:E:398:ARG:HH21	2.09	0.51
1:F:163:ARG:HA	1:F:164:ASP:HB2	1.93	0.51
1:B:69:HIS:HE1	1:B:117:HIS:HE1	1.59	0.51
1:D:309:SER:HA	1:D:313:GLU:HB3	1.91	0.51
1:D:392:SER:HA	1:F:433:ARG:NH2	2.26	0.51
1:F:213:THR:HB	1:F:255:TYR:HA	1.92	0.51
1:A:378:LEU:O	1:A:381:LEU:HB3	2.11	0.51
1:C:377:ASP:HA	1:C:380:LYS:HD2	1.93	0.51
1:B:351:ARG:HH12	1:B:371:ASP:HB2	1.75	0.50
1:B:377:ASP:HA	1:B:380:LYS:HD2	1.94	0.50
1:E:266:ALA:O	1:E:270:ILE:HG13	2.11	0.50
1:E:213:THR:HB	1:E:255:TYR:HA	1.93	0.50
1:E:144:ASP:HB2	1:E:153:ASP:HB2	1.93	0.50
1:E:298:ALA:HB3	1:E:381:LEU:CD1	2.37	0.50
1:B:273:CYS:SG	1:B:274:VAL:N	2.84	0.50
1:B:65:THR:CG2	1:D:49:GLN:OE1	2.57	0.50
1:B:55:PHE:CD2	1:B:283:LYS:HD3	2.41	0.50
1:C:391:PHE:CD1	1:C:391:PHE:N	2.77	0.50
1:E:309:SER:HA	1:E:313:GLU:CB	2.41	0.50
1:C:413:ILE:HG21	1:C:500:LEU:HD13	1.94	0.50
1:D:428:LEU:HD11	1:D:441:SER:HA	1.93	0.50
1:B:413:ILE:HG21	1:B:500:LEU:HD13	1.94	0.50
1:B:428:LEU:HD11	1:B:441:SER:HA	1.93	0.50
1:B:503:VAL:HG21	1:C:503:VAL:HG12	1.94	0.50
1:E:299:TRP:HB3	1:E:301:GLN:N	2.27	0.50
1:D:54:VAL:HG13	1:D:55:PHE:CD2	2.47	0.49
1:D:5:ASP:HB3	1:D:8:LYS:HD2	1.94	0.49
1:D:150:LEU:HD13	1:D:164:ASP:HB3	1.93	0.49
1:B:52:THR:HG21	1:B:56:PRO:HA	1.94	0.49
1:B:92:LYS:HB3	1:B:93:LEU:HD13	1.95	0.49
1:D:137:ARG:HH12	1:D:182:HIS:CE1	2.30	0.49
1:D:116:MET:HB2	1:D:209:ILE:HG21	1.95	0.49
1:A:5:ASP:HB3	1:A:8:LYS:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ALA:HA	1:A:233:PRO:HB3	1.94	0.49
1:C:133:ASN:O	1:C:137:ARG:HB2	2.12	0.49
1:E:5:ASP:HB3	1:E:8:LYS:HD2	1.94	0.49
1:F:352:PHE:HB2	1:F:368(A):LEU:HD21	1.94	0.49
1:F:118:ASP:HA	1:F:121:ASN:HD22	1.77	0.49
1:D:264:MET:HG3	1:D:265:GLU:N	2.27	0.49
1:C:5:ASP:HB3	1:C:8:LYS:HD2	1.95	0.49
1:D:213:THR:HB	1:D:255:TYR:HA	1.94	0.49
1:A:226:HIS:HA	1:A:365:ASN:ND2	2.25	0.48
1:B:150:LEU:N	1:B:150:LEU:CD1	2.73	0.48
1:B:52:THR:CB	1:B:56:PRO:HA	2.42	0.48
1:B:439:ILE:HD12	1:B:439:ILE:H	1.78	0.48
1:B:67:LEU:HG	1:B:71:MET:HE2	1.95	0.48
1:E:90:GLU:O	1:E:92:LYS:HD2	2.12	0.48
1:F:53:GLN:NE2	4:F:603:T8T:HO3'	2.01	0.48
1:A:282:GLU:C	1:A:284:ARG:H	2.14	0.48
1:B:11:ASN:H	1:B:204:ALA:HB2	1.78	0.48
1:E:150:LEU:HA	1:E:151:THR:CB	2.41	0.48
1:E:377:ASP:HA	1:E:380:LYS:HD2	1.96	0.48
1:A:145:ALA:HB1	1:A:174:ARG:HG2	1.94	0.48
1:F:87:ARG:O	1:F:91:LEU:HG	2.13	0.48
1:B:153:ASP:HB3	1:B:177:ARG:NH2	2.28	0.48
1:A:47:ARG:HA	1:F:61:ALA:HB1	1.94	0.48
1:A:381:LEU:C	1:A:381:LEU:HD12	2.32	0.48
1:B:166:GLU:HA	1:B:167:GLU:HB2	1.96	0.48
1:D:359:ILE:HG13	1:D:364:PHE:CD2	2.47	0.48
1:D:413:ILE:HG21	1:D:500:LEU:HD13	1.95	0.48
1:D:405:ARG:HD2	1:F:500:LEU:O	2.14	0.48
1:B:87:ARG:O	1:B:91:LEU:HG	2.13	0.48
1:D:304:LYS:H	1:D:305:GLY:HA2	1.78	0.48
1:B:158:ALA:HA	1:B:161:ARG:NH1	2.29	0.48
1:D:377:ASP:HA	1:D:380:LYS:HD2	1.95	0.48
1:D:442:ARG:CZ	1:E:400:GLU:OE1	2.62	0.48
1:F:228:TYR:O	1:F:231:LYS:HB2	2.14	0.48
1:A:228:TYR:O	1:A:231:LYS:HB2	2.14	0.47
1:B:5:ASP:HB3	1:B:8:LYS:HD2	1.95	0.47
1:B:56:PRO:O	1:B:58:GLU:N	2.47	0.47
1:D:24:THR:HB	1:D:27:GLU:H	1.80	0.47
1:E:289:GLU:HG3	1:E:316:TRP:HH2	1.79	0.47
1:A:67:LEU:HD21	1:F:71:MET:HE3	1.97	0.47
1:B:186:ASN:ND2	1:B:186:ASN:N	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:TRP:N	1:C:262:TRP:CD1	2.78	0.47
1:C:301:GLN:HB3	1:C:302:HIS:HA	1.96	0.47
1:D:307:LEU:HB2	1:D:374:GLU:HG2	1.95	0.47
1:E:299:TRP:HB3	1:E:300:GLY:C	2.35	0.47
1:A:24:THR:HB	1:A:27:GLU:H	1.79	0.47
1:D:433:ARG:HH21	1:D:442:ARG:HH22	1.61	0.47
1:F:148:GLN:H	1:F:149:PRO:CD	2.27	0.47
1:B:24:THR:HB	1:B:27:GLU:H	1.79	0.47
1:B:64:ARG:HH22	1:D:46:ARG:CZ	2.28	0.47
1:F:24:THR:HB	1:F:27:GLU:H	1.80	0.47
1:B:119:ILE:HD13	1:B:192:LEU:HD22	1.95	0.47
1:D:12:TRP:HZ2	1:D:23:LYS:HD3	1.80	0.47
1:A:69:HIS:CE1	1:A:272:TYR:HB3	2.49	0.47
1:C:23:LYS:HD2	1:C:31:ILE:HD11	1.97	0.47
1:D:503:VAL:O	1:D:504:GLU:CB	2.62	0.47
1:B:269:ASP:N	1:B:269:ASP:OD1	2.48	0.47
1:D:14:ARG:HB3	1:D:200:ASN:OD1	2.15	0.47
1:C:11:ASN:H	1:C:204:ALA:HB2	1.79	0.46
1:F:413:ILE:HG21	1:F:500:LEU:HD13	1.96	0.46
1:A:35:ASP:HA	1:A:38:ARG:HD2	1.97	0.46
1:C:287:THR:HG22	1:C:290:GLN:NE2	2.30	0.46
1:A:282:GLU:HG3	1:A:282:GLU:O	2.10	0.46
1:B:396:VAL:O	1:B:400:GLU:HG3	2.14	0.46
1:B:67:LEU:HD21	1:D:71:MET:CE	2.46	0.46
1:C:274:VAL:HG12	1:C:336:LEU:HD23	1.98	0.46
1:B:210:LEU:HD11	1:B:243:ILE:CD1	2.46	0.46
1:D:39:ILE:HD13	1:D:112:MET:HB3	1.97	0.46
1:E:170:ASN:HA	1:E:173:ARG:HD2	1.98	0.46
1:F:128:GLY:O	1:F:129:GLU:C	2.51	0.46
1:F:51:LYS:HE2	1:F:488:MET:O	2.16	0.46
1:C:35:ASP:HA	1:C:38:ARG:HD2	1.97	0.46
1:C:61:ALA:HB1	1:E:47:ARG:HA	1.97	0.46
1:B:400:GLU:OE1	1:C:442:ARG:CZ	2.61	0.46
1:D:446:LYS:HZ3	1:E:398:ARG:HH21	1.62	0.46
1:E:413:ILE:HG21	1:E:500:LEU:HD13	1.97	0.46
1:F:377:ASP:HA	1:F:380:LYS:HD2	1.96	0.46
1:E:228:TYR:O	1:E:231:LYS:HB2	2.15	0.46
1:C:283:LYS:O	1:C:284:ARG:HB2	2.15	0.46
1:C:422:LEU:CD1	1:C:473:GLU:HG3	2.46	0.46
1:E:226:HIS:HB2	1:E:230:MET:CE	2.44	0.46
1:D:304:LYS:N	1:D:305:GLY:CA	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ILE:HG21	1:A:500:LEU:HD13	1.97	0.45
1:A:67:LEU:HG	1:A:71:MET:CE	2.45	0.45
1:B:112:MET:C	1:B:114:CYS:H	2.19	0.45
1:C:228:TYR:O	1:C:231:LYS:HB2	2.16	0.45
1:F:69:HIS:CE1	1:F:272:TYR:HB3	2.51	0.45
1:F:5:ASP:HB3	1:F:8:LYS:HD2	1.97	0.45
1:B:170:ASN:HA	1:B:173:ARG:HD2	1.97	0.45
1:A:114:CYS:SG	1:A:264:MET:HB2	2.56	0.45
1:F:35:ASP:HA	1:F:38:ARG:HD2	1.99	0.45
1:B:94:LEU:HD13	1:B:99:LEU:HB3	1.98	0.45
1:C:347:TYR:HD2	1:C:369:LEU:HD23	1.81	0.45
1:D:301:GLN:HG3	1:D:304:LYS:HD2	1.98	0.45
1:E:127:PHE:CD2	1:E:400:GLU:HG2	2.51	0.45
1:A:370:GLU:HG3	1:A:371:ASP:CB	2.47	0.45
1:B:52:THR:HB	1:B:55:PHE:O	2.17	0.45
1:D:422:LEU:CD1	1:D:473:GLU:HG3	2.47	0.45
1:E:24:THR:HB	1:E:27:GLU:H	1.82	0.45
1:E:437:PHE:O	1:E:441:SER:HB2	2.17	0.45
1:D:111:GLU:O	1:D:114:CYS:HB2	2.17	0.45
1:B:54:VAL:CG2	1:B:55:PHE:N	2.79	0.44
1:D:262:TRP:CD1	1:D:359:ILE:HG23	2.52	0.44
1:D:88:LEU:HA	1:D:88:LEU:HD12	1.89	0.44
1:A:11:ASN:H	1:A:204:ALA:HB2	1.82	0.44
1:A:54:VAL:HB	1:A:55:PHE:CD1	2.52	0.44
1:A:145:ALA:HB3	1:A:219:ARG:NH2	2.32	0.44
1:C:150:LEU:HB2	1:C:152:ASP:N	2.32	0.44
1:C:163:ARG:HA	1:C:164:ASP:HB2	1.99	0.44
1:A:299:TRP:NE1	1:A:302:HIS:HD2	2.16	0.44
1:D:14:ARG:HD3	1:D:200:ASN:ND2	2.31	0.44
