



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:48 AM UTC

PDB ID : 4ZWE / pdb_00004zwe
Title : Crystal structure of the dGTP-bound catalytic core of SAMHD1 T592V mutant
Authors : Tang, C.; Ji, X.; Xiong, Y.
Deposited on : 2015-05-19
Resolution : 2.81 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

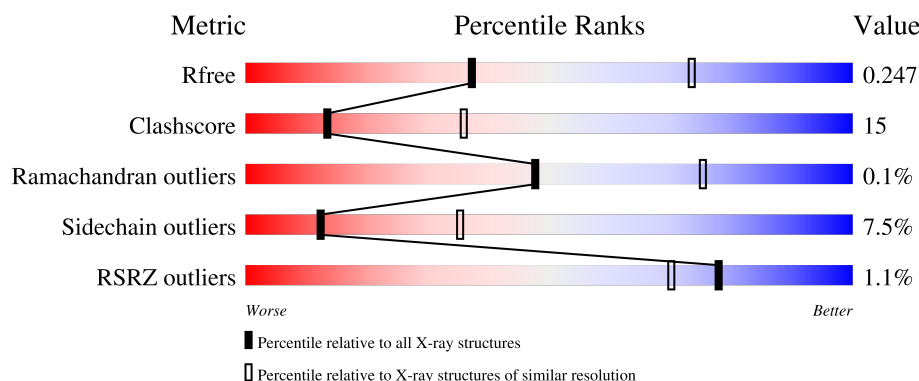
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	514	
1	B	514	
1	C	514	
1	D	514	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DGT	B	701	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16098 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.

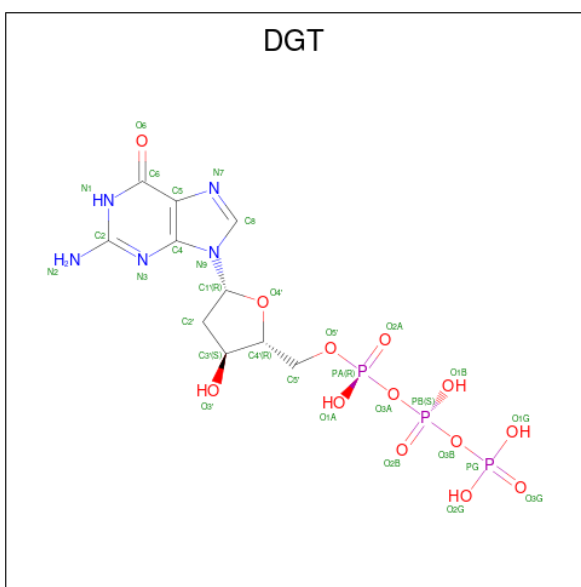
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3925	2514	684	707	20			
1	B	480	Total	C	N	O	S	0	1	0
			3934	2519	686	709	20			
1	C	480	Total	C	N	O	S	0	0	0
			3925	2514	684	707	20			
1	D	480	Total	C	N	O	S	0	1	0
			3934	2519	685	710	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
A	592	VAL	THR	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	592	VAL	THR	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	592	VAL	THR	engineered mutation	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
D	592	VAL	THR	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	B	2	Total 2	Mg 2	0	0
3	C	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0

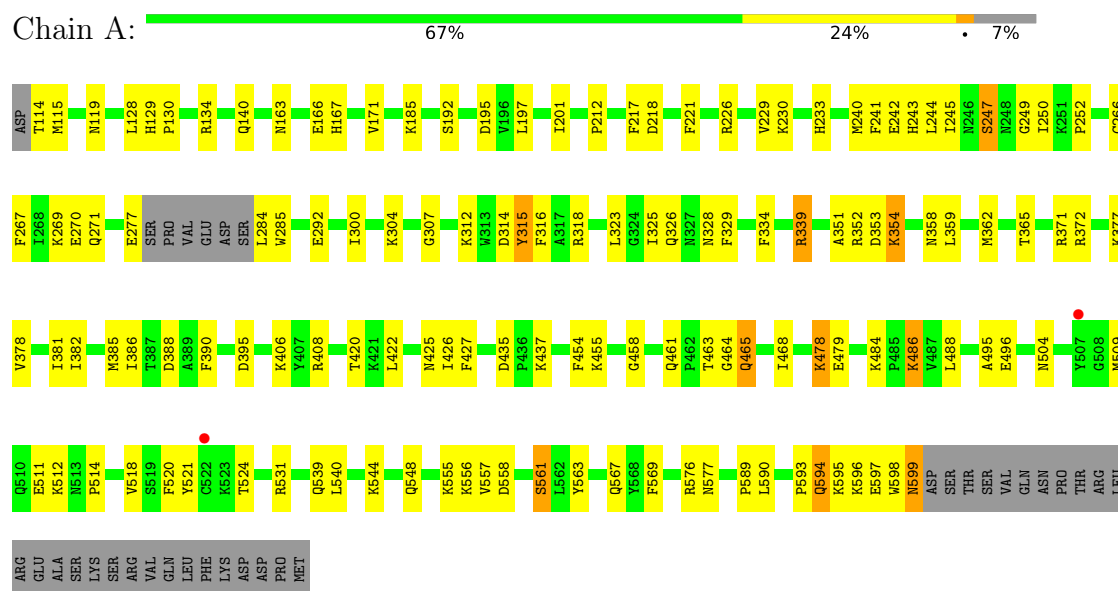
- Molecule 4 is water.

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

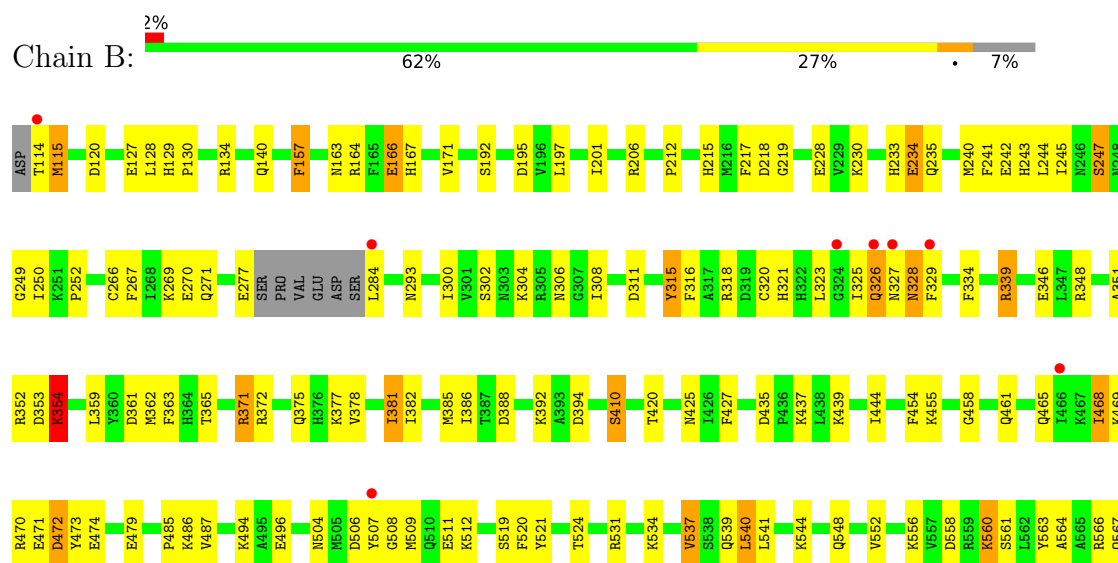
3 Residue-property plots

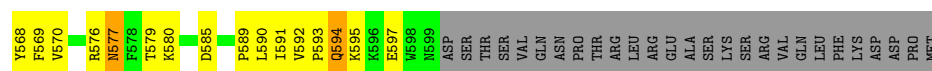
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

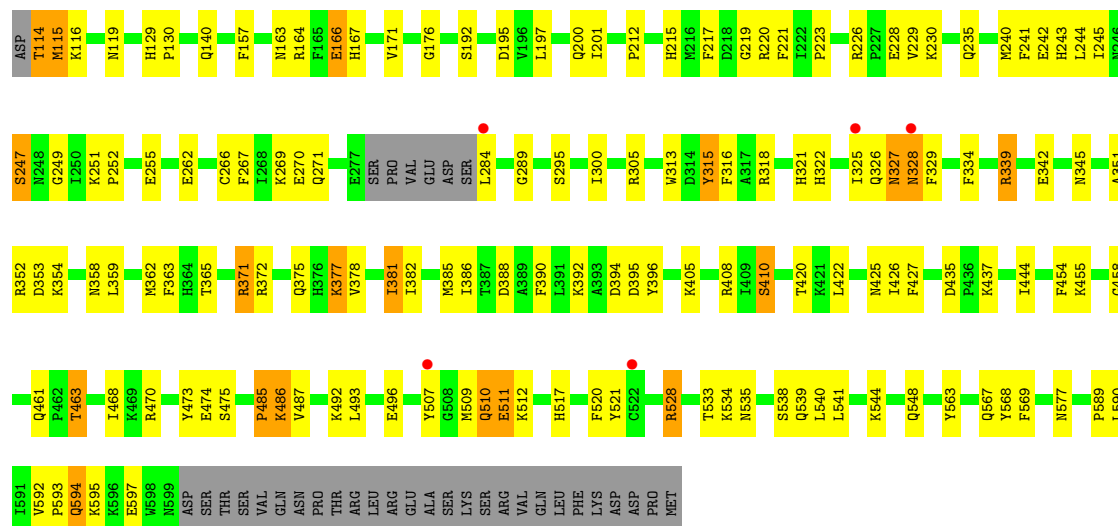


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

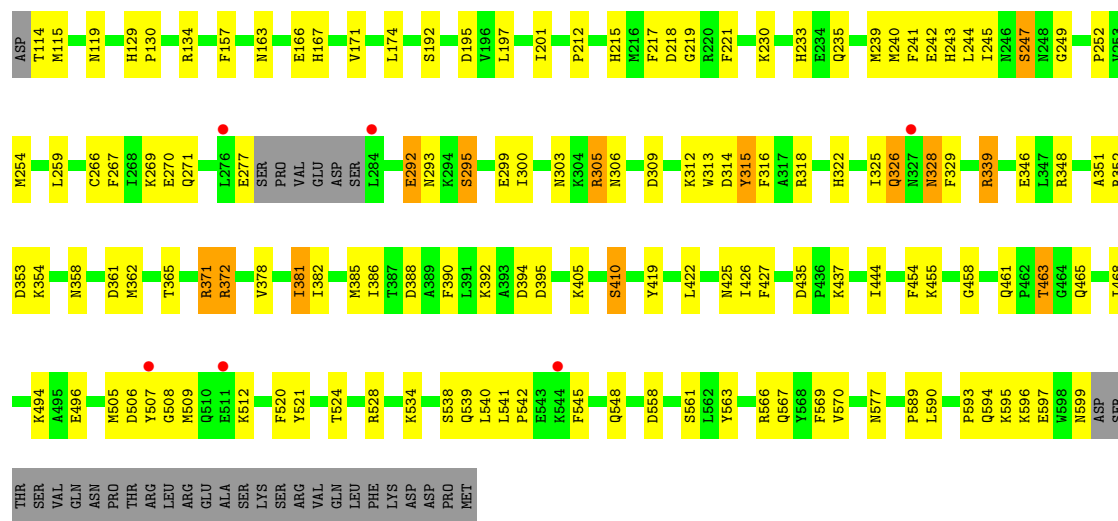




• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.08Å 146.09Å 98.46Å 90.00° 115.03° 90.00°	Depositor
Resolution (Å)	50.00 – 2.81 50.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.81) 98.4 (50.00-2.81)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.208 , 0.248 0.211 , 0.247	Depositor DCC
R_{free} test set	2790 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16098	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.80	0/4017	0.91	1/5422 (0.0%)
1	B	0.74	1/4026 (0.0%)	0.89	7/5434 (0.1%)
1	C	0.75	0/4017	0.89	4/5422 (0.1%)
1	D	0.79	0/4026	0.90	3/5434 (0.1%)
All	All	0.77	1/16086 (0.0%)	0.90	15/21712 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	234	GLU	C-O	-5.18	1.18	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	ILE	N-CA-C	8.44	118.47	110.53
1	D	300	ILE	N-CA-C	7.61	117.68	110.53
1	C	485	PRO	N-CA-C	7.53	123.99	113.53
1	C	300	ILE	N-CA-C	7.46	117.54	110.53
1	B	300	ILE	N-CA-C	7.12	117.22	110.53
1	B	157	PHE	CA-C-N	-6.04	113.46	119.56
1	B	157	PHE	C-N-CA	-6.04	113.46	119.56
1	C	157	PHE	CA-C-N	-5.67	113.83	119.56
1	C	157	PHE	C-N-CA	-5.67	113.83	119.56
1	B	354	LYS	CB-CG-CD	-5.62	98.38	111.30
1	B	234	GLU	CA-C-N	-5.54	112.80	120.38
1	B	234	GLU	C-N-CA	-5.54	112.80	120.38
1	B	327	ASN	N-CA-C	5.41	118.74	110.20
1	D	157	PHE	CA-C-N	-5.35	114.16	119.56
1	D	157	PHE	C-N-CA	-5.35	114.16	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3925	0	3919	103	0
1	B	3934	0	3922	157	0
1	C	3925	0	3919	123	0
1	D	3934	0	3923	99	0
2	A	124	0	48	4	0
2	B	93	0	36	23	0
2	C	62	0	24	9	0
2	D	93	0	36	7	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	3	0	0	0	0
All	All	16098	0	15827	468	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 15.