1:A:388:LYS:O	1:A:392:SER:OG	2.20	0.44
1:D:446:LYS:NZ	1:E:398:ARG:HE	2.16	0.44
1:A:316:TRP:CZ2	1:A:320:ARG:HD2	2.53	0.44
1:B:44:ALA:CB	1:B:119:ILE:HD11	2.47	0.44
1:B:35:ASP:HA	1:B:38:ARG:HD2	1.99	0.44
1:B:69:HIS:O	1:B:69:HIS:CG	2.70	0.44
1:D:228:TYR:O	1:D:231:LYS:HB2	2.18	0.44
1:B:197:MET:HA	1:B:197:MET:CE	2.48	0.44
1:D:146:GLU:HG2	1:D:219:ARG:HE	1.83	0.44
1:B:150:LEU:HA	1:B:151:THR:HA	1.59	0.43
1:B:222:THR:CB	1:B:223:PRO:HA	2.43	0.43
1:B:425:PHE:CE2	1:B:477:ARG:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:LEU:O	1:C:445:HIS:N	2.50	0.43
1:B:148:GLN:CD	1:B:148:GLN:H	2.06	0.43
1:B:53:GLN:HB2	1:B:66:ARG:HD3	1.99	0.43
1:D:12:TRP:CZ2	1:D:23:LYS:HD3	2.53	0.43
1:E:442:ARG:HG2	1:F:397:GLU:HB3	2.00	0.43
1:B:268:ASP:O	1:B:272:TYR:HD2	1.95	0.43
1:B:468:GLU:HB3	1:B:472:TRP:CD1	2.53	0.43
1:A:190:ILE:HG21	1:A:243:ILE:HD11	1.99	0.43
1:B:64:ARG:HH22	1:D:46:ARG:NH2	2.16	0.43
1:B:84:ILE:O	1:B:88:LEU:HB2	2.18	0.43
1:A:300:GLY:HA2	1:A:301:GLN:HG3	1.99	0.43
1:D:141:HIS:HB2	1:D:154:ARG:O	2.18	0.43
1:F:117:HIS:NE2	1:F:118:ASP:OD2	2.51	0.43
1:B:262:TRP:N	1:B:262:TRP:CD1	2.83	0.43
1:A:437:PHE:HB3	1:A:440:GLU:HB2	2.01	0.43
1:C:318:LYS:HB3	1:C:335:TYR:CE2	2.54	0.43
1:E:437:PHE:HB3	1:E:440:GLU:HB2	2.01	0.43
1:B:65:THR:HG21	1:D:49:GLN:CD	2.39	0.43
1:D:153:ASP:HB3	1:D:161:ARG:HG2	2.00	0.43
1:E:149:PRO:HA	1:E:150:LEU:CB	2.49	0.43
1:E:162:LEU:HD22	1:E:170:ASN:HB3	2.01	0.43
1:F:11:ASN:H	1:F:204:ALA:HB2	1.84	0.43
1:E:468:GLU:HB3	1:E:472:TRP:CD1	2.54	0.42
1:A:214:ARG:HE	1:A:218:TRP:HB3	1.84	0.42
1:A:232:LYS:HB2	1:A:233:PRO:CD	2.50	0.42
1:A:448:SER:HB2	1:A:451:HIS:CD2	2.54	0.42
1:B:175:LYS:HE2	1:B:217:TRP:CZ3	2.53	0.42
1:B:399:LEU:HD23	1:B:402:GLN:OE1	2.19	0.42
1:B:402:GLN:O	1:B:403:GLY:C	2.57	0.42
1:F:262:TRP:N	1:F:262:TRP:CD1	2.77	0.42
1:A:32:PHE:CE1	1:A:109:ILE:HD11	2.54	0.42
1:B:387:VAL:HG22	1:B:387:VAL:O	2.19	0.42
1:F:88:LEU:HD12	1:F:88:LEU:HA	1.90	0.42
1:C:32:PHE:CE1	1:C:109:ILE:HD11	2.55	0.42
1:E:214:ARG:HE	1:E:218:TRP:HB3	1.84	0.42
1:E:288:VAL:HG11	1:E:329:GLU:HA	2.02	0.42
1:B:127:PHE:CD2	1:B:400:GLU:HB3	2.54	0.42
1:B:437:PHE:HB3	1:B:440:GLU:HB2	2.00	0.42
1:C:422:LEU:HD13	1:C:473:GLU:HG3	2.01	0.42
1:C:310:LEU:H	1:C:310:LEU:HG	1.64	0.42
1:E:273:CYS:HB3	1:E:382:TYR:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:TYR:CD2	1:C:345:VAL:HG21	2.55	0.42
1:E:157:VAL:HG11	1:E:160:LEU:HD23	2.01	0.42
4:E:603:T8T:PA	4:E:603:T8T:O3G	2.77	0.42
1:A:140:LEU:HD23	1:A:157:VAL:HG21	2.02	0.41
1:A:217:TRP:HH2	1:A:240:GLU:HG3	1.85	0.41
1:A:316:TRP:CE2	1:A:320:ARG:HD2	2.56	0.41
1:B:295:LEU:HD23	1:B:385:VAL:HG21	2.02	0.41
1:D:437:PHE:HB3	1:D:440:GLU:HB2	2.01	0.41
1:B:71:MET:HE1	1:D:67:LEU:HD21	2.01	0.41
1:E:35:ASP:HA	1:E:38:ARG:HD2	2.02	0.41
1:A:262:TRP:CH2	1:A:364:PHE:O	2.73	0.41
1:B:60:ASN:HB3	1:B:63:VAL:CG2	2.51	0.41
1:A:54:VAL:HB	1:A:55:PHE:HD1	1.85	0.41
1:B:279:ASP:O	1:B:282:GLU:HB3	2.19	0.41
1:B:415:ARG:N	1:B:416:PRO:HD2	2.35	0.41
1:E:391:PHE:N	1:E:391:PHE:CD1	2.87	0.41
1:F:85:LEU:HD13	1:F:103:THR:HG23	2.03	0.41
1:A:184:GLU:HG2	1:A:233:PRO:O	2.20	0.41
1:A:87:ARG:HG2	1:A:353:ILE:CD1	2.51	0.41
1:B:228:TYR:O	1:B:231:LYS:HB2	2.20	0.41
1:D:73:VAL:HG12	1:D:114:CYS:SG	2.61	0.41
1:D:371:ASP:HA	1:D:380:LYS:NZ	2.35	0.41
1:D:392:SER:HA	1:F:433:ARG:HH21	1.86	0.41
1:F:295:LEU:HD22	1:F:381:LEU:HD11	2.01	0.41
1:A:146:GLU:HB2	1:A:219:ARG:HH11	1.84	0.41
1:B:69:HIS:C	1:B:69:HIS:ND1	2.73	0.41
1:C:468:GLU:HB3	1:C:472:TRP:CD1	2.56	0.41
1:D:468:GLU:HB3	1:D:472:TRP:CD1	2.55	0.41
1:E:287:THR:HG22	1:E:290:GLN:NE2	2.36	0.41
1:F:76:VAL:HG21	1:F:271:SER:HB3	2.02	0.41
1:A:61:ALA:HB1	1:F:47:ARG:HA	2.01	0.41
1:B:55:PHE:HD2	1:B:283:LYS:HD2	1.81	0.41
1:C:262:TRP:CH2	1:C:364:PHE:O	2.73	0.41
1:E:296:HIS:CE1	1:E:299:TRP:HE1	2.38	0.41
1:E:323:SER:HB3	1:E:326:ARG:O	2.20	0.41
1:F:150:LEU:HD23	1:F:153:ASP:HB2	2.02	0.41
1:F:83:GLU:O	1:F:87:ARG:HG2	2.20	0.41
1:E:295:LEU:HD23	1:E:385:VAL:HG21	2.02	0.41
1:C:191:ARG:HD2	1:C:239:GLU:OE2	2.21	0.41
1:D:53:GLN:OE1	1:D:69:HIS:CG	2.74	0.41
1:E:294:HIS:O	1:E:297:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ARG:HH12	1:B:182:HIS:CE1	2.39	0.41
1:B:399:LEU:HD23	1:B:399:LEU:HA	1.82	0.41
1:E:217:TRP:HH2	1:E:240:GLU:HG3	1.86	0.41
1:A:73:VAL:HG21	1:A:117:HIS:CE1	2.56	0.41
1:C:448:SER:HB2	1:C:451:HIS:CD2	2.56	0.41
1:C:46:ARG:O	1:C:49:GLN:HG2	2.20	0.41
1:E:11:ASN:H	1:E:204:ALA:HB2	1.85	0.41
1:E:127:PHE:CE2	1:E:400:GLU:CG	3.04	0.41
1:F:222:THR:O	1:F:223:PRO:C	2.58	0.41
1:F:468:GLU:HB3	1:F:472:TRP:CD1	2.56	0.41
1:B:468:GLU:HB3	1:B:472:TRP:HD1	1.85	0.41
1:D:438:PRO:O	1:D:442:ARG:HD2	2.21	0.41
1:D:232:LYS:NZ	4:D:602:T8T:O1G	2.44	0.41
1:B:448:SER:HB2	1:B:451:HIS:CD2	2.56	0.40
1:B:52:THR:CG2	1:B:57:LEU:H	2.08	0.40
1:F:211:LYS:HA	1:F:261:THR:HG21	2.03	0.40
1:F:344:LEU:CD2	1:F:375:CYS:HB3	2.51	0.40
1:B:112:MET:C	1:B:114:CYS:N	2.73	0.40
1:C:89:LYS:HE3	1:C:94:LEU:HD22	2.03	0.40
1:E:146:GLU:CD	1:E:219:ARG:HH11	2.24	0.40
1:E:46:ARG:O	1:E:49:GLN:HG2	2.21	0.40
1:A:468:GLU:HB3	1:A:472:TRP:CD1	2.56	0.40
1:C:47:ARG:HA	1:E:61:ALA:HB1	2.02	0.40
1:D:420:LEU:CD1	1:D:440:GLU:HG2	2.52	0.40
1:D:55:PHE:HA	1:D:56:PRO:HD3	1.91	0.40
1:E:48:LEU:HD22	1:E:66:ARG:HB3	2.03	0.40
1:F:232:LYS:HB3	1:F:233:PRO:CD	2.51	0.40
1:F:298:ALA:HB3	1:F:381:LEU:CD2	2.51	0.40
1:A:71:MET:CE	1:F:67:LEU:HD21	2.49	0.40
1:B:279:ASP:O	1:B:282:GLU:N	2.55	0.40
1:F:137:ARG:HH12	1:F:182:HIS:CE1	2.40	0.40
1:F:148:GLN:H	1:F:149:PRO:HD3	1.85	0.40
1:F:214:ARG:HE	1:F:218:TRP:HB3	1.86	0.40
1:F:17:ARG:HH12	1:F:38:ARG:HH22	1.67	0.40
1:C:262:TRP:CH2	1:C:364:PHE:HB3	2.55	0.40
1:D:425:PHE:CE2	1:D:477:ARG:HG3	2.56	0.40
1:E:269:ASP:O	1:E:270:ILE:C	2.59	0.40
1:F:497:TYR:O	1:F:501:MET:HG2	2.22	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/505 (99%)	463 (92%)	29 (6%)	10 (2%)	7	33
1	B	501/505 (99%)	460 (92%)	31 (6%)	10 (2%)	7	33
1	C	501/505 (99%)	457 (91%)	28 (6%)	16 (3%)	4	24
1	D	502/505 (99%)	456 (91%)	36 (7%)	10 (2%)	7	33
1	E	501/505 (99%)	455 (91%)	31 (6%)	15 (3%)	4	26
1	F	501/505 (99%)	452 (90%)	38 (8%)	11 (2%)	6	32
All	All	3008/3030 (99%)	2743 (91%)	193 (6%)	72 (2%)	6	30

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	SER
1	A	166	GLU
1	B	22	VAL
1	B	93	LEU
1	B	154	ARG
1	B	223	PRO
1	B	369	LEU
1	B	432	GLU
1	C	304	LYS
1	D	221	GLU
1	D	371	ASP
1	D	504	GLU
1	E	152	ASP
1	E	223	PRO
1	F	21	GLY
1	F	22	VAL
1	F	321	SER
1	F	371	ASP
1	B	23	LYS
1	C	21	GLY

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Mol	Chain	Res	Type
1	C	22	VAL
1	C	164	ASP
1	C	301	GLN
1	E	22	VAL
1	E	151	THR
1	E	225	THR
1	E	299	TRP
1	E	371	ASP
1	E	432	GLU
1	F	162	LEU
1	F	164	ASP
1	F	320	ARG
1	A	162	LEU
1	A	302	HIS
1	A	327	SER
1	A	432	GLU
1	C	23	LYS
1	C	166	GLU
1	C	300	GLY
1	C	328	THR
1	C	372	ALA
1	C	432	GLU
1	D	125	GLY
1	D	322	ASN
1	E	124	PHE
1	E	321	SER
1	A	57	LEU
1	B	301	GLN
1	C	371	ASP
1	D	200	ASN
1	D	325	SER
1	E	23	LYS
1	E	57	LEU
1	E	322	ASN
1	F	152	ASP
1	A	222(A)	THR
1	A	430	GLU
1	B	303	GLU
1	C	147	SER
1	C	149	PRO
1	C	430	GLU
1	D	319	SER