All (468) 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:D:303:ASN:ND2	1:D:306:ASN:OD1	1.56	1.37
1:B:329:PHE:CD2	1:B:362:MET:HB2	1.62	1.35
1:D:303:ASN:CG	1:D:306:ASN:OD1	1.71	1.30
1:B:328:ASN:CB	1:B:365:THR:OG1	1.82	1.28
1:B:354:LYS:HZ1	2:B:705:DGT:PA	1.58	1.24
1:D:242:GLU:OE1	1:D:269:LYS:NZ	1.74	1.21
1:C:242:GLU:OE1	1:C:269:LYS:NZ	1.75	1.20
1:B:469:LYS:N	1:B:472:ASP:OD2	1.74	1.18
1:B:354:LYS:NZ	2:B:705:DGT:PA	2.16	1.18
1:B:470:ARG:HA	1:B:473:TYR:CE2	1.80	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:ASP:CG	1:A:561:SER:OG	1.92	1.12
1:A:329:PHE:CD2	1:A:362:MET:HG3	1.92	1.04
1:B:215:HIS:CE1	2:B:701:DGT:O2B	2.11	1.04
1:B:242:GLU:OE1	1:B:269:LYS:NZ	1.89	1.04
1:B:328:ASN:HB3	1:B:365:THR:OG1	1.49	1.04
1:B:328:ASN:HB2	1:B:365:THR:OG1	1.54	1.03
1:A:395:ASP:OD1	1:A:408:ARG:NH1	1.91	1.03
1:B:375:GLN:NE2	2:B:701:DGT:O6	1.92	1.02
1:A:242:GLU:OE1	1:A:269:LYS:NZ	1.92	1.01
1:A:558:ASP:OD2	1:A:561:SER:OG	1.77	1.01
1:C:533:THR:OG1	1:C:535:ASN:OD1	1.80	1.00
1:B:577:ASN:ND2	1:B:595:LYS:NZ	2.10	0.99
1:A:558:ASP:OD1	1:A:561:SER:OG	1.75	0.98
1:D:315:TYR:OH	2:D:703:DGT:O3G	1.82	0.96
1:C:394:ASP:OD2	1:C:410:SER:OG	1.83	0.96
1:D:394:ASP:OD2	1:D:410:SER:OG	1.83	0.96
1:B:597:GLU:OE1	1:B:597:GLU:N	1.99	0.96
1:A:558:ASP:CG	1:A:561:SER:HG	1.67	0.95
1:B:394:ASP:OD2	1:B:410:SER:OG	1.82	0.95
1:A:314:ASP:OD1	1:A:318:ARG:NH2	2.00	0.94
1:D:597:GLU:N	1:D:597:GLU:OE1	2.00	0.94
1:B:425:ASN:ND2	1:C:425:ASN:OD1	2.01	0.94
1:A:425:ASN:OD1	1:D:425:ASN:ND2	2.01	0.94
1:B:329:PHE:CD2	1:B:362:MET:CB	2.49	0.93
1:A:597:GLU:N	1:A:597:GLU:OE1	2.00	0.93
1:C:328:ASN:OD1	1:C:365:THR:OG1	1.85	0.92
1:B:329:PHE:HD2	1:B:362:MET:HB2	1.22	0.91
1:B:328:ASN:HB3	1:B:365:THR:HG1	1.30	0.90
1:B:577:ASN:HD22	1:B:595:LYS:HZ3	1.19	0.90
1:A:354:LYS:NZ	2:A:704:DGT:O1A	2.04	0.89
1:B:354:LYS:NZ	2:B:705:DGT:O2A	2.01	0.89
1:A:328:ASN:HB3	1:A:365:THR:OG1	1.74	0.88
1:B:372:ARG:NH2	1:D:358:ASN:OD1	2.07	0.87
1:B:577:ASN:ND2	1:B:595:LYS:HZ3	1.71	0.87
1:A:479:GLU:OE1	1:A:576:ARG:NH2	2.11	0.84
1:B:469:LYS:N	1:B:472:ASP:CG	2.33	0.83
1:C:266:CYS:O	1:C:270:GLU:HG3	1.79	0.82
1:C:228:GLU:OE2	1:C:228:GLU:N	2.10	0.81
1:D:266:CYS:O	1:D:270:GLU:HG3	1.81	0.80
1:D:312:LYS:NZ	2:D:703:DGT:O1G	2.12	0.80
1:A:372:ARG:NH1	1:C:358:ASN:OD1	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:SER:OG	1:C:195:ASP:OD2	2.00	0.80
1:A:465:GLN:H	1:A:465:GLN:HE21	1.27	0.80
1:B:266:CYS:O	1:B:270:GLU:HG3	1.81	0.79
1:D:243:HIS:O	1:D:247:SER:OG	2.01	0.79
1:D:506:ASP:OD1	1:D:508:GLY:N	2.15	0.79
1:B:375:GLN:NE2	2:B:701:DGT:C6	2.46	0.79
1:B:329:PHE:CE2	1:B:362:MET:HB2	2.17	0.79
1:A:266:CYS:O	1:A:270:GLU:HG3	1.84	0.78
1:B:315:TYR:OH	2:B:701:DGT:O2G	2.00	0.78
1:D:558:ASP:OD1	1:D:561:SER:OG	2.03	0.77
1:A:486:LYS:HE2	1:A:594:GLN:NE2	1.99	0.76
1:C:509:MET:HE2	1:C:512:LYS:HD2	1.65	0.76
1:B:157:PHE:CD2	1:B:323:LEU:HD22	2.21	0.76
1:B:375:GLN:HE22	2:B:701:DGT:C6	1.99	0.76
1:C:371:ARG:NH1	1:C:372:ARG:HE	1.85	0.75
1:D:303:ASN:ND2	1:D:306:ASN:CG	2.43	0.74
1:B:577:ASN:HD22	1:B:595:LYS:NZ	1.76	0.74
1:B:479:GLU:OE2	1:B:576:ARG:NH2	2.19	0.74
1:B:325:ILE:HG22	1:B:326:GLN:N	2.02	0.73
1:C:342:GLU:OE2	1:C:345:ASN:N	2.19	0.73
1:A:329:PHE:HD2	1:A:362:MET:HG3	1.48	0.73
1:B:215:HIS:NE2	2:B:701:DGT:O2B	2.22	0.73
1:C:487:VAL:HG23	1:C:590:LEU:HD12	1.70	0.72
1:B:215:HIS:CD2	2:B:701:DGT:O4'	2.42	0.72
1:A:558:ASP:OD1	1:A:561:SER:N	2.20	0.72
1:D:534:LYS:NZ	1:D:541:LEU:O	2.22	0.71
1:C:243:HIS:O	1:C:247:SER:OG	2.08	0.70
1:C:485:PRO:O	1:C:486:LYS:HB2	1.92	0.69
1:B:487:VAL:HG23	1:B:590:LEU:HD12	1.74	0.69
1:B:577:ASN:ND2	1:B:595:LYS:HZ1	1.89	0.68
1:B:361:ASP:OD2	1:D:372:ARG:NH2	2.27	0.68
1:B:215:HIS:HE1	2:B:701:DGT:O2B	1.69	0.68
1:A:328:ASN:HB3	1:A:365:THR:HG1	1.60	0.67
1:A:329:PHE:CD2	1:A:362:MET:CG	2.75	0.67
1:C:378:VAL:O	1:C:381:ILE:HG22	1.95	0.67
1:B:469:LYS:CA	1:B:472:ASP:OD2	2.43	0.67
1:B:592:VAL:HG13	1:B:593:PRO:HD3	1.77	0.66
1:B:378:VAL:O	1:B:381:ILE:HG22	1.95	0.66
1:A:378:VAL:O	1:A:381:ILE:HG22	1.95	0.66
1:B:243:HIS:O	1:B:247:SER:OG	2.13	0.65
1:D:378:VAL:O	1:D:381:ILE:HG22	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:705:DGT:O6	1:D:372:ARG:HG2	1.96	0.65
1:B:506:ASP:OD1	1:B:508:GLY:N	2.25	0.65
1:B:487:VAL:CG2	1:B:590:LEU:HD12	2.28	0.64
1:C:408:ARG:HH11	1:C:408:ARG:HG2	1.62	0.64
1:B:325:ILE:HG22	1:B:326:GLN:H	1.62	0.64
1:C:487:VAL:CG2	1:C:590:LEU:HD12	2.28	0.64
1:A:328:ASN:CB	1:A:365:THR:OG1	2.46	0.63
1:B:140:GLN:HG3	1:B:240:MET:CE	2.28	0.63
1:D:339:ARG:HB2	1:D:521:TYR:CE1	2.34	0.63
1:C:226:ARG:HB3	1:C:229:VAL:HG12	1.81	0.63
1:A:140:GLN:HG3	1:A:240:MET:CE	2.28	0.62
1:A:339:ARG:HB2	1:A:521:TYR:CE2	2.33	0.62
1:C:509:MET:HE2	1:C:512:LYS:CD	2.29	0.62
1:A:243:HIS:O	1:A:247:SER:OG	2.16	0.62
1:D:594:GLN:HG3	1:D:595:LYS:N	2.12	0.62
1:C:140:GLN:HG3	1:C:240:MET:CE	2.29	0.62
1:C:528:ARG:HH21	1:C:528:ARG:HG3	1.65	0.62
1:B:558:ASP:OD1	1:B:561:SER:N	2.30	0.62
1:B:592:VAL:CG1	1:B:593:PRO:HD3	2.29	0.61
1:D:235:GLN:HG3	1:D:239:MET:HE3	1.82	0.61
1:B:352:ARG:NE	1:B:353:ASP:OD1	2.30	0.61
1:A:325:ILE:HG22	1:A:326:GLN:N	2.16	0.61
1:B:377:LYS:HG2	1:B:378:VAL:N	2.15	0.61
1:C:240:MET:HE1	1:C:420:THR:OG1	2.01	0.61
1:C:226:ARG:CB	1:C:229:VAL:HG12	2.30	0.61
1:B:470:ARG:O	1:B:473:TYR:CD2	2.55	0.60
1:D:509:MET:HE2	1:D:512:LYS:HE2	1.83	0.60
1:D:463:THR:OG1	1:D:577:ASN:O	2.18	0.60
1:B:240:MET:HE1	1:B:420:THR:OG1	2.02	0.60
1:B:385:MET:HG2	1:B:454:PHE:CE2	2.37	0.59
1:C:509:MET:HB3	1:C:512:LYS:HB2	1.84	0.59
1:B:215:HIS:CD2	2:B:701:DGT:C1'	2.86	0.59
2:B:704:DGT:O3G	1:C:455:LYS:NZ	2.35	0.59
1:D:352:ARG:NE	1:D:353:ASP:OD1	2.34	0.59
1:B:470:ARG:CA	1:B:473:TYR:CE2	2.73	0.58
1:C:352:ARG:NE	1:C:353:ASP:OD1	2.32	0.58
1:D:244:LEU:C	1:D:244:LEU:HD23	2.28	0.58
1:A:115:MET:HB2	1:A:128:LEU:O	2.04	0.58
1:C:315:TYR:CE1	1:C:316:PHE:CE1	2.90	0.58
1:B:534:LYS:NZ	1:B:541:LEU:O	2.37	0.58
1:C:244:LEU:C	1:C:244:LEU:HD23	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:GLU:O	1:D:295:SER:OG	2.15	0.58
1:D:315:TYR:CZ	2:D:703:DGT:O3G	2.55	0.58
1:B:339:ARG:HB2	1:B:521:TYR:CE2	2.38	0.58
1:A:465:GLN:HE21	1:A:465:GLN:N	2.01	0.58
1:B:244:LEU:HD23	1:B:244:LEU:C	2.28	0.58
1:B:306:ASN:OD1	1:B:308:ILE:HG13	2.04	0.58
1:B:315:TYR:CE1	1:B:316:PHE:CE1	2.91	0.58
1:A:486:LYS:HE2	1:A:594:GLN:HE22	1.68	0.58
1:A:377:LYS:HG2	1:A:378:VAL:N	2.19	0.57
1:C:119:ASN:ND2	2:D:702:DGT:HN2A	2.01	0.57
1:A:315:TYR:CE1	1:A:316:PHE:CE1	2.92	0.57
1:B:215:HIS:HD2	2:B:701:DGT:C1'	2.18	0.57
1:C:377:LYS:HG2	1:C:378:VAL:N	2.18	0.57
1:D:303:ASN:OD1	1:D:306:ASN:OD1	2.18	0.57
1:A:352:ARG:NE	1:A:353:ASP:OD1	2.35	0.57
1:D:351:ALA:O	1:D:520:PHE:HA	2.05	0.57
1:C:327:ASN:HB2	1:C:365:THR:HG21	1.86	0.56
1:D:240:MET:HE2	1:D:419:TYR:HD2	1.70	0.56
1:D:461:GLN:HG2	1:D:548:GLN:O	2.05	0.56
1:A:244:LEU:C	1:A:244:LEU:HD23	2.30	0.56
1:B:371:ARG:HH12	1:B:372:ARG:HE	1.52	0.56
1:A:354:LYS:HZ3	2:A:704:DGT:PA	2.28	0.56
1:B:351:ALA:O	1:B:520:PHE:HA	2.05	0.56
1:A:395:ASP:CG	1:A:408:ARG:NH1	2.63	0.56
1:B:577:ASN:HD21	1:B:595:LYS:NZ	2.02	0.56
1:C:251:LYS:O	1:C:255:GLU:HG3	2.05	0.56
1:B:157:PHE:CG	1:B:323:LEU:HD22	2.40	0.56
1:B:435:ASP:OD2	1:B:437:LYS:HE3	2.06	0.56
1:C:226:ARG:O	1:C:229:VAL:HG12	2.05	0.55
1:C:509:MET:CE	1:C:512:LYS:HD2	2.35	0.55
1:A:240:MET:HE1	1:A:420:THR:OG1	2.05	0.55
1:A:509:MET:HB3	1:A:512:LYS:HB2	1.89	0.55
1:D:325:ILE:HG22	1:D:326:GLN:N	2.22	0.55
1:D:315:TYR:CE1	1:D:316:PHE:CE1	2.94	0.55
1:A:351:ALA:O	1:A:520:PHE:HA	2.06	0.55
1:C:493:LEU:HD12	1:C:568:TYR:CD2	2.42	0.55
1:B:461:GLN:HG2	1:B:548:GLN:O	2.07	0.54
1:A:314:ASP:CG	1:A:318:ARG:HH21	2.09	0.54
1:C:315:TYR:CE1	1:C:316:PHE:CD1	2.94	0.54
1:B:215:HIS:NE2	2:B:701:DGT:O4'	2.40	0.54
1:B:470:ARG:HA	1:B:473:TYR:CD2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:LYS:CB	1:B:472:ASP:OD2	2.56	0.54
2:B:701:DGT:H5'A	2:B:701:DGT:O3B	2.07	0.54
1:B:363:PHE:HB3	1:B:507:TYR:CE2	2.43	0.54
1:D:534:LYS:HZ3	1:D:541:LEU:C	2.14	0.54
1:C:339:ARG:HB2	1:C:521:TYR:CE2	2.43	0.54
1:A:218:ASP:OD2	1:A:233:HIS:HD2	1.91	0.53
1:B:354:LYS:NZ	2:B:705:DGT:O1A	2.27	0.53
1:C:351:ALA:O	1:C:520:PHE:HA	2.08	0.53
1:B:164:ARG:HH22	2:B:701:DGT:H4'	1.73	0.53
1:C:325:ILE:HG22	1:C:326:GLN:N	2.24	0.53
1:C:509:MET:HE2	1:C:512:LYS:HB2	1.90	0.53
1:B:311:ASP:OD1	2:B:701:DGT:O1A	2.26	0.53
1:B:315:TYR:CE1	1:B:316:PHE:CD1	2.96	0.53
1:A:315:TYR:CE1	1:A:316:PHE:CD1	2.97	0.53
1:A:486:LYS:CE	1:A:594:GLN:NE2	2.71	0.53
1:B:589:PRO:O	1:B:593:PRO:HD3	2.08	0.53
1:C:461:GLN:HG2	1:C:548:GLN:O	2.07	0.53
1:A:385:MET:HG2	1:A:454:PHE:CE2	2.44	0.53
1:A:461:GLN:HG2	1:A:548:GLN:O	2.09	0.53
1:B:325:ILE:CG2	1:B:326:GLN:N	2.69	0.53
1:A:315:TYR:CD1	1:A:315:TYR:C	2.88	0.52
1:B:234:GLU:O	1:B:235[B]:GLN:C	2.47	0.52
1:D:235:GLN:HG3	1:D:239:MET:CE	2.39	0.52
1:B:485:PRO:O	1:B:486:LYS:HB2	2.09	0.52
1:D:422:LEU:CD1	1:D:426:ILE:HG13	2.40	0.52
1:B:120:ASP:CG	1:B:318:ARG:HH22	2.18	0.52
1:C:590:LEU:O	1:C:593:PRO:HD2	2.09	0.52
1:C:595:LYS:HE3	1:C:597:GLU:OE1	2.09	0.52
1:B:465:GLN:HG3	1:B:465:GLN:O	2.10	0.52
1:D:299:GLU:OE2	1:D:305:ARG:NH1	2.43	0.52
1:D:329:PHE:CD1	1:D:362:MET:HB2	2.45	0.52
1:D:167:HIS:ND1	1:D:314:ASP:OD2	2.36	0.51
1:D:218:ASP:OD2	1:D:233:HIS:HD2	1.93	0.51
1:D:427:PHE:CD1	1:D:427:PHE:C	2.88	0.51
1:B:234:GLU:O	1:B:235[A]:GLN:C	2.48	0.51
1:B:594:GLN:N	1:B:594:GLN:OE1	2.44	0.51
1:A:478:LYS:HD2	1:A:495:ALA:HB2	1.92	0.51
1:C:363:PHE:HB3	1:C:507:TYR:CE2	2.45	0.51
1:A:598:TRP:O	1:A:599:ASN:HB3	2.11	0.51
1:C:329:PHE:HB2	1:C:362:MET:HA	1.92	0.51
1:A:167:HIS:ND1	1:A:314:ASP:OD2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:GLU:OE1	1:C:289:GLY:N	2.43	0.51
1:B:590:LEU:O	1:B:593:PRO:HD2	2.11	0.51
1:C:385:MET:HG2	1:C:454:PHE:CE2	2.46	0.51
1:B:329:PHE:HB2	1:B:362:MET:HA	1.91	0.51
1:D:385:MET:HG2	1:D:454:PHE:CE2	2.45	0.51
1:A:589:PRO:O	1:A:593:PRO:HD3	2.10	0.51
1:B:215:HIS:CD2	2:B:701:DGT:N9	2.79	0.51
1:D:589:PRO:O	1:D:593:PRO:HD3	2.11	0.51
1:B:140:GLN:HG3	1:B:240:MET:HE2	1.93	0.50
1:B:218:ASP:OD2	1:B:233:HIS:HD2	1.94	0.50
1:B:392:LYS:HE2	1:B:444:ILE:HD11	1.93	0.50
1:C:589:PRO:O	1:C:593:PRO:HD3	2.10	0.50
1:D:371:ARG:HG3	1:D:505:MET:HE2	1.94	0.50
1:A:463:THR:HG22	1:A:464:GLY:N	2.26	0.50
1:D:329:PHE:HB2	1:D:362:MET:HA	1.92	0.50
1:D:394:ASP:CG	1:D:410:SER:OG	2.52	0.50
1:C:392:LYS:HE2	1:C:444:ILE:HD11	1.94	0.50
1:A:486:LYS:CD	1:A:594:GLN:NE2	2.75	0.50
1:A:435:ASP:OD1	1:A:437:LYS:HG3	2.12	0.50
1:C:119:ASN:HD21	2:D:702:DGT:HN2A	1.58	0.50
1:D:435:ASP:OD1	1:D:437:LYS:HG3	2.11	0.50
1:D:509:MET:HB3	1:D:512:LYS:HB2	1.94	0.50
1:B:504:ASN:OD1	1:B:548:GLN:NE2	2.28	0.50
1:D:318:ARG:O	1:D:322:HIS:HD2	1.95	0.49
1:B:325:ILE:CG2	1:B:326:GLN:H	2.24	0.49
1:C:470:ARG:NH1	1:C:470:ARG:HB2	2.27	0.49
1:C:140:GLN:HG3	1:C:240:MET:HE2	1.94	0.49
1:C:318:ARG:O	1:C:322:HIS:HD2	1.96	0.49
1:C:422:LEU:CD1	1:C:426:ILE:HG13	2.42	0.49
1:D:315:TYR:CE1	1:D:316:PHE:CD1	3.00	0.49
1:A:267:PHE:O	1:A:271:GLN:HG3	2.13	0.49
1:C:394:ASP:CG	1:C:410:SER:OG	2.53	0.49
1:C:427:PHE:CD1	1:C:427:PHE:C	2.90	0.49
1:A:326:GLN:HB3	1:C:327:ASN:O	2.13	0.49
1:B:206:ARG:HD3	1:B:311:ASP:OD2	2.13	0.49
1:B:315:TYR:CZ	2:B:701:DGT:O2G	2.66	0.49
1:B:329:PHE:HD2	1:B:362:MET:CB	2.05	0.49
1:C:396:TYR:CD2	1:C:437:LYS:HB3	2.48	0.49
1:A:422:LEU:CD1	1:A:426:ILE:HG13	2.43	0.49
1:B:267:PHE:O	1:B:271:GLN:HG3	2.13	0.49
1:B:315:TYR:CD1	1:B:315:TYR:C	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:ARG:HH11	1:C:372:ARG:HE	1.56	0.49
1:C:221:PHE:CE1	1:C:390:PHE:HB3	2.48	0.48
1:C:493:LEU:HD12	1:C:568:TYR:CE2	2.48	0.48
1:B:509:MET:HE2	1:B:512:LYS:HE2	1.94	0.48
1:A:518:VAL:O	1:A:531:ARG:NH1	2.46	0.48
1:B:577:ASN:ND2	1:B:595:LYS:CE	2.76	0.48
1:D:458:GLY:HA3	1:D:569:PHE:CE2	2.48	0.48
1:C:242:GLU:OE1	1:C:269:LYS:CE	2.59	0.48
1:A:455:LYS:HG2	1:A:557:VAL:HG12	1.95	0.48
1:A:509:MET:HE2	1:A:512:LYS:HB2	1.95	0.48
1:D:242:GLU:OE1	1:D:269:LYS:CE	2.59	0.48
1:B:394:ASP:CG	1:B:410:SER:OG	2.52	0.48
1:B:509:MET:HB3	1:B:512:LYS:HB2	1.96	0.48
1:A:221:PHE:CE1	1:A:390:PHE:HB3	2.49	0.48
1:A:463:THR:OG1	1:A:577:ASN:O	2.15	0.48
1:C:328:ASN:OD1	1:C:328:ASN:N	2.45	0.48
1:C:267:PHE:O	1:C:271:GLN:HG3	2.13	0.48
1:D:392:LYS:HE2	1:D:444:ILE:HD11	1.95	0.48
1:A:358:ASN:OD1	1:C:372:ARG:NH1	2.46	0.48
1:D:590:LEU:O	1:D:593:PRO:HD2	2.13	0.48
1:A:590:LEU:O	1:A:593:PRO:HD2	2.13	0.48
1:A:140:GLN:HG3	1:A:240:MET:HE2	1.94	0.47
1:A:323:LEU:O	1:D:119:ASN:ND2	2.47	0.47
1:B:519:SER:OG	1:B:531:ARG:NH1	2.47	0.47
1:C:116:LYS:NZ	2:C:702:DGT:O1G	2.47	0.47
1:C:215:HIS:CD2	2:C:703:DGT:N9	2.82	0.47
1:B:427:PHE:CD1	1:B:427:PHE:C	2.92	0.47
1:A:354:LYS:NZ	2:A:704:DGT:PA	2.87	0.47
1:B:580:LYS:NZ	1:B:585:ASP:OD2	2.46	0.47
1:C:241:PHE:O	1:C:245:ILE:HG12	2.15	0.47
1:C:315:TYR:CD1	1:C:315:TYR:C	2.91	0.47
1:B:469:LYS:HB2	1:B:472:ASP:CG	2.38	0.47
1:C:197:LEU:O	1:C:201:ILE:HG13	2.15	0.47
1:C:594:GLN:HG3	1:C:595:LYS:N	2.29	0.47
1:C:329:PHE:CD1	1:C:362:MET:HB2	2.49	0.47
1:D:267:PHE:O	1:D:271:GLN:HG3	2.14	0.47
1:D:422:LEU:HD12	1:D:426:ILE:HG13	1.97	0.47
1:C:539:GLN:HA	1:C:539:GLN:OE1	2.15	0.47
1:D:313:TRP:CD1	1:D:329:PHE:HE2	2.32	0.47
1:A:212:PRO:HD2	1:A:217:PHE:CD1	2.50	0.47
1:A:325:ILE:CG2	1:A:326:GLN:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:GLY:O	1:C:252:PRO:HD2	2.15	0.47
1:D:197:LEU:O	1:D:201:ILE:HG13	2.15	0.47
1:B:363:PHE:CB	1:B:507:TYR:CE2	2.97	0.47
1:B:577:ASN:HD21	1:B:595:LYS:HZ1	1.58	0.47
1:D:315:TYR:CD1	1:D:315:TYR:C	2.93	0.47
1:C:375:GLN:HE22	2:C:703:DGT:C6	2.28	0.46
1:C:212:PRO:HD2	1:C:217:PHE:CD1	2.49	0.46
1:D:539:GLN:OE1	1:D:539:GLN:HA	2.15	0.46
1:B:249:GLY:O	1:B:252:PRO:HD2	2.15	0.46
1:B:435:ASP:CG	1:B:437:LYS:HE3	2.41	0.46
1:B:563:TYR:O	1:B:567:GLN:HG2	2.15	0.46
1:C:226:ARG:CB	1:C:229:VAL:CG1	2.92	0.46
1:A:594:GLN:HG3	1:A:595:LYS:N	2.29	0.46
1:C:163:ASN:O	1:C:166:GLU:HG2	2.16	0.46
1:D:534:LYS:HZ2	1:D:541:LEU:HB2	1.81	0.46
1:A:458:GLY:HA3	1:A:569:PHE:CE2	2.50	0.46
1:A:496:GLU:O	1:A:555:LYS:HE3	2.16	0.46
1:B:241:PHE:O	1:B:245:ILE:HG12	2.16	0.46
1:D:241:PHE:O	1:D:245:ILE:HG12	2.15	0.46
1:B:157:PHE:CG	1:B:323:LEU:CD2	2.99	0.46
1:B:334:PHE:CE2	1:B:359:LEU:HD21	2.51	0.46
1:B:115:MET:HG3	1:B:128:LEU:O	2.16	0.46
1:B:197:LEU:O	1:B:201:ILE:HG13	2.16	0.46
1:A:241:PHE:O	1:A:245:ILE:HG12	2.16	0.46
2:A:703:DGT:H3'	2:A:703:DGT:O2A	2.16	0.46
1:B:326:GLN:OE1	1:D:326:GLN:HG2	2.15	0.46
1:B:552:VAL:HG21	1:B:569:PHE:CD1	2.51	0.46
1:A:427:PHE:CD1	1:A:427:PHE:C	2.94	0.45
1:B:435:ASP:OD1	1:B:437:LYS:HE3	2.16	0.45
1:A:197:LEU:O	1:A:201:ILE:HG13	2.16	0.45
1:B:461:GLN:H	1:B:579:THR:HG1	1.64	0.45
1:C:563:TYR:O	1:C:567:GLN:HG2	2.16	0.45
1:D:212:PRO:HD2	1:D:217:PHE:CD1	2.51	0.45
1:B:469:LYS:CB	1:B:472:ASP:CG	2.89	0.45
1:A:119:ASN:ND2	2:B:705:DGT:HN2A	2.14	0.45
1:B:372:ARG:CZ	1:D:358:ASN:OD1	2.64	0.45
1:A:563:TYR:O	1:A:567:GLN:HG2	2.16	0.45
1:D:221:PHE:CE1	1:D:390:PHE:HB3	2.52	0.45
1:B:564:ALA:O	1:B:568:TYR:HD1	1.98	0.45
1:C:129:HIS:CG	1:C:130:PRO:HD2	2.52	0.45
1:C:327:ASN:H	1:C:327:ASN:HD22	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASN:O	1:B:166:GLU:HG2	2.17	0.45
1:D:249:GLY:O	1:D:252:PRO:HD2	2.17	0.45
1:D:563:TYR:O	1:D:567:GLN:HG2	2.16	0.45
1:B:470:ARG:HG3	1:B:473:TYR:CE2	2.52	0.44
1:B:558:ASP:HB2	1:B:560:LYS:HD2	1.99	0.44
1:A:334:PHE:CE2	1:A:359:LEU:HD11	2.52	0.44
1:B:591:ILE:O	1:B:594:GLN:HG2	2.17	0.44
1:C:382:ILE:O	1:C:386:ILE:HG13	2.17	0.44
1:A:307:GLY:O	1:A:312:LYS:NZ	2.50	0.44
1:A:372:ARG:NE	1:C:358:ASN:OD1	2.50	0.44
1:B:140:GLN:CG	1:B:240:MET:CE	2.95	0.44
1:A:167:HIS:O	1:A:171:VAL:HG23	2.17	0.44
1:A:329:PHE:HB2	1:A:362:MET:HA	1.99	0.44
1:D:240:MET:HE2	1:D:419:TYR:CD2	2.51	0.44
1:A:382:ILE:O	1:A:386:ILE:HG13	2.18	0.44
1:B:315:TYR:CE1	1:B:316:PHE:HE1	2.36	0.44
1:B:329:PHE:CD2	1:B:362:MET:CG	3.01	0.44
1:D:134:ARG:HD2	1:D:134:ARG:HA	1.86	0.44
1:D:167:HIS:O	1:D:171:VAL:HG23	2.17	0.44
1:C:538:SER:HB3	1:C:541:LEU:HG	1.99	0.44
1:B:363:PHE:HB3	1:B:507:TYR:CD2	2.52	0.44
1:B:382:ILE:O	1:B:386:ILE:HG13	2.18	0.44
1:B:129:HIS:CG	1:B:130:PRO:HD2	2.53	0.43
1:B:167:HIS:O	1:B:171:VAL:HG23	2.17	0.43
1:C:167:HIS:O	1:C:171:VAL:HG23	2.17	0.43
1:A:465:GLN:H	1:A:465:GLN:NE2	2.05	0.43
1:B:371:ARG:NH2	1:D:361:ASP:OD2	2.44	0.43
1:B:563:TYR:CD1	1:B:563:TYR:C	2.96	0.43
1:C:315:TYR:OH	2:C:703:DGT:O2G	2.30	0.43
1:C:463:THR:OG1	1:C:577:ASN:O	2.35	0.43
1:A:163:ASN:O	1:A:166:GLU:HG2	2.18	0.43
1:A:315:TYR:CE1	1:A:316:PHE:HE1	2.37	0.43
1:A:422:LEU:HD12	1:A:426:ILE:HG13	2.00	0.43
1:B:212:PRO:HD2	1:B:217:PHE:CD1	2.54	0.43
1:D:163:ASN:O	1:D:166:GLU:HG2	2.18	0.43
1:C:313:TRP:CD1	1:C:329:PHE:HE2	2.36	0.43
1:C:334:PHE:CE2	1:C:359:LEU:HD11	2.54	0.43
1:D:346:GLU:OE1	1:D:348:ARG:NH2	2.50	0.43
1:B:293:ASN:OD1	1:B:293:ASN:N	2.52	0.43
1:C:325:ILE:O	1:C:326:GLN:OE1	2.36	0.43
1:A:372:ARG:CZ	1:C:358:ASN:OD1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ARG:HA	1:B:134:ARG:HD2	1.83	0.43
1:C:226:ARG:HB2	1:C:229:VAL:CG1	2.48	0.43
1:C:363:PHE:HB3	1:C:507:TYR:CD2	2.54	0.43
1:C:377:LYS:HG2	1:C:378:VAL:H	1.84	0.43
1:B:468:ILE:CG2	1:B:472:ASP:HB2	2.49	0.43
1:C:116:LYS:HZ1	2:C:702:DGT:PG	2.42	0.43
1:C:535:ASN:OD1	1:C:535:ASN:N	2.52	0.43
1:D:303:ASN:HD21	1:D:306:ASN:CG	2.22	0.43
1:D:309:ASP:C	1:D:309:ASP:OD1	2.62	0.43
1:D:593:PRO:HA	1:D:599:ASN:ND2	2.34	0.43
1:A:504:ASN:OD1	1:A:548:GLN:NE2	2.29	0.42
1:B:377:LYS:HG2	1:B:378:VAL:H	1.82	0.42
1:C:226:ARG:HB3	1:C:229:VAL:CG1	2.47	0.42
1:C:363:PHE:CB	1:C:507:TYR:CE2	3.02	0.42
1:A:114:THR:N	1:A:115:MET:HA	2.32	0.42
1:C:192:SER:O	1:C:195:ASP:HB2	2.19	0.42
1:C:244:LEU:HD23	1:C:244:LEU:O	2.19	0.42
1:B:566:ARG:O	1:B:570:VAL:HG23	2.20	0.42
1:A:192:SER:O	1:A:195:ASP:HB2	2.20	0.42
1:C:215:HIS:O	1:C:219:GLY:N	2.50	0.42
1:D:174:LEU:HD23	1:D:174:LEU:HA	1.89	0.42
1:D:129:HIS:CG	1:D:130:PRO:HD2	2.54	0.42
1:B:192:SER:O	1:B:195:ASP:HB2	2.19	0.42
1:D:382:ILE:O	1:D:386:ILE:HG13	2.20	0.42
1:D:538:SER:HB3	1:D:541:LEU:HG	2.02	0.42
1:A:226:ARG:NH1	1:A:229:VAL:HG21	2.35	0.42
1:A:249:GLY:O	1:A:252:PRO:HD2	2.20	0.42
1:B:320:CYS:HB3	1:B:325:ILE:O	2.20	0.42
1:D:315:TYR:CE1	1:D:316:PHE:HE1	2.38	0.42
1:D:315:TYR:CE2	2:D:703:DGT:O3G	2.73	0.42
1:C:164:ARG:HH22	2:C:703:DGT:H4'	1.84	0.42
1:D:192:SER:O	1:D:195:ASP:HB2	2.19	0.42
1:D:244:LEU:HD23	1:D:244:LEU:O	2.19	0.42
1:A:134:ARG:HA	1:A:134:ARG:HD2	1.84	0.42
1:A:244:LEU:HD23	1:A:244:LEU:O	2.19	0.42
1:A:285:TRP:CG	1:A:292:GLU:HG3	2.54	0.42
1:B:244:LEU:HD23	1:B:244:LEU:O	2.20	0.42
1:B:537:VAL:O	1:D:371:ARG:NH1	2.53	0.42
1:C:114:THR:HB	1:C:115:MET:H	1.72	0.42
1:B:228:GLU:N	1:B:228:GLU:OE1	2.53	0.42
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:TYR:CE1	1:C:316:PHE:HE1	2.35	0.42
1:D:303:ASN:HD21	1:D:306:ASN:ND2	2.18	0.42
1:C:470:ARG:HB2	1:C:470:ARG:HH11	1.84	0.41
1:C:509:MET:HE1	1:C:517:HIS:CE1	2.55	0.41
1:C:534:LYS:HE3	1:C:534:LYS:HB3	1.78	0.41
1:D:507:TYR:CD2	1:D:545:PHE:HD2	2.38	0.41
1:B:346:GLU:OE2	1:B:348:ARG:NH2	2.48	0.41
1:C:422:LEU:HD12	1:C:426:ILE:HG13	2.01	0.41
1:D:215:HIS:HD2	2:D:703:DGT:C4	2.33	0.41
1:B:215:HIS:O	1:B:219:GLY:N	2.48	0.41
1:A:304:LYS:HA	1:A:304:LYS:HD3	1.91	0.41
1:B:245:ILE:HG23	1:B:250:ILE:HB	2.02	0.41
1:C:176:GLY:HA3	1:C:200:GLN:HE21	1.86	0.41
1:A:486:LYS:CE	1:A:594:GLN:HE22	2.31	0.41
1:B:304:LYS:HA	1:B:304:LYS:HD3	1.94	0.41
1:C:116:LYS:NZ	2:C:702:DGT:O1A	2.45	0.41
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.84	0.41
1:A:486:LYS:HD2	1:A:594:GLN:NE2	2.35	0.41
1:C:215:HIS:NE2	2:C:703:DGT:O4'	2.54	0.41
1:A:129:HIS:CG	1:A:130:PRO:HD2	2.56	0.41
1:B:458:GLY:HA3	1:B:569:PHE:CE2	2.54	0.41
1:D:254:MET:HE2	1:D:259:LEU:HD23	2.03	0.41
1:D:558:ASP:CG	1:D:561:SER:OG	2.64	0.41
1:A:245:ILE:HG23	1:A:250:ILE:HB	2.03	0.41
1:A:509:MET:SD	1:A:514:PRO:HA	2.61	0.41
1:B:321:HIS:NE2	1:C:321:HIS:NE2	2.69	0.41
1:B:558:ASP:OD2	1:B:561:SER:OG	2.34	0.41
1:C:327:ASN:HB2	1:C:365:THR:CG2	2.49	0.41
1:C:435:ASP:OD1	1:C:437:LYS:N	2.38	0.41
1:C:470:ARG:HA	1:C:473:TYR:CE1	2.56	0.41
1:C:510:GLN:HB3	1:C:511:GLU:H	1.75	0.41
1:D:371:ARG:CG	1:D:505:MET:HE2	2.50	0.41
1:A:226:ARG:HB3	1:A:229:VAL:HG23	2.03	0.41
1:B:115:MET:HG2	1:B:127:GLU:HB3	2.03	0.41
1:B:470:ARG:HG3	1:B:473:TYR:HE2	1.84	0.41
1:C:220:ARG:C	1:C:223:PRO:HD2	2.46	0.41
1:C:592:VAL:N	1:C:593:PRO:CD	2.84	0.41
1:C:458:GLY:HA3	1:C:569:PHE:CE2	2.56	0.40
1:D:328:ASN:HB2	1:D:365:THR:OG1	2.21	0.40
1:D:566:ARG:O	1:D:570:VAL:HG23	2.21	0.40
1:B:540:LEU:O	1:D:542:PRO:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:HIS:CD2	2:C:703:DGT:C8	3.05	0.40
1:D:325:ILE:CG2	1:D:326:GLN:N	2.83	0.40
1:C:509:MET:HE2	1:C:509:MET:HB3	1.85	0.40
1:D:506:ASP:HA	1:D:545:PHE:O	2.21	0.40
1:A:509:MET:HB3	1:A:509:MET:HE2	1.87	0.40
1:B:534:LYS:O	1:B:537:VAL:HG23	2.21	0.40
1:D:215:HIS:O	1:D:219:GLY:N	2.49	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	476/514 (93%)	472 (99%)	4 (1%)	0	100	100
1	B	477/514 (93%)	471 (99%)	6 (1%)	0	100	100
1	C	476/514 (93%)	468 (98%)	7 (2%)	1 (0%)	43	71
1	D	477/514 (93%)	470 (98%)	7 (2%)	0	100	100
All	All	1906/2056 (93%)	1881 (99%)	24 (1%)	1 (0%)	48	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	486	LYS

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	426/459 (93%)	399 (94%)	27 (6%)	16	43
1	B	427/459 (93%)	392 (92%)	35 (8%)	10	31
1	C	426/459 (93%)	392 (92%)	34 (8%)	11	32
1	D	427/459 (93%)	396 (93%)	31 (7%)	13	36
All	All	1706/1836 (93%)	1579 (93%)	127 (7%)	12	36

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	LYS
1	A	230	LYS
1	A	247	SER
1	A	277	GLU
1	A	284	LEU
1	A	315	TYR
1	A	339	ARG
1	A	354	LYS
1	A	371	ARG
1	A	388	ASP
1	A	406	LYS
1	A	465	GLN
1	A	468	ILE
1	A	478	LYS
1	A	484	LYS
1	A	486	LYS
1	A	488	LEU
1	A	511	GLU
1	A	524	THR
1	A	539	GLN
1	A	540	LEU
1	A	544	LYS
1	A	556	LYS
1	A	561	SER
1	A	594	GLN
1	A	596	LYS
1	A	599	ASN
1	B	114	THR
1	B	115	MET
1	B	166	GLU

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Mol	Chain	Res	Type
1	B	230	LYS
1	B	247	SER
1	B	277	GLU
1	B	284	LEU
1	B	302	SER
1	B	315	TYR
1	B	326	GLN
1	B	328	ASN
1	B	339	ARG
1	B	354	LYS
1	B	371	ARG
1	B	381	ILE
1	B	388	ASP
1	B	410	SER
1	B	439	LYS
1	B	455	LYS
1	B	468	ILE
1	B	471	GLU
1	B	472	ASP
1	B	474	GLU
1	B	494	LYS
1	B	496	GLU
1	B	511	GLU
1	B	524	THR
1	B	537	VAL
1	B	539	GLN
1	B	540	LEU
1	B	544	LYS
1	B	556	LYS
1	B	560	LYS
1	B	577	ASN
1	B	594	GLN
1	C	114	THR
1	C	115	MET
1	C	166	GLU
1	C	230	LYS
1	C	235	GLN
1	C	247	SER
1	C	262	GLU
1	C	284	LEU
1	C	295	SER
1	C	305	ARG