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Mol	Chain	Res	Type
1	D	430	GLU
1	E	430	GLU
1	F	57	LEU
1	A	326	ARG
1	B	430	GLU
1	C	148	GLN
1	D	326	ARG
1	E	154	ARG
1	F	23	LYS
1	F	148	GLN

### 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	448/450 (100%)	408 (91%)	40 (9%)	9	34
1	B	448/450 (100%)	399 (89%)	49 (11%)	6	25
1	C	448/450 (100%)	405 (90%)	43 (10%)	8	30
1	D	448/450 (100%)	407 (91%)	41 (9%)	9	32
1	E	448/450 (100%)	411 (92%)	37 (8%)	11	37
1	F	448/450 (100%)	403 (90%)	45 (10%)	7	29
All	All	2688/2700 (100%)	2433 (90%)	255 (10%)	8	31

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	17	ARG
1	A	45	ILE
1	A	52	THR
1	A	83	GLU
1	A	88	LEU
1	A	140	LEU
1	A	143	GLU

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Mol	Chain	Res	Type
1	A	147	SER
1	A	151	THR
1	A	152	ASP
1	A	153	ASP
1	A	163	ARG
1	A	164	ASP
1	A	166	GLU
1	A	169	LEU
1	A	209	ILE
1	A	211	LYS
1	A	226	HIS
1	A	232	LYS
1	A	245	ARG
1	A	262	TRP
1	A	264	MET
1	A	282	GLU
1	A	310	LEU
1	A	320	ARG
1	A	334	MET
1	A	341	LEU
1	A	365	ASN
1	A	368(A)	LEU
1	A	370	GLU
1	A	379	LEU
1	A	430	GLU
1	A	431	LYS
1	A	449	THR
1	A	450	ARG
1	A	479	ARG
1	A	480	LEU
1	A	490	ASP
1	A	491	LEU
1	B	3	GLN
1	B	22	VAL
1	B	27	GLU
1	B	45	ILE
1	B	51	LYS
1	B	53	GLN
1	B	54	VAL
1	B	65	THR
1	B	66	ARG
1	B	83	GLU

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Mol	Chain	Res	Type
1	B	91	LEU
1	B	117	HIS
1	B	119	ILE
1	B	140	LEU
1	B	143	GLU
1	B	163	ARG
1	B	164	ASP
1	B	169	LEU
1	B	182	HIS
1	B	186	ASN
1	B	210	LEU
1	B	222	THR
1	B	225	THR
1	B	227	HIS
1	B	231	LYS
1	B	262	TRP
1	B	264	MET
1	B	269	ASP
1	B	272	TYR
1	B	274	VAL
1	B	283	LYS
1	B	310	LEU
1	B	317	GLU
1	B	324	LEU
1	B	341	LEU
1	B	368(A)	LEU
1	B	369	LEU
1	B	421	SER
1	B	430	GLU
1	B	431	LYS
1	B	432	GLU
1	B	435	LYS
1	B	442	ARG
1	B	449	THR
1	B	450	ARG
1	B	479	ARG
1	B	490	ASP
1	B	491	LEU
1	B	504	GLU
1	C	3	GLN
1	C	17	ARG
1	C	20	GLN

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Mol	Chain	Res	Type
1	C	45	ILE
1	C	63	VAL
1	C	83	GLU
1	C	87	ARG
1	C	88	LEU
1	C	89	LYS
1	C	138	GLN
1	C	140	LEU
1	C	143	GLU
1	C	150	LEU
1	C	152	ASP
1	C	153	ASP
1	C	163	ARG
1	C	164	ASP
1	C	182	HIS
1	C	190	ILE
1	C	249	GLU
1	C	262	TRP
1	C	264	MET
1	C	274	VAL
1	C	286	PHE
1	C	310	LEU
1	C	312	VAL
1	C	313	GLU
1	C	326	ARG
1	C	329	GLU
1	C	334	MET
1	C	368(A)	LEU
1	C	369	LEU
1	C	370	GLU
1	C	405	ARG
1	C	421	SER
1	C	430	GLU
1	C	431	LYS
1	C	449	THR
1	C	450	ARG
1	C	479	ARG
1	C	480	LEU
1	C	490	ASP
1	C	491	LEU
1	D	22	VAL
1	D	26	HIS

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Mol	Chain	Res	Type
1	D	45	ILE
1	D	83	GLU
1	D	88	LEU
1	D	94	LEU
1	D	114	CYS
1	D	138	GLN
1	D	140	LEU
1	D	143	GLU
1	D	148	GLN
1	D	152	ASP
1	D	156	SER
1	D	161	ARG
1	D	190	ILE
1	D	222	THR
1	D	225	THR
1	D	227	HIS
1	D	264	MET
1	D	296	HIS
1	D	297	GLU
1	D	301	GLN
1	D	307	LEU
1	D	310	LEU
1	D	312	VAL
1	D	316	TRP
1	D	320	ARG
1	D	328	THR
1	D	329	GLU
1	D	364	PHE
1	D	368(A)	LEU
1	D	405	ARG
1	D	430	GLU
1	D	431	LYS
1	D	433	ARG
1	D	441	SER
1	D	449	THR
1	D	450	ARG
1	D	479	ARG
1	D	480	LEU
1	D	491	LEU
1	E	45	ILE
1	E	66	ARG
1	E	83	GLU

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Mol	Chain	Res	Type
1	E	86	SER
1	E	88	LEU
1	E	92	LYS
1	E	101	GLU
1	E	140	LEU
1	E	146	GLU
1	E	150	LEU
1	E	151	THR
1	E	164	ASP
1	E	182	HIS
1	E	227	HIS
1	E	264	MET
1	E	272	TYR
1	E	299	TRP
1	E	310	LEU
1	E	312	VAL
1	E	324	LEU
1	E	334	MET
1	E	341	LEU
1	E	368(A)	LEU
1	E	369	LEU
1	E	415	ARG
1	E	430	GLU
1	E	431	LYS
1	E	432	GLU
1	E	433	ARG
1	E	436	ARG
1	E	441	SER
1	E	449	THR
1	E	450	ARG
1	E	479	ARG
1	E	480	LEU
1	E	490	ASP
1	E	491	LEU
1	F	3	GLN
1	F	17	ARG
1	F	45	ILE
1	F	59	ARG
1	F	83	GLU
1	F	88	LEU
1	F	117	HIS
1	F	138	GLN

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Mol	Chain	Res	Type
1	F	140	LEU
1	F	143	GLU
1	F	146	GLU
1	F	148	GLN
1	F	152	ASP
1	F	153	ASP
1	F	164	ASP
1	F	166	GLU
1	F	167	GLU
1	F	179	ASP
1	F	182	HIS
1	F	211	LYS
1	F	222	THR
1	F	227	HIS
1	F	240	GLU
1	F	262	TRP
1	F	264	MET
1	F	274	VAL
1	F	299	TRP
1	F	301	GLN
1	F	302	HIS
1	F	310	LEU
1	F	312	VAL
1	F	319	SER
1	F	328	THR
1	F	329	GLU
1	F	334	MET
1	F	341	LEU
1	F	351	ARG
1	F	368(A)	LEU
1	F	381	LEU
1	F	420	LEU
1	F	430	GLU
1	F	449	THR
1	F	480	LEU
1	F	490	ASP
1	F	491	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN