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Mol	Chain	Res	Type
1	C	315	TYR
1	C	327	ASN
1	C	328	ASN
1	C	339	ARG
1	C	354	LYS
1	C	371	ARG
1	C	377	LYS
1	C	381	ILE
1	C	388	ASP
1	C	395	ASP
1	C	405	LYS
1	C	410	SER
1	C	463	THR
1	C	468	ILE
1	C	474	GLU
1	C	475	SER
1	C	492	LYS
1	C	496	GLU
1	C	510	GLN
1	C	511	GLU
1	C	528	ARG
1	C	540	LEU
1	C	544	LYS
1	C	594	GLN
1	D	114	THR
1	D	115	MET
1	D	230	LYS
1	D	247	SER
1	D	277	GLU
1	D	292	GLU
1	D	293	ASN
1	D	295	SER
1	D	305	ARG
1	D	315	TYR
1	D	326	GLN
1	D	328	ASN
1	D	339	ARG
1	D	354	LYS
1	D	371	ARG
1	D	372	ARG
1	D	381	ILE
1	D	388	ASP

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Mol	Chain	Res	Type
1	D	395	ASP
1	D	405	LYS
1	D	410	SER
1	D	455	LYS
1	D	463	THR
1	D	465	GLN
1	D	468	ILE
1	D	494	LYS
1	D	496	GLU
1	D	524	THR
1	D	528	ARG
1	D	540	LEU
1	D	596	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	163	ASN
1	A	210	HIS
1	A	233	HIS
1	A	328	ASN
1	A	425	ASN
1	A	465	GLN
1	A	571	GLN
1	A	577	ASN
1	A	594	GLN
1	A	599	ASN
1	B	163	ASN
1	B	180	HIS
1	B	210	HIS
1	B	215	HIS
1	B	233	HIS
1	B	243	HIS
1	B	370	HIS
1	B	425	ASN
1	B	510	GLN
1	B	517	HIS
1	B	527	ASN
1	B	577	ASN
1	C	119	ASN
1	C	149	GLN

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Mol	Chain	Res	Type
1	C	163	ASN
1	C	200	GLN
1	C	207	ASN
1	C	210	HIS
1	C	322	HIS
1	C	327	ASN
1	C	364	HIS
1	C	425	ASN
1	C	517	HIS
1	C	577	ASN
1	C	594	GLN
1	D	119	ASN
1	D	149	GLN
1	D	163	ASN
1	D	210	HIS
1	D	233	HIS
1	D	248	ASN
1	D	322	HIS
1	D	326	GLN
1	D	425	ASN
1	D	571	GLN
1	D	577	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DGT	C	703	-	32,33,33	1.29	4 (12%)	48,52,52	1.66	8 (16%)
2	DGT	D	704	3	32,33,33	1.39	6 (18%)	48,52,52	1.82	10 (20%)
2	DGT	A	701	-	32,33,33	1.42	4 (12%)	48,52,52	1.79	9 (18%)
2	DGT	A	703	3	32,33,33	1.44	7 (21%)	48,52,52	1.75	10 (20%)
2	DGT	A	704	3	32,33,33	1.56	6 (18%)	48,52,52	1.62	6 (12%)
2	DGT	D	702	3	32,33,33	1.50	6 (18%)	48,52,52	1.59	6 (12%)
2	DGT	D	703	-	32,33,33	1.32	3 (9%)	48,52,52	1.77	8 (16%)
2	DGT	B	701	3	32,33,33	1.16	3 (9%)	48,52,52	1.73	6 (12%)
2	DGT	A	702	3	32,33,33	1.66	6 (18%)	48,52,52	1.59	8 (16%)
2	DGT	B	704	3	32,33,33	1.27	5 (15%)	48,52,52	1.75	8 (16%)
2	DGT	B	705	3	32,33,33	1.65	8 (25%)	48,52,52	1.63	7 (14%)
2	DGT	C	702	3	32,33,33	1.23	5 (15%)	48,52,52	1.90	9 (18%)

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	DGT	C	703	-	-	4/22/34/34	0/3/3/3
2	DGT	D	704	3	-	3/22/34/34	0/3/3/3
2	DGT	A	701	-	-	4/22/34/34	0/3/3/3
2	DGT	A	703	3	-	4/22/34/34	0/3/3/3
2	DGT	A	704	3	-	4/22/34/34	0/3/3/3
2	DGT	D	702	3	-	1/22/34/34	0/3/3/3
2	DGT	D	703	-	-	3/22/34/34	0/3/3/3
2	DGT	B	701	3	-	2/22/34/34	0/3/3/3
2	DGT	A	702	3	-	4/22/34/34	0/3/3/3
2	DGT	B	704	3	-	7/22/34/34	0/3/3/3
2	DGT	B	705	3	-	6/22/34/34	0/3/3/3
2	DGT	C	702	3	-	4/22/34/34	0/3/3/3

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	702	DGT	PA-O3A	5.55	1.65	1.59
2	A	704	DGT	PA-O3A	4.85	1.64	1.59
2	B	705	DGT	PB-O3B	4.29	1.64	1.59
2	D	704	DGT	PB-O3B	3.83	1.63	1.59
2	B	705	DGT	C5-N7	-3.72	1.31	1.39
2	B	705	DGT	PA-O3A	3.69	1.63	1.59
2	D	704	DGT	C6-N1	-3.66	1.32	1.38
2	A	703	DGT	C6-N1	-3.57	1.32	1.38
2	A	702	DGT	C5-C4	3.56	1.48	1.38
2	C	703	DGT	C5-C4	3.43	1.48	1.38
2	D	703	DGT	C5-C4	3.43	1.48	1.38
2	A	701	DGT	PA-O3A	3.38	1.63	1.59
2	A	701	DGT	C5-C4	3.37	1.48	1.38
2	D	702	DGT	PB-O3B	3.30	1.63	1.59
2	D	702	DGT	C5-C4	3.23	1.47	1.38
2	A	701	DGT	PB-O3A	3.15	1.62	1.59
2	B	701	DGT	C5-C4	3.11	1.47	1.38
2	D	702	DGT	PA-O3A	3.07	1.62	1.59
2	C	702	DGT	PB-O3B	3.04	1.62	1.59
2	D	702	DGT	PB-O3A	3.03	1.62	1.59
2	A	702	DGT	C4-N9	-3.01	1.30	1.38
2	A	704	DGT	C6-N1	-3.01	1.33	1.38
2	D	702	DGT	C6-N1	-2.85	1.33	1.38
2	A	703	DGT	C5-N7	-2.85	1.33	1.39
2	B	704	DGT	C5-C4	2.85	1.46	1.38
2	B	705	DGT	C4-N9	-2.83	1.30	1.38
2	A	703	DGT	C5-C4	2.78	1.46	1.38
2	B	704	DGT	C6-N1	-2.72	1.33	1.38
2	B	705	DGT	C6-N1	-2.72	1.33	1.38
2	B	704	DGT	C5-N7	-2.66	1.33	1.39
2	A	704	DGT	C5-C4	2.64	1.46	1.38
2	D	703	DGT	PA-O3A	2.63	1.62	1.59
2	C	703	DGT	PB-O3B	2.61	1.62	1.59
2	D	704	DGT	C5-C4	2.61	1.45	1.38
2	B	704	DGT	C4-N9	-2.59	1.31	1.38
2	A	703	DGT	PB-O3A	2.59	1.62	1.59
2	A	702	DGT	C6-N1	-2.58	1.34	1.38
2	C	703	DGT	PB-O3A	2.56	1.62	1.59
2	C	702	DGT	C6-N1	-2.54	1.34	1.38
2	D	703	DGT	PB-O3B	2.53	1.62	1.59
2	C	702	DGT	C5-C4	2.51	1.45	1.38
2	A	704	DGT	PB-O3B	2.50	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	704	DGT	C5-N7	-2.45	1.34	1.39
2	A	704	DGT	C5-N7	-2.42	1.34	1.39
2	A	702	DGT	PB-O3A	2.41	1.62	1.59
2	B	701	DGT	C6-N1	-2.39	1.34	1.38
2	D	702	DGT	C5-N7	-2.39	1.34	1.39
2	A	703	DGT	C4-N9	-2.39	1.32	1.38
2	A	702	DGT	C5-N7	-2.36	1.34	1.39
2	C	702	DGT	C5-N7	-2.31	1.34	1.39
2	A	703	DGT	PB-O3B	2.25	1.61	1.59
2	A	703	DGT	PA-O3A	2.23	1.61	1.59
2	B	705	DGT	C5-C4	2.23	1.44	1.38
2	B	705	DGT	PB-O3A	2.21	1.61	1.59
2	D	704	DGT	C4-N9	-2.19	1.32	1.38
2	A	704	DGT	C4-N9	-2.16	1.32	1.38
2	C	702	DGT	C4-N9	-2.14	1.32	1.38
2	A	701	DGT	C6-N1	-2.12	1.34	1.38
2	C	703	DGT	C6-N1	-2.06	1.35	1.38
2	B	701	DGT	C5-N7	-2.05	1.35	1.39
2	B	704	DGT	PB-O3B	2.04	1.61	1.59
2	B	705	DGT	C8-N9	-2.02	1.33	1.37
2	D	704	DGT	C8-N9	-2.00	1.33	1.37

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	702	DGT	C5-C4-N3	-6.00	118.84	128.39
2	B	701	DGT	C5-C4-N3	-5.99	118.85	128.39
2	D	704	DGT	C5-C4-N3	-5.73	119.27	128.39
2	A	703	DGT	C5-C4-N3	-5.66	119.39	128.39
2	D	703	DGT	C5-C4-N3	-5.53	119.58	128.39
2	B	704	DGT	C5-C4-N3	-5.23	120.06	128.39
2	A	701	DGT	C5-C4-N3	-5.13	120.22	128.39
2	C	702	DGT	C2-N3-C4	5.13	121.14	112.30
2	C	703	DGT	C5-C4-N3	-5.09	120.28	128.39
2	B	701	DGT	C2-N3-C4	5.02	120.94	112.30
2	D	702	DGT	C5-C4-N3	-4.91	120.57	128.39
2	A	704	DGT	C5-C4-N3	-4.84	120.68	128.39
2	B	705	DGT	C5-C4-N3	-4.84	120.69	128.39
2	A	703	DGT	C2-N3-C4	4.74	120.46	112.30
2	D	703	DGT	C2-N3-C4	4.67	120.35	112.30
2	C	702	DGT	N9-C4-N3	4.62	135.18	125.95
2	C	703	DGT	C2-N3-C4	4.60	120.22	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	704	DGT	C2-N3-C4	4.52	120.09	112.30
2	A	701	DGT	C2-N3-C4	4.48	120.01	112.30
2	D	703	DGT	N9-C4-N3	4.40	134.75	125.95
2	B	701	DGT	N9-C4-N3	4.40	134.75	125.95
2	B	704	DGT	C2-N3-C4	4.38	119.85	112.30
2	D	704	DGT	N9-C4-N3	4.31	134.56	125.95
2	D	702	DGT	C2-N3-C4	4.30	119.70	112.30
2	A	702	DGT	C5-C4-N3	-4.28	121.58	128.39
2	A	703	DGT	N9-C4-N3	4.23	134.41	125.95
2	C	702	DGT	O2G-PG-O1G	4.06	123.03	107.80
2	B	704	DGT	N9-C4-N3	4.03	134.02	125.95
2	A	704	DGT	C2-N3-C4	3.97	119.13	112.30
2	C	703	DGT	N9-C4-N3	3.92	133.80	125.95
2	A	701	DGT	N9-C4-N3	3.92	133.79	125.95
2	C	703	DGT	C6-C5-N7	3.91	137.40	130.29
2	A	704	DGT	N9-C4-N3	3.82	133.59	125.95
2	B	705	DGT	O4'-C1'-N9	-3.80	101.13	107.86
2	D	702	DGT	C6-C5-N7	3.73	137.07	130.29
2	B	705	DGT	N9-C4-N3	3.57	133.09	125.95
2	D	703	DGT	C6-C5-N7	3.56	136.77	130.29
2	A	702	DGT	C6-C5-N7	3.53	136.71	130.29
2	D	702	DGT	N9-C4-N3	3.35	132.66	125.95
2	A	701	DGT	C6-C5-N7	3.35	136.39	130.29
2	B	705	DGT	C2-N3-C4	3.35	118.06	112.30
2	D	704	DGT	C6-C5-N7	3.28	136.26	130.29
2	B	701	DGT	C6-C5-N7	3.24	136.19	130.29
2	A	702	DGT	C4-C5-N7	-3.10	105.75	110.67
2	B	704	DGT	O3A-PB-O2B	-3.08	101.44	110.70
2	A	704	DGT	C6-C5-N7	3.07	135.87	130.29
2	A	701	DGT	O6-C6-C5	-3.01	118.60	126.53
2	C	702	DGT	C6-C5-N7	2.98	135.71	130.29
2	B	705	DGT	O6-C6-C5	-2.91	118.86	126.53
2	D	702	DGT	O1A-PA-O2A	2.90	125.93	112.44
2	A	703	DGT	C6-C5-N7	2.88	135.54	130.29
2	B	704	DGT	C6-C5-N7	2.88	135.53	130.29
2	D	704	DGT	C4-C5-N7	-2.85	106.15	110.67
2	D	703	DGT	O4'-C1'-N9	2.84	112.91	107.86
2	A	704	DGT	O6-C6-C5	-2.84	119.05	126.53
2	A	702	DGT	C2-N3-C4	2.81	117.15	112.30
2	B	704	DGT	O3B-PG-O3G	-2.81	96.24	111.04
2	C	702	DGT	O3A-PB-O2B	-2.80	102.29	110.70
2	D	703	DGT	C4-C5-N7	-2.75	106.31	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	704	DGT	O1G-PG-O3G	2.72	121.44	110.83
2	B	705	DGT	O6-C6-N1	2.70	125.20	120.11
2	B	705	DGT	O3A-PB-O2B	-2.67	102.67	110.70
2	B	704	DGT	O1B-PB-O3A	2.57	114.21	107.27
2	D	704	DGT	O1A-PA-O5'	-2.56	95.95	107.57
2	A	702	DGT	N9-C4-N3	2.54	131.04	125.95
2	C	702	DGT	C4-C5-N7	-2.54	106.64	110.67
2	A	701	DGT	N2-C2-N1	2.53	122.10	116.76
2	C	703	DGT	O2G-PG-O1G	2.46	117.03	107.80
2	A	703	DGT	O6-C6-C5	-2.45	120.06	126.53
2	D	703	DGT	O2G-PG-O1G	2.42	116.87	107.80
2	B	701	DGT	C4-C5-N7	-2.41	106.86	110.67
2	D	703	DGT	C8-N7-C5	2.34	108.42	104.26
2	D	704	DGT	O1A-PA-O3A	2.30	113.49	107.27
2	A	702	DGT	N2-C2-N3	-2.30	115.19	119.67
2	A	703	DGT	N2-C2-N3	-2.30	115.19	119.67
2	D	702	DGT	C4-C5-N7	-2.28	107.06	110.67
2	A	701	DGT	C4-C5-N7	-2.27	107.07	110.67
2	A	701	DGT	N2-C2-N3	-2.27	115.25	119.67
2	B	701	DGT	O6-C6-C5	-2.26	120.56	126.53
2	C	703	DGT	C4-C5-N7	-2.26	107.09	110.67
2	C	703	DGT	C6-C5-C4	-2.21	115.51	118.83
2	A	702	DGT	O1B-PB-O3A	2.19	113.18	107.27
2	A	701	DGT	O3B-PG-O3G	-2.18	99.55	111.04
2	D	704	DGT	O1A-PA-O2A	2.16	122.49	112.44
2	A	704	DGT	C4-C5-N7	-2.13	107.29	110.67
2	A	703	DGT	O2G-PG-O1G	2.13	115.78	107.80
2	C	703	DGT	C5-C6-N1	2.12	118.65	113.25
2	A	703	DGT	N2-C2-N1	2.10	121.20	116.76
2	A	703	DGT	O1A-PA-O3A	2.09	112.92	107.27
2	C	702	DGT	O6-C6-C5	-2.08	121.04	126.53
2	D	704	DGT	O1B-PB-O2B	2.07	122.08	112.44
2	D	704	DGT	C8-N7-C5	2.07	107.94	104.26
2	A	702	DGT	O3B-PB-O2B	-2.05	104.52	110.70
2	C	702	DGT	O2G-PG-O3B	-2.04	97.78	104.64
2	A	703	DGT	C5-C6-N1	2.02	118.39	113.25

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	702	DGT	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
2	A	701	DGT	O4'-C4'-C5'-O5'
2	C	703	DGT	O4'-C4'-C5'-O5'
2	C	703	DGT	C3'-C4'-C5'-O5'
2	A	701	DGT	C3'-C4'-C5'-O5'
2	D	703	DGT	PB-O3B-PG-O3G
2	A	701	DGT	PA-O3A-PB-O2B
2	A	702	DGT	PG-O3B-PB-O2B
2	D	703	DGT	PA-O3A-PB-O2B
2	B	701	DGT	PB-O3A-PA-O5'
2	B	704	DGT	PB-O3B-PG-O1G
2	B	705	DGT	PB-O3B-PG-O1G
2	A	703	DGT	C4'-C5'-O5'-PA
2	A	702	DGT	PB-O3A-PA-O1A
2	A	704	DGT	PG-O3B-PB-O2B
2	B	705	DGT	PG-O3B-PB-O2B
2	C	703	DGT	PG-O3B-PB-O1B
2	B	704	DGT	C2'-C1'-N9-C8
2	B	704	DGT	PG-O3B-PB-O1B
2	D	703	DGT	PA-O3A-PB-O1B
2	A	703	DGT	C2'-C1'-N9-C4
2	B	704	DGT	C2'-C1'-N9-C4
2	C	702	DGT	C2'-C1'-N9-C4
2	B	704	DGT	C4'-C5'-O5'-PA
2	C	702	DGT	C4'-C5'-O5'-PA
2	A	703	DGT	C2'-C1'-N9-C8
2	C	702	DGT	C2'-C1'-N9-C8
2	B	704	DGT	PB-O3A-PA-O1A
2	C	703	DGT	PG-O3B-PB-O2B
2	B	705	DGT	PB-O3B-PG-O2G
2	D	704	DGT	C2'-C1'-N9-C8
2	A	701	DGT	PA-O3A-PB-O1B
2	A	702	DGT	PG-O3B-PB-O1B
2	A	704	DGT	PG-O3B-PB-O1B
2	A	704	DGT	PA-O3A-PB-O1B
2	A	704	DGT	PB-O3A-PA-O1A
2	B	704	DGT	PG-O3B-PB-O2B
2	B	705	DGT	PG-O3B-PB-O1B
2	B	705	DGT	PB-O3A-PA-O1A
2	C	702	DGT	PG-O3B-PB-O1B
2	D	704	DGT	PB-O3A-PA-O1A
2	D	704	DGT	C2'-C1'-N9-C4
2	A	702	DGT	PB-O3A-PA-O2A

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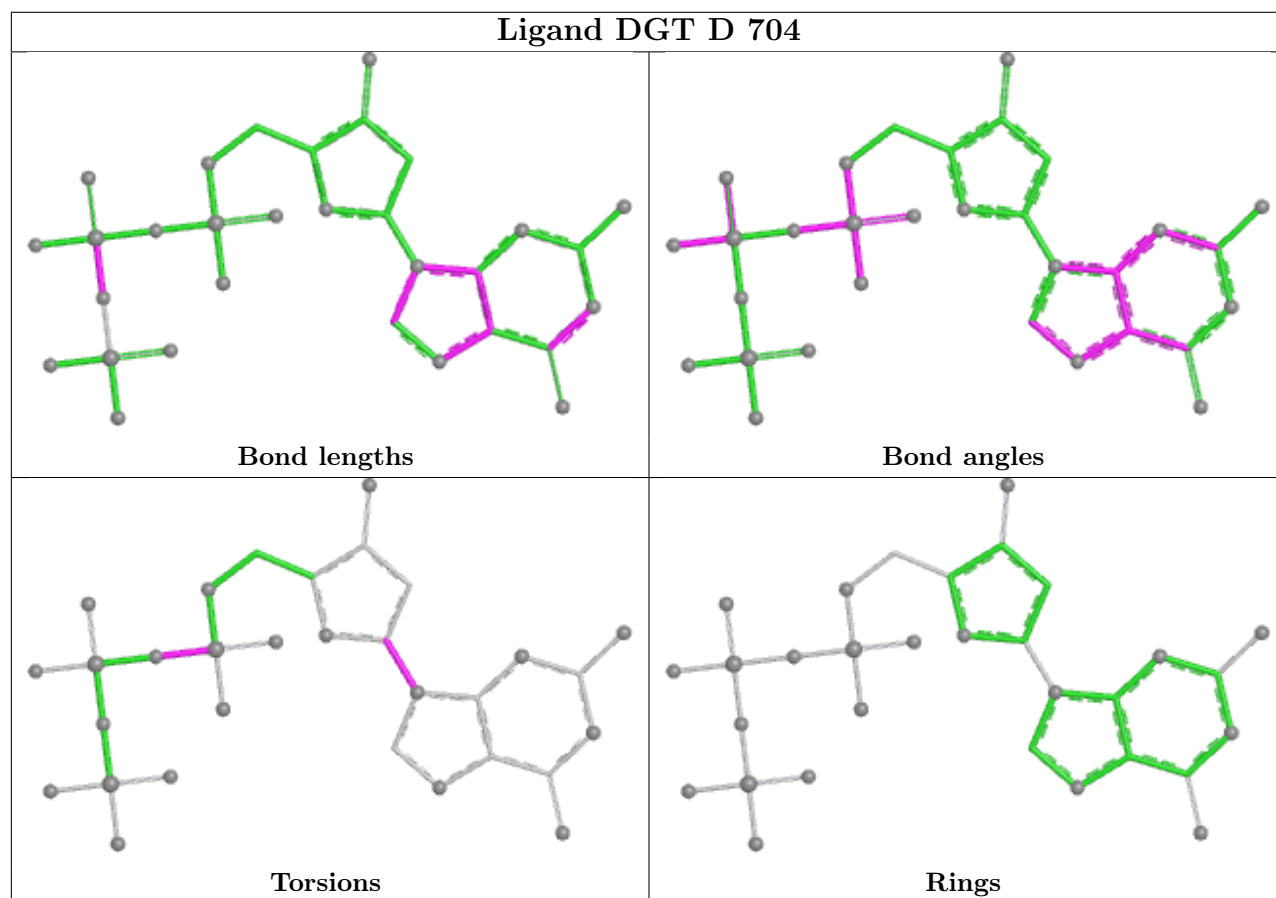
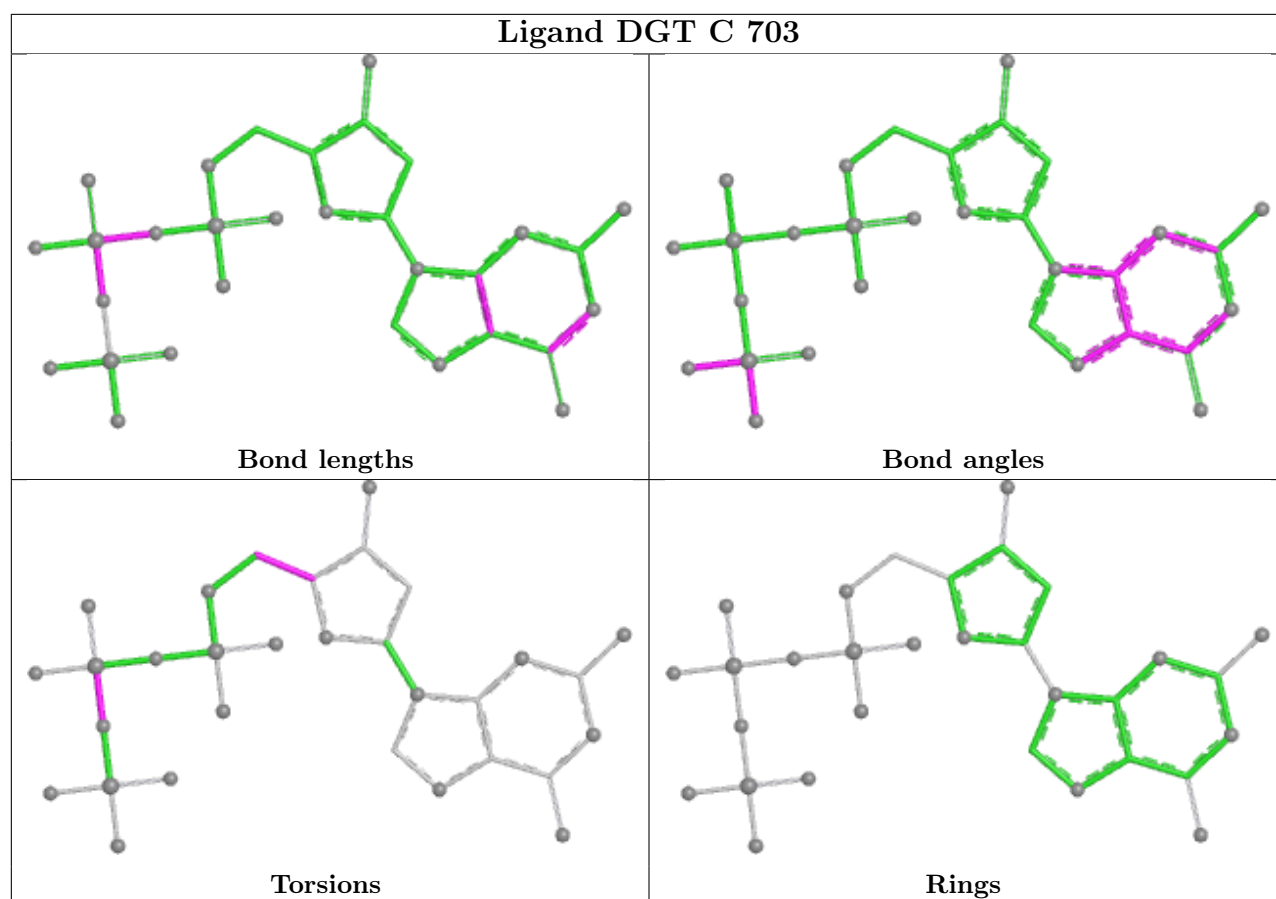
Mol	Chain	Res	Type	Atoms
2	A	703	DGT	PB-O3A-PA-O1A
2	B	701	DGT	PB-O3A-PA-O1A
2	B	705	DGT	PB-O3A-PA-O2A

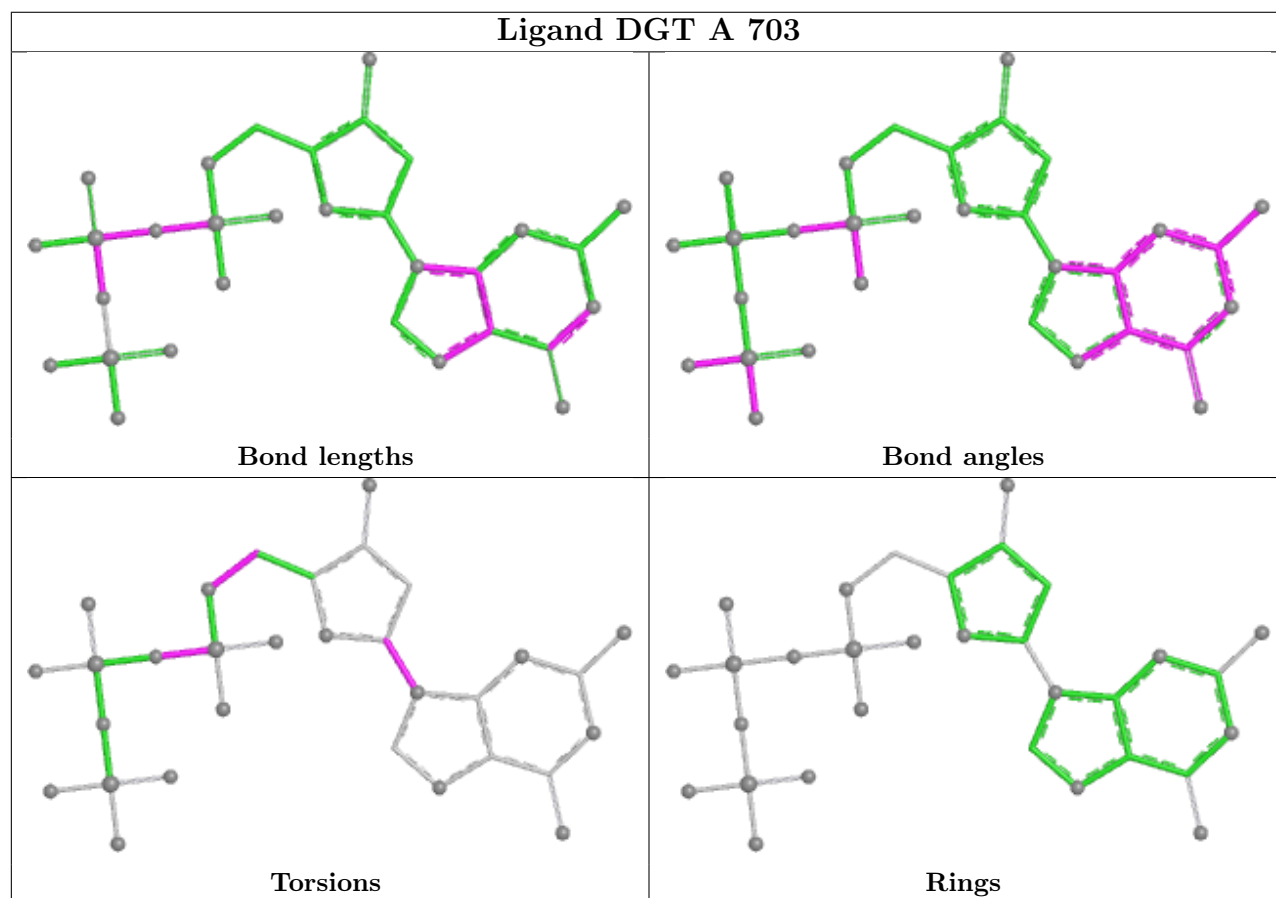
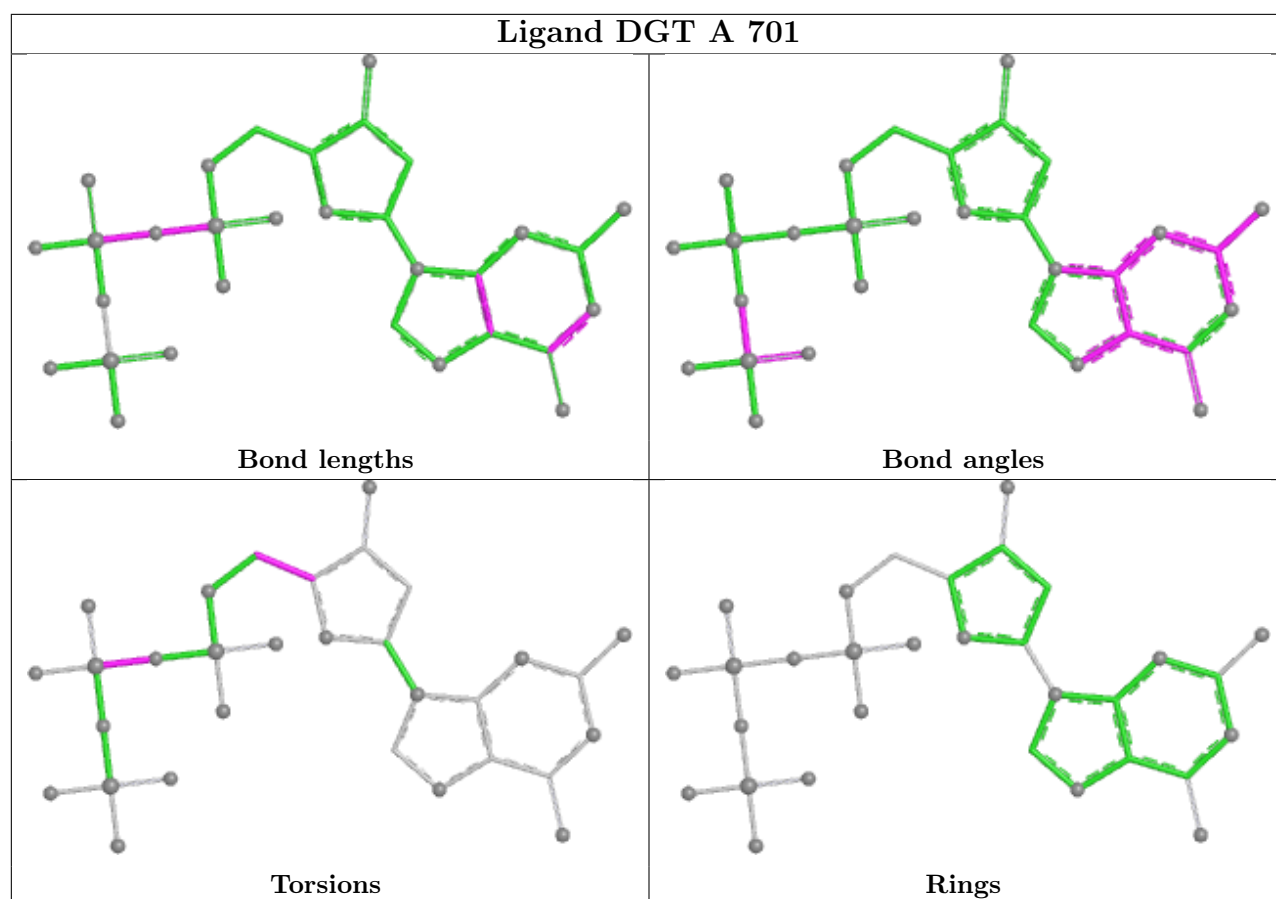
There are no ring outliers.