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Mol	Chain	Res	Type
1	A	20	GLN
1	A	49	GLN
1	A	60	ASN
1	A	182	HIS
1	A	205	GLN
1	A	290	GLN
1	A	296	HIS
1	A	301	GLN
1	A	302	HIS
1	A	314	ASN
1	A	505	GLN
1	B	3	GLN
1	B	49	GLN
1	B	53	GLN
1	B	60	ASN
1	B	69	HIS
1	B	121	ASN
1	B	170	ASN
1	B	186	ASN
1	B	290	GLN
1	B	331	GLN
1	B	445	HIS
1	C	49	GLN
1	C	53	GLN
1	C	121	ASN
1	C	290	GLN
1	C	314	ASN
1	C	402	GLN
1	C	445	HIS
1	D	60	ASN
1	D	69	HIS
1	D	148	GLN
1	D	182	HIS
1	D	314	ASN
1	D	322	ASN
1	D	331	GLN
1	D	445	HIS
1	E	53	GLN
1	E	74	GLN
1	E	290	GLN
1	E	331	GLN
1	E	339	ASN

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Mol	Chain	Res	Type
1	E	445	HIS
1	F	49	GLN
1	F	53	GLN
1	F	60	ASN
1	F	69	HIS
1	F	121	ASN
1	F	148	GLN
1	F	290	GLN
1	F	314	ASN
1	F	445	HIS
1	F	451	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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	$\# Z  > 2$
4	T8T	E	603	-	24,33,33	1.60	4 (16%)	30,52,52	2.43	6 (20%)
4	T8T	C	602	-	24,33,33	1.88	5 (20%)	30,52,52	1.99	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	T8T	B	602	-	24,33,33	1.54	6 (25%)	30,52,52	1.68	4 (13%)
4	T8T	D	602	-	24,33,33	1.17	2 (8%)	30,52,52	1.49	3 (10%)
4	T8T	F	603	-	24,33,33	1.24	3 (12%)	30,52,52	1.65	3 (10%)
4	T8T	A	603	2	24,33,33	1.78	4 (16%)	30,52,52	1.94	5 (16%)

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
4	T8T	E	603	-	-	1/14/34/34	0/3/3/3
4	T8T	C	602	-	-	6/14/34/34	0/3/3/3
4	T8T	B	602	-	-	3/14/34/34	0/3/3/3
4	T8T	D	602	-	-	4/14/34/34	0/3/3/3
4	T8T	F	603	-	-	2/14/34/34	0/3/3/3
4	T8T	A	603	2	-	5/14/34/34	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	T8T	PG-O3G	-6.18	1.30	1.50
4	E	603	T8T	C6-C5	5.41	1.50	1.41
4	C	602	T8T	PA-O5'	-5.26	1.49	1.57
4	C	602	T8T	PG-O3G	-4.06	1.37	1.50
4	B	602	T8T	PG-O3G	-3.55	1.39	1.50
4	B	602	T8T	PA-O5'	-3.45	1.52	1.57
4	A	603	T8T	PG-O2G	-3.27	1.42	1.54
4	C	602	T8T	PG-O2G	-3.14	1.42	1.54
4	C	602	T8T	C8-N7	-3.04	1.29	1.34
4	D	602	T8T	PA-O5'	-2.74	1.53	1.57
4	E	603	T8T	PG-O1G	-2.67	1.44	1.54
4	B	602	T8T	PG-O2G	-2.65	1.44	1.54
4	F	603	T8T	PG-O3G	-2.58	1.42	1.50
4	A	603	T8T	PG-O1G	-2.50	1.45	1.54
4	E	603	T8T	PG-O2G	-2.48	1.45	1.54
4	B	602	T8T	C6-C5	2.35	1.45	1.41
4	F	603	T8T	PG-O2G	-2.34	1.45	1.54
4	B	602	T8T	C8-N7	-2.27	1.30	1.34
4	A	603	T8T	C8-N7	-2.24	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	603	T8T	C8-N7	-2.17	1.30	1.34
4	D	602	T8T	C8-N7	-2.13	1.30	1.34
4	E	603	T8T	C8-N7	-2.12	1.30	1.34
4	C	602	T8T	C6-C5	2.12	1.45	1.41
4	B	602	T8T	PG-O1G	-2.01	1.47	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	603	T8T	C5-C6-N1	-7.31	113.44	123.43
4	C	602	T8T	C5-C6-N1	-6.27	114.85	123.43
4	B	602	T8T	C5-C6-N1	-5.83	115.46	123.43
4	F	603	T8T	C5-C6-N1	-5.75	115.57	123.43
4	A	603	T8T	C5-C6-N1	-5.62	115.75	123.43
4	E	603	T8T	PB-O3B-PG	-5.44	114.15	132.83
4	E	603	T8T	C6-N1-C2	5.27	124.31	115.93
4	E	603	T8T	O3A-PA-O5'	5.12	119.67	101.37
4	A	603	T8T	PA-O5'-C5'	4.85	135.47	120.16
4	D	602	T8T	C5-C6-N1	-4.68	117.03	123.43
4	B	602	T8T	C6-N1-C2	4.65	123.31	115.93
4	C	602	T8T	C6-N1-C2	4.45	123.00	115.93
4	F	603	T8T	C6-N1-C2	4.41	122.94	115.93
4	A	603	T8T	C6-N1-C2	4.37	122.88	115.93
4	D	602	T8T	C6-N1-C2	3.90	122.12	115.93
4	E	603	T8T	O5'-PA-O2A	-3.66	100.94	114.42
4	C	602	T8T	PB-O3B-PG	-3.55	120.65	132.83
4	A	603	T8T	O3A-PA-O5'	3.41	113.57	101.37
4	D	602	T8T	N3-C2-N1	-3.15	123.02	127.22
4	C	602	T8T	PA-O5'-C5'	3.12	130.03	120.16
4	F	603	T8T	N3-C2-N1	-3.05	123.15	127.22
4	C	602	T8T	N3-C2-N1	-3.05	123.16	127.22
4	A	603	T8T	N3-C2-N1	-3.02	123.19	127.22
4	B	602	T8T	N3-C2-N1	-3.01	123.21	127.22
4	E	603	T8T	N3-C2-N1	-2.73	123.58	127.22
4	B	602	T8T	C6-C5-C4	-2.19	118.71	120.80

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	602	T8T	PB-O3B-PG-O1G
4	D	602	T8T	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
4	C	602	T8T	PB-O3B-PG-O2G
4	A	603	T8T	PB-O3B-PG-O1G
4	A	603	T8T	C5'-O5'-PA-O2A
4	F	603	T8T	C3'-C4'-C5'-O5'
4	F	603	T8T	O4'-C4'-C5'-O5'
4	D	602	T8T	C5'-O5'-PA-O2A
4	C	602	T8T	PG-O3B-PB-O2B
4	A	603	T8T	C4'-C5'-O5'-PA
4	C	602	T8T	C5'-O5'-PA-O2A
4	B	602	T8T	PG-O3B-PB-O1B
4	D	602	T8T	PG-O3B-PB-O2B
4	B	602	T8T	PB-O3B-PG-O3G
4	D	602	T8T	PB-O3B-PG-O3G
4	A	603	T8T	PB-O3B-PG-O3G
4	C	602	T8T	PB-O3B-PG-O1G
4	A	603	T8T	PB-O3B-PG-O2G
4	E	603	T8T	PA-O3A-PB-O2B
4	C	602	T8T	PB-O3B-PG-O3G
4	C	602	T8T	PB-O3A-PA-O2A