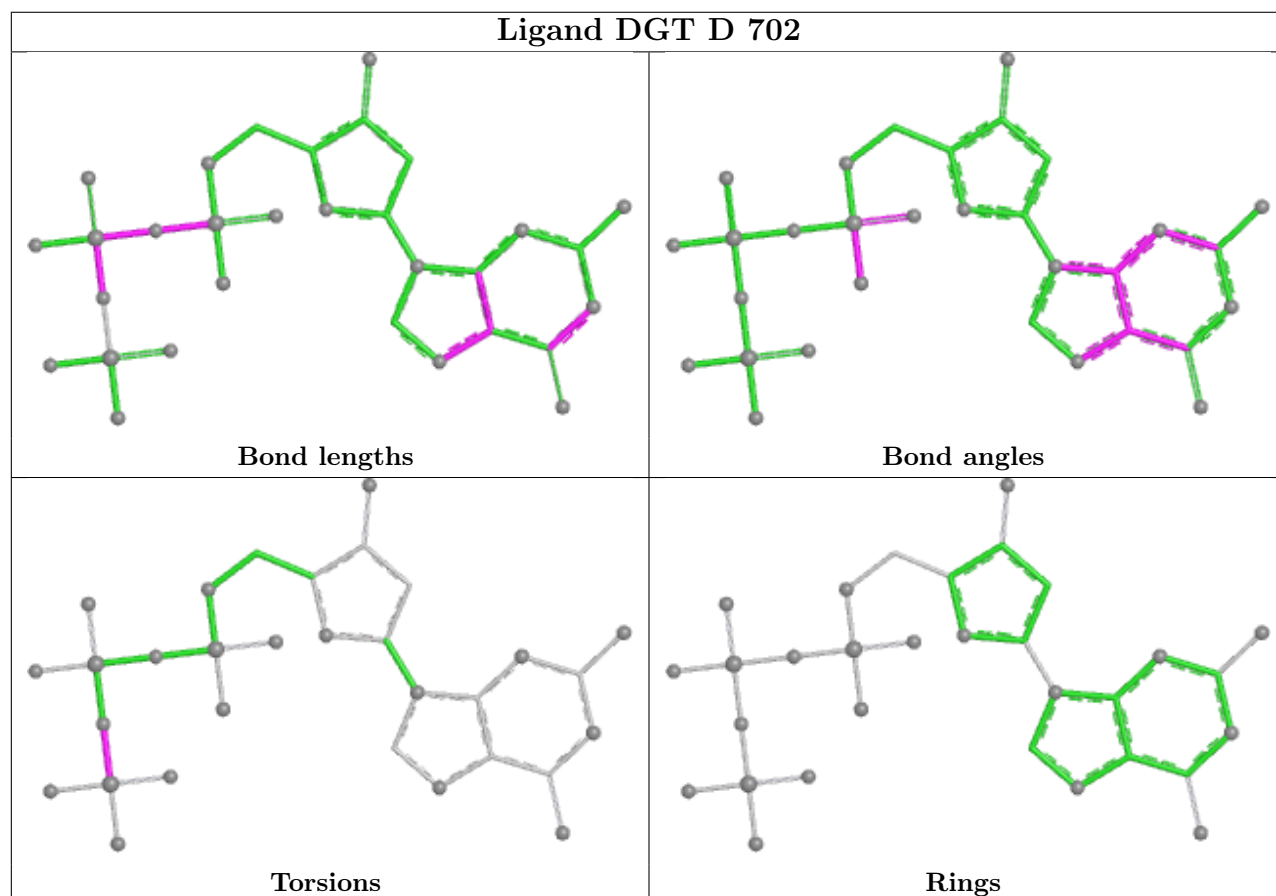
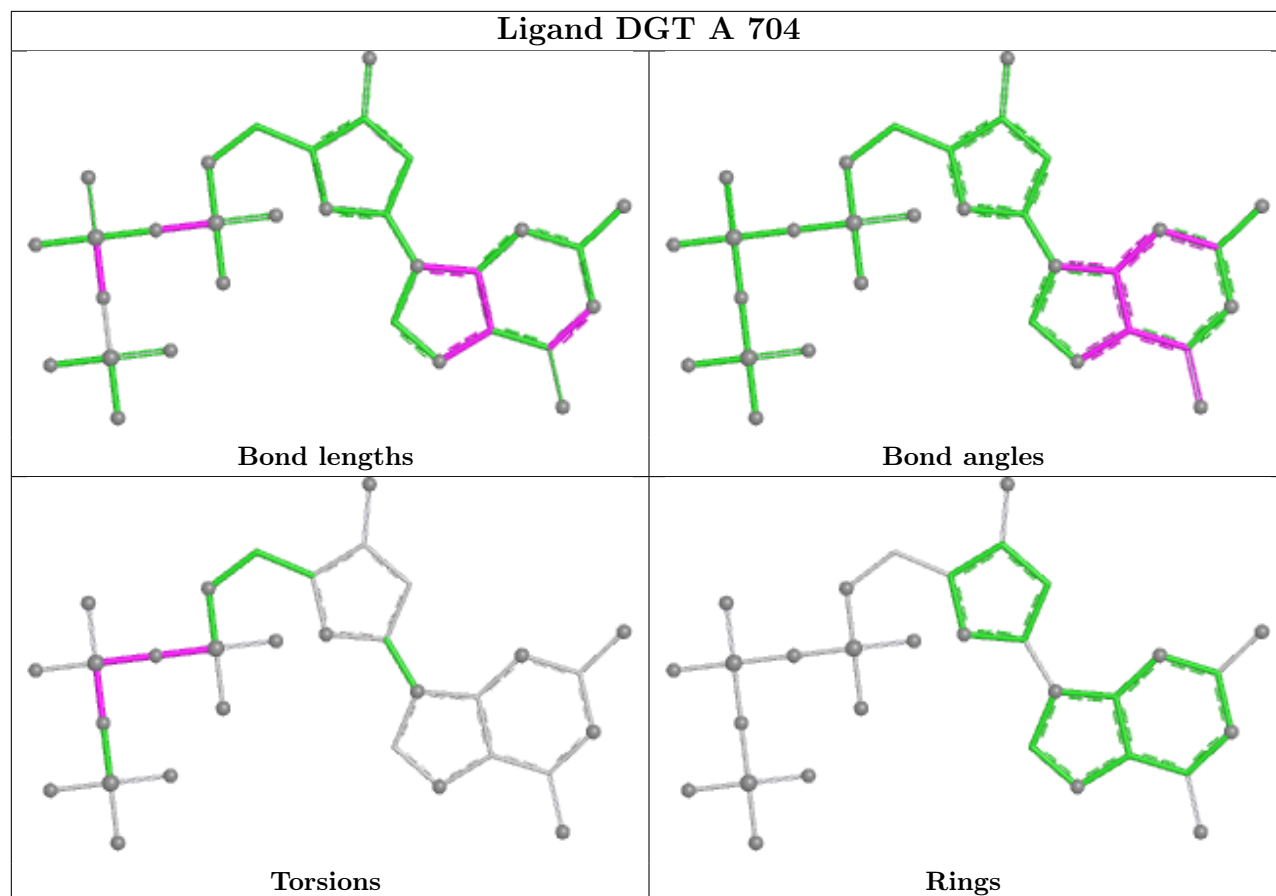
9 monomers are involved in 43 short contacts:

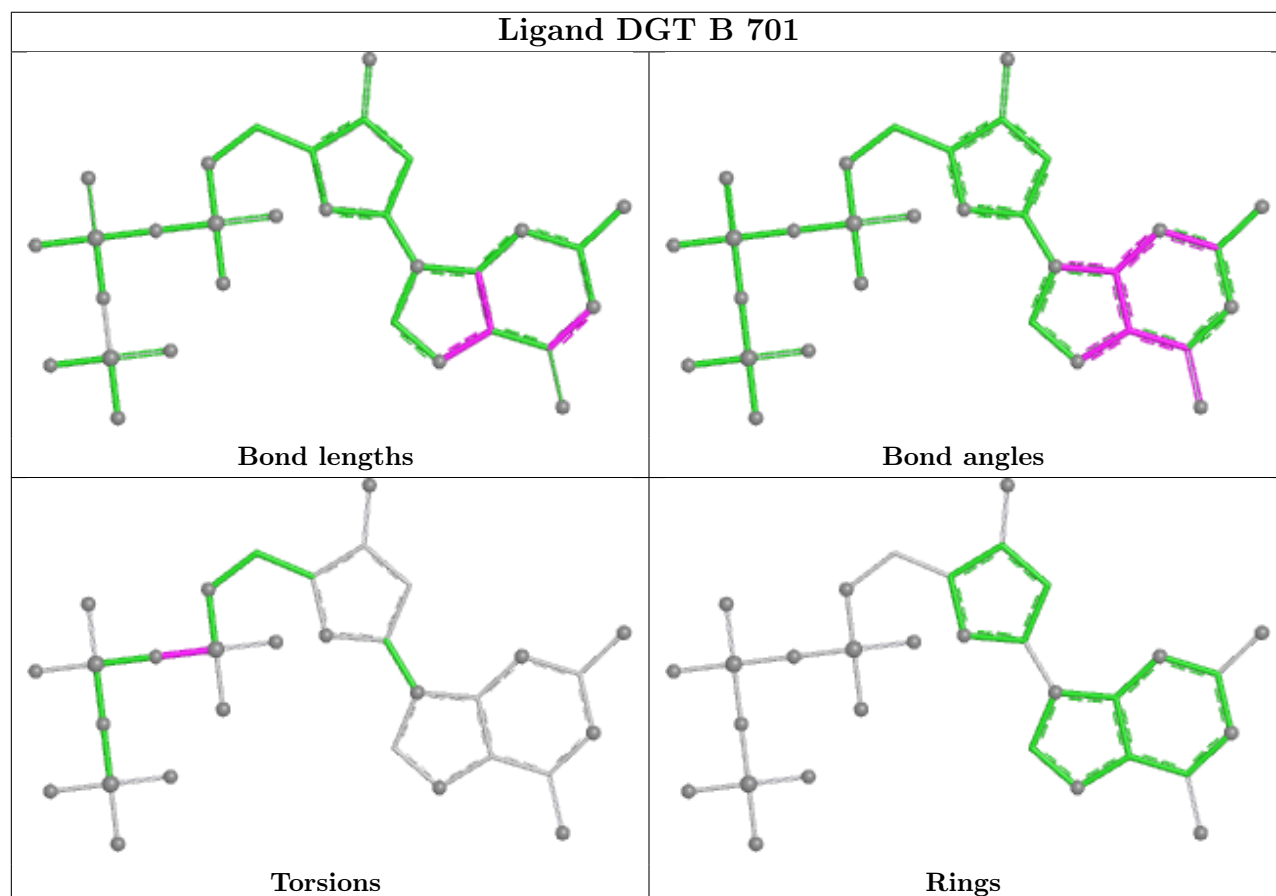
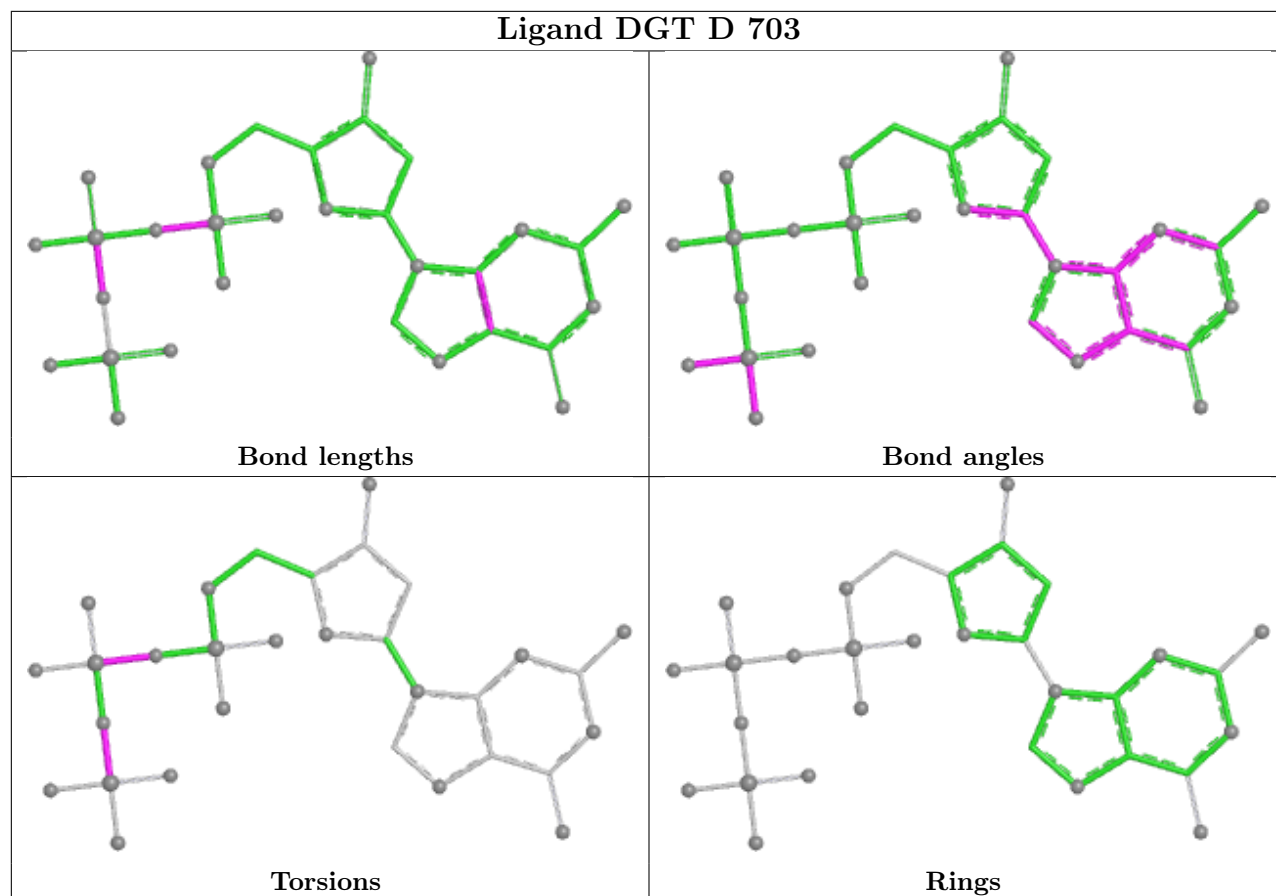
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	703	DGT	6	0
2	A	703	DGT	1	0
2	A	704	DGT	3	0
2	D	702	DGT	2	0
2	D	703	DGT	5	0
2	B	701	DGT	16	0
2	B	704	DGT	1	0
2	B	705	DGT	6	0
2	C	702	DGT	3	0

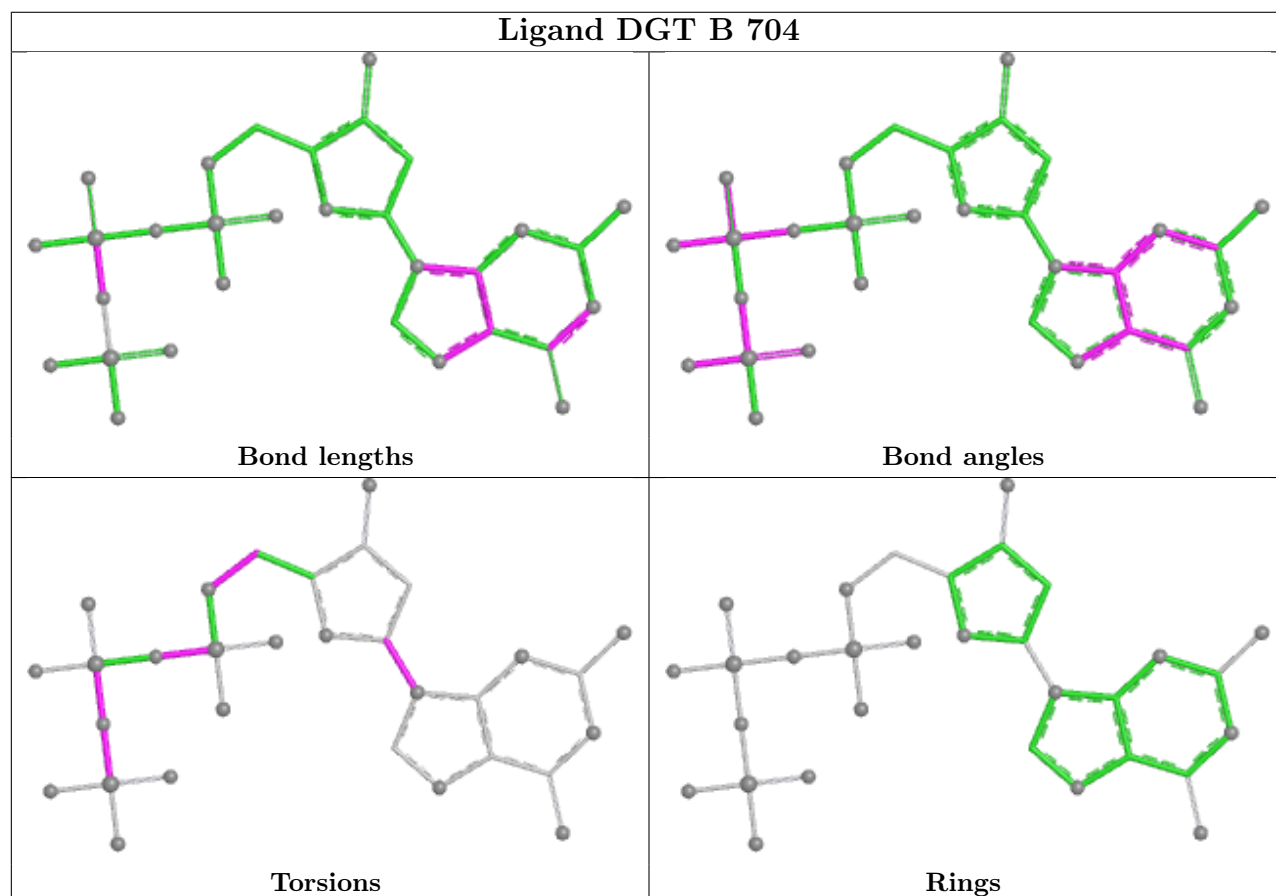
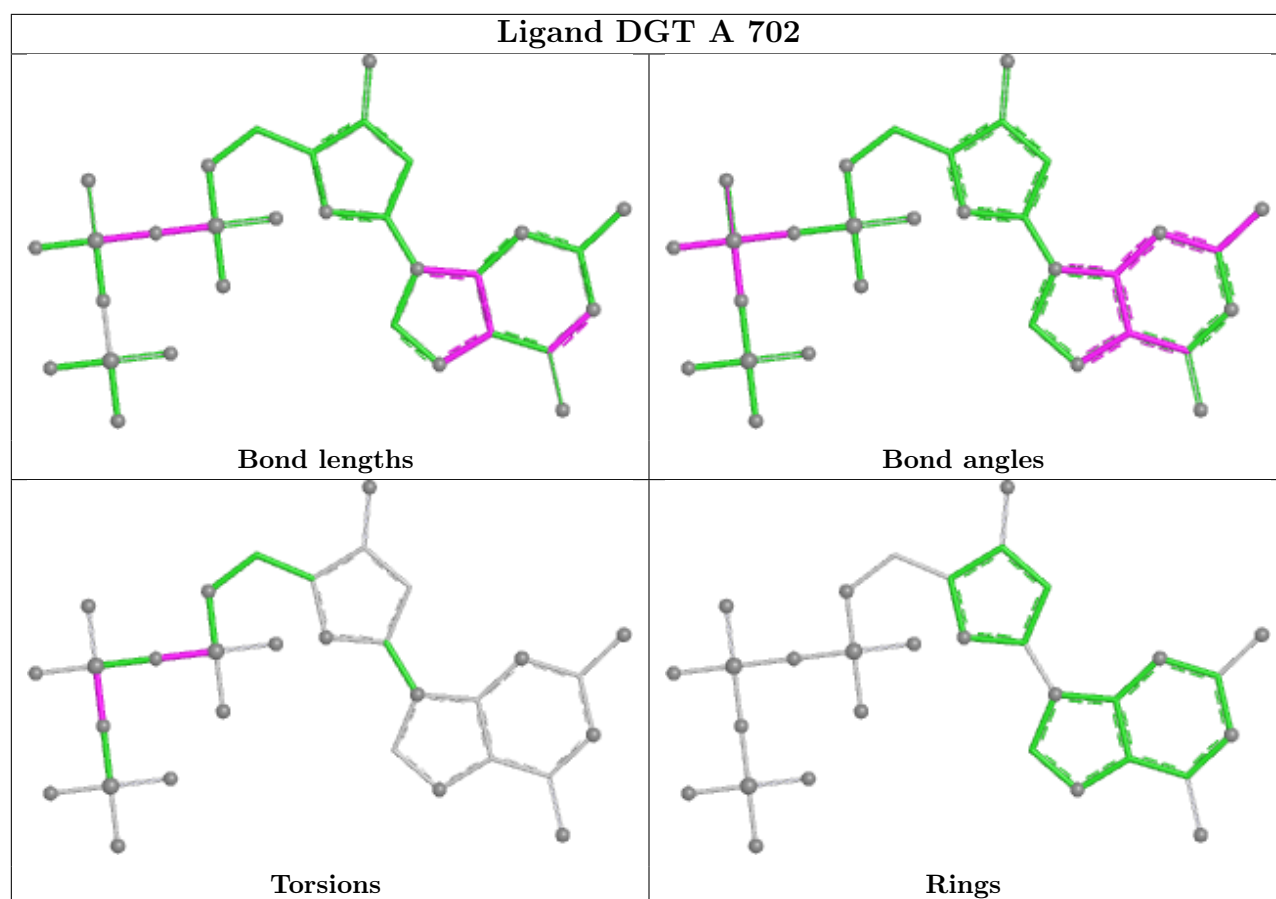
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

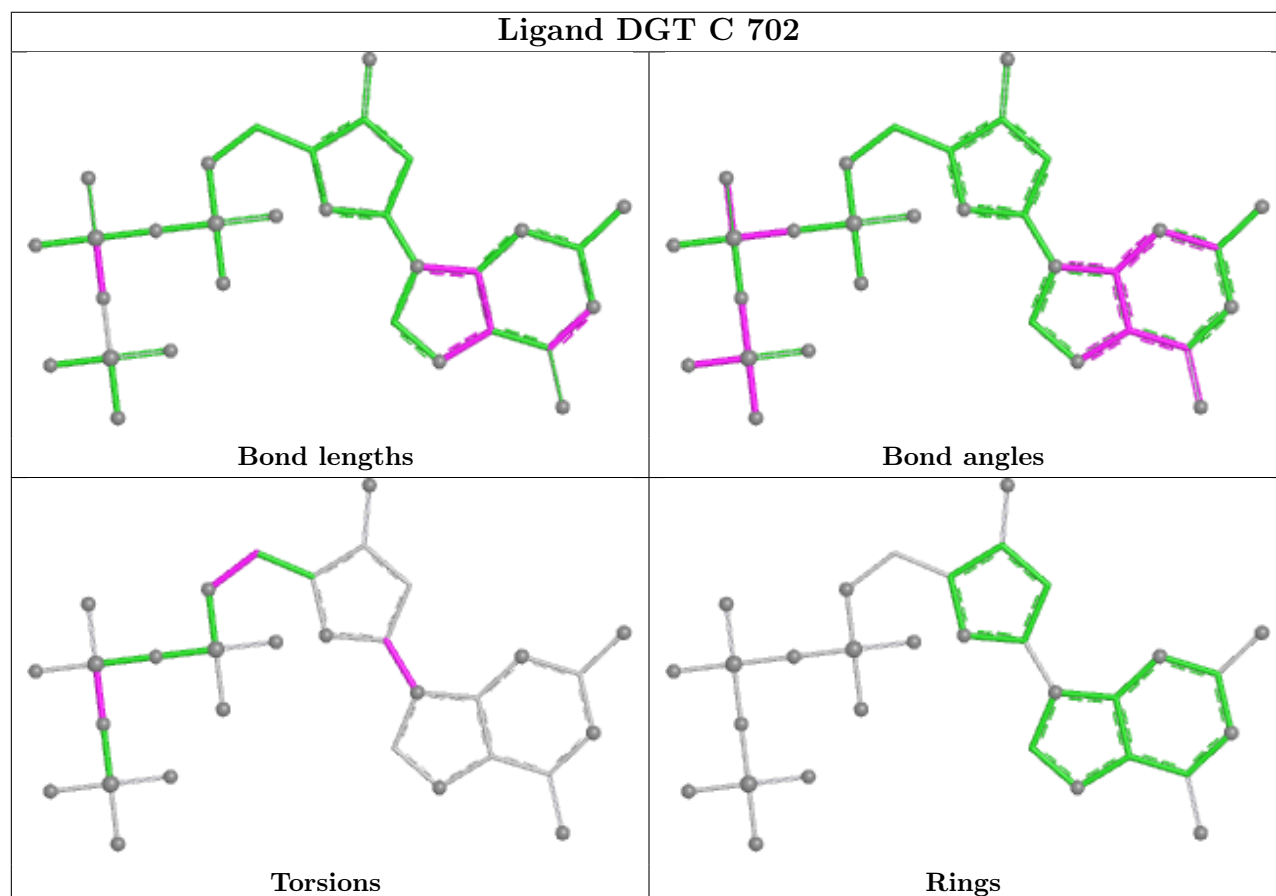
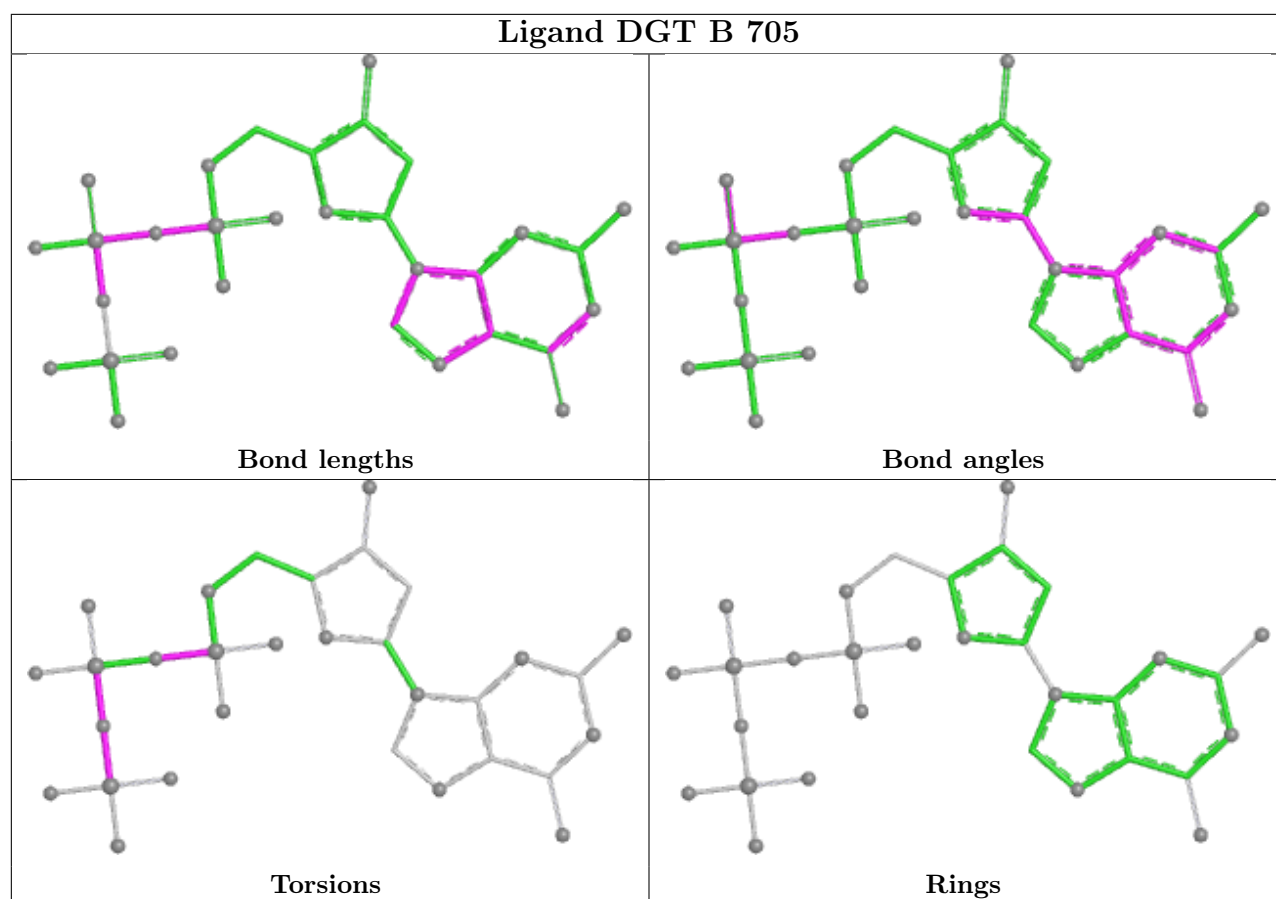












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	480/514 (93%)	-0.13	2 (0%) 88 84	39, 60, 95, 109	0
1	B	480/514 (93%)	0.09	8 (1%) 69 60	36, 73, 113, 143	1 (0%)
1	C	480/514 (93%)	-0.02	5 (1%) 79 72	48, 70, 98, 119	0
1	D	480/514 (93%)	-0.07	6 (1%) 75 66	39, 62, 100, 140	1 (0%)
All	All	1920/2056 (93%)	-0.03	21 (1%) 78 70	36, 66, 103, 143	2 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	507	TYR	3.6
1	D	544	LYS	2.9
1	B	327	ASN	2.9
1	D	511[A]	GLU	2.8
1	D	284	LEU	2.8
1	B	326	GLN	2.6
1	C	507	TYR	2.6
1	B	329	PHE	2.5
1	D	327	ASN	2.5
1	B	507	TYR	2.4
1	B	466	ILE	2.4
1	A	522	CYS	2.3
1	B	324	GLY	2.2
1	C	284	LEU	2.2
1	B	284	LEU	2.1
1	C	522	CYS	2.1
1	C	328	ASN	2.1
1	B	114	THR	2.1
1	C	325	ILE	2.1
1	A	507	TYR	2.1
1	D	276	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

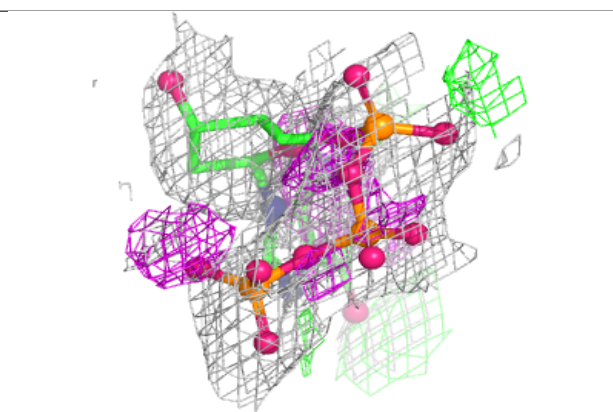
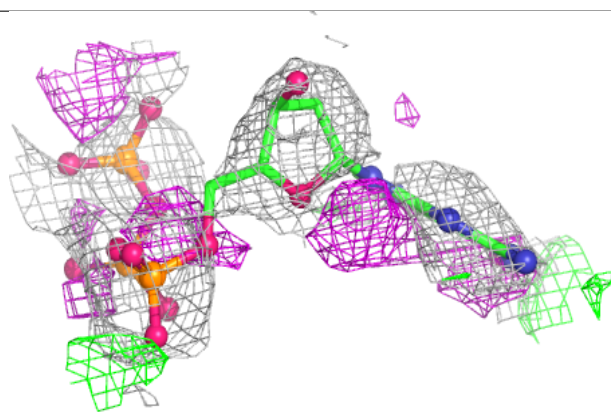
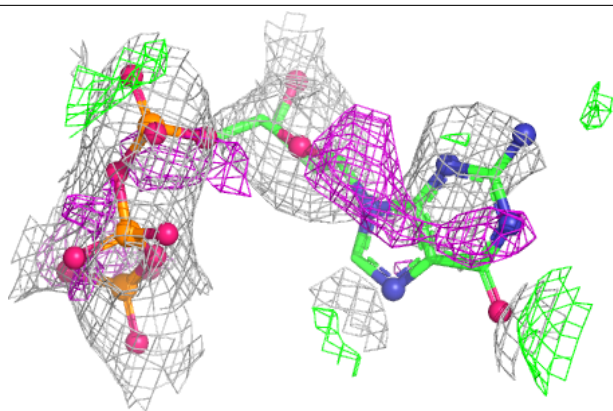
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DGT	D	703	31/31	0.69	0.17	82,124,149,155	0
2	DGT	B	701	31/31	0.74	0.14	79,121,143,148	0
2	DGT	C	703	31/31	0.75	0.13	80,113,136,141	0
3	MG	B	702	1/1	0.76	0.10	100,100,100,100	0
2	DGT	A	701	31/31	0.84	0.11	54,92,113,116	0
3	MG	C	701	1/1	0.92	0.10	60,60,60,60	0
3	MG	B	703	1/1	0.96	0.04	48,48,48,48	0
2	DGT	B	704	31/31	0.97	0.05	46,52,61,65	0
2	DGT	D	704	31/31	0.97	0.05	38,45,48,49	0
2	DGT	C	702	31/31	0.97	0.06	51,55,59,60	0
2	DGT	A	702	31/31	0.97	0.06	38,42,54,60	0
2	DGT	D	702	31/31	0.97	0.06	52,55,60,62	0
3	MG	A	705	1/1	0.98	0.05	46,46,46,46	0
2	DGT	B	705	31/31	0.98	0.04	40,44,48,53	0
2	DGT	A	703	31/31	0.98	0.05	41,44,51,51	0
2	DGT	A	704	31/31	0.98	0.04	47,51,60,62	0
3	MG	D	701	1/1	0.98	0.05	39,39,39,39	0

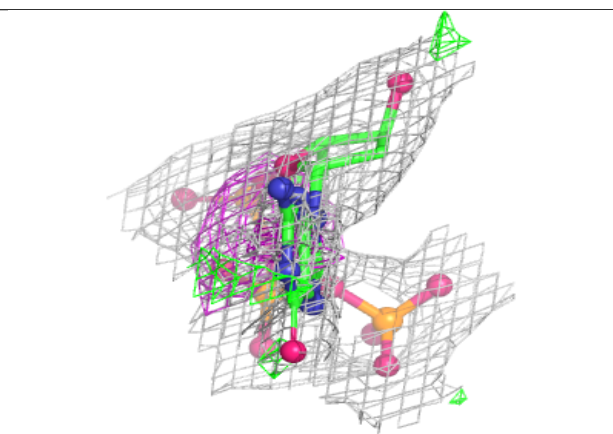
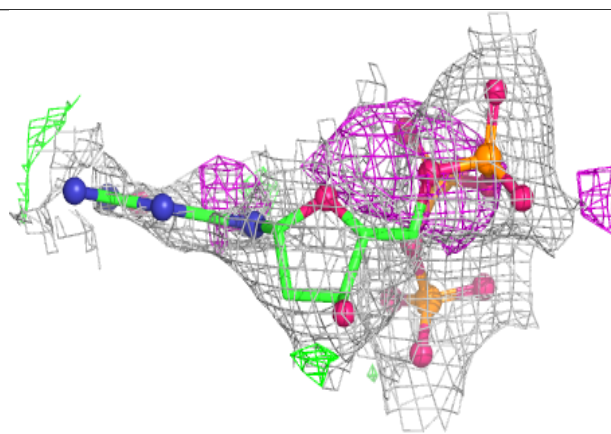
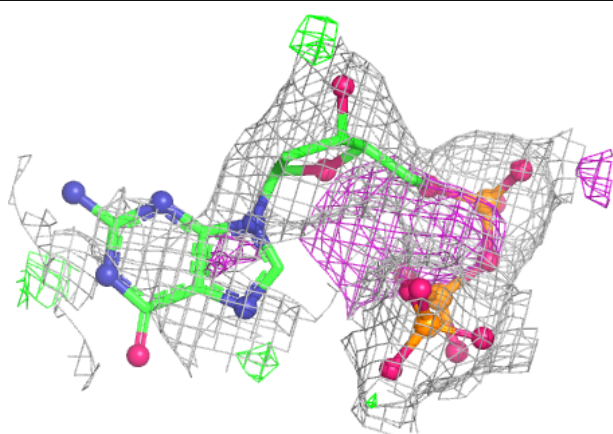
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGT D 703:

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

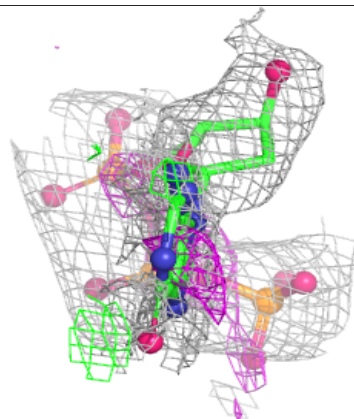
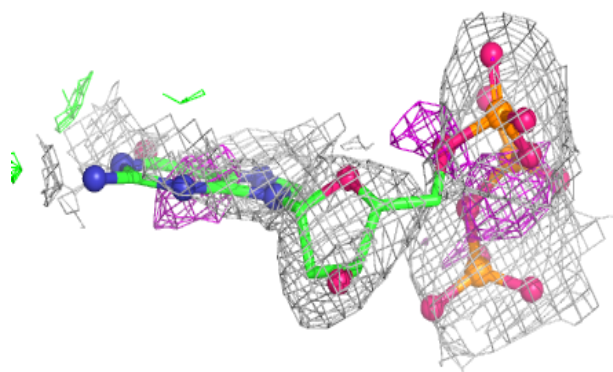
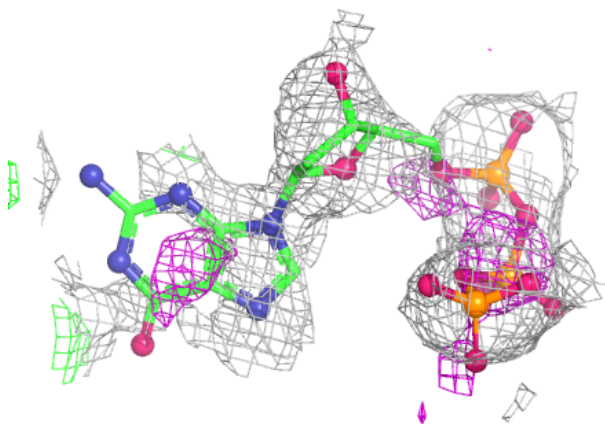
**Electron density around DGT B 701:**