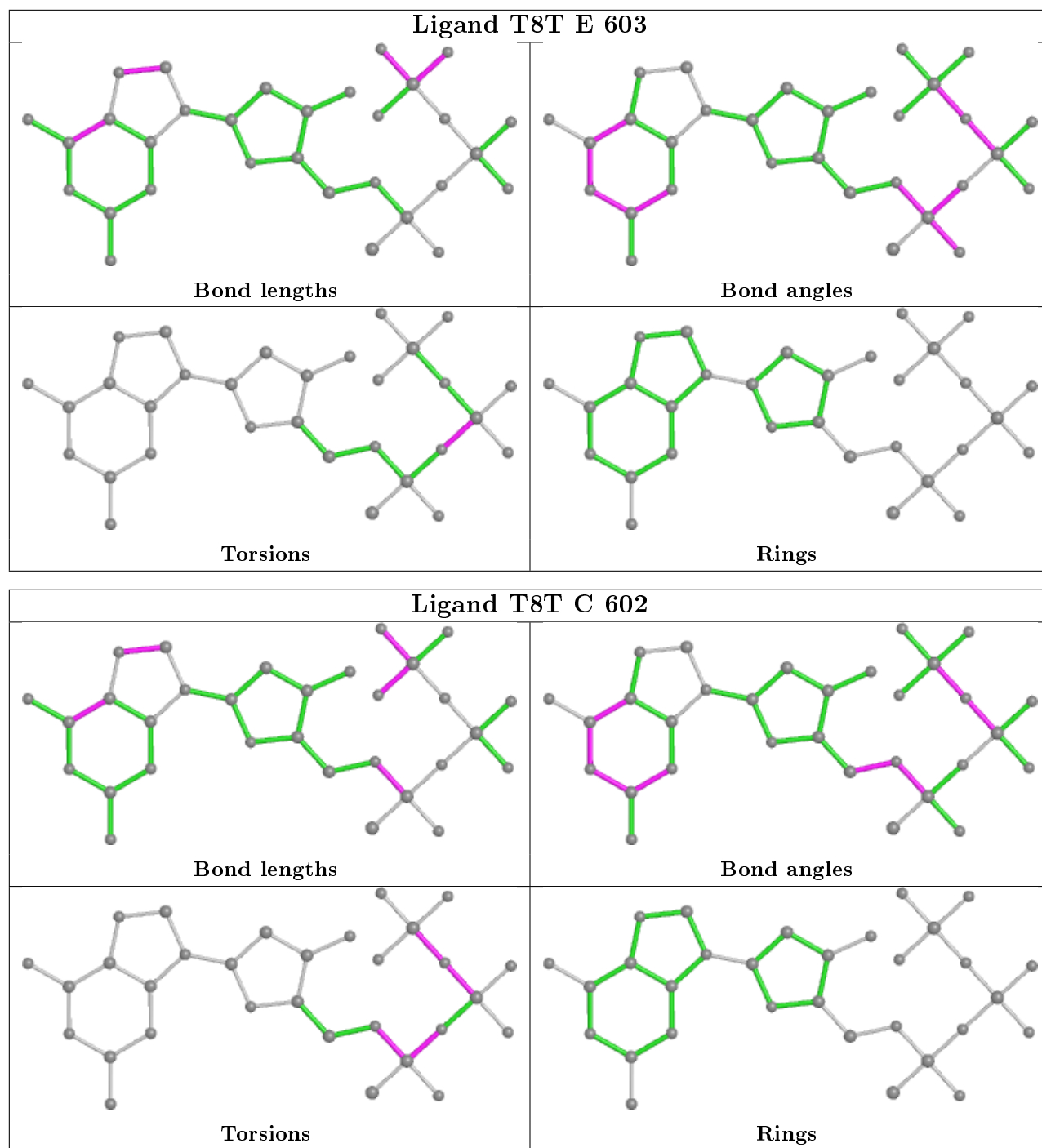
There are no ring outliers.

6 monomers are involved in 20 short contacts:

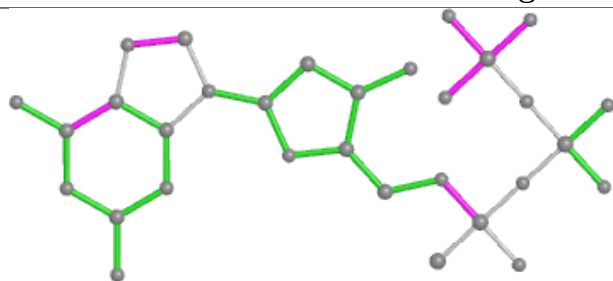
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	603	T8T	3	0
4	C	602	T8T	4	0
4	B	602	T8T	1	0
4	D	602	T8T	1	0
4	F	603	T8T	4	0
4	A	603	T8T	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

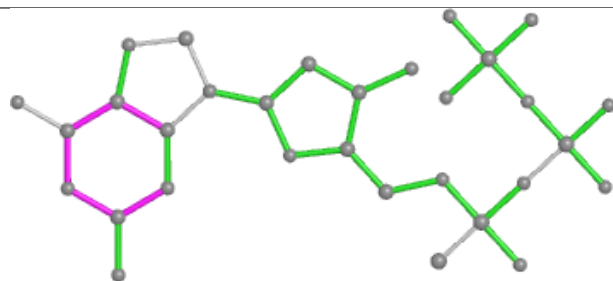
equivalents in the CSD to analyse the geometry.