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



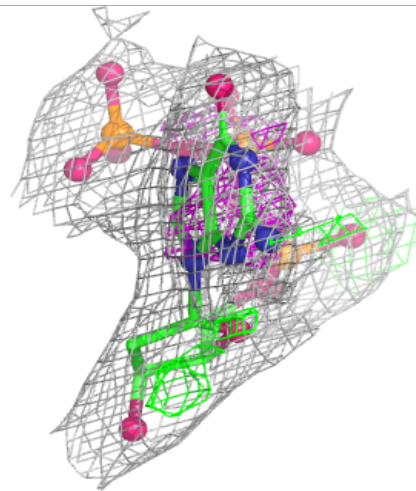
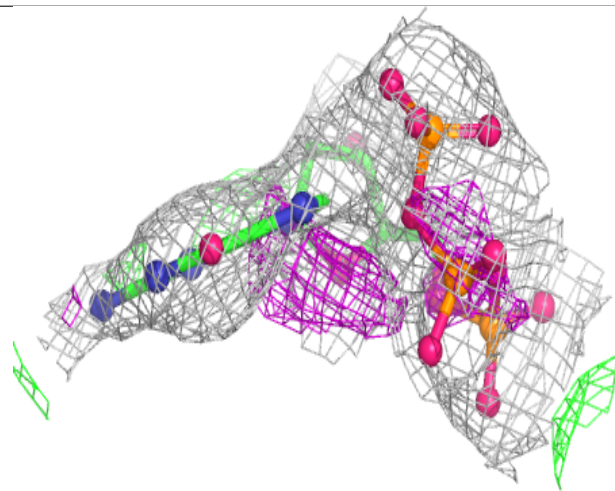
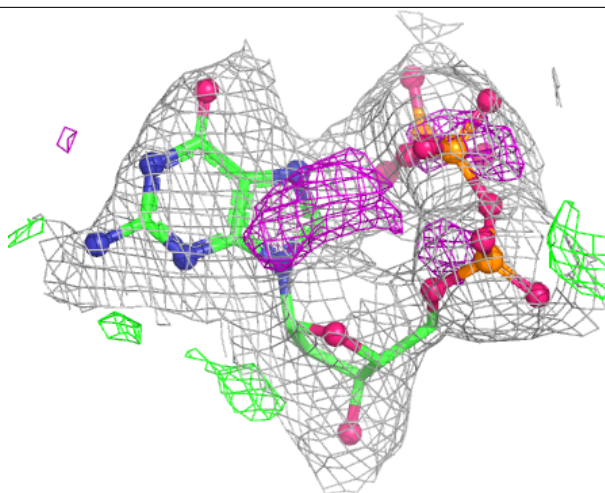
Electron density around DGT C 703:

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



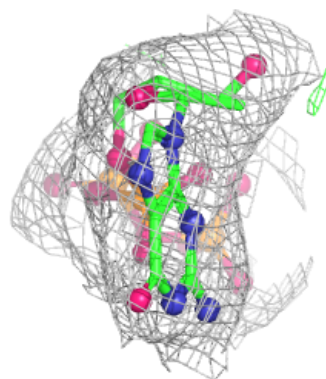
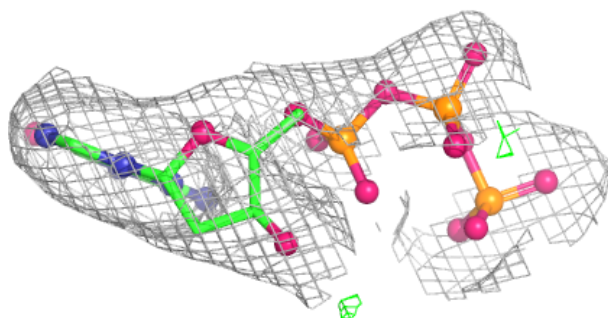
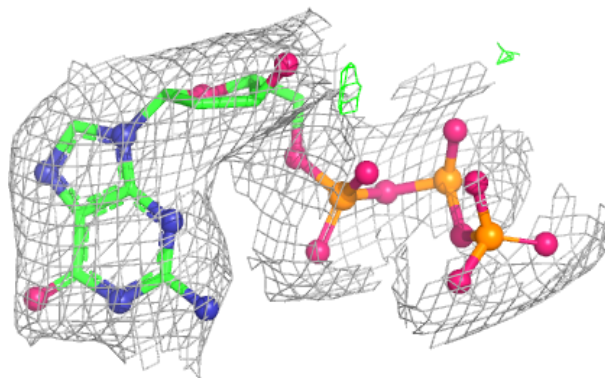
Electron density around DGT A 701:

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

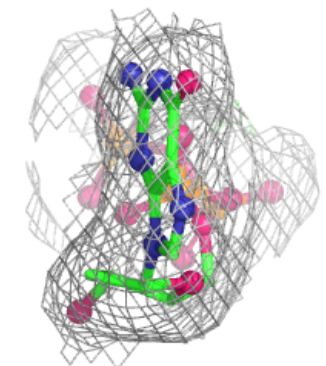
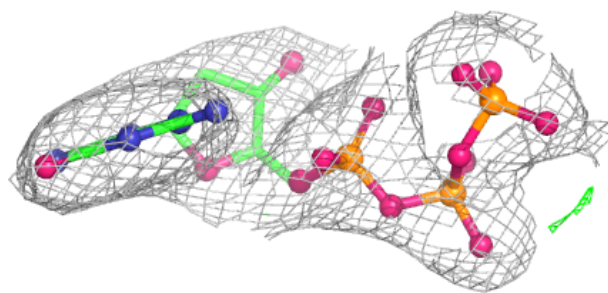
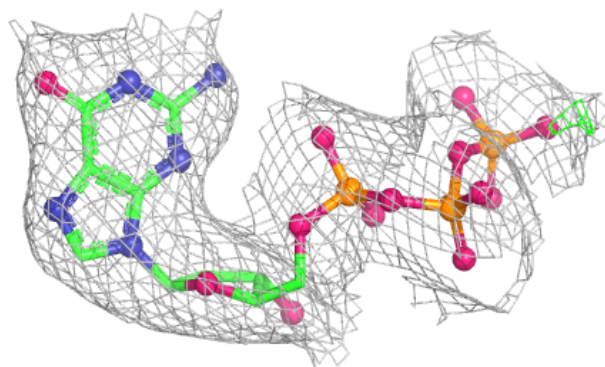


Electron density around DGT B 704:

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

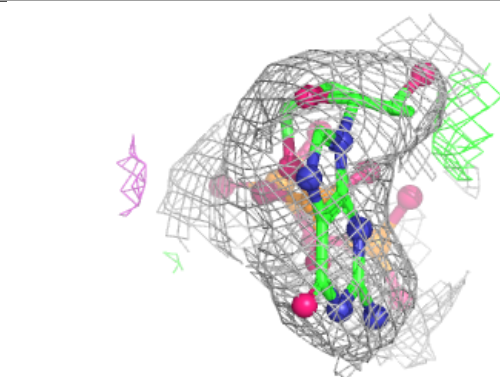
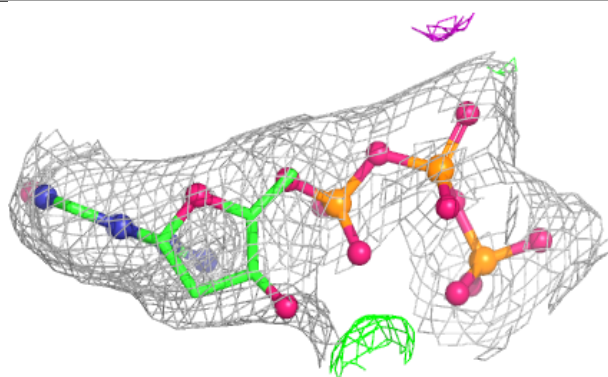
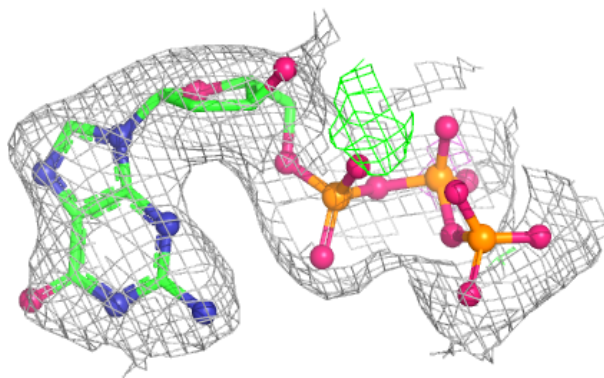
**Electron density around DGT D 704:**

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

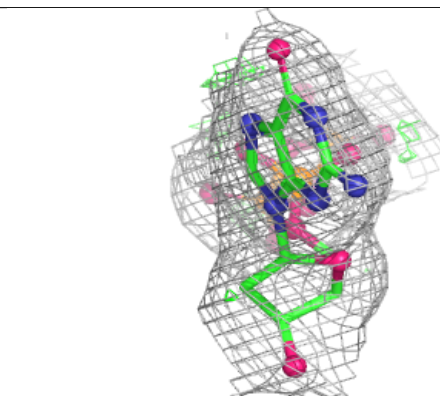
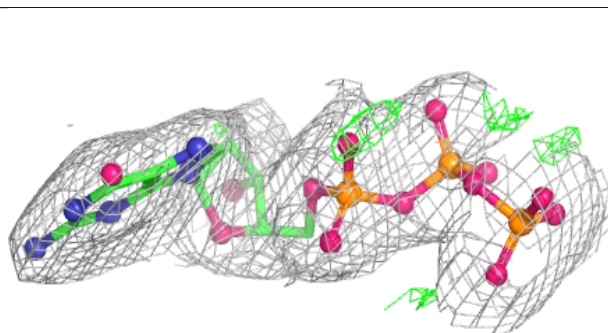
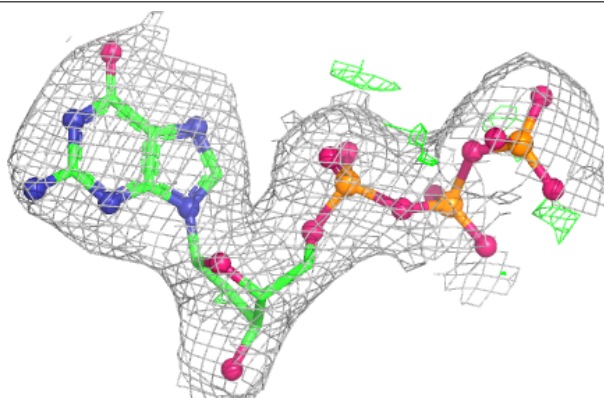


Electron density around DGT C 702:

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

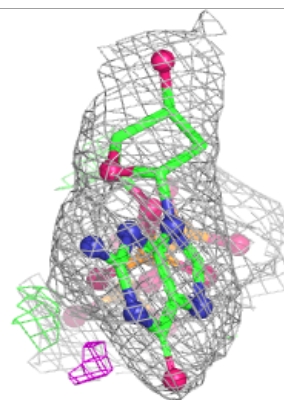
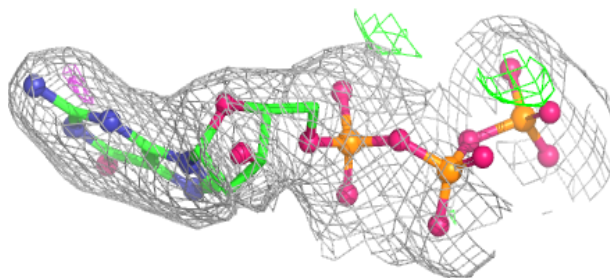
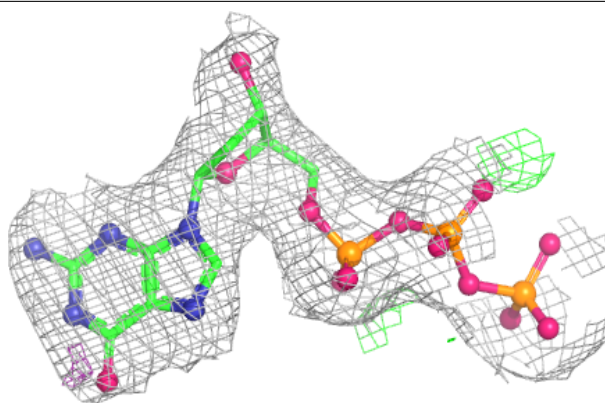
**Electron density around DGT A 702:**

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

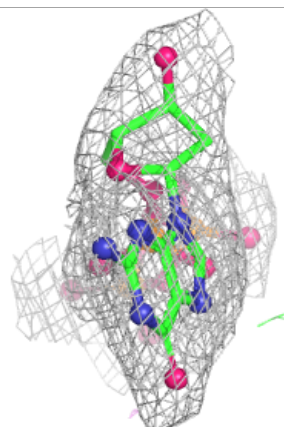
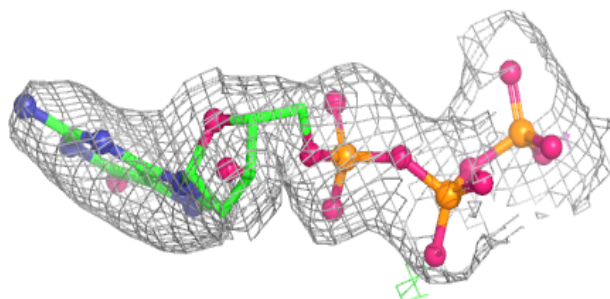
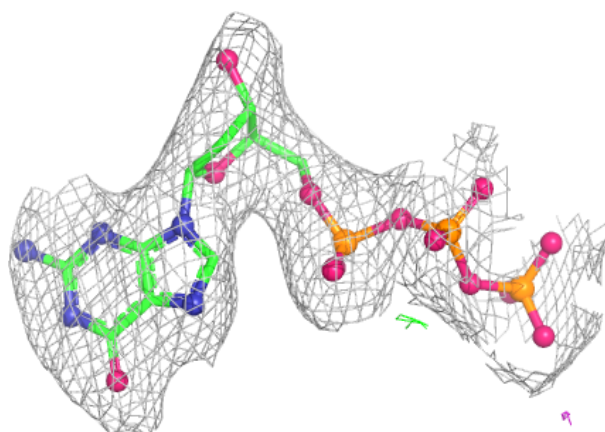


Electron density around DGT D 702:

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

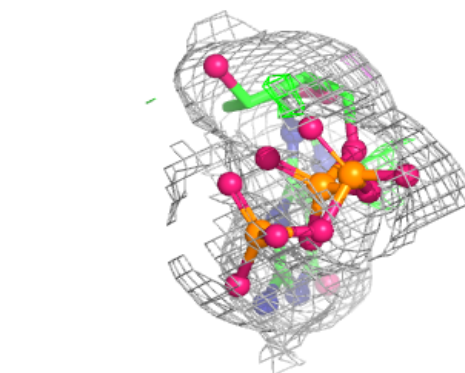
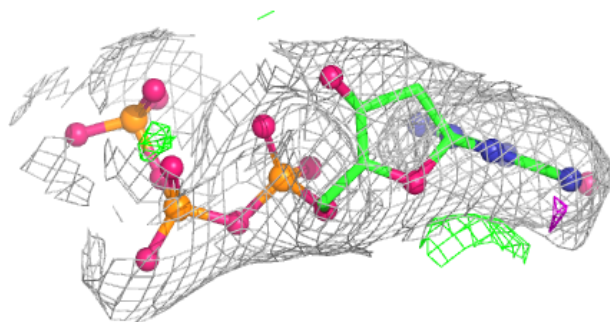
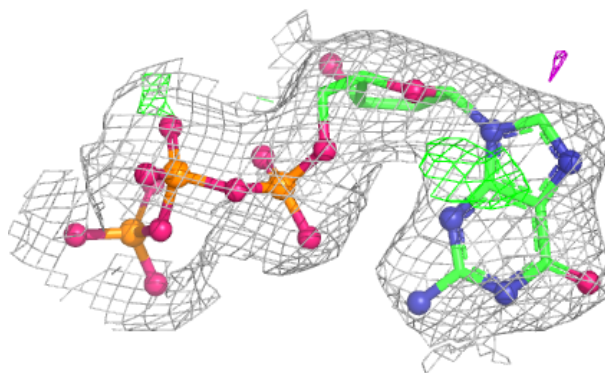
**Electron density around DGT B 705:**

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

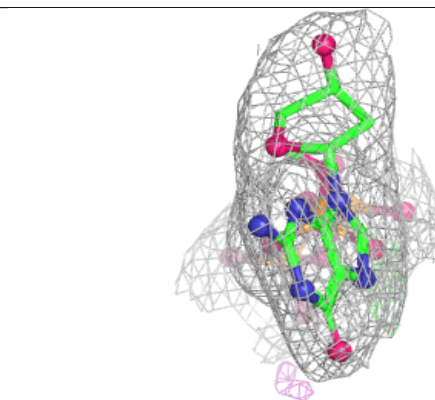
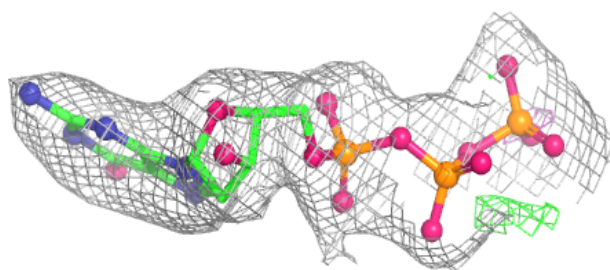
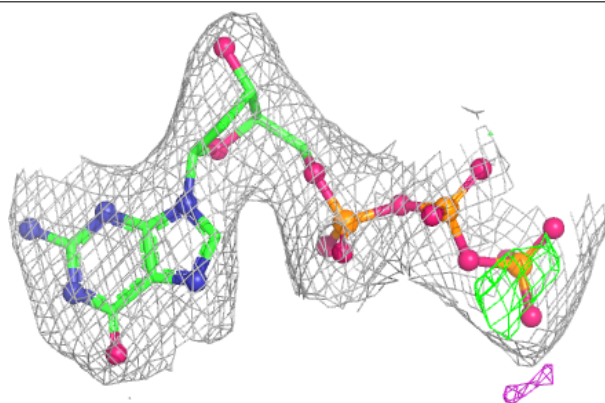


Electron density around DGT A 703:

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

**Electron density around DGT A 704:**

$2mF_o-DF_c$ (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.