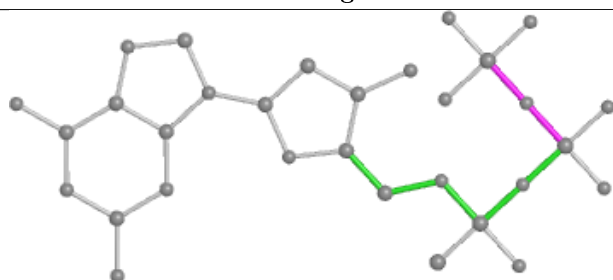
## Ligand T8T B 602



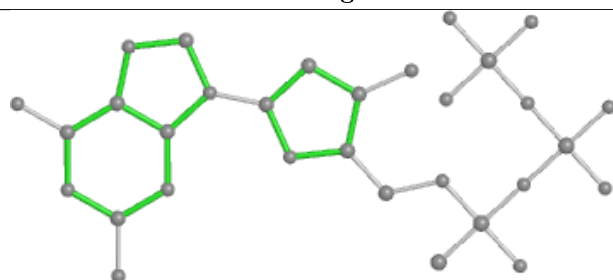
Bond lengths



Bond angles

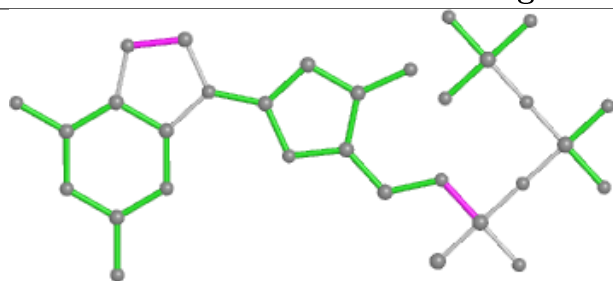


Torsions

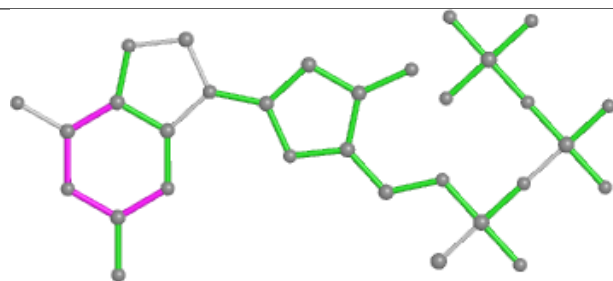


Rings

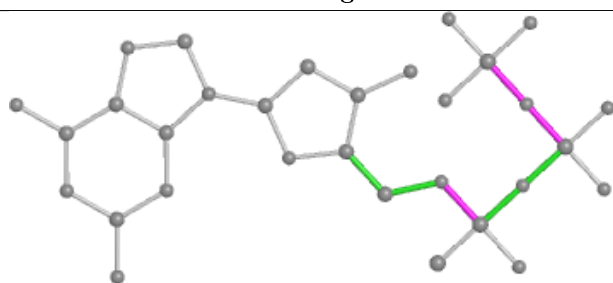
## Ligand T8T D 602



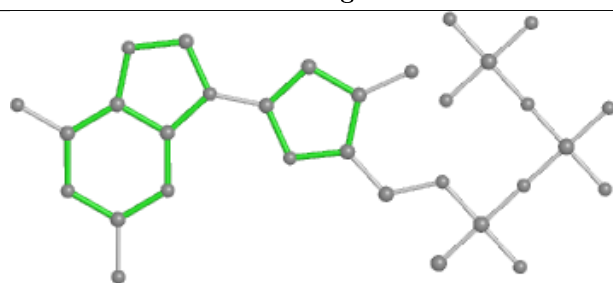
Bond lengths



Bond angles

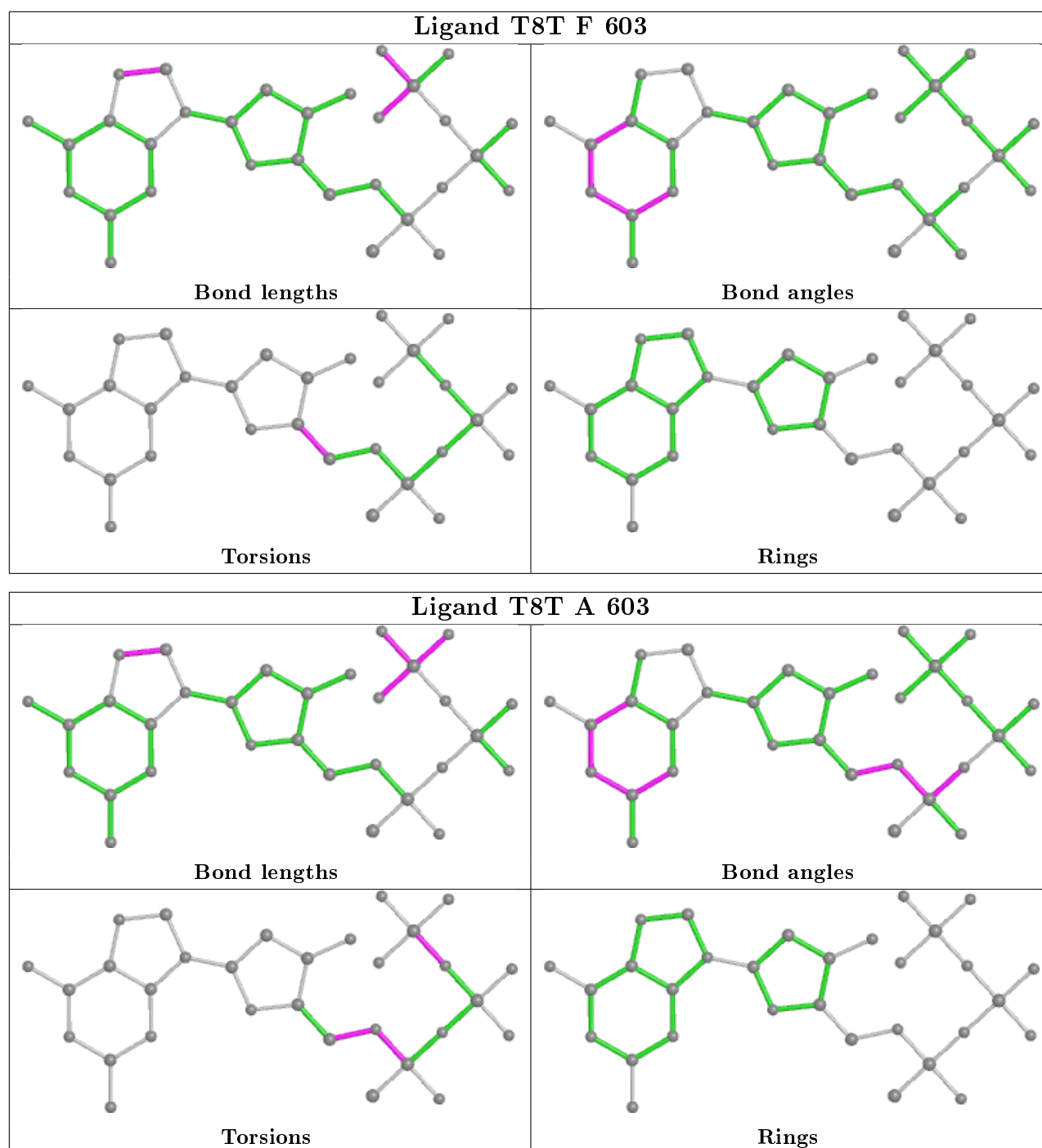


Torsions



Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

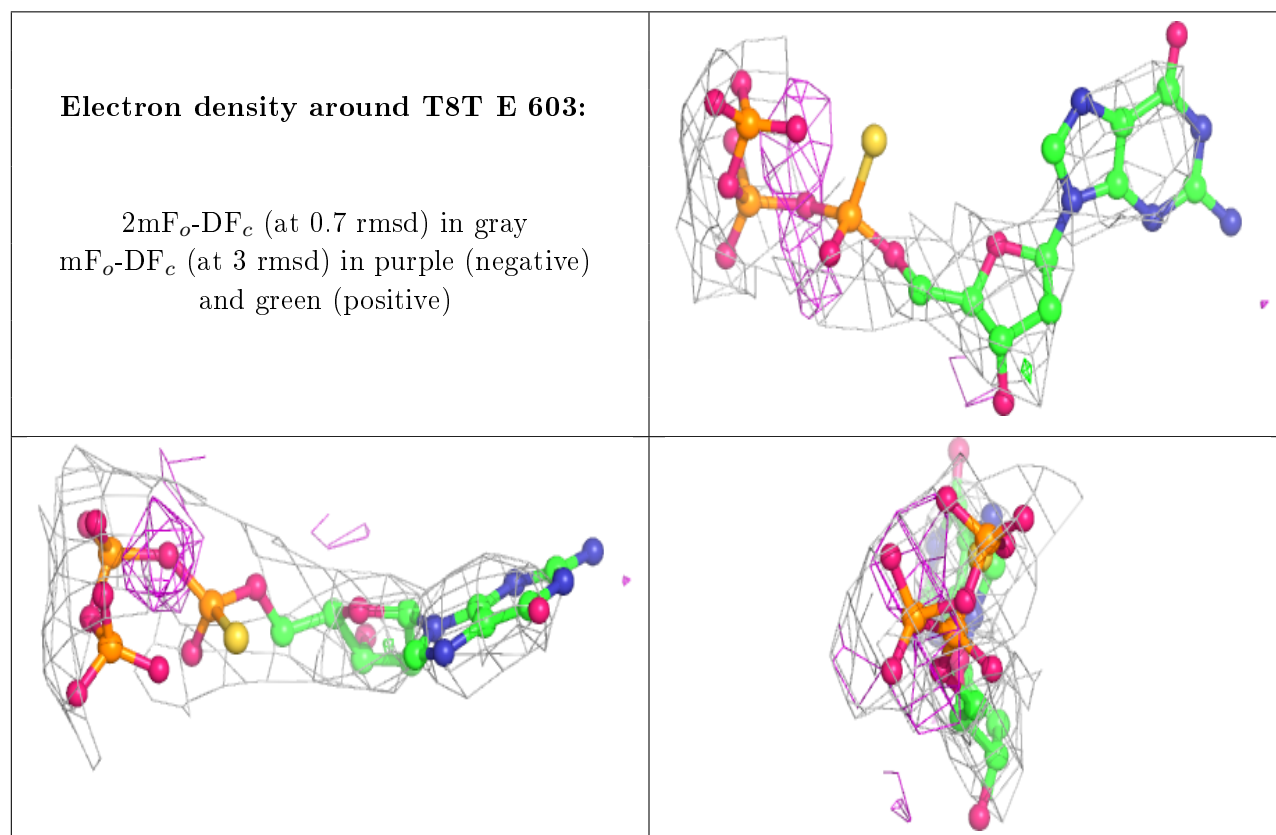
### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

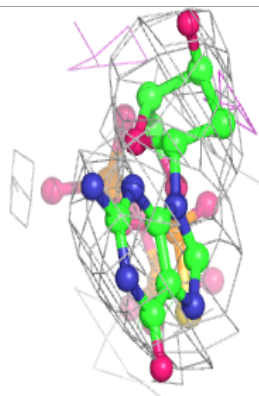
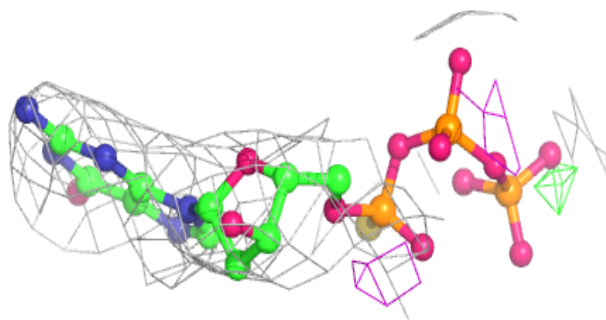
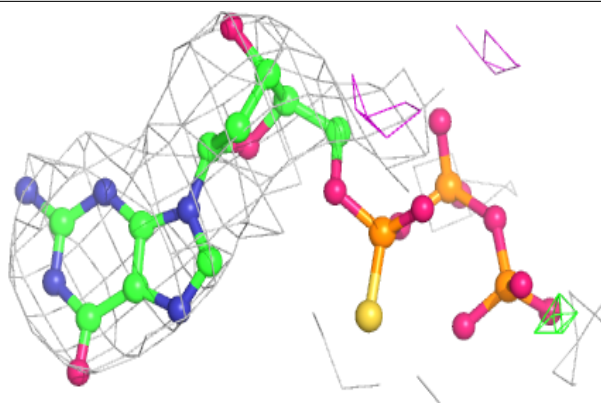
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

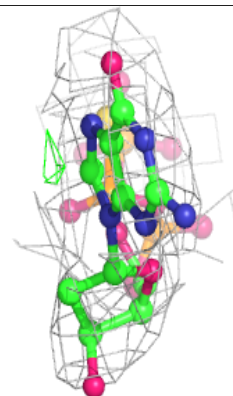
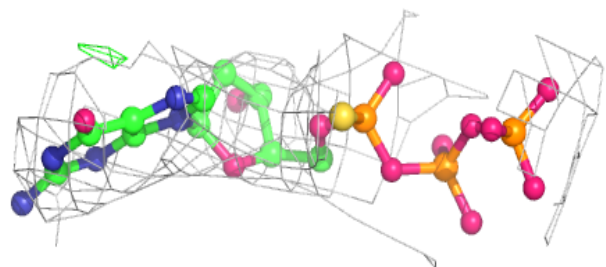
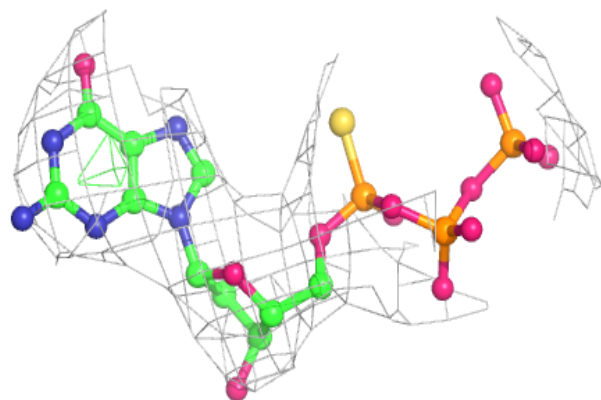


**Electron density around T8T B 602:**

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

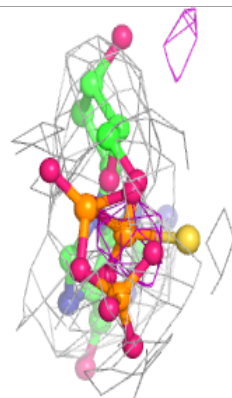
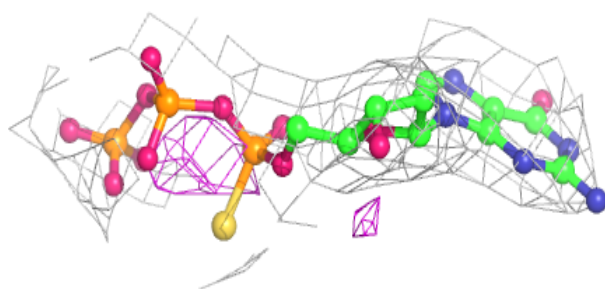
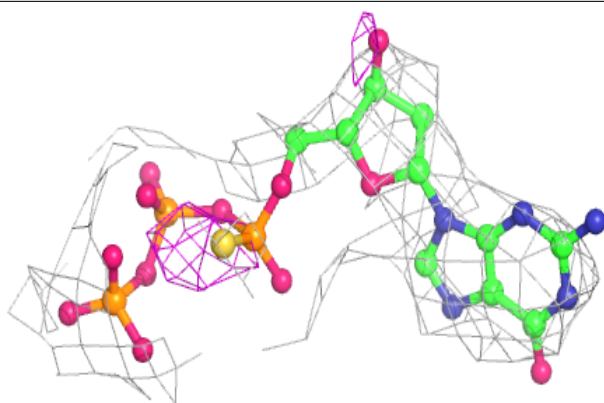
**Electron density around T8T D 602:**

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

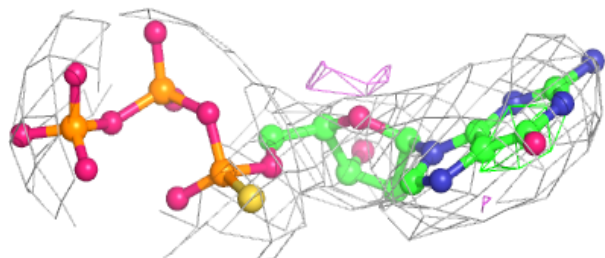
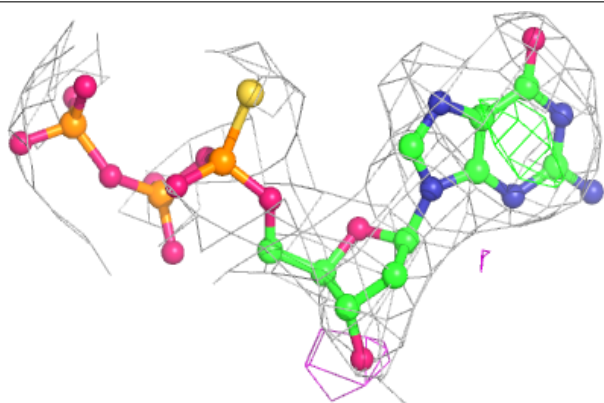


**Electron density around T8T C 602:**

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

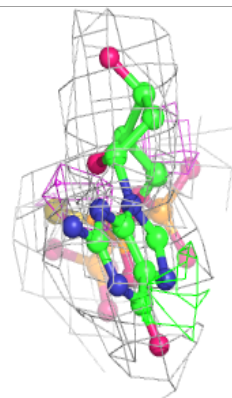
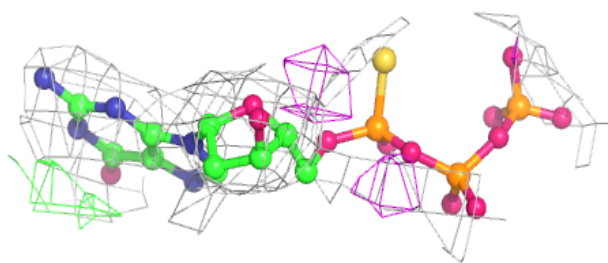
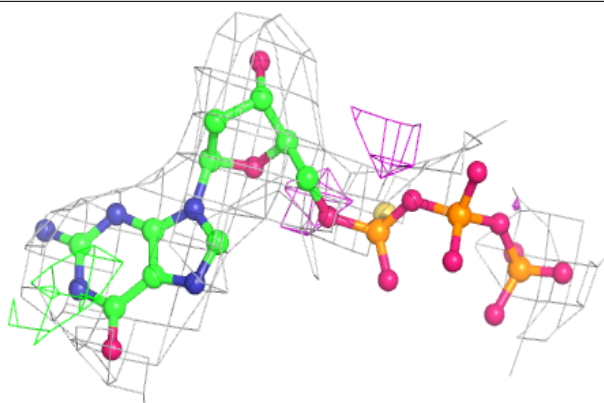
**Electron density around T8T F 603:**

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



**Electron density around T8T A 603:**

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



## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.